

THERMAL, SPECTROSCOPIC AND X-RAY
DIFFRACTION STUDIES OF COPPER(II)
1,2,4,5-BENZENETETRACARBOXYLATES AND
COPPER(II) OXALATE: A STUDY OF
METAL-ORGANIC FRAMEWORKS

THESIS

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“Another flaw in the human character is that everybody wants to build and nobody wants to do maintenance.”

— Kurt Vonnegut, Jr.

ABSTRACT

Novel and known metal organic frameworks with copper(II), sodium and 1,2,4,5-benzenetetracarboxylate were prepared by ambient precipitation, solvothermal and gel-synthesis methods, and characterized by single-crystal X-ray diffraction, X-ray powder diffraction, infrared spectroscopy, differential scanning calorimetry, and thermogravimetry with FTIR evolved-gas analysis. Some of these complexes were investigated for guest inclusion properties with water (the original guest species), methanol, ethanol and pyridine.

The gel-synthesis products were the most interesting. The novel three-dimensional metal-organic framework complex $\text{Cu}_2\text{Na}(\text{OH})\text{L}\cdot 7\text{H}_2\text{O}$ (where $\text{L}=1,2,4,5\text{-benzenetetracarboxylate}$) — formed by gel-synthesis — is a covalent three-dimensional metal organic framework polymer with open channels containing both guest water molecules and water molecules coordinated to sodium. The structure collapsed on dehydration, but was essentially restored to the original structure on rehydration in moist air. On exposure of the dehydrated material to methanol and ethanol vapour, significant uptake of these solvents was observed, and the resolvated structures closely resembled that of the parent material. On heating in dry nitrogen, small amounts of methanol and ethanol remained until about 280 °C, when loss of the remaining guest triggered decomposition of the framework.

The related complex, $\text{Cu}_{2\frac{1}{4}}(\text{OH})_{\frac{1}{2}}\text{L}\cdot 7\frac{1}{2}\text{H}_2\text{O}$ (or possibly $\text{Cu}_{2\frac{1}{3}}(\text{OH})_{\frac{2}{3}}\text{L}\cdot 8\text{H}_2\text{O}$) — formed by gel-synthesis — had a different physical appearance to $\text{Cu}_2\text{Na}(\text{OH})\text{L}\cdot 7\text{H}_2\text{O}$ above, but had nearly identical X-ray diffraction pattern, mid-infrared spectrum and thermal behaviour.

The novel complex $\text{Cu}_4\text{Na}_4\text{L}_3\cdot 14\text{H}_2\text{O}$ — formed by gel-synthesis — is a covalent three-dimensional metal-organic framework with small channels containing both guest water molecules and water coordinated to sodium and copper. Upon dehydration the structure collapsed, but on rehydration in moist air the original structure was partly restored. The dehydrated material did not absorb methanol.

Known two-dimensional polymeric complexes $[\text{Cu}_2\text{L}\cdot 6\text{H}_2\text{O}]\cdot 4\text{H}_2\text{O}$ and $[\text{Cu}_2\text{L}\cdot 4\text{H}_2\text{O}]\cdot 2\text{H}_2\text{O}$ were also obtained by gel-synthesis, and were characterized and investigated for guest inclusion properties. The structures of these complexes collapsed on dehydration, and were only partly restored on rehydration in saturated water vapour. The dehydrated materials did not absorb methanol.

The two-dimensional polymeric mixed-ligand complex $\text{Cu}_2(\text{pyridine})_4\cdot 6\text{H}_2\text{O}$ — formed very slowly by gel-synthesis — was characterized by TG-FTIR, and was shown to undergo a complicated decomposition involving the loss of water and pyridine, carbon dioxide and carbon monoxide in various stages.

Solvothermal synthesis did not yield materials suitable for single-crystal X-ray diffraction studies or inclusion studies, producing only an anhydrous or hemihy-

drate complex with the formula $\text{Cu}_2\text{L}\cdot 0.65\text{H}_2\text{O}$.

Ambient precipitation syntheses did not yield materials suitable for single-crystal diffraction studies, forming products approximately equivalent to the complexes $[\text{Cu}_2\text{L}\cdot 6\text{H}_2\text{O}]\cdot 4\text{H}_2\text{O}$ and $\text{Cu}_{2\frac{1}{4}}(\text{OH})_{\frac{1}{2}}\text{L}\cdot 7\frac{1}{2}\text{H}_2\text{O}$ above.

During the course of the above study it was discovered that, on changing the DSC purge from nitrogen to argon, the normally exothermic carboxylate decompositions appeared to become endothermic. The effects of the supposedly inert atmospheres of argon and nitrogen on the decomposition-mechanism of copper(II) oxalate — a well-studied copper carboxylate — were therefore studied by DSC, TG, TG-FTIR and XRPD. DSC experiments were performed in nitrogen and argon at different flow-rates, in various mixtures of nitrogen and argon, and at various heating rates. Regardless of the proportions of nitrogen and argon, the DSC residues consisted mainly of copper metal, a small amount of copper(I) oxide (cuprite) and, in some circumstances, traces of copper(II) oxide (tenorite). Also, regardless of whether TG-FTIR experiments were performed under argon or nitrogen, the gaseous decomposition products consisted mainly of carbon dioxide, with traces of carbon monoxide being detected over part of the decomposition period. Various explanations for the thermal behaviour are discussed, and it is possible that small amounts of O_2 or monatomic oxygen were given off during the decomposition under argon.

The design and implementation of a low-cost prototype X-ray proportional counter detector system, consisting of a hybrid analog-digital computer built using commonly available electronic components, is presented. This system was designed to replace ageing discrete-transistor designs still in use in earlier X-ray diffractometers. The prototype performs the functions of pulse-shaping, pulse-height discrimination, counting and scaling, and provides both digital and scaled analog outputs.

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Contents

I	Copper(II) 1,2,4,5-benzenetetracarboxylate studies	1
1	Introduction	2
1.1	Metal-organic frameworks (MOFs)	2
1.2	Copper(II) benzenepolycarboxylates	9
1.2.1	Copper 1,2,4,5-benzenetetracarboxylates	10
1.2.2	Copper(II) benzenehexacarboxylates and dinitrobenzenetetracarboxylates	31
1.3	The aims of this study	31
2	Experimental methods	48
2.1	Elemental analysis	48
2.1.1	Carbon, hydrogen and nitrogen (CHN) analysis	48
2.1.2	Complexometric titrations for copper determination	48
2.1.3	Metal analysis (instrumental)	49
2.1.4	Sodium fusion test for chlorides (Lassaigne test)	49
2.2	Thermal analysis	50
2.2.1	Differential scanning calorimetry (DSC)	50
2.2.2	Thermogravimetry (TG)	51
2.3	Fourier transform infrared spectroscopy (FTIR)	51
2.3.1	Mid-infrared spectroscopy	51
2.3.2	Gas-phase infrared spectroscopy for evolved-gas analysis	52
2.4	X-ray methods	52
2.4.1	X-ray powder diffractometry (XRPD)	52
2.4.2	X-ray fluorescence spectroscopy	53
2.4.3	Single-crystal X-ray diffractometry	53
3	Synthesis	56
3.1	Synthesis method overview	56
3.1.1	Ambient precipitation method	56
3.1.2	Solvothermal method	57
3.1.3	Gel-based method	57

3.2	Synthesis methods and products	59
3.2.1	Ambient precipitation syntheses and products	59
3.2.2	Solvothermal syntheses and products	60
3.2.3	Gel-based syntheses and products	61
4	Characterization	74
4.1	Group 1 products	74
4.1.1	Elemental analysis	75
4.1.2	Thermogravimetry and Differential scanning calorimetry	79
4.1.3	Crystal structure (xut-cu-b4c-acet-xtals only)	85
4.2	Group 2 products	93
4.2.1	Elemental analysis	93
4.2.2	Thermogravimetry and Differential scanning calorimetry .	95
4.2.3	Crystal structures	97
4.3	Group 3 products	103
4.3.1	Elemental analysis	103
4.3.2	Thermogravimetry and Differential scanning calorimetry .	105
4.3.3	Crystal structures	110
4.4	Group 4 products	119
4.4.1	XRPD and Mid-IR spectroscopy	119
4.4.2	Elemental analysis	121
4.4.3	Thermogravimetry and Differential scanning calorimetry .	123
4.4.4	Crystal structures	127
4.5	Group 5 products	132
4.6	Group 6 products	132
4.6.1	X-ray powder diffraction and infrared spectroscopy . . .	133
4.6.2	Elemental analysis	134
4.6.3	Thermogravimetry and Differential scanning calorimetry .	136
5	Desolvation-resolution experiments	143
5.1	Introduction and rationale	143
5.2	Specific methods	145
5.2.1	X-ray powder diffraction	145
5.3	xut-cu-b4c-acet-xtals	146
5.3.1	Single desolvation-resolution: water	146
5.3.2	Single desolvation-resolution: methanol	151
5.3.3	Single desolvation-resolution: ethanol	162
5.3.4	Single desolvation-resolution: pyridine	168
5.3.5	Multiple desolvation-resolution: water, water	168
5.3.6	Multiple desolvation-resolution: water, methanol	174
5.3.7	Multiple desolvation-resolution: methanol, methanol . .	179

5.3.8	Multiple desolvation-resolution: methanol, water	184
5.3.9	Discussion	188
5.4	xst-cu-b4c-no3-rhombi	193
5.4.1	Single desolvation-resolution: water	193
5.4.2	Single desolvation-resolution: methanol	202
5.4.3	Discussion	202
5.5	xst-cu-b4c-no3-lumps	205
5.5.1	Single desolvation-resolution: water	205
5.5.2	Discussion	212
5.6	xst-cu-b4c-so4-topxtals	213
5.6.1	Single desolvation-resolution: first step only, water . . .	213
5.6.2	Single desolvation-resolution: first and second steps, wa- ter	222
5.6.3	Single desolvation-resolution: methanol	230
5.6.4	Further discussion	230
5.7	Conclusion	231

II Copper(II) oxalate studies 235

6 Thermal behaviour of copper(II) oxalate 236

6.1	Introduction	236
6.2	Experimental	240
6.2.1	Preparation	240
6.2.2	Compositional analysis	240
6.2.3	X-ray powder diffraction	240
6.2.4	Spectroscopy	241
6.2.5	Thermal analysis	244
6.2.6	Evolved gas analysis	246
6.3	Results and discussion	246
6.3.1	TG-FTIR in inert atmospheres	246
6.3.2	DSC in inert atmospheres	255
6.3.3	DSC results in oxygen	278
6.3.4	Discussion	281
6.4	Concluding remarks	292

III X-ray diffractometer data system 297

7 X-Ray detector circuit 298

7.1	Introduction	298

7.2	A description of the original Philips powder diffractometer	298
7.2.1	Proportional counter probe (PW1965/40)	300
7.2.2	Pulse-shaping amplifier (in PW4620 unit)	304
7.2.3	Pulse-height discriminator (in Philips PW4620)	312
7.2.4	Counting ratemeter (in Philips PW4620)	314
7.3	Design and implementation of a replacement detector system . . .	321
7.4	Circuit Description	322
7.4.1	Analog section and pulse-height discriminator	322
7.4.2	Digital and analog DC output section	330
7.5	Concluding remarks	335
IV	Appendices	340
A	Complexometric titrations	341
A.1	Reagents and solutions	341
A.2	Procedure	342
B	Analysis for chlorine, sodium & potassium	344
B.1	Chemical analysis: sodium fusion test	344
B.2	X-ray fluorescence spectrometry	345
B.2.1	Test for chloride	346
B.2.2	Test for sodium	347
B.2.3	Test for potassium	349
C	CD-ROM	352

List of Figures

1.1	Drawing of the HKUST-1 structure.	5
1.2	A view of the framework of MOF-5, later named IRMOF-1. . . .	7
1.3	Non-catenated bis-1,10-phenanthroline-copper(II) complex with 1,2,4,5-benzenetetracarboxylic acid.	11
1.4	Double chain consisting of pairs of 1,10-phenanthroline copper(II) moieties doubly linked by 1,2,4,5-benzenetetracarboxylates.	12
1.5	Parallelogram motif in zig-zag covalent chains.	14
1.6	Staircase chains joined by π - π interactions to form a three-dimensional structure.	15
1.7	Hydrogen-bonded network, involving octameric guest-water clusters, linking monomeric units to form a three-dimensional structure.	16
1.8	Layered structure showing a covalently bound two-dimensional layer, consisting of copper(II) atoms and μ_6 -bridging 1,2,4,5-benzenetetracarboxylate ions.	19
1.9	Monomeric copper(II) complex with 3,10-bis(2-hydroxyethyl)-1,3,5,8,10,12-hexa-azacyclotetradecane and 1-carboxylato-2,4,5-benzenetetracarboxylic acid.	27
3.1	A typical straight-tube arrangement.	58
3.2	A typical U-tube arrangement.	59
3.3	The copper(II) nitrate/1,2,4,5-benzenetetracarboxylate straight-tube reaction after approximately three months.	63
3.4	The copper(II) sulfate/1,2,4,5-benzenetetracarboxylate straight-tube reaction after approximately three months.	65
3.5	The copper(II) chloride/1,2,4,5-benzenetetracarboxylate straight-tube reaction after approximately three months.	66
3.6	The copper(II) acetate/1,2,4,5-benzenetetracarboxylate straight-tube reaction after approximately six months.	68
4.1	TG curve for xut-cu-b4c-acet-xtals ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen.	79
4.2	TG curve for xst-cu-b4c-so4-needles ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen.	81

4.3	DSC and derivative DSC curves for (I.) xst-cu-b4c-no3-needles , (II.) xst-cu-b4c-so4-needles , (III.) xst-cu-b4c-cl-needles , and (IV.) xut-cu-b4c-acet-xtals	84
4.4	Secondary building unit (SBU) of xut-cu-b4c-acet-xtals	86
4.5	Schematic diagram of the binding in xut-cu-b4c-acet-xtals	89
4.6	Basic unit (I.) and an expanded unit (II.) of the structure of xut-cu-b4c-acet-xtals	90
4.7	Face A of the crystal structure of xut-cu-b4c-acet-xtals , showing large cavities containing guest water molecules.	91
4.8	Ray-traced diagram of face A of the crystal structure of xut-cu-b4c-acet-xtals , showing large cavities containing guest water molecules.	92
4.9	TG curve for xst-cu-b4c-no3-rhombi ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen.	95
4.10	DSC and derivative DSC curves for xst-cu-b4c-no3-rhombi , heated in a crimped (not sealed) aluminium pan at $10\text{ }^{\circ}\text{C min}^{-1}$ under flowing nitrogen (26 ml min^{-1}).	96
4.11	Schematic diagram of the binding in xst-cu-b4c-cl-rhombi	99
4.12	Basic unit of xst-cu-b4c-cl-rhombi	100
4.13	Face A of the crystal structure of xst-cu-b4c-cl-rhombi , showing cavities containing guest water molecules.	101
4.14	Ray-traced diagram of face A of the crystal structure of xst-cu-b4c-cl-rhombi , showing large cavities containing guest water molecules.	102
4.15	TG curve for xst-cu-b4c-so4-topxtals ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen.	106
4.16	DSC and derivative DSC curves for xst-cu-b4c-so4-topxtals , heated in a crimped (not sealed) aluminium pan at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen (26 ml min^{-1}).	106
4.17	TG curve for xst-cu-b4c-no3-lumps ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen.	109
4.18	DSC and derivative DSC curves for xst-cu-b4c-no3-lumps , heated in a crimped (not sealed) aluminium pan at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen (26 ml min^{-1}).	109
4.19	(I.) Basic unit, (II.) binding diagram and (III.) expanded diagram of xst-cu-b4c-so4-topxtals	112
4.20	Face C of the crystal structure of xst-cu-b4c-so4-topxtals , showing channels containing guest water molecules.	113
4.21	Ray-traced diagram of face C of the crystal structure of xst-cu-b4c-so4-topxtals , showing channels containing guest water molecules.	114

4.22	(<i>I.</i>) Basic unit, (<i>II.</i>) binding diagram and (<i>III.</i>) extended view of xst-cu-b4c-no3-lumps	116
4.23	Face A of the crystal structure of xst-cu-b4c-no3-lumps , showing channels containing guest water molecules.	117
4.24	Ray-traced diagram of face A of the crystal structure of xst-cu-b4c-no3-lumps , showing channels containing guest water molecules.	118
4.25	Experimental X-ray powder diffraction patterns of xut-cu-pyrX-b4c-no3-xtals and xut-cu-pyr2-b4c-no3-xtals , shown with the simulated pattern obtained from the crystal structure of xut-cu-pyr2-b4c-no3-xtals	120
4.26	Mid-infrared spectra of xut-cu-pyrX-b4c-no3-xtals and xut-cu-pyr2-b4c-no3-xtals , obtained in KBr.	121
4.27	<i>I.</i> TG curve for xut-cu-pyr2-b4c-no3-xtals , heated from 25–400 °C at 10 °C min ^{−1} under nitrogen (100 ml min ^{−1} .) <i>II.</i> Corresponding FTIR EGA profiles for various absorptions characteristic of pyridine and carbon dioxide.	125
4.28	TG-FTIR EGA stack-plot for xut-cu-pyr2-b4c-no3-xtals heated in a TG from 25–400 °C at 10 °C min ^{−1} under nitrogen (100 ml min ^{−1}).	126
4.29	DSC and derivative DSC curves for xut-cu-pyr2-b4c-no3-xtals , heated in a crimped (not sealed) aluminium pan at 10 °C min ^{−1} under nitrogen (26 ml min ^{−1}).	127
4.30	<i>I.</i> Binding diagram and <i>II.</i> basic unit of xut-cu-pyr2-b4c-no3-xtals	129
4.31	Face A of the crystal structure of xut-cu-pyr2-b4c-no3-xtals , showing the binding of two pyridine molecules — out of plane with each other — to each copper atom.	130
4.32	Ray-traced diagram of face A of the crystal structure of xut-cu-pyr2-b4c-no3-xtals , showing the binding of two pyridine molecules — out of plane with each other — to each copper atom.	131
4.33	X-ray powder diffraction patterns of hyd-cu-b4c-acet and hyd-cu-b4c-co3	133
4.34	Mid-infrared spectrum of hyd-cu-b4c-acet	134
4.35	TG curve for hyd-cu-b4c-acet (10 °C min ^{−1}) under nitrogen.	136
4.36	DSC and derivative DSC curves for hyd-cu-b4c-acet . The sample was heated in crimped (not sealed) aluminium pans from 25 °C to 400 °C at 10 °C min ^{−1} under flowing nitrogen (25 ml min ^{−1}).	138

5.1	X-ray diffraction patterns of xut-cu-b4c-acet-xtals (a) without pre-treatment, (b) after dehydration by heating in a DSC from 25 °C to 150 °C at 10 °C min ⁻¹ under nitrogen (25 ml min ⁻¹) and (c) after exposure of the dehydrated material to moist air for 2 hours.	149
5.2	X-ray diffraction patterns of a single sample of xut-cu-b4c-acet-xtals after dehydration, with the sample covered with a thin layer of paraffin oil. X-ray diffraction patterns were obtained (a) immediately after dehydration, (b) four hours later and (c) two days later.	150
5.3	X-ray diffraction patterns of xut-cu-b4c-acet-xtals (a) without pre-treatment, (b) after dehydration by heating in a DSC from 25 °C to 150 °C at 10 °C min ⁻¹ under nitrogen (25 ml min ⁻¹) and (c) after exposure of the dehydrated material to methanol vapour for 4 hours.	152
5.4	X-ray diffraction patterns of xut-cu-b4c-acet-xtals which had been dehydrated in a DSC (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 25–27 ml min ⁻¹) and exposed to methanol vapour. . . .	153
5.5	Infrared spectra of xut-cu-b4c-acet-xtals in the untreated, rehydrated and methanol-resolvated states (4000–2400 cm ⁻¹).	155
5.6	Infrared spectra of xut-cu-b4c-acet-xtals in the untreated, rehydrated and methanol-resolvated states (1800–1250 cm ⁻¹).	156
5.7	Infrared spectra of xut-cu-b4c-acet-xtals in the untreated, rehydrated and methanol-resolvated states (1250–450 cm ⁻¹).	157
5.8	TG and derivative TG curves (<i>I</i>) and corresponding time-resolved infrared spectra of the evolved gas (<i>II</i>) of xut-cu-b4c-acet-xtals , previously dehydrated (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) and exposed overnight to saturated methanol vapour.	159
5.9	Normalized intensity–TG temperature profiles for TG-FTIR of xut-cu-b4c-acet-xtals , previously dehydrated and exposed to saturated methanol vapour, showing two characteristic absorbance profiles for methanol and one for carbon dioxide.	160
5.10	Complex DSC response for the decomposition of xut-cu-b4c-acet-xtals , previously dehydrated and exposed to saturated methanol vapour. The sample was heated at 10 °C min ⁻¹ under nitrogen purge (26 ml min ⁻¹).	161

5.11	X-ray diffraction patterns of xut-cu-b4c-acet-xtals (a) without pre-treatment, (b) after dehydration by heating in a DSC from 25 °C to 150 °C at 10 °C min ⁻¹ under nitrogen (26 ml min ⁻¹) and (c) after exposure of the dehydrated material to ethanol vapour for 24 hours.	163
5.12	TG and derivative TG curves (<i>I</i>) and corresponding time-resolved infrared spectra of the evolved gas (<i>II</i>) of xut-cu-b4c-acet-xtals , previously dehydrated (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) and exposed for 24 hours to saturated ethanol vapour. The resolved material was heated in the TG (25 °C–350 °C at 10 °C min ⁻¹ under nitrogen, 100 ml min ⁻¹ total purge).	165
5.13	Normalized intensity–TG temperature profiles for TG-FTIR of xut-cu-b4c-acet-xtals , previously dehydrated and exposed to saturated ethanol vapour, showing two characteristic absorbance profiles for ethanol and one for carbon dioxide.	166
5.14	Complex DSC response for the decomposition of xut-cu-b4c-acet-xtals , previously dehydrated and exposed to saturated ethanol vapour. The sample was heated at 10 °C min ⁻¹ under nitrogen purge (26 ml min ⁻¹).	167
5.15	DSC (<i>I</i>) and derivative DSC (<i>II</i>) curves of xut-cu-b4c-acet-xtals (a) for the initial desolvation (water) (Desolv(1)), (b) for the second desolvation (water) (Desolv(2)), and (c) for the final desolvation (water) and subsequent decomposition (Decomp).	171
5.16	X-ray diffraction patterns of xut-cu-b4c-acet-xtals (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹), (c) dehydrated sample (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) exposed to moist air, and (d) a sample treated as in c, dehydrated again, (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) and exposed to moist air.	173
5.17	DSC (<i>I</i>) and derivative DSC (<i>II</i>) curves of xut-cu-b4c-acet-xtals (a) for the initial desolvation (water) (Desolv(1)), (b) for the second desolvation (water) (Desolv(2)), and (c) for the final desolvation (methanol) and subsequent decomposition (Decomp).	176
5.18	X-ray diffraction patterns of xut-cu-b4c-acet-xtals (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹), (c) dehydrated sample (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) exposed to moist air, and (d) a sample treated as in c, dehydrated (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) and exposed to methanol vapour.	178

5.19	DSC (<i>I</i>) and derivative DSC (<i>II</i>) curves of xut-cu-b4c-acet-xtals (a) for the initial desolvation (water) (Desolv(1)), (b) for the second desolvation (methanol) (Desolv(2)), and (c) for the final desolvation (methanol) and subsequent decomposition (Decomp). . . .	182
5.20	X-ray diffraction patterns of xut-cu-b4c-acet-xtals (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹), (c) dehydrated sample (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) exposed to methanol vapour, and (d) a sample treated as in c, desolvated, (25 °C–200 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) and exposed to methanol vapour.	183
5.21	DSC (<i>I</i>) and derivative DSC (<i>II</i>) curves of xut-cu-b4c-acet-xtals (a) for the initial desolvation (water) (Desolv(1)), (b) for the second desolvation (methanol) (Desolv(2)), and (c) for the final desolvation (water) and subsequent decomposition (Decomp).	185
5.22	X-ray diffraction patterns of xut-cu-b4c-acet-xtals (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹), (c) dehydrated sample (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) exposed to methanol vapour, and (d) a sample treated as in c, desolvated, (25 °C–200 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) and exposed to moist air.	187
5.23	Ray-traced drawing of the cavities within xut-cu-b4c-acet-xtals . .	191
5.24	DSC (<i>I</i>) and derivative DSC (<i>II</i>) of xst-cu-b4c-no3-rhombi (a) without pre-treatment and (b) after dehydration (25 °C–200 °C at 10 °C min ⁻¹ under nitrogen, 26 ml min ⁻¹) with subsequent exposure to open air (25 °C) overnight.	195
5.25	X-ray diffraction patterns for xst-cu-b4c-no3-rhombi (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–200 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹), and (c) dehydrated as above, and exposed to open air (12 hours).	196
5.26	Infrared spectra of xst-cu-b4c-no3-rhombi in the untreated, dehydrated and rehydrated states (4000–2400 cm ⁻¹).	199
5.27	Infrared spectra of xst-cu-b4c-no3-rhombi in the untreated, dehydrated and rehydrated states (1800–1250 cm ⁻¹).	200
5.28	Infrared spectra of xst-cu-b4c-no3-rhombi in the untreated, dehydrated and rehydrated states (1250–450 cm ⁻¹).	201
5.29	Ray-traced drawing of the cavities within xst-cu-b4c-no3-rhombi . .	204

5.30	DSC (I) and derivative DSC (II) of xst-cu-b4c-no3-lumps (a) without pre-treatment and (b) after dehydration (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 26 ml min ⁻¹) with subsequent exposure to open air (12 hours) and thereafter to saturated water vapour (25 °C) for 6 hours.	207
5.31	X-ray diffraction patterns for xst-cu-b4c-no3-lumps (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 26 ml min ⁻¹), and (c) dehydrated as above, and exposed to open air (12 hours) and thereafter to saturated water vapour (6 hours).	208
5.32	Infrared spectra of xst-cu-b4c-no3-lumps in the untreated, dehydrated and rehydrated states (4000–2400 cm ⁻¹).	209
5.33	Infrared spectra of xst-cu-b4c-no3-lumps in the untreated, dehydrated and rehydrated states (1800–1250 cm ⁻¹).	210
5.34	Infrared spectra of xst-cu-b4c-no3-lumps in the untreated, dehydrated and rehydrated states (1250–450 cm ⁻¹).	211
5.35	DSC (I) and derivative DSC (II) curves of xst-cu-b4c-so4-topxtals (a) without pre-treatment and (b) after dehydration (25 °C–95 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) with subsequent exposure to saturated water vapour (25 °C) for 6 hours.	214
5.36	X-ray diffraction patterns for xst-cu-b4c-so4-topxtals (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–95 °C at 10 °C min ⁻¹ under nitrogen, 26 ml min ⁻¹), and (c) dehydrated as above, and exposed to open air (12 hours) and thereafter to saturated water vapour (6 hours).	218
5.37	Infrared spectra of xst-cu-b4c-so4-topxtals in the untreated, dehydrated (by heating to 95 °C) and rehydrated states (4000–2400 cm ⁻¹).	219
5.38	Infrared spectra of xst-cu-b4c-so4-topxtals in the untreated, dehydrated (by heating to 95 °C) and rehydrated states (1800–1250 cm ⁻¹).	220
5.39	Infrared spectra of xst-cu-b4c-so4-topxtals in the untreated, dehydrated (by heating to 95 °C) and rehydrated states (1250–450 cm ⁻¹).	221
5.40	DSC (I) and derivative DSC (II) curves of xst-cu-b4c-so4-topxtals (a) without pre-treatment and (b) after dehydration (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 27 ml min ⁻¹) with subsequent exposure to open air (12 hours) and thereafter to saturated water vapour (25 °C) for 6 hours.	224

5.41	X-ray diffraction patterns for xst-cu-b4c-so4-topxtals (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min ⁻¹ under nitrogen, 26 ml min ⁻¹), and (c) dehydrated as above, and exposed to open air (12 hours) and thereafter to saturated water vapour (6 hours).	225
5.42	X-ray diffraction patterns of two dehydrated samples of xst-cu-b4c-so4-topxtals , heated to (a) 95 °C and (b) 150 °C.	226
5.43	Infrared spectra of xst-cu-b4c-so4-topxtals in the untreated, dehydrated (by heating to 150 °C) and rehydrated states (4000–2400 cm ⁻¹).	227
5.44	Infrared spectra of xst-cu-b4c-so4-topxtals in the untreated, dehydrated (by heating to 150 °C) and rehydrated states (1800–1250 cm ⁻¹).	228
5.45	Infrared spectra of xst-cu-b4c-so4-topxtals in the untreated, dehydrated (by heating to 150 °C) and rehydrated states (1250–450 cm ⁻¹).	229
6.1	X-ray powder diffraction patterns (Cu-K _α radiation) for undried and dried copper(II) oxalate.	242
6.2	Infrared spectra of undried and dried copper(II) oxalate, obtained in KBr pellets.	243
6.3	TG curves for copper(II) oxalate heated from 25 °C to 315 °C at 10 °C min ⁻¹ in argon and in nitrogen at flow rates of approximately 100 ml min ⁻¹	248
6.4	X-ray powder diffraction patterns (Cu-K _α radiation) of the residues of copper(II) oxalate heated in a TG in open platinum pans, from 25 °C to 320 °C at 10 °C min ⁻¹ under argon and nitrogen atmospheres.	249
6.5	TG-FTIR evolved gas analysis results for copper(II) oxalate heated in argon.	251
6.6	TG-FTIR evolved gas analysis results for copper(II) oxalate heated in argon: a greatly magnified spectrum slice at TG program temperature of 310.3 °C.	252
6.7	TG-FTIR evolved gas analysis results for copper(II) oxalate heated in nitrogen.	253
6.8	TG-FTIR evolved gas analysis results for copper(II) oxalate heated in nitrogen: a greatly magnified spectrum slice at TG program temperature of 309.8 °C.	254
6.9	DSC curves of copper(II) oxalate, run in crimped aluminium pans, in various mixed argon-nitrogen atmospheres.	256

6.10	Derivative DSC curves of copper(II) oxalate, run in crimped aluminium pans, in various mixed argon-nitrogen atmospheres. . . .	257
6.11	X-ray powder diffraction patterns of the residues of copper(II) oxalate heated in a DSC in crimped aluminium pans, from 25 °C to 350 °C at 10 °C min ⁻¹ under argon, mixed argon-nitrogen and nitrogen atmospheres.	258
6.12	DSC curves of copper(II) oxalate in argon and nitrogen atmospheres. Samples were heated from 25 °C to 350 °C at 10 °C min ⁻¹ in sealed, cold-welded pans perforated by a single pin-prick, in their specified atmospheres.	262
6.13	Derivative DSC curves of copper(II) oxalate in argon and nitrogen atmospheres. Samples were heated from 25 °C to 350 °C at 10 °C min ⁻¹ in sealed, cold-welded pans perforated by a single pin-prick, in their specified atmospheres.	263
6.14	DSC curves of copper(II) oxalate under argon at different heating rates. The samples (4 mg) were heated in crimped aluminium pans from 25 °C to 360 °C at the specified heating rates.	267
6.15	X-ray powder diffraction patterns of the residues of copper(II) oxalate heated under argon (25 ml min ⁻¹) at different heating rates. .	268
6.16	DSC curves of copper(II) oxalate under nitrogen at different heating rates. The samples (4 mg) were heated in crimped aluminium pans from 25 °C to 360 °C at the specified heating rates.	269
6.17	X-ray powder diffraction patterns of the residues of copper(II) oxalate heated under nitrogen (24 ml min ⁻¹) at different heating rates.	270
6.18	DSC curves of copper(II) oxalate samples (4 mg) heated in crimped aluminium pans at 10 °C min ⁻¹ under argon purge at various flow rates.	273
6.19	X-ray powder diffraction patterns of the residues of copper(II) oxalate heated as indicated under argon at various flow rates. . . .	274
6.20	DSC curves of copper(II) oxalate samples (4 mg) heated in crimped aluminium pans at 10 °C min ⁻¹ under nitrogen purge at various flow rates.	275
6.21	X-ray powder diffraction patterns of the residues of copper(II) oxalate heated as indicated under nitrogen at various flow rates. . . .	276
6.22	DSC and derivative DSC curves of copper(II) oxalate in oxygen. .	279
6.23	X-ray powder diffraction pattern (Cu-K _α radiation) of the residue of copper(II) oxalate heated in the DSC from 25 °C to 350 °C at 10 °C min ⁻¹ in oxygen.	280
6.24	Three-dimensional plot of $\Delta H_r^\circ(\beta, \omega)$ for proposed mechanisms involving the loss of $\frac{1}{2}\text{O}_2(g)$ (surface a) and $\text{O}(g)$ (surface b). . .	287

7.1	A simplified schematic diagram illustrating the various component parts of the original Philips X-ray detector.	301
7.2	An idealized preamplifier output pulse, shown in terms of its exponential decay constant.	304
7.3	A shorted delay-line used to generate a short pulse from a step input.	306
7.4	Illustrating the concept of single delay-line pulse-clipping.	307
7.5	A simplified schematic of a CR-RC pulse-shaping amplifier.	308
7.6	Traces at various stages of CR-RC-CR pulse shaping.	309
7.7	AC-coupled unipolar pulse trains (A) undergoing zero-line shifts with changing count-rate.	311
7.8	A simplified schematic of a CR-RC-CR pulse-shaper with pole-zero cancellation.	311
7.9	Diagrammatic representation of the various operations involved in pulse-height discrimination for three input pulses.	313
7.10	A simplified diagram of a ratemeter.	314
7.11	Pulse-height discriminator timing diagram of the outputs at the various stages of the circuit, for pulses which cross both the upper and lower discriminator thresholds.	328
7.12	Pulse-height discriminator timing diagram of the outputs at the various stages of the circuit, for pulses which cross only the lower discriminator threshold.	329
7.13	A schematic diagram of the new pulse-shaping amplifier and single-channel analyzer.	333
7.14	A schematic diagram of the new digital ratemeter/scaler and analog ratemeter output section.	334
B.1	X-ray fluorescence spectra for KRF-13 rock standard, KRF-13 with xst-cu-b4c-cl-rhombi , KRF-13 with xst-cu-b4c-no3-rhombi (prepared in chloride-free medium), and the NIM-L reference standard.	347
B.2	X-ray fluorescence spectra for boric acid (binder), KRF-13 rock standard, and boric acid with xst-cu-b4c-cl-rhombi	348
B.3	X-ray fluorescence spectra for KRF-13 rock standard, and KRF-13 with xst-cu-b4c-cl-rhombi	349

List of Tables

3.1	Copper-containing reagent solutions (in 30 ml deionized water) for straight-tube and U-tube syntheses.	62
3.2	Products recovered from the copper(II) nitrate/1,2,4,5-benzenetetracarboxylate straight-tube reaction.	64
3.3	Products recovered from the copper(II) sulfate/1,2,4,5-benzenetetracarboxylate straight-tube reaction.	66
3.4	Products recovered from the copper(II) chloride/1,2,4,5-benzenetetracarboxylate straight-tube reaction.	67
3.5	Products recovered from the copper(II) acetate/1,2,4,5-benzenetetracarboxylate straight-tube reaction.	68
3.6	Products recovered from the copper(II) acetate/1,2,4,5-benzenetetracarboxylate U-tube reaction	70
4.1	Results of elemental analyses of the needle-like products and their calculated metal-to-ligand ratios.	75
4.2	Experimental and calculated analyses for Group 1 products.	78
4.3	Experimental and calculated analysis figures for Group 2 products.	94
4.4	Experimental and calculated elemental analyses for Group 3 products.	104
4.5	Experimental and calculated elemental analyses for Group 4 products.	122
4.6	Experimental and calculated elemental analyses for Group 6 products.	135
5.1	Experimental parameters and data for multiple desolvation-resolution experiments (water, water) on xut-cu-b4c-acet-xtals.	169
5.2	Experimental parameters and data for multiple desolvation-resolution experiments (water, methanol) on xut-cu-b4c-acet-xtals.	174

5.3	Experimental parameters and data for multiple desolvation-resolution experiments (methanol, methanol) on xut-cu-b4c-acet-xtals	180
5.4	Experimental parameters and data for multiple desolvation-resolution experiments (methanol, water) on xut-cu-b4c-acet-xtals	184
5.5	Selected physical properties, in the liquid phase at room temperature, of potential guest species.	189
6.1	Analytical data for undried and dried copper(II) oxalate.	240
6.2	Specifications of the inert purge gases used.	244
6.3	DSC results of copper(II) oxalate heated in crimped aluminium pans, under 100% argon and 100% nitrogen atmospheres.	259
6.4	DSC results of copper(II) oxalate heated in crimped aluminium pans under mixed argon-nitrogen atmospheres.	260
6.5	DSC results of copper(II) oxalate heated under 100% argon and 100% nitrogen atmospheres. The samples were run in sealed aluminium pans of the cold-welded type, which were perforated with a single pin-prick.	261
6.6	DSC results for copper(II) oxalate heated under argon and nitrogen atmospheres at various heating rates.	271
6.7	DSC results for copper(II) oxalate heated at 10 °C min ⁻¹ under argon and nitrogen atmospheres at various flow rates.	277
6.8	DSC results of copper(II) oxalate heated in crimped aluminium pans under oxygen atmosphere.	281
6.9	DSC results of recent studies of the decomposition of copper(II) oxalate in different atmospheres and at various heating rates. . . .	288
6.10	Physical properties of selected gases.	291
7.1	Selected specifications of the Philips 18511 (Centronic ZP1610) proportional counter tube.	303
7.2	Selected specifications of the preamplifier and pulse characteristics of the Philips PW1965/40 proportional detector probe.	305
7.3	Pseudo-code illustrating the basic digital ratemeter execution cycle.	320

Part I

Copper(II)

1,2,4,5-benzenetetracarboxylate

studies

Chapter 1

Introduction

1.1 METAL-ORGANIC FRAMEWORKS (MOFs)

Metal-organic frameworks are a relatively new class of porous materials, which are the subject of a large and burgeoning field of research, which has yielded a large number of new materials, many of which have interesting characteristics. The desired outcome of this research is to make it possible for materials to be prepared, to order, with specific chemical and physical properties.

At the most basic level, metal organic frameworks are polymeric crystal lattices which contain metal centres linked by organic bridging ligands. This simple definition includes materials which contain voids, possibly containing guest molecules, and those which do not. Materials which do contain voids may be described as porous, but those porous materials which allow exchange of guest molecules (either with the original guest or by different guest species) are termed open-framework materials. A review of the basic terminology, synthetic strategies, structure types and sub-units, properties and future prospects of metal-organic frameworks is given in [1].

An extensive overview of the development of microporous materials — starting with the discovery of natural zeolites in the 17th century, the synthesis of artificial zeolites in the mid-1800s, the synthesis of zeolite-like aluminophosphates in the 1980s, the emergence of porous metal-organic complexes, and through to the creation of metal organic framework materials with extremely large pores by

the linking together of larger “secondary building units” (SBUs) — appears in in [2]. In a tutorial article focusing on the geometric aspects of network materials [3], three important strategies for producing materials with large open pores are summarized. These are *decoration*, *augmentation* and *expansion*.

To understand *decoration*, imagine a tetrahedral structure consisting of five identical spheres, one at the centre of the tetrahedron, and the other four at the vertices (corners); the central sphere is linked to the four outer spheres. Such a tetrahedron may be described as a TX_4 tetrahedron, where T signifies the centre sphere and X_4 the four outer spheres. As is well-known, the perfect diamond structure consists of sp^3 -hybridized carbon atoms arranged in such a way that each is tetrahedrally bound to four of its neighbours. Owing to the nature of the packing, there are open spaces between the spheres. Four tetrahedra can be stacked in the form of a larger tetrahedron, with three tetrahedra in the form of a triangular base, and the fourth resting on the apices of the three lower tetrahedra. In this example, this entails sharing the inner vertices, so that there is one sphere at the centre of each small tetrahedron, and ten others at the outer vertices of the small tetrahedra. The large tetrahedron may be termed a T_4X_{10} tetrahedron. In a similar way, this tetrahedron may be expanded to form a $T_{10}X_{20}$ tetrahedron¹ by placing it on a triangular base consisting of six tetrahedra. In this way, so-called supertetrahedra are built up. *Decoration* of a lattice might involve replacing every point in that lattice with a supertetrahedron, as illustrated for the sodalite and tetragonal (CrB_4) lattice-types in [4]. In these examples, the decorated lattice has extremely large cavities. For a given lattice type, the larger the SBU (i.e., the tetrahedra in the above examples), the larger the cavities within the structure.

Augmentation is a special case of decoration. To illustrate the point, consider the well-known CsCl crystal lattice, in which the Cs^+ and Cl^- lattices are of the simple cubic type. In the Cs^+ lattice, each Cs^+ ion is surrounded by six Cs^+ ions. Likewise, in the Cl^- lattice, each Cl^- ion is surrounded by six Cl^- ions. The CaB_6 crystal lattice is analogous to a simple cubic lattice, with Ca^{2+} corresponding to the Cs^+ ions in the CsCl lattice, but with hexameric octahedral B_6^{2-} anions occupying the Cl^- sites. Placing the hexameric cluster in the octahedral hole (connected to six other clusters) of the lattice is an example of *augmentation*. In

¹Erroneously designated T_8X_{20} in [3, Fig. 8].

general, augmentation involves replacing the vertices of an N -connected network (in which each vertex is connected to six others) with groups of N vertices. An example of this is the porous diamond-like lattice reported in [5] (with discussion, and more examples in [3]).

Expansion is the commonly-employed strategy to construct porous materials from metal ions and organic building blocks. For example, a diamond-like structure for a silver(I) complex with 4,4'-bipyridine was reported [6] in which tetrahedral silver(I) cations are bound together by μ_2 -bridging 4,4'-bipyridine molecules. Here, the single covalent bonds of the diamond structure have effectively been replaced by a series of bonds. It might be expected that the longer the linking unit (here, 4,4'-bipyridine), the larger will be the cavities in the structure. However, it often happens that pore-size is undermined by growth patterns such as interpenetration, where two networks form within each other, decreasing the overall pore-volume, or interweaving, where two networks form in such a way that they are in close contact with each other, possibly leading to mutual reinforcement [1].

Decoration (including augmentation as a special case) and expansion form a two-pronged approach in the present state of the art in the design of microporous materials. The often-cited three-dimensional microporous polymer "HKUST-1" [7], with formula $[\text{Cu}_3(1,3,5\text{-benzenetricarboxylate})_2 \cdot (\text{H}_2\text{O})_3]_n$ (excluding guest water molecules), provides an apt example. Figure 1.1 shows a diagram of the porous structure. Inset A shows the classic paddle-wheel motif, consisting two square-based pyramidal copper(II) cations bridged by four pairs of carboxyl groups as shown, with the apical water molecules on the coppers pointing in opposite directions. The SBU, shown in inset B, makes up the repeating unit of a decorated lattice, and the relatively large size of the SBU gives rise to large voids or pores within the structure. These pores contain ten lattice water molecules per formula unit, as determined by TG. Complete dehydration of this structure (i.e., including removal of the coordinated waters) and exposure to pyridine resulted in pyridine uptake to give $[\text{Cu}_3(1,3,5\text{-benzenetricarboxylate})_2 \cdot (\text{pyr})_3]_n \cdot 0.5(\text{pyr}) \cdot 2\text{H}_2\text{O}$. The X-ray diffraction pattern of this material is similar to that of the untreated HKUST-1, showing that the guest was exchanged, and the functional groups within the pore changed, without loss of structural integrity.

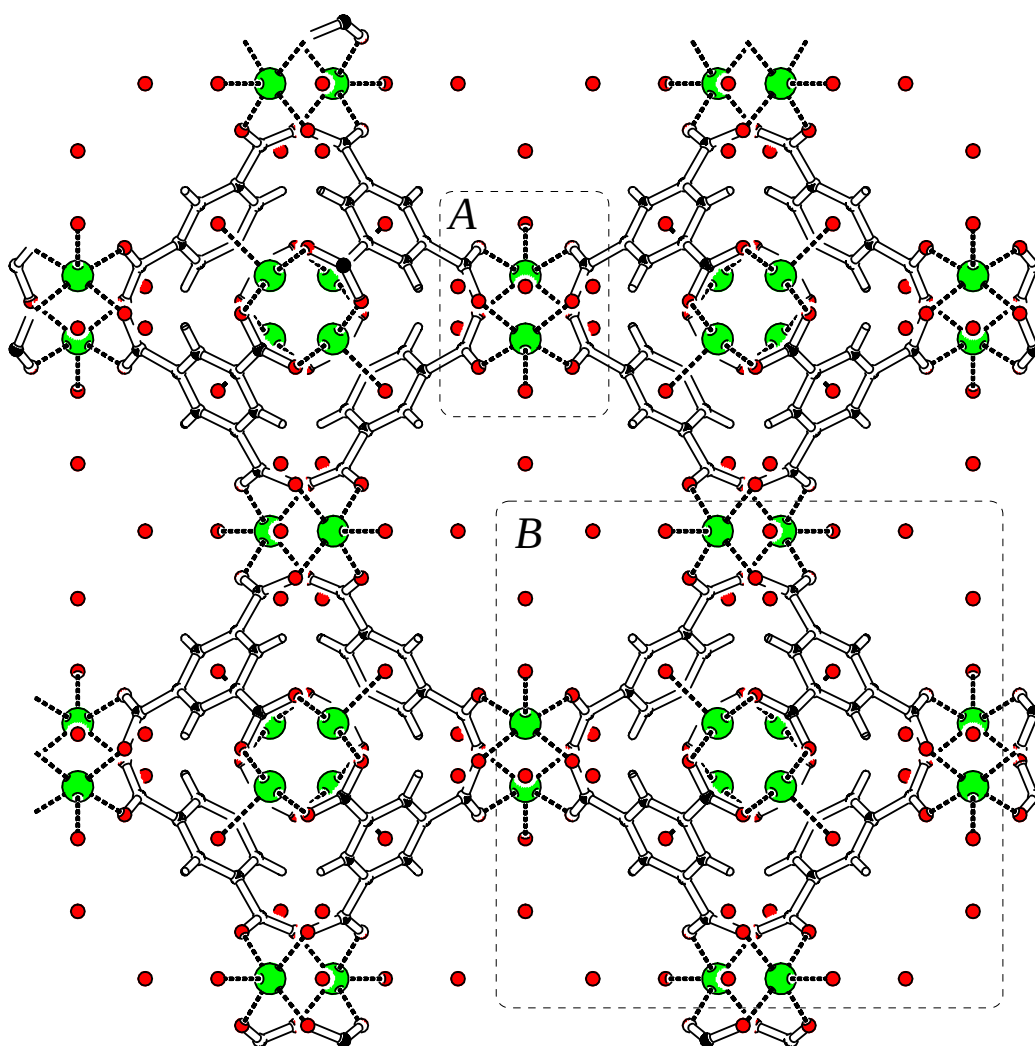


Figure 1.1: Drawing of the HKUST-1 structure [7]: (A) the “paddle-wheel” moiety, and (B) the SBU.

Subsequently, the gas-sorption properties of HKUST-1 (with a different synthesis) were investigated, and the results showed that it can be used for gas separation and air-purification [8]. This material also acts as a heterogeneous catalysis in the cyanosilation of benzaldehyde [9]. The presence of coordinatively unsaturated metal centres has been cited as the reason for the considerable ability of the dehydrated form of this material to adsorb hydrogen gas at low pressures [10] (at 77 K, up to 1 atm), while other metal organic frameworks are shown to surpass it greatly in gravimetric uptake at higher pressures [11] (at 77 K, up to 80 atm). A neutron powder-diffraction study (with Rietveld analysis) of D₂ (i.e., deuterium) into the dehydrated framework showed the positions of the D₂ molecules within the framework, and the order of filling of the six sites [12]. The first sites filled are at the apical positions of the coordinatively unsaturated copper(II) centres, and the others lie at various points within the voids in the structure.

One striking and famous example of how the the decoration—expansion strategy can be used to assemble a number of microporous materials — known as *isorecticular* MOFs, or IRMOFs — with successively larger pores from a given SBU is the series of metal-organic frameworks based on the tetrahedral μ_4 -oxo-bridged zinc-carboxyl cluster [13] shown in Figure 1.2. Inset (A) has one carboxyl group removed to show the central tetrahedral μ_4 -bridging oxide. Many larger frameworks have been constructed from this SBU by linking through longer linear or quasi-linear organic linking units [14], and also through large ligands of greater dimensionality such as 1,3,5-benzenetribenzoate [15]; such frameworks have large enough pores to accommodate polycyclic organic molecules. These materials have also been investigated as potential hydrogen absorbers [10, 11].

An early three-dimensional zinc dicarboxylate methanol solvate — without the Zn₄O cluster, but featuring a carboxyl-bridged cluster of three zinc atoms — showed interesting selective inclusion behaviour for alcohols (methanol, ethanol and *n*-propanol), ammonia and secondary amines, possibly due to the presence of coordinatively unsaturated metal centres in the dehydrated material [16]. The X-ray diffraction pattern of the dehydrated material showed some loss of peaks, peak-broadening and peak-shifts compared to that of the original material, but on the re-introduction of methanol, the X-ray diffraction pattern returns to that of the original material.

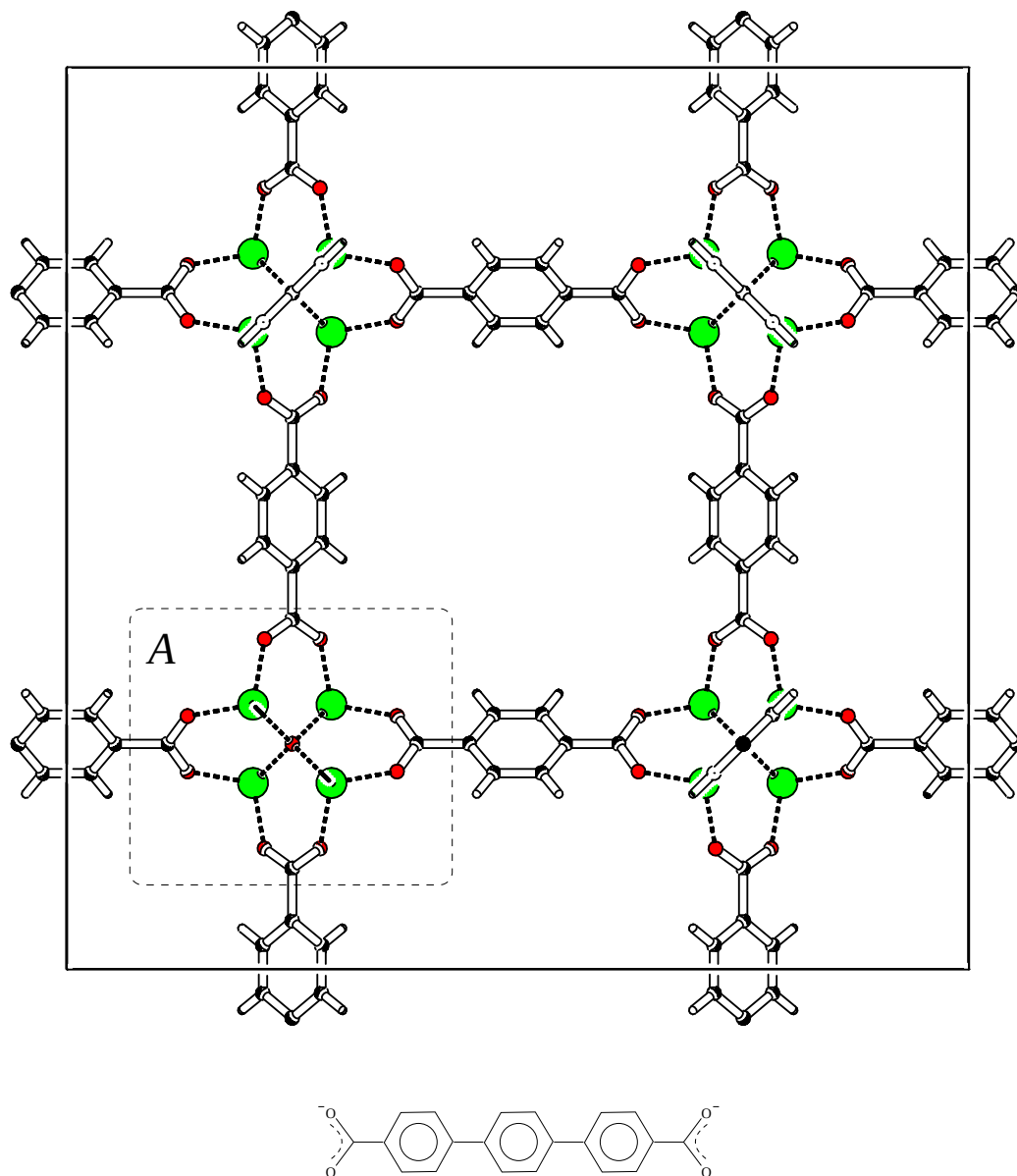


Figure 1.2: A view of the framework of MOF-5 [13], later named IRMOF-1. Tetrahedral zinc clusters are shown in green. Inset (A) has one carboxyl group removed to show the μ_4 -bridging oxide. Beneath this is drawn an example of the larger organic linking units employed to produce more open versions of this framework [14].

HKUST-1 and the IRMOF series are clearly examples of highly porous, three-dimensional open-frame metal-organic framework which have remarkable guest-exchange capability. By contrast, the three-dimensional mixed-valence Cu(I)–Cu(II) polymer, $[\text{Cu}_4(1,4\text{-benzenedicarboxylate})_3(4,4'\text{-bipy})_2]_n$ — which features a distorted three-quarter paddle-wheel bound to three μ_2 -bridging 1,4-benzenedicarboxylates with a pair of μ_2 -bridging 4,4'-bipyridine moieties attached at the “hub”, forming an “axle” by coordination to neighbouring paddle-wheels — has no unbound guest molecules and has very little porosity [17]. Not all metal-organic three-dimensional networks are microporous, although it is sometimes taken for granted that they are.

Likewise, polymers of lesser dimensionality (in terms of the covalently bound framework) have also shown interesting inclusion properties. Two-dimensional frameworks can also exhibit remarkable desolvation-resolvation behaviour. An early, but significant and much-cited, example is the layered polymer $\text{CoC}_6\text{H}_3(\text{COOH}_{\frac{1}{3}})_3(\text{pyr})_2 \cdot \frac{2}{3}(\text{pyr})$ [18]. This structure consists of flat sheets made up of monodentate and bidentate-bridging 1,3,5-benzenetricarboxylate units bound to in-plane coordination sites of octahedral Co(II) centres, the latter having pyridine molecules (disordered) coordinated at the two remaining sites above and below the sheet. The layers are held together by π -stacking of these coordinated pyridine molecules, forming three-dimensional cavities which contain guest pyridine molecules. This structure survives the removal (by heating to 200 °C) of the non-coordinated pyridine guests, as shown by X-ray powder diffraction, and remains crystalline after guest-removal. The remaining desolvated framework has the ability to selectively take up aromatic molecules (benzene and substituted benzenes) from mixtures of aromatic and non-aromatic liquids. Upon removal (by heating to 350 °C) of the coordinated pyridine molecules, which bind together the two-dimensional layers of the framework, the structure collapses, but on re-introduction of pyridine the original structure is restored. In certain circumstances, two-dimensional polymers held together by intermolecular interactions involving guest molecules can collapse, on desolvation, in such a way as to form covalently bound three-dimensional structures [19], thus creating robust frameworks which may have interesting guest-inclusion properties.

The examples cited above represent only a tiny fragment of the vast litera-

ture of open framework materials, a class which includes metal-organic frameworks. This literature has been surveyed recently, with the important metal-organic frameworks reported to date classified as magnetic, chiral, conducting, optical or sensing materials [20]. A concise review of current developments in the applications of coordination framework materials, with reference to their chemical, electronic/magnetic, and thermal/mechanical functions is given in [21]. A review of many metal-organic frameworks and other materials which have been found to have significant hydrogen absorption ability, with a summary of the metals and ligands employed, pore volumes, surface areas, gas-absorption properties and geometric characteristics, has been published recently [22].

1.2 COPPER(II) BENZENEPOLYCARBOXYLATES

A survey of the literature reveals that there are more than 1100 reported crystal structures of benzenepolycarboxylates of the transition elements from manganese through zinc, mainly coordination compounds plus a few ionic salts [23]. The compounds surveyed include salts and complexes of the various anions of the isomers of benzenedicarboxylic acid, benzenetricarboxylic acid, benzenetetracarboxylic acid, benzenepentacarboxylic acid and benzenehexacarboxylic acid. The copper compounds are most common, at about 30 % of the total number.

Benzenetetracarboxylates account for about 17 % of all polycarboxylate crystal structures of the transition elements manganese—zinc. Copper(II) benzenetetracarboxylates account for 23 % of the surveyed benzenetetracarboxylates, making the copper(II) compounds next most common after the cobalt(II) compounds, at about 30 %.

Copper(II) benzenetetracarboxylates account for fewer than 3 % of the surveyed benzenepolycarboxylate structures. Besides the monomeric complexes, most of these structures are one-dimensional chain polymers or two-dimensional layer structures, linked together by hydrogen-bonding and/or π - π interactions. About 20 % of the reported copper(II) benzenetetracarboxylate structures are three-dimensional covalent structures, of which nearly all can be said to contain one or more guest molecules in voids or channels in the structure.

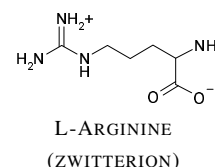
This section contains a detailed review of the reported crystal structures of

copper(II) compounds with the 1,2,4,5-benzenetetracarboxylate moiety. This includes the various protonated anions, and certain substituted forms such as benzenhexacarboxylate.

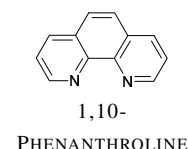
1.2.1 Copper 1,2,4,5-benzenetetracarboxylates

Relatively few crystal structures of copper(II) 1,2,4,5-benzenetetracarboxylates have been reported. The majority of these are mixed-ligand complexes, featuring organic bases coordinated to at least one of the copper atoms in the structure, mostly through nitrogen atoms.

One monomeric copper complex [24] contains 1,2,4,5-benzenetetracarboxylate (deprotonated) only as a counterion to a pair of aqua-bis(L-arginine)-copper(II) moieties. The arginines — as zwitterions [25] — are bound bidentately to copper(II) in a *trans* equatorial formation via the nitrogen and one carboxyl oxygen of the deprotonated α -amino acid group. The structure contains one guest water molecule per bis(aqua-bis(L-arginine))-copper(II) moiety, and is held together by hydrogen bonding.



The base which features most commonly in known 1,2,4,5-benzenetetracarboxylate structures is 1,10-phenanthroline, appearing in both monomeric and catenated complexes. One monomeric structure [26] is reported to contain a di-protonated 1,2,4,5-benzenetetracarboxylate unit as a counterion to a pair of bis-1,10-phenanthrolinechloro-copper(II) cations. In each of these, the copper(II) ion is in a distorted trigonal bipyramidal coordination sphere, with chloride in one of the equatorial positions, displaced by about 30 ° from the equatorial plane. The structure is built up of pairs of π -stacked bis-1,10-phenanthrolinechloro-copper(II) units, alternating with out-of-plane di-protonated 1,2,4,5-benzenetetracarboxylate units. The phenanthroline moieties face each other in such a way that the stacking involves three pairs of rings. The structure is hydrated, with water molecules forming linear hydrogen-bonded chains with the benzenetetracarboxylate units.



A similar motif occurs in another non-catenated structure [27], which has both coordinated and non-coordinated 1,2,4,5-benzenetetracarboxylate units. Two bis-1,10-phenanthroline-copper(II) cations — which are approximate inversions of

each other — are bridged by binding to diagonally-opposite carboxyl groups of a 1,2,4,5-benzenetetracarboxylate group, as shown schematically in Figure 1.3. The bis-1,10-phenanthroline copper(II) moiety shown on the left of this diagram is equivalent to the bis-1,10-phenanthrolinechloro-copper(II) moiety in the above complex, with the coordinated carboxyl oxygen being in a position roughly equivalent to that of the chlorine atom. As before, the structure is held together by π -stacking of pairs of bis-1,10-phenanthroline-copper(II) moieties, but here the stacking involves only two pairs of rings. A very similar structure was also re-

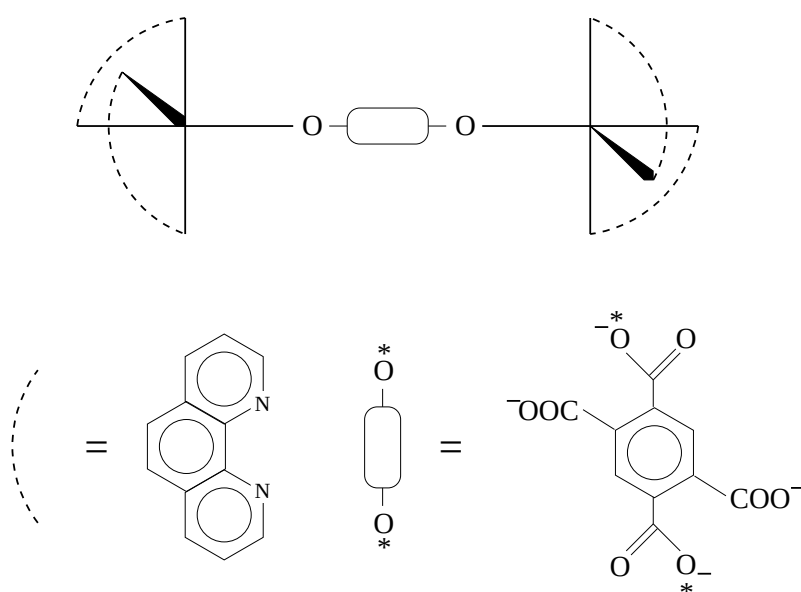


Figure 1.3: Non-catenated bis-1,10-phenanthroline-copper(II) complex with 1,2,4,5-benzenetetracarboxylic acid [27]. A non-coordinated, fully-protonated 1,2,4,5-benzenetetracarboxylate unit is also present, but is not shown in the diagram.

ported [28], at a lower temperature. In this structure, the coordinated (i.e., bridging) 1,2,4,5-benzenetetracarboxylate unit is reported to be mono-protonated, and the ionic 1,2,4,5-benzenetetracarboxylate is tri-protonated.

Polymeric structures can be constructed by catenation of 1,10-phenanthroline-copper(II) moieties through the 1,2,4,5-benzenetetracarboxylate unit, structures with types μ_2 -bridging [29]- and μ_4 -bridging [30, 31] (duplicate structures) having been reported. In the μ_2 -bridged structure, phenanthroline-copper(II) (dis-

torted square-planar) and non-planar 1,2,4,5-benzenetetracarboxylate units form zig-zag covalent chains. The three-dimensional structure is built up by hydrogen-bonding between neighbouring chains, and by π -stacking of the aromatic rings between alternating 1,2,4,5-benzenetetracarboxylate and phenanthroline rings.

In the μ_4 -bridged structure, pairs of the 1,10-phenanthroline copper(II) moieties are doubly linked by the 1,2,4,5-benzenetetracarboxylates to form a double-chain, as shown in Figure 1.4. The chains are linked to form two-dimensional layers by π - π interactions between the phenanthroline rings attached to the neighbouring chains. These layers are bound together by hydrogen-bonding between non-coordinated carboxyl oxygens in the layers and non-coordinated water molecules between the layers, forming a three-dimensional hydrogen-bonded framework [31].

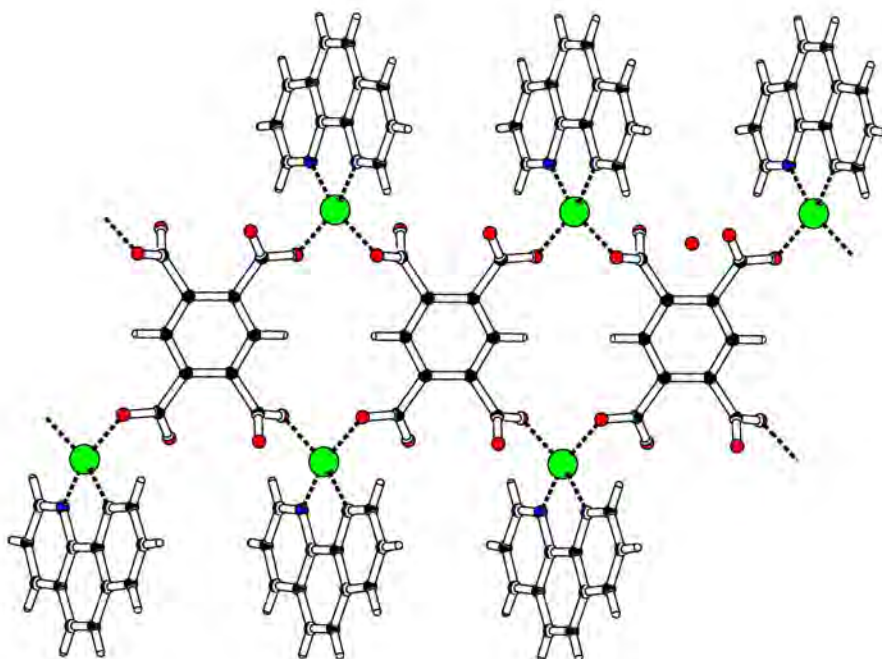


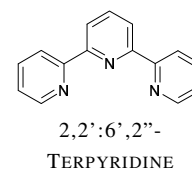
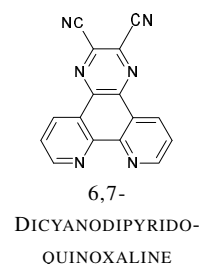
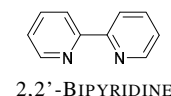
Figure 1.4: Double chain consisting of pairs of 1,10-phenanthroline copper(II) moieties doubly linked by 1,2,4,5-benzenetetracarboxylates [30].

A very similar structure — with 2,2'-bipyridine instead of 1,10-phenanthroline

— has been reported [32, 33]. As before, linear chains — made up of four-coordinate copper(II) ions μ_4 -bridged by fully-deprotonated 1,2,4,5-benzenetetracarboxylate units — are arranged in two-dimensional layers, held together by π - π interactions between 2,2'-bipyridine moieties bound to neighbouring chains. However, unlike the 1,10-phenanthroline analogue, this structure is not hydrated, and it is said [33] that the layers are held together by hydrogen-bonding interactions between hydrogens on the bipyridine rings belonging to one layer and carboxyl oxygens belonging to the next ($d(\text{C}-\text{H}\cdots\text{O}) \approx 2.5 \text{ \AA}$). Likewise, it can be seen from the crystal structure of the 1,10-phenanthroline analogue [30] that several hydrogen-oxygen interactions, shorter than or equal to $2.5 \text{ \AA}$, of the same type exist between phenanthroline hydrogens and aqua-oxygens ($d(\text{C}-\text{H}\cdots\text{O}) \approx 2.4 \text{ \AA}$), and between phenanthroline hydrogens and carboxyl oxygens (two sets, $d(\text{C}-\text{H}\cdots\text{O}) \approx 2.4 \text{ \AA}$ and $d(\text{C}-\text{H}\cdots\text{O}) \approx 2.5 \text{ \AA}$).

1,10-Phenanthroline and 2,2'-bipyridine share a common bidentate “bite” with 6,7-dicyanodipyridoquinoxaline, which appears in a μ_2 -bridging 1,5-diprotonated 1,2,4,5-benzenetetracarboxylate complex with copper(II) [34]. Each deprotonated carboxylate group bridges two copper(II) ions through one carboxyl oxygen. Each pair of copper(II) ions is bound in this way to two 1,2,4,5-benzenetetracarboxylate units, giving rise to a parallelogram motif (see Figure 1.5, p. 14) with a pair of copper atoms on the major diagonal and a pair of carboxyl oxygens on the minor diagonal. The non-equivalent square-based pyramidal copper(II) ions are each bound equatorially to a pair of heterocyclic nitrogens, a carboxyl oxygen and a bromide ion, and bound axially to a second carboxyl oxygen. The structure consists of a zig-zag three-strand coordination chain, within which there is π -stacking of alternating heterocyclic and 1,2,4,5-benzenetetracarboxylate rings. Methanol within the structure forms hydrogen-bonds to the carboxylic protons, and also to the non-coordinated oxygens of the carboxylate groups of neighbouring chains, thereby forming two-dimensional layers. These layers are π -stacked to form a three-dimensional structure.

2,2':6',2''-Terpyridine features in another anhydrous μ_4 -bridging 1,2,4,5-benzenetetracarboxylate complex [35]. The basic unit consists of a square-based pyramidal copper(II) ion, with three of the equatorial coordination sites occupied by the nitrogen donors from one, very nearly planar, terpyridyl moe-



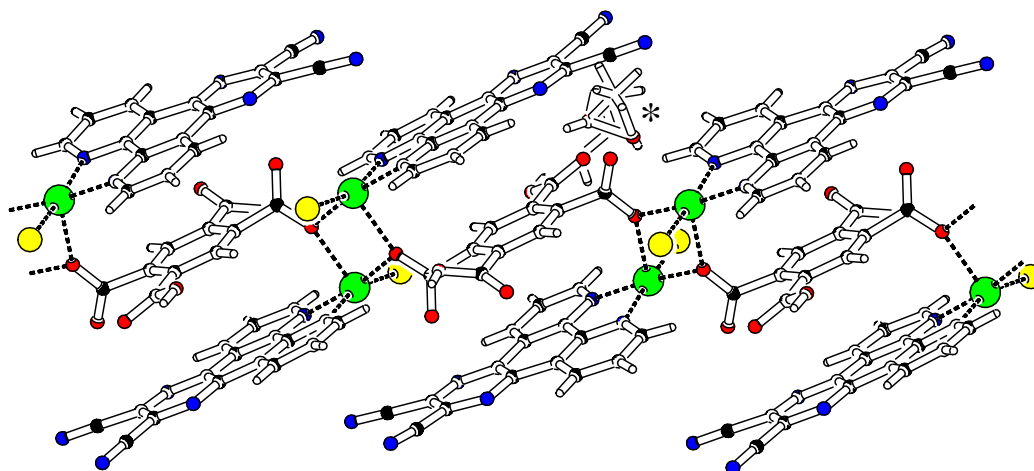
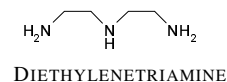


Figure 1.5: Parallelogram motif in the zig-zag covalent chains in [34]. Bromine ions are shown in yellow, and the asterisk indicates a disordered guest methanol molecule. The chains are hydrogen-bonded together — via guest methanol molecules — to form layers, which, in turn, form a three-dimensional structure by π -stacking of alternating 1,2,4,5-benzenetetracarboxylate and 6,7-dicyanodipyridoquinoxaline moieties.

ity. The remaining equatorial site and the axial site are occupied by carboxyl oxygens from staggered 1,2,4,5-benzenetetracarboxylate groups. The 1,2,4,5-benzenetetracarboxylate group bridges as follows: in both pairs of ortho-carboxylate groups, one carboxyl group binds axially to one terpyridyl-copper(II) moiety, and the other binds equatorially to another terpyridyl-copper(II) moiety. The carboxyl groups are out of plane with the phenolic ring to which they are bound, and the phenolic ring of the 1,2,4,5-benzenetetracarboxylate ion is out of plane with the terpyridine rings. Thus a zig-zag chain — described as a staircase [35] — is formed. These chains are linked to form a three-dimensional network via π - π interactions between the terpyridine rings of neighbouring chains, as shown in Figure 1.6 (p. 15).

Non-aromatic multifunctional chelating ligands can also function as terminal ligands. In one three-dimensional network polymer [36] with copper(II) and 1,2,4,5-benzenetetracarboxylate, diethylenetriamine binds to copper(II) in the same manner as terpyridine above, occupying three coordination sites roughly in plane. In this structure there are two crystallographically distinct copper(II) ions.



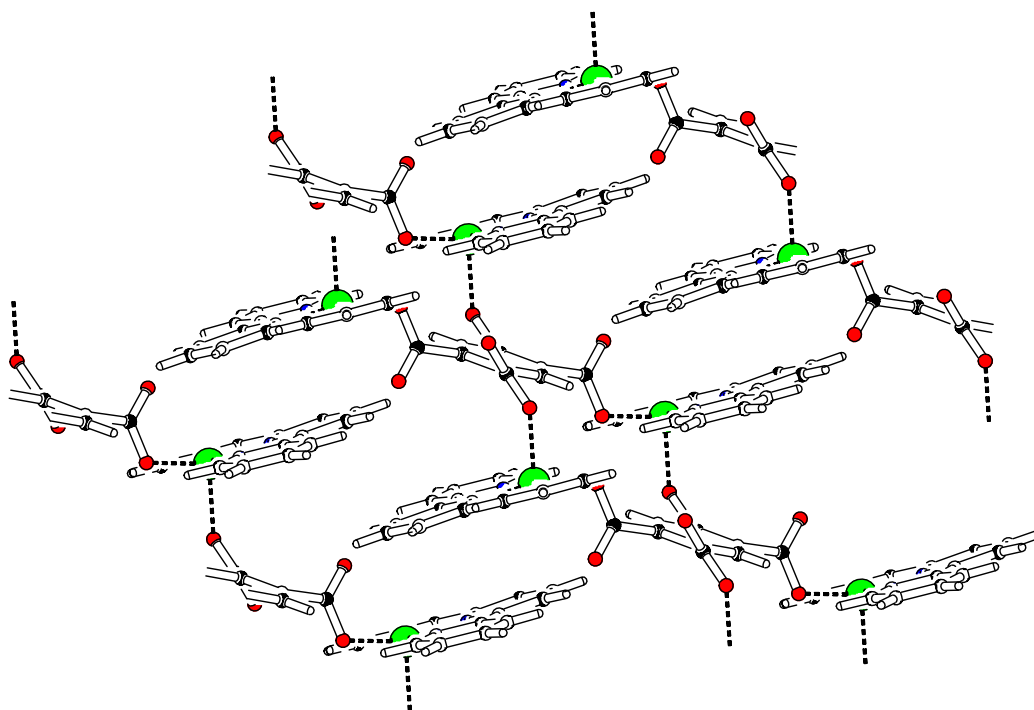


Figure 1.6: Staircase chains joined by π - π interactions to form a three-dimensional structure [35].

One type has an octahedral coordination sphere, being bound to three diethyletri-amine nitrogens and water in plane, with the remaining (diametrically opposite) coordination sites being occupied by carboxyl oxygens from monodentate carboxyl groups. The second type has a square-based pyramidal coordination sphere, being bound in-plane to three diethylentriamine nitrogens and a carboxyl oxygen on a bridging carboxyl group, and in the apical position to a non-equivalent carboxyl oxygen from a bridging carboxyl on a neighbouring unit. Each benzenetetracarboxylate unit functions as a μ_6 -bridging ligand, and has two types of carboxyl groups (*ortho* to each other): one type is singly bound to an octahedral copper(II) ion, and the other bridges two square-based pyramidal copper(II) ions. The benzenetetracarboxyl group is symmetrical about the axis running through the non-carboxyl carbons. The structure can be viewed as consisting of layers joined together by covalent bridging via the square-based pyramidal copper(II) atoms. The structure contains perchlorate counterions, and does not contain any guest water molecules.

The related ligand, 1,7-diamino-4-azaheptane, whose alkyl chains are longer by one carbon, acts as a terminal ligand in a monomeric dinuclear copper(II) complex with monodentate μ_2 -bridging 1,2,4,5-benzenetetracarboxylate (deprotonated) [37]. Each square-based pyramidal copper(II) ion is bound to three amine nitrogens and one carboxyl oxygen, and is bound to water in the apical position. An extensive hydrogen bonding network, involving all the amine nitrogens, both guest and coordinated water, and carboxyl oxygens², links the monomeric units to form a three-dimensional structure. The guest water molecules are arranged in a box-like octameric hydrogen-bonded cluster, which links adjacent monomeric units via hydrogen-bonding to waters at the corners of the box (see Figure 1.7, p. 16).

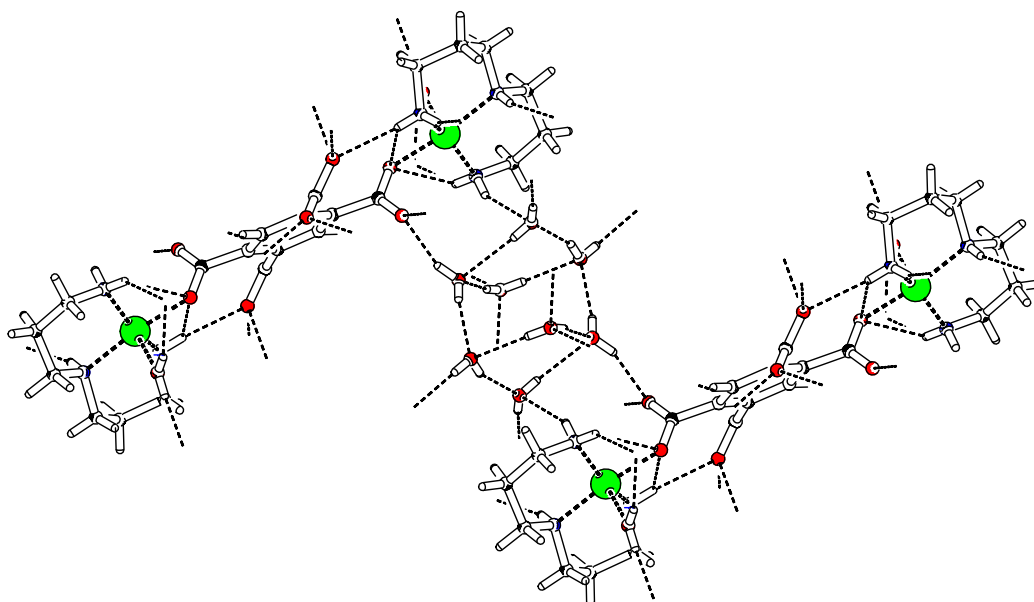
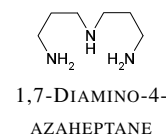
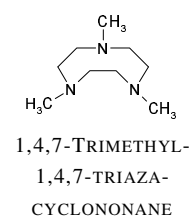


Figure 1.7: Hydrogen-bonded network, involving octameric guest-water clusters, linking monomeric units of the structure reported in [37].

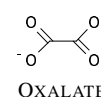
1,4,7-Trimethyl-1,4,7-triazacyclononane binds to copper(II) ions linked by μ_2 -bridging 1,2,4,5-benzenetetracarboxylate (deprotonated) to form a dinuclear monomeric complex [39]. Unlike terpyridine above, 1,4,7-trimethyl-1,4,7-



²According to calculations performed using PLATON [38], only the uncoordinated oxygens of the bridging carboxyl groups are involved in hydrogen bonding, although the original authors state (in the abstract) that all the carboxyl oxygens participate in hydrogen bonding.

triazacyclononane binds to the square-based pyramidal copper(II) ions through two equatorial and one apical site, with the remaining two equatorial sites being occupied by monodentate-bound *ortho* carboxyl groups. The dinuclear monomeric unit has a centre of inversion. The monomeric units are linked together by an extensive hydrogen-bonding network involving guest water molecules.

Several structures have been reported which show, in addition to bridging by the 1,2,4,5-benzenetetracarboxylate ligand, bridging by a second multifunctional ligand. One copper(II) complex is reported³ to have μ_{10} -bridging 1,2,4,5-benzenetetracarboxylate μ_2 -bridging oxalate and μ_2 -bridging water [40].



μ_2 -Bridging by pyrazine, in one structure [41], together with μ_4 -bridging by 1,2,4,5-benzenetetracarboxylate, forms two-dimensional layers. Each layer is bound by hydrogen bonding⁴ to the layer above and the layer below. One coordinated water hydrogen-bonds directly to a carboxyl oxygen from the neighbouring layer above. A second coordinated water hydrogen-bonds to the oxygen of a free water molecule, which itself hydrogen-bonds to a carboxyl oxygen of the same layer, as well as to a carboxyl oxygen of another neighbouring layer below. There is also hydrogen bonding between the coordinated water molecules and the carboxyl oxygens within the same layer. In this structure, there is a single crystallographically unique copper(II) ion, in a distorted octahedral coordination sphere, bound *cis* to two water molecules and to oxygens of a chelating carboxyl group roughly in plane, and bound also to a single carboxyl oxygen and a pyrazine nitrogen.



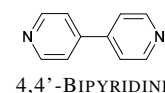
μ_2 -Bridging by pyrazine is the sole form of covalent bridging in another copper(II)-1,2,4,5-benzenetetracarboxylate complex [42], in which three of the four carboxyl groups on each 1,2,4,5-benzenetetracarboxylate unit are protonated. Each six-coordinate molecule is coordinated to two pyrazine moieties at 180 ° to each other, with the remaining four coordination sites occupied by opposite pairs of coordinated water molecules and carboxyl oxygens. Thus, there are one-dimensional chains made up of alternating pyrazine and copper(II) links. These chains are bound to each other by hydrogen bonding, both of the carboxylic-dimer

³No atom coordinates are given in the crystallographic data file.

⁴As determined from the crystal structure [41] using PLATON [38].

type to form layers of 1,2,4,5-benzenetetracarboxylate ions, and by bridging of the carboxyl oxygens of one layer and the coordinated water molecules of its neighbouring layer by uncoordinated water molecules. There are also π -stacking interactions between 1,2,4,5-benzenetetracarboxylate the layers.

Unlike 2,2'-bipyridine above, 4,4'-bipyridine can participate in bridging rather than chelation. This is exemplified by [43], a complicated three-dimensional structure in which two-dimensional layers made up of copper(II) and μ_6 -bridging 1,2,4,5-benzenetetracarboxylates are linked together by μ_2 -bridging 4,4'-bipyridine moieties. This complex has three non-equivalent copper(II) ions. Two are tetrahedral and are bound to 4,4'-bipyridine, with the remaining three sites being occupied by carboxyl oxygens. They differ in that they are bound to non-equivalent 1,2,4,5-benzenetetracarboxylates. The third is square-based pyramidal, with the axial site occupied by water and the other four by a 4,4'-bipyridyl nitrogen and three carboxyl oxygens.



There are two non-equivalent 4,4'-bipyridine moieties: both are μ_2 -bridging, but only one has the two rings in-plane. There are also two non-equivalent 1,2,4,5-benzenetetracarboxylate moieties. Both have one pair of *para* carboxyl groups, each bridging a pair of copper(II) ions to form linear chains. The remaining pair of carboxyl groups bridges (by monodentate binding) the copper(II) ions of separate chains to form a sheet. The 4,4'-bipyridine moieties tie neighbouring sheets together to form a three-dimensional structure. Guest water molecules occupy voids within the structure. The guest waters are hydrogen-bonded (as acceptors) to the coordinated water, and bridge (as donors) carboxyl oxygens of neighbouring sheets. In addition, the coordinated water hydrogen-bonds to a carboxyl oxygen in the same layer. This structure is thus held together by covalent bonds, assisted by inter-layer hydrogen-bonded bridging by guest water molecules.

4,4'-bipyridine, monoprotonated, acts as a terminal ligand in one structure [44] — a two-dimensional network polymer — which has 1,2,4,5-benzenetetracarboxylate in both μ_6 - and μ_4 -bridging modes. In this structure, there are two distinct copper(II) atoms (both square-based bipyramidal, one type bound only to carboxyl groups and the other bound also to monoprotonated 4,4'-bipyridine through the deprotonated nitrogen) and two 1,2,4,5-benzenetetracarboxylate units (deprotonated μ_6 -bridging and monoprotonated μ_4 -

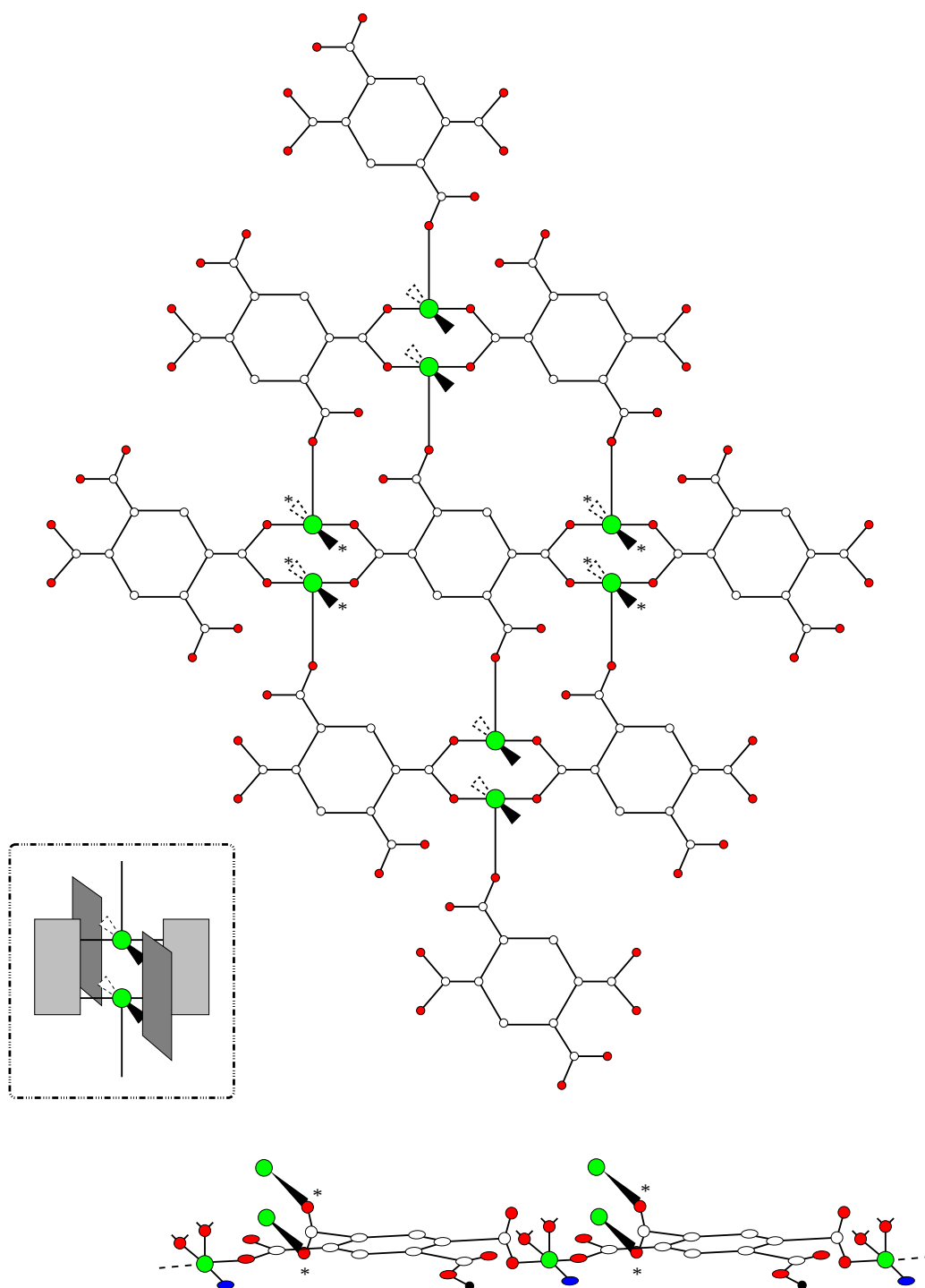


Figure 1.8: Layered structure [44], showing the covalently bound two-dimensional layer, consisting of copper(II) atoms and μ_6 -bridging 1,2,4,5-benzenetetracarboxylate ions. Each pair of open bonds to copper (marked with *) joins to a similarly-bound monoprotonated μ_4 -bridging 1,2,4,5-benzenetetracarboxylate ion and associated sub-structure (shown at the bottom of the figure). The asterisks indicate where the chain joins the layer. The monoprotonated 4,4'-bipyridine are omitted, except for the nitrogens bound to copper, which are shown in blue. The “paddle-wheel” moiety is illustrated in the inset.

bridging). The structure is made up of covalently-bound two-dimensional layers. Each layer consists of equivalent pairs of square-based pyramidal copper(II) ions bound together by the μ_6 -bridging 1,2,4,5-benzenetetracarboxylate ions as shown in Figure 1.8. (p. 19). The copper(II) atoms shown are also bound together by bidentate bridging involving μ_4 -bridging 1,2,4,5-benzenetetracarboxylate units, with carboxyl groups directed out of and into the plane of the paper (indicated as triangles in the figure), forming a structure known as a “paddle-wheel” (see figure inset). The μ_4 -1,2,4,5-benzenetetracarboxylates, in addition to being part of the paddle-wheels, also form zig-zag chains with copper(II) ions of the second type, i.e., bound to monoprotonated 4,4'-bipyridine. These chains run alongside the layers, linking neighbouring paddle-wheel structures as shown in the figure. The distance between the copper(II) ions in the paddle-wheel is 2.693 Å [44].

The chains bound to alternating layers are interpenetrated, and are joined together by hydrogen bonding to form a three-dimensional structure. Hydrogen bonding occurs between the protonated 4,4'-bipyridine (proton donor) moieties of one layer and a carboxyl oxygen from the μ_6 -1,2,4,5-benzenetetracarboxylate unit in the next (N—H...O = 1.902 Å). Hydrogen bonding can also occur between the protonated 1,2,4,5-benzenetetracarboxylate groups bound to neighbouring layers (O—H...O = 1.665 Å).

Imidazole — mainly, but not exclusively, as imidazolate [23] — has the potential for μ_2 -bridging through its two heterocyclic nitrogen atoms, but in the only reported crystal structure of a copper(II) complex with imidazole and 1,2,4,5-benzenetetracarboxylate [45], it acts as a terminal ligand only. In this structure, there are two crystallographically distinct octahedral copper(II) atoms. The first is the centre of a complex diaqua-tetrakis(imidazole) copper(II) cation, being bound to four imidazole moieties in plane and to two water molecules at the remaining two sites. The second has *trans* pairs of water molecules, imidazole molecules and carboxyl oxygens, and catenation of these bis(imidazole) copper(II) units by μ_2 -bridged 1,2,4,5-benzenetetracarboxylate moieties (completely deprotonated) form infinite one-dimensional chains. The diaqua-tetrakis(imidazole) copper(II) cations are packed between parallel chains, and it is reported⁵ that the structure is held together by hydrogen bonding between the imidazole nitrogens, water coordinated to the complex cations and uncoordinated carboxyl oxygens [45]. Ex-



IMIDAZOLE

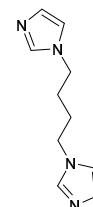
tensive hydrogen bonding is also reported to exist between the complexes and uncoordinated guest water molecules.

In contrast to imidazole, no crystal structure involving μ_2 -bridging methylimidazole has been reported. It appears as a terminal ligand in an anhydrous two-dimensional coordination polymer [46] with square-planar *trans*-methylimidazole copper(II) moieties forming layers with monodentate μ_4 -bridging 1,2,4,5-benzenetetracarboxylate anions (deprotonated). The layers are held together by interlayer π - π interactions between methylimidazole rings.



METHYLMIDAZOLE

The 1,1'-(1,4-butanediyl)-bis(imidazole) moiety is a flexible potential μ_2 -bridging ligand which has been reported in several structures with transition metals such as zinc(II) [47, 48], cadmium(II) [47, 49], cobalt(II) [48] and copper(II) [50, 51]. It appears in a three-dimensional polymeric copper(II) complex with μ_2 -bridging 1,2,4,5-benzenetetracarboxylate (deprotonated) [52]. There are three non-equivalent copper(II) cations. Two are square-planar, each bound in a *trans* configuration to two μ_4 -bridging 1,2,4,5-benzenetetracarboxylate ions (monodentate) and to two μ_2 -bridging 1,1'-(1,4-butanediyl)-bis(imidazole) moieties. The two differ slightly in the Cu–O and, to a lesser extent, the Cu–N bond lengths. The copper that has the longer Cu–O and Cu–N bonds has long-range tetragonal interactions with water (2.719 Å), possibly as a result of Jahn-Teller effects. The third type of copper(II) atom is in a square-based pyramidal configuration, binding to three μ_2 -bridging imidazole nitrogens, to one carboxyl oxygen from μ_4 -bridging 1,2,4,5-benzenetetracarboxylate, and to water in the apical position. The structure contains uncoordinated water molecules in large pores. There is potentially⁶ an extensive hydrogen bonded network involving carboxylate oxygens, uncoordinated guest waters and waters coordinated to copper, which bridges across the pores and which may play a role in stabilizing the structure.

1,1'-(1,4-BUTANE-
DIYL)-BIS(IMID-
AZOLE)

μ_2 -bridging 4-aminopyridine is rare but not unknown [53, 54] (both silver(I) complexes). However, it acts as a terminal ligand in a hydrated chain polymer [55] consisting of square-planar *trans* bis-4-aminopyridine-*N*-copper(II) moieties linked together by monodentate μ_2 -bridging 1,2,4,5-benzenetetracarboxylate an-



4-AMINOPYRIDINE

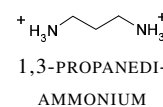
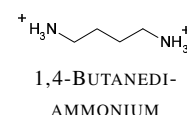
⁵The hydrogen bonding could not be calculated independently because the reported structure does not list hydrogen atoms.

⁶These could not be identified because no information about the positions of hydrogen atoms on guest water molecules was provided in the crystal structure.

ions (deprotonated). In addition, there are two water molecules 2.9 Å and 2.6 Å away from the Cu(II) cation, above and below the remaining two sites associated with the octahedral geometry. Protonated 4-aminopyridinium cations are interspersed between the chains, and the three-dimensional structure is held together by extensive networks of hydrogen bonding and π - π interactions.

1,4-Butanediamine has two nitrogen donor sites, and appears as a μ_2 -bridging ligand in crystal structures with copper(II) [56], with the copper(II) the dicyanoargentato(I) moiety [57], and with copper(I) [58] (all polymeric). However, it appears as a counterion — the 1,4-butanediammonium di-cation — in an anionic three-dimensional covalent network polymer [59] with copper(II) and μ_6 -bridging 1,2,4,5-benzenetetracarboxylate (deprotonated). In this structure, there are two crystallographically unique copper(II) ions: one is octahedral, and bound *trans* to two pairs of water and one pair of monodentate carboxyl groups); the other is square-based pyramidal, bound to five carboxyl groups (one monodentate, four μ_2 -bridging to neighbouring equivalent copper). Each 1,2,4,5-benzenetetracarboxylate unit is monodentately bound to copper(II) via the oxygens of *para* carboxyl groups, while each of the remaining pair of carboxyl groups bridges a pair of equivalent square-based pyramidal copper(II) ions ($d(\text{Cu}-\text{Cu}) = 2.67$ Å). This pair of copper(II) ions, together with the coordinated 1,2,4,5-benzenetetracarboxylate moieties, forms a “paddle-wheel” similar to the one shown in Figure 1.3 (inset, p. 11). The 1,4-butanediammonium cation occupies channels within the structure, and non-equivalent pores are occupied by non-coordinated water. Although the structure extends via coordination between copper(II) and 1,2,4,5-benzenetetracarboxylate, there is a hydrogen-bonded network stretching across the pores, involving the $-\text{NH}_3^+$ groups (donors only), carboxyl oxygens, and uncoordinated and coordinated water molecules.

1,3-Diaminopropane can act both as a chelating ligand and as a μ_2 -bridge with copper — see [60] for an example where both types of binding appear in the same structure. It has also been reported as a μ_2 -bridging ligand in polymeric copper(II) complexes, for example in [61]. However, like the 1,4-butanediammonium ion, it acts as a counterion (1,3-propanediammonium) in an anionic three-dimensional covalent polymeric copper(II) complex [62] with μ_4 -bridging 1,2,4,5-benzenetetracarboxylate (deprotonated). The structure can be viewed as a series

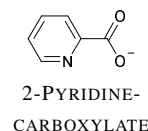
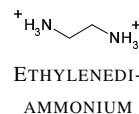


of criss-cross intersecting two-dimensional sheets made up of square-planar copper(II) ions, each bound to four 1,2,4,5-benzenetetracarboxylate anions via monodentate carboxyl groups. The structure has two sets of large rhombic channels, one set housing non-coordinated guest water molecules, and the other, the 1,3-propanediammonium cations. As before, with 1,4-butanediammonium, the channels are traversed by a hydrogen-bonding network. This network involves both bound and unbound carboxyl oxygens, -NH_3^+ groups (donors only) and guest water molecules.

Simultaneous DSC-TG⁷ (heating at $10\text{ }^\circ\text{C min}^{-1}$) in dry nitrogen (100 ml min^{-1}) revealed that this complex loses its guest waters (two per copper atom) in a single broad step between $44\text{ }^\circ\text{C}$ and $150\text{ }^\circ\text{C}$, remains stable until $219\text{ }^\circ\text{C}$, at which temperature it decomposes in two steps ($219\text{ }^\circ\text{C}$ — $339\text{ }^\circ\text{C}$ and $339\text{ }^\circ\text{C}$ — $458\text{ }^\circ\text{C}$), with mass-loss continuing until $1000\text{ }^\circ\text{C}$ was reached, to a final mass slightly heavier than the calculated masses for Cu_2O or CuO residues. All the thermal events are reported to be endothermic.

Ethylenediamine also appears in mixed μ_2 -bridging and chelating coordination modes in complexes with copper(II) [63] and copper(I) [64]. As ethylenediammonium, it appears as a counterion in two anionic two-dimensional copper(II) complexes with 1,2,4,5-benzenetetracarboxylate (deprotonated). Both complexes [65] consist of alternating layers, one of copper(II) and μ_4 -bridging 1,2,4,5-benzenetetracarboxylate and the next of water and ethylenediammonium ions. In both complexes, copper(II) is bound to four 1,2,4,5-benzenetetracarboxylate ions via monodentate carboxyl groups. The two complexes differ in that in one, the copper(II) adopts a square-pyramidal geometry (water in the apical position), and in the other, it adopts a square-planar geometry.

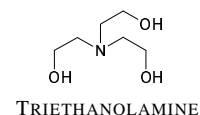
2-Pyridinecarboxylate is an obvious *N,O*-chelator, and appears as such in a one-dimensional network polymer [66] with completely protonated 1,2,4,5-benzenetetracarboxylic acid. Octahedral bis(2-pyridinecarboxylato-*N,O*)copper(II) moieties form a zig-zag chain with monodentate μ_2 -bridging 1,2,4,5-benzenetetracarboxylic acid, via *para* carboxylic acid groups. The zig-zag chains are held together by a hydrogen-bonding network involving non-coordinated guest water molecules (acting as bridges between chains),



⁷Results are as discussed in the original paper; the DSC-TG curves were not shown.

pyridinecarboxylate oxygens and benzenetetracarboxylate oxygens.

Triethanolamine, as triethylaminolate, acts as both a chelating and a μ_3 -bridging ligand in a recently reported [67] water-soluble two-dimensional bimetallic copper(II) complex, also including sodium, with μ_2 -bridging water and μ_4 -bridging 1,2,4,5-benzenetetracarboxylate (deprotonated). Each 1,2,4,5-benzenetetracarboxylate unit is bound symmetrically about the axis which passes through the ring-hydrogens. In each adjacent pair of carboxylate groups, one group is bound monodentately to a distorted octahedral sodium ion, and the other bridges this sodium ion to a distorted octahedral copper(II) ion. The copper(II) ion is tetradentately bound to a triethanolaminato anion (singly deprotonated): nitrogen is bound *cis* to the carboxyl oxygen and the O^- occupies the site *trans* to the carboxyl oxygen. These three sites define a plane. The two OH groups occupy sites above and below the plane. The remaining octahedral coordination site is occupied by an O^- from a neighbouring equivalent triethanolaminato. One of the triethanolamine OH groups functions as a third μ_2 -bridge between the copper(II) and sodium ions. The sodium ion is doubly bridged to its equivalent neighbour by two μ_2 -bridging water molecules, and the remaining octahedral coordination site, opposite the carboxyl oxygen, is occupied by terminal water. Similarly, the copper(II) ion is also doubly bridged to its equivalent neighbour by a pair of μ_2 -bridging triethanolaminato O^- groups (the one belonging to the neighbouring unit, mentioned above).



Thus the metal-to-metal bridging can be described in terms of four-membered rings:

Na-to-Na : Na to water to Na to a second water and back to Na,

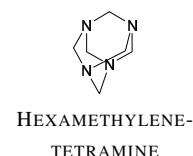
Cu-to-Cu : Cu to triethylaminato O^- to Cu to a second triethylaminato O^- back to Cu,

Na-to-Cu : Na to carboxyl O^- to Cu to triethylaminato OH and back to Na.

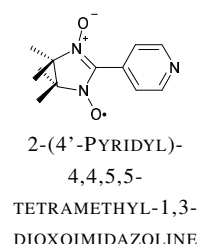
There are also nine- and ten-membered rings involving these two metal atoms and carbon chains of the organic ligands. The copper-sodium units, bridged by 1,2,4,5-benzenetetracarboxylate, form two-dimensional layers. These are

bound together by hydrogen-bonding interactions involving carboxyl groups, triethanolamine oxygens, coordinated water molecules and guest water molecules. The guest water molecules are arranged in decameric units, consisting of nearly-planar eight-membered rings, with two dangling water molecules at opposite ends, resembling a chair-conformation. This complex has shown catalytic activity in the oxidation of cyclohexane and cyclopentane by hydrogen peroxide in aqueous acetonitrile. A very recent study of the catalytic behaviour of this complex is given in [68].

Hexamethylenetetramine can act as a μ_4 -bridging ligand with gallium [69] (other bridging modes also reported with Ga and Al), silver [70] (many other structures reported with silver) and others. However, it acts as a μ_2 -bridging ligand with square-based pyramidal copper(II) and μ_4 -bridging 1,2,4,5-benzenetetracarboxylate (deprotonated) [71]. Each carboxyl group is bound to one copper in monodentate fashion. Each copper(II) is bound equatorially to two carboxyl groups (*trans*), one water and one hexamethylenetetramine nitrogen, and axially to water. Copper(II) ions, bridged by 1,2,4,5-benzenetetracarboxylate ions, form two-dimensional layers, which are bound together by μ_2 -bridging hexamethylenetetramine moieties to create a three-dimensional covalent structure. The covalent layers are similar to those found in the two-dimensional network polymer reported in [72] (discussed on p. 29), but in the present complex, these are linked together by covalent bonds, not hydrogen bonds. Guest water molecules — four per copper(II) ion — are contained in rhombic channels, and the original authors report many hydrogen bonding interactions involving carboxyl groups and water molecules ⁸.



2-(4'-pyridyl)-4,4,5,5-tetramethyl-1,3-dioxoimidazoline has been reported both as a μ_2 -bridging ligand [73] and a μ_3 -bridging ligand [74] with copper(II). However, it acts as a terminal ligand in one reported copper(II) complex with μ_2 -bridging 1,5-diprotonated 1,2,4,5-benzenetetracarboxylate [75]. The structure is made up of one-dimensional chains of distorted square-based pyramidal copper(II) atoms bridged by coordination (equatorially) to the *meta* carboxyl groups of the 1,5-diprotonated 1,2,4,5-benzenetetracarboxylate ions. The remain-



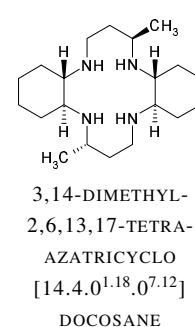
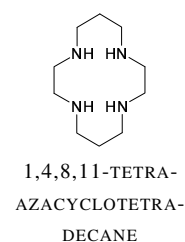
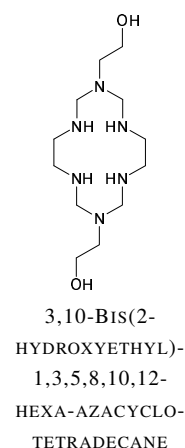
⁸The crystal structure does not list the positions of the hydrogen atoms, so the hydrogen bonds could not be inspected independently.

ing equatorial position is occupied by water, and the two axial positions are occupied by the heterocyclic nitrogens of two 2-(4'-pyridyl)-4,4,5,5-tetramethyl-1,3-dioxoimidazoline moieties. Each chain is bound to its neighbouring chains by a hydrogen-bonded network, involving hydrogen-bonding between protonated carboxyl groups via bridging guest water molecules, and between 2-(4'-pyridyl)-4,4,5,5-tetramethyl-1,3-dioxoimidazoline-*N*-oxide oxygens and protonated carboxyl groups via bridging guest water molecules.

3,10-bis(2-hydroxyethyl)-1,3,5,8,10,12-hexa-azacyclotetradecane is a macrocyclic polyaza ligand analogous to a crown ether, but has nitrogen donors instead of oxygens. It forms both monomeric [76] and polymeric [77] complexes — both anhydrous — with copper and partly-protonated 1,2,4,5-benzenetetracarboxylate ions. The monomeric complex (see Figure 1.9) is unusual in that it has a tri-protonated benzenetetracarboxylic acid moiety, and also because it features coordination of the carbonyl oxygen of a carboxylic acid group to copper(II) (as assigned by the original authors on the basis of Cu–O bond length, hydrogen bonding properties and vibrational spectra). In the polymeric complex, 3,10-bis(2-hydroxyethyl)-1,3,5,8,10,12-hexa-azacyclotetradecane copper(II) moieties are linked by monodentate binding to μ_2 -bridging diprotonated 1,2,4,5-benzenetetracarboxylate anions, which coordinate to copper(II) via deprotonated, *para* carboxyl groups. The chains are held together by intermolecular hydrogen bonding between the hydroxyethyl groups of adjacent chains.

The related 1,4,8,11-tetraazacyclotetradecane copper(II) moiety, similarly, forms a hydrated chain polymer due to monodentate μ_2 -bridging by diprotonated 1,2,4,5-benzenetetracarboxylate ions [78]. This structure also has the unusual property that copper(II) is coordinated to the carbonyl oxygens of protonated carboxyl groups (as assigned by the original authors on the basis of bond distances). It is also unusual in that the μ_2 -bridging takes place via *meta* carboxyl groups (see also [75] for a similar binding motif).

Another related crown-like ligand is 3,14-dimethyl-2,6,13,17-tetraazatricyclo[14.4.0^{1.18}.0^{7.12}]docosane, which forms a monomeric complex with copper(II) and 1,5-diprotonated 1,2,4,5-benzenetetracarboxylic acid [79]. The square-based pyramidal copper(II) ion is bound axially to the four nitrogens, and also via the apical position to one of the carboxyl oxy-



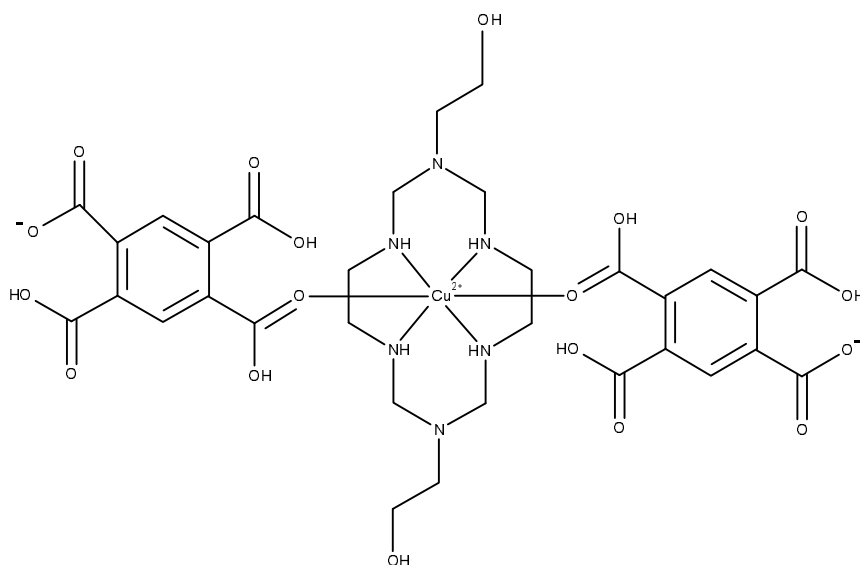
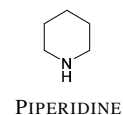


Figure 1.9: Monomeric copper(II) complex with 3,10-bis(2-hydroxyethyl)-1,3,5,8,10,12-hexa-azacyclotetradecane and 1-carboxylato-2,4,5-benzenetetracarboxylic acid. This complex shows unusual coordination of the carbonyl oxygen to copper [76].

gens of one of the deprotonated carboxyl groups. Each guest water bridges three 1,2,4,5-benzenetetracarboxylato-(3,14-dimethyl-2,6,13,17-tetraazatri-cyclo[14.4.0^{1.18}.0^{7.12}]docosane)-copper(II) moieties by acting as a proton donor to two carboxyl oxygens and as a proton acceptor to one aza nitrogen. There is additional intermolecular hydrogen bonding between carboxylic acid groups and aza groups and between the carboxylic acid groups of different monomeric units.

Piperidine, although it acts as a ligand with copper(II) in several compounds, including a catenated copper(II)-1,2-benzenedicarboxylate [80] complex, appears as a guest in channels in a copper chain polymer with diprotonated 1,2,4,5-benzenetetracarboxylate [81]. Each square-based pyramidal copper(II) is equatorially bound to *trans* pairs of carboxyl oxygens and water molecules, and to water in the apical position. Chains of alternating copper(II) and 1,5-diprotonated 1,2,4,5-benzenetetracarboxylate units are linked by hydrogen bonding to form a porous three-dimensional polymer⁹. Large open channels exist within the structure, and these are occupied by guest water and piperidine molecules.



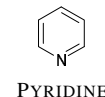
PIPERIDINE

⁹Atom positions were not given in the crystal structure data.

For the formula $\{[\text{Cu}(\text{H}_2\text{B4C})(\text{H}_2\text{O})_3]_2(\text{H}_4\text{B4C})(\text{pip})_2 \cdot \text{H}_2\text{O}\}_n$ (B4C = 1,2,4,5-benzenetetracarboxylate and pip = piperazine, $\text{C}_5\text{H}_{11}\text{N}$), the results of TG experiments¹⁰ (heating at $10\text{ }^\circ\text{C min}^{-1}$ in nitrogen) indicate that the structure loses its three water and two piperidine guests in two steps when heated to $127\text{ }^\circ\text{C}$. The six coordinated water molecules are lost between $127\text{ }^\circ\text{C}$ and $225\text{ }^\circ\text{C}$. Two further mass losses occur between $225\text{ }^\circ\text{C}$ and $370\text{ }^\circ\text{C}$ which correspond to the loss of two 1,2,4,5-benzenetetracarboxylic acid molecules, leaving a residue of mass which corresponds to $[\text{Cu}_2(\text{B4C})]$, which slowly loses mass on further heating to $600\text{ }^\circ\text{C}$.

On heating to $130\text{ }^\circ\text{C}$ for one hour, to drive off the guest water and piperidine molecules, the structure was shown by XRPD to collapse. XRPD studies of the rehydrated material showed that the original structure was not completely regained on rehydration¹¹. Similar studies after dehydration by heating to $210\text{ }^\circ\text{C}$, to drive off the coordinated water molecules, followed by rehydration, showed that the rehydrated material did not regain its original structure.

Pyridine appears in one copper(II) 1,2,4,5-benzenetetracarboxylate complex as a nitrogen donor [82] in a two-dimensional copper(II) complex with monodentate μ_4 -bridging 1,2,4,5-benzenetetracarboxylate. Each copper is bound axially to water and equatorially to *trans* pairs of pyridine (out of plane) and carboxyl oxygens. Cavities within the structure contain guest water clusters, and these are hydrogen bonded to each other, to the coordinated water molecules and to carboxyl oxygens. Thus the water molecules present in the structure form hexameric clusters which bridge the two-dimensional layers of the structure by hydrogen bonding via the carboxyl groups of neighbouring layers. These hexameric clusters adopt a puckered boat conformation similar to the formation found in hexagonal ice [83, 84] (and other references cited in [82]). XRPD and FTIR evidence suggested that, after dehydration at $140\text{ }^\circ\text{C}$ under vacuum, long exposure to water vapour did not lead to the reabsorption of water into the crystal lattice, and that



¹⁰TG curves not shown in the reference.

¹¹The term “rehydration” appears in the original reference, and no attempt to re-introduce piperidine into the dehydrated material is mentioned. Considering that the three-dimensional structure consists of one-dimensional chains held together by hydrogen bonding, in which piperidine can participate, it is not surprising that the structure of the rehydrated material shows significant differences to that of the original material.

the host lattice broke down due to the removal of water. An identical structure was obtained as part of this study, and this is described in more detail in Section 4.4.4 (p. 127).

Of particular importance to the present study are those copper(II) 1,2,4,5-benzenetetracarboxylates which contain no ligands or counterions aside from 1,2,4,5-benzenetetracarboxylate itself and OH^- . μ_2 -Bridging of square-based pyramidal copper(II) ions via *para* monodentate carboxyl groups of 1,5-diprotonated 1,2,4,5-benzenetetracarboxylate groups forms linear chains in a 1:1 copper:1,2,4,5-benzenetetracarboxylate complex [85, 86]. The one-dimensional chains are built up into a three-dimensional structure by hydrogen bonding involving protonated carboxyl groups, coordinated water and non-coordinated guest water as donors, and guest water, carbonyl oxygens and carboxylate oxygens as acceptors. Thermal analysis and kinetic models for decomposition are reported in [86].

In one 2:1 copper:1,2,4,5-benzenetetracarboxylate complex [72], square-based pyramidal copper(II) ions — each bound equatorially to *trans* pairs of water and carboxyl oxygens (monodentate) and also to water in the apical position — form neutral covalent two-dimensional layers with monodentate μ_4 -bridging 1,2,4,5-benzenetetracarboxylate. These layers are linked together by hydrogen bonding, the proton donors being mostly coordinated water molecules but also non-coordinated guest waters¹², and the acceptors being mainly bound and unbound carboxyl oxygens, but also guest and coordinated water molecules. This structure is discussed in greater detail in Section 4.3.3 (p. 110).

Another two-dimensional layered polymer, with less hydration, has been reported in [87]. In this structure, square-based pyramidal copper(II) centres are linked to form uncharged layers by μ_6 -bridging 1,2,4,5-benzenetetracarboxylate anions (deprotonated). The substituents are distributed on the ring in *para* pairs of singly bound and bridging carboxyl groups. Each square-based pyramidal copper(II) ion is bound equatorially a *cis* pair of water, to one oxygen from a bridging carboxyl group, and to one oxygen from a monodentate carboxyl group on a different 1,2,4,5-benzenetetracarboxylate ligand; it is also bound in the ax-

¹²The crystal structure lists the hydrogen positions of only one of the two guest water molecules (per copper).

ial position to an oxygen from a bridging carboxyl group on a third 1,2,4,5-benzenetetracarboxylate ion. The copper(II)-1,2,4,5-benzenetetracarboxylate layers thus formed are linked by hydrogen bonding. There are a large number of potential hydrogen-bonding contacts between carboxyl oxygens and water molecules (coordinated and non-coordinated), and between water molecules and each other ¹³. This structure is discussed in greater detail in Section 4.3.3, (p. 115).

Also of particular interest is an anhydrous three-dimensional 3:1 copper:1,2,4,5-benzenetetracarboxylate complex [88] which features not only μ_6 -bridging 1,2,4,5-benzenetetracarboxylate, but also μ_3 -bridging hydroxide. There are two non-equivalent copper(II) ions. One is perfectly square-planar, bound to *para* pairs of carboxyl oxygens (equivalent bridging groups) and μ_3 -hydroxyl groups. The other is in a distorted square-planar configuration, and is bound to a *cis* pair of μ_3 -hydroxyl groups, one carboxyl oxygen from a monodentate group and one carboxyl oxygen from a bridging group. The 1,2,4,5-benzenetetracarboxylate group (deprotonated) is symmetrical about the axis joining the ring hydrogens, and each *ortho* pair of carboxyl groups has one bridging and one monodentate carboxyl group. Each hydroxyl oxygen is coordinated to two distorted and one regular square-planar copper(II) ions. The parallelogram-motif, previously noted in the structure containing 6,7-dicanodipyridoquinoxaline [34] (p. 13), occurs here again, but with hydroxyl oxygens instead of carboxyl oxygens. In the present structure, alternating distorted square-planar copper(II) atoms and hydroxyl groups make up a parallelogram. The three-dimensional structure is made up of two-dimensional covalent layers of copper(II) and 1,2,4,5-benzenetetracarboxylate, linked together to form a three-dimensional structure by hydroxyl oxygens bridging distorted copper(II) ions of neighbouring layers. The shortest copper-copper distance is between pairs of distorted copper(II) ions (2.951 Å).

¹³The positions of the hydrogen atoms on water molecules are not listed in the crystal structure. These potential hydrogen-bonding sites are inferred from oxygen-oxygen distances.

1.2.2 Copper(II) benzenhexacarboxylates and dinitrobenzenetetra-carboxylates

Relatively few copper(II) benzenhexacarboxylate complexes have been reported. All those which do not have additional ligands besides OH^- or water are in the form of two-dimensional layers consisting of copper(II) and benzenhexacarboxylate, with the link between layers being provided by hydrogen bonding involving guest and coordinated water molecules, carboxyl groups, etc. [89–91]. Of these, the one reported in [91] is particularly important to this study because it contains *both* μ_2 -bridging water and μ_2 -bridging OH^- . The only three-dimensional covalent copper(II) benzenhexacarboxylate polymer [92] consists of two-dimensional anionic layers of octahedral copper(II) and μ_4 -bridging benzenhexacarboxylate (deprotonated), linked to form a three-dimensional structure by μ_2 -bridging 4,4'-bipyridine. Channels within the structure contain chains of alternating octahedral tetraaquacopper(II) and 4,4'-bipyridine moieties. In addition, a one-dimensional polymeric copper(II) complex with μ_2 -bridging 1,4-dinitro-2,3,5,6-benzenetetra-carboxylate¹⁴ — containing both coordinated and guest dimethylformamide molecules — has been reported [93].

1.3 THE AIMS OF THIS STUDY

The main aims of this study were to:

- attempt to synthesize novel metal-organic framework materials from copper(II) ions and 1,2,4,5-benzenetetra-carboxylate;
- determine the crystal structures of novel materials wherever possible;
- characterize the materials obtained using X-ray powder diffraction, infrared spectroscopy and thermal analysis techniques; and
- investigate the guest-inclusion properties of likely candidates.

¹⁴Mis-named 3,6-dinitrobenzene-1,2,5,6-tetra-carboxyl[ate]" in the Cambridge Structural Database

This study is reported in Part I.

During the course of the above study, some seemingly anomalous thermal behaviours were observed for the copper(II) 1,2,4,5-benzenetetracarboxylates under investigation. On changing the purge gas from nitrogen to argon during thermal analysis experiments, the main decomposition events of the complexes changed from being exothermic to being endothermic. This effect was investigated further by studying a simpler system copper(II) oxalate, a well-studied copper(II) carboxylate. This study is reported in Part II.

It became necessary to replace the proportional-counter detector electronics of the X-ray diffractometer employed in this study, owing to repeated failures. To this end, an inexpensive electronic detector circuit — consisting of a hybrid analog-digital computer made from readily available off-the-shelf electronic components — was designed to replace the existing system. The design and implementation of this new system is described in Part III.

References

- [1] **J. L. C. Rowsell and O. M. Yaghi.** “Metal-organic frameworks: a new class of porous materials”. *Microporous and Mesoporous Mater.* **73** (2004), 3–14.
- [2] **G. Férey.** “Microporous Solids: From Organically Templated Inorganic Skeletons to Hybrid Frameworks... Ecumenism in Chemistry”. *Chem. Mater.* **13** (2001), 3084–3098.
- [3] **M. O’Keeffe, M. Eddaoudi, H. Li, T. Reineke and O. M. Yaghi.** “Frameworks for Extended Solids: Geometrical Design Principles”. *J. Solid State Chem.* **152** (2000), 3–20.
- [4] **H. Li, A. Laine, M. O’Keeffe and O. M. Yaghi.** “Supertetrahedral Sulfide Crystals With Giant Cavities and Channels”. *Science* **283** (1999), 1145–1147.
- [5] **O. M. Yaghi, Z. Sun, D. A. Richardson and T. L. Groy.** “Directed Transformation of Molecules to Solids: Synthesis of a Microporous Sulfide from Molecular Germanium Sulfide Cages”. *J. Am. Chem. Soc.* **116** (1994), 807–808.
- [6] **L. Carlucci, G. Ciani, D. M. Prosperio and A. Sironi.** “Interpenetrating Diamondoid Frameworks of Silver(I) Cations Linked by N,N’-Bidentate Molecular Rods”. *J. Chem. Soc., Chem. Commun.* pp. 2755–2756.
- [7] **S. S. Chui, S. M. Lo, J. P. H. Charmant, A. G. Orpen and I. D. Williams.** “A Chemically Functionalizable Nanoporous Material $[\text{Cu}_3(\text{TMA})_3 \cdot (\text{H}_2\text{O})_3]_n$ ”. *Science* **283** (1999), 1148–1150. Cited in the Cambridge Structural Database, structure FIQCEN.

- [8] **Q. M. Wang, D. Shen, M. Bülow, S. D. Miu Ling Lau, F. R. Fitch, N. O. Lemcoff and J. Semanscin.** “Metallo-organic molecular sieve for gas separation and purification”. *Microporous and Mesoporous Mater.* **55** (2002), 217–230.
- [9] **K. Schlichte, T. Kratzke and S. Kaskel.** “Improved synthesis, thermal stability and catalytic properties of the metal-organic framework, $\text{Cu}_3(\text{BTC})_2$ ”. *Microporous and Mesoporous Mater.* **73** (2004), 81–88.
- [10] **J. L. C. Rowsell and O. Yaghi.** “Effects of functionalization, Catenation, and Variation of the Metal Oxide and Organic Linking Units on the Low-Pressure Hydrogen Adsorption Properties of Metal-Organic Frameworks”. *J. Am. Chem. Soc.* **128** (2006), 1304–1315.
- [11] **A. G. Wong-Foy, A. J. Matzger and O. M. Yaghi.** “Exceptional H_2 saturation uptake in microporous metal-organic frameworks”. *J. Am. Chem. Soc.* **128** (2006), 3494–3495.
- [12] **V. K. Peterson, Y. Liu, C. M. Brown and C. J. Kepert.** “Neutron Powder Diffraction Study of D_2 Sorption in $\text{Cu}_3(1,3,5\text{-benzenetricarboxylate})_2$ ”. *J. Am. Chem. Soc.* **128** (2006), 15578–15579.
- [13] **H. Li, M. Eddaoudi, M. O’Keeffe and O. M. Yaghi.** “Design and synthesis of an exceptionally stable and highly porous metal-organic framework”. *Nature (London)* **402** (1999), 276–279. Cited in the Cambridge Structural Database, structure SAHY0Q.
- [14] **M. Eddaoudi, J. Kim, N. Rosi, D. Vodak, J. Wachter, M. O’Keeffe and O. M. Yaghi.** “Systematic Design of Pore Size and Functionality in Isoreticular MOFs and Their Application in Methane Storage”. *Science* **295** (2002), 469–472. Cited in the Cambridge Structural Database, structure EDUSIF.
- [15] **H. K. Chae, D. Y. Siberio-Pérez, J. Kim, Y. Go, M. Eddouadi, A. J. Matzger, M. O’ Keeffe and O. M. Yaghi.** “A route to high surface area, porosity and inclusion of large molecules in crystals”. *Nature* **427** (2004), 523–527.

- [16] **H. Li, C. E. Davis, T. L. Groy, D. G. Kelley and O. M. Yaghi.** “Establishing Microporosity in Open Metal-Organic Frameworks: Gas Sorption Isotherms for Zn(BDC) (BDC = 1,4-Benzenedicarboxylate)”. *J. Am. Chem. Soc.* **120** (1998), 2186–2187. Cited in the Cambridge Structural Database, structure PURSOK.
- [17] **S. M. F. Lo, S. S. Y. Chui, L.-Y. Shek, Z. Lin, X. X. Zhang, G. hei Wen and I. D. Williams.** “Solvothermal Synthesis of a Stable Coordination Polymer with Copper(I)–Copper(II) Dimer Units: $[\text{Cu}_4\{1,4\text{-C}_6\text{H}_4(\text{COO})_2\}_3(4,4'\text{-bipy})_2]_n$ ”. *J. Am. Chem. Soc.* **122** (2000), 6293–6294. Cited in the Cambridge Structural Database, structure LOLQOS.
- [18] **O. M. Yaghi, G. Li and H. Li.** “Selective binding and removal of guests in a microporous metal-organic framework”. *Nature* **378** (1995), 703–706. Cited in the Cambridge Structural Database, structure ZUWET.
- [19] **H. Li, M. Eddaoudi, T. L. Groy and O. M. Yaghi.** “Coordinatively Unsaturated Metal Centers in the Extended Porous Framework of $\text{Zn}_3(\text{BDC})_3 \cdot 6\text{CH}_3\text{OH}$ (BDC = 1,4-Benzenedicarboxylate)”. *J. Am. Chem. Soc.* **120** (1998), 8571–8572. Cited in the Cambridge Structural Database, structure GECXUH.
- [20] **D. Maspoch, D. Ruis-Molina and J. Veciana.** “Old materials with new tricks: multifunctional open-framework materials”. *Chem. Soc. Rev.* **36** (2007), 770–818.
- [21] **C. J. Kepert.** “Advanced functional properties in nanoporous coordination framework materials”. *Chem. Commun.* pp. 695–700.
- [22] **V. I. Isaeva and L. M. Kustov.** “Metal-Organic Frameworks — New Materials for Hydrogen Storage”. *Russ. J. General Chem.* **77**(4) (2007), 56–72.
- [23] **F. H. Allen.** “The cambridge structural database: a quarter of a million structures and rising”. *Acta Crystallogr.* **B58** (2002), 380–388.
- [24] **N. Ohata, H. Masuda and O. Yamauchi.** “Aromatic carboxylate-controlled self-organization of copper(II)-L-arginine complexes”. *Inorg. Chim. Acta*

- 286** (1999), 37–45. Cited in the Cambridge Structural Database, structure FEQLES.
- [25] **T. Mallik, T. Kar, G. Bocelli and A. Musatti.** “Structural and thermal characterization of L-arginine dihydrate — a nonlinear optic material”. *Cryst. Res. Technol.* **41**(3) (2006), 280–284.
- [26] **H.-P. Xiao, M.-L. Hu and X.-H. Li.** “Bis(bis(1,10-phenanthroline)-chloro-copper(ii)) benzene-1,2,4,5-tetracarboxylate dihydrate”. *Acta Crystallogr., Sect. E: Struct. Rep. Online* **60** (2004), m71–m72. Cited in the Cambridge Structural Database, structure IROKEF.
- [27] **J.-X. Yuan, H.-P. Xiao and M.-L. Hu.** “Crystal structure of μ -benzene-1,2,4,5-tetracarboxylato-bis[bis(1,10-phenanthroline)-copper(II)] benzene-1,2,4,5-tetracarboxylic acid solvate [Cu(C₁₂H₈N₂)₂]₂(C₁₀H₂O₈).(C₁₀H₆O₈)”. *Z. Kristallogr.–New Cryst. Struct.* **219**(3) (2004), 224–226. Cited in the Cambridge Structural Database, structure DAMRUF, CAN 142:306753.
- [28] **Ji-xin Yuan, Mao-lin Hu, Ju-xia Li and Xin-yuan Song.** “Hydrothermal synthesis and crystal structure of binuclear copper(II) complex bridged by 1,2,4,5-benzenetetracarboxylato trivalent anion.” *Chem. Res. Chin. Univ.* **21** (2005), 21–23. Cited in the Cambridge Structural Database, structure DAMRUF01, CAN 143:205068.
- [29] **M.-L. Hu, H.-P. Xiao, S. Wang and X.-H. Li.** “catena-Poly[[(1,10-phenanthroline- κ^2 N,N')copper(II)- μ -(dihydrogen benzene-1,2,4,5-tetracarboxylato)- κ^2 O1:O4]”. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **59** (2003), m454–m455. Cited in the Cambridge Structural Database, structure BEBC0B.
- [30] **Q. Shi, R. Cao, D.-F. Sun, M.-C. Hong and Y.-C. Liang.** “Solvothermal syntheses and crystal structures of two metal coordination polymers with double-chain structures”. *Polyhedron* **20** (2001), 3287. Cited in the Cambridge Structural Database, structure MEVLII.

- [31] **L.-J. Zhang, J.-Q. Xu, Z. Shi, X.-L. Zhao and T.-G. Wang.** “Hydrothermal synthesis, structures and properties of coordination polymers based on μ_4 -bridging benzene-1,2,4,5-tetracarboxylate: $[\text{Co}(\text{Him})(\mu_4\text{-bta})_{1/2}]_n$ and $\{[\text{Cu}(\text{phen})(\mu_4\text{-4bta})_{1/2}]\cdot\text{H}_2\text{O}\}_n$ (bta = benzene-1,2,4,5-benzenetetracarboxylate, Him = imidazole, phen = 1,10-phenanthroline)”. *J. Solid State Chem.* **32** (2003), 32–39. Cited in the Cambridge Structural Database, structure MEVLII01.
- [32] **H.-P. Xiao, X.-H. Li, J.-X. Yuan and M.-L. Hu.** “catena-Poly[bis[(2,2-bipyridine- κ^2N,N')copper(II)]- μ_4 -1,2,4,5-benzenetetracarboxylato- $\kappa^4O^1:O^2:O^3:O^4$]”. *Acta Crystallogr., Sect. C:Cryst. Struct. Commun.* **60** (2004), m63–m64. Cited in the Cambridge Structural Database, structure INIYEJ.
- [33] **N. Hao, Y. Li, E. Wang, E. Shen, C. Hu and L. Xu.** “Hydrothermal synthesis and crystal structure of an infinite 1D ladderlike metal-organic compound: $[\text{Cu}_2(\text{btec})(2,2'\text{-bipy})_2]_\infty$ (btec = 1,2,4,5-benzenetetracarboxylate)”. *J. Mol. Struct.* **697** (2004), 1–8. Cited in the Cambridge Structural Database, structure INIYEJ01.
- [34] **M. D. Stephenson and M. J. Hardie.** “Extended Structures of Transition Metal Complexes of 6,7-Dicyanodipyridoquinoxaline: π -Stacking, Weak Hydrogen Bonding and $\text{CN}\cdots\pi$ Interactions”. *Cryst. Growth Des.* **6** (2006), 423–432. Cited in the Cambridge Structural Database, structure SEFQAW.
- [35] **P. Wang, C. N. Moorefield, M. Panzer and G. R. Newkome.** “Helical and polymeric nanostructures assembled from benzene tri- and tetracarboxylic acids associated with terpyridine copper(II) complexes”. *Chem. Commun.* pp. 465–467. Cited in the Cambridge Structural Database, structure FERCIP.
- [36] **J.-Z. Zou, Q. Liu, Z. Xu, X.-Z. You and X.-Y. Huang.** “TCB bridged binuclear and polynuclear copper(II) complexes: a novel three dimensional network structure complex $[(\text{Cudien})_2(\text{Cudien}\cdot\text{H}_2\text{O})\text{TCB}(\text{ClO}_4)_2\cdot\text{H}_2\text{O}]_2$ (TCB = tetracarboxylatobenzene, dien = 3-azapentane-1,5-diamine)”. *Polyhedron* **17** (1998), 1863–1869. Cited in the Cambridge Structural Database, structure VAQDAS.

- [37] **W. Chen, N. H. Tioh, J.-Z. Zou, Z. Xu and X.-Z. You.** “A Tetracarboxylatobenzene-Bridged Binuclear Copper(II) Complex”. *Acta Crystallogr. ,Sect. C:Cryst. Struct. Commun.* **52** (1996), 43–45. Cited in the Cambridge Structural Database, structure ZITV0N, CAN 124:161006.
- [38] **A. L. Spek.** *PLATON: A Multipurpose Crystallographic Tool*. Utrecht University, Utrecht, The Netherlands 2001.
- [39] **P. Chaudhuri, K. Oder, K. Wieghardt, S. Gehring, W. Haase, B. Nuber and J. Weiss.** “Moderately Strong Intramolecular Magnetic Exchange Interaction between the Copper(II) Ions Separated by 11.25 Å in $[\text{L}_2\text{Cu}_2(\text{OH}_2)_2(\mu\text{-terephthalato})](\text{ClO}_4)_2$ (L = 1,4,5-Trimethyl-1,4,7-triazacyclononane)”. *J. Am. Chem. Soc.* **110** (1988), 3657–3658. Cited in the Cambridge Structural Database, structure GECNIL.
- [40] **C.-B. Li, J.-Q. Xu, L.-J. Zhang, Y.-H. Sun, C. Su and T.-G. Wang.** “Hydrothermal synthesis and crystal structure of compound $[\text{Cu}_3(\mu\text{-10-bta})(\mu\text{-2-C}_2\text{O}_4)(\text{H}_2\text{O})_2]_n$ ”. *Gaodeng Xuexiao Huaxue Xuebao(Chin.)(Chem. J. Chin. Univ. (Chinese Edition))* **24** (2003), 785–787. Cited in the Cambridge Structural Database, structure YATLUB.
- [41] **R. Kofenstein and C. Robl.** “The layered structure of $\text{Cu}_2(\text{H}_2\text{O})_4[\text{C}_4\text{H}_4\text{N}_2][\text{C}_6\text{H}_2(\text{COO})_4]\cdot 2\text{H}_2\text{O}$ ”. *Z. Anorg. Allg. Chem.* **631** (2005), 1756–1758. Cited in the Cambridge Structural Database, structure WARYIY, CAN 144:160623.
- [42] **A. Majumder, V. Gramlich, G. M. Rosair, S. R. Batten, J. D. Masuda, M. S. E. Fallah, J. Ribas, J. P. Sutter, C. Desplanches and S. Mitra.** “Five New Cobalt(II) and Copper(II)-1,2,4,5-benzenetetracarboxylate Supramolecular Architectures: Syntheses, Structures and Magnetic Properties”. *Cryst. Growth Des.* **6** (2006), 2355–2368. Cited in the Cambridge Structural Database, structure XESS0E.
- [43] **E. Yang, J. Zhang, Y.-H. Wen, Y.-B. Chen, Y. Kang, Z.-J. Li and Y.-G. Yao.** “Poly[[diaquatrakis(μ_6 -benzene-1,2,4,5-tetracarboxylato)tris(μ_2 -4,4'-bipyridine)hexacopper(II)] dihydrate]”. *Acta Crystallogr., Sect. C:Cryst.*

- Struct. Commun.* **60** (2004), m280–m282. Cited in the Cambridge Structural Database, structure EV0MEH.
- [44] **R. Cao, Q. Shi, D. Sun, M. Hong, W. Bi and Y. Zhao.** “Syntheses and Characterizations of Copper(II) Polymeric Complexes Constructed from 1,2,4,5-Benzenetetracarboxylic Acid”. *Inorg. Chem.* **41** (2002), 6161–6168. Cited in the Cambridge Structural Database, structure MURBUW.
- [45] **D. Cheng, C. Feng, M. Hu, Y. Zheng, D. Xu and Y. Xu.** “Synthesis and crystal structure of a polymeric 1,2,4,5-benzenetetracarboxylato complex of Cu(II) with imidazole, $\text{Cu}_2(\text{C}_{10}\text{H}_2\text{O}_8)(\text{C}_3\text{H}_4\text{N}_2)_6(\text{H}_2\text{O})_4 \cdot 4\text{H}_2\text{O}$ ”. *J. Coord. Chem.* **52** (2001), 245–51. Cited in the Cambridge Structural Database, structure AH0LAK.
- [46] **D. Cheng, M. A. Khan and R. P. Houser.** “Copper(II) and cobalt(II) coordination polymers with bridging 1,2,4,5-benzenetetracarboxylate and *N*-methylimidazole: coordination number-determined sheet topology.” *J. Chem. Soc., Dalton Trans.* pp. 4555–4560. Cited in the Cambridge Structural Database, structure MUMKUA.
- [47] **J.-F. Ma, J.-F. Liu, Y. Xing, H.-Q. Jia and Y.-H. Lin.** “Networks with hexagonal circuits in co-ordination polymers of metal ions (Zn^{II} , Cd^{II}) with 1,1’-(1,4-butanediyl)bis(imidazole)”. *J. Chem. Soc., Dalton Trans.* pp. 2403–2407. Cited in the Cambridge Structural Database, structures DOVHAX, DOVHEB and DOVKAA.
- [48] **Y.-Y. Liu, J.-F. Ma, J. Yang and Z.-M. Su.** “Synthesis and Characterization of Six Coordination Polymers of Zinc(II) and Cobalt(II) with 1,3,5-Benzenetricarboxylate Anion and Bis(imidazole) Ligands”. *Inorg. Chem.* **46** (2007), 3027–3037. Cited in the Cambridge Structural Database, structure HICJUZ, HICKAG and HICKIO.
- [49] **L. Wen, Z. Lu, J. Lin, Z. Tian, H. Zhu and Q. Meng.** “Syntheses, Structures and Physical Properties of Three Novel Metal-Organic Frameworks Constructed from Aromatic Polycarboxylic Acids and Flexible Imidazole-

- Based Synthons”. *Cryst. Growth. Des.* **7**(1), 93–99. Cited in the Cambridge Structural Database, structure QETWIW.
- [50] **Yang, Yin; Ma, Jian-Fang; Liu, Ying-Ying; Ma, Ji-Cheng; Jia, Heng-Qing; Hu, Ning-Hai.** “Two new CuII coordination polymers: studies of topological networks and water clusters”. *Eur. J. Inorg. Chem.* **6** (2006), 1208–1215. CAN 146:92028.
- [51] **J.-F. Ma, J. Yang, G.-L. Zheng, L. Li, Y.-M. Zhang, F.-F. Li and J.-F. Liu.** “Four new coordination polymers of Cu(II) with 1,1’-(1,4-butanediyl)bis(imidazole)”. *Polyhedron* **23** (2004), 553–559. Cited in the Cambridge Structural Database, structure EXUYAX and EXUYIF.
- [52] **J. Yang, J.-F. Ma, Y.-Y. Liu, S.-L. Li and G.-L. Zheng.** *Eur. J. Inorg. Chem.* p. 2174. Cited in the Cambridge Structural Database, structure WASNOU.
- [53] **R. P. Feazell, C. E. Carson and K. K. Klausmeyer.** “Variability in the Structures of [4-(Aminomethyl)pyridine]silver(I) Complexes through Effects of Ligand Ratio, Anion, Hydrogen Bonding, and π -Stacking”. *Inorg. Chem.* **45** (2006), 935–944. Cited in the Cambridge Structural Database, structure DECNEF.
- [54] **S. Sailaja and M. V. Rajasekharan.** “Synthesis and Structure of Coordination Polymers of Ag(I) with Isomeric (Aminomethyl)pyridines. Formation of A Novel Circular Helicate and 2-D Networks via Ag $\cdots$ Ag Contacts and Coordination Shell Expansion under Anion Control”. *Inorg. Chem.* **42** (2003), 5675–5684. Cited in the Cambridge Structural Database, structure ULADEQ.
- [55] **A. Majumder, V. Gramlich, G. M. Rosair, S. R. Batten, J. D. Masuda, M. S. E. Fallah, J. Ribas, J. P. Sutter, C. Desplanches and S. Mitra.** “Five New Cobalt(II) and Copper(II)-1,2,4,5-benzenetetracarboxylate Supramolecular Architectures: Syntheses, Structures and Magnetic Properties”. *Cryst. Growth Des.* **6** (2006), 2355–2368. Cited in the Cambridge Structural Database, structure XESSUK.

- [56] **J. Du, G. Wei, J. He, B. Han and Z. Dong.** “[Cu(1,4-C₄H₁₂N₂)₂(ClO₄)₂]_n(H₂O)_{2n}, a novel butane-1,4-diamine-bridged two-dimensional copper(II) square network: Synthesis, structure and magnetic properties”. *Mater. Let.* **60** (2006), 2248–2251. Cited in the Cambridge Structural Database, structure WEYNUK.
- [57] **I. Potocnák, L. Triscíková and C. Wagner.** “Low-dimensional compounds containing cyano groups. VI. A unique two- and one-dimensional structure in amminebis(1,4-diaminobutane)tetrakis[dicyanoargentato(I)]dicopper(II) dihydrate”. *Acta Crystallogr., Sect. C:Cryst. Struct. Commun.* **59**, m249–m251. Cited in the Cambridge Structural Database, structure JAGWUK.
- [58] **F. B. Stocker, T. P. Staeva, C. M. Rienstra and D. Britton.** “Crystal Structures of a Series of Complexes Produced by Reaction of Copper(I) Cyanide”. *Inorg. Chem.* **38** (1999), 984–991. Cited in the Cambridge Structural Database, structure HIWHOK.
- [59] **R. Kofenstein and C. Robl.** “Cu₂[Cu(H₂O)₄][(CH₂)₄(NH₃)₂][C₆H₂(COO)₄]₂·4H₂O. A 3-dimensional coordination polymer with negative excess charge and channel-like voids”. *Z. Anorg. Allg. Chem.* **629** (2003), 1374–1378. Cited in the Cambridge Structural Database, structure KABNIL, CAN 139:390070.
- [60] **C. Bazzicalupi, A. Bencini, A. Bianchi, V. Fusi, P. Paoletti and B. Valtancoli.** “Unusual complexation behaviour of 1,3-diaminopropane”. *Inorg. Chim. Acta* **244** (1996), 255–258. Cited in the Cambridge Structural Database, structure DEDDUL01.
- [61] **X.-P. Shen, Y.-Z. Li, A.-H. Yuan and Z. Xu.** “A novel three-dimensional mixed bridged-ligand complex [Cu₂^{II}(tn)₂][Fe^{II}(CN)₆]·H₂O”. *J. Mol. Struct.* **754** (2005), 106–110. Cited in the Cambridge Structural Database, structure KAWQOP.
- [62] **D. Poletti and L. Karanović.** “1,3-Propanediammonium [μ -1,2,4,5-benzenetetracarboxylato(4-)]copper(II) dihydrate with a microporous struc-

- ture". *J. Serb. Chem. Soc.* **70** (2005), 1441–1450. Cited in the Cambridge Structural Database, structure MEMGAN.
- [63] **N. Habermann, M. Klaassen and P. Klüfers.** “Ethylenediamin–Kupfer(II)-Komplexe mit Polyolat-Ionen aus *rac-trans*-Cyclohexan-1,2-diol, Erythritol und Methyl- α -D-mannopyranosid. Herstellung und Kristallstrukturen von $[(\text{Ethylenediamin})\text{Cu}(\text{C}_6\text{H}_{10}\text{O}_2)]\cdot\text{H}_2\text{O}$, $[(\mu\text{-Ethylenediamin})\{\text{Cu}_2(\text{Ethylenediamin})_2(\mu'\text{-meso-Butantetraolat}(4-))\}]\cdot 8\text{H}_2\text{O}$ und $[(\text{Ethylenediamin})\text{Cu}(\alpha\text{-D-Man } p\text{OMeH}_2^{[2,3]2-})]\cdot 2\text{H}_2\text{O}$ ". *Carbohydr. Res.* **241** (1993), 9–23. Cited in the Cambridge Structural Database, structure YASJEH (abstract, paper in German).
- [64] **M. Pasquali, C. Floriani and A. Gaetani-Manfredotti.** “Copper-Amine-Carbonyl Chemistry. Solution and Solid-State Studies of the Copper(I)-Ethylenediamine-Carbon Monoxide System: Synthesis and X-ray Structures of Mononuclear and Binuclear Copper(I)-Carbonyl Complexes". *Inorg. Chem.* **19** (1980), 1191–1197. Cited in the Cambridge Structural Database, structure KAWQOP.
- [65] **J.-H. Luo, C.-C. Huang, X.-H. Huang and X.-J. Chen.** “Two pseudopolymorphic copper-benzene-tetracarboxylate complexes". *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **63** (2007), m273–m276. Cited in the Cambridge Structural Database, structures HIFPOC and HIFPUI, ISSN 0108-2701.
- [66] **L. Wang, D.-H. Zhou and J.-P. Zhang.** “catena-Poly[[[bis(2-pyridinecarboxylato- κ^2N, O)-copper(II)- μ -benzene-1,2,4,5-tetracarboxylic acid] dihydrate] (*sic.*)". *Acta Crystallogr., Sect. E: Struct. Rep. Online* **61** (2005), m958–m960. Cited in the Cambridge Structural Database, structure SAPBER.
- [67] **Y. Y. Karabach, A. M. Kirillov, M. F. C. G. da Silva, M. N. Kopylovich and A. J. L. Pombeiro.** “An Aqua-Soluble Copper(II)-Sodium Two-Dimensional Coordination Polymer with Intercalated Infinite Chains of Decameric Water Clusters". *Cryst. Growth Des.* **6** (2006), 2200–2203. Cited in the Cambridge Structural Database, structure RERPUA.

- [68] **Y. Y. Karabach, A. M. Kirillov, M. Haukka, M. N. Kopylovich and A. J. L. Pombeiro.** “Copper(II) coordination polymers derived from triethanolamine and pyromellitic acid for bioinspired mild peroxidative oxidation of cyclohexane”. *J. Inorg. Biochem.* Manuscript in press.
- [69] **J. B. Hill, S. J. Eng, W. T. Pennington and G. H. Robinson.** “Reaction of Me_3Ga and Me_3Al with the tertiary-tetraaza analog of adamantane, hexamethylenetetramine ($\text{N}_4\text{-Ada}$). Syntheses and molecular structures of $[(\text{Me}_3\text{M})_n\cdot\text{N}_4\text{-Ada}]$ ($n = 1\text{--}4$, $\text{M} = \text{Ga}$ or Al)”. *J. Organomet. Chem.* **445**. Cited in the Cambridge Structural Database, structure PESPEI.
- [70] **M. Bertelli, L. Carlucci, G. Ciani, D. M. Proserpio and A. Sironi.** “Structural studies of molecular-based nanoporous materials. Novel networks of silver(I) cations assembled with polydentate N-donor bases hexamethylenetetramine and 1,3,5-triazine”. *J. Mater. Chem.* **7**(7) (1997), 1271–1276. Cited in the Cambridge Structural Database, structure ROPVEX.
- [71] **R. Cao, Q. Shi, D. Sun, M. Hong, W. Bi and Y. Zhao.** “Syntheses and Characterizations of Copper(II) Polymeric Complexes Constructed from 1,2,4,5-Benzenetetracarboxylic Acid”. *Inorg. Chem.* **41** (2002), 6161–6168. Cited in the Cambridge Structural Database, structure MURCAD.
- [72] **B. T. Usubaliev, A. N. Shnulin and K. S. Mamedov.** “Crystal and molecular structure of a decahydrate complex of copper with 1,2,4,5-benzenetetracarboxylic acid.” *Koord. Khim. (Russ.) (Coord. Chem.)* **8** (1982), 1532–1538. Cited in the Cambridge Structural Database, structure BOVTAH, CAN 98:81758.
- [73] **I. Yeltsov, V. Ovcharenko, V. Ikorskii, G. Romanenko and S. Vasilevsky.** “Copper(II) thenoyltrifluoroacetate as acceptor matrix in design of heterospin complexes”. *Polyhedron* **20** (2001), 1215–1222. Cited in the Cambridge Structural Database, structure RAMLUM.
- [74] **A. Caneschi, F. Ferraro, D. Gatteschi, P. Rey and R. Sessoli.** “Structure and Magnetic Properties of a Chain Compound Formed by Copper(II) and a

- Tridentate Nitronyl Nitroxide Radical”. *Inorg. Chem.* **30** (1991), 3162–3166. Cited in the Cambridge Structural Database, structure S0LBAW.
- [75] **L.-Y. Wang, L.-C. Li, D.-Z. Liao, Z.-H. Jiang and S.-P. Yan.** “Synthesis, crystal structure and magnetic properties of a 1-D polymer, [Cu(NITpPy)₂(H₂TCB)(H₂O)]·2H₂O”. *Chin. J. Chem.* **21** (2003), 500–504. Cited in the Cambridge Structural Database, structure ESEQIC, CAN 139:373609.
- [76] **J. Cho, A. J. Lough and J. C. Kim.** “Monomeric and polymeric copper(II) hexaaza macrocyclic complexes with btc anions (btc-1,2,4,5-benzenetetracarboxylic acid”. *Inorg. Chim. Acta* **342** (2003), 305–310. Cited in the Cambridge Structural Database, structure BASNAL.
- [77] **J. Cho, A. J. Lough and J. C. Kim.** “Monomeric and polymeric copper(II) hexaaza macrocyclic complexes with btc anions (btc-1,2,4,5-benzenetetracarboxylic acid”. *Inorg. Chim. Acta* **342** (2003), 305–310. Cited in the Cambridge Structural Database, structure BASNEP.
- [78] **J. C. Kim, H. Jo, A. J. Lough, J. Cho, U. Lee and S. Y. Pyun.** “Polymeric nickel(II) and copper(II) complexes with btc²⁻ ions as bridging ligands (btc²⁻ = 1,2,4,5-benzenetetracarboxylic acid dianion”. *Inorg. Chem. Commun.* **6** (2003), 474–477. Cited in the Cambridge Structural Database, structure OMECE0.
- [79] **J. C. Kim, A. J. Lough and H. Jo.** “Syntheses and X-ray crystal structures of 14-membered tetraaza macrocyclic copper(II) complexes with polycarboxylate ligands”. *Inorg. Chem. Commun.* **5** (2002), 616–620. Cited in the Cambridge Structural Database, structure X0PS0K.
- [80] **E. G. Bakalbassis and A. Terzis.** “Antiferromagnetism tuned by the topology of the intervening bridging ligand. Crystal structure and magnetic properties of the (μ-phthalato)[bis(piperidine)]Cu(II) chain complex”. *Inorg. Chim. Acta* **218** (1994), 167–172. Cited in the Cambridge Structural Database, structure HEHPEP.

- [81] **S.-F. Si, R.-J. Wang and Y.-D. Li.** “Synthesis and crystal structure of three dimensional complex from copper(II) and 1,2,4,5-benzenetetracarboxylate”. *Inorg. Chem. Commun.* **6** (2003), 1152–1155. Cited in the Cambridge Structural Database, structure NEHRAU.
- [82] **S. K. Ghosh and P. K. Bharadwaj.** “Puckered-Boat Conformation Hexameric Water Clusters Stabilized in a 2D Metal–Organic Framework Structure Built from Cu(II) and 1,2,4,5-Benzenetetracarboxylic Acid”. *Inorg. Chem.* **43** (2004), 5180–5182. Cited in the Cambridge Structural Database, structure PADPIU.
- [83] **M. Matsumoto, S. Saito and I. Ohmine.** “Molecular dynamics simulation of the ice nucleation and growth process leading to water freezing”. *Nature* **416** (2002), 409–413.
- [84] **N. H. Fletcher.** *The Chemical Physics of Ice.* Cambridge University Press, Cambridge 1970.
- [85] **R. Diniz, H. A. de Abreu, W. B. de Almeida, M. T. C. Sansiviero and N. G. Fernandes.** “X-ray crystal structure of triaquacopper(II) dihydrogen 1,2,4,5-benzenetetracarboxylate trihydrate and raman spectra of Cu^{2+} , Co^{2+} and Fe^{2+} salts of 1,2,4,5-benzenetetracarboxylic (pyromellitic) acid.” *Eur. J. Inorg. Chem.* p. 1115. Cited in the Cambridge Structural Database, structure MOFJEW.
- [86] **J.-Y. Guo, T.-L. Zhang, J.-G. Zhang, X.-J. Qiao, L. Yang, W. Yu and R.-F. Wu.** “Non-isothermal kinetics and crystal structure of one-dimensional coordination polymer $\{[\text{Cu}(\text{H}_2\text{btcc})(\text{H}_2\text{O})_3]\cdot 3\text{H}_2\text{O}\}$ ”. *Wuji Huaxue Xuebao(Chin.)(Chin. J. Inorg. Chem.)* **22** (2006), 2179–2185. Cited in the Cambridge Structural Database, structure MOFJEW01, CAN 147:393316.
- [87] **R. Cao, Q. Shi, D. Sun, M. Hong, W. Bi and Y. Zhao.** “Syntheses and Characterizations of Copper(II) Polymeric Complexes Constructed from 1,2,4,5-Benzenetetracarboxylic Acid”. *Inorg. Chem.* **41** (2002), 6161–6168. Cited in the Cambridge Structural Database, structure MURB0Q.

- [88] **R. Cao, Q. Shi, D. Sun, M. Hong, W. Bi and Y. Zhao.** “Syntheses and Characterizations of Copper(II) Polymeric Complexes Constructed from 1,2,4,5-Benzenetetracarboxylic Acid”. *Inorg. Chem.* **41** (2002), 6161–6168. Cited in the Cambridge Structural Database, structure MURCEH.
- [89] **M.-G. Zhao, C.-Q. Liu, J.-M. Shi and W. Xu.** “Synthesis, crystal structure and magnetic behaviour of a two-dimensional copper(II) complex with mellitic anion as bridging ligand”. *Transition Met. Chem.* **28** (2003), 525–528. Cited in the Cambridge Structural Database, structure AKIWAS.
- [90] **H. Tamura and K. Ogawa.** “Crystal structure of copper(II) mellitate, β -type, $[\text{Cu}_4\{\text{C}_6(\text{COO})_5(\text{COOH})\}_2(\text{H}_2\text{O})_{12}\text{Cu}(\text{H}_2\text{O})_4]\cdot 6\text{H}_2\text{O}$ ”. *J. Crystallogr. Spectrosc. Res.* **22** (1992), 237–247. Cited in the Cambridge Structural Database, structure VUGBUU, CAN 117:17746.
- [91] **H. Tamura, K. Ogawa and W. Mori.** “Crystal structure of copper(II) mellitate, $[\text{Cu}_3.5\text{C}_6(\text{COO})_5(\text{COOH})(\text{OH}_2)(\text{H}_2\text{O})_{8.5}]\cdot 4.5\text{H}_2\text{O}$ ”. *J. Crystallogr. Spectrosc. Res.* **19** (1989), 203–13. Cited in the Cambridge Structural Database, structure VAPLED, CAN: 110:224450.
- [92] **E. Yang, J. Zhang, Z.-J. Li, S. Gao, Y. Kang, Y.-B. Chen, Y.-H. Wen and Y.-G. Yao.** “Interweaving 3D Network with Double-Helical Tubes Filled by 1D Coordination Polymer Chains”. *Inorg. Chem.* **43** (2004), 6525–6527. Cited in the Cambridge Structural Database, structure RAHMAP.
- [93] **J.-M. Shi, X. Zhang and H.-L. Yin.** “Synthesis, crystal structure and ferromagnetic interaction of a binuclear copper(II) complex with the 1,4-dinitro-2,3,5,6-tetracarboxylatobenzenic anion as bridging ligand”. *Transition Met. Chem.* **29** (2004), 671–674. Cited in the Cambridge Structural Database, structure SALTIJ.

Note: Where structure codes are given in MONOTYPE FACE, the cited crystal structure in the Cambridge Structural Database should be regarded as the primary reference, although the original papers were consulted wherever possible. Depending on relative positions within the text, a given paper may have been cited more than

once with different structure codes. Titles are formatted as in the original references. References to abstracts contain CAN or ISSN numbers, and for these the titles given above are rendered as they were in the Chemical Abstracts entries.

Chapter 2

Experimental methods

In this chapter, a brief description of the physical methods employed in this study is given. Detailed procedures are given in appendices.

2.1 ELEMENTAL ANALYSIS

2.1.1 Carbon, hydrogen and nitrogen (CHN) analysis

Analyses for carbon, hydrogen and nitrogen were performed by Ms B. Soko of the School of Pure and Applied Chemistry at the University of KwaZulu-Natal in Durban (using a LECO CHNS-932 analyzer), and by Mr P. Benincasa of the Department of Chemistry at the University of Cape Town (Fisons EA 1108 CHNS-O).

2.1.2 Complexometric titrations for copper determination

Preliminary copper determinations were done by means of complexometric titration, using a method given in [1]. The complete procedure is given in Appendix A (p. 341).

2.1.3 Metal analysis (instrumental)

Inductively coupled plasma mass spectrometry (ICP-MS)

ICP results were obtained by Dr E. Hosten of the Nelson Mandela Metropolitan University, using a Perkin-Elmer Sciex ELAN 6100 ICP spectrometer.

Atomic absorption spectroscopy (AAS)

AAS results (for copper determination) were obtained using a Varian 1275 spectrometer with a laminar acetylene burner. Standards were prepared by diluting commercially available standard 1000 ppm metal solutions. Samples were digested in nitric acid (with a few drops of sulfuric acid) and diluted appropriately with distilled water. A common standard addition method [2], was employed for these analyses.

Combustion analysis

Weighed samples were heated in an aluminium DSC pan (covered but not crimped) at $5\text{ }^{\circ}\text{C min}^{-1}$ in a DSC furnace in an oxygen atmosphere (approx. 25 ml min^{-1}) well past the main decomposition point. Residues were identified as CuO by XRPD, and by noting that CuO contains 79.89 % copper, the copper percentages of the samples were calculated. Experiments were performed in duplicate.

2.1.4 Sodium fusion test for chlorides (Lassaigne test)

To confirm the absence of chloride in certain samples, sodium fusion tests were performed as described in a more complex form for organic compounds in standard textbooks such as [3] and [4]. The complete procedure is given in Appendix B (p. 344).

2.2 THERMAL ANALYSIS

Brief summaries of the thermal analysis techniques employed in this study are given below. A complete introduction to the methods discussed can be found in [5] (and references therein), and the manufacturer's literature (for later-model instruments) is available on the Internet at [6].

2.2.1 Differential scanning calorimetry (DSC)

The instrument employed in this study was a Perkin-Elmer DSC 7 differential scanning calorimeter (power-compensating type), with Pyris Version 4.01 software.

In power-compensating DSC, a sample and an inert reference are subjected to a common temperature programme by heating in separate furnaces, each equipped with its own heater and temperature sensor. In a typical DSC experiment, the sample and reference are both heated from a starting temperature to a final temperature at a pre-determined heating rate, while the instrument control system continually attempts to keep the sample and reference temperatures equal to each other. The difference between the power supplied to the sample furnace and that supplied to the reference furnace is recorded and plotted against time or programme temperature. In this way, an endothermic event in the sample results in a positive peak on the DSC plot, and an exothermic event results in a negative peak¹. The area of the plot can be related to the enthalpy change associated with the thermal event by calibration.

The furnaces are purged by means of an inert gas (normally nitrogen), but a reactive atmosphere (oxygen, for example) may be used if desired. Nitrogen, argon and oxygen were used as purge gases in this study. The instrument was calibrated using indium (temperature and heat flow) and zinc (temperature) standards, using a nitrogen atmosphere except where noted.

¹In the related technique, differential thermal analysis (DTA), and also in heat-flux DSC, the sample and reference are heated in a common furnace, and the difference between the sample and reference temperatures is plotted as a function of time or programme temperature. For these techniques, endothermic events give rise to negative peaks, and exothermic events give rise to positive peaks.

An early introduction to power-compensating DSC, with technical details, can be found in [7], with critique and cautions given in [8].

2.2.2 Thermogravimetry (TG)

A Perkin-Elmer TGA 7 thermogravimetric analyzer — as modified by the manufacturer to allow evolved gas analysis by Fourier transform infrared spectroscopy (see Section 2.3.2 below), and with Pyris Version 4.01 software — was employed in this study.

In thermogravimetry, a sample is subjected to a pre-determined temperature programme in a furnace, and the mass of the sample is recorded and plotted as a function of time or programme temperature. As with DSC, the furnace is purged with either an inert or a reactive gas. The TG furnace is equipped with a separate thermocouple, located close to the position of the sample during operation, to record the sample temperature during the run. Temperature control is based on the furnace temperature as measured using the furnace resistance.

The instrument was calibrated for mass using a standard 20 mg mass piece, and for temperature using the magnetic calibration kit provided by the manufacturer (nickel and perkalloy standards). Furnace calibration was performed whenever necessary, following the built-in procedures.

2.3 FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR)

A Perkin-Elmer FTIR2000 spectrometer — with Spectrum Version 3.02.01 (for Windows) software for mid-infrared spectroscopy, and Spectrum TimeBase Version 2.0 for time-resolved infrared spectroscopy — was used in this study. The manufacturer's literature is available on the Internet at [6].

2.3.1 Mid-infrared spectroscopy

Infrared spectra were obtained either by mounting samples on sodium chloride plates in the form of mulls (nujol and hexachlorobutadiene, HCBd) or by forming

disks by compression with potassium bromide.

Spectra were treated using the standard baseline correction and smoothing routines provided in software by the manufacturer. Using a custom-written computer program, spectrum pairs obtained using nujol and hexachlorobutadiene mulls were combined appropriately to give composite spectra free from interference by the mulling agents. The spectrum windows were as follows:

Nujol: 2400–1500 cm^{-1} , 1300–747 cm^{-1} , 701–400 cm^{-1}

HCBD: 4000–2400 cm^{-1} , 1500–1300 cm^{-1} , 747–701 cm^{-1}

Peak coordinates, where shown, were obtained using the automatic software routines as far as possible, and these were supplemented manually when necessary.

2.3.2 Gas-phase infrared spectroscopy for evolved-gas analysis

Evolved gas analysis was performed using the equipment provided by the manufacturers [9]. The TG is interfaced to a heated gas-cell fitted inside the sample compartment of the infrared spectrometer by means of a heated line. Gases evolved by the sample are flushed by the purge gas stream from the TG furnace, along this line and into the gas-cell, and from there to the exhaust. Infrared spectra of the gas-cell contents were obtained at regular intervals (about three spectra per minute).

The heated gas-cell and interface line were kept at a constant 150 °C during operation. Except where noted, nitrogen was used as a purge gas (100 ml min^{-1} total purge rate). Infrared bands for qualitative analysis of various evolved gases are given in [10].

2.4 X-RAY METHODS

2.4.1 X-ray powder diffractometry (XRPD)

The X-ray powder diffraction patterns were recorded on a Philips upright X-ray powder diffractometer (Philips PW1050/25 goniometer with accessories), using copper K_{α} radiation (nickel filter). The X-ray tube was operated at 40 kV

(20 mA). The detector was a Xenon-filled proportional counter, operated at 1600 V, equipped with a CR-RC-CR pulse-shaping amplifier and pulse-height discriminator. The ratemeter filter time constant was 1 second. Except where indicated, the goniometer was scanned at 1° min^{-1} .

Samples were mounted on glass slides with petroleum jelly. For moisture-sensitive substances, the samples were pre-coated either with liquid paraffin or with a 4:1 mixture of liquid paraffin and petroleum ether.

The instrument was substantially re-built during the course of the study (see Chapter 7 on p. 298).

2.4.2 X-ray fluorescence spectroscopy

The X-ray fluorescence spectroscopy results were obtained by Prof. G. S. Marsh of the Department of Geology, Rhodes University, using a Philips PW1480 wavelength dispersive spectrometer with a Rh-target 3 kW X-ray tube.

2.4.3 Single-crystal X-ray diffractometry

The crystal structures were obtained by Prof. S. A. Bourne of the Department of Chemistry at the University of Cape Town, by means of a Nonius KappaCCD diffractometer using graphite-monochromated Mo-K α radiation ($0.7107 \text{ \AA}$) at 110–113 K.

The crystal structure data were examined using PLATON [11]. See full PLATON output on attached CD-ROM (Appendix C, p. 352).

References

- [1] **H. A. Flaschka.** *EDTA Titrations*. Pergamon Press, Inc., New York 1959. P. 78.
- [2] **M. Bader.** “A systematic approach to standard addition methods in instrumental analysis”. *J. Chem. Ed.* **57**(10) (1980), 703–706. (Method used was as described in Case 1, p. 703.).
- [3] **B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell.** *Vogel’s Textbook of Practical Organic Chemistry*. 5th ed. Addison Wesley Longman Ltd., England 1989.
- [4] **F. G. Mann and B. C. Saunders.** *Practical Organic Chemistry*. 3rd ed. Longmans, Green and Co., London 1952.
- [5] **M. E. Brown.** *Introduction to Thermal Analysis: Techniques and Applications*, vol. 1 of *Hot Topics in Thermal Analysis and Calorimetry*. 2nd ed. Kluwer Academic Publishers, Dordrecht, The Netherlands 2001.
- [6] **PerkinElmer Life and Analytical Sciences.** “web-site and included links”. URL: <http://las.perkinelmer.com>. (last accessed Dec. 2006).
- [7] **E. S. Watson, M. J. O’Neill, J. Justin and N. Brenner.** “A differential scanning calorimeter for quantitative differential thermal analysis”. *Analytical Chem.* **36**(7) (1964), 1233–1238.
- [8] **G. W. H. Höhne and E. Glöggler.** “Some peculiarities of the DSC-2/-7 (Perkin-Elmer) and their influence on accuracy and precision of the measurements”. *Thermochim. Acta* **151** (1989), 195–304.

- [9] **PerkinElmer Life and Analytical Sciences.** “TG/IR Interface”. URL: <http://las.perkinelmer.com>. Part no. L1200502/L1200503 (last accessed Dec. 2006).
- [10] **R. H. Pierson, A. N. Fletcher and E. S. C. Gantz.** “Catalog of infrared spectra for qualitative analysis of gases”. *Analytical Chem.* **28**(7) (1956), 1218–1239.
- [11] **A. L. Spek.** *PLATON: A Multipurpose Crystallographic Tool*. Utrecht University, Utrecht, The Netherlands 2001.

Chapter 3

Synthesis

This chapter describes the synthesis and characterisation of various copper(II) complexes with 1,2,4,5-benzenetetracarboxylic acid. Synthesis took place by ambient precipitation, solvothermal and gel-based methods.

3.1 SYNTHESIS METHOD OVERVIEW

This section provides a brief overview of the synthesis methods used, in general terms. The specific syntheses will be discussed in a later section, each under an individual sub-heading. Except where indicated, AR-grade reagents were used, as obtained from the manufacturers.

3.1.1 Ambient precipitation method

For a chemical reaction of the form,



where M is a metal cation and L is a charged or uncharged ligand, if the reaction is very fast and the precipitate, ML_n , is insoluble, the simplest possible synthesis method is simply to mix solutions of M and L in sufficient quantities to provide the desired metal-to-ligand ratio, and to stir the reaction mixture for a few minutes

to ensure completeness of reaction. In reactions of the form,



where the source of M is a sparingly soluble salt, it is necessary to stir the reaction for several days. Carbonates are especially useful when used in reactions with the acidic (i.e., protonated) form of an anionic ligand, because the carbonate ion is released as carbon dioxide and water, leaving no other anions besides the ligand to balance the charge of the metal cations.

3.1.2 Solvothermal method

This method is similar to the ambient precipitation reaction, except that the reaction mixture (usually *after* precipitation has taken place under ambient conditions) is placed in an autoclave whose internal temperature is regulated to some value above ambient, and often higher than the normal boiling point of the solvent. The reaction vessel is not pressurized artificially. Thus the reaction is performed at an elevated temperature and at the natural pressure of the sealed reaction vessel at this temperature.

A review of the role of hydrothermal methods in chemical synthesis appears in [1].

3.1.3 Gel-based method

Gel-based synthesis methods [2] may be advantageous when conventional methods of crystal growth fail. Whenever an insoluble product forms rapidly, methods involving the evaporation of solvent cannot be used. Instead, a way of slowing down the reaction itself must be found if slow crystal growth is to take place.

For the chemical reaction in Equation 3.1, if solutions of M and L are separated by a gel barrier, then immediate mixing of the solutions is prevented, although mixing within the gel takes place after a period of time. Henisch [2] asserts that convection currents do not occur in gels, except possibly at the sub-microscopic level, and thus that the chief mechanism of transport within the gel is diffusion. Rates of diffusion in gels are similar to those in liquids, and the true function of the

gel is to inhibit mixing by convection currents rather than to slow down diffusion.

Two forms of gel methods were employed in this study, viz., the *straight-tube form* and the *U-tube form*. Sodium metasilicate gel was used in this study, but methods employing silica gel [3–5], gelatin and Cab-O-Sil [2] have also been described. Solvothermal gel methods have been employed in zeolite synthesis [6].

Straight-tube method

In this method, the gel, impregnated with L (dissolved, not merely in suspension), is formed in the lower half of a cylindrical vessel such as a boiling tube. A solution of M is placed in the vessel above the gel. The arrangement is shown in Figure 3.1. Crystal growth begins almost immediately, and crystals may grow either at the

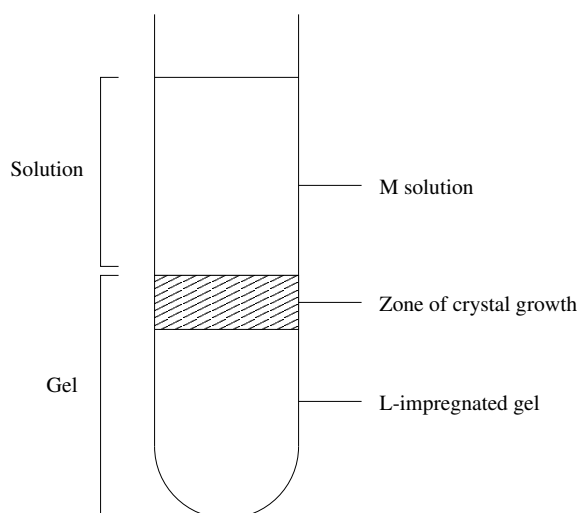


Figure 3.1: A typical straight-tube arrangement.

liquid-side or the gel-side of the interface, or both. Different products may form in various zones of the gel. The placement of the reagents may sometimes be inverted, but because the gel must be formed with one of the reagents *in situ*, the gel formation procedure may exclude one of the arrangements.

U-tube Method

In this method, the “blank” gel barrier is formed in the lower arc-shaped region of a U-tube, and solutions of M and L are placed in opposite legs. Figure 3.2 shows

the arrangement. Unlike in the straight-tube arrangement, the reaction takes much

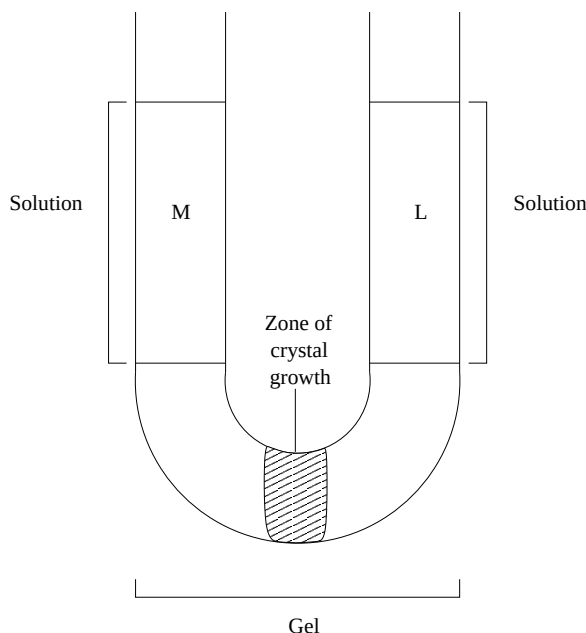


Figure 3.2: A typical U-tube arrangement.

longer to begin because of the greater distance through which the reagents must diffuse. Crystals begin to form approximately in the centre of the gel-region, and the reaction zone gradually increases in size until it encompasses practically the whole gel-region. Although multiple products may form, the emergence of secondary products is much delayed, compared to the straight-tube method.

3.2 SYNTHESIS METHODS AND PRODUCTS

3.2.1 Ambient precipitation syntheses and products

Two ambient syntheses were employed, neither of which gave products suitable for single-crystal X-ray diffraction. These products were not taken beyond initial characterization (see Section 4.5, p. 132, for details).

Copper(II) acetate/1,2,4,5-benzenetetracarboxylic acid Copper(II) acetate monohydrate (0.9920 g, 4.969 mmol) was dissolved in 20 ml deionized water.

1,2,4,5-benzenetetracarboxylic acid (0.6723 g, 2.645 mmol) was dissolved in 5 ml ethanol. The two solutions were mixed and swirled, and left standing for a few minutes. The product was filtered using a Buchner funnel and washed with 60 ml ethanol, and dried by the suction of air through the filter for one hour. The product was a fine light-blue powder, of which 1.0126 g was recovered. This product was named **ppt-cu-b4c-acet**.

Copper(II) basic carbonate/1,2,4,5-benzenetetracarboxylic acid Copper(II) basic carbonate¹ (0.3896 g, 1.762 mmol) and 1,2,4,5-benzenetetracarboxylic acid (0.5094 g, 2.004 mmol) were added to 50 ml deionized water. Slight bubbling of the heterogeneous mixture was observed on mixing, indicating a chemical reaction. The heterogeneous mixture was stirred continuously for five days. A colour-change from blue-green to light blue suggested a conversion of the solid copper basic carbonate to a copper-1,2,4,5-benzenetetracarboxylate complex. The product was filtered using a Buchner funnel and washed with 50 ml water, and after drying by suction of air through the filter, a mass of 0.8473 g was obtained. This product was name **ppt-cu-b4c-co3**.

3.2.2 Solvothermal syntheses and products

Two types of solvothermal synthesis were attempted, giving identical products which were not suitable for single-crystal X-ray diffraction. These products were not taken beyond initial characterization (see Section 4.6, p. 132).

Copper(II) acetate/1,2,4,5-benzenetetracarboxylic acid Copper(II) acetate monohydrate (1.292 g, 6.471 mmol) and 1,2,4,5-benzenetetracarboxylic acid (0.8222 g, 3.23 mmol) were added to 15 ml deionized water, and heated with stirring in an autoclave at 140 °C for 24 hours, 120 °C for 5 hours and 100 °C for 5 hours, followed by cooling to room temperature at the natural rate of the autoclave. The product was filtered using a Buchner funnel and washed with 50 ml water. The product — a dense medium-blue powder — was dried by suction

¹ Approximate formula, $\text{CuCO}_3 \cdot \text{Cu}(\text{OH})_2$.

of air through the filter, and 1.024 mg was recovered. This product was named **hyd-cu-b4c-acet**.

Copper(II) basic carbonate/1,2,4,5-benzenetetracarboxylic acid Copper(II) basic carbonate (0.4709 g, 2.130 mmol) and 1,2,4,5-benzenetetracarboxylic acid (0.6710 g, 2.640 mmol) were added to 50 ml deionized water, and heated with stirring in an autoclave at 140 °C for 24 hours, 120 °C for 5 hours and 100 °C for 5 hours, followed by cooling to room temperature at the natural rate of the autoclave. The product was filtered using a Buchner funnel and washed with 50 ml water. The product — a dense medium-blue powder — was dried by suction of air through the filter, and 0.6710 mg was recovered. This product was named **hyd-cu-b4c-co3**.

3.2.3 Gel-based syntheses and products

The sodium metasilicate stock solution referred to in the following descriptions contained 488 g of technical-grade sodium metasilicate ($\text{Na}_2\text{SiO}_3 \cdot 9\text{H}_2\text{O}$) per litre of deionized water, as described by Henisch [2]. Monoprotic acids used in gel-preparation were diluted to 1:1 acid-water, while diprotic acids were diluted to 1:3 acid-water. A dilute solution of sodium hydroxide (0.2 M) was kept on hand to raise the pH of slightly over-acidified sodium metasilicate solutions and so to “fine-tune” the gel pH.

Straight-tube Syntheses

Four straight-tube syntheses were performed using solutions of the nitrate, sulfate, chloride and acetate salts of copper(II); and a sodium metasilicate gel impregnated with 1,2,4,5-benzenetetracarboxylic acid. For each copper(II) salt:

- 5 ml of sodium metasilicate stock solution was added to 25 ml of an aqueous solution containing 1.0 g (3.9 mmol) of 1,2,4,5-benzenetetracarboxylic acid, (previously heated to dissolve the acid and expel dissolved air, and allowed to cool to slightly above ambient temperature);

- the resulting (basic) solution was then acidified to the desired pH of approximately 6.5² by adding the diluted acid whose conjugate base is the counter-ion to copper(II) in the specific copper(II) salt;
- the resulting solution (at this point exhibiting the slight turbidity that indicates the beginning of the gelling process) was poured into the lower half of a boiling tube, and the reaction vessel was covered (but *not* sealed), placed in a thermostatted water bath at 45 °C and left overnight to allow setting of the gel to its proper consistency;
- a solution of the copper(II) salt, containing, in terms of molar amounts, twice as much copper(II) as the amount of 1,2,4,5-benzenetetracarboxylate present in the gel, in 30 ml deionized water was prepared (see Table 3.1, p. 62), and poured into the boiling tube above the gel, taking care not to damage the gel;
- the boiling tube was covered (but *not* sealed) and placed back in the thermostatted water bath.

Table 3.1: Copper-containing reagent solutions (in 30 ml deionized water) for straight-tube and U-tube syntheses.

Compound	Molar Mass/g mol ⁻¹	Required mass/g
Cu(NO ₃)·3H ₂ O	241.60	1.90
CuSO ₄ ·5H ₂ O	249.69	1.96
CuCl ₂ ·2H ₂ O	170.48	1.34
Cu(CH ₃ COO) ₂ ·H ₂ O	199.65	1.57

²The optimum pH for rapid gelling of sodium metasilicate solutions is 8 [2]. Although our initial *U-tube* experiments with copper(II) had some success, *straight-tube* experiments with other metals at this pH, and slightly higher, failed, apparently because the metals were being trapped by the formation of insoluble hydroxides. Better results were obtained for these metals at a pH of 6.5, and thus 6.5 was chosen as a starting pH for all gel-based syntheses with sodium metasilicate gels.

Copper(II) nitrate/1,2,4,5-benzenetetracarboxylate straight-tube reaction The state of this reaction after three months is illustrated in Figure 3.3. The following

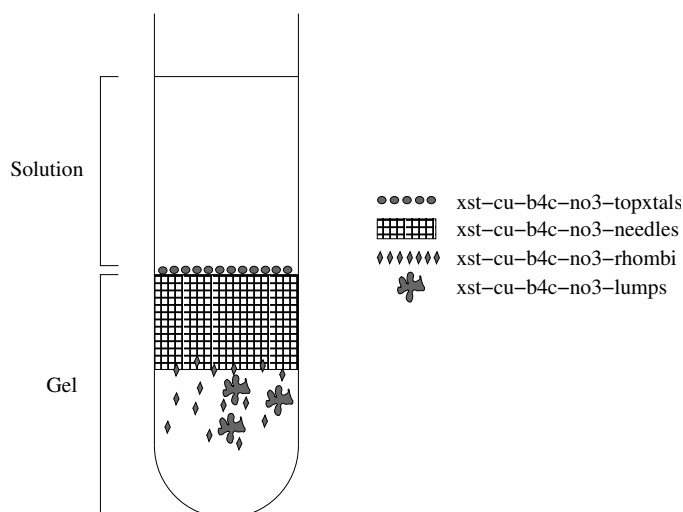


Figure 3.3: The copper(II) nitrate/1,2,4,5-benzenetetracarboxylate straight-tube reaction after approximately three months.

products were obtained for this reaction:

xst-cu-b4c-no3-topxtals Occurring at the interface between the copper(II) nitrate solution and gel, growing on the surface of the gel in the supernatant solution, this product consists of large clear light-blue crystals with a spherical diameter of 3-4 mm, with some larger than 5 mm. This product began to form immediately after the copper(II) nitrate solution was placed over the gel.

xst-cu-b4c-no3-needles This product consisted of fine blue-green needles occurring in clumps, shaped like large three-dimensional asterisks as large as 10 mm from end to end, growing within the gel from the solution-gel interface down to slightly below the halfway-point between the bottom of the tube and the solution-gel interface. This product began to form within a day or two after the copper(II) nitrate solution was placed over the gel.

xst-cu-b4c-no3-rhombi This product consisted of light-blue flat rhombi measuring between 2 and 4 mm from corner to corner, this product occurred

exclusively in the lower half of the gel-region. It formed relatively late in the course of the reaction, after more than a month had elapsed.

xst-cu-b4c-no3-lumps This product consisted of large clumps of light-blue crystals, growing exclusively in the lower half of the gel-region. It was the last product to form, beginning to do so only after more than two months had elapsed.

Very soon after the moment which Figure 3.3 depicts, first **xst-cu-b4c-no3-rhombi** and soon afterwards **xst-cu-b4c-no3-needles** began to deteriorate, change colour slightly, and redissolve. **xst-cu-b4c-no3-topxtals** was immediately removed, and this disturbance caused the redissolution process to speed up. Within a few days, **xst-cu-b4c-no3-needles** and **xst-cu-b4c-no3-rhombi** had almost completely redissolved, and **xst-cu-b4c-no3-lumps** was growing rapidly. From this reaction, only **xst-cu-b4c-no3-topxtals** and **xst-cu-b4c-no3-lumps** could be recovered in sufficient quantities to permit characterization, but replicate syntheses were later performed. Table 3.2 shows the relative amounts of products obtained³.

Table 3.2: Products recovered from the copper(II) nitrate/1,2,4,5-benzenetetracarboxylate straight-tube reaction.

Compound code	Mass recovered/mg
xst-cu-b4c-no3-topxtals	0.2784
xst-cu-b4c-no3-needles ^{*†}	0.2701
xst-cu-b4c-no3-rhombi [*]	0.2910
xst-cu-b4c-no3-lumps	0.4479

^{*} Isolated in replicate synthesis.

[†] Large additional amount was discarded.

³The mass figures are not significant in the usual way, because completeness of reaction, in the sense of the limiting reagent or reagents having been used up, is never attained. Even after standing for approximately a year, the characteristic colours of the metal ions are still visible in the solutions above the gel, although it should be mentioned that the status of the reagent in the gel is impossible to gauge without disturbing the reaction.

Copper(II) sulfate/1,2,4,5-benzenetetracarboxylate straight-tube reaction The state of this reaction after three months is illustrated in Figure 3.4. The following

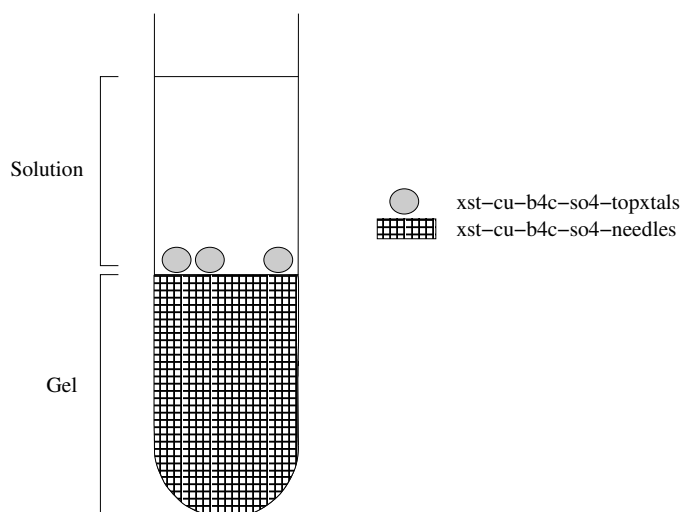


Figure 3.4: The copper(II) sulfate/1,2,4,5-benzenetetracarboxylate straight-tube reaction after approximately three months.

products were obtained for this reaction:

xst-cu-b4c-so4-topxtals These very large light-blue crystals, one greater than 10 mm in spherical diameter, began to form on the gel surface, in the solution zone, immediately after the copper(II) sulfate solution was placed over the gel.

xst-cu-b4c-so4-needles This product consists of very fine blue-green needles growing in star-like clumps, some as long as 20 mm. Formation began within a day or two of the copper(II) sulphate solution being placed over the gel. The product formed throughout the entire volume of the gel-region. Denser growth of shorter needles occurred towards the top of the gel-region, with longer needles forming towards the middle. Both the density of the growth and the size of the needles decreased from the middle of the gel region towards the bottom of the tube.

These products appeared to be very stable within the reaction system, and were removed intact.

Table 3.3: Products recovered from the copper(II) sulfate/1,2,4,5-benzenetetracarboxylate straight-tube reaction.

Compound code	Mass recovered/g
xst-cu-b4c-so4-topxtals	0.2245
xst-cu-b4c-so4-needles	0.4934

Copper(II) chloride/1,2,4,5-benzenetetracarboxylate straight-tube reaction

The state of this reaction after three months is illustrated in Figure 3.5. The fol-

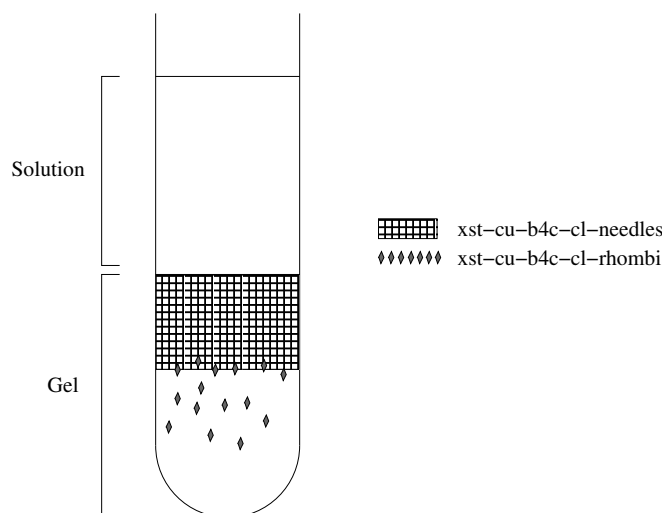


Figure 3.5: The copper(II) chloride/1,2,4,5-benzenetetracarboxylate straight-tube reaction after approximately three months.

lowing products were obtained for this reaction:

xst-cu-b4c-cl-needles This product occurred throughout mainly the top third of the gel region, and consisted of fine blue-green needles occurring in star-like clumps. It began to form almost immediately after the copper(II) chloride solution was placed above the gel.

xst-cu-b4c-cl-rhombi This product, composed of flat rhombi 2-5 mm from corner to corner, began to form approximately one week after the copper(II) chloride solution was placed above the gel.

xst-cu-b4c-cl-lumps Visually identical to, and confirmed by XRPD to be the same as, **xst-cu-b4c-no3-lumps**, this product formed occasionally in replicate syntheses. It formed above the gel in the supernatant metal-salt solution. When this material formed, other products — starting with **xst-cu-b4c-cl-rhombi** — would slowly be converted to this product.

These products appeared to be very stable in the reaction system, and were removed intact.

Table 3.4: Products recovered from the copper(II) chloride/1,2,4,5-benzenetetracarboxylate straight-tube reaction.

Compound code	Mass recovered/g
xst-cu-b4c-cl-needles	0.6660
xst-cu-b4c-cl-rhombi	0.0756
xst-cu-b4c-cl-lumps*	0.1511

* Obtained in replicate synthesis.

Copper(II) acetate/1,2,4,5-benzenetetracarboxylate straight-tube reaction

Only one product, viz., **xst-cu-b4c-acet-xtals**, was obtained for this reaction. Formation began within a week of the copper(II) acetate solution being placed over the gel, and grew very slowly over the ensuing months. Relatively few crystals formed at first, but as these grew slowly, more formed throughout the reaction zone. The dark blue-green crystals grew either individually (this is the dominant pattern at first), as rectangular formations up to 3 mm from end to end, or in star-shaped clusters. Figure 3.6 shows the reaction at the end of approximately six months. This product appeared to be stable in the reaction system, but examination by means of an optical microscope showed some slight surface degradation at a room temperature of approximately 30 °C.

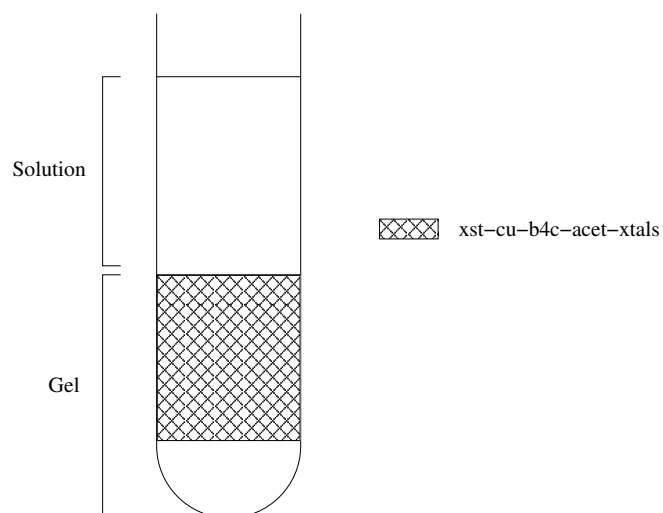


Figure 3.6: The copper(II) acetate/1,2,4,5-benzenetetracarboxylate straight-tube reaction after approximately six months.

Table 3.5: Products recovered from the copper(II) acetate/1,2,4,5-benzenetetracarboxylate straight-tube reaction.

Compound code	Weight recovered
xst-cu-b4c-acet-xtals	0.8373 g

U-tube Syntheses

Four U-tube syntheses were performed, one for each of the nitrate, sulphate, chloride and acetate of copper(II). For each copper(II) salt:

- a “blank” sodium metasilicate gel was prepared by diluting 5 ml of sodium metasilicate stock solution to 30 ml with deionized water (previously heated to expel dissolved air, and allowed to cool to slightly above ambient temperature), and acidifying to the desired pH of approximately 6.5 by the addition of the diluted acid whose conjugate base is the counter-ion to copper(II) in the copper(II) salt in question;
- the resulting gel-mixture (slightly turbid at this point, indicating the start of the gelling process) was poured into the lower semicircular portion of a U-tube, and the vessel was covered (but *not* sealed) and placed overnight in a thermostatted water bath at 45 °C to allow the gel to cure to its full consistency;
- a solution of 1,2,4,5-benzenetetracarboxylate was prepared by dissolving 1 g (3.9 mmol) of 1,2,4,5-benzenetetracarboxylic acid in deionized water, adding an equivalent of sodium bicarbonate (1.3 g, 16 mmol) to aid in dissolution;
- a solution of the copper(II) salt (details in Table 3.1, p. 62) was prepared, containing (in molar terms) twice the amount of copper(II) as the amount of 1,2,4,5-benzenetetracarboxylic acid;
- the copper(II) and 1,2,4,5-benzenetetracarboxylate solutions were poured into opposite legs of the U-tube, taking care not to damage the gel, and the reaction vessel was covered (but *not* sealed) and placed back in the thermostatted water bath.

The U-tube syntheses gave simpler sets of products than the corresponding straight-tube syntheses. Secondary product formation in U-tubes occurred to a much lesser extent, and was much delayed, compared that in straight-tubes. Thus, Figure 3.2 on page 59 is sufficient to illustrate all examples. Only the major products are discussed below.

Copper(II) nitrate, sulfate and chloride/1,2,4,5-benzenetetracarboxylate reactions The major products of these reactions were identical in appearance, formed in the same parts of the tube, and at approximately the same time. They consisted of fine blue-green needles up to 20 mm long, occurring in clumps, some star-like in shape. The major products of the copper(II) nitrate, sulfate and chloride reactions were named **xut-cu-b4c-no3-needles**, **xut-cu-b4c-so4-needles**, and **xut-cu-b4c-cl-needles**, respectively. These products appeared to be identical to the corresponding straight-tube products, and had similar properties. It proved to be very difficult to remove these products because of the fragility of the needle-like crystals, and isolation of the products was accompanied by much loss of material. About 0.6 g could be retrieved from each reaction. The products of these U-tube reactions were not employed further in this study.

Copper(II) acetate/1,2,4,5-benzenetetracarboxylate U-tube reaction. A single product was obtained for this reaction, consisting of large rectangular-shaped dark blue-green crystals, occurring both individually and in star-like clumps⁴. The crystals appeared very similar to the corresponding straight-tube product, **xst-cu-b4c-acet-xtals**, but for the present reaction the crystals were larger and appeared to be of better quality. Therefore, **xut-cu-b4c-acet-xtals** was employed in further studies rather than **xst-cu-b4c-acet-xtals**.

Table 3.6: Products recovered from the copper(II) acetate/1,2,4,5-benzenetetracarboxylate U-tube reaction

Compound code	Mass recovered/g
xut-cu-b4c-acet-xtals	1.1878

⁴In the first attempt at this reaction, the product began to form much later than in the corresponding copper(II) nitrate, sulfate and chloride reactions, and formed in the gel near the copper(II) acetate solution/gel interface, not near the centre of the gel regions, as with the other U-tube reactions. However, in two subsequent repetitions of this reaction under identical conditions, the same product formed towards the centre of the gel region.

Mixed-ligand syntheses

Several attempts at gel-based, mixed-ligand syntheses were made, but only two produced useful results. Both of these were U-tube syntheses involving pyridine as the second ligand. These syntheses were intended to be preliminary trials, and were done on a much smaller scale than the reactions described above, in small U-tubes with a diameter of about 8mm. When they did not produce any products for several weeks, they were placed in storage. After several months they were found to have formed products. Although two methods described are quite different, they resulted in the formation of identical products.

Cu-pyridine/1,2,4,5-benzenetetracarboxylate synthesis A sodium metasilicate gel was prepared using the same method as above, acidifying to a final pH of 7–8 (by pH paper) but only about 5 ml was placed in the tube. Two solutions were prepared:

- 1,2,4,5-benzenetetracarboxylic acid (0.0981 g, 0.386 mmol) and sodium bicarbonate (0.1254 g, 1.492 mmol) were dissolved in 7 ml deionized water;
- $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (0.2323 g, 0.9617 mmol) was dissolved in 7 ml water, to which was added pyridine (310 μl , approx. 4 mmol).

These solutions were placed on either side of the gel-barrier. Several months later, large purple crystals appeared both in the gel and above the gel in the supernatant liquid. In all, 0.0740 g of crystals were obtained. Based on analysis and crystal structure information (see Section 4.4, p. 119), it was later shown that two pyridine molecules were coordinated to each copper in this product, which was named **xut-cu-pyr2-b4c-no3-xtals**.

Cu/pyridine-1,2,4,5-benzenetetracarboxylate synthesis A sodium metasilicate gel was prepared using the same method as above, acidifying to a final pH of 8–9 (by pH paper) but only about 5 ml was placed in the tube. Two solutions were prepared:

- 1,2,4,5-benzenetetracarboxylic acid (0.1062 g, 0.4186 mmol) and sodium

bicarbonate (0.1482 g, 1.764 mmol) were dissolved in 7 ml of aqueous pyridine (1:1 by volume);

- $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (0.2162 g, 0.8949 mmol) was dissolved in 7 ml deionized water.

These solutions were placed on either side of the gel-barrier. Several months later, large clumps of purple crystals appeared at the interfaces between the gel and the supernatant liquids. In all, 0.1503 g of crystals were obtained. Although this product was subsequently shown to be identical to **xut-cu-pyr2-b4c-no3-xtals** (see Section 4.4, p. 119), it was called **xut-cu-pyrX-b4c-no3-xtals** to distinguish it from the other product.

References

- [1] **Albrecht Rabenau.** “The Role of Hydrothermal Synthesis in Preparative Chemistry”. *Angew. Chem. Int. Ed. Engl.* **24** (1985), 1026–1040.
- [2] **H. K. Henisch.** *Crystal Growth in Gels*. Dover Publications, Mineola, New York 1996.
- [3] **N. C. Martin and W. Clegg.** “Synthesis and Structures of Complexes of Pyromellitic Acid with First Row Transition Metals”. British Crystallographic Association Conference: BCA 2001, 7–10 April 2001, Reading, England. URL: <http://www.isis.rl.ac.uk/BCA2001/Abstract%20files/bca3.pdf> (Last accessed September 2007, apparently no longer available).
- [4] **R. Kofenstein and C. Robl.** “The layered structure of $\text{Cu}_2(\text{H}_2\text{O})_4[\text{C}_4\text{H}_4\text{N}_2][\text{C}_6\text{H}_2(\text{COO})_4]\cdot 2\text{H}_2\text{O}$ ”. *Z. Anorg. Allg. Chem.* **631** (2005), 1756–1758. Cited in the Cambridge Structural Database, structure WARYIY, CAN 144:160623.
- [5] **I. Stein and U. Ruschewitz.** “Polymeric diaquatetrakis(μ -1,2-benzenedicarboxylato)di- μ -nitrate-pentastrontium(II)”. *Acta Crystallogr., Sect. E: Struct. Rep. Online* **E61**(1) (2005), m141–m143. CAN 142:420308.
- [6] **Julius Ciric.** “Synthetic Zeolites: Growth of Larger Single Crystals”. *Science* **155** (1967), 689.

Chapter 4

Characterization

In this chapter, the compounds synthesized by the methods reported in Chapter 3 (p. 56) are characterized by means of X-ray powder diffraction (XRPD), Fourier transform mid-infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), thermogravimetry with evolved gas analysis by FTIR (TG-FTIR), various methods of elemental analysis and single-crystal X-ray diffraction. The compounds are grouped according to their physical appearance, and this grouping is discussed.

4.1 GROUP 1 PRODUCTS

This group consists of the three needle-like products, **xst-cu-b4c-no3-needles**, **xst-cu-b4c-so4-needles** and **xst-cu-b4c-cl-needles** (all three from straight-tube syntheses), and the product of the U-tube synthesis with copper(II) acetate **xut-cu-b4c-acet-xtals**. See Section 3.2.3 (p. 61 *et seq.*) for synthesis details.

On the strength of XRPD and mid-IR studies, the product **xut-cu-b4c-acet-xtals** was initially thought to be identical to the needle-like products, **xst-cu-b4c-no3-needles**, **xst-cu-b4c-so4-needles** and **xst-cu-b4c-cl-needles**, and results of a preliminary analysis suggested a formula of $\text{Cu}_2\text{L}\cdot x\text{H}_2\text{O}$. A crystal structure was obtained for **xut-cu-b4c-acet-xtals** which agreed with this formula, but it proved to be impossible to reconcile this with the TG results, and further investigations were necessary to determine the compositions of these compounds.

4.1.1 Elemental analysis

Results of the elemental analyses for **xut-cu-b4c-acet-xtals** and for the needle-like products, with the metal-to-ligand (M:L) ratios calculated from these, are given in Table 4.1 (p. 75). The Cu:L ratio is lower for **xut-cu-b4c-acet-xtals** than for the three needle-like products¹. Also, the sodium content for **xut-cu-b4c-acet-xtals** corresponds to one sodium per ligand, whereas the sodium content is less than 0.6 % (less than $\frac{1}{7}$ of a sodium atom per ligand) for all three needle-like products. The sodium content of the needle-like products is most likely due to surface contamination by traces of sodium metasilicate gel, and was therefore discounted from Table 4.1.

Table 4.1: Results of elemental analyses of the needle-like products and their calculated metal-to-ligand ratios. (Cu and Na determined by ICP-MS.)

Product	% C	% H	% Cu	% Na	Cu:L	Na:L
xut-cu-b4c-acet-xtals	22.27	3.26	23.20	4.13	1.97:1	0.97:1
xst-cu-b4c-no3-needles	21.82	3.25	26.95	—	2.33:1	—
xst-cu-b4c-so4-needles	21.99	3.21	26.18	—	2.25:1	—
xst-cu-b4c-cl-needles	21.99	3.16	26.66	—	2.29:1	—

The analytical data for **xut-cu-b4c-acet-xtals**, for which the crystal structure was determined (see Section 4.1.3, p. 85), was fed into a spreadsheet and compared to the calculated analytical data for formulas of the form $\text{Cu}_2 \text{Na}(\text{OH})\text{L}\cdot x\text{H}_2\text{O}$ — where L stands for the fully deprotonated 1,2,4,5-benzenetetracarboxylate unit, and the OH is assumed for balance of charge — for $x = 0, \frac{1}{4}, \frac{1}{2}, \dots$. The sum of the squares of the residuals (SSR) between the experimental and calculated values of the Cu, Na, C and H percentages were computed for the different values of x , and the formula with the smallest SSR-value was found. This was $\text{Cu}_2 \text{Na}(\text{OH})\text{L}\cdot 7\text{H}_2\text{O}$, with an SSR value of 0.09. See Table 4.2 (p. 78) for details.

¹While the Q-test for outliers [1, p. 57–58] would not reject the lower Cu:L ratio for **xut-cu-b4c-acet-xtals** as an outlier even at the 90 % confidence level (4 points), it should be noted that the Cu:L ratios reported here are *not* replicate analyses, but the averages of separate sets of replicate analyses. Furthermore, the same trend was observed in preliminary analysis by complexometric titration (see Appendix A, p. 341).

Interpretation of the analysis data for the three needle-like products proved to be more difficult. Their Cu:L ratios, reported above, are consistently greater than or equal to $2\frac{1}{4} : 1$. These higher metal-to-ligand ratios are consistent with preliminary results obtained by copper determination by complexometric titration.

The arithmetic mean and the median of the experimental Cu:L ratios are both equal to 2.29:1. This figure was considered to be too far from 2.00:1 (for a completely deprotonated benzenetetracarboxylate unit and no other anions²), and too closely reproducible, for the difference to be ascribed to experimental error. The mean/median is equally close to $2\frac{1}{4}$ as to $2\frac{1}{3}$, and neither could be excluded as the correct figure.

To calculate the most likely compositions of the three needle-like products, the following four formulas were employed: $\text{Cu}_2\text{L}\cdot x\text{H}_2\text{O}$, $\text{Cu}_{2\frac{1}{4}}(\text{OH})_{\frac{1}{2}}\text{L}\cdot x\text{H}_2\text{O}$, $\text{Cu}_{2\frac{1}{3}}(\text{OH})_{\frac{2}{3}}\text{L}\cdot x\text{H}_2\text{O}$, and $\text{Cu}_{2\frac{1}{2}}(\text{OH})\text{L}\cdot x\text{H}_2\text{O}$, where L is the completely deprotonated 1,2,4,5-benzenetetracarboxylate ion and the hydroxyl groups are assumed for balance of charge. The compositions for each formula with $x = 0, \frac{1}{2}, 1, \dots$ were calculated and compared to the experimental data obtained for each of the three products. For each formula, the sum of the squares of the residuals (SSR) between the calculated and experimental data (expressed as percentages) was computed for the different values of x , giving rise to twelve sets of computations (four formulas, and three sets of experimental data). Each computation has an associated x for which the SSR is at a minimum, within the “granularity” of half a water. The hydrates of each proposed formula which best fit the experimental data for each product are shown, with each associated SSR, in Table 4.2 (p. 78).

For all three needle-like products, the minimum SSR values are obtained for formulas of the type $\text{Cu}_{2\frac{1}{4}}(\text{OH})_{\frac{1}{2}}\text{L}\cdot x\text{H}_2\text{O}$ or $\text{Cu}_{2\frac{1}{3}}(\text{OH})_{\frac{2}{3}}\text{L}\cdot x\text{H}_2\text{O}$, with much larger SSR values being obtained for the other two formula-types. It is not possible to decide between $\text{Cu}_{2\frac{1}{4}}(\text{OH})_{\frac{1}{2}}\text{L}\cdot x\text{H}_2\text{O}$ and $\text{Cu}_{2\frac{1}{3}}(\text{OH})_{\frac{2}{3}}\text{L}\cdot x\text{H}_2\text{O}$ for each needle-like product by using such methods. Of the two formulas, $\text{Cu}_{2\frac{1}{4}}(\text{OH})_{\frac{1}{2}}\text{L}\cdot x\text{H}_2\text{O}$ may

²Anions other than 1,2,4,5-benzenetetracarboxylate and hydroxyl ions were not considered in this study because for **xst-cu-b4c-so4-needles** and **xst-cu-b4c-cl-needles**, preliminary, qualitative XRF experiments, similar to those reported in Appendix B (p. 344), suggested that no significant quantities of sulfur, chloride or silicon could be detected in these needle-like products. The presence of carbonate ions was considered to be unlikely because they were not found in the crystal structure of **xut-cu-b4c-acet-xtals**.

be justified as being analogous to **xut-cu-b4c-acet-xtals** ($\text{Cu}_2 \text{Na} (\text{OH}) \text{L} \cdot 7\text{H}_2\text{O}$), with every fourth site, occupied by sodium in this structure, being occupied by copper in the needle-like product. Various elemental formulas of this type have been proposed previously, on the strength of elemental analyses, in early reports of preparations of copper(II)-1,2,4,5-benzenetetracarboxylate compounds (in powder form) [2, 3], but the infrared spectra reported in these studies [2] are very poorly resolved and could not be used for comparison.

Table 4.2: Experimental and calculated analyses for Group 1 products. The copper and sodium percentages were obtained by ICP-MS.

Product	Formula	Form. mass /g mol ⁻¹	Calculated				Experimental				SSR
			%C	%H	%Cu	%Na	%C	%H	%Cu	%Na	
xut-cu-b4c-acet-xtals	Cu ₂ Na (OH) L·7H ₂ O	543.33	22.10	3.15	23.39	4.23	22.27	3.26	23.20	4.13	0.09
xst-cu-b4c-no3-needles	Cu ₂ L·7H ₂ O	503.33	23.86	3.20	25.25	—	21.82	3.25	26.95	—	7.05
	Cu _{2$\frac{1}{4}$} (OH) _{$\frac{1}{2}$} L·7 $\frac{1}{2}$ H ₂ O	536.73	22.38	3.29	26.64	—				—	0.41
	Cu _{2$\frac{1}{3}$} (OH) _{$\frac{2}{3}$} L·8H ₂ O	553.87	21.68	3.40	26.77	—				—	0.07
	Cu _{2$\frac{1}{2}$} (OH) L·8H ₂ O	570.13	21.07	3.36	27.87	—				—	1.42
xst-cu-b4c-so4-needles	Cu ₂ L·7 $\frac{1}{2}$ H ₂ O	512.34	23.44	3.34	24.81	—	21.99	3.21	26.18	—	4.01
	Cu _{2$\frac{1}{4}$} (OH) _{$\frac{1}{2}$} L·8H ₂ O	545.74	22.01	3.42	26.20	—				—	0.04
	Cu _{2$\frac{1}{3}$} (OH) _{$\frac{2}{3}$} L·8H ₂ O	553.87	21.68	3.40	26.77	—				—	0.48
	Cu _{2$\frac{1}{2}$} OH L·8 $\frac{1}{2}$ H ₂ O	579.14	20.74	3.48	27.43	—				—	3.21
xst-cu-b4c-cl-needles	Cu ₂ L·7H ₂ O	503.33	23.86	3.20	25.25	—	21.99	3.16	26.66	—	5.49
	Cu _{2$\frac{1}{4}$} (OH) _{$\frac{1}{2}$} L·7 $\frac{1}{2}$ H ₂ O	536.73	22.38	3.29	26.64	—				—	0.17
	Cu _{2$\frac{1}{3}$} (OH) _{$\frac{2}{3}$} L·8H ₂ O	553.87	21.68	3.40	26.77	—				—	0.16
	Cu _{2$\frac{1}{2}$} OH L·8 $\frac{1}{2}$ H ₂ O	579.14	20.74	3.48	27.43	—				—	2.27

4.1.2 Thermogravimetry and Differential scanning calorimetry

The TG curve for **xut-cu-b4c-acet-xtals** ($\text{Cu}_2\text{Na}(\text{OH})\text{L} \cdot 7\text{H}_2\text{O}$)— in conjunction with the EGA results — suggests that water is lost in three steps, marked on Figure 4.1 (p. 79) as follows:

- i. Loss of 0.5 water molecules (1.67 %) between 25 °C and 48 °C overlapping with the next step,
- ii. Loss of a further 5.5 water molecules (total loss, 19.89 %) in one clear step, between 48 °C and 105 °C and
- iii. Loss of a further water molecule over the broad range between 105 °C and about 289 °C (total loss, 23.21 %), overlapping to some extent with the decomposition step which follows.

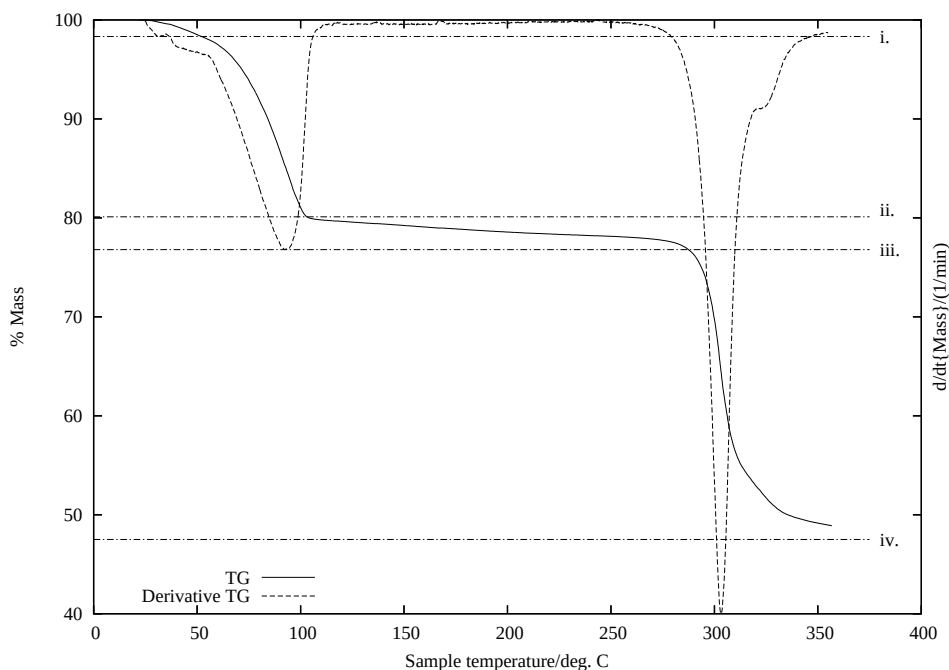
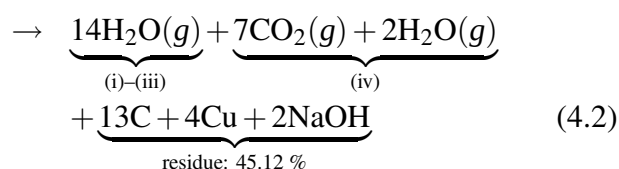
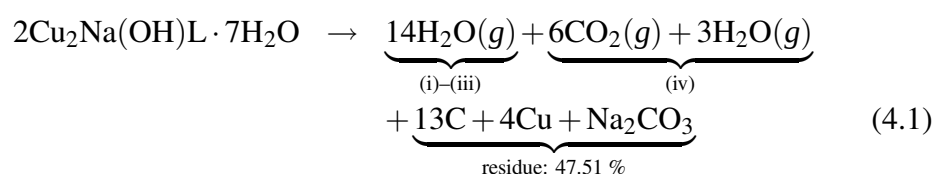


Figure 4.1: TG curve for **xut-cu-b4c-acet-xtals** ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen.

The final decomposition, step iv, is difficult to interpret. If two formula units, i.e., $2(\text{Cu}_2\text{Na}(\text{OH})\text{L} \cdot 7\text{H}_2\text{O})$, are assumed to decompose to some combination of

$\text{H}_2\text{O}(g)$, $\text{CO}(g)$, $\text{CO}_2(g)$, $\text{Cu}(s)$, $\text{C}(s)$, $\text{Na}_2\text{CO}_3(s)$ and/or $\text{NaOH}(s)$, and it is assumed that the seven waters in the formula unit are evolved as such, then there are fifteen non-equivalent ways in which the decomposition may proceed. Of these, the one with the greatest proportion of solid residue (47.51 % of formula mass) is also one of only two which do not involve the evolution of carbon monoxide. The second such reaction has a solid residue amounting to 45.12 % of the formula mass. These reactions are:



The steps for reaction 4.1 are indicated on Figure 4.1 (p. 79), and they agree reasonably well with the mass data. In addition, no carbon monoxide evolution was evident in the EGA results. The DSC residues (see below) were examined by X-ray powder diffraction, and only peaks from copper metal (see Chapter 6 on p. 236 and references therein) could be observed³. The powder patterns of Na_2CO_3 (various anhydrous and hydrated forms) and NaOH all have their major peaks in the range $2\theta = 15 - 55^\circ$ [4], but none of these could be distinguished meaningfully from noise in the experimental patterns.

The TG curves of the needle-like products, *viz.*, **xst-cu-b4c-no3-needles**, **xst-cu-b4c-so4-needles** and **xst-cu-b4c-cl-needles**, are more difficult to interpret. Assuming a formula of the type $\text{Cu}_{2\frac{1}{4}}(\text{OH})_{\frac{1}{2}}\text{L} \cdot x\text{H}_2\text{O}$, the best fit for the analytical data of **xst-cu-b4c-so4-needles** is obtained with $x = 8$, the calculated guest wa-

³TG (nitrogen purge) results for anhydrous product, **hyd-cu-b4c-acet**, as well as for the crystalline products **xst-cu-b4c-so4-topxtals** and **xst-cu-b4c-no3-lumps**, show that the residue masses cannot be accounted for by copper metal alone, and that carbon must be present in measurable quantities. No powder diffraction peaks for anything other than copper metal were observed for the DSC residues of these materials (which have relative masses similar to the final TG masses), so the carbon must be present in an amorphous form.

ter content making up 26.41 % of the sample mass. The other likely formula, $\text{Cu}_{2\frac{1}{3}}(\text{OH})_{\frac{2}{3}}\text{L} \cdot x\text{H}_2\text{O}$ provides the best match for **xst-cu-b4c-no3-needles** and, by a very small margin, **xst-cu-b4c-cl-needles** with $x = 8$, gives rise to a calculated guest water content of 26.02 %.

The dehydration steps, assuming the formula, $\text{Cu}_{2\frac{1}{4}}(\text{OH})_{\frac{1}{2}}\text{L} \cdot 8\text{H}_2\text{O}$, are marked on the TG curve (Figure 4.2, p. 81) for **xst-cu-b4c-so4-needles** as follows:

- i. loss of 5 water molecules per formula unit (16.51 %) in a step between 25 °C and 89 °C, overlapping with the next step, and
- ii.–iv. loss of a further 3 water molecules (total loss, 26.41 %) in a broad step from 89 °C to 302 °C, overlapping with the main decomposition.

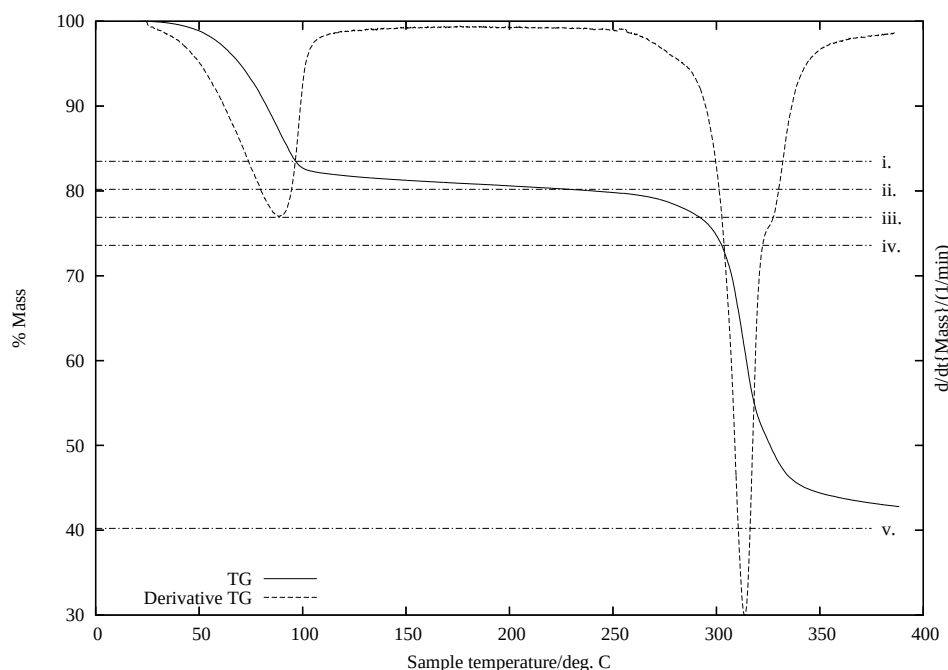
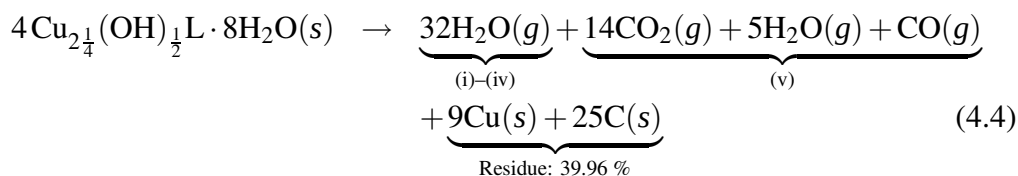
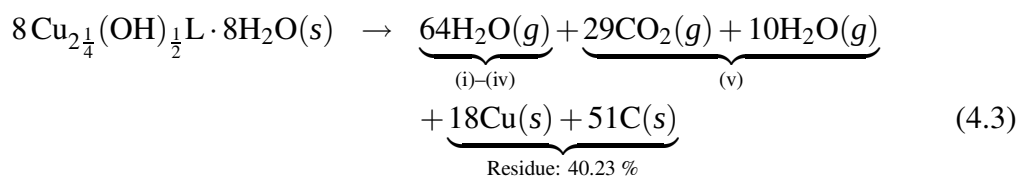


Figure 4.2: TG curve for **xst-cu-b4c-so4-needles** ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen. TG curves of the other needle-like products were nearly identical, although for **xst-cu-b4c-no3-needles** the final mass was in slightly better agreement with step (v.).

If one assumes instead the formula, $\text{Cu}_{2\frac{1}{3}}(\text{OH})_{\frac{2}{3}}\text{L} \cdot 8\text{H}_2\text{O}$, the corresponding total mass losses would, at 16.26 % (i.) and 26.02 % (iv.), be very similar to those

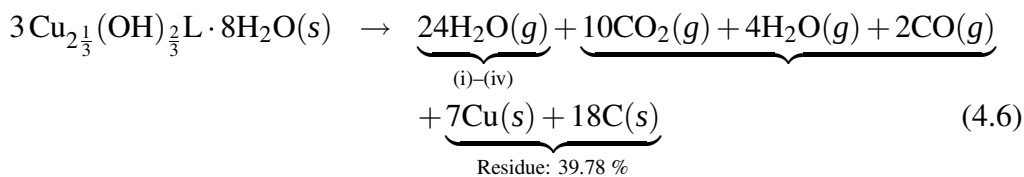
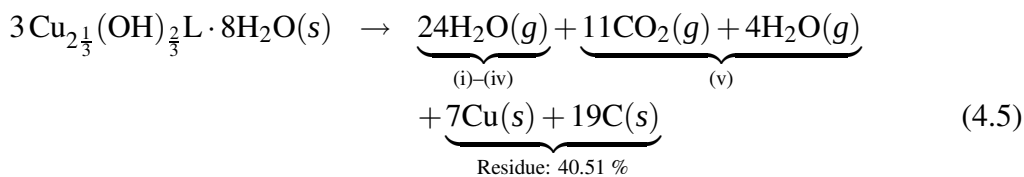
for the earlier formula. Given the small difference in the relative residue masses, these formulas cannot be distinguished from each other using TG.

There are 30 possible non-equivalent decomposition reactions given a maximum of 8 units of the formula, $\text{Cu}_{2\frac{1}{4}}(\text{OH})_{\frac{1}{2}}\text{L} \cdot 8\text{H}_2\text{O}$, of which the two most likely are:



Reaction 4.4 involves the evolution of CO (in a small amount), whereas Reaction 4.3 does not. No carbon monoxide was observed by EGA of the TG exhaust stream, and examination of the DSC residues (see below) by XRD indicated copper metal only (no oxides). It is, however, possible that CO might not have been detected in the quantities that would be evolved in Reaction 4.4 and, given the nearly identical calculated relative residue masses, TG cannot be used to distinguish between the two proposed reactions.

Given three units of the formula, $\text{Cu}_{2\frac{1}{3}}(\text{OH})_{\frac{2}{3}}\text{L} \cdot 8\text{H}_2\text{O}$, there are 12 possible decomposition reactions, of which the most likely are:



Reaction 4.5 is the more likely because the amount of carbon monoxide evolved in Reaction 4.6 is proportionally much higher than it was in Reaction 4.4, and should therefore have been observable by EGA.

The DSC and derivative DSC curves for **xst-cu-b4c-no3-needles**, **xst-cu-b4c-so4-needles** and **xst-cu-b4c-cl-needles**, as well as **xut-cu-b4c-acet-xtals**, are shown in Figure 4.3 (p. 84). The curves for the three needle-like products are very similar. Each shows a single broad endotherm corresponding to dehydration, and a complex series of overlapping endo- and exotherms corresponding to thermal decomposition. The minor differences observed in the range 275–295 °C — slightly more pronounced on the curve for **xst-cu-b4c-cl-needles** — do not appear to be reproducible, and may depend on sample packing. The other features of the decomposition responses for the three needle-like products are reproducible, with minor variations in relative peak sizes, from scan to scan.

The decomposition exotherm (from about 275 °C onwards) for **xut-cu-b4c-acet-xtals** is slightly, though reproducibly, different to those of the needle-like products. The initial endothermic response is very much less pronounced. The second rising edge of the decomposition peak also does not show the shoulder present for the needle-like products.

Neglecting the small initial endotherms, the decomposition peaks for the needle-like products closely resemble the corresponding derivative TG peaks (compare Figure 4.2 on p. 81), particularly the shoulder on the rising edge. This suggests that the shoulder on the derivative TG peak is *not* due to some interference by residual air in the TG furnace. The shoulder is absent —perhaps masked — in the decomposition exotherm for **xut-cu-b4c-acet-xtals**, but present (reproducibly) in the corresponding DTG signal (see Figure 4.1, p. 79), albeit diminished in size.

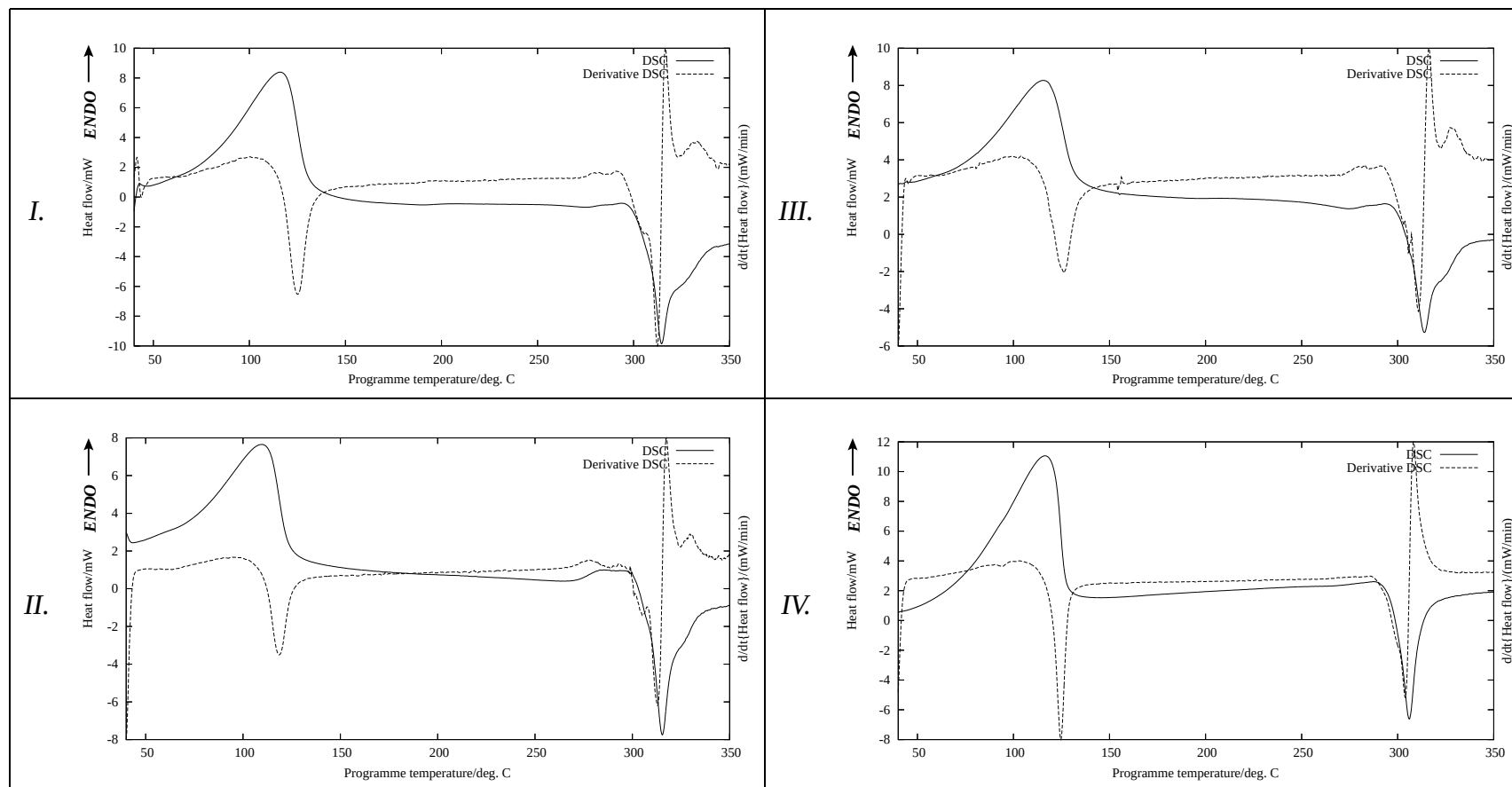


Figure 4.3: DSC and derivative DSC curves for (I.) **xst-cu-b4c-no3-needles**, (II.) **xst-cu-b4c-so4-needles**, (III.) **xst-cu-b4c-cl-needles**, and (IV.) **xut-cu-b4c-acet-xtals**. Samples were heated in crimped (not sealed) aluminium pans from 25 °C to 350 °C at 10 °C min⁻¹ under flowing nitrogen (26 ml min⁻¹).

4.1.3 Crystal structure (**xut-cu-b4c-acet-xtals** only)

Figure 4.5 (p. 89) is a schematic diagram of the binding in the crystal structure of **xut-cu-b4c-acet-xtals**, which is shown more fully in Figures 4.6–4.8 (pp. 90–92). Full crystal structure details are given in Appendix C (p. 352).

This material is a three-dimensional covalent polymer, consisting of tetrameric copper(II) clusters linked together by 1,2,4,5-benzenetetracarboxylate ligands. The structure is traversed by channels which contain guest water molecules, as shown in Figures 4.7–4.8 (pp. 91–92). There are two types of 1,2,4,5-benzenetetracarboxylate anion: one type is μ_{10} -bridging (designated A) and makes up the floor of the channels as drawn; the other is μ_8 -bridging (designated B), and makes up the walls of the channels.

The SBU of this metal organic framework is shown in Figure 4.4 (p. 86). Two crystallographically equivalent copper(II) ions (2) are doubly linked by μ_3 -bridging oxygens, believed to be hydroxides, which also link this pair of coppers to non-equivalent copper(II) atoms (1) as shown. The interatomic distance for the hydroxo-bridged Cu(2)–Cu(2) pair is 2.912 Å. Cu(1) and (2) pairs are linked together by bridging carboxyl groups, as shown, to form the 16-membered ring, Cu1–O11A–C–O12A–Cu2–...–O21A.

This motif has a precedent in the Cambridge Structural Database, in the form of a carboxyl-bridged isonicotinate-N-oxide copper(II) complex [5], which features in addition a μ_2 -sulfato-bridge between the Cu2-pair. In this complex, the μ_3 -bridging oxygens are taken as hydroxides, but the authors stated that only carbon and heavier atoms could be located in the crystal structure investigation. The copper-copper distance between the hydroxo-bridged copper(II) ions was 2.855 Å.

Each type-2 copper is also doubly-bridged to sodium via μ_2 -bridging carboxyl oxygens O11B and O22A, forming the four-membered ring, Cu2–O11B–Na–O22A. This motif can also be seen in other copper(II) carboxylates [6–14].

Two copper atoms, Cu1 and Cu2, are bridged by an oxygen atom, O1, which is itself bound to a copper atom equivalent to Cu2 in the next unit behind. Each copper atom is in a square-based pyramidal configuration. 1,2,4,5-Benzenetetracarboxylate units A and B are both bound to the bridged pair of copper atoms through one carboxylate group each. Cu1 is bound axially to the carboxylate oxygen atom O12B on ligand B. Going clockwise around the bond Cu1—O12B, Cu1 is bound to:

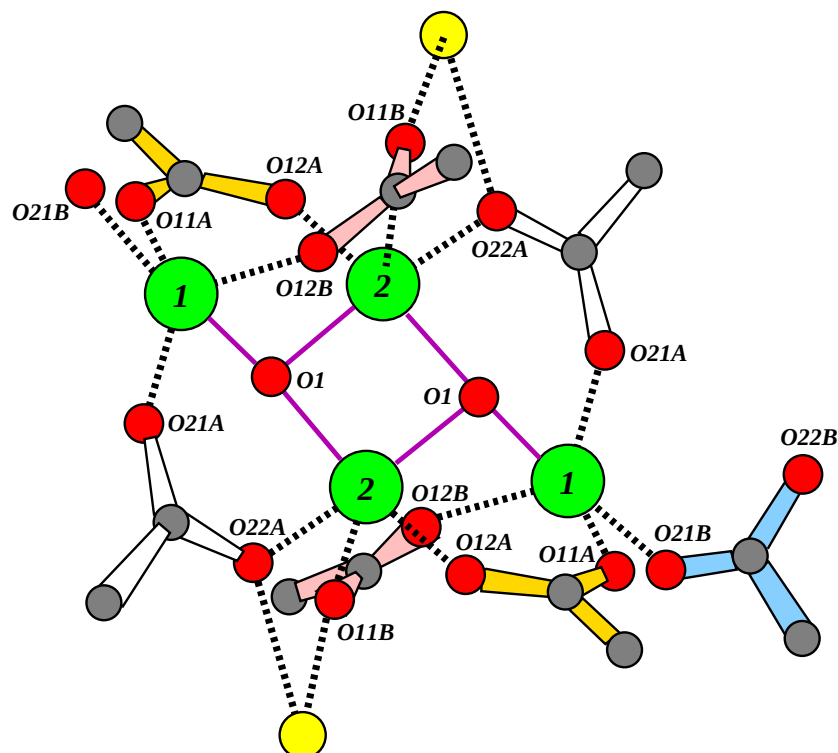


Figure 4.4: SBU of **xut-cu-b4c-acet-xtals**. The carboxyl group at the bottom right, shown in blue, has a crystallographic equivalent at the top right, shown only as the oxygen O21B. Green spheres indicate copper(II) ions; yellow, Na^+ ions; red, oxygen atoms; and black, carbon atoms. Some atom positions are slightly displaced to clearly show the binding.

1. O1, the oxygen atom bridging Cu1 and Cu2;
2. O11A, a carboxylate oxygen atom on ligand A;
3. O21B(b), a carboxylate oxygen atom on ligand B of a neighbouring unit;
and
4. O21A(e), a carboxylate oxygen atom on ligand A of a different neighbouring unit.

Likewise, Cu2 is bound axially to the carboxylate oxygen O11B on ligand B, and going clockwise around this bond as before, also to

1. O12A, a carboxylate oxygen atom on ligand A;

2. O1, the bridging oxygen;
3. O1(c), the bridging oxygen from a neighbouring unit; and
4. O22A(a), a carboxylate oxygen on ligand A of a different neighbouring unit.

Ligand A is bound to Cu2(b) from a neighbouring unit through the carboxylate oxygen O21A and, similarly, ligand B is bound to Cu1(a) of a neighbouring unit through O21B. The sodium atom Na1 — in a square-based pyramidal arrangement with an axial bond to water molecule O5W (disordered) — is bound to the carboxylate oxygen atom O22A, to water molecules O4W and O6W, and to the carboxylate oxygen atom O11B(b) in a neighbouring unit.

The bridging oxygen, O1, is bound to Cu1, Cu2 and Cu2(c) from a neighbouring cell, with bond distances of 1.92Å, 1.96Å and 1.94Å respectively, and since this binding would require three lone pairs, O1 cannot be a water molecule.

If O1 were a bridging oxide, then one of the ligand carboxyl oxygens would have to be protonated for balance of charge. Because O22B is unbound, this would be the most likely site for protonation. From common correlation charts for carboxylic acids, the following characteristic bands [15, p. 1418] would be expected:

C–O stretch: weak-to-medium band at 1440–1395 cm⁻¹

O–H in-plane bend: strong band at 1320–1211 cm⁻¹

The infrared spectrum of **xut-cu-b4c-acet-xtals** has a weak band in the former region (at 1417 cm⁻¹) but not in the latter (the band at 1332 cm⁻¹ falls within the range for the carboxylate ion [16, p. F-173]). However, both **xst-cu-b4c-so4-topxtals** and **xst-cu-b4c-no3-lumps** — which are not expected to have protonated carboxyl groups — have bands in the region 1440–1395 cm⁻¹. Therefore the existence of a protonated carboxyl group in **xut-cu-b4c-acet-xtals** cannot be proved.

It also cannot be established beyond a doubt whether O1 is a bridging hydroxide. Nakamoto [17, pp. 229–230] refers to a vibrational study of various copper complexes in which a pair of copper atoms is bridged by two hydroxyl groups [18], which states that the OH vibration of the bridging hydroxyl group

is at 955 cm^{-1} . This paper, citing [19], also mentions that the bending OH vibrations in basic copper compounds are in the region $1000\text{--}677\text{ cm}^{-1}$. In the region $1000\text{--}900\text{ cm}^{-1}$, **xut-cu-b4c-acet-xtals** (spectra shown in Figures 5.5–5.7, pp. 155–157) has three clear bands at 996 cm^{-1} , 973 cm^{-1} and 930 cm^{-1} , plus a small shoulder at 918 cm^{-1} . **xst-cu-b4c-so4-topxtals** has clear bands at 998 cm^{-1} and 929 cm^{-1} , and **xst-cu-b4c-no3-lumps** has bands at 966 cm^{-1} , 932 cm^{-1} , and 917 cm^{-1} . Thus **xut-cu-b4c-acet-xtals** has no unique bands in this region which may correspond to a bridging OH group. Below 900 cm^{-1} the spectra are complex and a band corresponding to bridging OH cannot be assigned.

The crystal structure shows five non-coordinated water molecules (labelled O1W, O2W, O3W, O7W and O8W) per basic unit (i.e., for each two copper atoms) and three water molecules coordinated to the sodium atom (labelled O4W, O5W and O6W). O5W is disordered, and O6W has a longer bond to sodium ($2.42\text{ \AA}$) than the other two coordinated water molecules ($2.34\text{ \AA}$ and $2.35\text{ \AA}$, respectively). The analysis data (see Section 4.1.1, p. 75) strongly suggest the presence of seven waters in total, and this is well supported by TG evidence (see Section 4.1.2, p. 79).

Nevertheless, it is not impossible to reconcile the TG results with a crystal structure containing eight water molecules per formula unit. Steps i. and ii. in the TG curve (Figure 4.1, p. 79) cannot be accounted for as the loss of five non-coordinated water molecules out of a total of eight, because this loss would correspond to only 16 % of the total sample mass. However, the loss of six water molecules (five non-coordinated plus one coordinated) makes up 19.3 % of the total sample mass, and fits well with the end of step ii. in the TG curve. The loss of a further one coordinated water molecule to give a total loss of seven would make up 22.5 % of the total sample mass, which is a good fit to step iii. The loss of the final water molecule might trigger the final decomposition ending in step iv. Both this alternative interpretation and the interpretation given in Section 4.1.2 (p. 79) involve the loss of one or more coordinated water molecules before $150\text{ }^{\circ}\text{C}$, the dehydration temperature selected for dehydration/resolution studies discussed later (Section 5.3, p. 146). As discussed there, the structure collapses after the loss of six (out of eight or seven) water molecules, including at least one of the coordinated waters, and returns to the original structure upon

rehydration or resolution with other solvents.

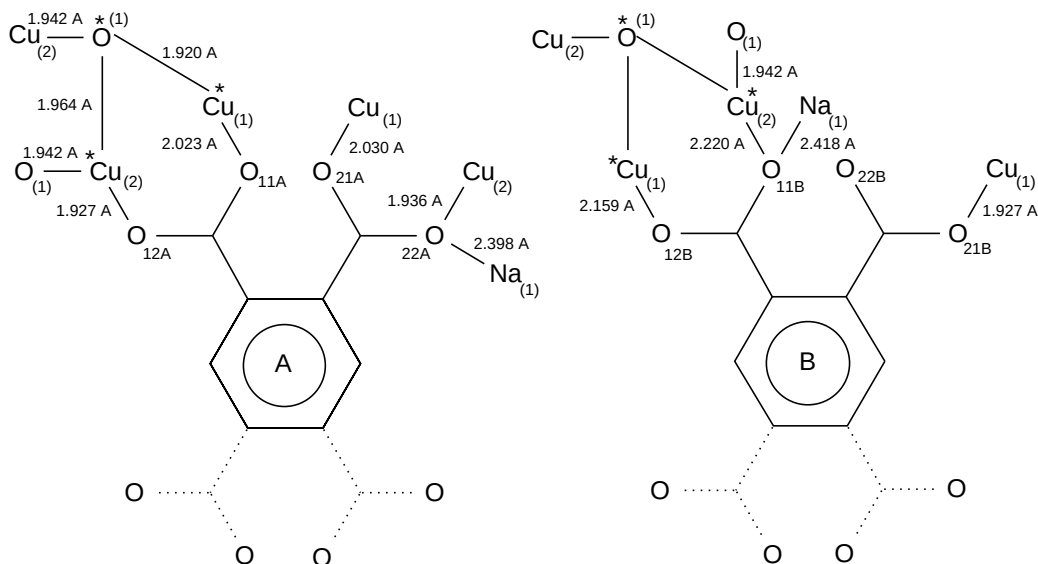


Figure 4.5: Schematic diagram of the binding in **xut-cu-b4c-acet-xtals**. Asterisks indicate the same atoms shown twice, bound to different parts of the structure. The lower halves of ligands A and B — shown in dotted lines — are symmetrical with the upper halves shown.

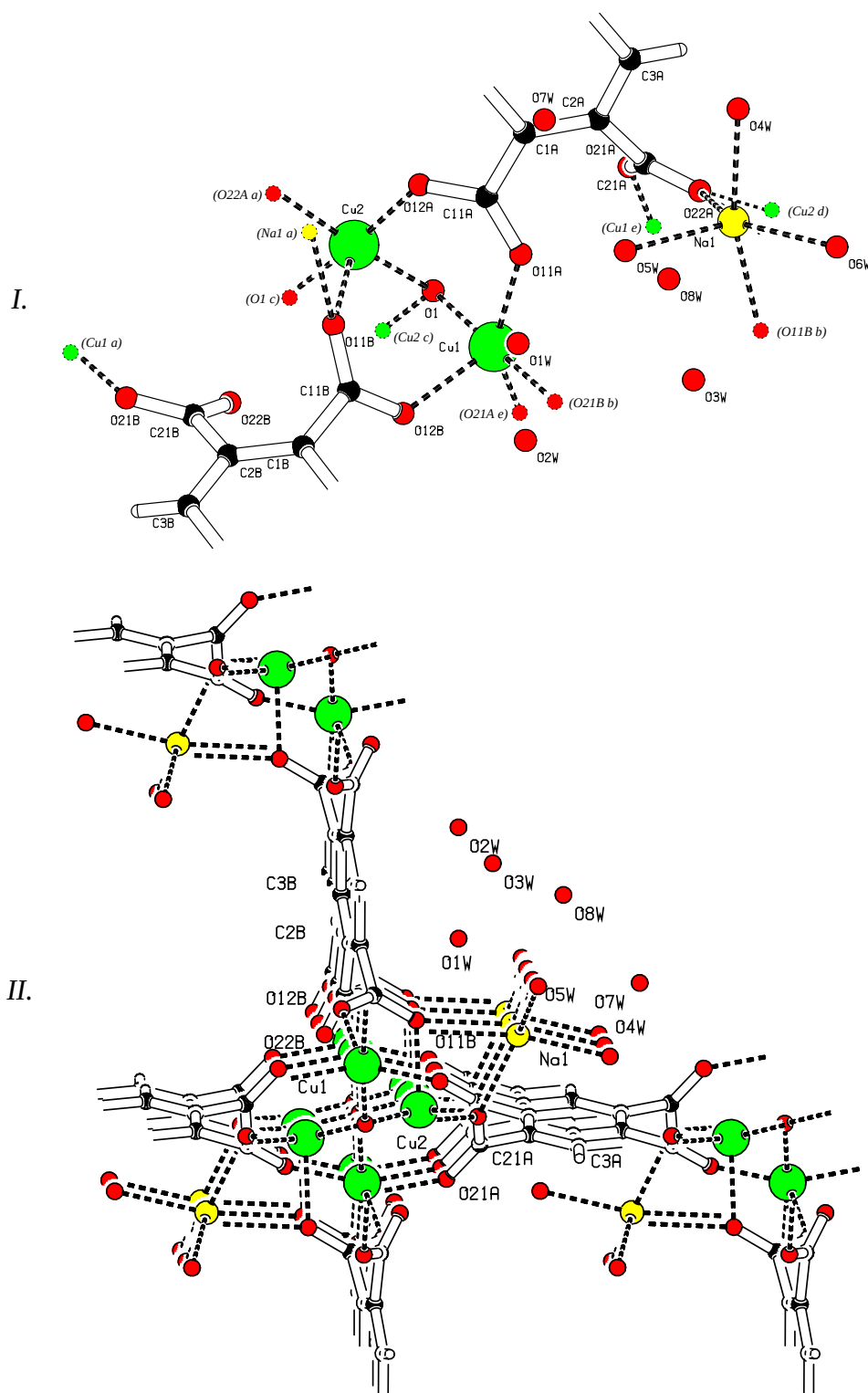


Figure 4.6: Basic unit (*I.*) and an expanded unit (*II.*) of the structure of **xut-cu-b4c-acet-xtals**. Oxygen atoms labelled ‘A’ and ‘B’ are on different ligands, and those labelled ‘W’ are water molecules. Atoms drawn with dotted outlines and italic labels are part of neighbouring units.

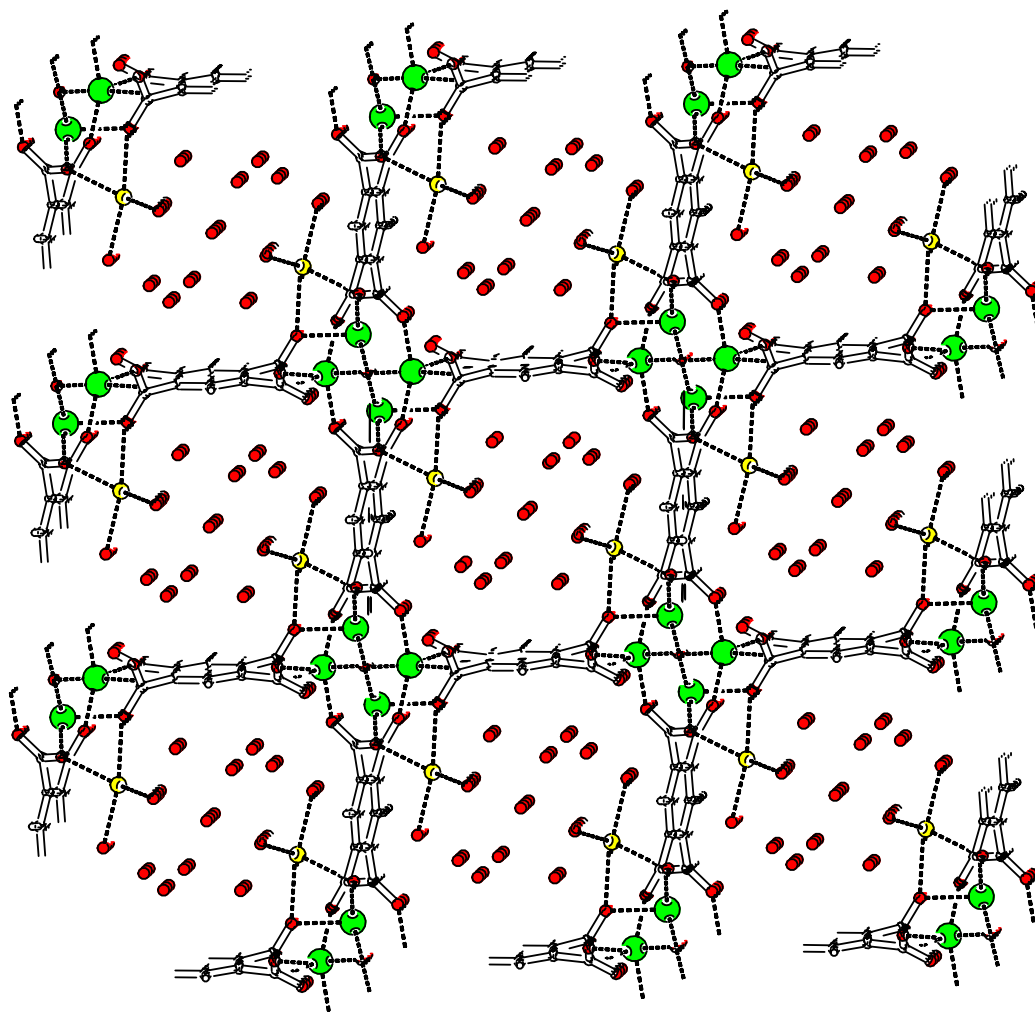


Figure 4.7: Face A of the crystal structure of **xut-cu-b4c-acet-xtals**, showing large cavities containing guest water molecules.

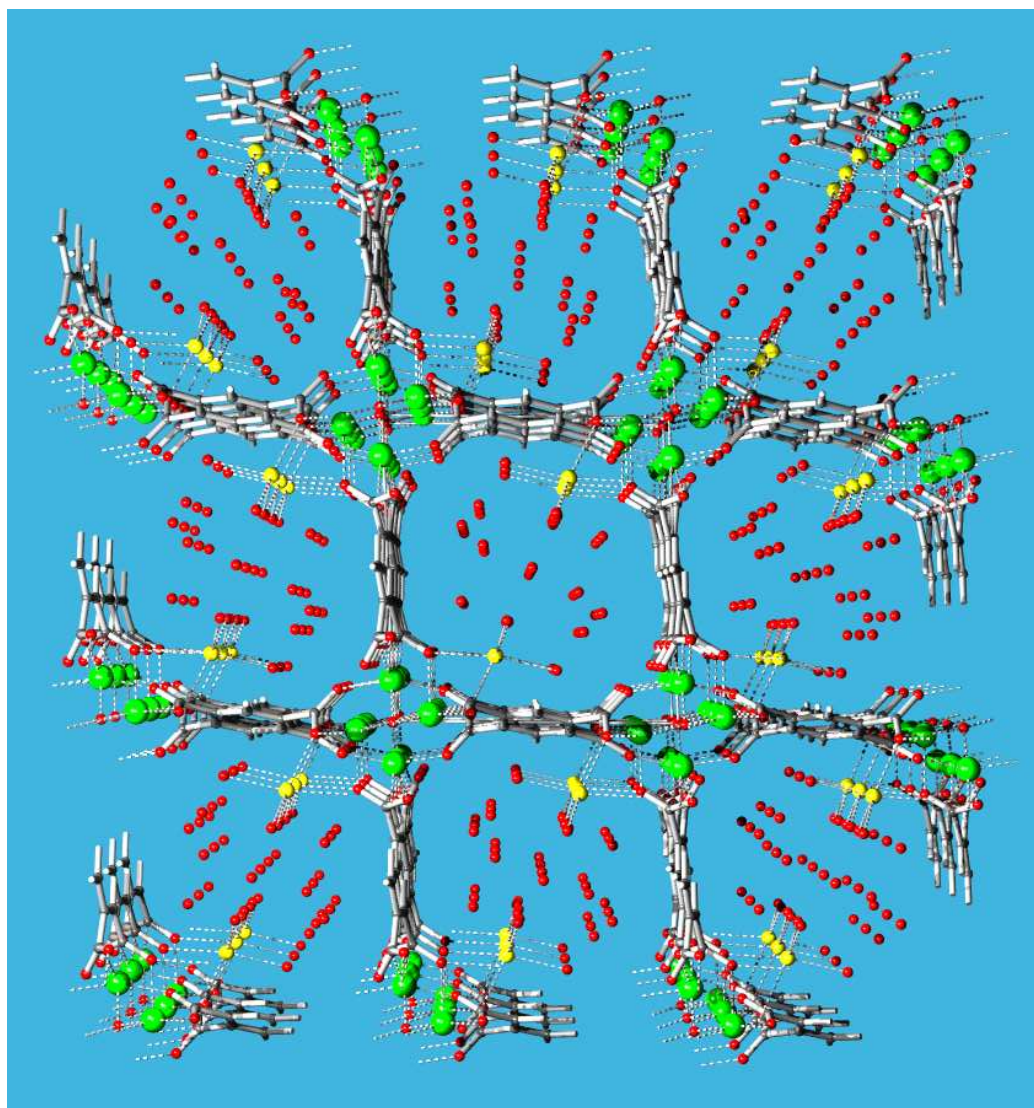


Figure 4.8: Ray-traced diagram of face A of the crystal structure of **xut-cu-b4c-acet-xtals**, showing large cavities containing guest water molecules.

4.2 GROUP 2 PRODUCTS

When the products, **xst-cu-b4c-no3-rhombi** and **xst-cu-b4c-cl-rhombi** were first synthesized, the former could not be isolated at first, as explained on p. 63. A crystal structure for **xst-cu-b4c-cl-rhombi** was obtained and it was initially thought to contain chloride ions. In repeat syntheses, **xst-cu-b4c-no3-rhombi** was successfully isolated and XRPD and mid-IR results showed that these two structures were very similar.

Assuming that **xst-cu-b4c-no3-rhombi** was analogous to **xst-cu-b4c-cl-rhombi** with nitrate present instead of chloride, a crystal structure was obtained for **xst-cu-b4c-no3-rhombi** (see Section 4.2.3, p. 97). This structure proved to be identical to that of **xst-cu-b4c-cl-rhombi**, including the presence of chlorides. This was unexpected, because no significant amount of chloride could have been present in the synthesis of **xst-cu-b4c-no3-rhombi**. The reagents were spot-tested for chloride contamination using 1 M silver chloride solution, and it was concluded that the presence of chloride in **xst-cu-b4c-no3-rhombi** was highly unlikely.

The absence of chloride was confirmed in *both* structures using a sodium fusion test and later also by semi-quantitative XRF experiments (see Appendix B on p. 344). The XRF work showed the presence of sodium in significant quantities, and further analysis (see below) showed that, what were thought initially to be chloride ions are, in fact, sodium ions.

4.2.1 Elemental analysis

The crystal structures (see Section 4.2.3, p. 97) of these compounds suggested the formula, $\text{Cu}_{1\frac{1}{3}} \text{Na}_{1\frac{1}{3}} \text{L} \cdot 4\frac{2}{3} \text{H}_2\text{O}$, or $\text{Cu}_4 \text{Na}_4 \text{L}_3 \cdot 14 \text{H}_2\text{O}$. These proposed structures agree well with the analysis data (see Table 4.3, p. 94), although it appears that $\text{Cu}_{1\frac{1}{3}} \text{Na}_{1\frac{1}{3}} \text{L} \cdot 4\frac{1}{3} \text{H}_2\text{O}$, or $\text{Cu}_4 \text{Na}_4 \text{L}_3 \cdot 13 \text{H}_2\text{O}$, is a slightly better match for both compounds.

Table 4.3: Experimental and calculated analysis figures for Group 2 products.

Product	Formula	Form. mass /g mol ⁻¹	Calculated				Experimental				SSR
			%C	%H	%Cu	%Na	%C	%H	%Cu	%Na	
xst-cu-b4c-no3-rhombi	$\text{Cu}_{1\frac{1}{3}} \text{Na}_{1\frac{1}{3}} \text{L} \cdot 4\frac{2}{3} \text{H}_2\text{O}$ ($\text{Cu}_4 \text{Na}_4 \text{L}_3 \cdot 14 \text{H}_2\text{O}$)	449.58 1348.7	26.71	2.54	18.85	6.82	26.70	2.52	18.15*	6.71*	1.29
xst-cu-b4c-cl-rhombi	$\text{Cu}_{1\frac{1}{3}} \text{Na}_{1\frac{1}{3}} \text{L} \cdot 4\frac{2}{3} \text{H}_2\text{O}$ ($\text{Cu}_4 \text{Na}_4 \text{L}_3 \cdot 14 \text{H}_2\text{O}$)	449.58 1348.7	26.71	2.54	18.85	6.82	27.41	2.49	18.34†	—‡	0.74

*Metal concentration as determined by ICP-MS

†Metal concentration as determined in preliminary work by complexometric titration.

‡Metal concentration not determined in preliminary work.

4.2.2 Thermogravimetry and Differential scanning calorimetry

The TG curve for **xst-cu-b4c-no3-rhombi** shows water loss in at least three overlapping steps to a flat plateau, followed by thermal decomposition. The dehydration steps are marked (assuming $\text{Cu}_2 \text{Na}_2 \text{L}_{1\frac{1}{2}} \cdot 6.5 \text{H}_2\text{O}$, or equivalently $\text{Cu}_4 \text{Na}_4 \text{L}_3 \cdot 13 \text{H}_2\text{O}$, based on the analysis data) on the TG curve (Figure 4.9, p. 95) as follows:

- i. loss of 1.5 water molecules per formula unit (4.06 %) in a step from 25 °C to 95 °C overlapping with the next step
- ii. loss of a further 4 water molecules (total loss, 14.89 %) in a step from 95 °C to 138 °C overlapping with the next step, and
- iii. loss of a further water molecule (total loss, 17.60 %) in a step starting at 138 °C and ending at 165 °C in a level plateau.

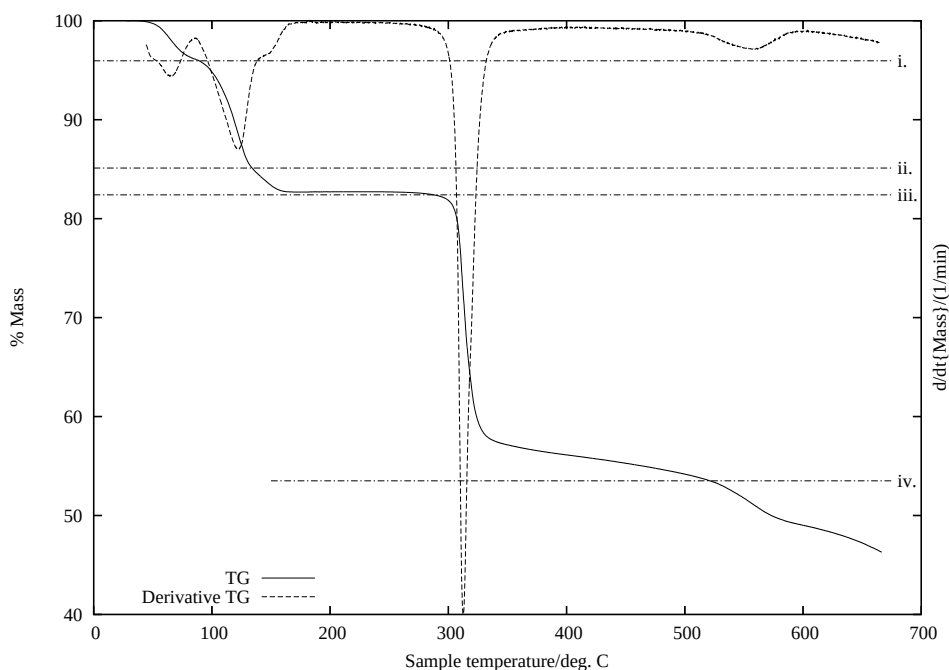


Figure 4.9: TG curve for **xst-cu-b4c-no3-rhombi** ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen.

The decomposition step at about $300\text{ }^{\circ}\text{C}$ does not end in a level plateau, but continues in a slow mass-loss extending to the operating temperature limit of the TG furnace. No carbon monoxide could be detected by FTIR in the exhaust stream

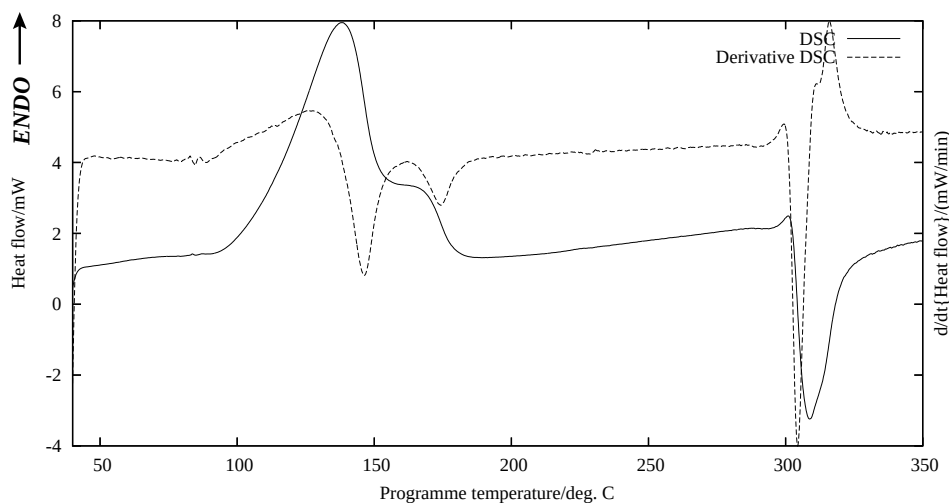
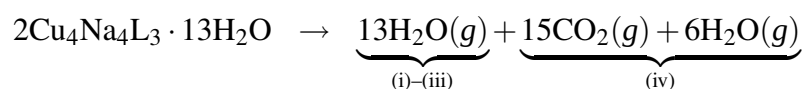
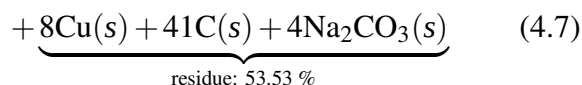


Figure 4.10: DSC and derivative DSC curves for **xst-cu-b4c-no3-rhombi**, heated in a crimped (not sealed) aluminium pan at $10\text{ }^{\circ}\text{C min}^{-1}$ under flowing nitrogen (26 ml min^{-1}). The corresponding curves for the similar structure, **xst-cu-b4c-cl-rhombi** are identical to these.

of the TG. XRPD examination of the DSC residues (see below) showed mainly copper metal present, with a small amount of copper(I) oxide present in some of the residues. Rapid mass gain was observed on exposure of these residues to air, and it is possible that part of this mass gain may be attributed to oxidation of the finely divided copper residue. As with the residues of **xut-cu-b4c-acet-xtals** (see section 4.1.2, p. 79), no X-ray diffraction peaks for the various anhydrous and hydrated forms of sodium carbonate, or for sodium hydroxide, could be distinguished from noise in the experimental patterns.

Assuming that one unit of $\text{Cu}_4\text{Na}_4\text{L}_3 \cdot 13\text{H}_2\text{O}$ decomposes to some combination of $\text{Cu}(s)$, $\text{C}(s)$, $\text{NaOH}(s)$, $\text{Na}_2\text{CO}_3(s)$, $\text{CO}(g)$, $\text{CO}_2(g)$ and $\text{H}_2\text{O}(g)$, and assuming also that the 13 H_2O molecules leave as such, there are 27 possible reactions, all of which involve the loss of carbon monoxide. For two formula units, there are 90 possible reactions, five of which do not involve the loss of CO . Of these, the reaction with the highest mass-proportion of solid residue is





although, owing to the sloping plateau at the end of the decomposition, agreement of this proposed reaction with the mass data is difficult to judge.

If a stoichiometric amount of $\text{Cu}_2\text{O}(s)$ is allowed as well, then the possible reactions number in the hundreds, so this type of reaction was not considered further.

The DSC and derivative DSC curves show only two major peaks, the first beginning at approximately 100 °C. These correspond to steps ii. and iii. of the TG curve. The absence of a visible endotherm for step i. suggests that the water lost in this step is very weakly bound⁴.

4.2.3 Crystal structures

Identical crystal structures were obtained for **xst-cu-b4c-no3-rhombi** and **xst-cu-b4c-cl-rhombi**, although — as previously mentioned — the atoms now known to be sodium atoms were initially thought to be chlorines. The structure discussed here is the corrected structure as obtained for **xst-cu-b4c-cl-rhombi**. The basic unit of the crystal structure is shown schematically in Figure 4.11 (p. 99), and more fully in Figure 4.12 (p. 100).

This material is a covalent three-dimensional metal organic framework with two crystallographically distinct copper(II) ions and two sodium cations. It also has two fully-deprotonated 1,2,4,5-benzenetetracarboxylate units, namely a μ_{11} -type (designated A) and a μ_{10} -type, designated B.

Cu1 and Cu2 — both in a distorted octahedral (or possibly square-based pyramidal) configuration — are bound to one carboxyl group on each of ligand A and B, forming a puckered octagon with copper(II) ions at opposite vertices ($d(\text{Cu1}-\text{Cu2}) = 4.505 \text{ \AA}$). The carboxyl groups, with carbons at opposite vertices of the octagon, are approximately in the same plane.

⁴The standard practice for all the DSC runs reported here was to purge the instrument for a brief period between loading the sample and beginning the temperature programme, to aid the removal of residual air. To maintain uniform conditions, this was done prior to all runs, except where noted. When this pre-purging was omitted for this sample, a very small endotherm was noted between 50 °C and 100 °C, corresponding to this first mass loss.

Cu1 is bound to the carboxyl oxygen O11B on ligand B (eight-membered ring formation) and to carboxyl oxygens O11A on ligand A, forming part of the eight-membered ring. It is bound also to carboxyl oxygens O51A(f) and O22B(g) from neighbouring units, and to water (O7W). In addition, there is a long-range distorted interaction between Cu1 and carboxyl oxygen O52A(f) from a neighbouring unit. The interatomic distance is 2.805 Å, and O52A(f) is elevated considerably from the plane defined by O11A, O7W and O11B. An equivalent interaction exists between O52A and Cu1(f), and the distortion of the oxygen from the sp^3 geometry can be seen clearly in Figure 4.12 (p. 100).

Likewise, Cu2 is bound to O12A and O12B forming part of the eight-membered ring. It is also bound to carboxyl oxygens O42A(b) and O21A(e) from neighbouring units, and to water (O6W). In addition, a long-range interaction exists between Cu2 and O41A(b) (inter-atomic distance, 2.674 Å), with considerable downward displacement of O41A(b) from the plane defined by O6W, O12B and O12A. As before, O41A, being equivalently bound to Cu2(a), shows considerable distortion from the tetrahedral orbital geometry.

Like the copper atoms, the sodium atoms Na1 and Na2 are both in a distorted octahedral arrangement. Na1 is bound to four carboxyl oxygens from four different ligands — O52A plus O11A(f) (longest bond, 2.449 Å), O21B(d) and O41A(e) from neighbouring units — and to two water molecules, O4W and O5W. Note that O52A links Na1, Na2(e) and Cu1(f), with the bond to Cu1(f) being unusually long. Likewise, Na2 is also bound to four ligand oxygens from four different ligands — O41A, O52A(g), O12B(a) (longest bond, 2.538 Å) and O22A(i) — and to two water molecules (O3W and O1W). Carboxyl oxygen O41A also links together two sodium atoms (Na1(g) and Na2) and Cu2(a), with the bond to Cu2(a) being unusually long, as before.

Several ring formations can be distinguished besides the eight-membered ring mentioned above. There are four-membered rings consisting of bridging carboxyl oxygens and Na, i.e., Na1–O52A–Na2(e)–O41A(e). There are also puckered five-membered bimetallic rings Na1–O52A–Cu1A–O51A–Cu1(f)–O11A.

The carboxyl groups centred on carbon atoms C21A and C21B are similar, with one oxygen in each group binding to a copper atom and the other binding to a sodium atom. These two carboxyl groups are orientated approximately in the

same plane, but pointing in opposite directions.

Face A of the crystal structure is shown in Figures 4.13–4.14 (pp. 101–102), and although there appear to be channels through the structure, these are smaller than those of **xut-cu-b4c-acet-xtals**. A non-coordinated guest water molecule, O2W, is located in a pore within the structure.

Given this crystal structure information, the TG curve and DSC curves for this material (see Section 4.2.2, p. 95 *et seq.*) can be interpreted more closely. This is most conveniently done while considering the formula unit $\text{Cu}_2 \text{Na}_2 \text{L}_{1\frac{1}{2}} \cdot 6.5 \text{H}_2\text{O}$. If the guest water site O2W is considered to be half-occupied, then the loss of $\frac{1}{2}\text{O2W}$ and O3W (longest Na–OH₂ bond) would account for the step i. (not visible on the DSC curve). The order in which water molecules are lost in steps ii. and iii. cannot be assigned unambiguously because of the likelihood of internal rearrangements in the crystal structure during dehydration, but it is clear that all the coordinated water molecules are lost during these dehydration steps. It is likely, however, that step iii. corresponds to the loss of a water molecule coordinated to copper(II).

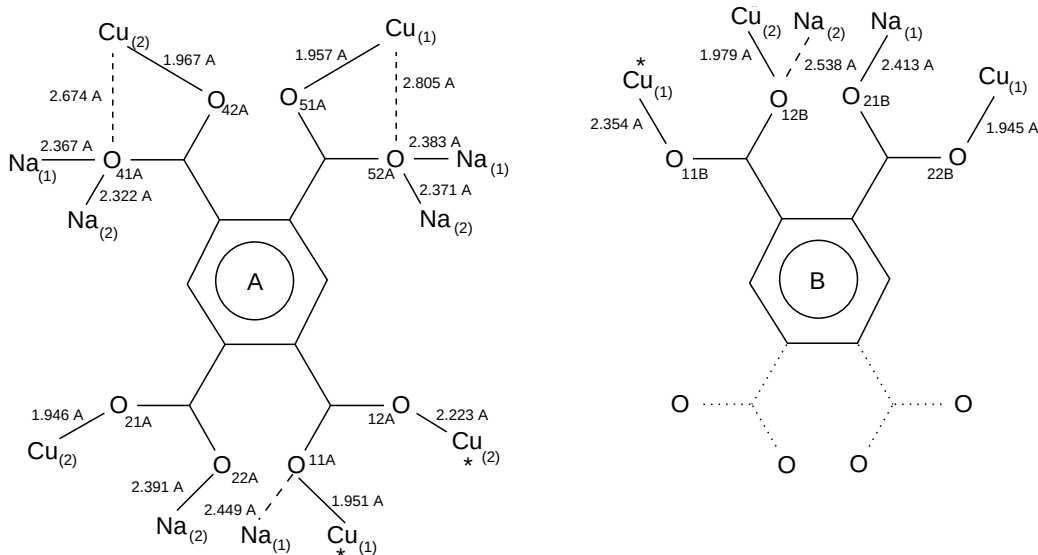


Figure 4.11: Schematic diagram of the binding in **xst-cu-b4c-cl-rhombi**. Asterisks indicate the same atom shown twice, bound to different parts of the structure. Dashed lines show long-range interactions discussed in text. The lower half of ligand B — drawn with dotted lines — is symmetrical with the upper half shown.

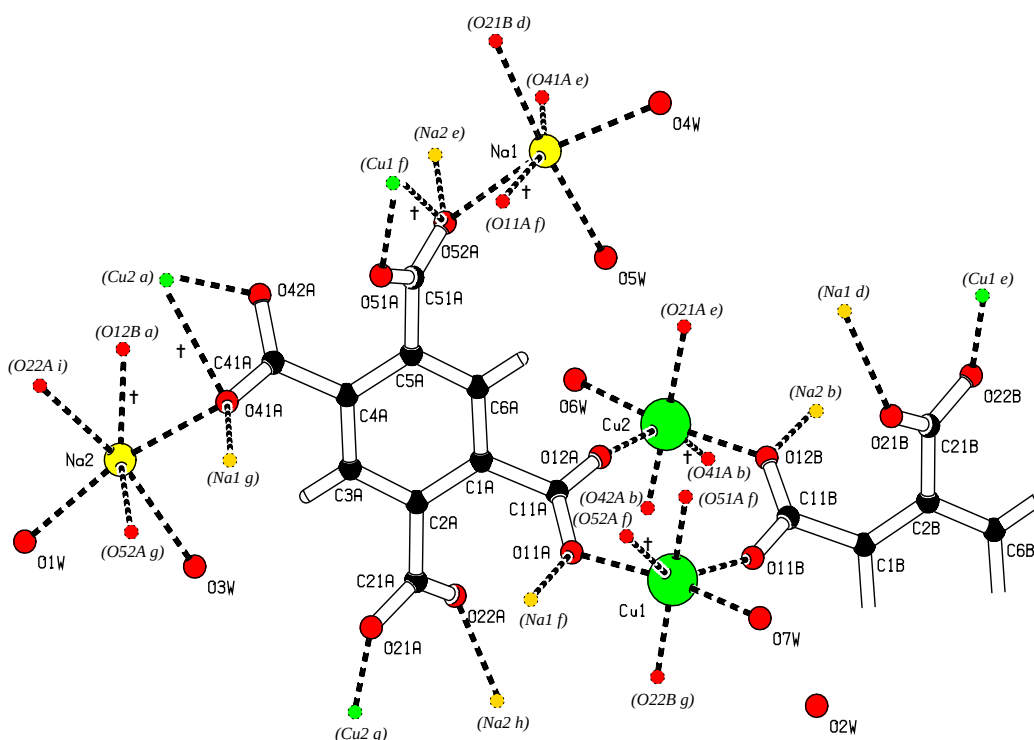


Figure 4.12: Basic unit of **xst-cu-b4c-cl-rhombi**. Oxygen atoms labelled ‘A’ and ‘B’ are on different ligands, and those labelled ‘W’ are water molecules. Atoms drawn with dotted outlines and italic labels are part of neighbouring units. Bent, elongated bonds are labelled with the symbol ‘†’.

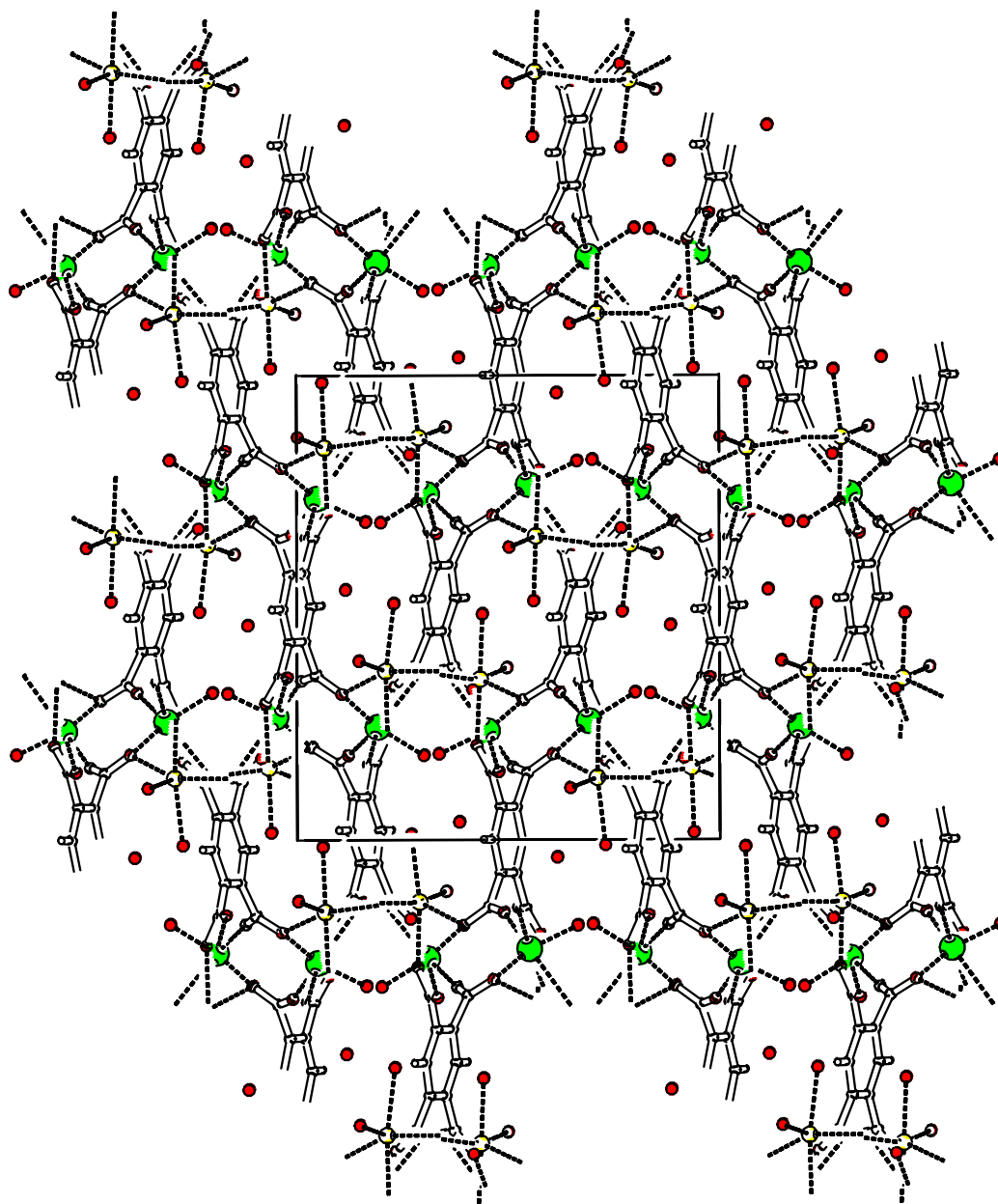


Figure 4.13: Face A of the crystal structure of **xst-cu-b4c-cl-rhombi**, showing cavities containing guest water molecules.

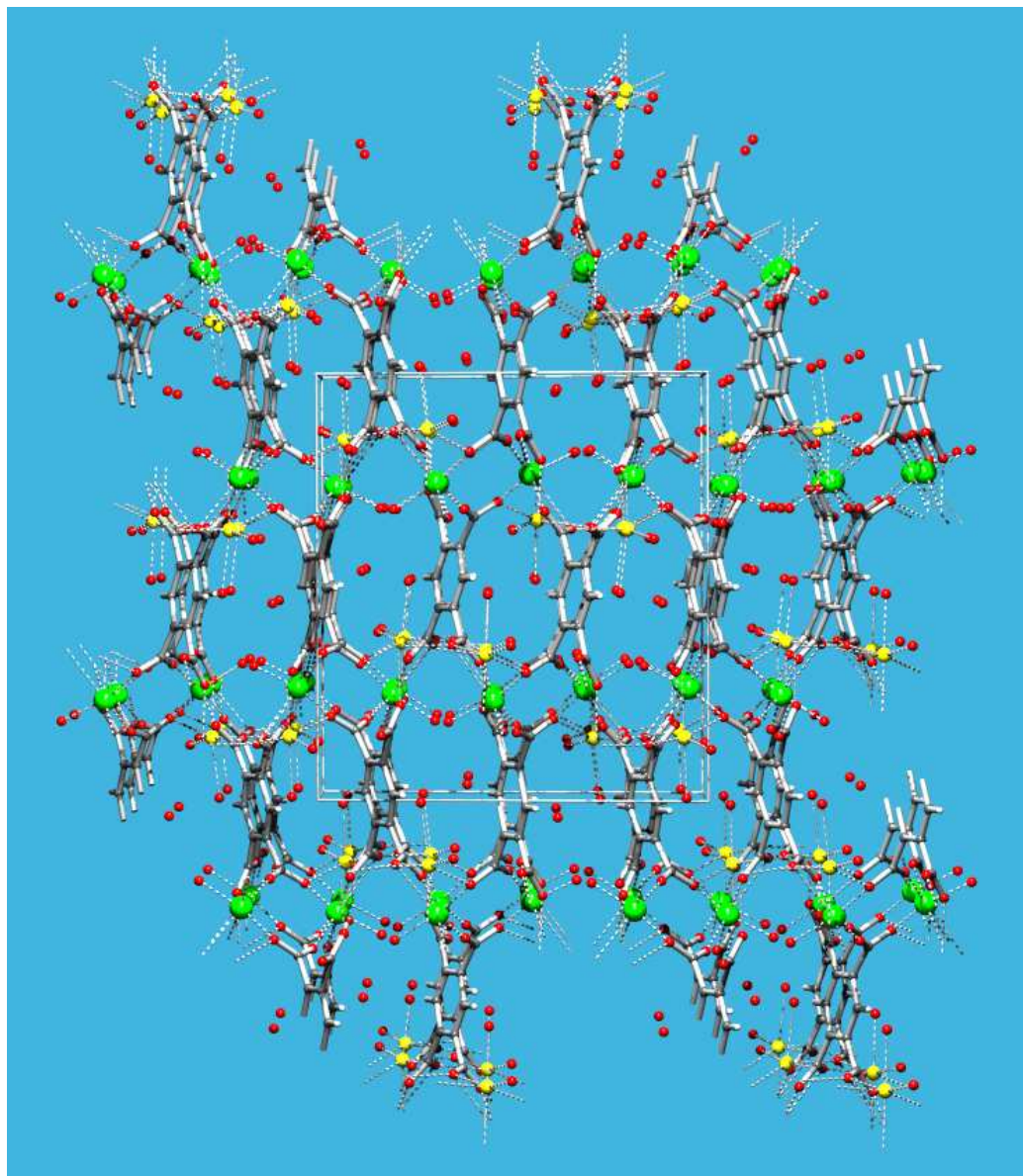


Figure 4.14: Ray-traced diagram of face A of the crystal structure of **xst-cu-b4c-cl-rhombi**, showing large cavities containing guest water molecules.

4.3 GROUP 3 PRODUCTS

This group consists of the products **xst-cu-b4c-no3-topxtals**, **xst-cu-b4c-so4-topxtals** and **xst-cu-b4c-no3-lumps**. The first two were shown to be identical by X-ray powder diffraction, mid-IR spectroscopy and thermal analysis (including metal content from combustion analysis). Owing to the paucity of this material, **xst-cu-b4c-so4-topxtals** was not sent for carbon and hydrogen analysis. The third product is a 2:1 metal-to-ligand complex which is distinct from the first two in structure (see discussion on p. 115), extent of hydration and thermal properties.

4.3.1 Elemental analysis

The results of elemental analyses for these compounds are summarized in Table 4.4 (p. 104). The experimental data agree well with the calculated data for the formulas suggested by the corresponding crystal structures (see discussions on pp. 110 & 115).

Table 4.4: Experimental and calculated elemental analyses for Group 3 products. (Metal determinations by combustion analysis.)

Product	Formula	Form. mass	Calculated			Experimental			SSR
		/g mol ⁻¹	%C	%H	%Cu	%C	%H	%Cu	
xst-cu-b4c-no3-topxtals	Cu ₂ L·6H ₂ O ·4H ₂ O	557.38	21.55	3.98	22.80	22.15	3.40	22.30	0.96
xst-cu-b4c-no3-lumps	Cu ₂ L·4H ₂ O ·2H ₂ O	485.31	24.75	2.91	26.19	25.10	2.57	26.00	0.27

4.3.2 Thermogravimetry and Differential scanning calorimetry

xst-cu-b4c-so4-topxtals

The TG curve for **xst-cu-b4c-so4-topxtals** shows a complex dehydration, involving the loss of water in at least five overlapping steps, followed by a complex decomposition to a fairly flat plateau. The dehydration steps are marked on the TG curve (Figure 4.15, p. 106) as follows:

- i. the loss of 5 water molecules per formula unit (16.16 %), between 25 °C and 91 °C, overlapping with the next step
- ii. the loss of a further 2.5 water molecules (total loss, 24.24 %), between 91 °C and 122 °C in an indistinct step
- iii. the loss of a further 1 water molecule (total loss, 27.47 %), between 122 °C and 154 °C in another indistinct step
- iv. the loss of a further 1 water molecule (total loss, 30.71 %), between 154 °C and 265 °C in a very broad, indistinct step, and
- v. the loss of a further 0.5 water molecule (total loss, 32.32 %), between 265 °C and 292 °C, overlapping with the complex decomposition which follows.

The DSC curves (Figure 4.16, p. 106) show two clear transitions, corresponding to steps i. and ii. above. Step iii. may be represented by small shoulder at around 150 °C. This shoulder is not always well-resolved. The DSC response for the final decomposition, starting at about 320 °C, does not show the complexity revealed by the TG curves, although the small preliminary endothermic response may correspond to the water-loss in step iv. The DSC residues were identified as copper metal with no trace of oxidation.

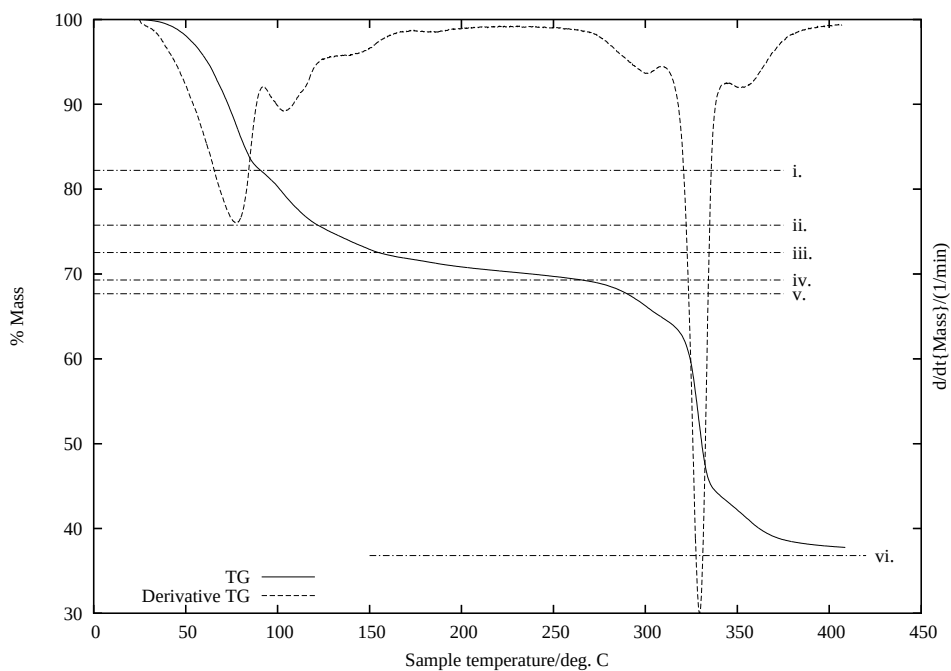


Figure 4.15: TG curve for **xst-cu-b4c-so4-topxtals** ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen.

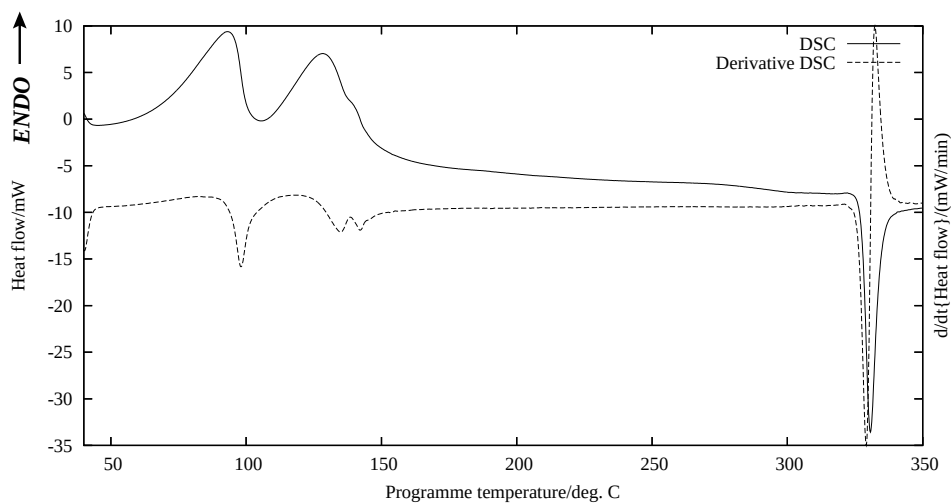
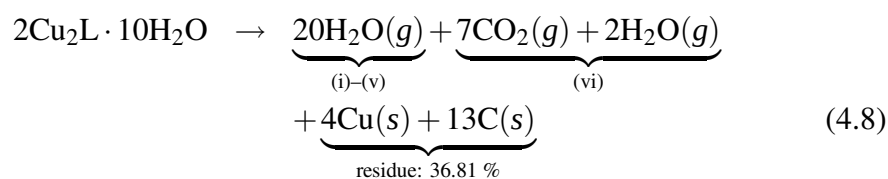


Figure 4.16: DSC and derivative DSC curves for **xst-cu-b4c-so4-topxtals**, heated in a crimped (not sealed) aluminium pan at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen (26 ml min^{-1}). The corresponding curves for **xst-cu-b4c-no3-topxtals** are very similar.

No clear signs of carbon monoxide evolution were observed by FTIR in the TG exhaust stream, and examination of the DSC residues (see below) by XRPD showed diffraction peaks for copper metal only. If it is assumed that the ten water molecules per formula unit depart as such, and further that the decomposition products are $\text{CO}_2(g)$, $\text{H}_2\text{O}(g)$, $\text{Cu}(s)$ and $\text{C}(s)$, then two formula units of **xst-cu-b4c-so4-topxtals** decompose stoichiometrically in eight different ways. Only one of these reactions does not involve the loss of carbon monoxide:



This reaction agrees well with the reported mass data.

xst-cu-b4c-no3-lumps

The TG curve for **xst-cu-b4c-no3-lumps** shows dehydration in two steps, followed by a complex decomposition at relatively high temperature to a fairly flat plateau. The dehydration steps are marked on the TG curve (Figure 4.17, p. 109) as follows:

- i. the loss of 5.5 water molecules per formula unit (20.42 %) in one step between 25 °C and 155 °C overlapping with the next step, and
- ii. the loss of a further 0.5 water molecule (total loss, 22.27 %) in a very broad step between 155 °C and 313 °C, overlapping with the main decomposition.

The DSC curve shows a large endotherm at a relatively high temperature corresponding to dehydration. A small shoulder is visible against the falling edge, which corresponds to the early part of step ii above, perhaps accounting for the loss of about 0.25 water molecules per formula unit.

Although the exothermic DSC response returns to the baseline well before the final DSC temperature (360 °C), the residue mass — which, at 47 % of the sample mass, is somewhat higher than the relative final mass of corresponding TG residue — showed that the decomposition was not yet complete at this temperature. The DSC residue showed characteristic X-ray diffraction peaks for copper metal, but none for copper oxides.

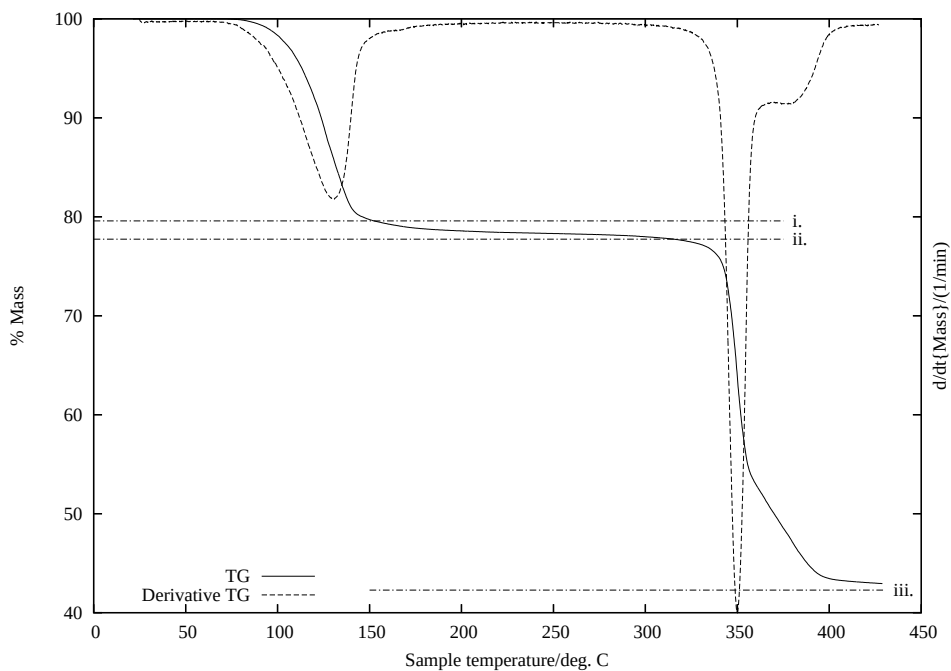


Figure 4.17: TG curve for **xst-cu-b4c-no3-lumps** ($10\text{ }^{\circ}\text{C min}^{-1}$) under nitrogen.

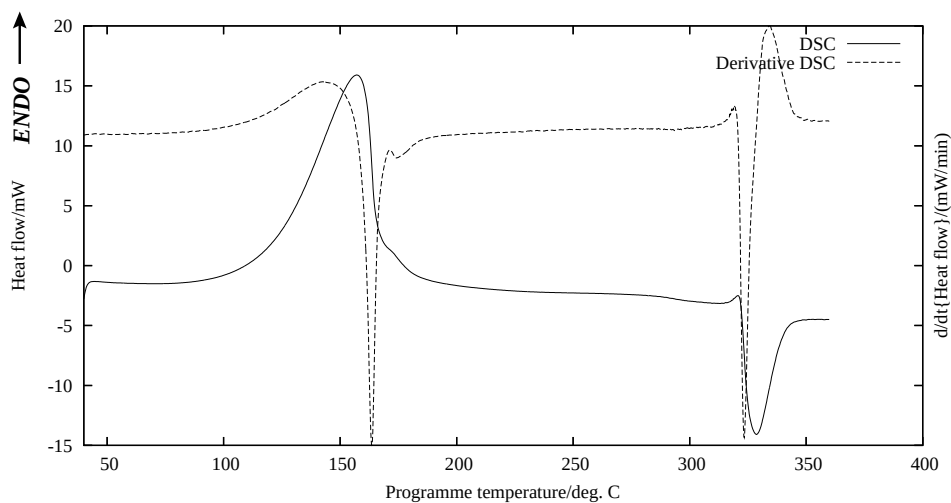
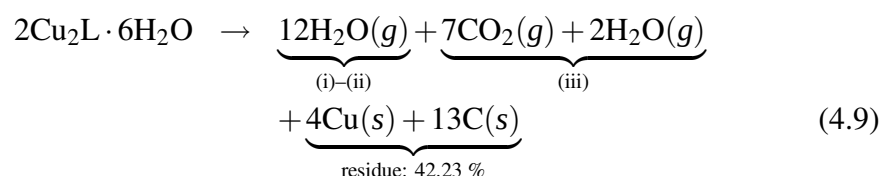


Figure 4.18: DSC and derivative DSC curves for **xst-cu-b4c-no3-lumps**, heated in a crimped (not sealed) aluminium pan at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen (26 ml min^{-1}).

As with **xst-cu-b4c-so4-topxtals**, no carbon monoxide evolution or copper oxide formation could be detected. The decomposition is therefore proposed to proceed as:



This reaction agrees well with the reported mass data.

4.3.3 Crystal structures

xst-cu-b4c-so4-topxtals

Using X-ray powder diffraction, this structure was matched to the known structure reported in [20]. The discussion which follows is based on the reported crystal structure.

A brief outline of this crystal structure has already been given on p. 29, and this discussion is quoted here.

In [this] 2:1 copper:1,2,4,5-benzenetetracarboxylate complex, square-based pyramidal copper(II) ions — each bound equatorially to *trans* pairs of water and carboxyl oxygens (monodentate) and also to water in the apical position — form neutral covalent two-dimensional layers with monodentate μ_4 -bridging 1,2,4,5-benzenetetracarboxylate. These layers are linked together by hydrogen bonding, the proton donors being mostly coordinated water molecules but also non-coordinated guest waters⁵, and the acceptors being mainly bound and unbound carboxyl oxygens, but also guest and coordinated water molecules.

Figure 4.19 (p. 112) shows the basic unit of **xst-cu-b4c-so4-topxtals** and an expanded view of the packing. The basic unit is highly symmetrical, and the three-dimensional structure arises from the orientation of the carboxyl groups, as shown

in the opposite directions of bonds C1—O4 and C5—O6. As with **xst-cu-b4c-cl-rhombi**, there is a long interaction between O7 and Cu1(b) from a neighbouring cell (2.70 Å). An equivalent bond exists between Cu1 and O7(c), and it is clear that this bond is significantly displaced downwards from the plane defined by O1W, O2W and O3W, showing that Cu1 would be significantly distorted from normal octahedral geometry if O7(c) were regarded as being bound to it. In this case, the carboxyl group centred on C5 may be regarded as chelating to Cu1(b), with equivalent chelation to Cu1 by a neighbouring 1,2,4,5-benzenetetracarboxylate unit (through carboxyl oxygens O6(c) and O7(c)). The shortest Cu—Cu distance, visible between copper(II) ions shown bound to the right-hand half of the 1,2,4,5-benzenetetracarboxylate units in Figure 4.19(III), is 4.958 Å.

This structure contains both coordinated and “free” guest water molecules. Figures 4.20–4.21 (p. 113–114) show face C of the crystal structure and the guest water molecules in channels.

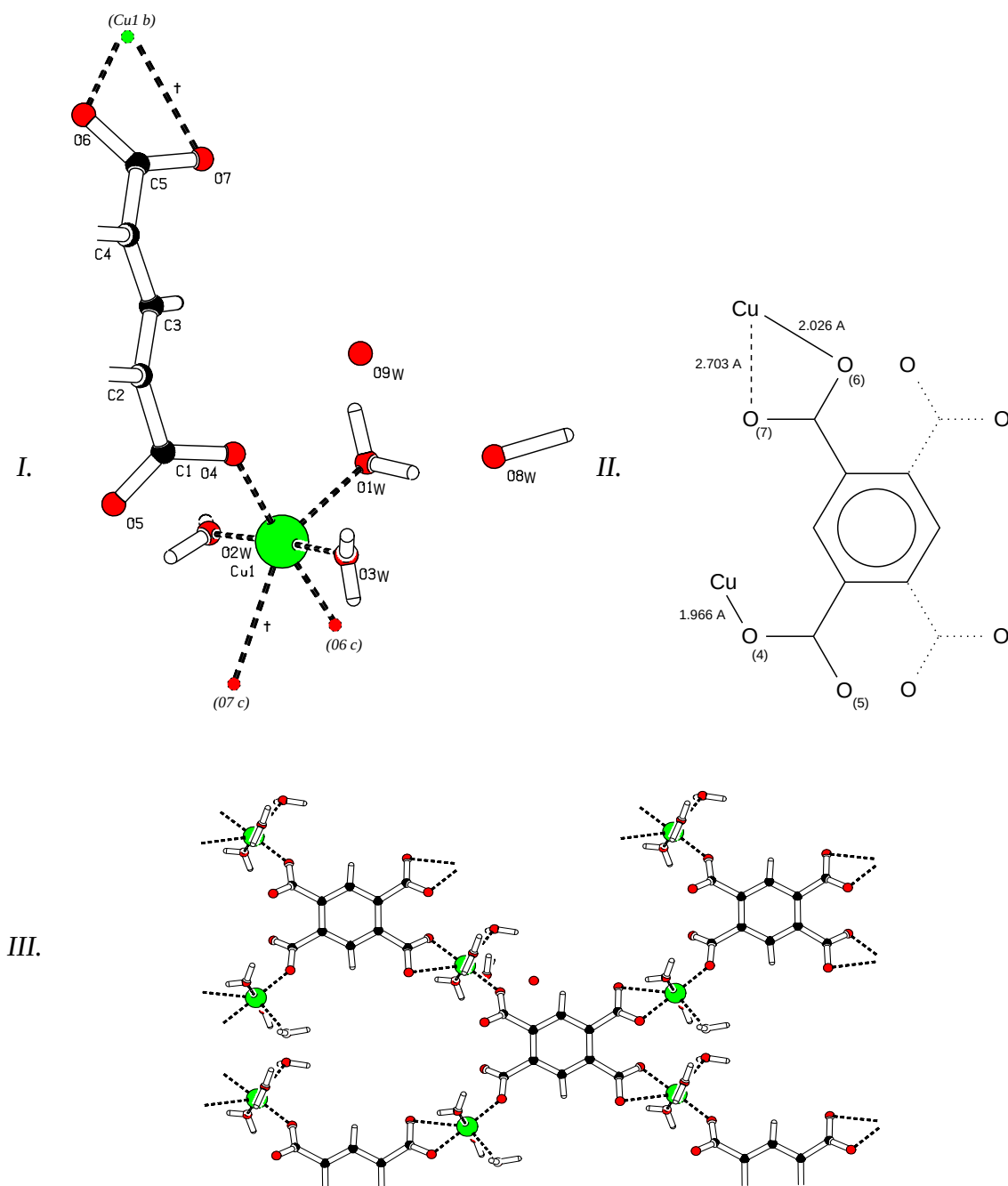


Figure 4.19: (I.) Basic unit, (II.) binding diagram and (III.) expanded diagram of **xst-cu-b4c-so4-topxtals**. In I, the long bent bonds discussed in text are marked with the symbol †. In II, the right-hand part of the ligand, drawn in dotted lines, is symmetrical with the left-hand part, and the dashed line represents an unusually long bent bond.

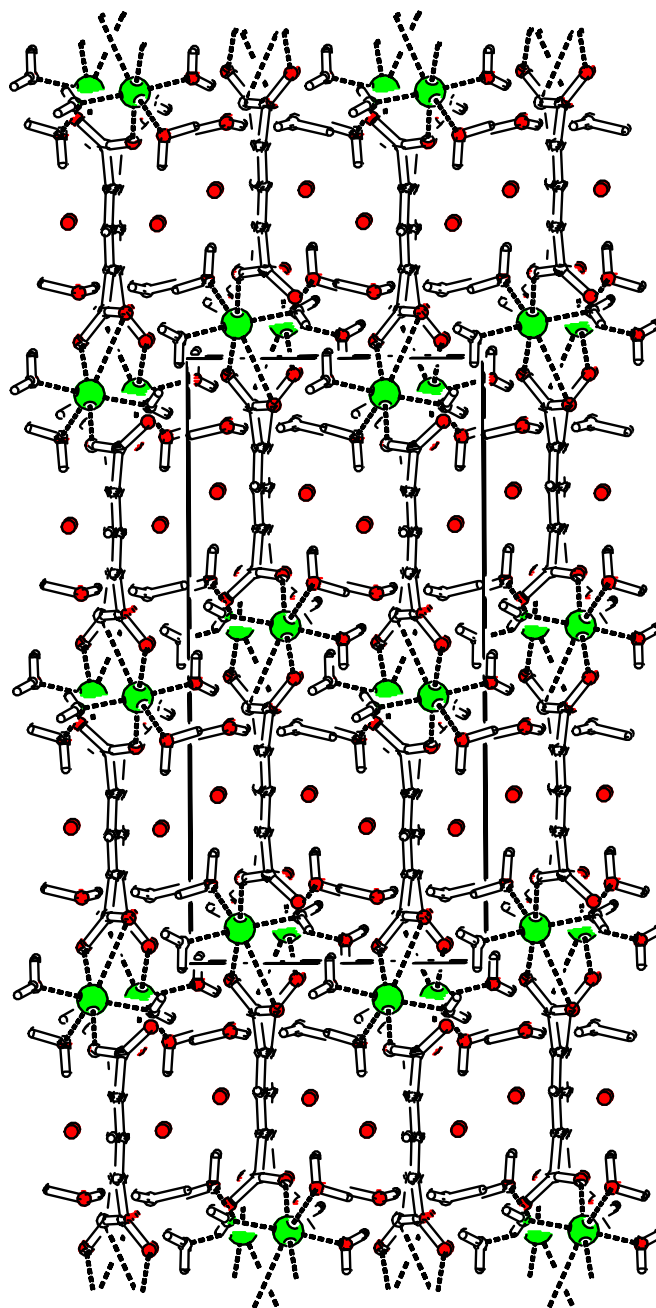


Figure 4.20: Face C of the crystal structure of **xst-cu-b4c-so4-topxtals**, showing channels containing guest water molecules.

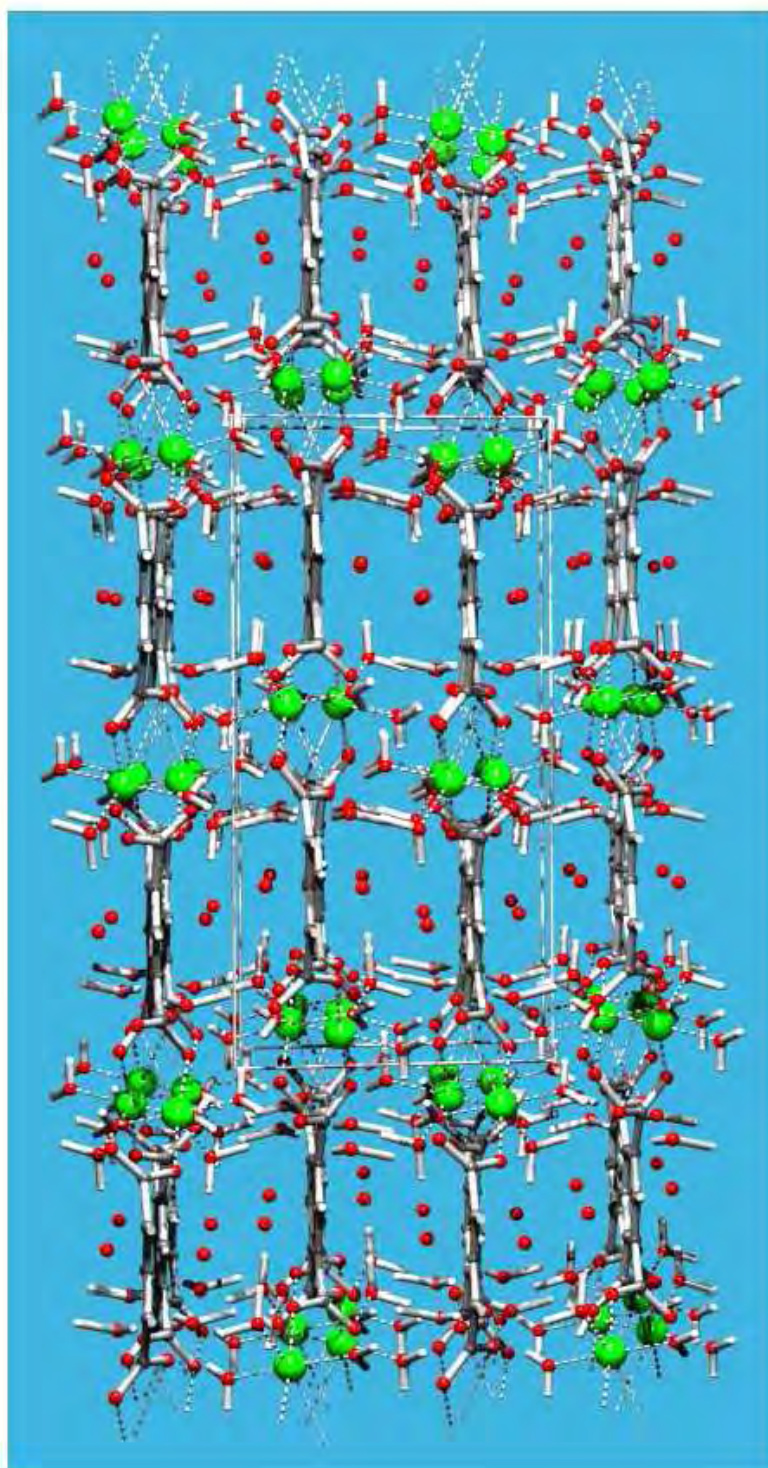


Figure 4.21: Ray-traced diagram of face C of the crystal structure of **xst-cu-b4c-so4-topxtals**, showing channels containing guest water molecules.

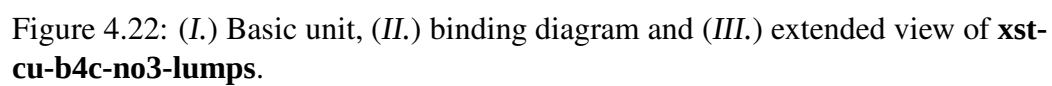
xst-cu-b4c-no3-lumps

Using X-ray powder diffraction, this structure was matched to a known structure reported in [21]. The discussion which follows is based on the reported crystal structure.

A basic outline of this structure has already been given earlier on p. 29, and this discussion is quoted here.

In this [two-dimensional layered polymeric] structure, square-based pyramidal copper(II) centres are linked to form uncharged layers by μ_6 -bridging 1,2,4,5-benzenetetracarboxylate anions (deprotonated). The substituents are distributed on the ring in *para* pairs of singly bound and bridging carboxyl groups. Each square-based pyramidal copper(II) ion is bound equatorially a *cis* pair of water, to one oxygen from a bridging carboxyl group, and to one oxygen from a monodentate carboxyl group on a different 1,2,4,5-benzenetetracarboxylate ligand; it is also bound in the axial position to an oxygen from a bridging carboxyl group on a third 1,2,4,5-benzenetetracarboxylate ion. The copper(II)-1,2,4,5-benzenetetracarboxylate layers thus formed are linked by hydrogen bonding. There are a large number of potential hydrogen bonding contacts between carboxyl oxygens and water molecules (coordinated and non-coordinated), and between water molecules and each other.

Figure 4.22 (p. 116) shows the basic unit, binding diagram and an expanded view of the crystal structure of **xst-cu-b4c-no3-lumps**. This is another highly symmetrical structure, with each half-ligand unit bound to three copper atoms as shown. The copper atom is in a slightly distorted square-based pyramidal configuration, with water molecules coordinated equatorially at right angles as shown. In addition to the coordinated water molecules, this structure contains guest waters in channels, as shown in Figures 4.23–4.24 (pp. 117–118). As shown in Figure 4.22(III), copper(II) ions are bridged by carboxyl groups (via carboxyl oxygens O3 and O4) ($d(\text{Cu}-\text{Cu}) = 4.281 \text{ \AA}$).



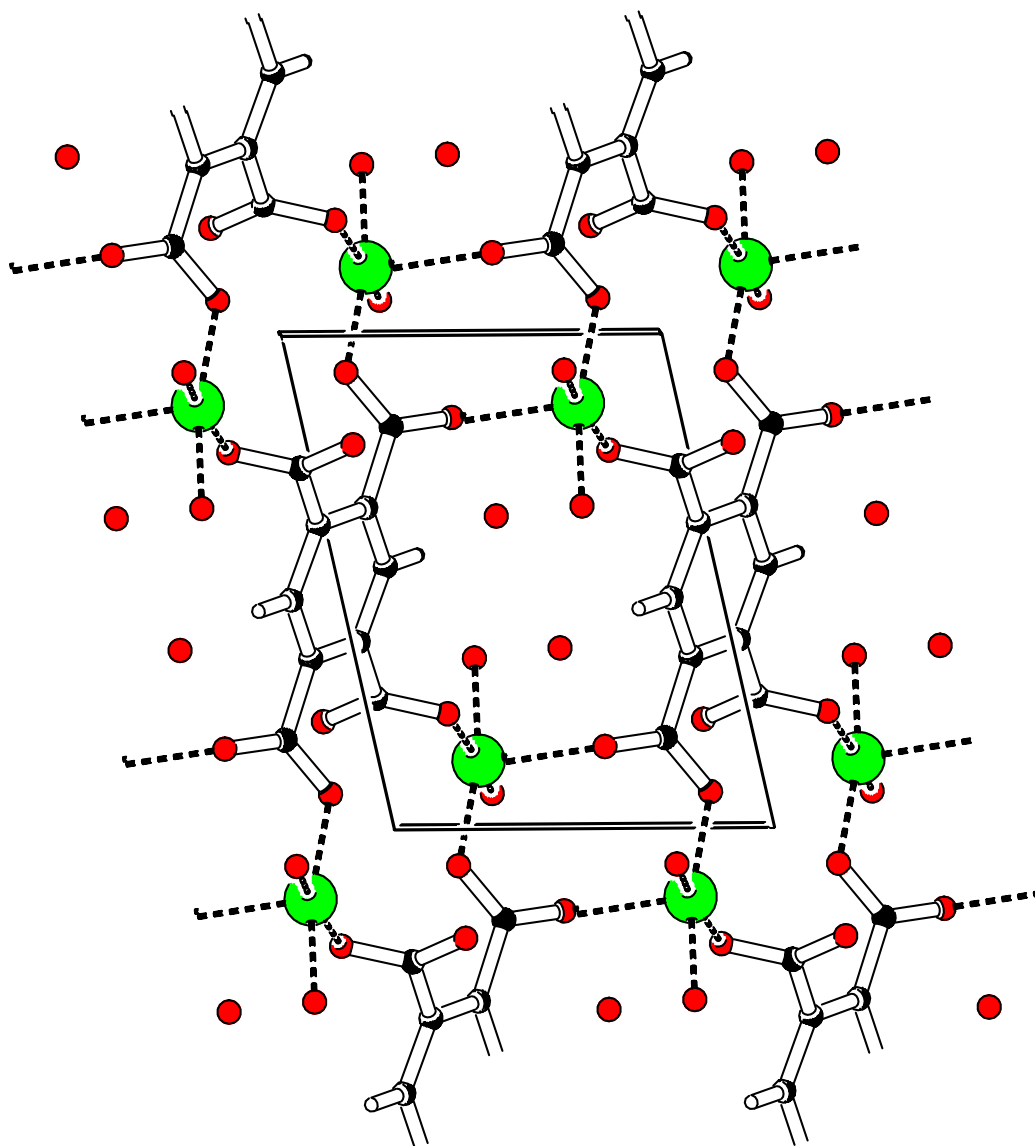


Figure 4.23: Face A of the crystal structure of **xst-cu-b4c-no3-lumps**, showing channels containing guest water molecules.

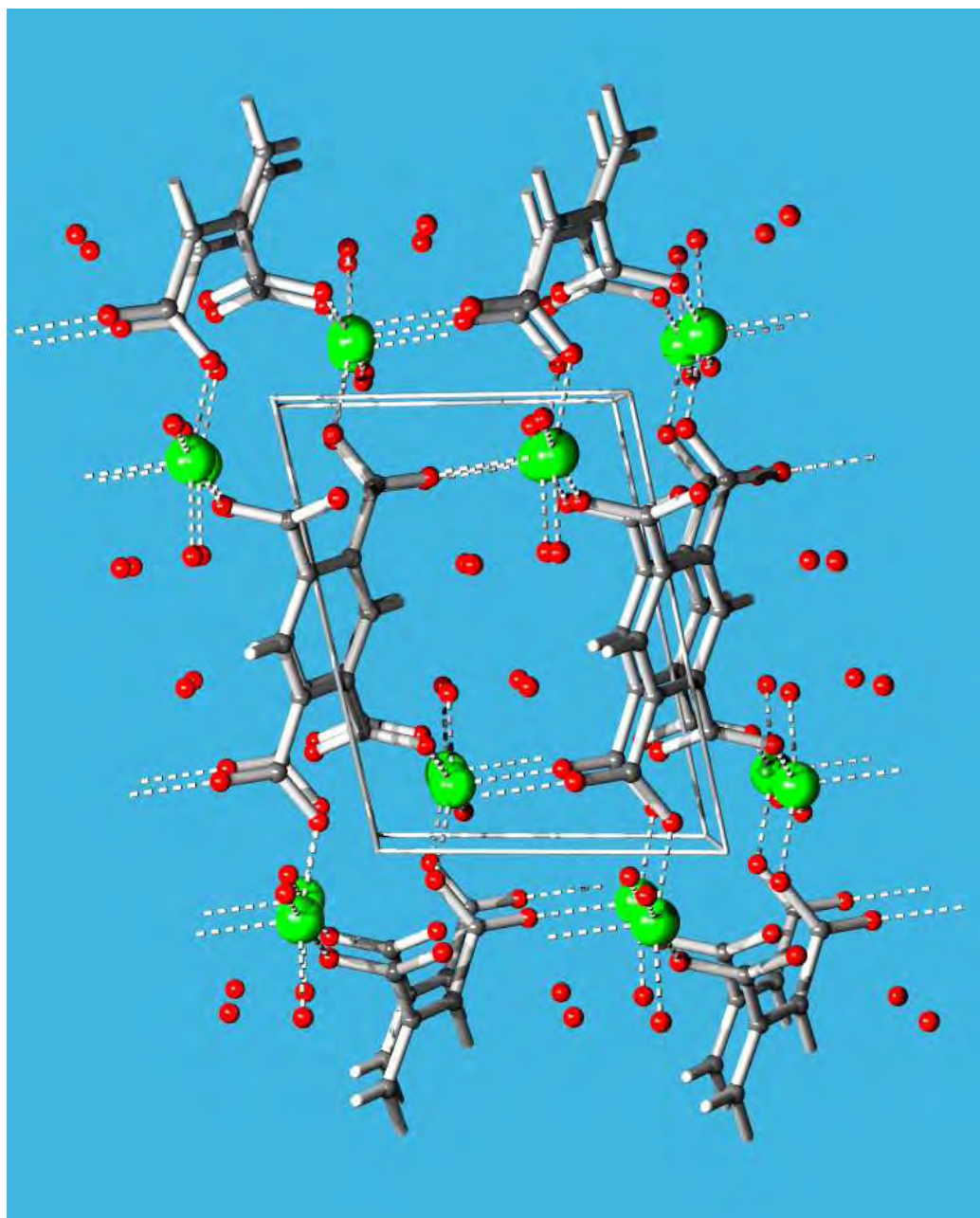


Figure 4.24: Ray-traced diagram of face A of the crystal structure of **xst-cu-b4c-no3-lumps**, showing channels containing guest water molecules.

4.4 GROUP 4 PRODUCTS

This group consists of **xut-cu-pyrX-b4c-no3-xtals** and **xut-cu-pyr2-b4c-no3-xtals**, which were visually identical. See Section 3.2.3 (p. 71) for synthesis details.

4.4.1 XRPD and Mid-IR spectroscopy

Figure 4.25 (p. 120) shows the X-ray powder diffraction patterns of **xut-cu-pyrX-b4c-no3-xtals** and **xut-cu-pyr2-b4c-no3-xtals**, together with the the simulated diffraction pattern obtained from the crystal structure of **xut-cu-pyr2-b4c-no3-xtals** using PLATON [22]. The experimental patterns are very poor, and cannot be matched beyond doubt to the simulated pattern. This may suggest that the samples decomposed partly during preparation or during exposure to air in the diffractometer, perhaps by loss of water and/or pyridine. The experimental diffraction patterns do, however, suggest that **xut-cu-pyrX-b4c-no3-xtals** and **xut-cu-pyr2-b4c-no3-xtals** are very similar. The infrared spectra of **xut-cu-pyrX-b4c-no3-xtals** and **xut-cu-pyr2-b4c-no3-xtals** — shown in Figure 4.26 (p. 121) — are identical.

It was therefore concluded that these two compounds are identical. All further characterization was performed on **xut-cu-pyr2-b4c-no3-xtals** only.

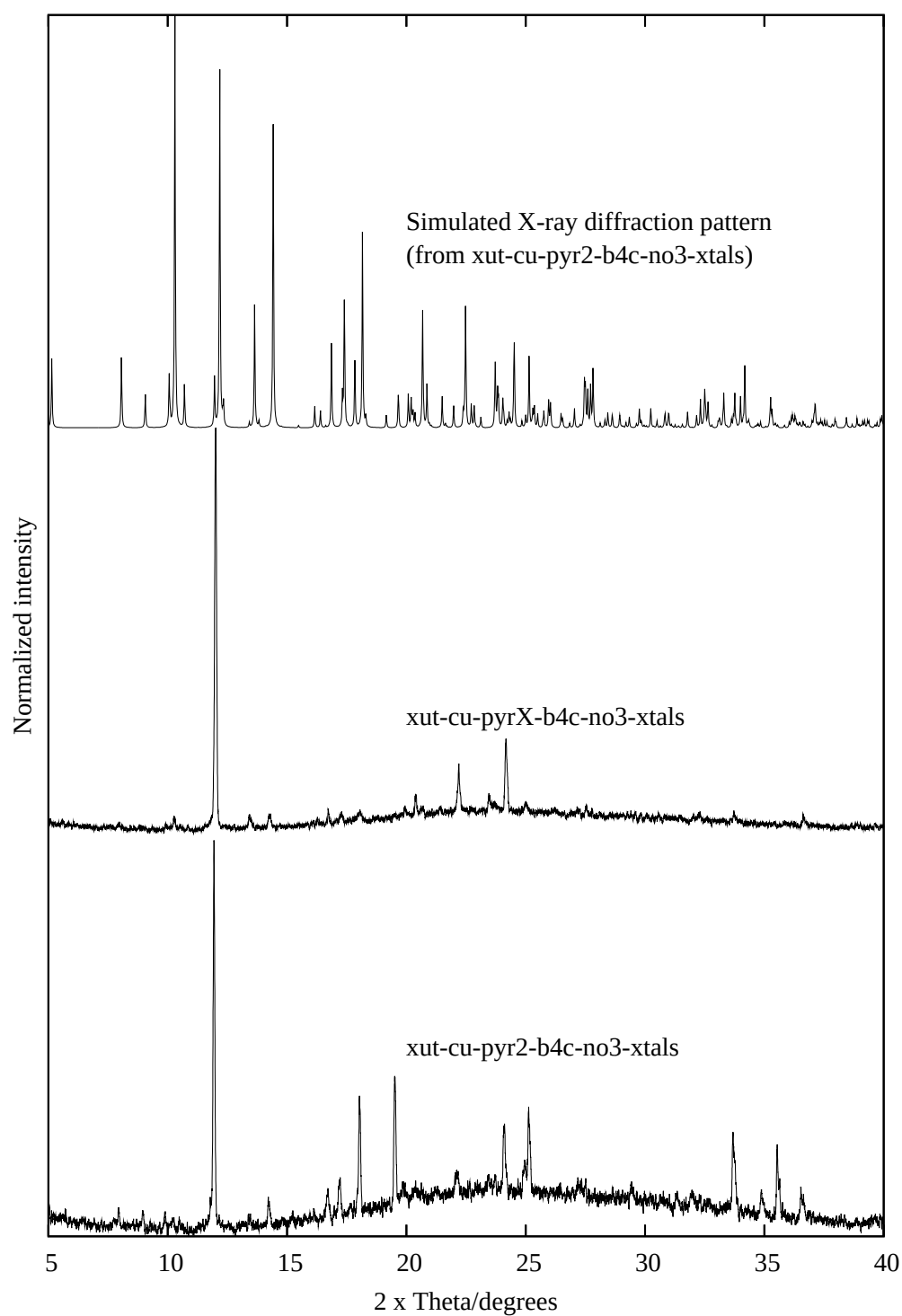


Figure 4.25: Experimental X-ray powder diffraction patterns of **xut-cu-pyrX-b4c-no3-xtals** and **xut-cu-pyr2-b4c-no3-xtals**, shown with the simulated pattern obtained from the crystal structure of **xut-cu-pyr2-b4c-no3-xtals**.

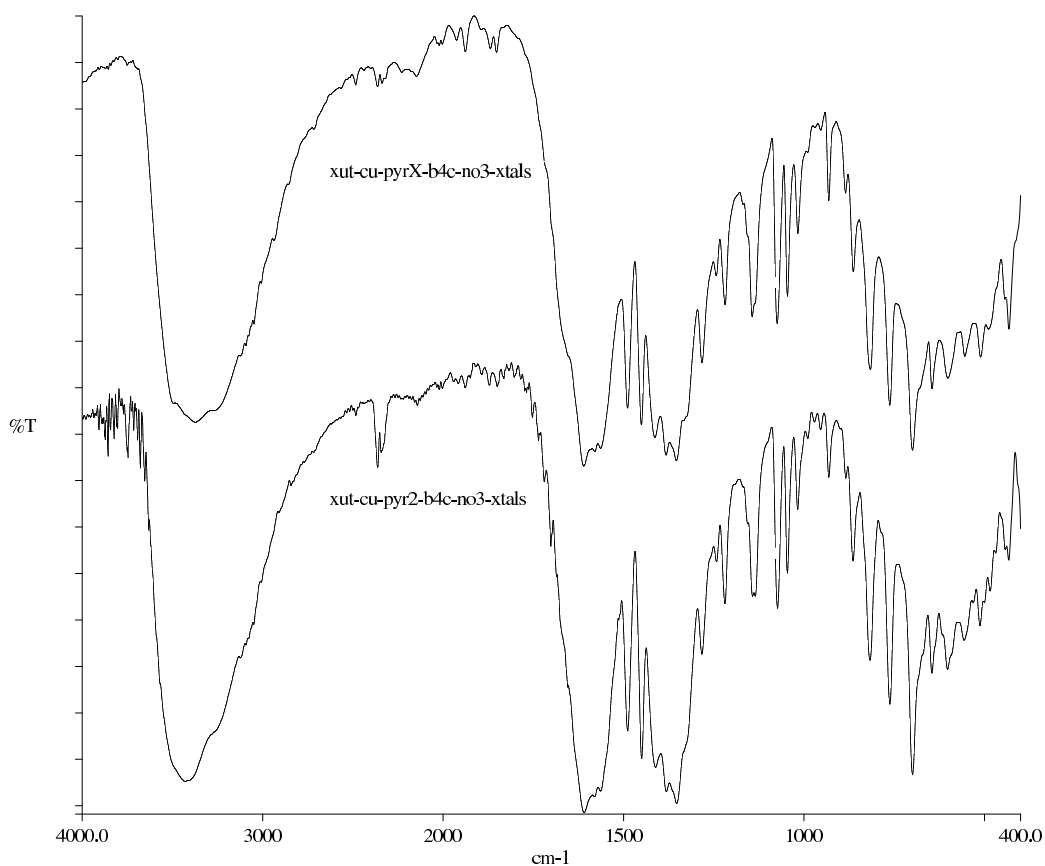


Figure 4.26: Mid-infrared spectra of **xut-cu-pyrX-b4c-no3-xtals** and **xut-cu-pyr2-b4c-no3-xtals**, obtained in KBr.

4.4.2 Elemental analysis

The results of the carbon, hydrogen and nitrogen analysis for this compound are shown in Table 4.5 (p. 122). The experimental results are a good match for the calculated formula based on the proposed crystal structure (see Section 4.4.4, p. 127).

Table 4.5: Experimental and calculated elemental analyses for Group 4 products.

Product	Formula	Form. mass	Calculated			Experimental			SSR
		/g mol ⁻¹	%C	%H	%N	%C	%H	%N	
xut-cu-pyr2-b4c-no3-xtals	Cu ₂ (C ₅ H ₅ N) ₄ L·6H ₂ O	801.71	44.94	4.27	6.99	45.07	3.99	6.86	0.12

4.4.3 Thermogravimetry and Differential scanning calorimetry

The TG curve for **xut-cu-pyr2-b4c-no3-xtals** and EGA profiles for pyridine and carbon dioxide are shown in Figure 4.27 (p. 125). A time-resolved stack-plot of the EGA data is shown in Figure 4.28 (p. 126). The TG curve shows at least five partly-overlapping steps, which are marked on the TG curve (Figure 4.27 (I), p. 125) as follows:

- i. the loss of 6 water molecules (13.48 %) per formula unit in one step between 25 °C and 85 °C (TG temperatures)
- ii. the loss of 0.5 pyridine molecules (total loss, 18.42 %) in one broad step from 85 °C to 150 °C
- iii. the loss of a further 1.5 pyridine molecules (total loss, 33.22 %) in one step between 150 °C to 197 °C
- iv. the loss of 2 pyridine molecules, 1.5 carbon dioxide molecules and 1 water molecule (total loss, 63.43 %) in a broad step from 197 °C to 303 °C, overlapping somewhat with the previous one, and
- v. the loss of a further 0.5 carbon dioxide molecules and 3 carbon monoxide molecules (total loss, 76.66 %) in a broad step from 303 °C to 400 °C, overlapping somewhat with the previous one. Mass loss continues beyond this point, and this is thought to be due to loss of carbon through slow oxidation with residual air.

This interpretation agrees quite well with the EGA results, if a delay of about 2 minutes between a TG mass loss and the corresponding EGA signal is allowed for. Curves b and c in the EGA graphs show a noisy upward peak between about 70 °C and 120 °C (corresponding to the range 50 °C and 100 °C) which may signal earlier loss of pyridine, but because they are absent from the other pyridine traces (curves a and d), they are most likely background noise due to water.

Although a satisfactory EGA profile could not be obtained owing to the weakness of the signals, carbon monoxide was seen to be present in the exhaust stream

from about 300 °C (corrected) onwards by the observation of its characteristic doublet-envelope, centred at 2143 cm^{-1} [23, pp. 80 & 82], in the individual time-resolved spectra.

The TG residues were examined by XRPD and were found, reproducibly, to contain copper metal with a significant amount of copper(I) oxide. This is believed to be due to oxidation by residual air, because the DSC residues (heated in nitrogen to 500 °C) showed copper metal with no traces of oxidation. Some or all of the above-mentioned carbon monoxide in the TG exhaust stream may stem from slow oxidation of the carbonaceous residue by residual air, making it impossible to obtain a quantitative interpretation of the final stages of decomposition.

The DSC curve, although not amenable to close interpretation in the decomposition region owing to the complex baseline response at higher temperatures, nevertheless shed light on the desolvation processes. Steps i., ii. and iii. above all have corresponding DSC responses, and step iv. — at about 250 °C — is resolved into two, or possibly three, small peaks.

As noted below, a crystal structure identical to the one obtained for this material was reported independently [24] during the course of this study (see 28 and Section 4.4.4 on p. 127). This report stated that this material did not survive an attempted dehydration/rehydration cycle. Therefore, no guest inclusion studies were done on this material. However, in retrospect, it was noted that the desolvation method employed in [24] — that is, heating to 140 °C under vacuum — may have also driven off pyridine (see EGA profiles in Figure 4.27, p. 125). Further work is necessary to determine whether this substance can, indeed, be dehydrated without causing irreversible breakdown of the structure.

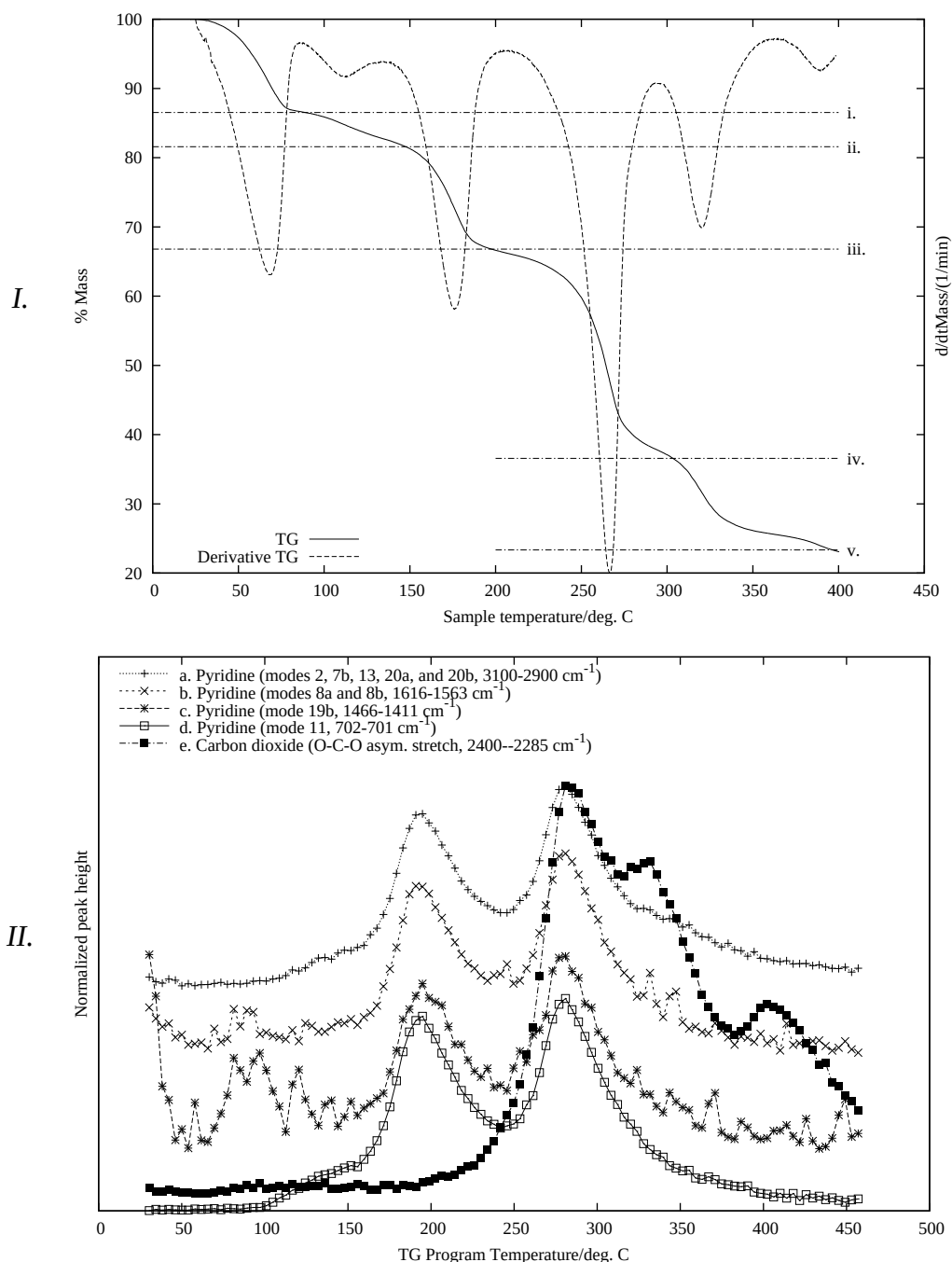


Figure 4.27: *I.* TG curve for **xut-cu-pyr2-b4c-no3-xtals**, heated from 25–400 °C at 10 °C min^{−1} under nitrogen (100 ml min^{−1}.) *II.* Corresponding FTIR EGA profiles for various absorptions characteristic of pyridine and carbon dioxide. The temperature range from 400 to 450 °C does not correspond to real heating, but encompasses the approximately 2-minute delay between the TG mass loss and the corresponding EGA signals. The modes labelled a.–d. refer to the well-known Wilson’s modes of vibration for pyridine, as assigned in [25].

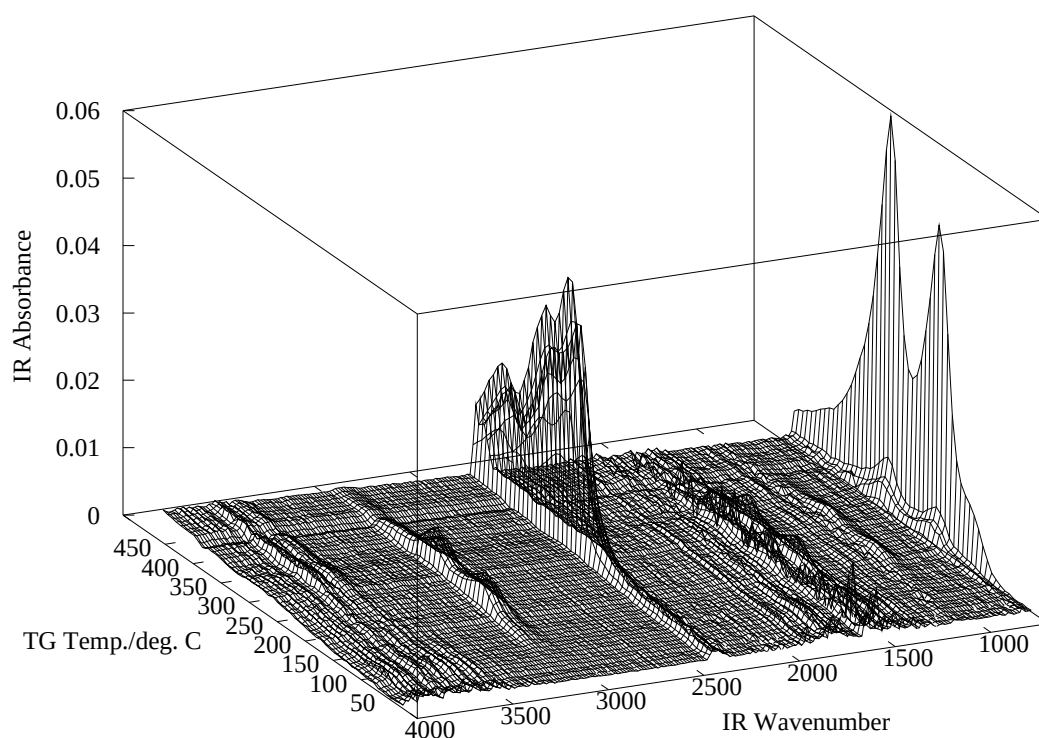


Figure 4.28: TG-FTIR EGA stack-plot for **xut-cu-pyr2-b4c-no3-xtals** heated in a TG from 25–400 °C at 10 °C min⁻¹ under nitrogen (100 ml min⁻¹). The interval from 400 °C to 450 °C is plotted only to overcome the lag between the TG and IR responses. **Linear IR wavenumber scale.**

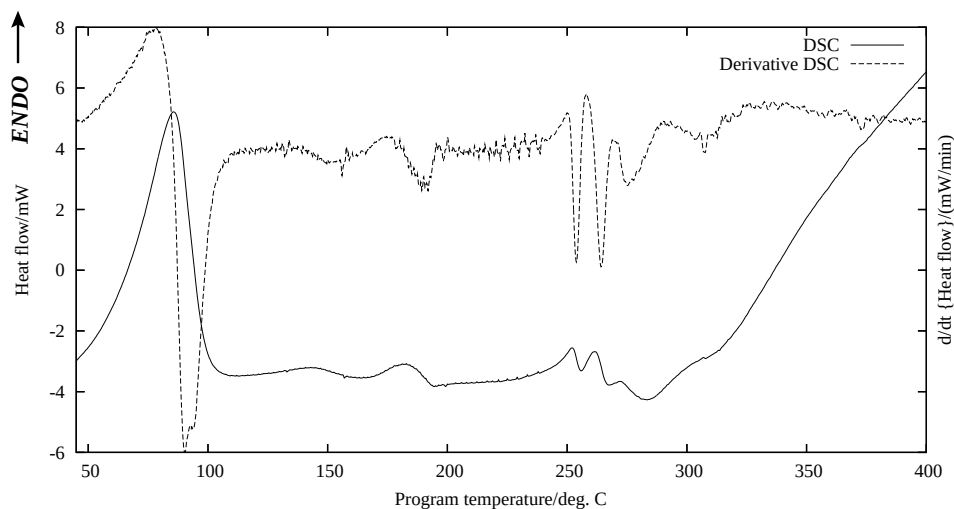


Figure 4.29: DSC and derivative DSC curves for **xut-cu-pyr2-b4c-no3-xtals**, heated in a crimped (not sealed) aluminium pan at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen (26 ml min^{-1}).

4.4.4 Crystal structures

During the course of this study, a similar crystal structure was reported independently in [24]. The discussion which follows is based on the crystal structure obtained as part of this study, but the one reported in [24] has already been discussed on p. 28. This description is quoted below.

Pyridine appears in [this] copper(II) 1,2,4,5-benzenetetracarboxylate complex as a nitrogen donor in a two-dimensional copper(II) complex with monodentate μ_4 -bridging 1,2,4,5-benzenetetracarboxylate. Each copper is bound axially to water and equatorially to *trans* pairs of pyridine (out of plane) and carboxyl oxygens. Cavities within the structure contain guest water clusters, and these are hydrogen bonded to each other, to the coordinated water molecules and to carboxyl oxygens. Thus the water molecules present in the structure form hexameric clusters which bridge the two-dimensional layers

of the structure by hydrogen bonding via the carboxyl groups of neighbouring layers. These hexameric clusters adopt a puckered boat conformation similar to the formation found in hexagonal ice.

The binding diagram and basic unit of the crystal structure of **xut-cu-pyr2-b4c-no3-xtals** is shown in Figure 4.30 (p. 129). Each half of each 1,2,4,5-benzenetetracarboxylate unit shown bridges two copper atoms together by unidentate binding of one carboxyl group to each copper. Cu1 and Cu2 are both in the square-based pyramidal configuration, and each is bound to:

- two carboxyl oxygens, equatorially: Cu1 to O11A and O11B, Cu2 to O21A and O21B(d) from a neighbouring unit
- two out-of-plane pyridine rings, equatorially, and
- one water molecule, axially.

In addition there are two guest water molecules present per copper atom, making up six water molecules per unit as shown. This agrees well with the analysis data.

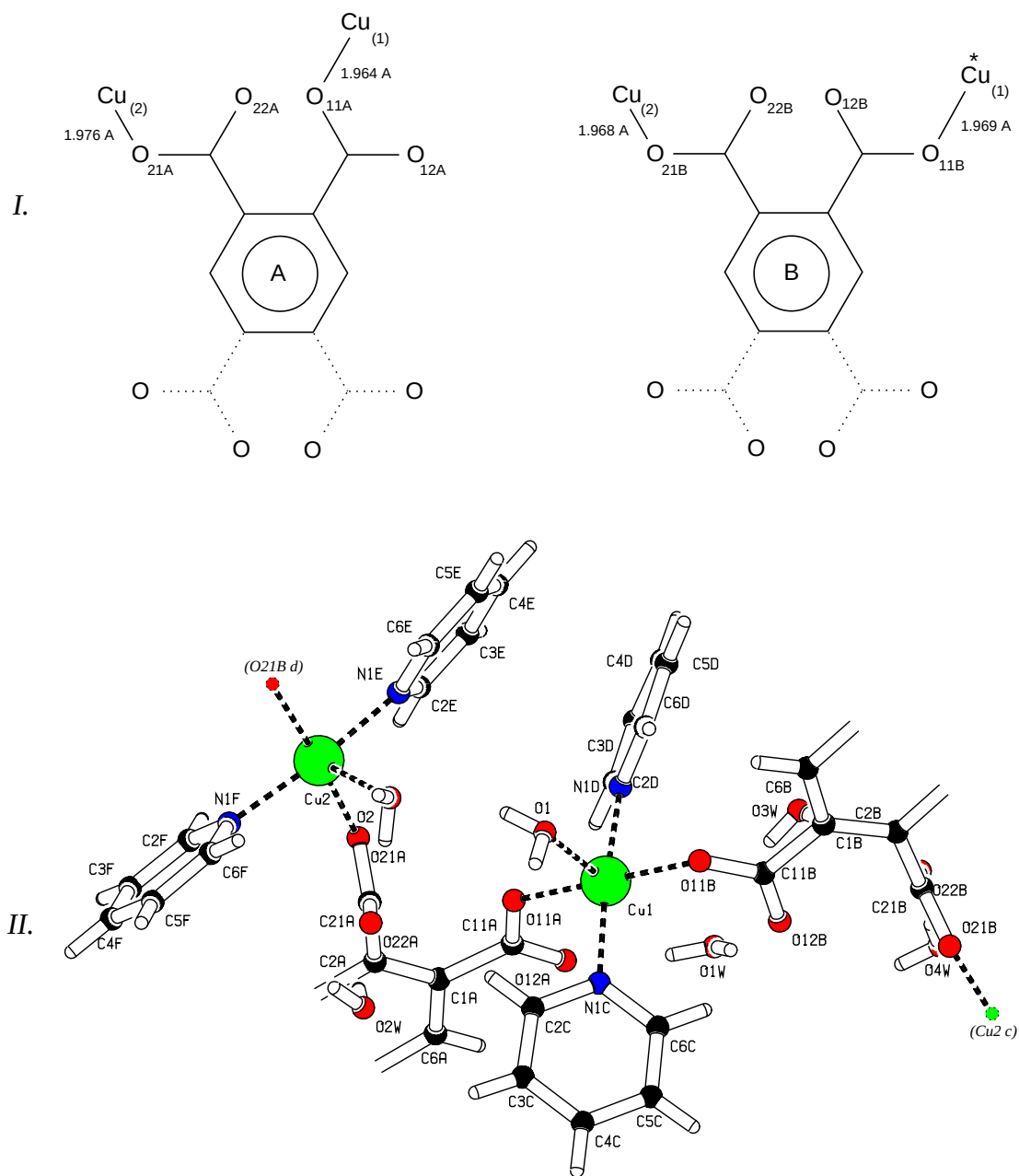


Figure 4.30: *I.* Binding diagram and *II.* basic unit of **xut-cu-pyr2-b4c-no3-xtals**. In *I*, the lower halves of 1,2,4,5-benzenetetracarboxylate units A and B — drawn with dotted lines — are symmetrical with the upper halves shown.

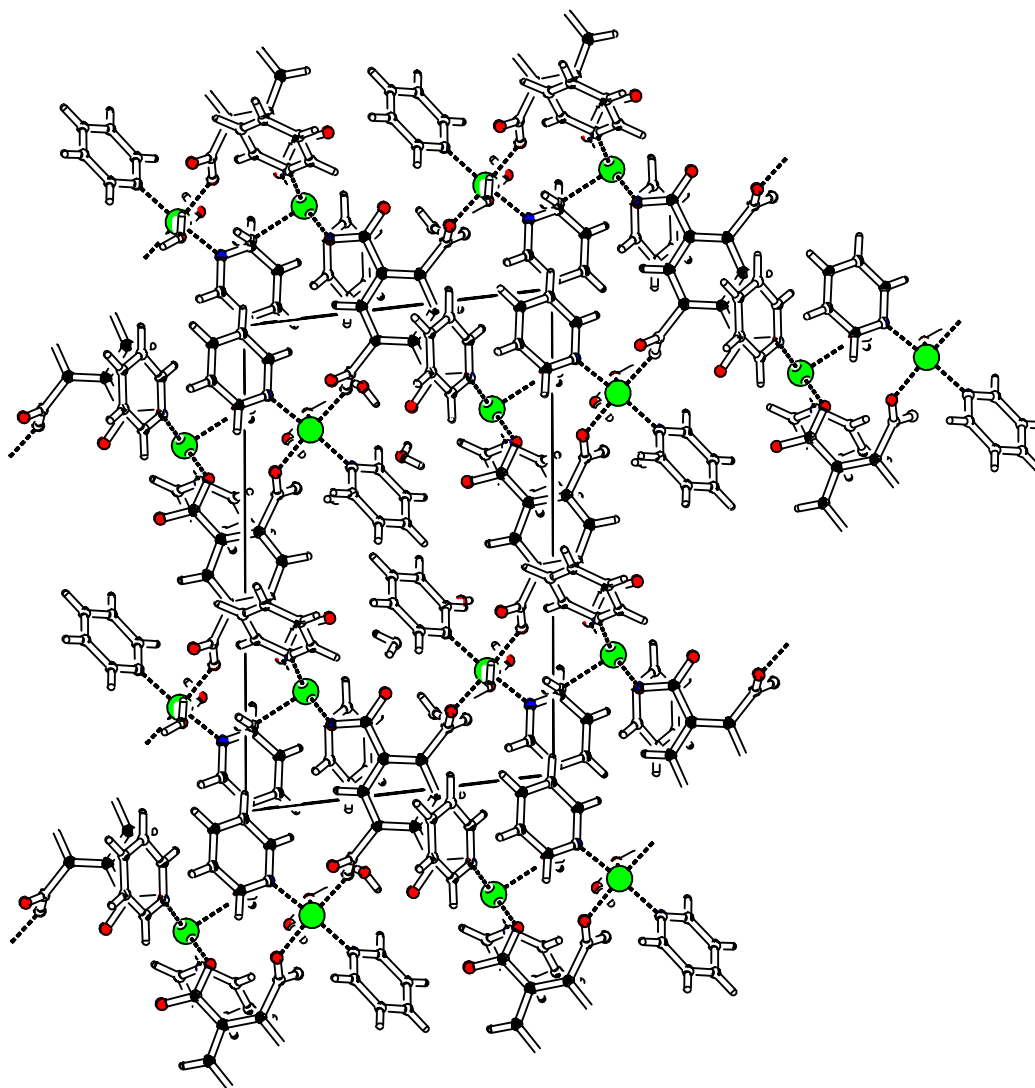


Figure 4.31: Face A of the crystal structure of **xut-cu-pyr2-b4c-no3-xtals**, showing the binding of two pyridine molecules — out of plane with each other — to each copper atom.

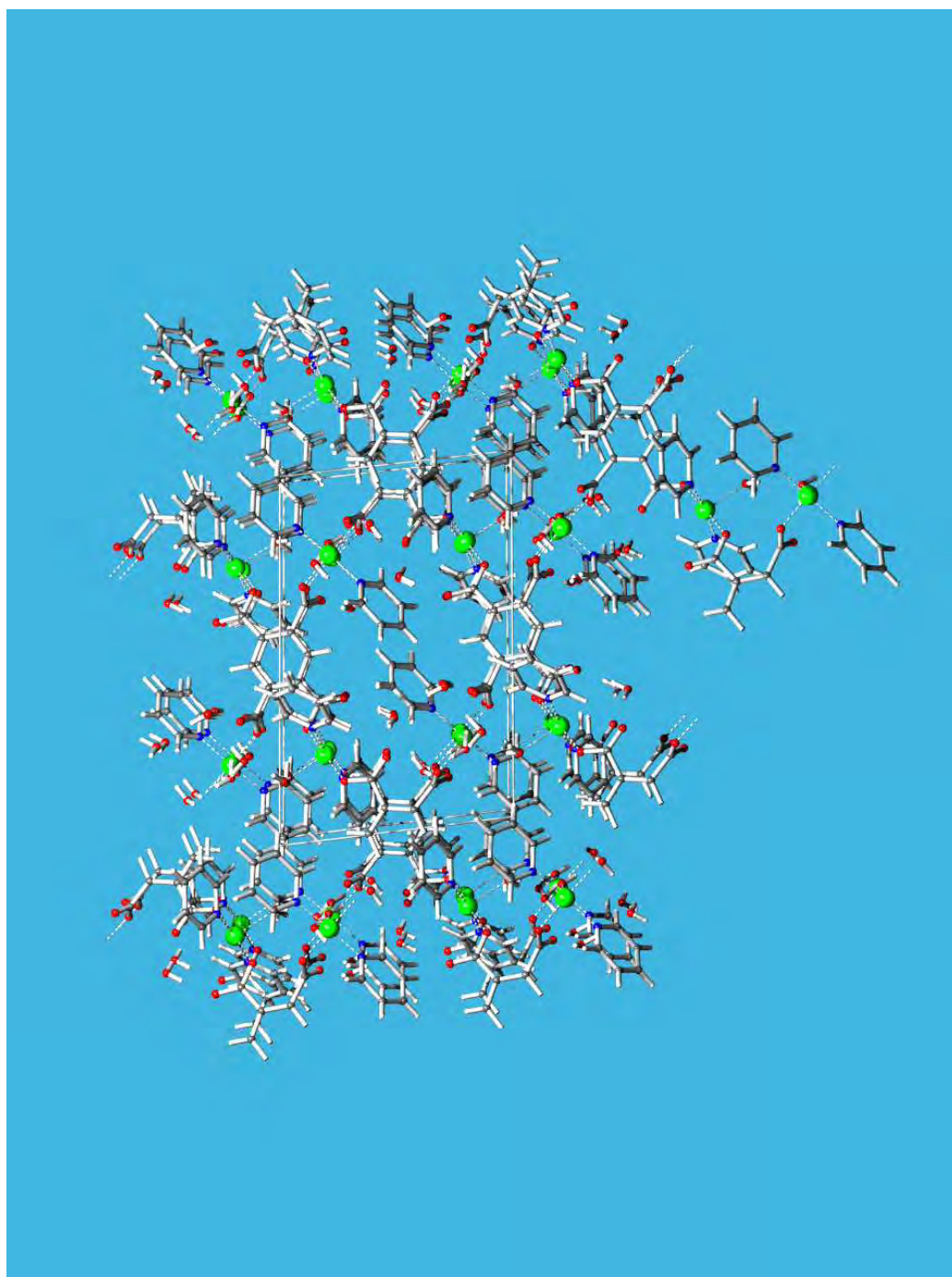


Figure 4.32: Ray-traced diagram of face A of the crystal structure of **xut-cu-pyr2-b4c-no3-xtals**, showing the binding of two pyridine molecules — out of plane with each other — to each copper atom.

4.5 GROUP 5 PRODUCTS

No materials suitable for single-crystal X-ray diffraction were obtained from the ambient precipitation syntheses (see Section 3.2.1, p. 59), and the materials were not taken beyond initial characterization.

A satisfactory elemental composition could not be determined from the material obtained from the precipitation synthesis with copper acetate, **ppt-cu-b4c-acet**, although copper (by AAS) and carbon-hydrogen determinations suggested the formulas $\text{Cu}_2 \text{L} \cdot 8\text{H}_2\text{O}$ (SSR = 2.13) or $\text{Cu}_{2\frac{1}{4}} (\text{OH})_{\frac{1}{2}} \text{L} \cdot 8.5\text{H}_2\text{O}$ (SSR = 0.55). The latter formula agrees better with the metal-to-ligand ratio obtained (2.2:1) for **ppt-cu-b4c-acet**, although the large relative error in the metal determination by AAS ($\pm 11\%$) means that neither of these formulas can be excluded. The X-ray powder diffraction pattern was similar to the ones obtained for **xst-cu-b4c-no3-needles**, **xst-cu-b4c-so4-needles** and **xst-cu-b4c-cl-needles**, but peak-broadening and mismatches in peak-intensity suggested poor crystallinity.

The material obtained from the copper carbonate synthesis, **ppt-cu-b4c-co3**, has the same X-ray powder diffraction pattern, and similar metal content and thermal behaviour to **xst-cu-b4c-no3-topxtals** and **xst-cu-b4c-so4-topxtals** (see discussions in Section 4.3, p. 103 *et seq.*). The TG transitions for the powder product are less well-defined than for the single crystals, suggesting that the product of the ambient precipitation synthesis is not as pure as the single crystals obtained by gel methods.

4.6 GROUP 6 PRODUCTS

No single crystals could be obtained from the hydrothermal syntheses (see Section 3.2.2, p. 60), and the materials were not taken beyond initial characterization. The two synthesis types yielded identical products — as shown by X-ray powder diffraction, thermal analysis and metal determination (AAS) — namely, **hyd-cu-b4c-acet** and **hyd-cu-b4c-co3**.

4.6.1 X-ray powder diffraction and infrared spectroscopy

The X-ray diffraction patterns of **hyd-cu-b4c-acet** and **hyd-cu-b4c-co3** — obtained from packed samples, i.e., not using the grease-smear method — were identical, and are shown in Figure 4.33.

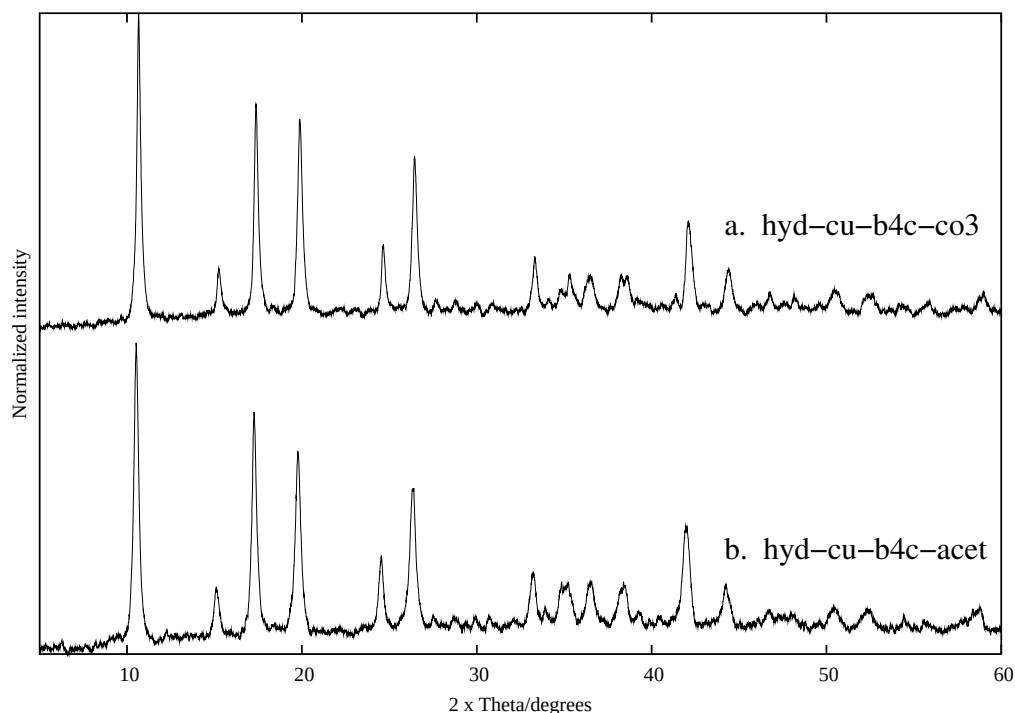


Figure 4.33: X-ray powder diffraction patterns of **hyd-cu-b4c-acet** and **hyd-cu-b4c-co3**

The mid-infrared spectra of **hyd-cu-b4c-acet** and **hyd-cu-b4c-co3** (obtained in KBr) were identical, except for differences in relative peak-height near 1500 cm^{-1} . The possibility of contamination of **hyd-cu-b4c-co3** by copper basic carbonate was eliminated because both forms — malachite, the form employed in synthesis, and azurite — exhibit strong absorptions (at 950 cm^{-1} and 1050 cm^{-1} , respectively [26]) which are absent from the spectrum of **hyd-cu-b4c-co3**. Variable interference from KBr during sample-preparation could account for these differences. The infrared spectrum of **hyd-cu-b4c-acet** — obtained in nujol and hexachlorobutadiene — is shown in Figure 4.34.

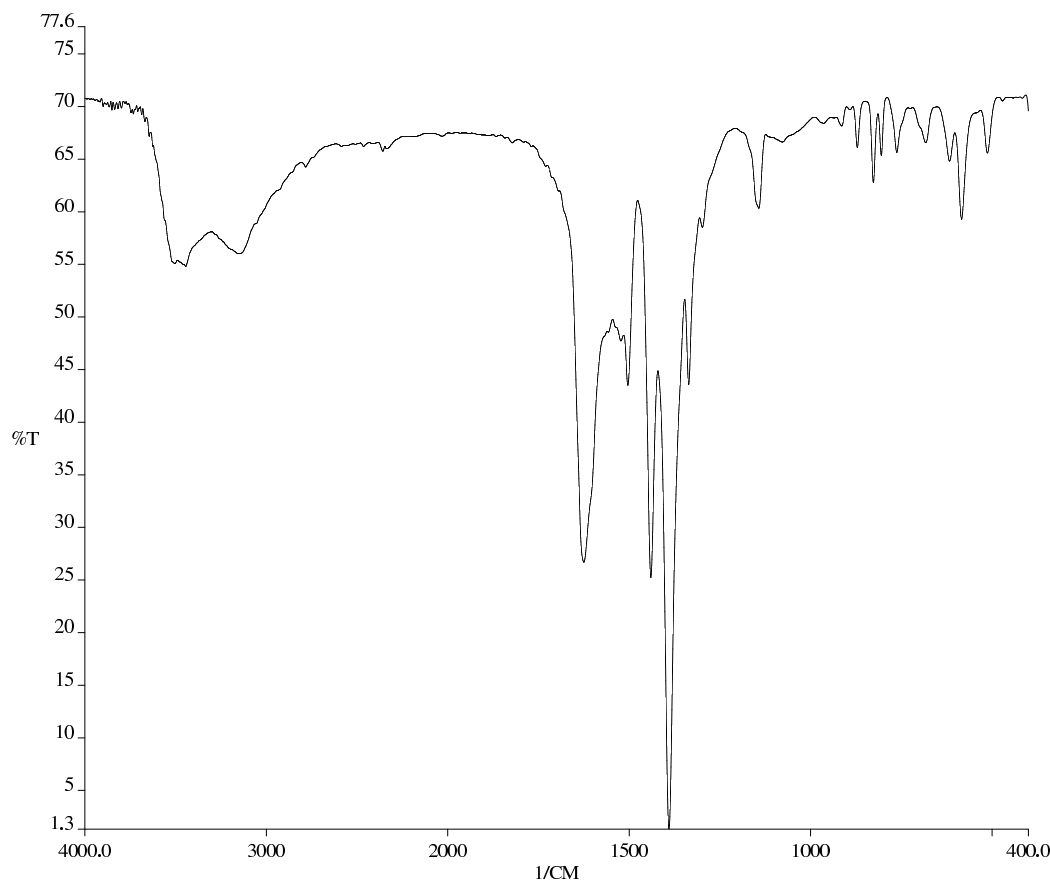


Figure 4.34: Mid-infrared spectrum of **hyd-cu-b4c-acet**.

4.6.2 Elemental analysis

The analytical data in Table 4.6 (p. 135) suggest a 2:1 metal-to-ligand ratio with very little hydration: 0.6–0.7 water molecules per formula unit. This is similar to the level of hydration normally reported for copper(II) oxalate (see Chapter 6 on p. 236). By minimizing SSR values, using increments of $\frac{1}{20}$ H₂O, the formula Cu₂ L·0.65H₂O was obtained for **hyd-cu-b4c-acet**. Metal analysis (AAS) of **hyd-cu-b4c-co3** gave a copper content of 32.54 %, which is within acceptable error of the metal content determined for **hyd-cu-b4c-acet**, i.e., 33.05 %.

Table 4.6: Experimental and calculated elemental analyses for Group 6 products. (Metal determination by AAS within ± 2 %.)

Product	Formula	Form. mass	Calculated			Experimental			SSR
		/g mol ⁻¹	%C	%H	%Cu	%C	%H	%Cu	
hyd-cu-b4c-acet	Cu ₂ L·0.65H ₂ O	388.93	30.88	0.86	32.68	30.43	0.67	33.05	0.37

4.6.3 Thermogravimetry and Differential scanning calorimetry

The TG curve in Figure 4.35 (p. 136) shows two indistinct steps, marked on the graph as follows:

- i. loss of $0.65 \text{ H}_2\text{O}$ (3.01 %), but because of the sloping plateau this step is not clearly visible, and
- ii. decomposition to $6\text{C} + 2\text{Cu}$ (51.20 %)

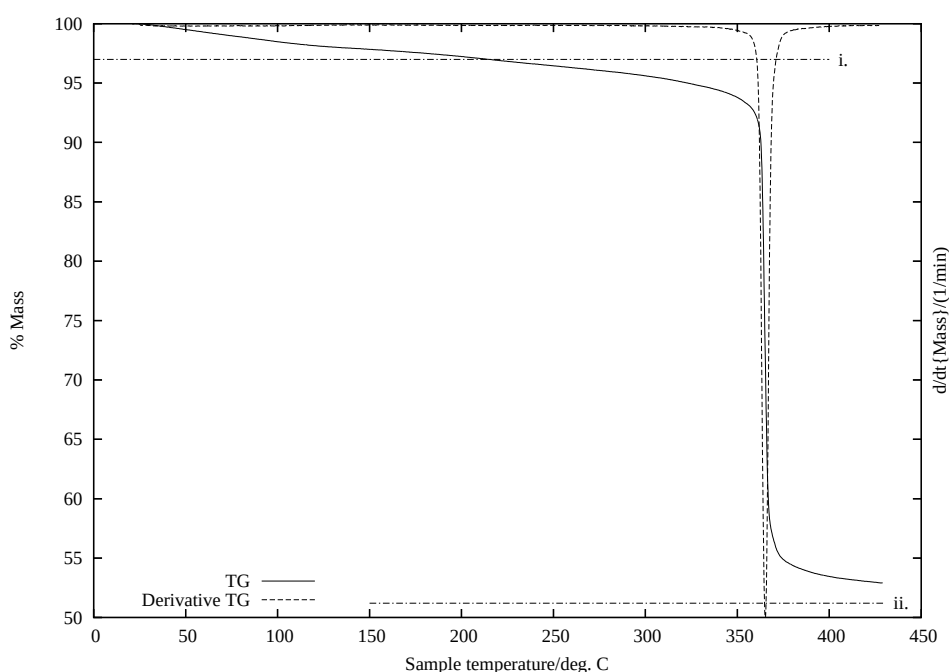
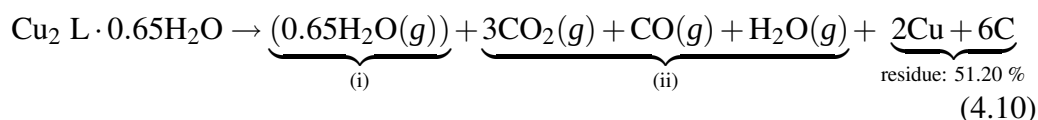


Figure 4.35: TG curve for **hyd-cu-b4c-acet** ($10 \text{ }^\circ\text{C min}^{-1}$) under nitrogen.

The interpretation of this dehydration/decomposition is somewhat arbitrary because of the sloping plateaux before and after the main mass-loss. Assuming that two formula units of $\text{Cu}_2\text{L} \cdot 0.65\text{H}_2\text{O}$ decompose to give off CO , CO_2 , and H_2O , leaving carbon and copper as residues, and assuming also that the 2×0.65 water molecules are given off as such, there are eight possible net decomposition reactions, with calculated solid residue masses in the range of 52.75–41.94 % of the original sample mass. If the formation of Cu_2O in stoichiometric quantities is

allowed, twenty-two possible reactions exist, the heaviest solid residue mass now being 58.41 %.

No evidence of copper oxides could be found in the DSC residues by XRPD. Furthermore, evolved gas analysis (TG-FTIR) showed evidence of large amounts of carbon dioxide in the exhaust stream, and indicated the presence of carbon monoxide at some stages of the decomposition. Therefore, the field is narrowed slightly to six possible reactions, involving the loss of 1,2,...,6 carbon monoxide molecules per formula unit, respectively. The reaction in which the least carbon monoxide is evolved (and, hence, the most solid carbon residue remains) is:



This reaction is in reasonable agreement with the observed mass losses, evolved gas analysis and residue analysis.

The DSC curve (see Figure 4.36) shows a single sharp exotherm at the same temperature as the TG mass-loss, and the mass of the residue after heating to 400 °C corresponded to 54.5 % of the original sample mass, which is considerably higher than the final TG mass. This suggests that the decomposition was not complete at this temperature. The XRPD pattern for the DSC residue showed very weak peaks characteristic of copper metal, and the material appeared to be very finely divided.

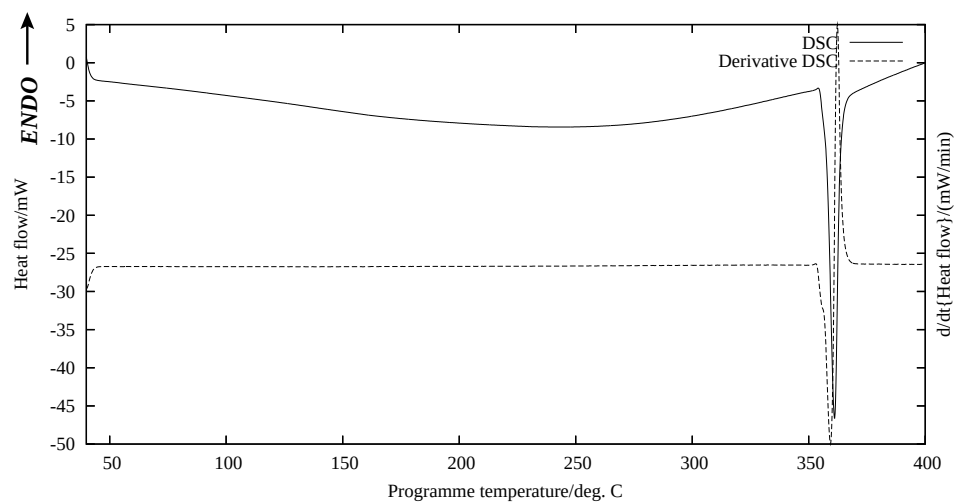


Figure 4.36: DSC and derivative DSC curves for **hyd-cu-b4c-acet**. The sample was heated in crimped (not sealed) aluminium pans from 25 °C to 400 °C at 10 °C min⁻¹ under flowing nitrogen (25 ml min⁻¹).

References

- [1] **D. A. Skoog, D. M. West and F. J. Holler.** *Fundamentals of Analytical Chemistry*. 7th ed. Saunders College Publishing, Orlando, Florida, USA 1996.
- [2] **T. OTA and H. IMAI.** “Synthesis of Pyromellitic Acid-Copper(II) Complex”. *Technol. Rep. Kansai Univ.* **13** (1972), 25–37.
- [3] **T. OTA and H. IMAI.** “Studies of Pyromellitic Acid-Copper(II) Complex Synthesized From Water-Ethanol Solution”. *Technol. Rep. Kansai Univ.* **15** (1974), 61–69.
- [4] *Powder Diffraction File: Alphabetical Index Inorganic Phases*. Swarthmore, Philadelphia, USA 1989.
- [5] **P. Knuuttila.** “The Preparation, IR Spectrum and Structure of the Di- μ_3 -hydroxo- μ -sulphato-tetrakis- μ -(isonicotinato-N-oxide)tetraaqua-tetracopper(II)”. *Inorganica Chimica Acta* **58** (1982), 201–206. Cited in the Cambridge Structural Database, structure BEGZA0.
- [6] **M. E. Bluhm, M. Ciesielski, H. Górls, O. Walter and M. Döring.** “Complexes of Schiff Bases and Intermediates in the Copper-Catalyzed Oxidative Heterocyclization by Atmospheric Oxygen”. *Inorg. Chem.* **42** (2003), 8878–8885. Cited in the Cambridge Structural Database, structure AQEDIJ.
- [7] **M. Du, X.-H. Bu, Y.-M. Guo and J. Ribas.** “Ligand design for alkali-metal-templated self-assembly of unique high-nuclearity CuII aggregates with diverse coordination cage units: crystal structures and properties”. *Chem.-Eur.*

- J.* **10** (2004), 1345–1354. Cited in the Cambridge Structural Database, structure IXELUS, CAN 140:433247.
- [8] **J. S. Park, K.-T. Youm and M.-J. Jun.** “A new spherical metallacryptate compound $[\text{Na}\text{C}]\{\text{Cu}_6(\text{Thr})_8(\text{H}_2\text{O})_2(\text{ClO}_4)_4\}\cdot\text{ClO}_4\cdot\text{H}_2\text{O}$: Magnetic properties and DFT calculations”. *Polyhedron* **21** (2002), 1273–1278. Cited in the Cambridge Structural Database, structure MUBCOB.
- [9] **S. W. Ng, X.-M. Chen and G. Yang.** “Metallo-Ligand $[\text{Cu}^{\text{II}}(\text{carboxylato})_4]^{2+}$ Cores: Tetrakis(trimethylammonioacetato-*O*)copper Diperchlorate and its 1,1 Complex with Sodium Perchlorate”. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **54** (1998), 1389–1393. Cited in the Cambridge Structural Database, structure POTR0F, abstract only.
- [10] **H.-L. Liu, H.-Y. Mao, H.-Y. Zhang, C. Xu, Q.-A. Wu, G. Li, Y. Zhu and H.-W. Hou.** “Two novel heterometallocrowns: syntheses and crystal structures of two copper(II) complexes with malonate and *o*-phthalate”. *Polyhedron* **23** (2004), 943–948. Cited in the Cambridge Structural Database, structure RUWMUR02.
- [11] **D. Ghoshal, T. K. Maji, T. Mallah, T.-H. Lu, G. Mostafa and N. R. Chaudhuri.** “Synthesis of a metal-dicarboxylate hybrid with three dimensional Na-O-Cu connectivity: structure, magnetic property and controlled solid state thermolysis leading to CuO nanorod”. *Inorg. Chim. Acta* **358** (2005), 1027–1033. Cited in the Cambridge Structural Database, structure RUWMUR03.
- [12] **J. Tercero, C. Diaz, J. Ribas, M. Maestro, J. Mahia and H. Stoeckli-Evans.** “Oxamato-bridged Trinuclear $\text{Ni}^{\text{II}}\text{Cu}^{\text{II}}\text{Ni}^{\text{II}}$ Complexes: A New $(\text{Ni}^{\text{II}}\text{Cu}^{\text{II}}\text{Ni}^{\text{II}})_2$ Hexanuclear Complex and Supramolecular Structures. Characterization and Magnetic Properties”. *Inorg. Chem.* **42** (2003), 3366–3373. Cited in the Cambridge Structural Database, structure VAJWIN.
- [13] **I. Gautier-Luneau, D. Phanon, C. Duboc, D. Luneau and J. L. Pierre.** “Electron delocalization in a trinuclear copper(II) complex: high field EPR characterization and magnetic properties of $\text{Na}_3[\text{Cu}_3(\text{mal})_3(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}$ ”.

- Dalton Trans.* pp. 3795–3799. Cited in the Cambridge Structural Database, structure XAXVU0.
- [14] **F. S. Delgado, C. Ruiz-Perez, J. Sanchiz, F. Lloret and M. Julve.** “Versatile supramolecular self-assembly. Part I. Network formation and magnetic behaviour of alkaline salts of the bis(malonate)cuprate(II) anion”. *CrystEngComm* **8** (2006), 507–529. Cited in the Cambridge Structural Database, structure RUWMUR04.
- [15] **B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell.** *Vogel’s Textbook of Practical Organic Chemistry*. 5th ed. Addison Wesley Longman Limited, Harlow, England 1989.
- [16] **R. C. Weast** (editor). *CRC Handbook*. 49th ed. Chemical Rubber Co., Cleaveland, Ohio, USA 1969.
- [17] **K. Nakamoto.** *Infrared and Raman Spectra of Inorganic and Coordination Compounds*. 3rd ed. John Wiley and Sons, Inc., New York 1978.
- [18] **J. R. Ferraro and W. R. Walker.** “Infrared spectra of hydroxy-bridged copper(II) compounds”. *Inorg. Chem.* **4**(10) (1965), 1382–1386.
- [19] **P. Tarte.** “Recherches sur les fréquences de déformation OH–I: Spectre infrarouge des seils basiques de cuivre”. *Spectrochim. Acta* **13** (1958), 107–119. Note: Original paper in French.
- [20] **B. T. Usubaliyev, A. N. Shnulin and K. S. Mamedov.** “Crystal and molecular structure of a decahydrate complex of copper with 1,2,4,5-benzenetetracarboxylic acid”. *Koord. Khim.* **8** (1982), 1532–1538. Cited in the Cambridge Structural Database, structure B0VTAH.
- [21] **R. Cao, Q. Shi, D. Sun, M. Hong, W. Bi and Y. Zhao.** “Synthesis and characterizations of copper(II) polymeric complexes constructed from 1,2,4,5-benzenetetracarboxylic acid”. *Inorg. Chem.* **41** (2002), 6161–6168. Cited in the Cambridge Structural Database, structure MURB0Q.
- [22] **A. L. Spek.** *PLATON: A Multipurpose Crystallographic Tool*. Utrecht University, Utrecht, The Netherlands 2001.

- [23] **C. N. Banwell.** *Fundamentals of Molecular Spectroscopy.* 2nd ed. McGRAW-HILL Book Company (UK) Limited, Maidenhead, Berkshire, England 1972.
- [24] **S. K. Ghosh and P. K. Bharadwaj.** “Puckered-boat conformation hexameric water clusters stabilized in a 2D metal-organic framework structure built from Cu(II) and 1,2,4,5-benzenetetracarboxylic acid.” *Inorg. Chem.* **43** (2004), 5180–5182. Cited in the Cambridge Structural Database, structure PADPIU.
- [25] **K. N. Wong and S. D. Colson.** “The FT-IR spectra of pyridine and pyridine- d_5 ”. *J. Mol. Spec.* **104** (1984), 129–151. Note: summary table on p. 148.
- [26] **R. A. Nyquist and R. O. Kagel.** *Handbook of Infrared and Raman Spectra of Inorganic Compounds and Organic Salts*, vol. 4. Academic Press, Inc., Chestnut Hill, Massachusetts, USA 1997.

Chapter 5

Desolvation-resolution experiments

5.1 INTRODUCTION AND RATIONALE

The compounds discussed above which contain significant numbers of guest water molecules per formula unit were considered to be suitable candidates for dehydration-resolution studies. **xut-cu-b4c-acet-xtals** and **xst-cu-b4c-no3-rhombi** were of particular interest because of their novelty and also because of the clear microporous nature of their structures. In particular, the structure of **xut-cu-b4c-acet-xtals** is traversed by large channels (see Section 4.1.3, p. 85) and was judged to have the greatest potential for inclusions studies. The other complexes were studied mainly for comparison to **xut-cu-b4c-acet-xtals**.

The studies involved dehydrating the parent material and attempting to bring about the inclusion of guest solvent molecules by exposing the dehydrated material to vapours of different solvents. The most obvious choice of guests was the series R-OH where R is H-, CH₃-, or CH₃CH₂-. These provide a convenient series of straight-chain molecules of increasing size. Initial work with **xut-cu-b4c-acet-xtals** as a host and pyridine as a guest did not show promise and these studies were discontinued at the preliminary stage.

Samples of each material were dehydrated to a temperature at which the DSC signal had clearly returned to the baseline after the main dehydration peak, and

allowed to cool under anhydrous conditions. Each material was then exposed to water vapour — as explained below — to investigate whether significant structural changes took place on dehydration, and to show whether the structure of the rehydrated material was the same as that of the untreated parent material. Dehydrated samples of the materials for which the dehydration process was reversible were then exposed to methanol vapour and ethanol vapour to see whether these substances could be included in voids in the dehydrated host structures. In most experiments, the dehydrated host materials were exposed to the saturated vapour above the guest in liquid form, although in some cases ambient air was sufficiently humid for rapid rehydration to occur.

The compound **xut-cu-b4c-acet-xtals**, in dehydrated form, was found to accept H_2O , CH_3OH and $\text{CH}_3\text{CH}_2\text{OH}$ as guests. The interactions with H_2O and CH_3OH were rapid and reproducible, and so the reversibility of these processes was studied in greater detail. The uptake of $\text{CH}_3\text{CH}_2\text{OH}$ was much slower and less reproducible, and the guest-inclusion study was therefore limited. In addition, as the size of the guest molecules increased, there was a large increase in the broadness of the DSC endotherms for the desolvation of these guests. For ethanol, the desolvation endotherm was too broad even for semi-quantitative investigation.

Dehydrated **xst-cu-b4c-no3-rhombi**, like dehydrated **xut-cu-b4c-acet-xtals**, rapidly absorbed water even from the atmosphere. However, close examination of the infrared spectra and X-ray diffraction patterns of the original and rehydrated materials showed that the dehydration was not wholly reversible. Small, but reproducible, differences were observed also in the DSC curves corresponding to the dehydration of the untreated and rehydrated materials. The dehydrated material did not take up methanol as a guest even after many hours of exposure to the saturated vapour.

Dehydrated samples of **xst-cu-b4c-so4-topxtals** and **xst-cu-b4c-no3-lumps** did not take up water readily from the atmosphere, but did so after some hours of exposure to saturated water vapour. DSC studies showed very significant differences in thermal behaviour between the dehydrated and rehydrated materials for **xst-cu-b4c-no3-lumps**, so this compound was not considered for further guest inclusion studies. The dehydration of **xst-cu-b4c-so4-topxtals** was shown to be at least partly reversible, but preliminary resolution experiments with methanol did

not indicate methanol uptake.

5.2 SPECIFIC METHODS

5.2.1 X-ray powder diffraction

In the course of this study, it was necessary to obtain the X-ray diffraction patterns of dehydrated samples which absorb water readily from the atmosphere. The X-ray diffractometer employed in this study was not equipped with any means to purge the sample compartment with dry inert gas, and it was considered impractical to enclose the instrument in an airtight case.

In an attempt to exclude moisture from the sample compartment of the X-ray diffractometer, the lower part of the compartment was packed with small desiccant-bags filled with indicating silica-gel and the instrument left for several hours. To test this method, a small sample (4.099 mg) of **xut-cu-b4c-acet-xtals** was dehydrated in a DSC to 78 % of its original sample mass and, after being allowed to cool, was placed in the sample compartment together with the desiccant. After one hour, the sample was found to have absorbed water to a final mass of 87 % of the original sample mass. This method of excluding water was therefore considered to be inadequate.

Dehydrated samples were then coated with hydrophobic substances after mounting. Light machine oil, soya lecithin (in aerosol form) and paraffin oil were tested by placing a drop onto anhydrous copper sulfate. Under paraffin oil, anhydrous copper sulfate remained white for several hours, but the oil was found to be too viscous for easy handling. A 4:1 blend of paraffin oil and petroleum ether was found to spread over the sample rapidly, and to exclude atmospheric moisture.

All samples related to the inclusion study were therefore mounted on glass slides smeared with petroleum jelly, and coated with either 4:1 paraffin oil–petroleum ether or undiluted paraffin oil (as indicated) immediately after mounting. The slides were then mounted in the diffractometer with a paper spacer to compensate for the thickness of the petroleum jelly.

The following are possible limitations of this method:

- The dehydrated sample has to be mounted very quickly to minimize exposure to moisture in the air.
- The sample size, i.e., the amount of sample actually in the path of the incident X-ray beam, is not easily reproducible, and is likely to differ considerably from one run to the next. Thus, the reproducibility of peak heights is bound to be poor, even for identical samples.
- It is difficult to mount the sample evenly, especially the dehydrated sample. Uneven mounting would influence the relative peak heights in an X-ray diffraction pattern.
- Coating the samples with paraffin oil after mounting may increase preferred-orientation effects by allowing the crystalline particles greater mobility. This would also affect relative peak heights.
- The possibility of an interaction between some component of the paraffin oil and the dehydrated sample cannot be excluded.

Other attempts at excluding water included sandwiching the sample between a glass slide greased with petroleum jelly and a layer of greased laboratory film (Parafilm), and also covering the sample with a layer of silicone oil. Parafilm, in its normal unstretched form, has a clear X-ray diffraction pattern which interferes with the peaks of interest, and silicone oil appears to strongly absorb the X-rays used in this study. It was found that the thickness of paraffin oil influenced the intensity of the X-ray peaks of the sample, so great care was taken to ensure uniformity of sample preparation.

5.3 xut-cu-b4c-acet-xtals

5.3.1 Single desolvation-resolution: water

The sample was crushed lightly and a small quantity (3.353 mg) was packed into an aluminium DSC pan and covered with a lid (not crimped). The sample was then subjected to the following treatment:

1. Heating from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen purge (25 ml min⁻¹) to drive off water. The sample mass after heating corresponded to 78.5 % of the original sample mass.
2. Exposure to moist air for 2 hours. The mass of the sample after exposure corresponded to 100 % of the original sample mass.

The sample was removed for examination by X-ray powder diffraction. More samples of similar size were dried as above to obtain a dehydrated sample for X-ray diffraction. The dehydrated samples were a darker blue than the blue-green crushed original and rehydrated materials. On removal of the DSC pan lid, the dehydrated material began to turn blue-green immediately, and the darker blue colour disappeared in under three minutes.

The X-ray diffraction patterns of the untreated, dehydrated and rehydrated samples are shown in Figure 5.1 (p. 149). The patterns are similar, but there are some points of difference that are not immediately apparent from the figure.

The intensities of the leftmost pair of reflections are significantly lower in pattern b than in patterns a and c and, except for the peaks at $2\theta \approx 11^\circ$, all the peaks in pattern b are somewhat less well-defined than in the other patterns.

Pattern b is the X-ray diffraction pattern of the partly hydrated material. The leftmost pair of peaks in the range 5–10° and the peak at the rightmost dotted line are from the hydrated material, and the peak at the leftmost dotted line is from the dehydrated material. To verify this, X-ray diffraction patterns were obtained from a sample of the dehydrated material, covered immediately after dehydration with a drop of undiluted paraffin oil.. The excess oil was wiped away, and the X-ray diffraction pattern was obtained immediately. In addition, X-ray diffraction patterns of the same sample were obtained after four hours and after two days. The X-ray diffraction patterns obtained are shown — with the intensities *not* normalized as in normal practice, but expressed proportionally, in arbitrary units, to the actual count-rates obtained from the instrument — in Figure 5.2, p. 150).

It is clear from the figure that peaks i and ii in curve a increase in intensity as the sample slowly takes up moisture from the atmosphere. At the same time, peak iii in curve a decreases in intensity so that it is hardly visible as iii' in curve b, and totally disappears in curve c. Also, peak iv is scarcely distinguishable in curve a,

but is prominent in curves b and c. Other peaks in curve a are not clearly visible, and the pattern, as a whole, is much less distinct than b and c.

Peaks i, ii, and iv are attributed to the hydrated structure, as has been confirmed by comparing these X-ray diffraction patterns to the simulated pattern obtained from the crystal structure (crystal structure discussed in Section 4.1.3, p. 85). They would be absent if it were possible to obtain a pattern of the material before rehydration began. The appearance of peak iii (absent in the simulated diffraction pattern) is evidence of the formation of a new structure — probably by partial collapse of the framework — on dehydration.

In Figure 5.1 (p. 149), pattern c bears a very close resemblance to pattern a, with no peak at the leftmost dotted line. The rehydrated structure thus appears to be practically identical to the original, despite having passed through a dehydrated intermediate with a collapsed structure, as shown by the different X-ray diffraction pattern of the dehydrated material.

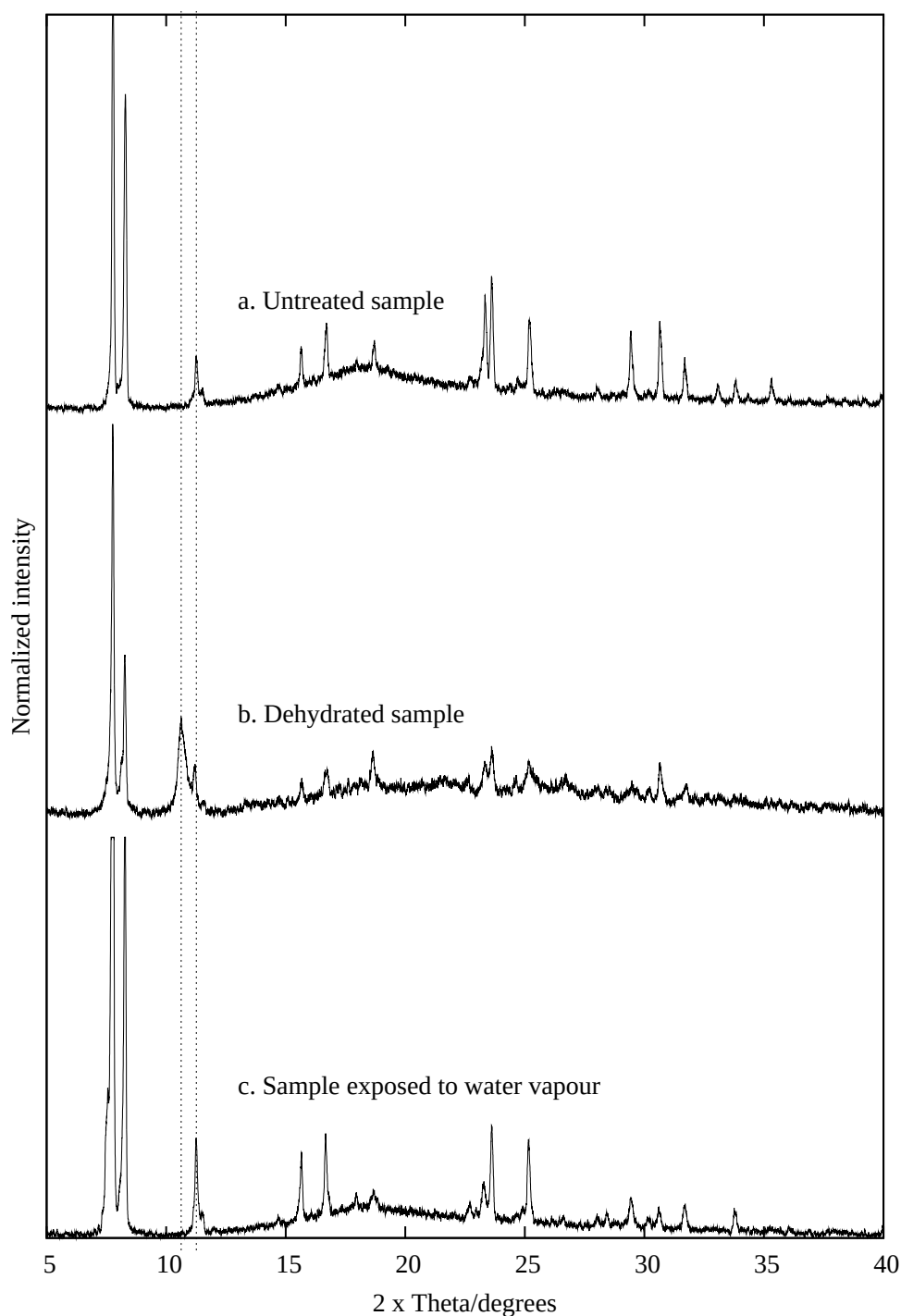


Figure 5.1: X-ray diffraction patterns of **xut-cu-b4c-acet-xtals** (a) without pre-treatment, (b) after dehydration by heating in a DSC from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen (25 ml min⁻¹) and (c) after exposure of the dehydrated material to moist air for 2 hours. The dotted lines are to indicate peak-shifts. The samples were all coated prior to running with a thin layer of a 4:1 mixture of paraffin-oil and petroleum ether.

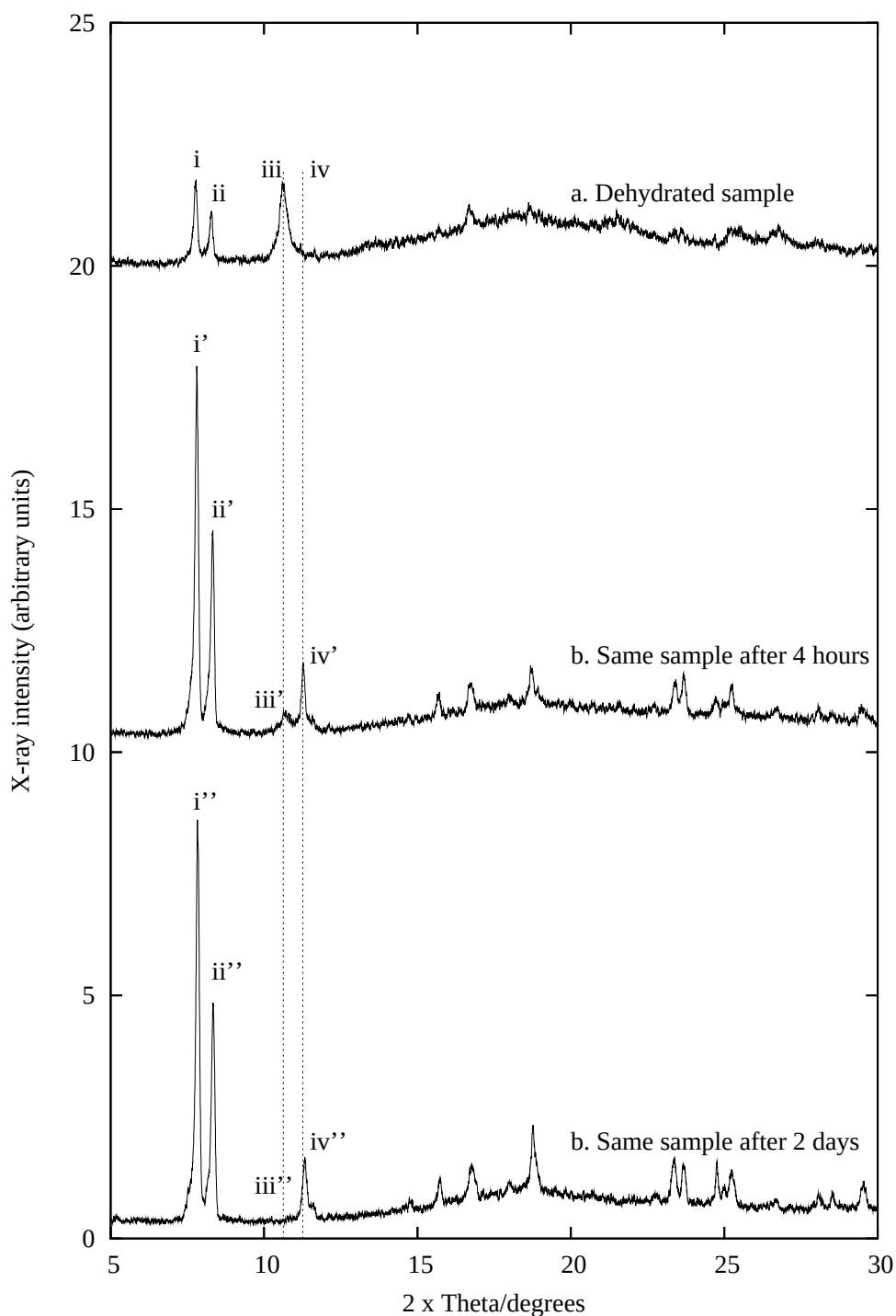


Figure 5.2: X-ray diffraction patterns of a single sample of **xut-cu-b4c-acet-xtals** after dehydration, with the sample covered with a thin layer of paraffin oil. X-ray diffraction patterns were obtained (a) immediately after dehydration, (b) four hours later and (c) two days later.

5.3.2 Single desolvation-resolvation: methanol

The sample was crushed lightly and a small quantity (4.218 mg) was packed into an aluminium DSC pan and covered with a lid (not crimped). The sample was then subjected to the following treatment:

1. Heating from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen purge (25 ml min⁻¹) to drive off water. The sample mass after heating corresponded to 78.1 % of the original sample mass.
2. Exposure to saturated methanol vapour (25 °C) for 4 hours. The mass of the sample after exposure corresponded to 96.4 % of the original sample mass.

The sample was removed for examination by X-ray powder diffraction. More samples of similar size were dried as above to obtain a dehydrated sample for X-ray diffraction, and to obtain samples for TG-FTIR studies.

The X-ray diffraction patterns of the untreated, dehydrated and resolvated samples are shown in Figure 5.3 (p. 152). As with the rehydrated sample (Section 5.3.1, p. 146), the X-ray diffraction pattern of the material exposed to methanol vapour (curve c) is very similar to that of the original material, and bears little resemblance to the diffraction pattern of the dehydrated material (Figure 5.2, curve a, p. 150). In agreement with the observations for the rehydrated material, the material exposed to methanol shows no peak at the leftmost dotted line, indicating that the dehydrated material is not present. As was found above with the rehydrated material, the structure of the material exposed to methanol vapour seems to be very similar to that of the original material.

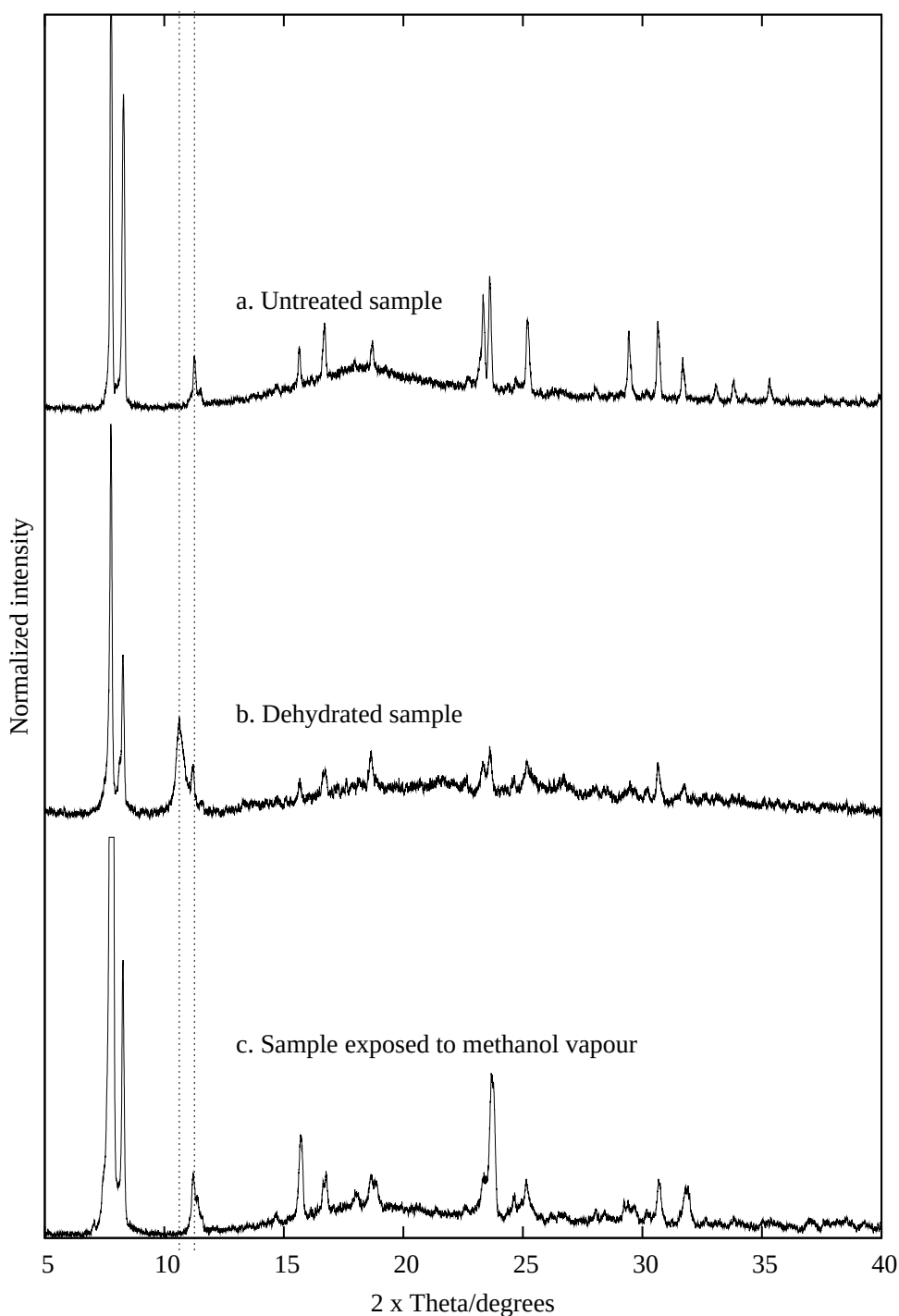


Figure 5.3: X-ray diffraction patterns of **xut-cu-b4c-acet-xtals** (a) without pre-treatment, (b) after dehydration by heating in a DSC from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen (25 ml min⁻¹) and (c) after exposure of the dehydrated material to methanol vapour for 4 hours. The dotted lines are to indicate peak-shifts. The samples were all coated prior to running with a thin layer of a 4:1 mixture of paraffin oil and petroleum ether.

The X-ray diffraction pattern of a dehydrated sample which had been exposed to methanol vapour was also obtained under paraffin oil, to compare with that of the sample coated with 4:1 paraffin oil and petroleum ether. The patterns are shown in Figure 5.4, (p. 153) and although the peaks under paraffin oil (curve a) are weaker than under the diluted oil (curve b), there is a one-to-one correspondence between the peaks in curve a and those in curve b. There is no observable peak beneath the leftmost dotted line, indicating that no trace of the dehydrated structure could be detected.

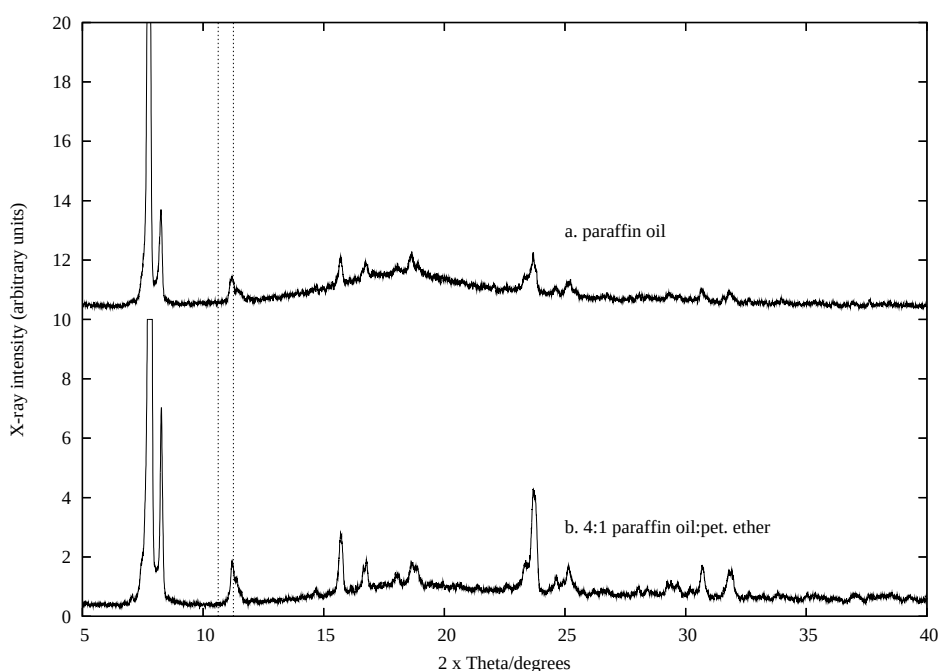


Figure 5.4: X-ray diffraction patterns of **xut-cu-b4c-acet-xtals** which had been dehydrated in a DSC (25 °C–150 °C at 10 °C min⁻¹ under nitrogen, 25–27 ml min⁻¹) and exposed to methanol vapour. Patterns were obtained (a) under paraffin oil and (b) under a 4:1 mixture of paraffin oil and petroleum ether.

To attempt to prove that the included host was indeed methanol, and not simply water in a different environment, and to study the nature of the inclusion, the mid-infrared spectrum of the untreated material and that of a sample which had been dehydrated and exposed to methanol vapour were obtained. The mid-infrared spectra of **xut-cu-b4c-acet-xtals** in untreated form, as well as of samples **xut-cu-b4c-acet-xtals** which had been dehydrated and exposed to moist air or methanol

vapour, are shown in Figure 5.5, 5.6 and 5.7 (pp. 155–157). The spectra are almost indistinguishable, except for a few minor changes noted below:

- In Figure 5.5 the maximum of the very broad peak at 3014 cm^{-1} appears unchanged for the rehydrated material, but shifts to 2956 cm^{-1} for the methanol-resolvated material. While this shift may be an artifact owing to peak-broadening, there may be some influence by the methanol C–H stretch at around 2900 cm^{-1} [1, p. 63].
- In Figure 5.7 the peak at 996 cm^{-1} in the spectrum of the untreated material is present only as a small shoulder in the spectrum of the rehydrated material (not marked) and appears to shift to 1005 cm^{-1} , perhaps under the influence of the methanol C–O stretch at around 1035 cm^{-1} [1, p. 63].

Thus the infrared spectra gave no information about the host inclusions¹, except that no major changes in the framework as a result of dehydration and resolution could be detected. This was unexpected, and contrasts with the early studies of guest-inclusion in metal-organic frameworks (for example [2] and brief suggestions in [3]).

DSC evidence, presented later in Sections 5.3.7 and 5.3.8 (pp. 179 and 184, respectively), and the mass-data given above, strongly suggest that methanol is taken up by the dehydrated material, to form — judging by the X-ray diffraction and mid-infrared data given above — a structure very similar to the untreated parent. Nevertheless, it remained to be proved conclusively that methanol is taken up in the structure. The effects of methanol inclusion on the thermal decomposition characteristics of the material were also examined.

Figure 5.8 (p. 159) shows the TG/derivative TG (part *I*) and evolved gas analysis results (part *II*) of the material exposed to methanol. The TG-curve is similar to that of the parent material (Figure 4.3 (*I.*), p. 84), but with broader mass-loss

¹In preliminary investigations, mid-infrared spectra of the methanol-resolvated material were obtained in KBr pellets, also showing no characteristic bands for methanol. To prove that methanol could be observed in the presence of the matrix, small amounts of liquid methanol were added during sample preparation. Methanol bands could only be observed, weakly, over the spectrum of the complex when the sample was visibly moist with methanol. Furthermore, the infrared spectrum of the dehydrated material was also nearly identical to that of the parent material, suggesting that the sample rehydrates too quickly in air to be able to obtain a spectrum for the truly dehydrated material.

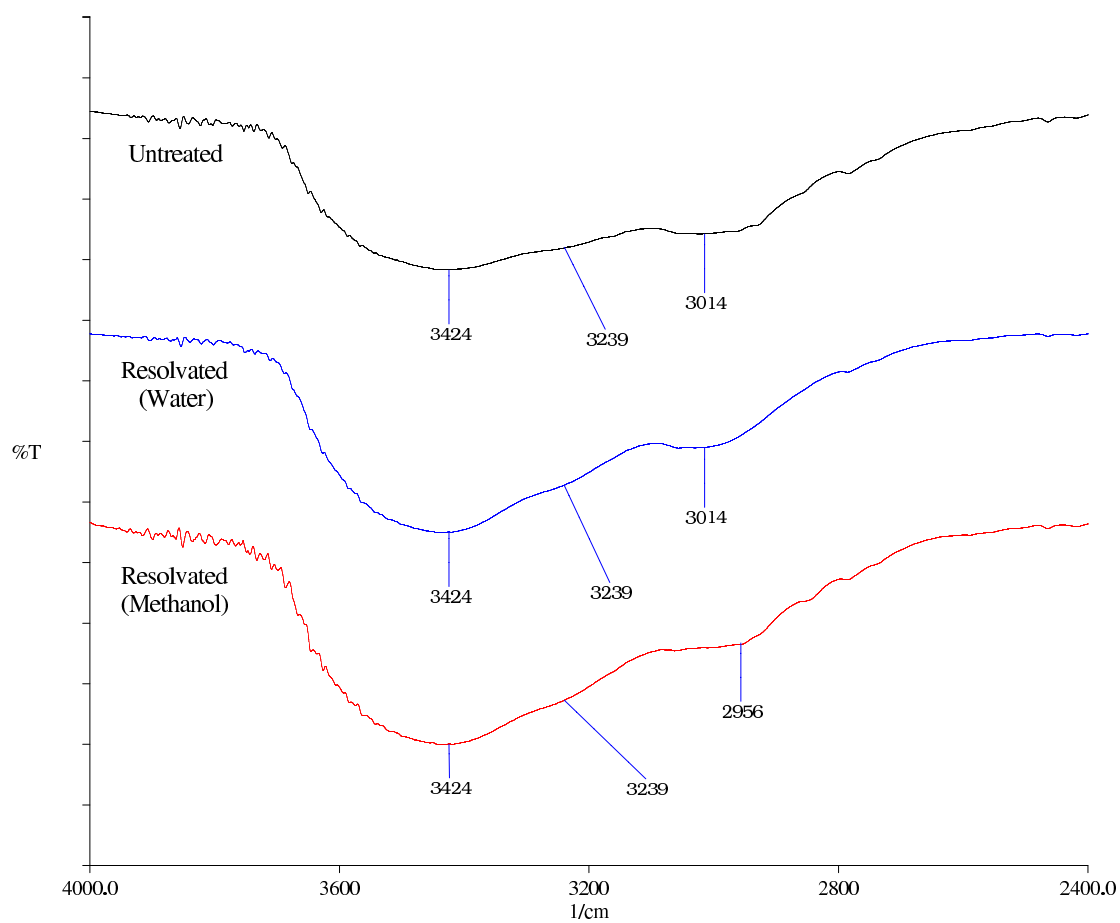


Figure 5.5: Infrared spectra of **xut-cu-b4c-acet-xtals** in the untreated, rehydrated and methanol-resolvated states ($4000\text{--}2400\text{ cm}^{-1}$).

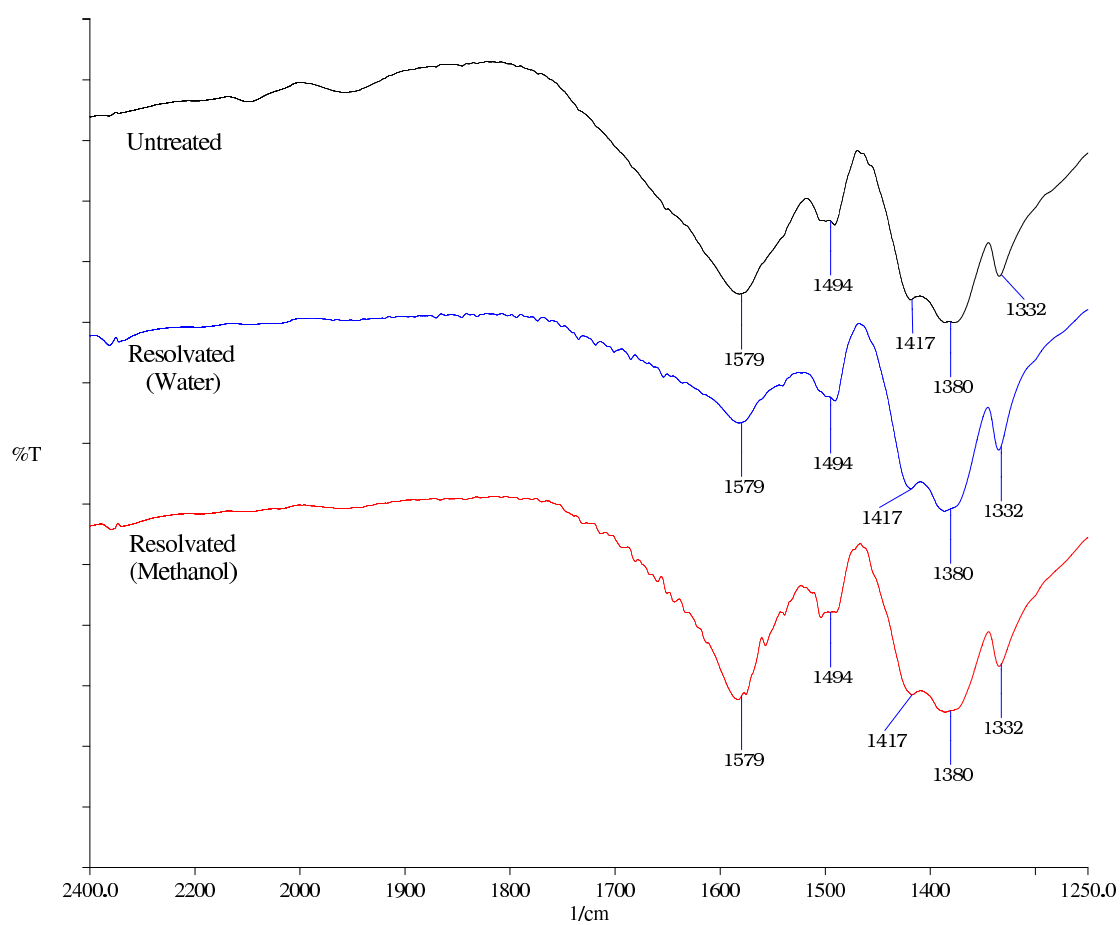


Figure 5.6: Infrared spectra of **xut-cu-b4c-acet-xtals** in the untreated, rehydrated and methanol-resolvated states (1800–1250 cm^{-1}).

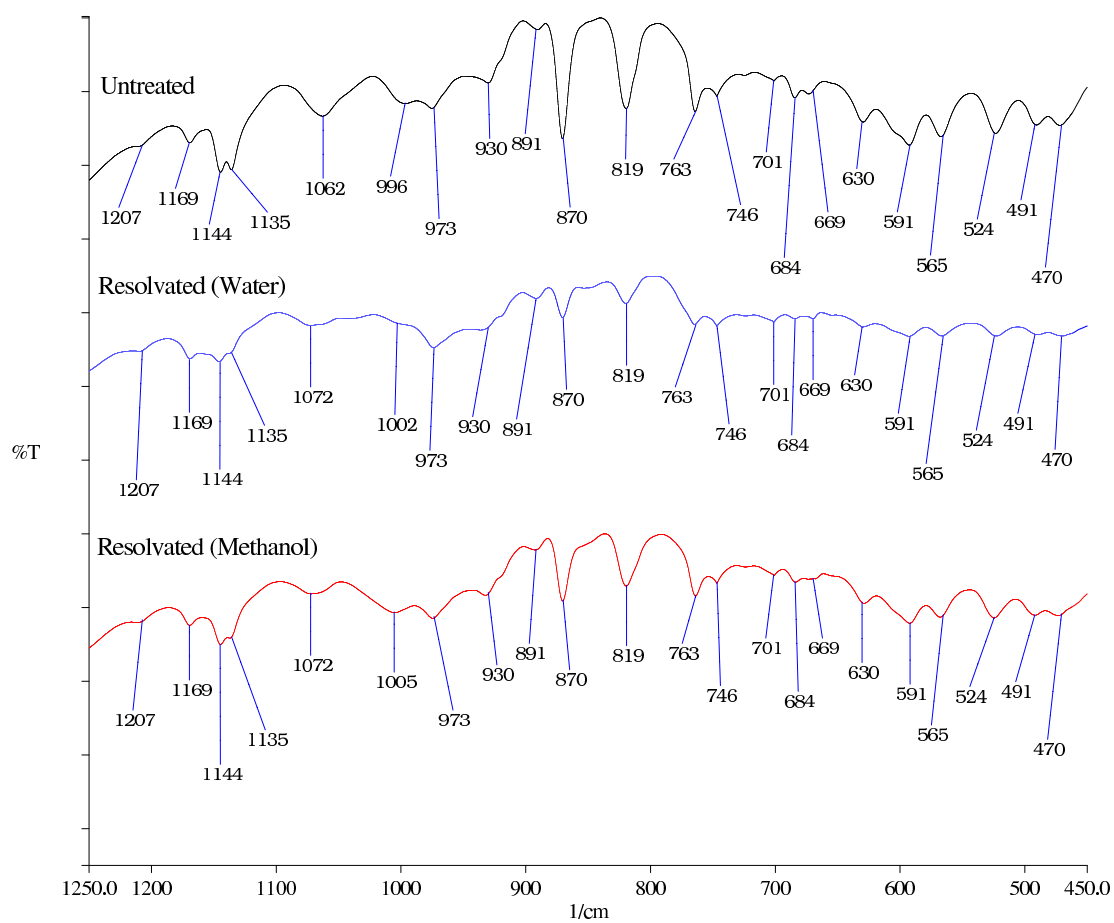


Figure 5.7: Infrared spectra of **xut-cu-b4c-acet-xtals** in the untreated, rehydrated and methanol-resolvated states ($1250\text{--}450\text{ cm}^{-1}$).

curves, and — as shown clearly on the derivative TG curve — a more complex final decomposition. The main features of the TG and, particularly, the derivative TG curves are reproducible from one experiment to another, but the details of these features (e.g., peak height and resolution) are not. Clear indications of methanol in the exhaust gas stream can be seen in the time-resolved infrared spectra.

The evolved gas analysis results are presented differently in Figure 5.9 (p. 160) which shows two absorbance–programme temperature profiles in regions characteristic of methanol and one region characteristic of carbon dioxide (details on the figure). The absorbance at each point is simply the peak-height in the spectral region specified for the corresponding profile at the time corresponding to the TG-programme temperature given for that point on the *x*-axis. The profiles for methanol show the expected response between 45 °C and 125 °C, corresponding to the TG-mass loss of 15 % in a similar temperature region. A second response in the methanol region is seen between 185 °C and 280 °C. Corresponding responses can be seen in the derivative TG curve in Figure 5.8 *I* (p. 159), in the form of a small peak followed by a shoulder on the main decomposition peak. Moreover, it is apparent from the absorbance surface in Figure 5.8 *I* (p. 159), that loss of methanol occurs almost continuously, albeit at different rates, from the beginning of the TG-run until the programme temperature has reached 260–280 °C. It appears that a final loss of methanol at this point triggers the final decomposition of the sample, and this suggests that some methanol may be coordinated to sodium or copper in the (largely) desolvated material.

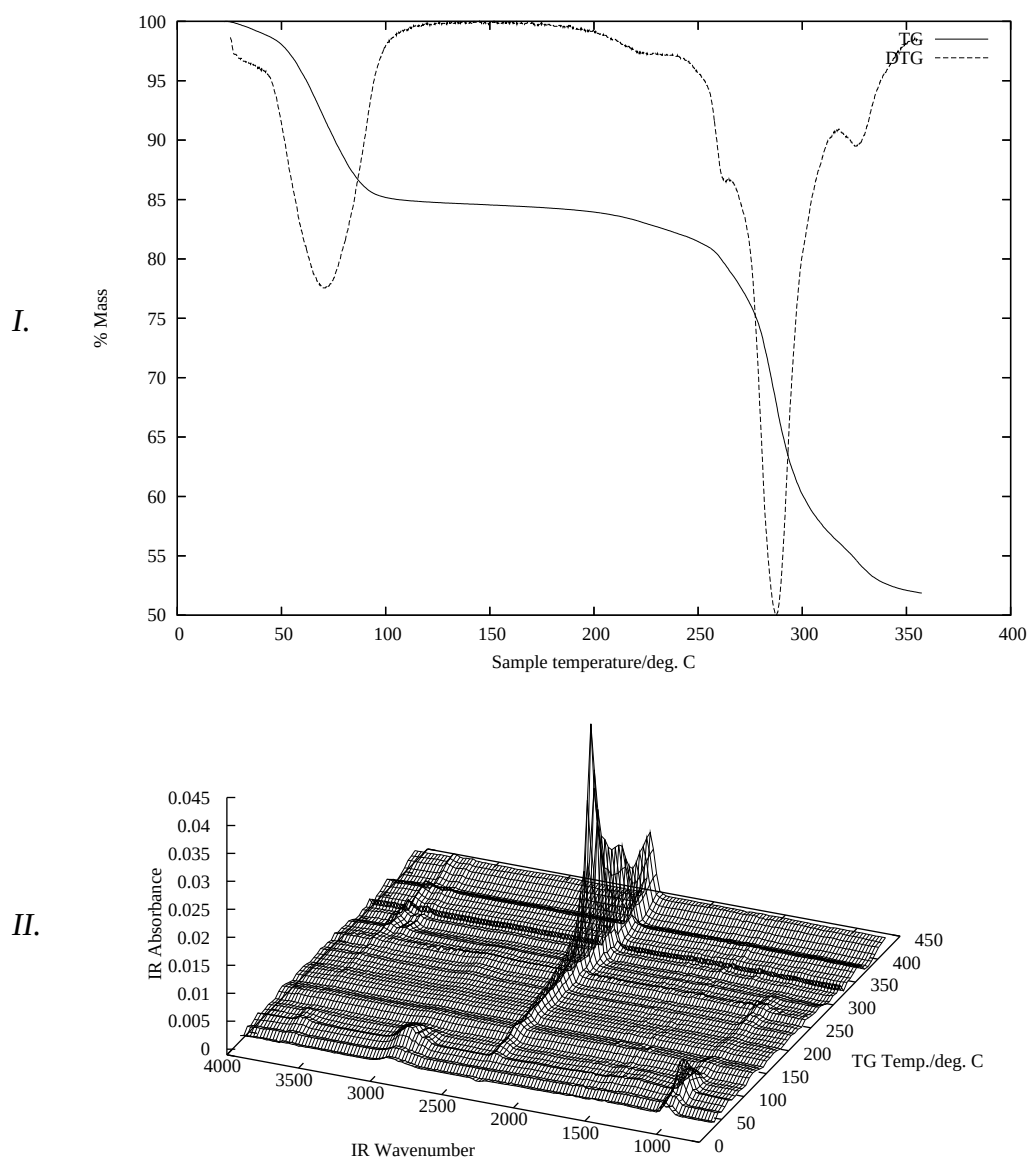


Figure 5.8: TG and derivative TG curves (I) and corresponding time-resolved infrared spectra of the evolved gas (II) of **xut-cu-b4c-acet-xtals**, previously dehydrated ($25\text{ }^{\circ}\text{C}$ – $150\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 27 ml min^{-1}) and exposed overnight to saturated methanol vapour. The resolved material was heated in the TG ($25\text{ }^{\circ}\text{C}$ – $350\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 100 ml min^{-1} total purge). The final TG mass reading was 51.9 %. On the stack-plot, II, the interval from $350\text{ }^{\circ}\text{C}$ to $450\text{ }^{\circ}\text{C}$ is plotted only to overcome the lag between the the TG and IR responses, owing to the length of the connecting tube. **Linear IR wavenumber scale.**

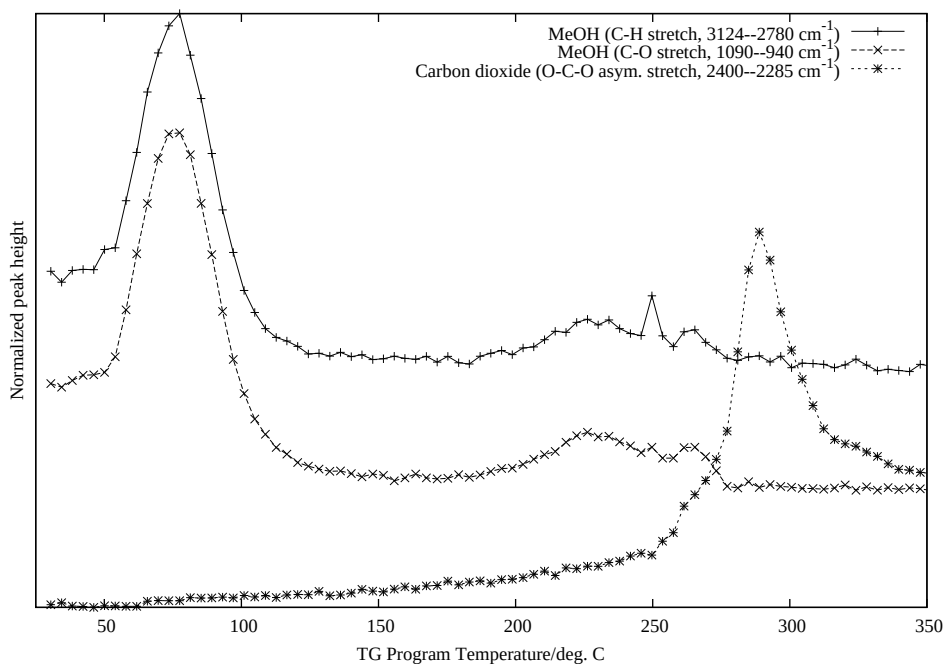


Figure 5.9: Normalized intensity–TG temperature profiles for TG-FTIR of **xut-cu-b4c-acet-xtals**, previously dehydrated and exposed to saturated methanol vapour, showing two characteristic absorbance profiles for methanol (cf. [1, p. 63]) and one for carbon dioxide (cf. [4, p. 90]). The profiles were straightened by linear subtraction.

The DSC curve of the main decomposition step in Figure 5.10 (p. 161) is considerably more complex than the one reported for the parent material in Figure 4.3 (p. 84), and the weak broad endotherm in the region 235–280 °C corresponds to the loss of methanol in the TG-FTIR curves.

In summary, the results indicate that methanol, taken into a structure that had been dehydrated by heating to 150 °C, remains in this structure until it is heated to about 260–280 °C. The methanol remaining in the structure after the main desolvation peak at 45–125 °C is thus trapped in some way during the collapse of the structure accompanying the main desolvation step, either by the physical effect of the framework collapsing, or by changes in binding concomitant with structural collapse (for example, coordination of methanol to sodium or perhaps to copper).

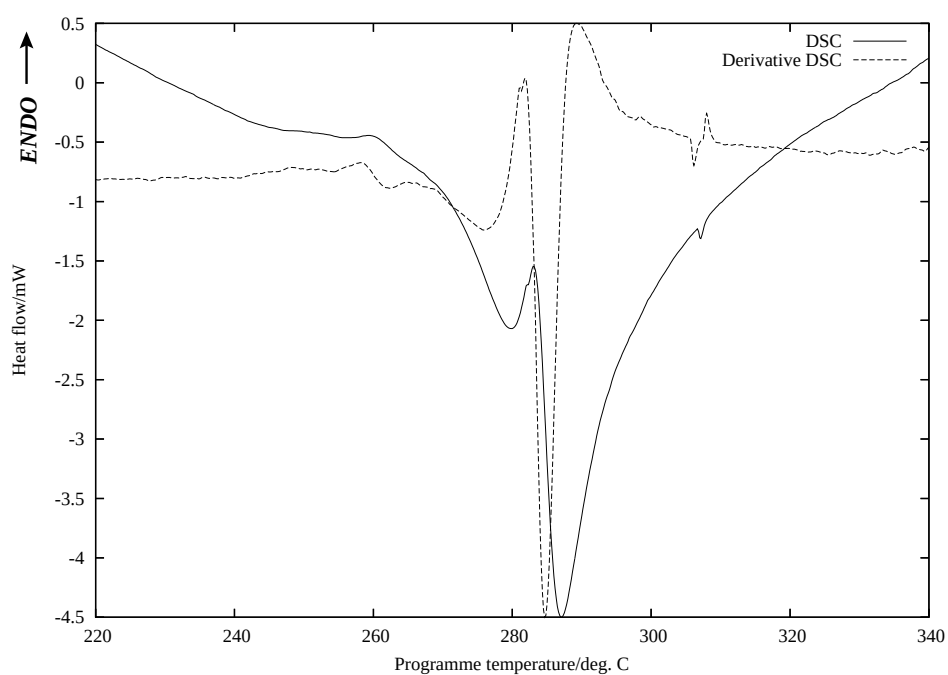


Figure 5.10: Complex DSC response for the decomposition of **xut-cu-b4c-acet-xtals**, previously dehydrated and exposed to saturated methanol vapour. The sample was heated at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen purge (26 ml min^{-1}).

5.3.3 Single desolvation-resolution: ethanol

The sample was crushed lightly and a small quantity (3.381 mg) was packed into an aluminium DSC pan and covered with a lid (not crimped). The sample was then subjected to the following treatment:

1. Heating from 25 °C to 150 °C under nitrogen purge (26 ml min⁻¹ to drive off water. The sample mass after heating corresponded to 78.3 % of the original sample mass.
2. Exposure to saturated ethanol vapour (25°C) for approximately 24 hours in total. The mass of the sample after exposure corresponded to 96.72 % of the original sample mass.

The sample was removed for examination by X-ray powder diffraction. More samples were dried as above to obtain a dehydrated sample for X-ray diffraction, and to obtain samples for TG-FTIR studies.

Figure 5.11 (p. 163) shows the X-ray diffraction patterns of the untreated, dehydrated and resolvated samples. As found for samples resolvated in methanol vapour (compare Section 5.3.2, p. 151), the material resolvated in ethanol vapour has a structure very similar to that of the untreated material, with the X-ray diffraction pattern again showing slightly broader peaks for the resolvated material than for the untreated parent material.

The mass data for the resolution of this material showed greater variability for ethanol than for methanol, and the process was much slower for ethanol than for methanol. The vapour pressure of ethanol is only about half that of methanol at room temperature (as calculated using the method and data given in [5, p. 5.30 *et seq.*]), but the greater size of ethanol relative to the pore-size of the dehydrated material must also play a role. The poor reproducibility of the resolvated mass may be related to variations in sample-handling and packing.

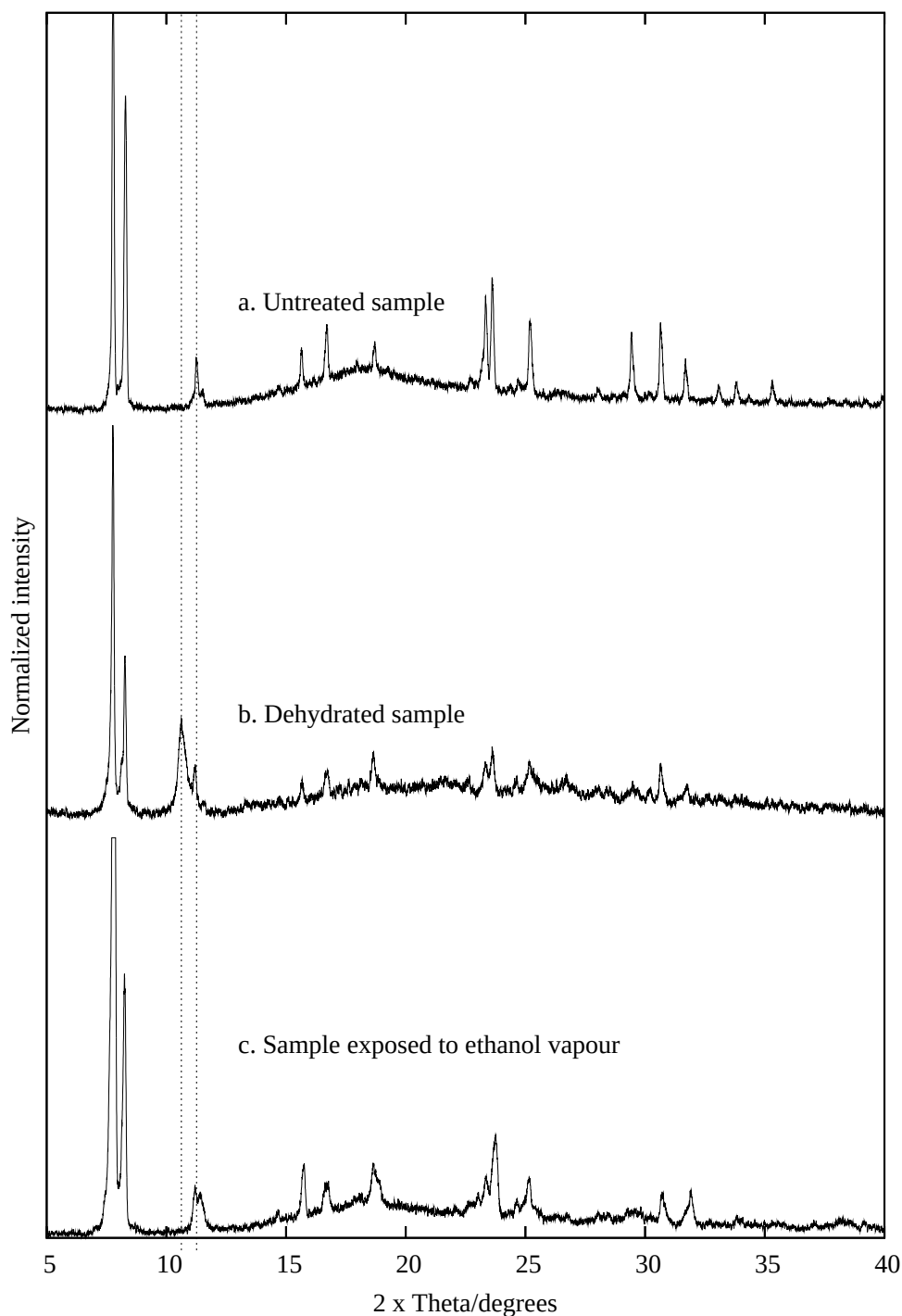


Figure 5.11: X-ray diffraction patterns of **xut-cu-b4c-acet-xtals** (a) without pre-treatment, (b) after dehydration by heating in a DSC from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen (26 ml min⁻¹) and (c) after exposure of the dehydrated material to ethanol vapour for 24 hours. The dotted lines indicate major peak-shifts. The samples were all pre-coated with a thin layer of a 4:1 mixture of paraffin oil and petroleum ether.

Figures 5.12 and 5.13 (pp. 165 & 166) show the TG-FTIR results for the material resolvated in ethanol². As found for the material resolvated in methanol (see Section 5.3.2, p. 151), infrared absorbances characteristic of ethanol can be seen in the evolved gas analysis results both in the initial desolvation step and also just prior to the main decomposition at TG programme temperatures of 190–250 °C. Because of the variability in the final mass in the resolvated compounds, no strong quantitative meaning can be ascribed to the TG information, but the overall trends are the same for the material resolvated in ethanol as for that in methanol. The main decomposition step, beginning at about 190 °C, is very complex, consisting of as many as five incompletely resolved stages, and is significantly broader than for methanol. The evolved gas analysis signals were much weaker for ethanol than those shown above for methanol. The background for this scan was problematic in the carbon dioxide region, which was exacerbated by the weakness of the signal in general.

The DSC and derivative DSC curves for ethanol being driven off a sample of material which had been previously dehydrated and exposed to saturated ethanol vapour, is shown in Figure 5.14 (p. 167). There are significant differences between these and the DSC responses for the parent material in Figure 4.3 (p. 84), and there are strong contributions from ethanol being given off in the complicated main decomposition curve at temperatures higher than 200 °C. Although the TG-FTIR results (Figures 5.12–5.13, pp. 165–166) clearly indicate loss of ethanol prior to 100 °C, the DSC responses (Figure 5.14, p. 167) in this region are too weak and broad to interpret.

²The mass of the resolvated sample for this run corresponded to just 90.39 % of the original sample mass after about 48 hours in saturated ethanol vapour. The dehydrated sample (dehydrated mass, 78.06 % of the original sample mass) was — as was the usual method employed in this study — placed in ethanol vapour in the DSC pans in which they were dried, with the (uncrimped) lids in place to eliminate rehydration during handling, which would otherwise take place very rapidly. The rehydrated sample appeared to be somewhat inhomogeneous: the centre of the sample showed the blue colour of the dehydrated compound, while the outer region showed the blue-green colour of the parent material. The sample was left to resolvate to an approximately constant mass. It is believed that sample-size and packing play a significant role in the rate of resolution.

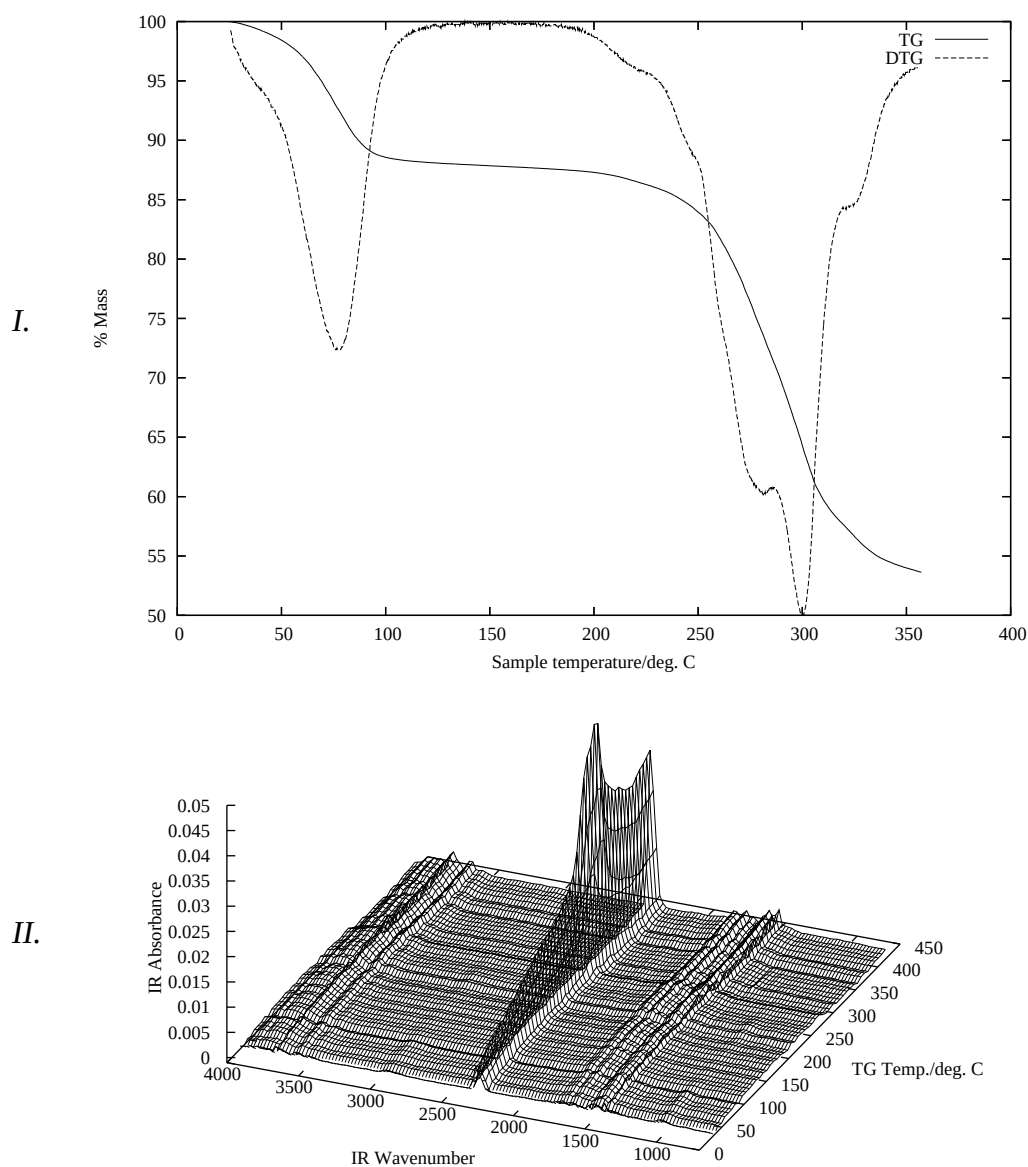


Figure 5.12: TG and derivative TG curves (I) and corresponding time-resolved infrared spectra of the evolved gas (II) of **xut-cu-b4c-acet-xtals**, previously dehydrated ($25\text{ }^{\circ}\text{C}$ – $150\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 27 ml min^{-1}) and exposed for 24 hours to saturated ethanol vapour. The resolvated material was heated in the TG ($25\text{ }^{\circ}\text{C}$ – $350\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 100 ml min^{-1} total purge). The final TG mass reading was 53.63 %. On the stack-plot, II, the interval from $350\text{ }^{\circ}\text{C}$ to $450\text{ }^{\circ}\text{C}$ is plotted only to overcome the lag between the the TG and IR responses, owing to the length of the connecting tube. **Linear IR wavenumber scale.**

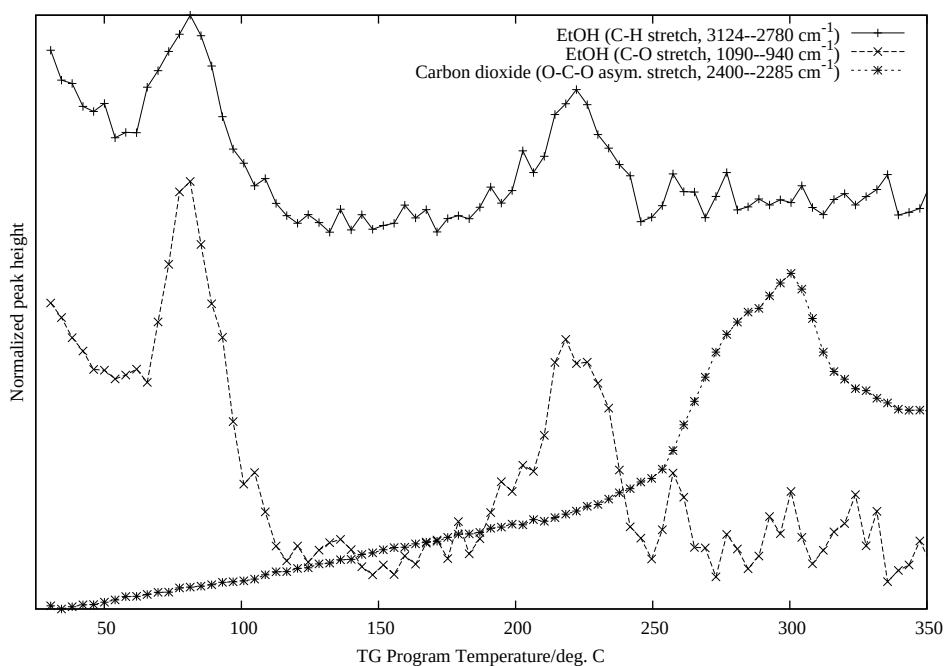


Figure 5.13: Normalized intensity–TG temperature profiles for TG-FTIR of **xut-cu-b4c-acet-xtals**, previously dehydrated and exposed to saturated ethanol vapour, showing two characteristic absorbance profiles for methanol (cf. [1, p. 63]) and one for carbon dioxide (cf. [4, p. 90]). The profiles were straightened by linear subtraction.

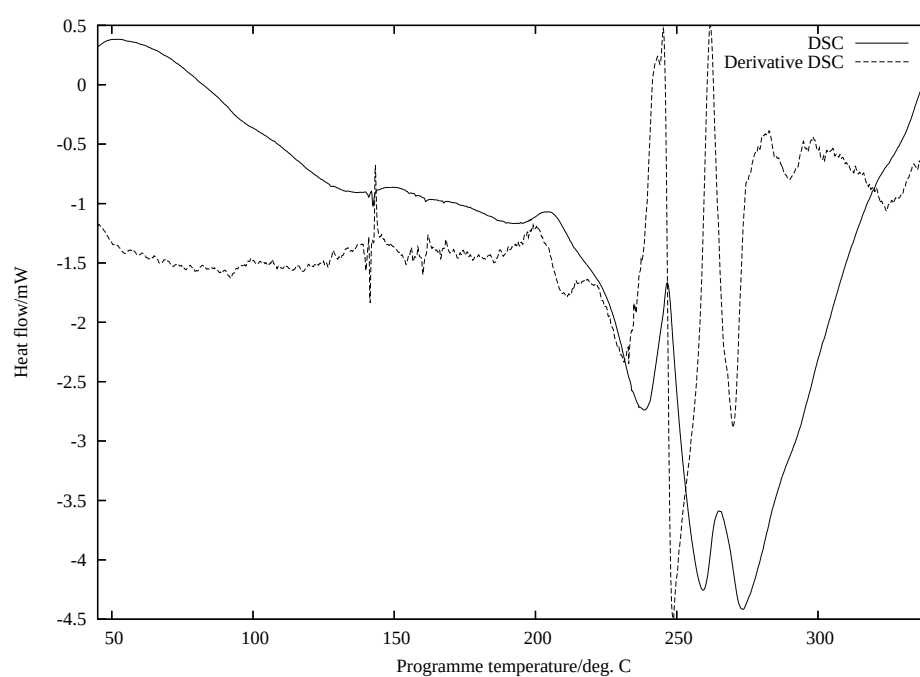


Figure 5.14: Complex DSC response for the decomposition of **xut-cu-b4c-acet-xtals**, previously dehydrated and exposed to saturated ethanol vapour. The sample was heated at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen purge (26 ml min^{-1}).

5.3.4 Single desolvation-resolution: pyridine

Similar attempts with pyridine as a potential guest species met with no success. The dehydrated samples did gain mass very slightly on exposure to pyridine vapour, but the samples were inhomogeneous in appearance. A purple tinge in part of the sample suggested coordination of pyridine to copper, which would alter the coordination sphere of the copper and potentially alter the binding holding the framework together. This investigation was not pursued further.

5.3.5 Multiple desolvation-resolution: water, water

The sample was crushed lightly and a small quantity (2.868 mg) was packed into an aluminium DSC sample pan and covered with a lid (not crimped). The sample was then subjected to the following treatment (see Table 5.1 [set 1] for details):

1. [Desolv(1)] Heating from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to drive off water.
2. [Expose(1)] Exposure to moist (i.e., open) air (25 °C) for 12 hours.
3. [Desolv(2)] Heating from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to drive off water.
4. [Expose(2)] Exposure to moist (i.e., open) air (25 °C) for 6 hours.
5. [Decomp] Heating from 25 °C to 350 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to decompose the sample.

Table 5.1: Experimental parameters and data for multiple desolvation-resolution experiments (water, water) on **xut-cu-b4c-acet-xtals**. ΔH refers, in all cases, to the enthalpy change associated with the desolvation process, per gram of the parent material.

No.	Step	Parameters		Results				
		$T_{\text{start}}/^{\circ}\text{C}$	$T_{\text{end}}/^{\circ}\text{C}$	$T_i/^{\circ}\text{C}$	$T_p/^{\circ}\text{C}$	$T_f/^{\circ}\text{C}$	$\Delta H/\text{J g}^{-1}$	$\%m_{\text{res}}$
SET 1								
1.	Desolv(1)	25	150	78.4	113.8	123.3	420.5	77.86
2.	Expose(1)	Guest= H ₂ O, as moist air (12 hours)						99.86
3.	Desolv(2)	25	150	76.6	113.0	122.3	428.4	76.60
4.	Expose(2)	Guest= H ₂ O, as moist air (6 hours)						99.58
5.	Decomp	25	350	74.8	113.0	122.5	427.3	49.30
SET 2								
1.	Desolv(1)	25	150	79.2	115.5	125.3	423.3	77.98
2.	Expose(1)	Guest= H ₂ O, as moist air (12 hours)						99.68
3.	Desolv(2)	25	150	77.6	115.5	125.4	442.0	77.82
4.	Expose(2)	Guest= H ₂ O, as moist air (6 hours)						99.78

The DSC and derivative DSC curves (Figure 5.15, p.171) show that the DSC responses after one and two cycles of dehydration with subsequent re-hydration (curves b & c) are very similar to those for the original dehydration of the untreated sample (curve a). The DSC curves are practically superimposable, with only very slight differences in onset, peak and final temperatures (T_i , T_p and T_f , respectively).

The ΔH for the dehydration of the untreated material (step Desolv(1), curve a) is slightly smaller than the ΔH for the two subsequent dehydrations (steps Desolv(2) & Decomp, curves b & c) whose ΔH values are very close to each other. By contrast, the mass data shows that the mass of water absorbed during each of the two re-hydration (steps Expose(1) and Expose(2)) is slightly less than the mass of water driven off in the first dehydration of the untreated sample (step Desolv(1)). The mass effects may be attributed to the loss of moisture — in the form of condensation owing to storage of the sample in a refrigerator — prior to the main dehydration of the untreated sample. Although the small increase in ΔH from the first to the final dehydration may, in principle, be attributable to greater compaction of the sample during handling between DSC runs, with consequent improvement in thermal contact between the DSC furnace and the sample material, this trend in the thermal data was not always observed.

The reproducibility of the thermal responses for duplicate sets of runs was not of the highest order. Differences of up to 3.4 % for corresponding ΔH values were observed. These differences are significantly greater than one would expect for repeated runs with a standard calibrant with this instrument, and could be related to inevitable variations in grinding and packing the samples, to the effect of variations in the purging rate, and to the subjectiveness of the process by which the temperature and enthalpy data are extracted from the DSC curves. As far as could be determined, the thermal information suggests that the sample is unchanged by cycles of dehydration and re-hydration.

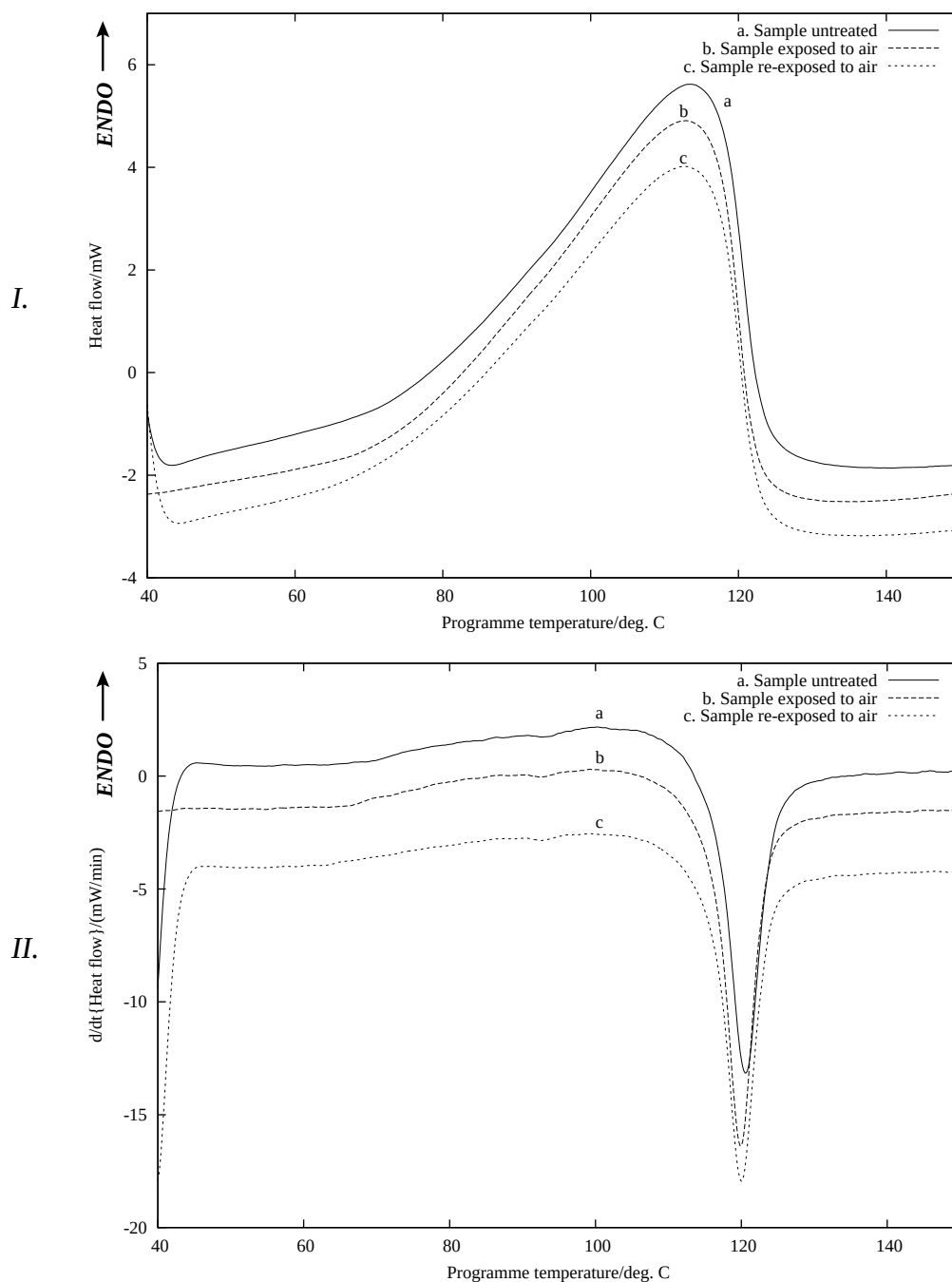


Figure 5.15: DSC (*I*) and derivative DSC (*II*) curves of **xut-cu-b4c-acet-xtals** (a) for the initial desolvation (water) (Desolv(1)), (b) for the second desolvation (water) (Desolv(2)), and (c) for the final desolvation (water) and subsequent decomposition (Decomp). See Table 5.1 for details. All DSC curves were obtained under nitrogen purge (27 ml min^{-1}).

Steps Desolv(1)–Expose(2) were repeated on a new sample (Table 5.1 [set 2], p. 169) in order to obtain a sample of the material obtained after step Expose(2) for examination by XRPD. The X-ray diffraction pattern is shown, with others for comparison, in Figure 5.16 (p. 173). Within the limits of reproducibility inherent in the method, there is a clear peak-for-peak correspondence between the X-ray diffraction patterns of the untreated material (curve a), the material after one cycle of dehydration and rehydration (curve c) and the material after two such cycles (curve d). Some peak-broadening is evident in curves c and d, but no trace of the peak under the leftmost dotted line (curve b) — observed for the dehydrated sample, and believed to be due to partial collapse of the structure on dehydration — is observable in these curves. Thus the framework appears to survive the dehydration–rehydration cycles largely intact. The peak-broadening observed may be due to larger-scale effects such as damage to the crystalline particles during the escape of the guest molecules, and differences in grinding from one sample to the next.

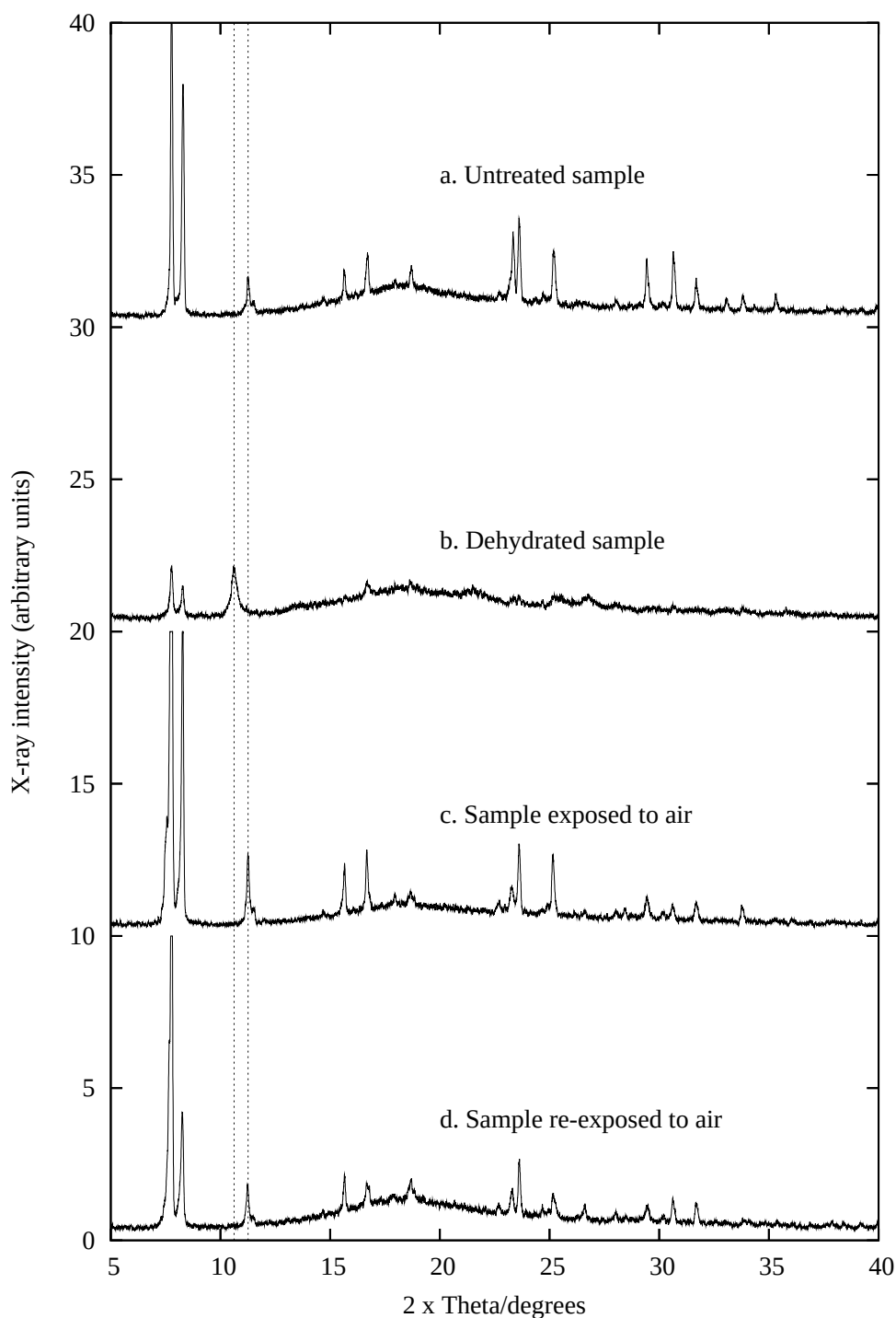


Figure 5.16: X-ray diffraction patterns of **xut-cu-b4c-acet-xtals** (a) without pre-treatment, (b) dehydrated by heating in a DSC ($25\text{ }^{\circ}\text{C}$ – $150\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 27 ml min^{-1}), (c) dehydrated sample ($25\text{ }^{\circ}\text{C}$ – $150\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 27 ml min^{-1}) exposed to moist air, and (d) a sample treated as in c, dehydrated again, ($25\text{ }^{\circ}\text{C}$ – $150\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 27 ml min^{-1}) and exposed to moist air. Pattern b was obtained with the sample under a thin layer of paraffin oil, and all others under a thin layer of a 4:1 mixture of paraffin oil and petroleum ether.

5.3.6 Multiple desolvation-resolution: water, methanol

The sample was crushed lightly and a small quantity (3.502 mg) was packed into an aluminium DSC sample pan and covered with a lid (not crimped). The sample was then subjected to the following treatment (see Table 5.2 [set 1] for details):

1. [Desolv(1)] Heating from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to drive off water.
2. [Expose(1)] Exposure to moist (i.e., open) air for 12 hours.
3. [Desolv(2)] Heating from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to drive off water.
4. [Expose(2)] Exposure to saturated methanol vapour (25 °C) for 6 hours.
5. [Decomp] Heating from 25 °C to 350 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to decompose the sample.

Table 5.2: Experimental parameters and data for multiple desolvation-resolution experiments (water, methanol) on **xut-cu-b4c-acet-xtals**. ΔH refers, in all cases, to the enthalpy change associated with the desolvation process, per gram of the parent material.

No.	Step	Parameters		Results				
		$T_{\text{start}}/^{\circ}\text{C}$	$T_{\text{end}}/^{\circ}\text{C}$	$T_i/^{\circ}\text{C}$	$T_p/^{\circ}\text{C}$	$T_f/^{\circ}\text{C}$	$\Delta H/\text{J g}^{-1}$	$\%m_{\text{res}}$
SET 1								
1.	Desolv(1)	25	150	81.0	118.3	129.3	432.2	78.01
2.	Expose(1)	Guest= H ₂ O, as moist air (12 hours)						99.54
3.	Desolv(2)	25	150	78.9	117.2	127.9	431.5	76.96
4.	Expose(2)	Guest= MeOH, saturated vapour(6 hours)						96.09
5.	Decomp	25	350	65.2	100.3	131.0	147.7	50.46
SET 2								
1.	Desolv(1)	25	150	79.0	116.3	126.7	439.3	77.80
2.	Expose(1)	Guest= H ₂ O, as moist air (12 hours)						99.62
3.	Desolv(2)	25	150	79.9	116.3	126.5	423.7	77.68
4.	Expose(2)	Guest= MeOH, saturated vapour(6 hours)						96.11

As found before, the thermal responses, shown in Figure 5.17 (p. 176), for the dehydration of the untreated material (step Desolv(1), curve a) and the rehydrated material (step Desolv(2), curve b) were very similar. Upon further dehydration and exposure to methanol vapour (steps Desolv(2) & Expose(2)), significantly less mass was gained than on exposure to water vapour. A final heating cycle (step Decom) revealed a much weaker, much broader endotherm (curve c), attributed to methanol being driven from the sample. Although the mass gained on exposure to methanol (step Expose(2)) was approximately 80 % of the mass of water lost in the dehydration of the untreated sample (step Desolv(1)), the ΔH value for desolvation of methanol (step Decom) was only about 34 % of that obtained in the first dehydration.

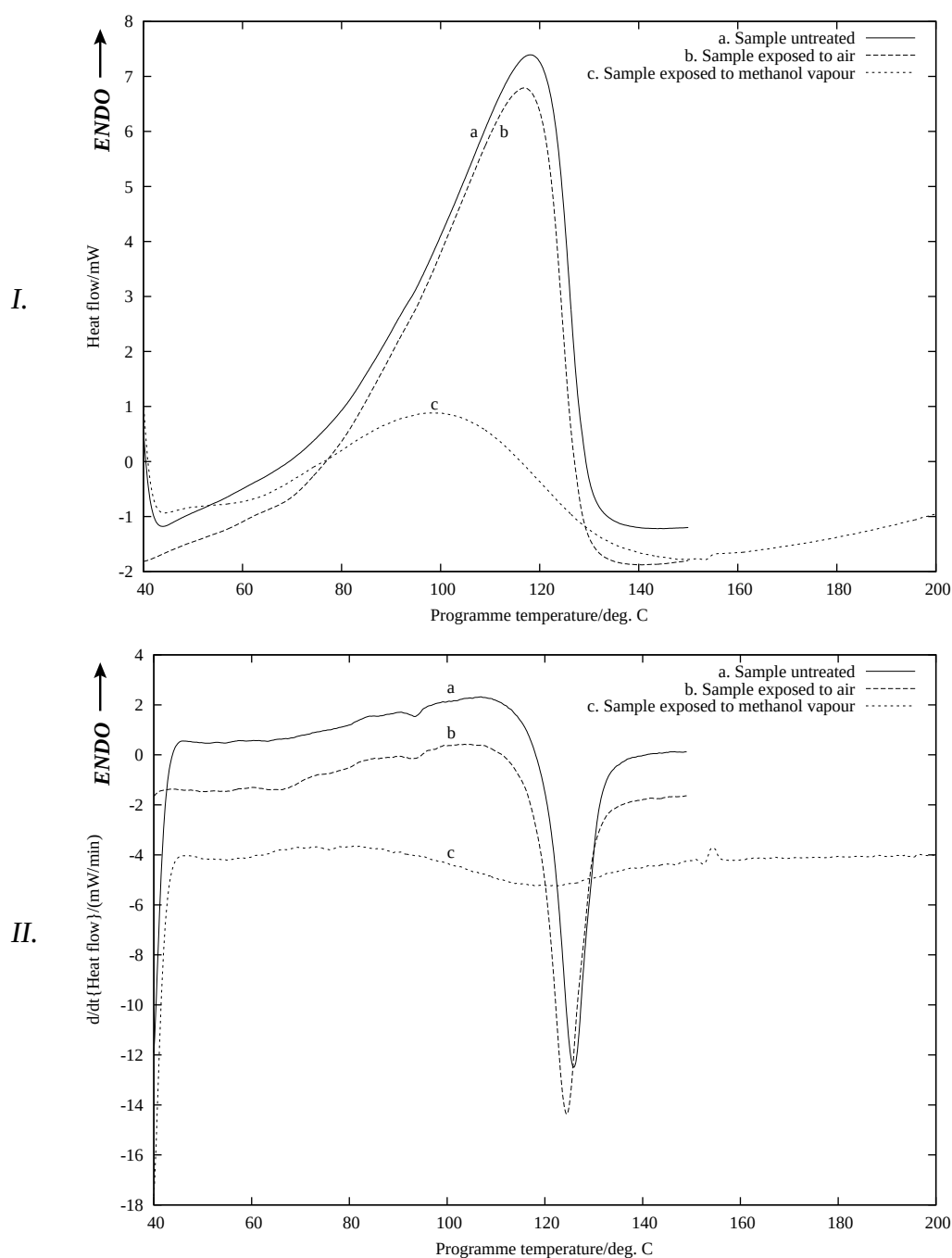


Figure 5.17: DSC (*I*) and derivative DSC (*II*) curves of **xut-cu-b4c-acet-xtals** (a) for the initial desolvation (water) (Desolv(1)), (b) for the second desolvation (water) (Desolv(2)), and (c) for the final desolvation (methanol) and subsequent decomposition (Decomp). See Table 5.2 for details. All DSC curves were obtained under nitrogen purge (27 ml min^{-1}).

Steps Desolv(1)–Expose(2) were repeated on a new sample (Table 5.2 [set 2], p. 174) to obtain a sample of the material obtained after step Expose(2) for examination by XRPD. The X-ray diffraction pattern is shown, with others for comparison, in Figure 5.18 (p. 178). As found before, the X-ray diffraction pattern of the untreated material (curve a) was very similar to the pattern of the material after dehydration and exposure to moist air (curve c), and to that of the material after a second dehydration and exposure to methanol vapour (curve d). This, together with the fact that in curves a, c and d, no peak was observed under the leftmost dotted line (cf. curve b, dehydrated material), suggests that the structure survives two cycles of desolvation and resolution, and that the structure of the final material is very similar to that of the untreated material. There is minor peak broadening in curves c and d, perhaps suggesting that damage to the crystallites occurs during successive dehydration–resolution cycles.

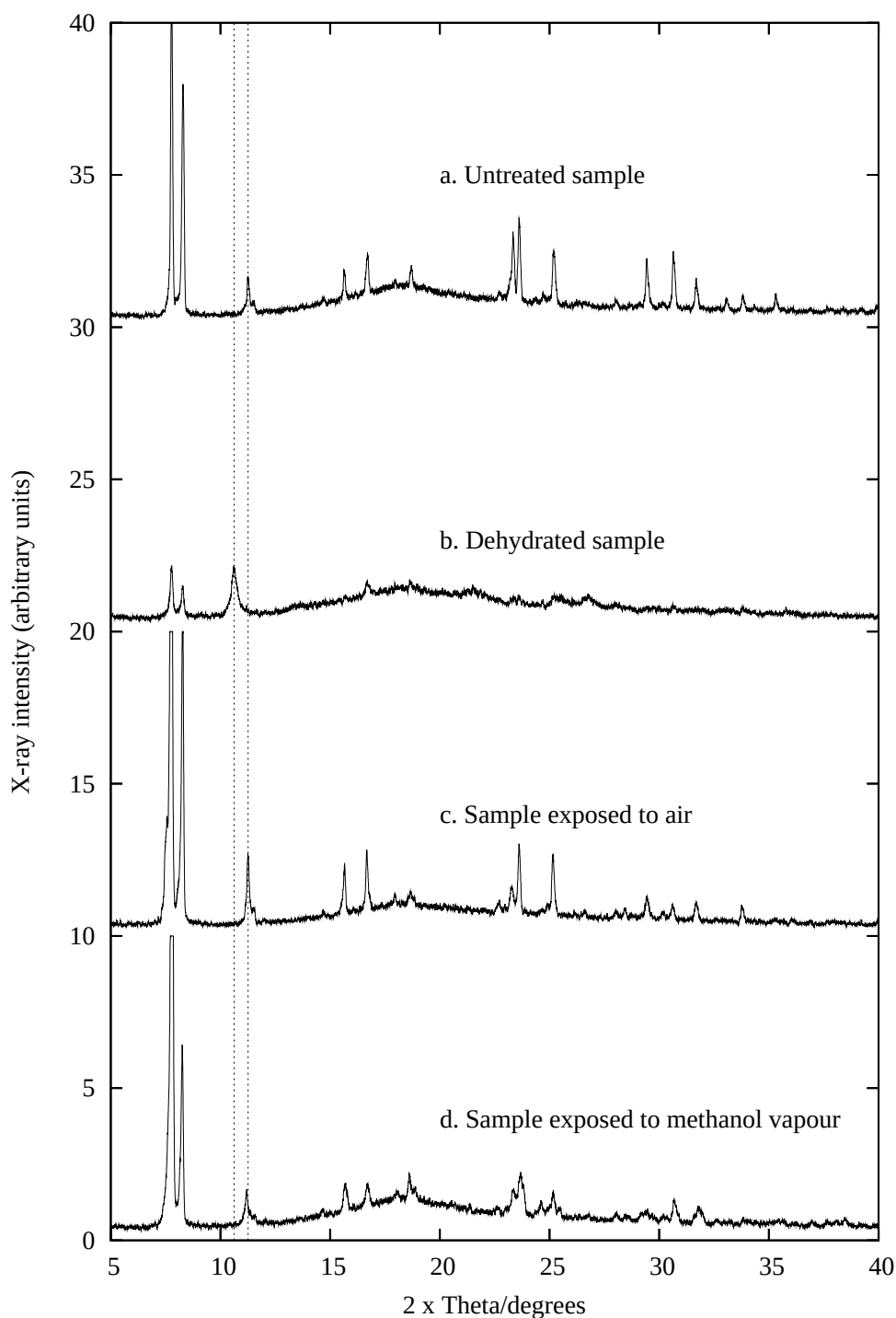


Figure 5.18: X-ray diffraction patterns of **xut-cu-b4c-acet-xtals** (a) without pre-treatment, (b) dehydrated by heating in a DSC ($25\text{ }^{\circ}\text{C}$ – $150\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 27 ml min^{-1}), (c) dehydrated sample ($25\text{ }^{\circ}\text{C}$ – $150\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 27 ml min^{-1}) exposed to moist air, and (d) a sample treated as in c, dehydrated ($25\text{ }^{\circ}\text{C}$ – $150\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen, 27 ml min^{-1}) and exposed to methanol vapour. Pattern b was obtained with the sample under a thin layer of paraffin oil, and all others under a thin layer of a 4:1 mixture of paraffin oil and petroleum ether.

5.3.7 Multiple desolvation-resolution: methanol, methanol

The sample was crushed lightly and a small quantity (3.082 mg) was packed into an aluminium DSC sample pan and covered with a lid (not crimped). The sample was then subjected to the following treatment (see Table 5.3 [set 1] for details):

1. [Desolv(1)] Heating from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to drive off water.
2. [Expose(1)] Exposure to saturated methanol vapour (25 °C) for 12 hours.
3. [Desolv(2)] Heating from 25 °C to 200 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to drive off methanol.
4. [Expose(2)] Exposure to saturated methanol vapour (25 °C) for 6 hours.
The mass of the sample after exposure was 2.972 mg, corresponding to 96.43 % of the original sample mass.
5. [Decomp] Heating from 25 °C to 350 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to decompose the sample.

The mass gained after the initial dehydration (step Desolv(1)) and first exposure to methanol (step Expose(1)) was 83 % of the mass lost in the initial dehydration, and the ΔH attributed to desolvation of methanol (step Desolv(2)) was 40 % of that corresponding to the loss of water in the original dehydration (step Desolv(1)). Despite heating to the higher temperature of 200 °C in step Desolv(2), a comparison of the residual sample masses after this step and after the initial dehydration (step Desolv(1)) showed that not all the methanol was driven off. This was also evident in the TG-FTIR results discussed in Section 5.3.2, p. 151.

Table 5.3: Experimental parameters and data for multiple desolvation-resolution experiments (methanol, methanol) on **xut-cu-b4c-acet-xtals**. ΔH refers, in all cases, to the enthalpy change associated with the desolvation process, per gram of the parent material.

No.	Step	Parameters		Results				
		$T_{\text{start}}/^{\circ}\text{C}$	$T_{\text{end}}/^{\circ}\text{C}$	$T_i/^{\circ}\text{C}$	$T_p/^{\circ}\text{C}$	$T_f/^{\circ}\text{C}$	$\Delta H/\text{J g}^{-1}$	$\%m_{\text{res}}$
SET 1								
1.	Desolv(1)	25	150	77.5	115.0	124.6	432.2	78.13
2.	Expose(1)	Guest= MeOH, saturated vapour(12 hours)						96.30
3.	Desolv(2)	25	200	63.6	98.0	127.3	172.3	79.66
4.	Expose(2)	Guest= MeOH, saturated vapour(6 hours)						96.43
5.	Decomp	25	350	63.9	101.7	128.0	210.1	48.48
SET 2								
1.	Desolv(1)	25	150	81.0	117.8	127.8	425.2	78.34
2.	Expose(1)	Guest= MeOH, saturated vapour(12 hours)						96.42
3.	Desolv(2)	25	200	60.4	100.2	129.4	195.8	79.83
4.	Expose(2)	Guest= MeOH, saturated vapour(6 hours)						96.53

Comparison of steps Desolv(2) and Decomp (Figure 5.19, curves b & c, p. 182) shows that the corresponding two thermal responses are not as similar to each other as the ones for repeated dehydration in Section 5.3.5 (p. 168). The peak temperature in step Decomp (curve c) is shifted nearly four degrees to higher temperatures, and the ΔH is 18 % higher than in step Desolv(2) (curve b). There is also relatively poor agreement between the ΔH values of these desolvation events and the ones corresponding to methanol being driven off in Section 5.3.6, step Decomp (p. 174) and Section 5.3.8, step Desolv(2) (p. 184).

Steps Desolv(1)–Expose(2) were repeated on a new sample (Table 5.3 [set 2], p. 180) to obtain a sample of the material obtained after step Expose(2) for examination by XRPD. The X-ray diffraction pattern is shown, with others for comparison, in Figure 5.20 (p. 183). Apart from differences in peak-broadening, the X-ray diffraction patterns of the samples after one and two cycles of desolvation and exposure to methanol vapour (curves c and d, respectively) are very similar to each other, and very similar to that of the original material (curve a). Peak intensities decrease slightly from one cycle to the next, perhaps because of damage to crystallites during desolvation–exposure cycles. It would appear from XRPD evidence that the sample survives, for the most part, multiple cycles of desolvation and exposure to methanol.

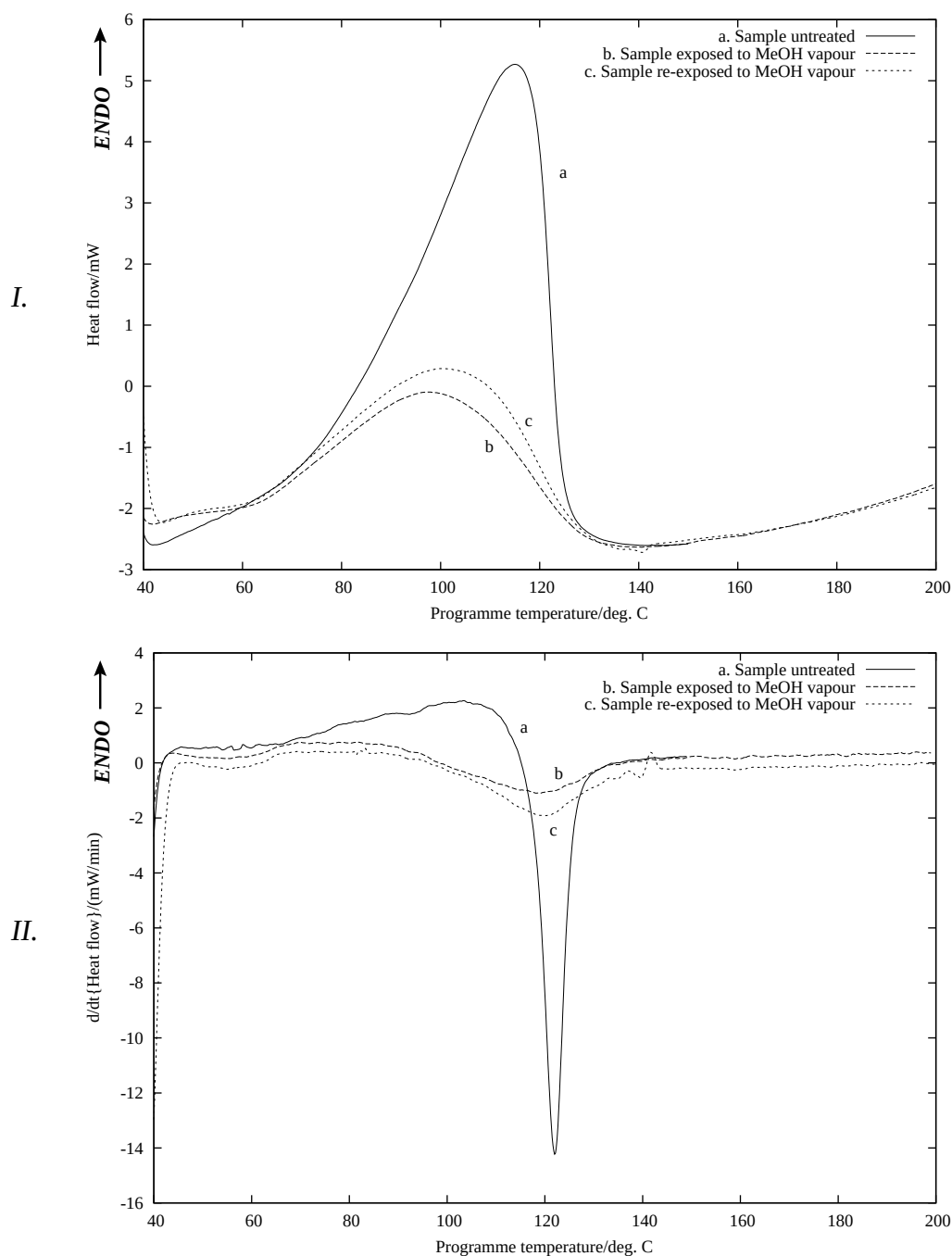


Figure 5.19: DSC (*I*) and derivative DSC (*II*) curves of **xut-cu-b4c-acet-xtals** (a) for the initial desolvation (water) (Desolv(1)), (b) for the second desolvation (methanol) (Desolv(2)), and (c) for the final desolvation (methanol) and subsequent decomposition (Decomp). See Table 5.3 for details. All DSC curves were obtained under nitrogen purge (27 ml min^{-1}).

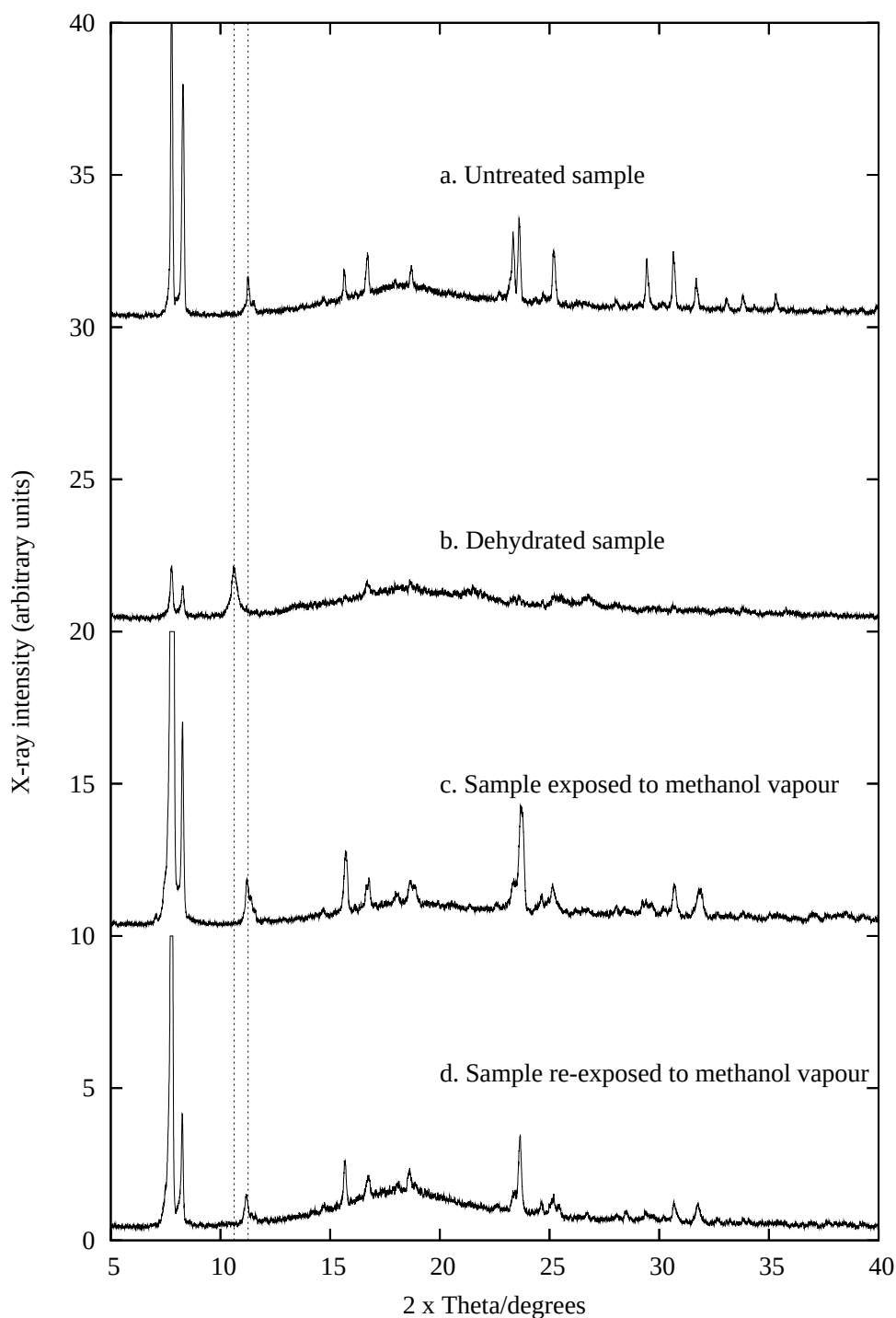


Figure 5.20: X-ray diffraction patterns of **xut-cu-b4c-acet-xtals** (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹), (c) dehydrated sample (25 °C–150 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹) exposed to methanol vapour, and (d) a sample treated as in c, desolvated, (25 °C–200 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹) and exposed to methanol vapour. Pattern b was obtained with the sample under a thin layer of paraffin oil, and all others under a thin layer of a 4:1 mixture of paraffin oil and petroleum ether.

5.3.8 Multiple desolvation-resolution: methanol, water

The sample was crushed lightly and a small quantity (3.292 mg) was packed into an aluminium DSC sample pan and covered with a lid (not crimped). The sample was then subjected to the following treatment (see Table 5.4 [set 1] for details):

1. [Desolv(1)] Heating from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to drive off water.
2. [Expose(1)] Exposure to saturated methanol vapour (25 °C) for 12 hours.
3. [Desolv(2)] Heating from 25 °C to 200 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to drive off methanol.
4. [Expose(2)] Exposure to moist (i.e., open) air for 6 hours.
5. [Decomp] Heating from 25 °C to 350 °C at 10 °C min⁻¹ under nitrogen purge (27 ml min⁻¹) to decompose the sample.

Table 5.4: Experimental parameters and data for multiple desolvation-resolution experiments (methanol, water) on **xut-cu-b4c-acet-xtals**. ΔH refers, in all cases, to the enthalpy change associated with the desolvation process, per gram of the parent material.

No.	Step	Parameters		Results				
		$T_{\text{start}}/^{\circ}\text{C}$	$T_{\text{end}}/^{\circ}\text{C}$	$T_i/^{\circ}\text{C}$	$T_p/^{\circ}\text{C}$	$T_f/^{\circ}\text{C}$	$\Delta H/\text{J g}^{-1}$	$\%m_{\text{res}}$
SET 1								
1.	Desolv(1)	25	150	79.0	115.0	124.5	414.2	77.89
2.	Expose(1)	Guest= MeOH, saturated vapour (12 hours)						96.26
3.	Desolv(2)	25	200	66.9	97.0	127.4	148.5	78.34
4.	Expose(2)	Guest= H ₂ O, as moist air (6 hours)						99.33
5.	Decomp	25	350	82.1	117.5	126.4	415.4	49.54
SET 2								
1.	Desolv(1)	25	150	74.0	111.0	120.8	436.9	78.00
2.	Expose(1)	Guest= MeOH, saturated vapour (12 hours)						96.41
3.	Desolv(2)	25	200	61.5	100.3	129.6	186.07	79.86
4.	Expose(2)	Guest= H ₂ O, as moist air (6 hours)						99.48

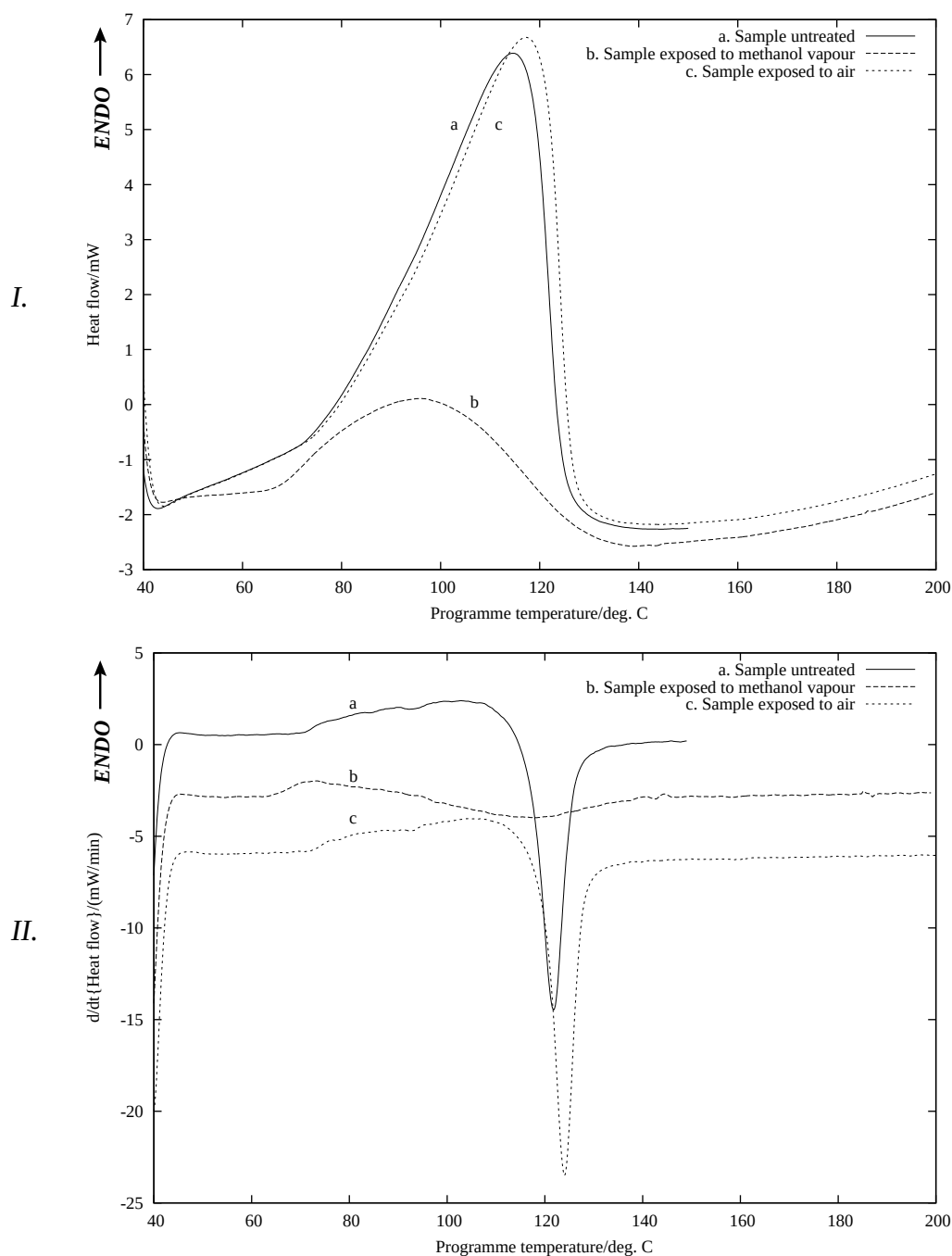


Figure 5.21: DSC (*I*) and derivative DSC (*II*) curves of **xut-cu-b4c-acet-xtals** (a) for the initial desolvation (water) (Desolv(1)), (b) for the second desolvation (methanol) (Desolv(2)), and (c) for the final desolvation (water) and subsequent decomposition (Decomp). See Table 5.4 for details. All DSC curves were obtained under nitrogen purge (27 ml min^{-1}).

The DSC and derivative DSC curves in Figure 5.21 (p. 185) show similar trends to those noted above. After dehydration (step Desolv(1), curve a) and exposure to methanol vapour (step Expose(1)), the sample regained approximately 84 % of the mass lost during the initial dehydration.

The DSC and derivative DSC responses for methanol being driven off (Desolv(2), curve b) show the same broad, relatively weak endotherm as was observed in Sections 5.3.6 and 5.3.7 (pp. 174 & 179, respectively).

After subsequent desolvation and exposure to moist air (Desolv(2) & Expose(2)), the mass returned to nearly the original sample mass. The DSC response for water being driven off (step DeComp, curve c) is nearly superimposable with that of the initial dehydration (curve a). The peak temperature of curve c is shifted slightly to higher temperatures, compared to the responses reported for repeated dehydration-re-hydration (Section 5.3.5, p. 168).

Steps Desolv(1)–Expose(2) were repeated on a new sample (Table 5.4 [set 2], p. 184) to obtain a sample of the material obtained after step Expose(2) for examination by XRPD. The X-ray diffraction pattern of this sample is shown, together with others for comparison, in Figure 5.22 (p. 187). The X-ray diffraction patterns of a sample which had been dehydrated and exposed to methanol (curve c), and a sample which had been treated in the same way with subsequent dehydration and exposure to water vapour (curve d), are very similar, except for differences in peak-broadening and some differences in peak intensity. These may be due to damage to the crystallites during repeated cycles of desolvation and exposure to methanol and moist air. It would appear, from X-ray diffraction evidence, that these structures are very similar to each other, and to the untreated sample (curve a).

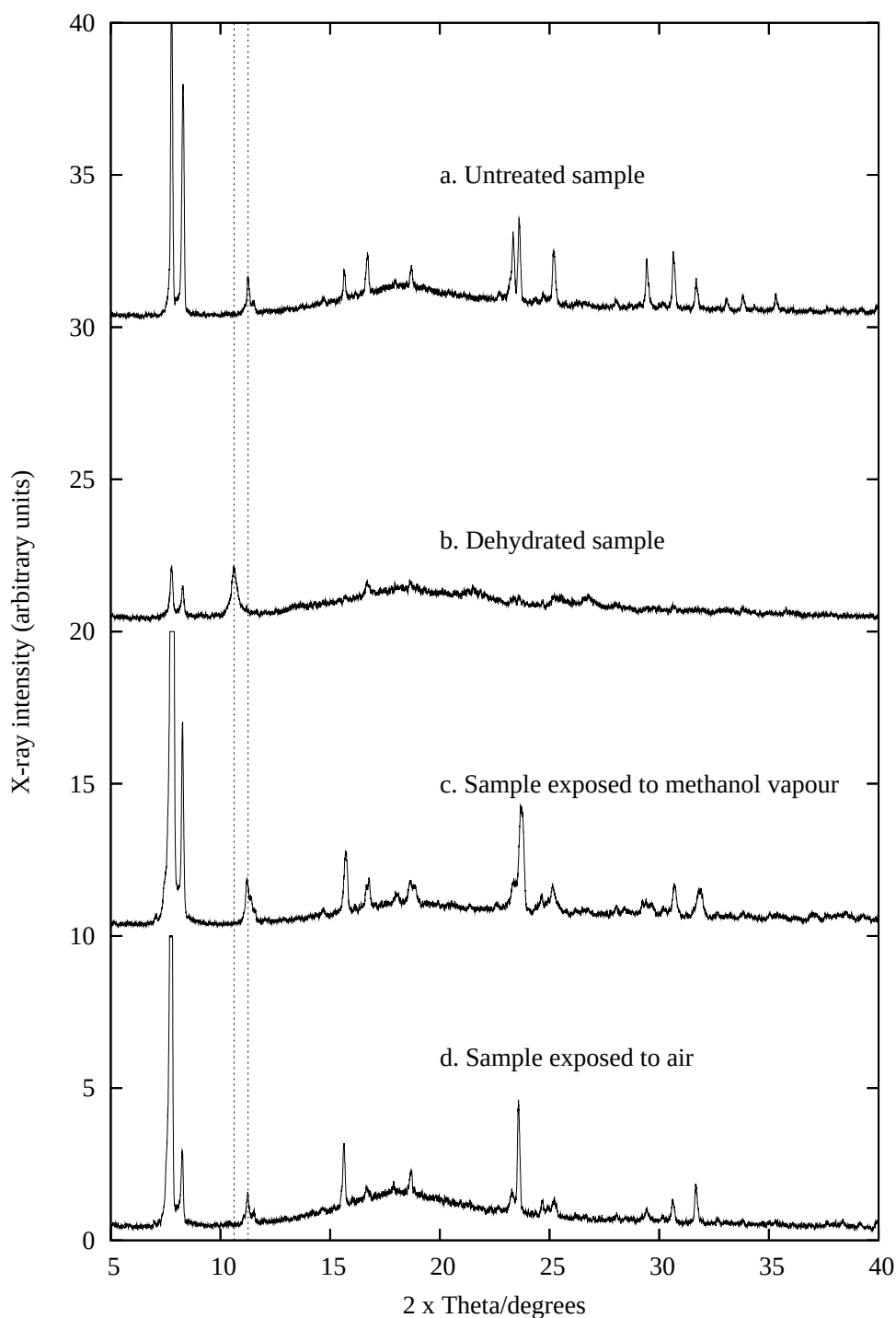


Figure 5.22: X-ray diffraction patterns of **xut-cu-b4c-acet-xtals** (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹), (c) dehydrated sample (25 °C–150 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹) exposed to methanol vapour, and (d) a sample treated as in c, desolvated, (25 °C–200 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹) and exposed to moist air. Pattern b was obtained with the sample under a thin layer of paraffin oil, and all others under a thin layer of a 4:1 mixture of paraffin oil and petroleum ether.

5.3.9 Discussion

It is clear from the above that the covalent three-dimensional metal-organic framework **xut-cu-b4c-acet-xtals** has the following properties:

- the structure collapses on dehydration, as indicated by XRPD evidence;
- on exposure of the dehydrated material to water vapour, the original structure is, to a great extent, regained, as shown by DSC, XRPD and mid-infrared spectral evidence;
- on exposure of the dehydrated material to saturated methanol and ethanol vapours, a large uptake of these solvents occurs, and the structure of the resolvated material is similar to that of the parent, hydrated, material, as shown by DSC, XRPD and mid-infrared spectral evidence;
- on exposure to pyridine the dehydrated material does not significantly gain mass, although a colour change occurs which suggests some changes to the copper(II) coordination sphere, possibly only on the surface;
- the framework survives multiple desolvation/resolution cycles, with water and methanol as guest species, largely intact, as shown by DSC and XRPD (owing to DSC peak-broadening, multiple resolution with ethanol could not be studied); and
- on heating of the resolvated material, a small amount of the guest species remains in the structure well past the first dehydration temperature, and can be seen to be evolved right up to the final decomposition temperature, as evidenced by TG-FTIR.

The results of desolvation/resolution experiments with different guest species warrant further comment. The physical properties of the potential guest species, in the liquid phase, are summarized in Table 5.5 (p. 189). To a first approximation, each molecule within the bulk solvent may be regarded as being inside a box with the volume given under particle volume. Using the mass data for the multiple methanol resolution experiment (Section 5.3.7, p. 179), the ratio of the number of water molecules *lost* during dehydration (step 1) to the number of methanol

Table 5.5: Selected physical properties, in the liquid phase at room temperature, of potential guest species.

Substance	Density* / g cm ⁻³	Molar mass / g mol ⁻¹	Molar volume** / cm ³ mol ⁻¹	Particle volume / Å ³
Water	0.997	18.02	18.07	30.01
Methanol	0.7913	32.04	40.49	67.26
Ethanol	0.7894	46.07	58.36	96.94
Pyridine	0.9827	79.10	80.49	133.71

* Values taken from [5, pp. 5.87, 1.255 & 1.211]

** Molar volume = molar mass / density

molecules *gained* during exposure to methanol (step 2) is 2.14:1. Since the ratio of the particle volume of methanol to that of water can be calculated as 2.24:1, this implies that the pore volume of the material is slightly more than sufficient to accommodate this amount of methanol.

The TG data for this compound (Section 4.1.2, p. 79 *et seq.*) suggests the loss of 6–6.5 water molecules from the formula unit $\text{Cu}_2\text{Na}(\text{OH})\text{L}\cdot 7\text{H}_2\text{O}$ ³ during heating to 150 °C, which would correspond to the loss of 12–13 water molecules (out of 14) from each pore. Therefore, according to the mass data, the number of methanol molecules gained during the first resolution would be between about 5.6 and 6 per pore.

The “CALC SOLV” routine in PLATON [6] was used to calculate the solvent accessible voids within the structure. To do this, the structure was artificially “dehydrated” by deleting water molecules from the structure prior to calculation. The removal of six water molecules per formula unit $\text{Cu}_2\text{Na}(\text{OH})\text{L}\cdot 7\text{H}_2\text{O}$ (i.e., twelve from the pore, out of a total of fourteen) would involve the loss of the four⁴ non-coordinated guest water molecules plus two of the coordinated molecules.

If guest water molecules O1W, O2W, O3W and O7W, plus coordinated water molecules O5W and O6W (those with the two longest bonds to sodium) are

³Although the crystal structure was solved with the formula $\text{Cu}_2\text{Na}(\text{OH})\text{L}\cdot 8\text{H}_2\text{O}$, analysis and TG suggested $\text{Cu}_2\text{Na}(\text{OH})\text{L}\cdot 7\text{H}_2\text{O}$, and the latter formula was used in this discussion.

⁴That is, the removal of the *five* guest molecules of a total of eight water molecules listed per formula unit in the crystal structure. In this discussion, the water molecule O8W is assumed to be absent.

deleted, PLATON detects a single pore with a volume of $348 \text{ \AA}^3$ (37 %). Figure 5.23 (p. 191) shows an approximate representation of the pores within the structure. With the further removal of coordinated water O4W, it detects a single pore with a volume of $385 \text{ \AA}^3$ (41 %).

According to the data in Table 5.5, 12–13 water molecules in the bulk liquid should have a volume of $360 \text{ \AA}^3$ – $390 \text{ \AA}^3$. Likewise, the calculated 5.6–6 methanol molecules, replacing the departed water molecules, should occupy $377 \text{ \AA}^3$ – $404 \text{ \AA}^3$. These volumes are slightly larger than the calculated pore volumes above. While it is tempting to ascribe these differences to tighter packing of water and methanol within the pore volume than within the bulk solvent, perhaps attributing this to coordination of the solvent species to sodium, the use of a smaller probe-radius setting in PLATON significantly increases the calculated void sizes⁵. These pore volumes are also *not* the pore volumes of the dehydrated material, which has been shown by XRPD to collapse on dehydration, but rather the volumes occupied by guests in the solvated structures.

In Section 5.3.2 (p. 151 *et seq.*), methanol was found to be evolved by the resolvated material well past the dehydration temperature and right up to the final decomposition (see Figures 5.8–5.9, pp. 159–160). The mass data for the second desolvation in step 3 (Section 5.3.7, p. 179) show that the desolvated material ($\%m_{\text{res}} = 79.66$) has a slight excess mass compared to the dehydrated material ($\%m_{\text{res}} = 78.13$). Assuming that 12–13 water molecules were lost during the initial dehydration, and assuming also that this small excess mass is due to methanol trapped in the collapsed structure, the excess mass corresponds to approximately 0.5 methanol molecules per collapsed pore, i.e., one trapped methanol molecule in every second collapsed pore of the desolvated material.

The ΔH value associated with the second desolvation of methanol (see Table 5.3, p. 180) is about 22 % larger than for the first desolvation of methanol in the first experiment. While there is doubt that this difference is statistically significant⁶, this, together with the change in the shape of the DSC peak (Figure 5.19 curves b and c, p. 5.19), suggests some subtle change in the pore environment

⁵For the removal of five and six waters (out of seven) per formula unit, i.e., 10 and 12 from the pore, PLATON detects pore volumes of $397 \text{ \AA}^3$ and $432 \text{ \AA}^3$, respectively, using a $0.6 \text{ \AA}$ probe instead of the default $1.2 \text{ \AA}$.

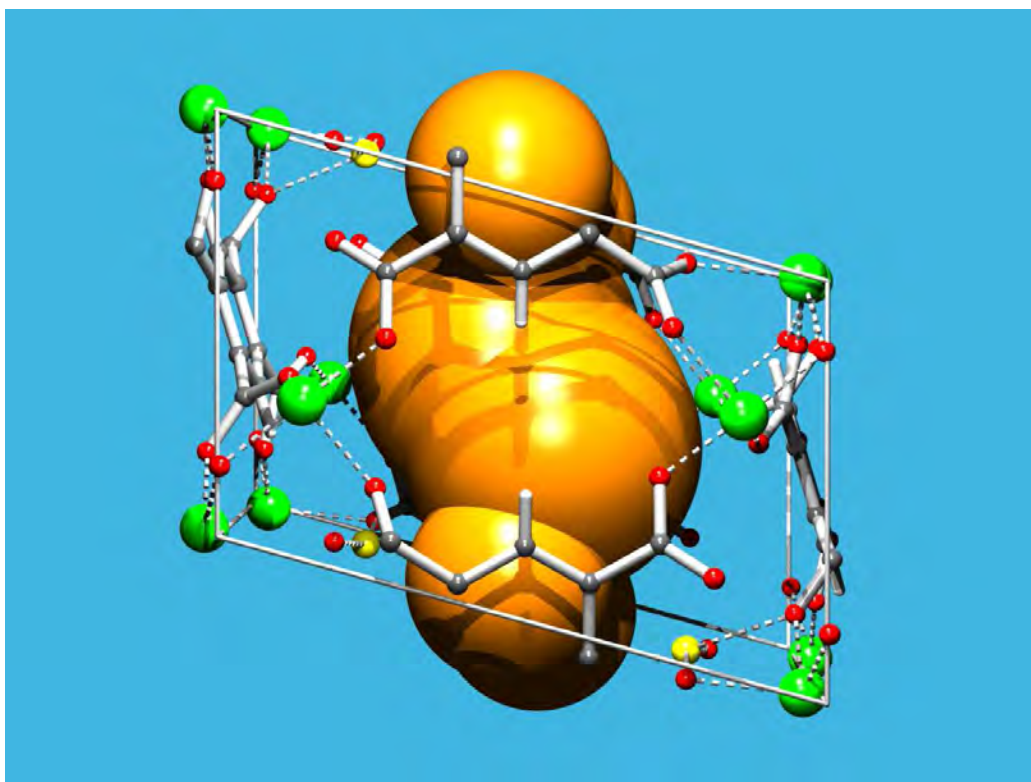


Figure 5.23: Ray-traced drawing of the cavities within **xut-cu-b4c-acet-xtals** (12 waters deleted from the pore out of a total of 14), showing the cavities in orange. Cavities were determined using PLATON, with the default 1.2 Å probe.

over the desolvation/resolution cycles. For example, if 13 water molecules are lost from a pore in the untreated material, leaving one coordinated water attached to one of the two sodium ions in the pore, then the coordination of this water molecule to sodium may be lost over repeated desolvation/resolution cycles, and replaced by coordination to methanol. For the water-water and methanol-water cycles, the increases in ΔH between the first and third desolvations are relatively much smaller at about 1 % (see set 1 of Tables 5.1 & 5.4 on pp. 169 & 184, respectively), and this supports this suggestion.

⁶The two ΔH values for the removal of methanol as the *second* solvent to which the individual samples had been exposed — i.e., for Section 5.3.6 step 5 (p. 174) and for Section 5.3.7 step 5 (p. 179) — are, respectively, the smallest and the largest of all six ΔH values for the removal of methanol reported above. These ΔH values are thus the outliers in the set of all six ΔH values obtained for the removal of methanol (as first or second solvent) in the studies on this compound. This raises the question of whether the two outliers can be judged, objectively, to be significantly

For ethanol as a guest molecule (Section 5.3.3, p. 162 *et seq.*), the DSC mass data (see p. 162) suggests (assuming the loss of 12–13 water molecules per pore in the original dehydration) that about one third of an ethanol molecule remains within each pore of the collapsed ethanol-desolvated material. The collapsed ethanol-desolvated material thus contains one ethanol molecule in every third pore.

It is clear from the TG-FTIR results (Figures 5.12–5.13, pp. 165–166) that upon heating of the ethanol-resolvated material, ethanol — like methanol — remains in the structure well past the first desolvation temperature, right up to the main decomposition.

Although, to a first approximation, pyridine’s calculated particle-volume of $139 \text{ \AA}^3$, suggests that this potential guest should be capable of being absorbed into the pores of the dehydrated **xut-cu-b4c-acet-xtals**, significant inclusion of pyridine was not observed. A colour change in the dehydrated material on exposure to pyridine was observed, suggesting that a small amount of pyridine had coordinated to copper(II). This may have caused a significant structural change which does not permit restoration of the original material.

different from the other four members of the set.

The mean of the four ΔH values reported above for the removal of methanol as the *first* solvent to which the individual samples had been exposed is calculated to be 180.5 J g^{-1} , with a sample standard deviation of 19.0 J g^{-1} . Using the Student’s t values [7, p. 50], the confidence limits may be reported at the 95 % and 99 % confidence intervals as follows:

$$180.5 \pm 30.2 \text{ J g}^{-1} \quad (95 \% \text{ confidence interval})$$

$$180.5 \pm 55.4 \text{ J g}^{-1} \quad (99 \% \text{ confidence interval})$$

So, at the stricter 95 % confidence interval, the ΔH value of 153.7 J g^{-1} obtained for the removal of methanol as a *second solvent*, after water (Section 5.3.6, p. 174), falls within the limits of error, but the ΔH value of 217.9 J g^{-1} for the removal of methanol as a *second solvent* after methanol (Section 5.3.7, p. 179), does not. However, at the less strict 99 % confidence interval, both of the outliers fall within the limits of error.

5.4 xst-cu-b4c-no3-rhombi

The DSC and TG curves (Section 4.2.2, p. 95 *et seq.*) showed that this compound undergoes dehydration in two main steps which are insufficiently resolved to be examined separately.

5.4.1 Single desolvation-resolution: water

The sample was crushed lightly and a small quantity (3.371 mg) was packed into an aluminium DSC pan and covered with a lid (not crimped). The sample was then subjected to the following treatment:

1. Heating from 25 °C to 200 °C at 10 °C min⁻¹ under nitrogen purge (26 ml min⁻¹) to drive off water. The mass of sample after heating was 2.778 mg, corresponding to 82.41 % of the original sample mass.
2. Exposure to moist (i.e., open) air overnight. The mass of the sample after exposure was 3.366 mg, corresponding to 99.85 % of the original sample mass.
3. Heating from 25 °C to 350 °C at 10 °C min⁻¹ under nitrogen purge (26 ml min⁻¹) to decompose the sample. The mass of the residue was 1.996 mg, corresponding to 59.21 % of the original sample mass.

More samples were treated as above to obtain dehydrated and rehydrated samples for X-ray diffraction and infrared studies.

The DSC curves for the untreated and rehydrated materials in Figure 5.24 (p. 195) were superficially similar, but showed some significant, and repeatable, changes, suggesting that there are some non-reversible changes to the structure on dehydration. All the peaks shifted to lower temperatures for the dehydrated material, and there is peak-broadening, which may indicate that the porous environments in which the guest and coordinated water molecules reside are slightly different and less well-defined in the rehydrated material than in the parent material. Because of the peak overlap, comparison of the enthalpies associated with the dehydrations was not attempted.

The X-ray diffraction patterns for the untreated, dehydrated and rehydrated materials, shown in Figure 5.25 (p. 196), indicate that there are significant structural changes on dehydration, and there is some restoration of the original framework on rehydration. However, the powder diffraction pattern for the rehydrated material is significantly poorer in quality than that of the untreated material, and there are many peaks — e.g., in the ranges $20\text{--}25^\circ$ and $30\text{--}50^\circ$ which suffer loss of intensity as a result of the sample treatment.

The infrared spectra (Figure 5.26–5.28, pp. 199–201) show the presence of extended hydration, as shown by the broad bands between 3400 cm^{-1} and 3000 cm^{-1} , which indicate strong hydrogen bonding. This would mask any sharp $\nu\text{O-H}$ band between 3400 cm^{-1} and 3300 cm^{-1} that would be expected [8, p. 310] if coordinated water were present. Coordinated water would also give rise to a medium-to-weak infrared band between 1200 cm^{-1} and 1050 cm^{-1} due to the $\delta\text{M-O-H}$ bend, a weak infrared-allowed rock between 800 cm^{-1} and 600 cm^{-1} , and a medium-to-weak infrared-allowed wag between 650 cm^{-1} and 400 cm^{-1} . The infrared spectra of the complexes obtained in this study are complicated in these regions.

There is a common profile for the carbonyl regions for the 1,2,4,5-benzenetetracarboxylate complexes obtained in this study and in others prepared by this group [9]. Between 1680 cm^{-1} and 1500 cm^{-1} there is a strong, broad band, often with a higher-wavenumber and a lower-wavenumber shoulder. Between 1500 cm^{-1} and 1450 cm^{-1} can be found a band of medium intensity, often split. Finally, between 1450 cm^{-1} and 1300 cm^{-1} there are three intense bands, the lower of which is quite separate from the other two. These bands often have shoulders. The first region is commonly associated with the asymmetric carbonyl stretch, $\nu_a\text{C=O}$. The second and third regions are associated with the symmetric carbonyl stretch, $\nu_s\text{C=O}$. In protonated systems, this vibration reflects a coupled $\delta\text{C-O-H}$ bend and $\nu_s\text{C-O}$ stretch [9].

The vibrational behaviour of carboxyl groups is well-known [10, 11]. The following points are relevant to this study:

- A non-coordinated protonated carboxyl group (i.e., a free carboxylic acid group) is expected to have a $\nu_a\text{C=O}$ vibration between 1595 cm^{-1} and 1575 cm^{-1} , whereas a non-coordinated deprotonated carboxyl group (i.e.,

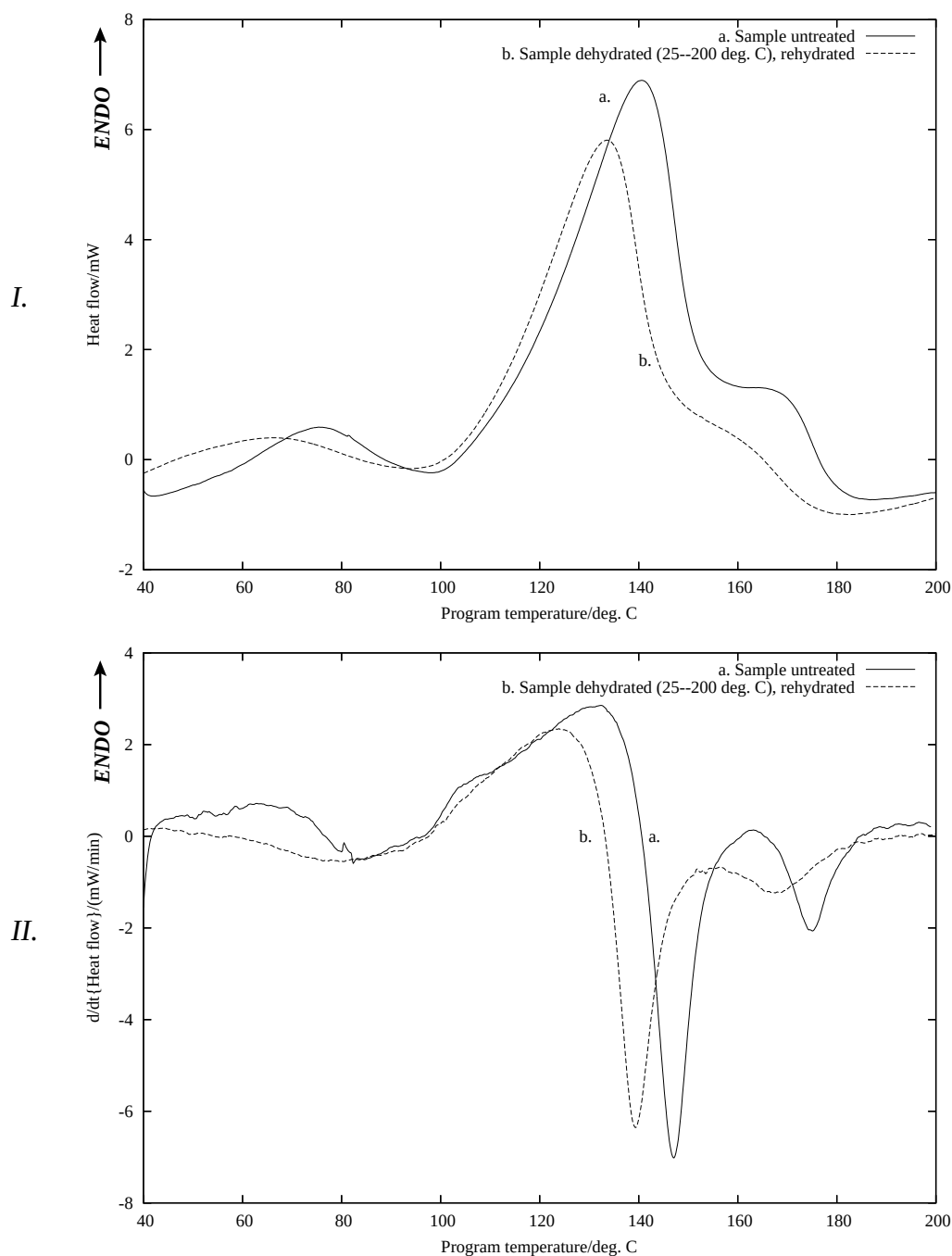


Figure 5.24: DSC (I) and derivative DSC (II) of **xst-cu-b4c-no3-rhombi** (a) without pre-treatment and (b) after dehydration (25 °C–200 °C at 10 °C min⁻¹ under nitrogen, 26 ml min⁻¹) with subsequent exposure to open air (25 °C) overnight. In (b), the sample was decomposed by heating in the DSC (25 °C–360 °C at 10 °C min⁻¹ under nitrogen, 26 ml min⁻¹).

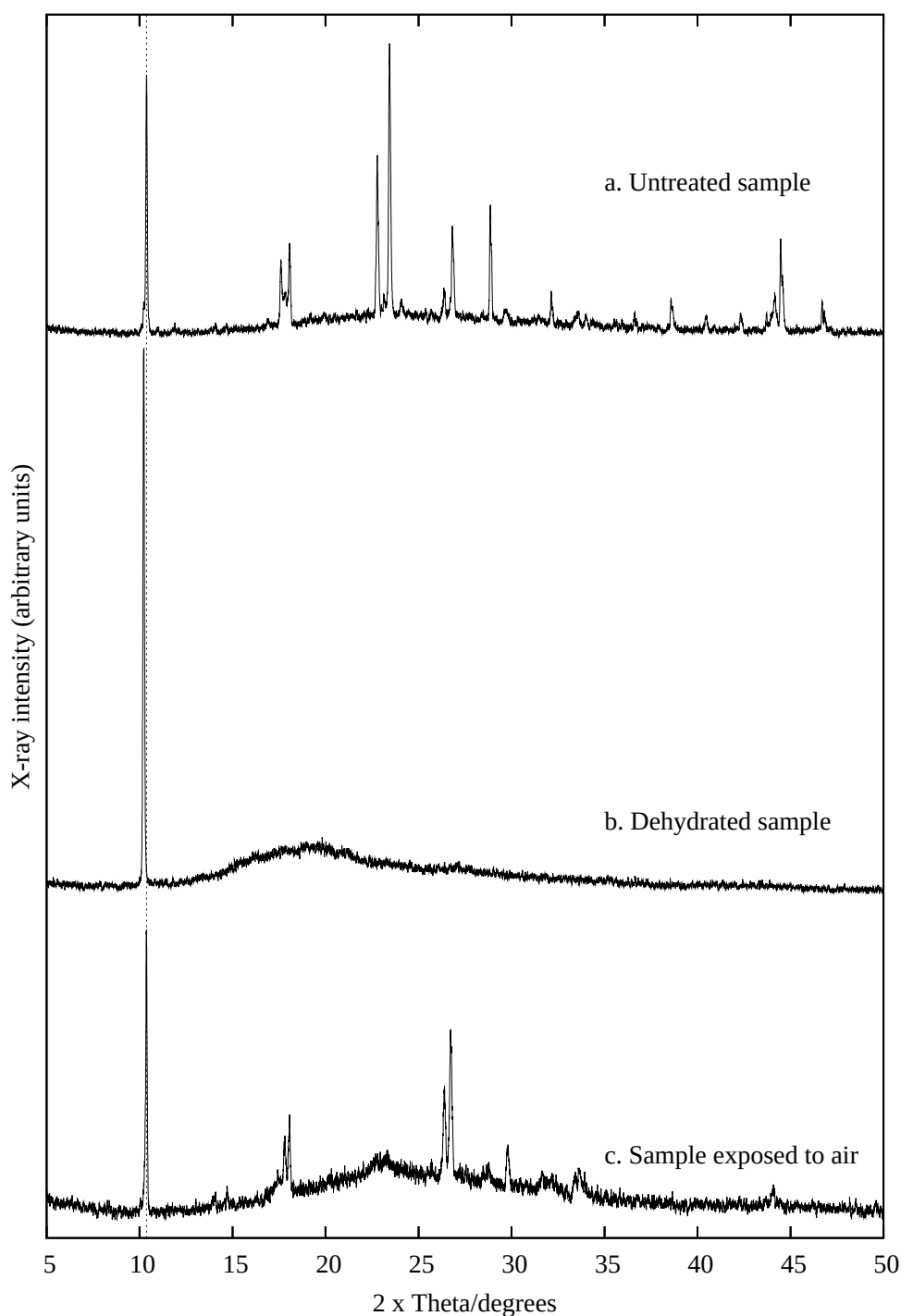


Figure 5.25: X-ray diffraction patterns for **xst-cu-b4c-no3-rhombi** (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–200 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹), and (c) dehydrated as above, and exposed to open air (12 hours). Pattern (b) was obtained under a 4:1 mixture of paraffin oil and petroleum ether, and the rest with no oil covering.

a free carboxylate group) has $\nu_a\text{C=O}$ between 1730 cm^{-1} and 1700 cm^{-1} .

- The position of the $\nu_a\text{C=O}$ band for a coordinated carboxyl group depends on the degree of covalency of the coordination: if it appears between 1650 cm^{-1} and 1620 cm^{-1} , the coordination has a covalent character, but if it appears between 1630 cm^{-1} and 1575 cm^{-1} the coordination has an ionic character.
- For a carboxyl group which is coordinated unidentately, $\nu_a\text{C=O}$ will be shifted to higher wavenumbers relative to its position for a non-coordinated carboxyl group in the free ligand, and will have $\nu_s\text{C=O}$ shifted to lower wavenumbers. Consequently, the distance between these bands, ΔCO_2^- , increases on monodentate coordination, typically to values greater than 200 cm^{-1} .
- By contrast, on chelation, $\nu_a\text{C=O}$ will be shifted to lower wavenumbers, and $\nu_s\text{C=O}$ to lower wavenumbers. Consequently, ΔCO_2^- decreases on chelation, typically to values less than 100 cm^{-1} .
- For a carboxyl group which is coordinated to two metals in a bridging fashion, both $\nu_a\text{C=O}$ and $\nu_s\text{C=O}$ shift to higher wavenumbers, with ΔCO_2^- having a value of 150 cm^{-1} , typically.

Given the known crystal structures, a comparison of all the infrared spectra reported in this work indicates that the above principles cannot readily be applied. For 1,2,4,5-benzenetetracarboxylates, these regions overlap some of the fundamental vibrational modes of the 1,2,4,5-tetrasubstituted benzene ring, specifically [9] (using those of Varsányi and Szöke [12]) :

Wavenumbers/ cm^{-1}	Mode
1650–1540	$\nu(\text{ring})$, 8a & 8b
1540–1420	$\nu(\text{ring})$, 19a
1440–1300	$\nu(\text{ring})$, 19b
1380–1260	$\nu(\text{C-CO}_2)$, 7a
1280–1240	$\delta(\text{C-H})$, 9b
1260–1200	$\nu(\text{ring})$, 14

This makes unambiguous interpretation of the carbonyl vibrations tentative in the absence of crystal structure data. Consequently, vibrational spectra have been used only as a fingerprint technique, to flag structural changes due to sample treatments.

Although the carbonyl regions are commonly reported in the characterizations of metal polycarboxylates, it is the region below the carbonyls — specifically, $1200\text{--}1050\text{ cm}^{-1}$, $800\text{--}600\text{ cm}^{-1}$ and $650\text{--}400\text{ cm}^{-1}$ — that shows the greatest variability between different materials, and materials that have undergone various treatments. These regions might prove to be fruitful areas of investigation once a full vibrational assignment for 1,2,4,5-benzenetetracarboxylates has been done. Such work is beyond the scope of this study.

The infrared spectra of the untreated, dehydrated and rehydrated materials show significant differences. The broad O–H region ($3500\text{--}3000\text{ cm}^{-1}$) cannot be interpreted easily, but the appearance of peaks at around 2782 cm^{-1} in spectrum of the dehydrated material, which do not disappear on rehydration, suggests an irreversible change. Similarly, an examination of the peaks in the regions associated with carboxyl symmetric and asymmetric stretches — from 1780 cm^{-1} to 1260 cm^{-1} (see below) — shows that the spectrum of the rehydrated structure contains a “mixture” of the bands associated with the original and dehydrated materials. However, the fingerprint region, from 1250 cm^{-1} to 450 cm^{-1} more strongly suggests some restoration of the original structure on rehydration.

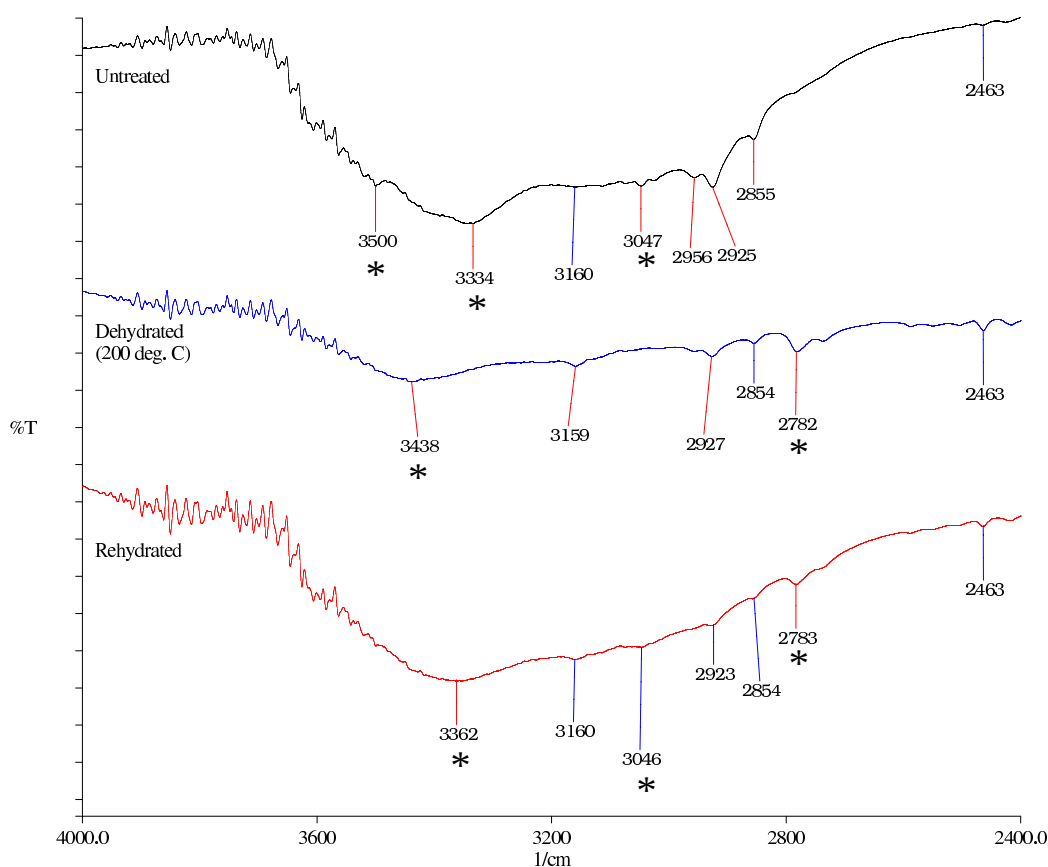


Figure 5.26: Infrared spectra of **xst-cu-b4c-no3-rhombi** in the untreated, dehydrated and rehydrated states ($4000\text{--}2400\text{ cm}^{-1}$). Asterisks indicate bands sensitive to change.

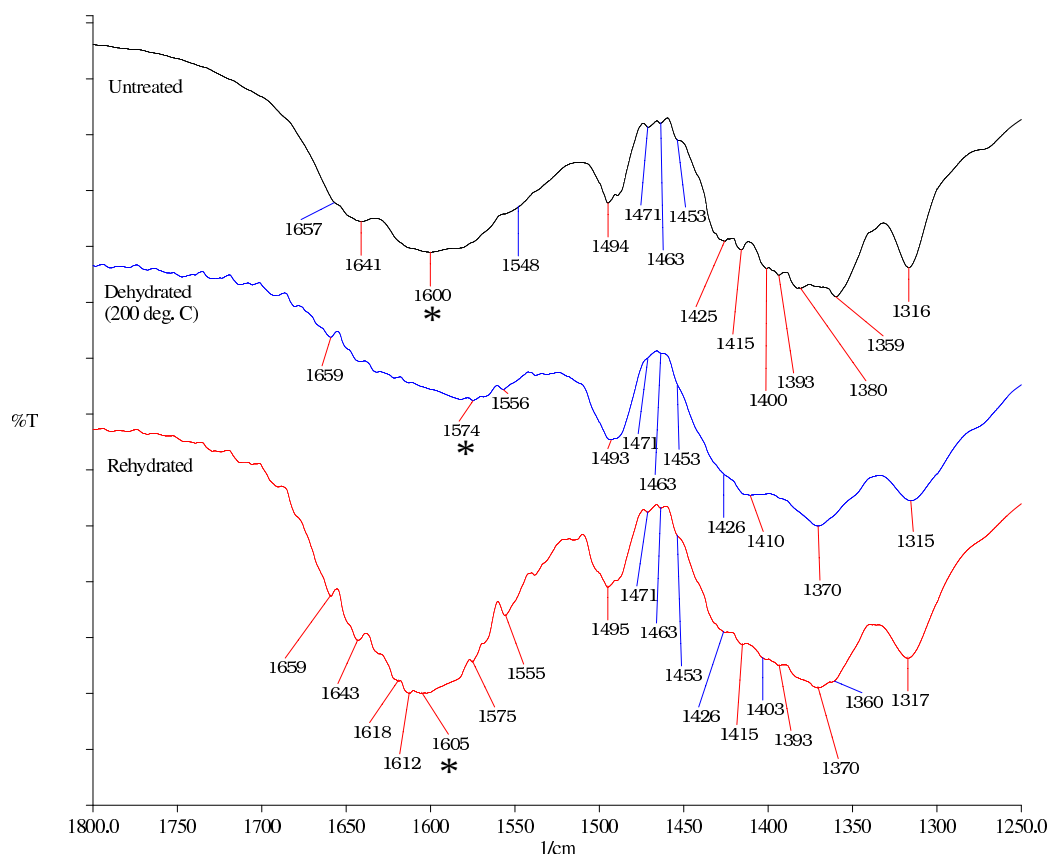


Figure 5.27: Infrared spectra of **xst-cu-b4c-no3-rhombi** in the untreated, dehydrated and rehydrated states ($1800\text{--}1250\text{ cm}^{-1}$). Asterisks indicate important bands sensitive to change. This region contains significant fine-structure due to rotational bands associated with water.

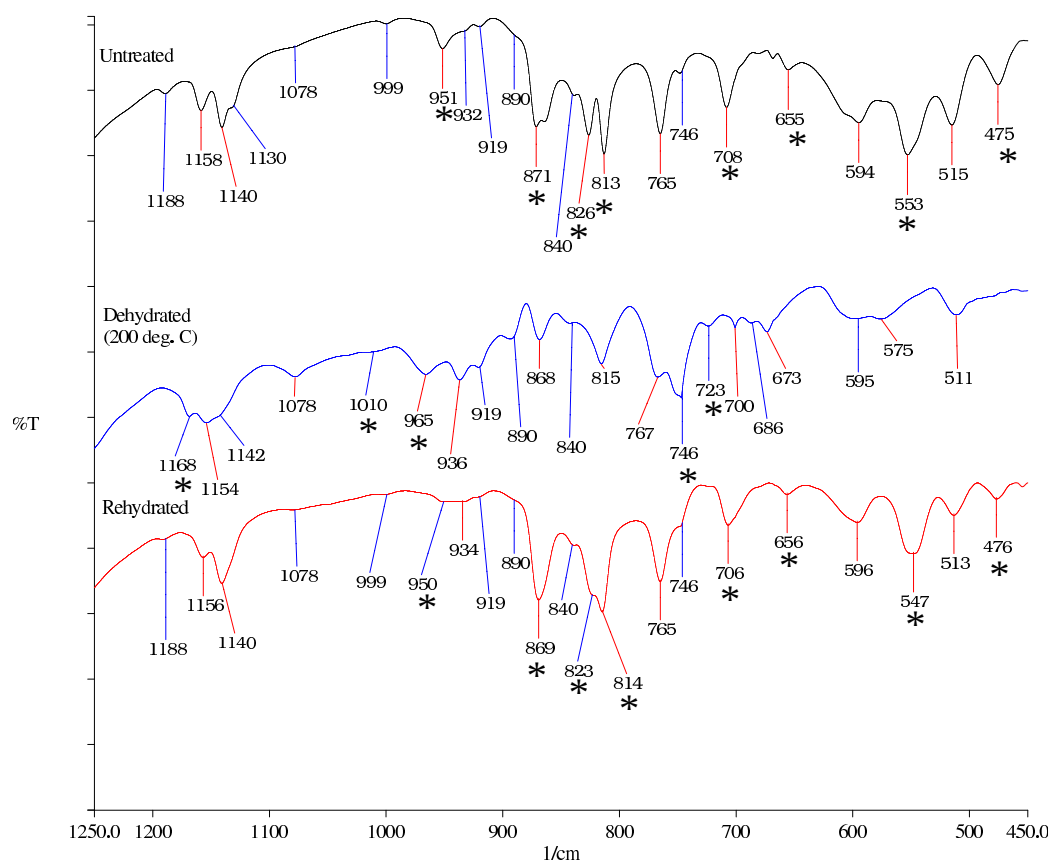


Figure 5.28: Infrared spectra of **xst-cu-b4c-no3-rhombi** in the untreated, dehydrated and rehydrated states ($1250\text{--}450\text{ cm}^{-1}$). Asterisks indicate important bands sensitive to change.

5.4.2 Single desolvation-resolution: methanol

In similar experiments with methanol as a potential guest species, the dehydrated material showed nearly no mass gain in the presence of saturated methanol vapour. Therefore this substance was not considered for further guest-inclusion studies.

5.4.3 Discussion

The three-dimensional metal organic framework, **xst-cu-b4c-no3-rhombi**, collapses on dehydration as shown by XRPD and FTIR results, and is incompletely restored to its original structure on exposure to water vapour. There is some evidence from these, and also the DSC results, that the structure is partly restored on rehydration, and that the environment in which the guest waters reside within the rehydrated material is comparable, but not identical, to that in which the guest waters reside within the parent. Collapse of the structure on loss of water may result in the formation of coordinate bonds — perhaps the potential interactions indicated by ‘†’ in Figure 4.12 (p. 100) — causing changes in the framework which are not reversed on exposure to water vapour.

Although the dehydration steps were not sufficiently resolved to allow the selective removal of differently bound waters by heating alone, it may be possible to do so by more gentle heating under vacuum. This may provide an avenue for further work with this compound.

Calculation of the pore volume, using PLATON, of the crystal structure from which all water molecules have been deleted, provides further insights. According to the crystal structure, each unit cell contains two of the formula units $\text{Cu}_4\text{Na}_4\text{L}_3 \cdot 14\text{H}_2\text{O}$, i.e., 28 waters in total. If these are deleted, then according to calculations using PLATON (using the default 1.2 Å probe), there are six small cavities per unit cell, four of them each with a volume of 54 Å³ and two each with a volume of 44 Å³ (see Figure 5.29, p. 204). The total pore volume is therefore 304 Å³ (14.5 % of the unit cell volume), which is insufficient to accommodate the 26–28 departed guest water molecules (calculated volume, 780 Å³–840 Å³) as determined by TG (see Table 5.5, p. 189). Although this may be accounted for partly by tighter packing of the coordinated water molecules compared to the hydrogen-bonded molecules in bulk water⁷, it should be borne in mind PLATON’s pore-

volume calculations are dependent on the probe-size parameter used. In other studies of metal-organic frameworks [13], it was suggested that the calculated pore volume for small voids would be more greatly dependent on the probe-tip size used by PLATON in the calculation than for larger pores.

According to these calculations, none of these pores, individually, would be large enough to accommodate a methanol molecule. Although no definite significance can be attached to the numerical values of these calculated pore-sizes, these results do suggest that the space within the structure is partitioned in such a way that methanol cannot be accommodated in any one site. However, using a finer probe ($0.8 \text{ \AA}$) for the calculations produces two pores, each with a volume of $242 \text{ \AA}^3$, giving a total pore volume of $484 \text{ \AA}^3$ (24 %). It is important to remember that these calculated results do not describe the pores in the dehydrated material, which has been shown to collapse on dehydration. They describe the space occupied by the guest water molecules in the parent material, and, perhaps, to some extent, also in the rehydrated material.

In spite of the small pore size and the differences in structure between the rehydrated and parent materials, the presence of unsaturated copper(II) sites in the dehydrated material make this compound (strictly speaking, the dehydrated variant) a potential candidate for hydrogen sorption studies.

⁷Compare, for example, the structure of copper(II) sulfate pentahydrate [14], which contains ten water molecules per unit cell, of which eight are coordinated to copper and the remaining two are uncoordinated guests. If all ten waters are deleted, PLATON finds a void with a volume of $167 \text{ \AA}^3$, sufficient to hold 5.6 bulk water molecules. This suggests that the coordinated water molecules occupy just over half the volume of bulk water molecules. A simple visualization of this is a space-filling model of a copper(II) ion bound to an aqua oxygen: if the copper and oxygen are viewed as intersecting spheres, about half the volume of the oxygen sphere is “inside” the copper sphere. On decreasing the probe volume from the default $1.2 \text{ \AA}$ to $0.6 \text{ \AA}$, the volume of the detected pore increased to $219 \text{ \AA}^3$, which is sufficient to hold 7.3 bulk water molecules. On reducing the probe radius further, the pore volume began to decrease.

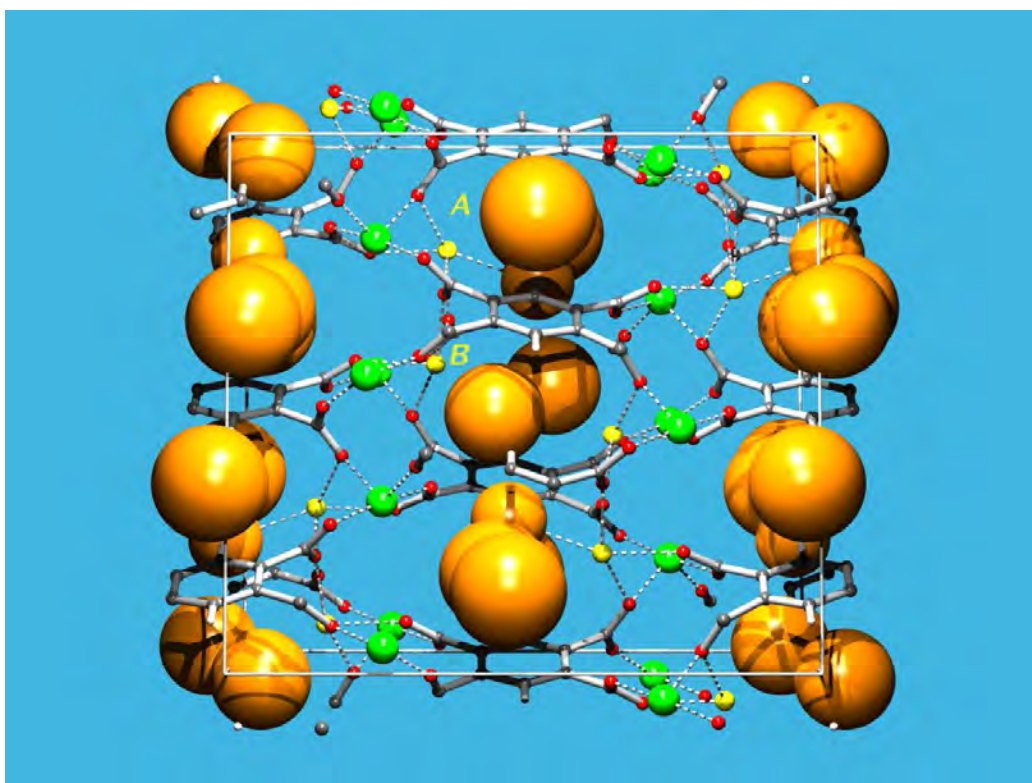


Figure 5.29: Ray-traced drawing of the cavities within **xst-cu-b4c-no3-rhombi** (all water molecules deleted), showing the cavities in orange. Cavities were determined using PLATON, with the default 1.2 Å probe. The cavities labelled A and B have volumes of 54 Å³ and 44 Å³, respectively.

5.5 xst-cu-b4c-no3-lumps

Preliminary experiments showed that this material — when dehydrated — does not re-hydrate significantly in open air. Even after exposures as long as 14 days, only a small fraction of the mass lost on dehydration is regained. On exposure to saturated water vapour, the dehydrated sample regains mass more rapidly, and so this method of rehydration was used for this sample.

5.5.1 Single desolvation-resolution: water

The sample was crushed lightly and a small quantity (3.130 mg) was packed into an aluminium DSC pan and covered with a lid (not crimped). The sample was then subjected to the following treatment:

1. Heating from 25 °C to 180 °C at 10 °C min⁻¹ under nitrogen purge (26 ml min⁻¹) to drive off water. The mass of the residue after heating was 78.76 % of the original sample mass. Visual examination showed that the dehydrated material was a dull green colour.
2. Exposure to moist (i.e., open) air for 12 hours. The mass of the sample after exposure was 80.35 % of the original sample mass.
3. Exposure to saturated water vapour (25 °C) for 6 hours. The mass of the sample after exposure was 95.47 % of the original sample mass.
4. Heating from 25 °C to 360 °C at 10 °C min⁻¹ under nitrogen purge (26 ml min⁻¹) to decompose the sample. The residue mass was 46.11 % of the original sample mass.

DSC and derivative curves are shown in Figure 5.30 (p. 207) for the untreated (curve a) and rehydrated (curve b) materials. X-ray diffraction patterns for these materials are given in Figure 5.31, (p. 208). The DSC and X-ray diffraction results show clearly that the residue is different to the untreated parent material, i.e., that the structure does not survive the dehydration–rehydration cycle intact. The infrared spectrum of the rehydrated structure (Figures 5.32–5.34, pp. 209–211) contains peaks from both the spectra of the parent material and the dehydrated

intermediate, suggesting incomplete restoration of the original structure on rehydration.

Because of the marked differences between the original and resolvated materials, the very weak DSC signals for dehydration of the resolvated material and the very poor powder diffraction pattern for of the resolvated material (suggesting poor crystallinity), this material was not considered for further guest-inclusion studies.

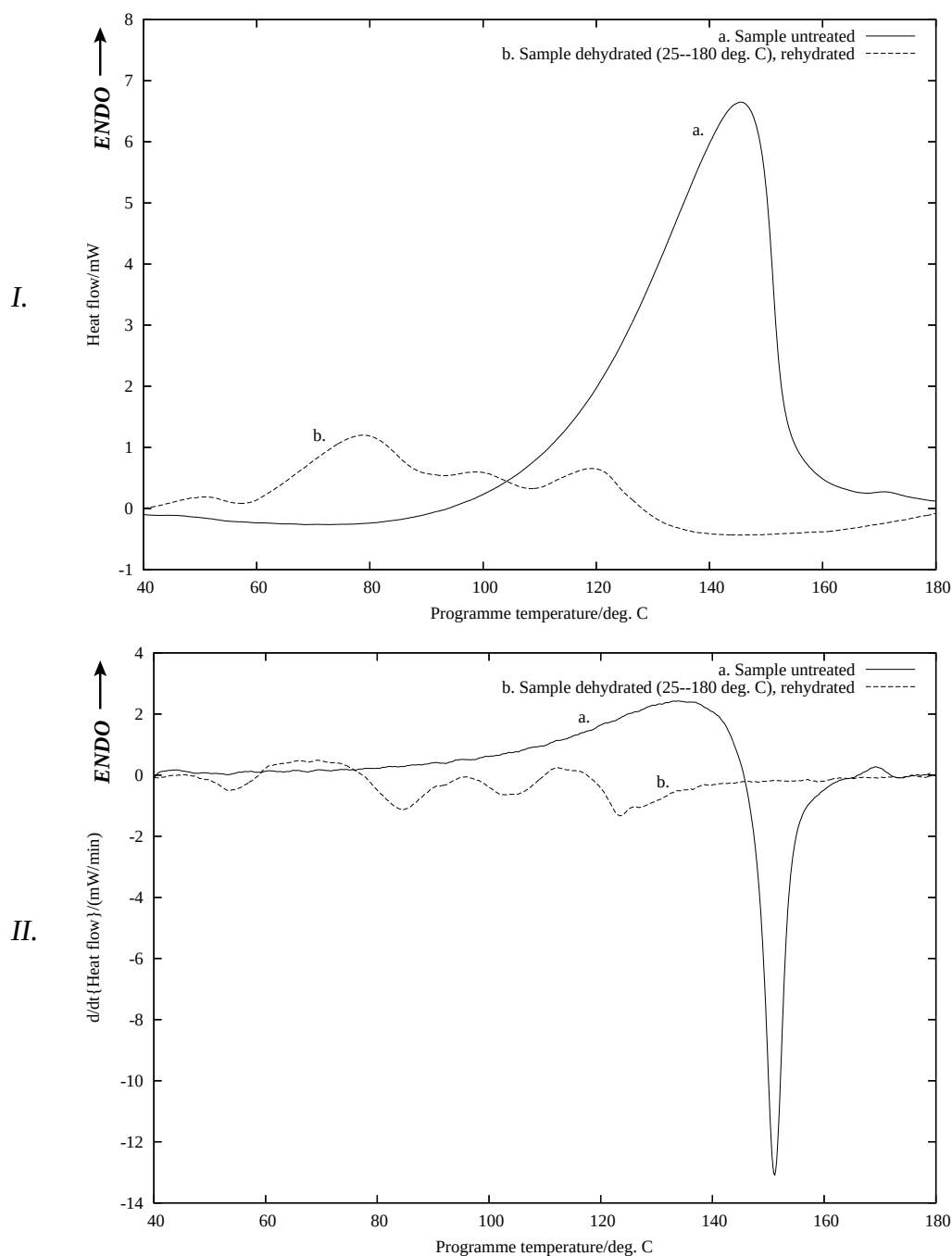


Figure 5.30: DSC (I) and derivative DSC (II) of **xst-cu-b4c-no3-lumps** (a) without pre-treatment and (b) after dehydration (25 °C–150 °C at 10 °C min⁻¹ under nitrogen, 26 ml min⁻¹) with subsequent exposure to open air (12 hours) and thereafter to saturated water vapour (25 °C) for 6 hours. In (b), the sample was decomposed by heating in the DSC (25 °C–360 °C at 10 °C min⁻¹ under nitrogen, 26 ml min⁻¹).

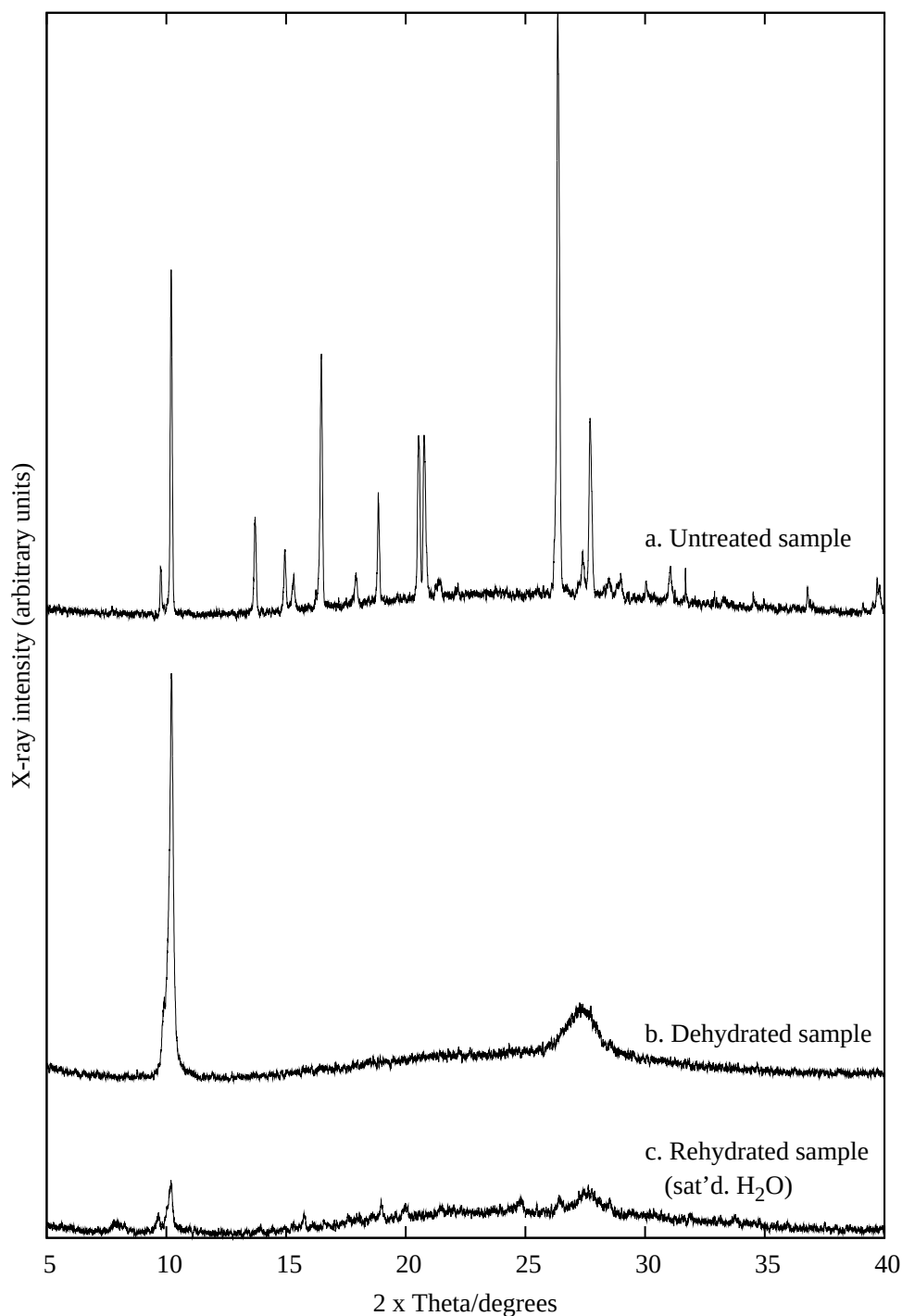


Figure 5.31: X-ray diffraction patterns for **xst-cu-b4c-no3-lumps** (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min⁻¹ under nitrogen, 26 ml min⁻¹), and (c) dehydrated as above, and exposed to open air (12 hours) and thereafter to saturated water vapour (6 hours). The patterns were obtained without any oil covering.

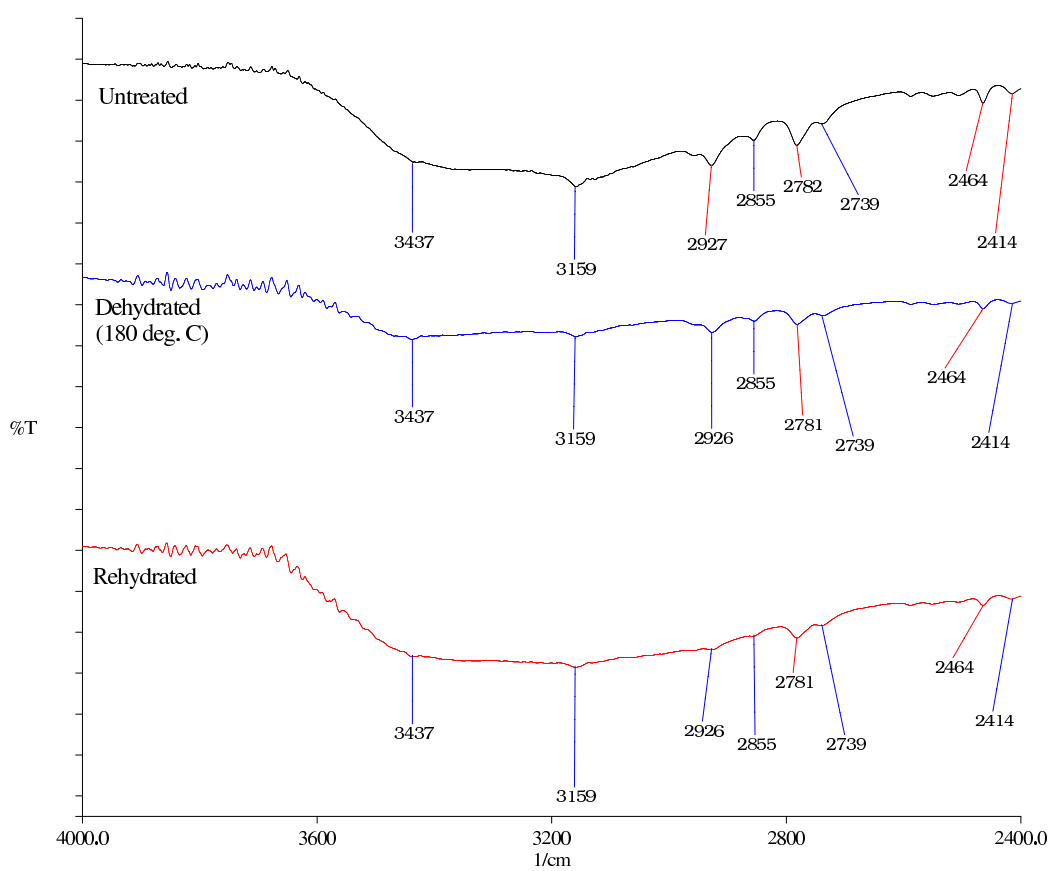


Figure 5.32: Infrared spectra of **xst-cu-b4c-no3-lumps** in the untreated, dehydrated and rehydrated states (4000–2400 cm^{-1}).

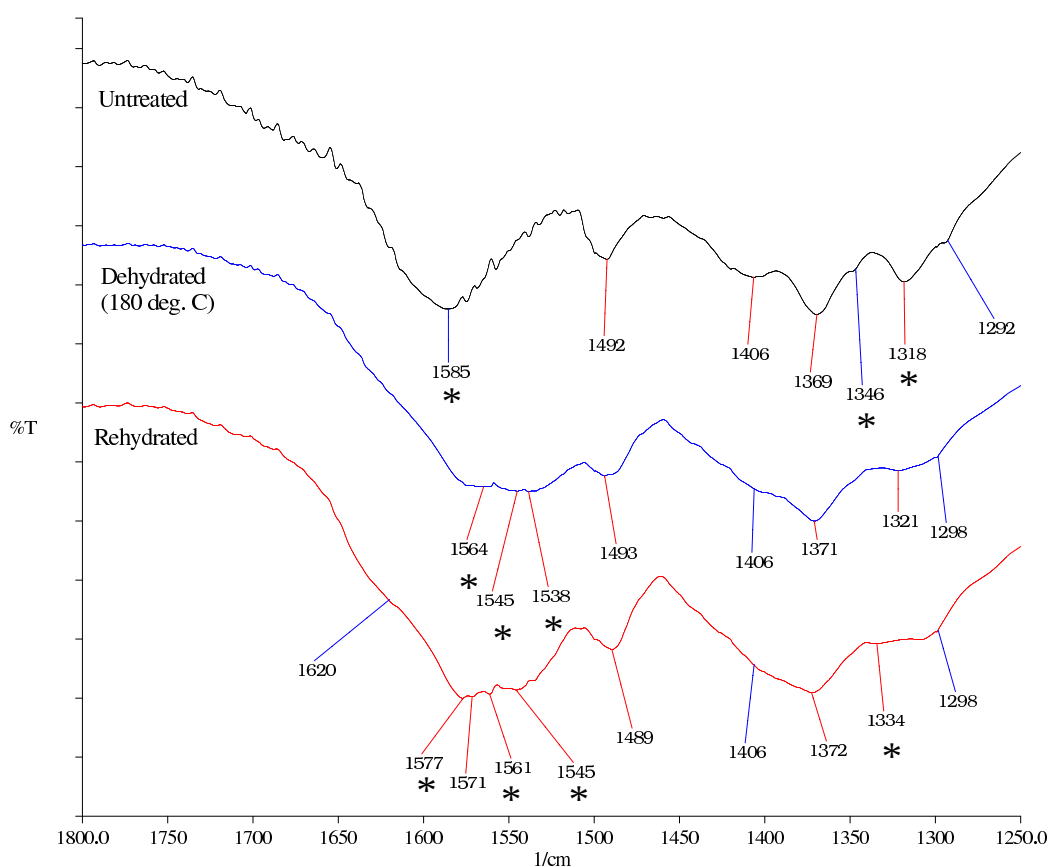


Figure 5.33: Infrared spectra of **xst-cu-b4c-no3-lumps** in the untreated, dehydrated and rehydrated states ($1800\text{--}1250\text{ cm}^{-1}$). Asterisks indicate important bands sensitive to change.

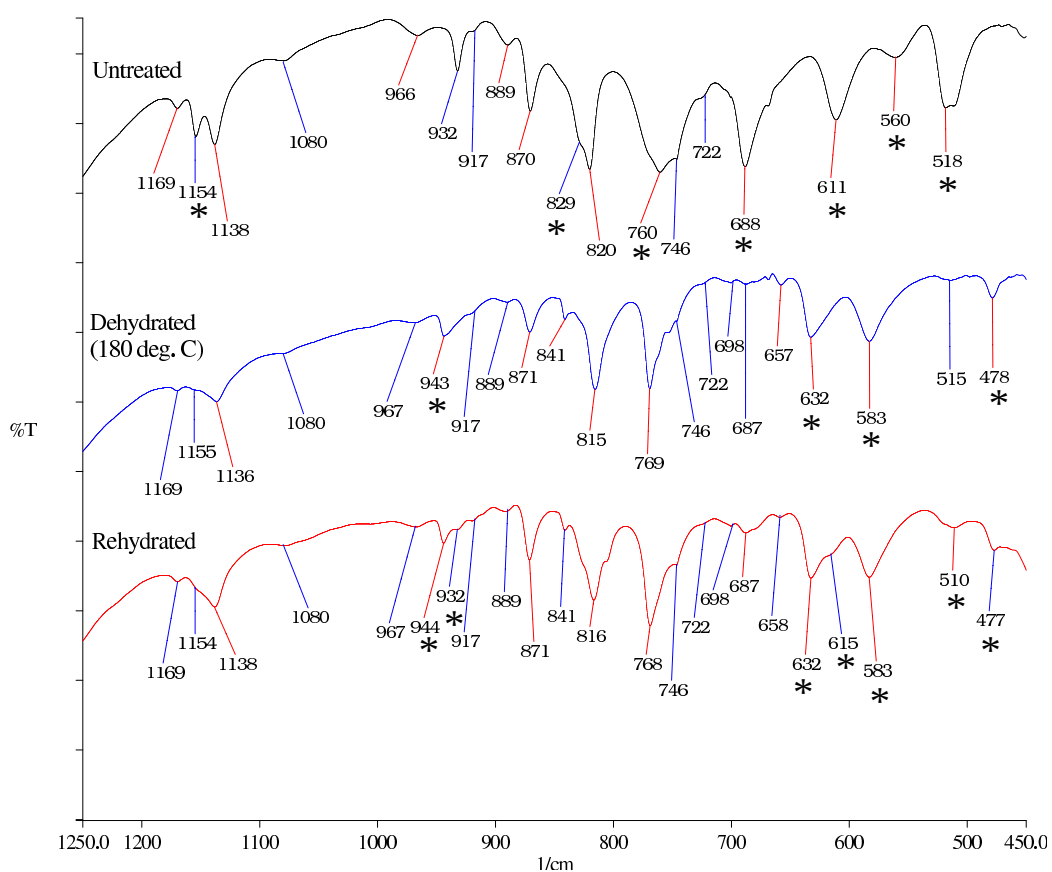


Figure 5.34: Infrared spectra of **xst-cu-b4c-no3-lumps** in the untreated, dehydrated and rehydrated states ($1250\text{--}450\text{ cm}^{-1}$). Asterisks indicate important bands sensitive to change.

5.5.2 Discussion

The XRPD, FTIR and especially the DSC results, including the mass data, show that this material collapses on dehydration, and is not restored to its original structure on exposure to water vapour. As a result of dehydration, the coordination sphere of the copper(II) ions is probably altered, and the structural collapse accompanying loss of water may provide opportunities for coordination to the unsaturated copper(II) centres by carboxyl oxygens in adjacent layers, causing changes in binding which are not reversed on exposure to water vapour. In other words, on dehydration, the two-dimensional covalent framework is thus changed, perhaps incompletely, into a three-dimensional covalent framework of lesser porosity, which does not revert to the original structure on rehydration.

PLATON was again used to calculate the volume of the pore occupied by guest water molecules in the structure. Deletion of all the water molecules leaves a pore of volume $121 \text{ \AA}^3$ (33 % of unit cell). This pore is too small to accommodate the six deleted water molecules per formula unit, $\text{Cu}_2 \text{L} \cdot 4\text{H}_2\text{O} \cdot 2\text{H}_2\text{O}$ (also the unit-cell formula), having a volume equivalent to 56 % of the volume occupied by six bulk-liquid water molecules. As the probe-tip setting in PLATON is decreased, the reported volume of the pore increases. For example, with a probe radius of $0.6 \text{ \AA}$, the calculated pore volume is $157 \text{ \AA}^3$, or 87 % of the bulk-liquid volume.

Although the calculated pore volume of $121 \text{ \AA}^3$ is, to a first approximation, large enough to accommodate both methanol and ethanol, no methanol inclusion was observed (and hence no ethanol-inclusion studies were performed). However, it is important to note that this pore volume describes only the size of the cavity occupied by water in the untreated material. As indicated by DSC results (including mass data) the pore environment in the rehydrated material is very different from that of the untreated material, and it is likely that the irreversibly-altered dehydrated material cannot form pores large enough to accommodate methanol molecules.

5.6 xst-cu-b4c-so4-topxtals

The DSC and TG curves (Section 4.3.2, p. 105 *et seq.*) show that this compound undergoes dehydration in two main steps which are sufficiently resolved to be examined separately. Two types of dehydration–resolution experiments were performed on this compound: the first involved only the first dehydration step, and the second involved both the first and second steps.

Preliminary studies showed that the dehydrated samples did not gain mass significantly in open air, so the rehydration experiments reported here were performed in saturated water vapour, in the manner previously described.

5.6.1 Single desolvation-resolution: first step only, water

The sample was crushed lightly and a small quantity (1.705 mg) was packed into an aluminium DSC pan and covered with a lid (not crimped). The sample was then subjected to the following treatment:

1. Heating from 25 °C to 95 °C at 10 °C min⁻¹ under nitrogen purge (26 ml min⁻¹) to drive off water. The sample mass after heating was 81.88 % of the original sample mass.
2. Exposure to moist (i.e., open) air for 12 hours. The mass of the sample after exposure was 83.46 % of the original sample mass.
3. Exposure to saturated water vapour (25 °C) for 6 hours. The mass of the sample after exposure was 91.67 % of the original sample mass.
4. Heating from 25 °C to 350 °C at 10 °C min⁻¹ under nitrogen purge (26 ml min⁻¹) to decompose the sample. The mass of the residue was 0.692 mg, corresponding to 40.59 % of the original sample mass.

The DSC and derivative DSC curves in Figure 5.35 (curves b, p. 214) are for the dehydration part of step 4 above — i.e., for the dehydration of the rehydrated material. Curves a are for the *complete* dehydration (25–150 °C) of an untreated sample of similar size, shown for comparison.

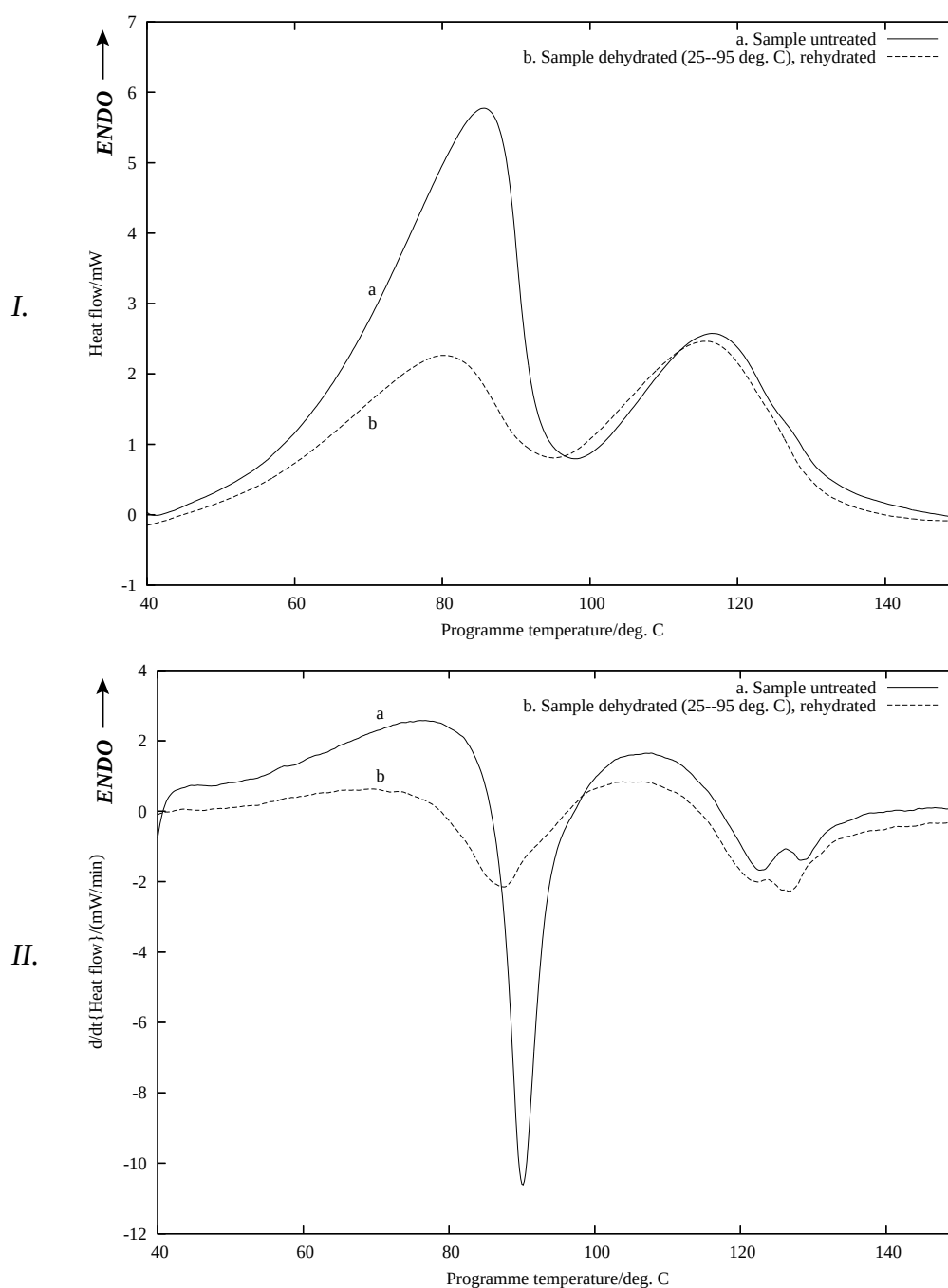


Figure 5.35: DSC (I) and derivative DSC (II) curves of **xst-cu-b4c-so4-topxtals** (a) without pre-treatment and (b) after dehydration (25 °C–95 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹) with subsequent exposure to saturated water vapour (25 °C) for 6 hours. In (b), the sample was decomposed by heating in the DSC (25 °C–350 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹).

The second dehydration step in curve b is superimposable on the corresponding step in curve a. In contrast, the endotherm corresponding to the first step is much smaller for the rehydrated material (curve b) than for the untreated material. To provide a semi-quantitative comparison of the peaks, pairs of bifurcated gaussian functions⁸ were fitted to the experimental dehydration curves. The curve-fitting involved the following steps:

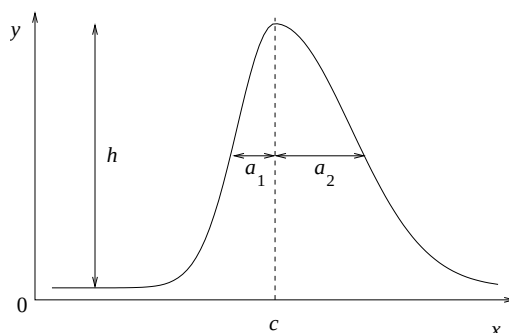
- subtracting a “dead run” (of the residue of a previous run on similar material) to remove baseline-curvature
- baseline-straightening by linear subtraction
- fitting to the experimental data two bifurcated gaussian functions using the freely available `fityk` software package⁹.

For all curve-fitting operations reported here, R^2 was better than 0.99, and while visual inspection of the residual plots showed small deviations from the experimental data which may be systematic, the combined areas of the fitted curves

⁸A bifurcated (or split) gaussian curve consists of the left and right halves of two gaussian curves of different widths but identical heights, joined together. The curve is described by the equation [15] (see also [16, p. 97]):

$$y(x) = \begin{cases} h \exp \left[-\ln 2 \left(\frac{x-c}{a_1} \right)^2 \right] & x \leq c \\ h \exp \left[-\ln 2 \left(\frac{x-c}{a_2} \right)^2 \right] & x > c \end{cases}$$

where h is the height of the peak, c is the so-called centre (indicated by a vertical line in the diagram below) and a_1 and a_2 are constants — the *half-width at half-maximum* values — related to the width of the left and right gaussians, respectively.



⁹Versions earlier than 0.7.6 are unsuitable for the tasks described above.

agreed with the numerical integration of the experimental data to within 0.5 % or better.

For the experimental curves in Figure 5.35(I) (p. 214), the ratio of the areas of the two bifurcated gaussians fitted to curve a — left peak : right peak — is 1.9 . The ratio of corresponding mass-losses is 1.7 (second mass loss obtained in Section 5.6.2), showing that the enthalpy changes corresponding to the first and second dehydration steps are very similar per unit mass of water lost.

Repeating this procedure for curve b — assuming that the second mass loss has the same magnitude as for curve a above — gives a peak-area ratio of 0.86 and a mass-loss ratio of 0.93, again showing that the enthalpy changes for the first and second dehydration steps are similar per unit mass of water lost.

This suggests that, although less water is gained on rehydration than was lost on dehydration (to 95 °C), the water gained on rehydration enters a similar environment to that occupied by the water originally present. The rehydration step thus causes a partial restoration of the original structure.

Steps 1–3 were repeated on a new sample to obtain some of the rehydrated material obtained after step 3 for examination by X-ray powder diffraction. The thermal and mass data for the corresponding steps were in good agreement with those reported above. In addition, samples of the dehydrated material were obtained in the same manner as above. The X-ray diffraction patterns of the untreated, dehydrated and partly rehydrated samples are shown in Figure 5.36 (p. 218). The X-ray diffraction pattern of the dehydrated material (pattern b) consists of some of the peaks from the untreated material (pattern a) and some new peaks which have appeared as a result of dehydration. The pattern for the rehydrated material (pattern c) shows a stronger contribution from the peaks from the untreated material, indicating that the dehydrated material returns, at least partly, to the structure of the untreated material upon rehydration. That it does not do so completely is clear from the X-ray diffraction patterns and from the mass data reported above. In addition to peaks from patterns a and b, pattern c also shows peaks which are unique to the rehydrated material at $2\theta = 49.9^\circ$ and 50° . It is uncertain whether the intensities of these peaks are due to the formation of a new structure, or whether they are due to a structure formed because of dehydration and are not visible in pattern b because of preferred orientation effects.

The infrared spectra (Figures 5.37–5.39, pp. 5.37–5.39) suggest that the dehydrated and rehydrated materials are very similar, and that they show marked differences to the parent material.

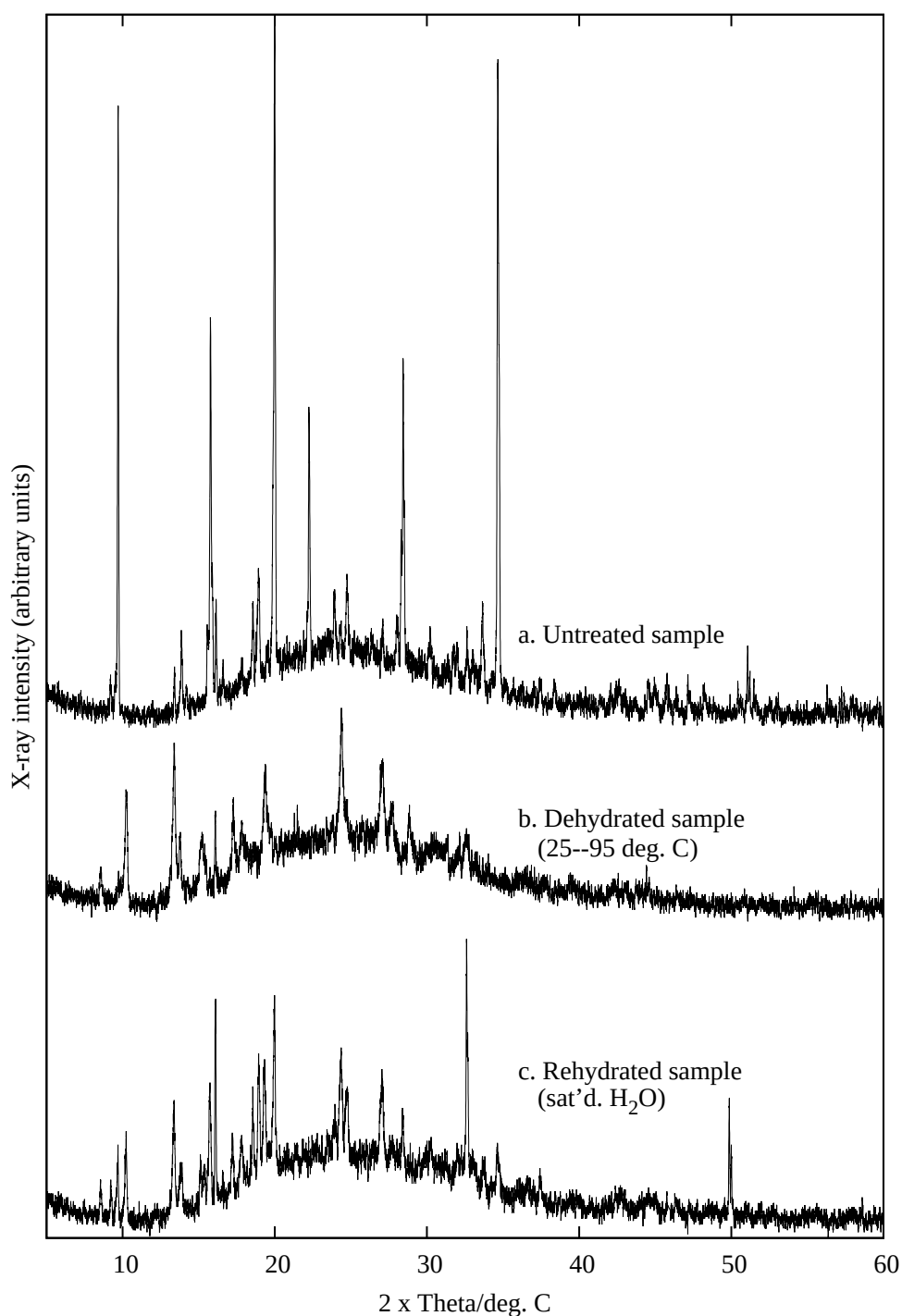


Figure 5.36: X-ray diffraction patterns for **xst-cu-b4c-so4-topxtals** (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–95 °C at 10 °C min⁻¹ under nitrogen, 26 ml min⁻¹), and (c) dehydrated as above, and exposed to open air (12 hours) and thereafter to saturated water vapour (6 hours). The patterns were obtained without any oil covering.

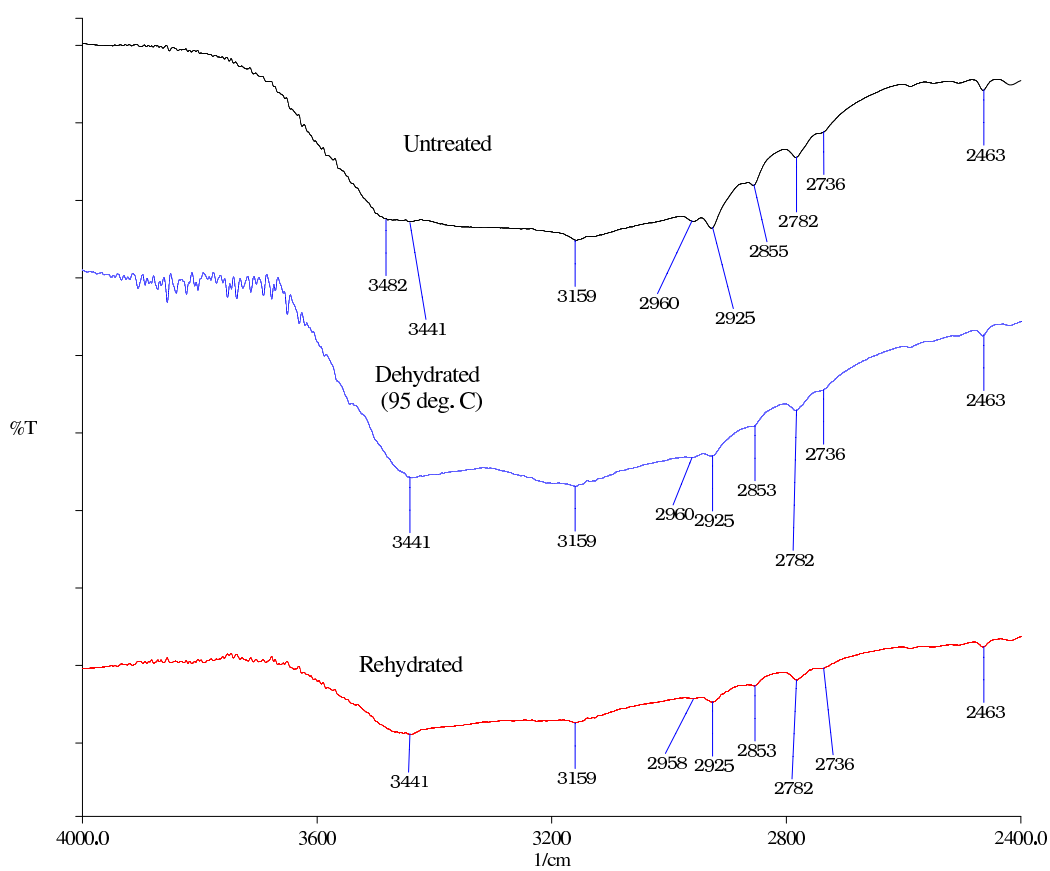


Figure 5.37: Infrared spectra of **xst-cu-b4c-so4-topxtals** in the untreated, dehydrated (by heating to 95 °C) and rehydrated states (4000–2400 cm^{-1}).

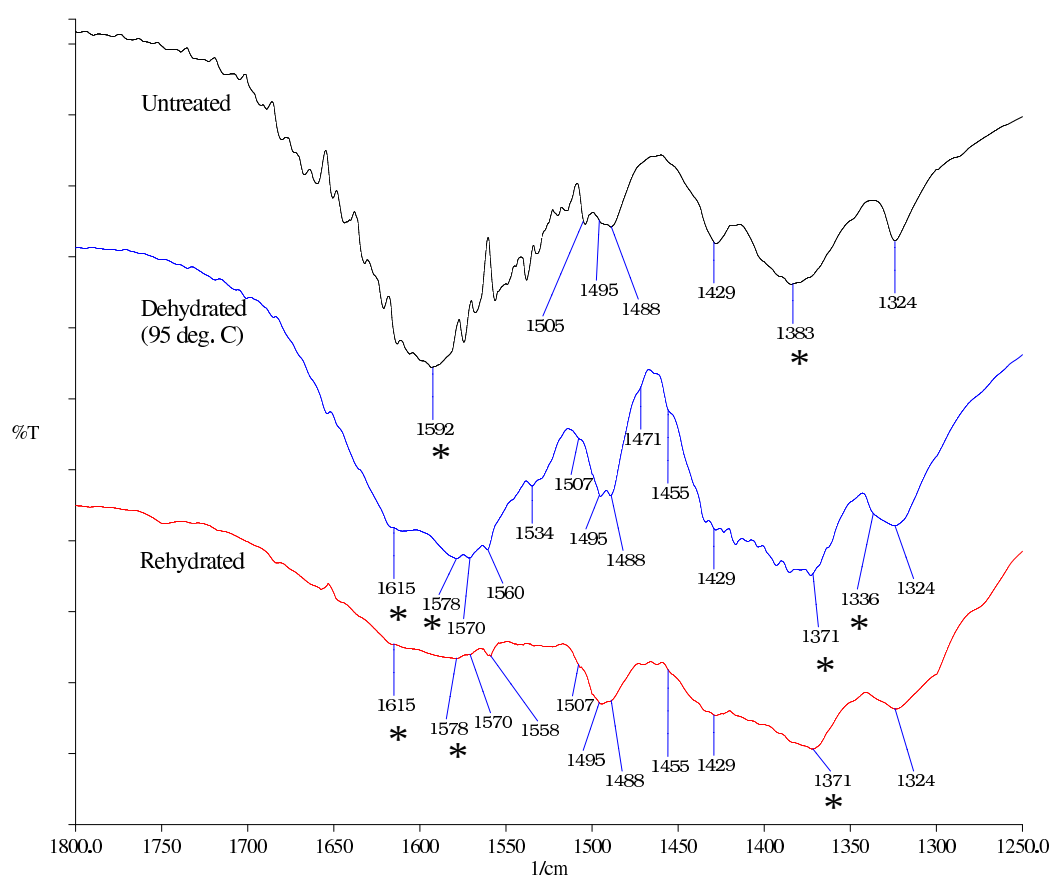


Figure 5.38: Infrared spectra of **xst-cu-b4c-so4-topxtals** in the untreated, dehydrated (by heating to 95 °C) and rehydrated states (1800–1250 cm^{-1}). Asterisks indicate important bands sensitive to change.

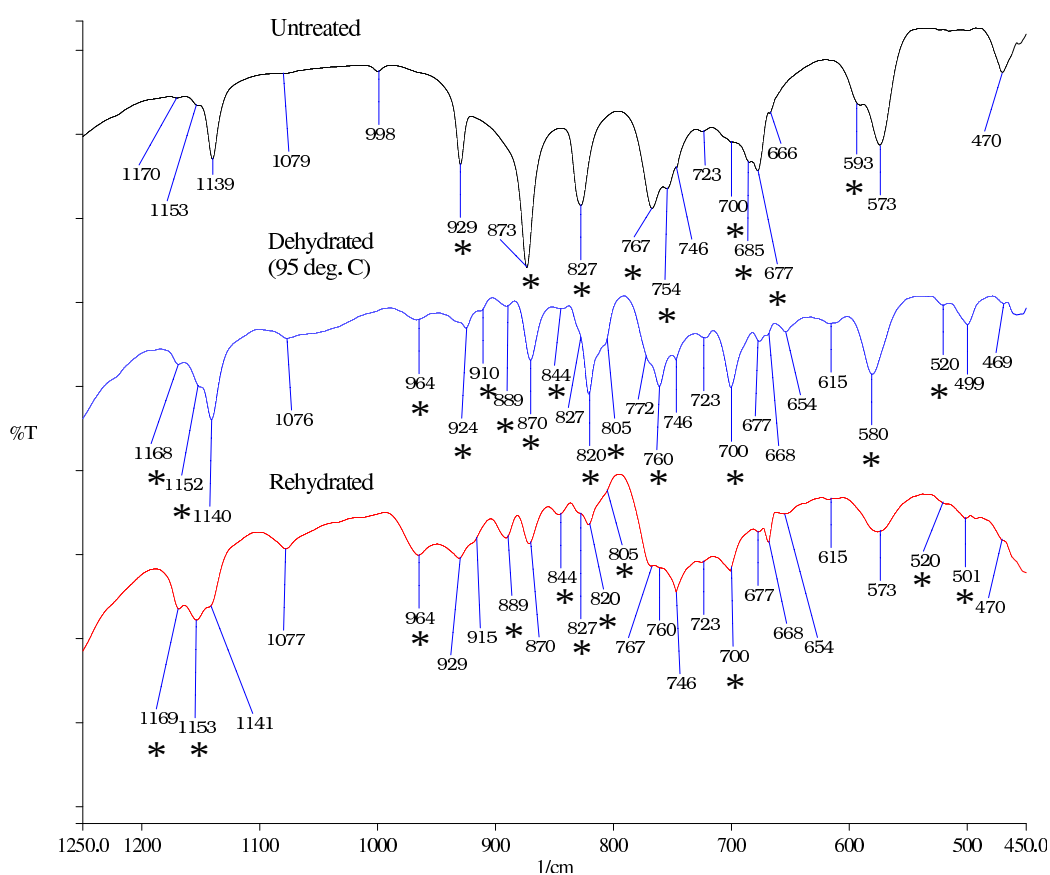


Figure 5.39: Infrared spectra of **xst-cu-b4c-so4-topxtals** in the untreated, dehydrated (by heating to 95 °C) and rehydrated states (1250–450 cm^{-1}). Asterisks indicate bands sensitive to change.

5.6.2 Single desolvation-resolution: first and second steps, water

The sample was crushed lightly and a small quantity (2.541 mg) was packed into an aluminium DSC pan and covered with a lid (not crimped). The sample was then subjected to the following treatment:

1. Heating from 25 °C to 150 °C at 10 °C min⁻¹ under nitrogen purge (26 ml min⁻¹) to drive off water. The sample mass after heating was 71.19 % of the original sample mass.
2. Exposure to saturated water vapour (25 °C) for 5 hours. The mass of the sample after exposure was 86.27 % of the original sample mass.
3. Heating from 25 °C to 350 °C at 10 °C min⁻¹ under nitrogen purge (26 ml min⁻¹) to decompose the sample. The mass of the residue was 0.692 mg, corresponding to 40.93 % of the original sample mass.

The DSC and derivative DSC curves are shown in Figure 5.40 (p. 224). The DSC curve of the rehydrated material resembles that of the original material in that the endotherm for the first dehydration step is much larger than the second, but the peaks are greatly reduced in intensity.

Dehydrated and rehydrated samples were obtained in the manner outlined above for comparison to the parent material by X-ray powder diffraction, and the powder patterns of these samples are shown in Figure 5.41 (p. 225). The X-ray powder diffraction patterns of the dehydrated and rehydrated materials are very much less intense than for the parent material, although this may be partly due to sample-handling. The pattern of the dehydrated material is clearly different to that of the parent material. The pattern of the rehydrated material is a superposition of the pattern of the dehydrated material and a few major peaks from the pattern of the untreated material. The rehydrated material is probably a mixture of the dehydrated and untreated structures. Thus, the dehydrated material is, on rehydration, partly restored to the structure of the untreated material, with poor crystallinity. The infrared spectra in Figures 5.43–5.45 (pp. 227–229) confirm that the rehydrated material is similar to the dehydrated material, with partial restoration to the original structure.

Figure 5.42 (p. 226) shows the X-ray diffraction patterns for the dehydrated material heated to 95 °C (curve a, discussed in the previous section) and the dehydrated material heated to 150 °C (curve b). The patterns are quite different. Several major peaks curve b do not have corresponding peaks in curve a, and many major peaks in curve a do not have corresponding peaks in curve b, so it is unlikely that curve b is a superposition of peaks from curve a and peaks corresponding to a second substance. The two dehydrated substances are therefore not identical. This agrees with the mass data, which indicates that dehydration to 150 °C entails significantly more loss of water than dehydration to 95 °C.

To see whether the dehydrated structure discussed in the previous section (dehydrated to 95 °C) might be present as an intermediate during rehydration of the present dehydrated structure, the X-ray diffraction pattern of the present rehydrated substance was compared to that of the dehydrated substance discussed in the previous section, in the range 5–20 degrees. There are some overlapping peaks, but the results are inconclusive because of the low signal intensities.

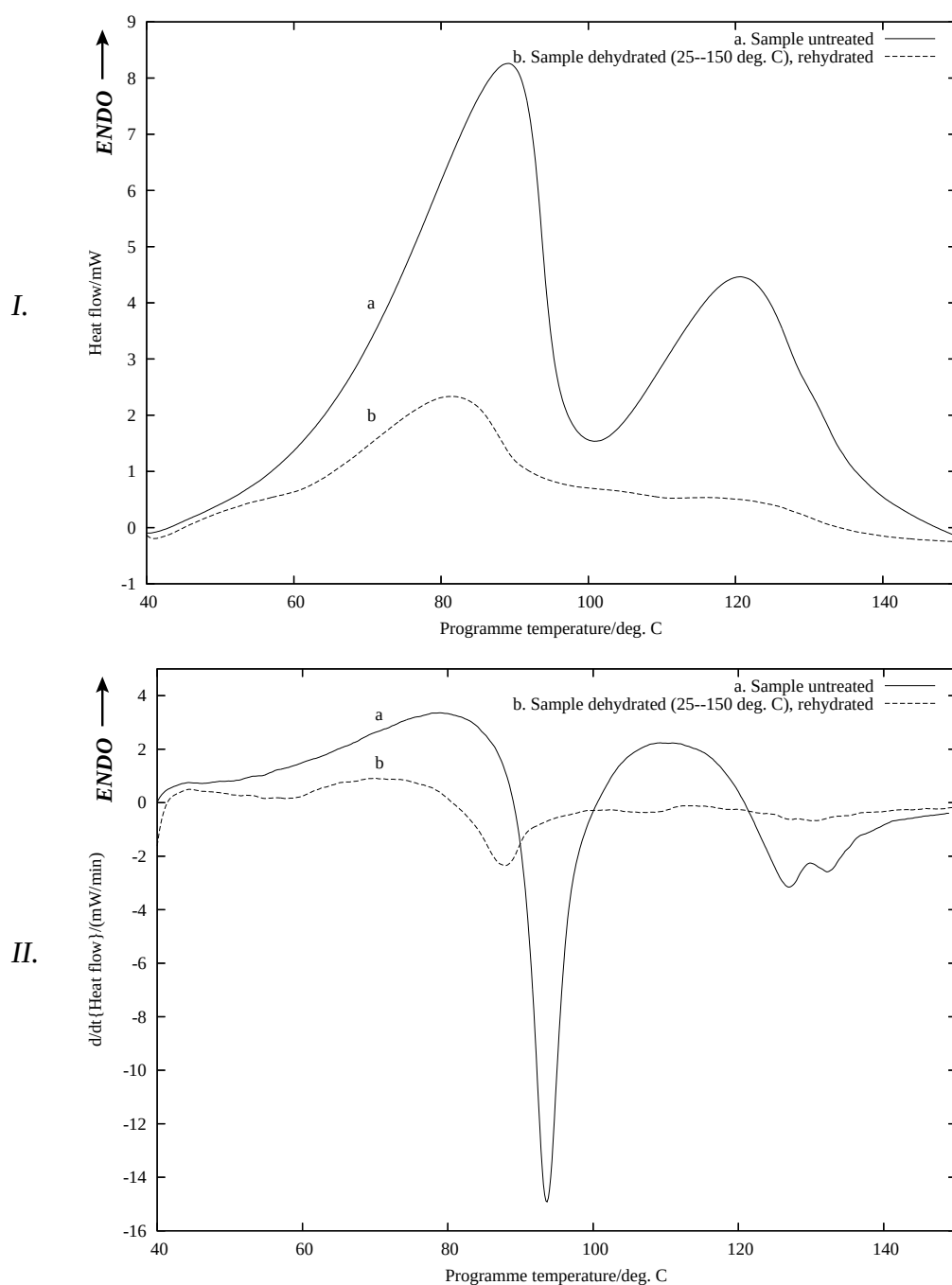


Figure 5.40: DSC (*I*) and derivative DSC (*II*) curves of **xst-cu-b4c-so4-topxtals** (a) without pre-treatment and (b) after dehydration (25 °C–150 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹) with subsequent exposure to open air (12 hours) and thereafter to saturated water vapour (25 °C) for 6 hours. In (b), the sample was decomposed by heating in the DSC (25 °C–350 °C at 10 °C min⁻¹ under nitrogen, 27 ml min⁻¹).

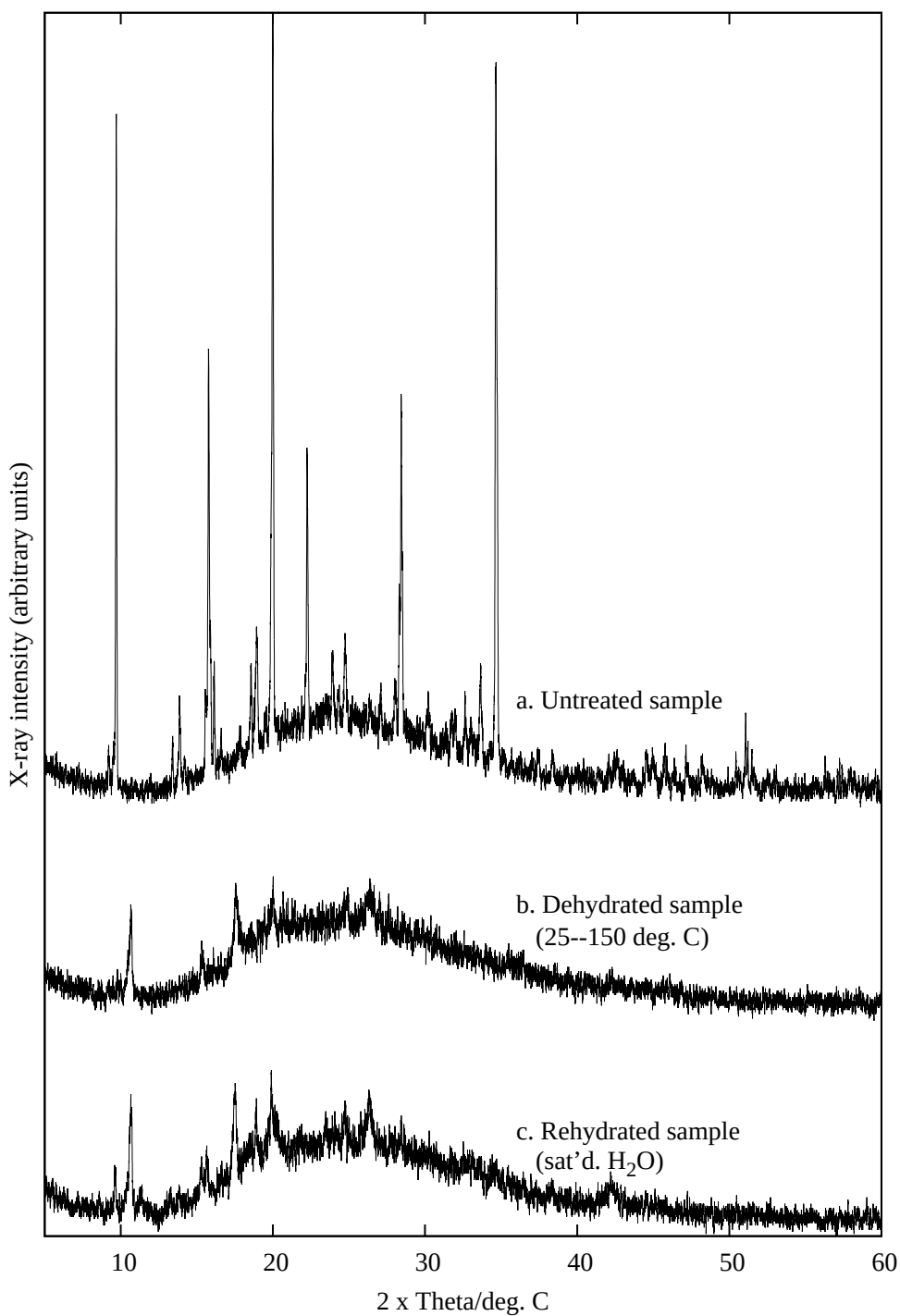


Figure 5.41: X-ray diffraction patterns for **xst-cu-b4c-so4-topxtals** (a) without pre-treatment, (b) dehydrated by heating in a DSC (25 °C–150 °C at 10 °C min⁻¹ under nitrogen, 26 ml min⁻¹), and (c) dehydrated as above, and exposed to open air (12 hours) and thereafter to saturated water vapour (6 hours). The patterns were obtained without any oil covering.

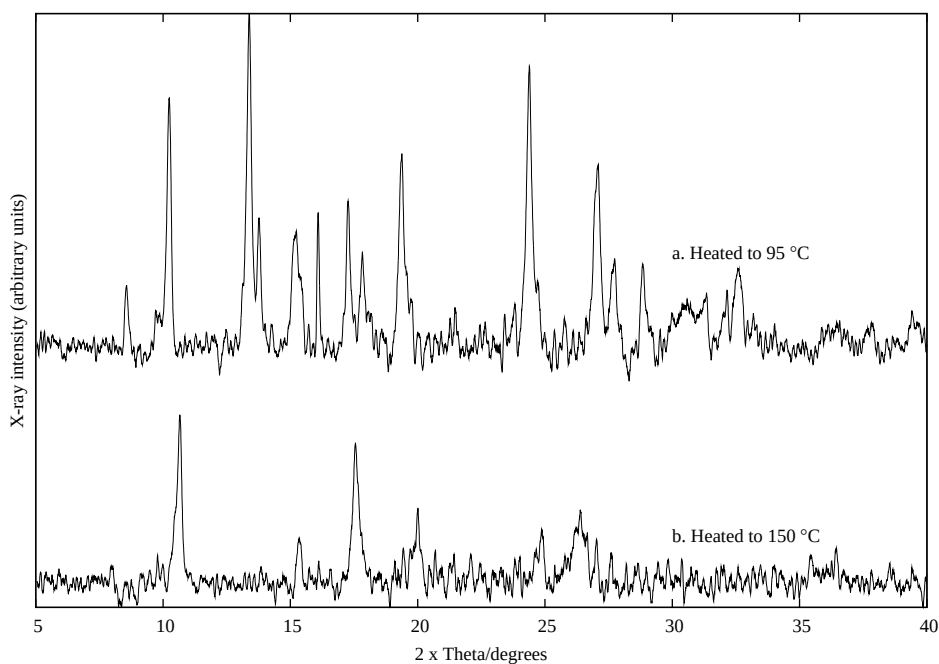


Figure 5.42: X-ray diffraction patterns of two dehydrated samples of **xst-cu-b4c-so4-topxtals**, heated to (a) 95 °C and (b) 150 °C. For ease of comparison, the patterns were obtained without any oil covering. The data sets were smoothed by means of a 20-point boxcar algorithm and, in both curves, the glass background was subtracted digitally as an interpolated spline.

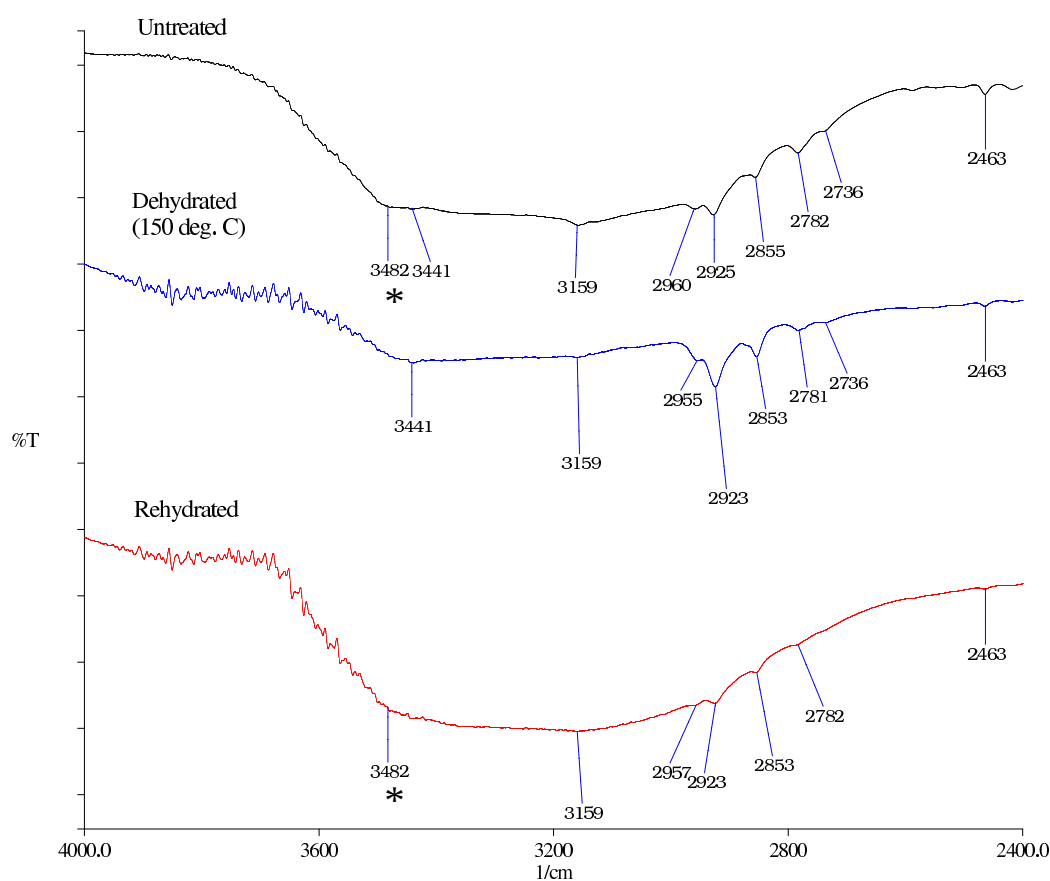


Figure 5.43: Infrared spectra of **xst-cu-b4c-so4-topxtals** in the untreated, dehydrated (by heating to 150 °C) and rehydrated states (4000–2400 cm^{-1}). Asterisks indicate important bands sensitive to change.

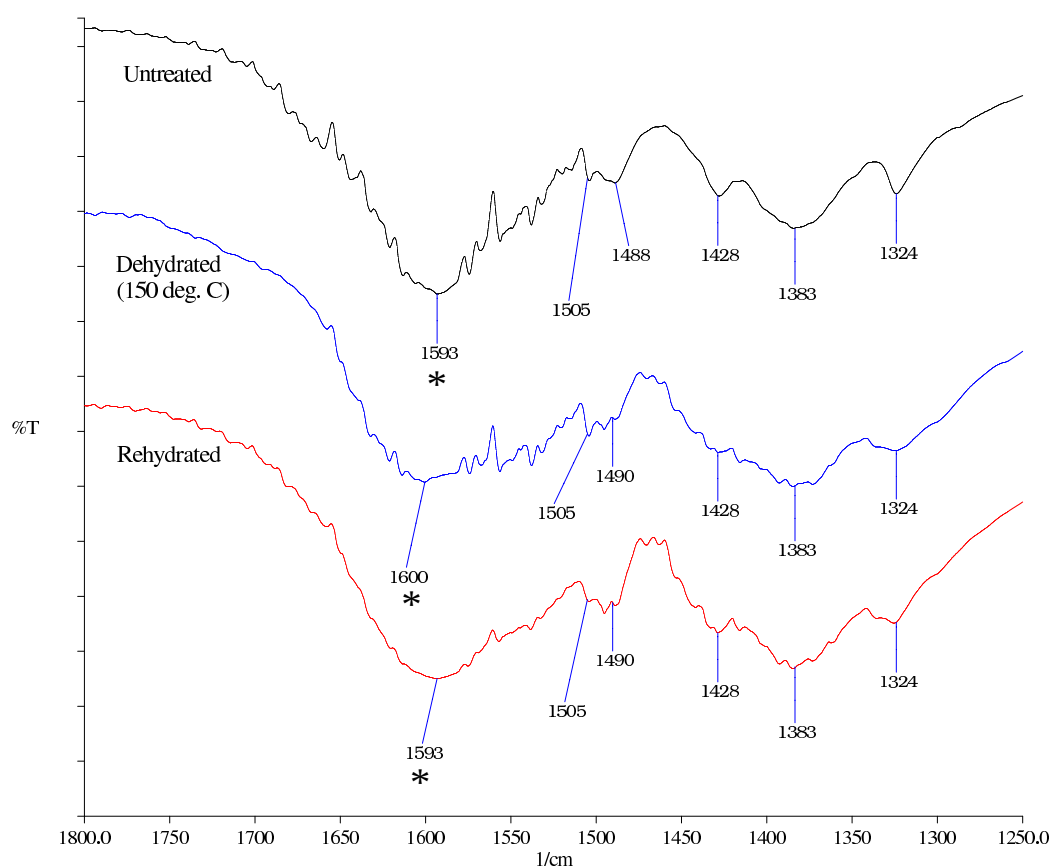


Figure 5.44: Infrared spectra of **xst-cu-b4c-so4-topxtals** in the untreated, dehydrated (by heating to 150 °C) and rehydrated states (1800–1250 cm^{-1}). Asterisks indicate important bands sensitive to change.

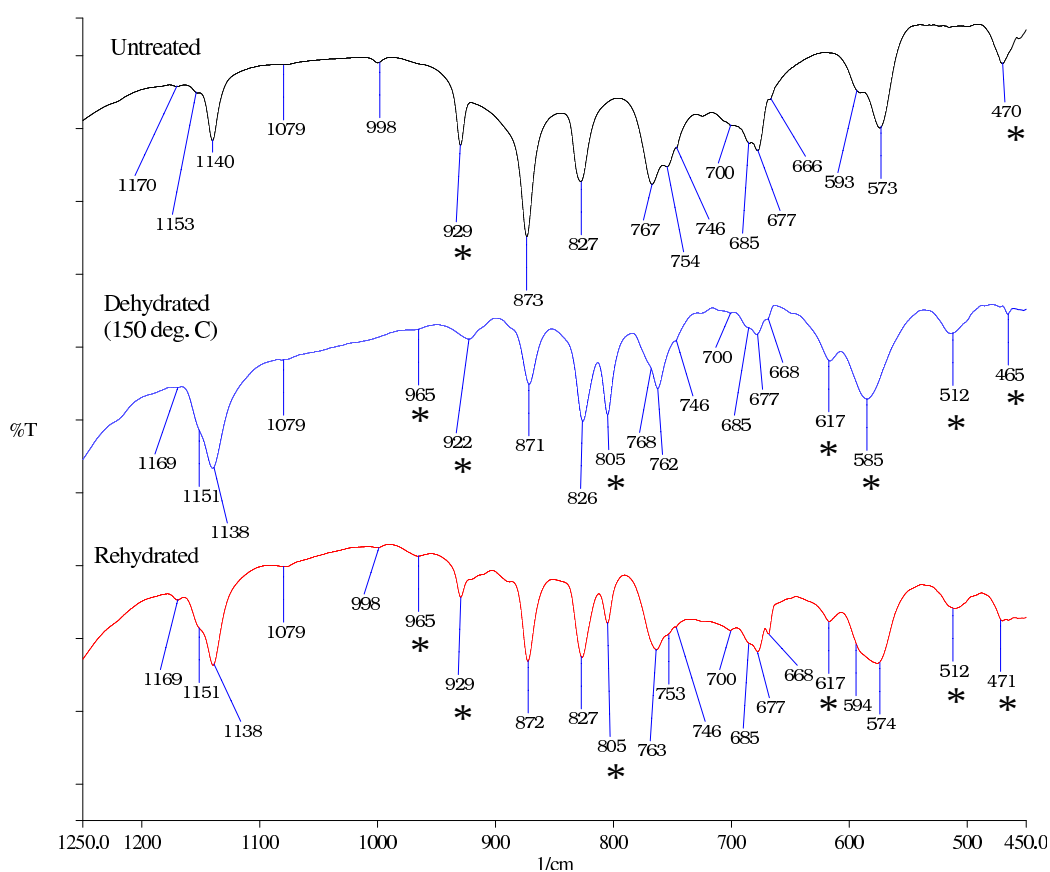


Figure 5.45: Infrared spectra of **xst-cu-b4c-so4-topxtals** in the untreated, dehydrated (by heating to 150 °C) and rehydrated states (1250–450 cm^{-1}). Asterisks indicate important bands sensitive to change.

5.6.3 Single desolvation-resolution: methanol

Similar experiments with methanol as a potential guest solvent were performed. Material that had been dehydrated to 95 °C showed no mass increase in the presence of methanol vapour, suggesting that no methanol uptake occurred. Therefore this material was not considered for further dehydration-resolution studies.

5.6.4 Further discussion

The TG and DSC data (Figures 4.15 & 4.16, p. 106) show that between 25 °C and 91 °C, five waters are lost out of a total of ten (formula unit $[\text{Cu}_2\text{L}\cdot 6\text{H}_2\text{O}] \cdot 4\text{H}_2\text{O}$). This corresponds to the loss of 20 waters out of a total of 40 per unit cell. These are most likely to be the guest water molecules O8W and O9W (and their symmetry-equivalents), and one of the symmetry equivalents of O1W, the most weakly-held coordinated water molecule. All of these are involved in the hydrogen-bonding that holds the structure together and, as shown by XRPD and FTIR, their loss results in the collapse of the structure. Also accompanying dehydration would be the creation of a vacant coordination site on every second copper(II) ion, possibly allowing for interlayer coordination via the the potential bonding interactions flagged by ‘‡’ in Figure 4.19 (p. 112). Changes in the coordination to the carboxyl group, even if incomplete, may lead to changes in geometry of the layers, leading to irreversible changes on dehydration. Partial restoration of the parent material on rehydration indicates some survival of the original binding modes, and hence the restoration of some of the original pore sites. Further dehydration, involving the loss of further coordinated water molecules, would cause similar rearrangements, perhaps to a greater extent, and on rehydration, fewer of the original pore sites would be restored.

The pore-volumes calculated using PLATON were again smaller than the approximated volumes for the equivalent amounts of bulk water (see Table 5.5). For deletion of *six*¹⁰ water molecules per formula unit of $[\text{Cu}_2\text{L}\cdot 6\text{H}_2\text{O}] \cdot 4\text{H}_2\text{O}$ (i.e., 24 from the unit cell), two pores each with a volume of 239 Å³ (total porosity, 24 %) were found, equivalent to four bulk water molecules (i.e., 16 per unit cell). For deletion of *ten* water molecules per formula unit, one pore with a volume of 967 Å³ (total porosity, 49 %) was found, equivalent to 8 bulk water molecules

(i.e., 32 per unit cell). This disparity may be explained by more dense packing of coordinated water molecules, but it is important to note that these pore volumes do not describe the porosity of the dehydrated material or of the rehydrated material, but only the volumes occupied by water molecules in the parent structures. Also, the calculated pore volumes are again heavily dependent on the probe-radius setting used in the calculation.

The calculated pore volumes do, however, suggest that methanol inclusion should have been possible, had the collapse of the structure been reversible, confirming that the size of the guest is not the only factor here.

5.7 CONCLUSION

Four metal organic framework compounds (two novel) were investigated for their host-inclusion properties with water, methanol, ethanol and pyridine, for each framework. The guests were tried in order of increasing size until inclusion did not occur.

The structure of **xut-cu-b4c-acet-xtals** collapsed on dehydration, but on exposure to water, methanol and ethanol (in turn) there was significant guest-uptake, and the original structure was almost completely restored. No significant guest-uptake was observed with pyridine, and coordination to the copper(II) ions by a small amount of pyridine may cause irreversible changes to the structure, preventing re-opening of the collapsed pores. This material survives repeated desolvation/resolution cycles with water and methanol. For the methanol-resolvated material, a small amount of methanol remains within the collapsed structure after desolvation, and this trapped methanol is slowly evolved on heating until the main decomposition temperature is reached. The loss of all the trapped guest molecules appears to trigger the final decomposition. The space occupied by the guest species inside the framework, as calculated using PLATON, correlated well with the equivalent volumes of these species in the bulk liquid phase.

The structure of **xst-cu-b4c-no3-rhombi** collapses on dehydration, and is

¹⁰Deletion of five waters is not possible here, because, crystallographically, the formula unit is made up by doubling of an asymmetric residue unit consisting of one copper, half a 1,2,4,5-benzenetetracarboxylate and three water molecules.

partly restored on rehydration. No methanol uptake was observed for this material. The volume occupied by the guest water molecules in the framework, as calculated using PLATON, was significantly smaller than the equivalent volume of bulk water. This may be due to tight packing of coordinated water molecules bound to copper(II) and sodium ions in the pores.

The structure of **xst-cu-b4c-no3-lumps** collapses on dehydration, but is not restored on rehydration. The water molecules within the framework occupy less space than they would in bulk water, possibly due to tight packing of coordinated water molecules bound to copper(II) ions in the pores. The collapse of the two-dimensional layer-structure on the loss of water molecules coordinated to copper(II) may result in the formation of interlayer coordination between carboxyl oxygens and coordinatively unsaturated copper centres, partly forming a three-dimensional covalent network which cannot be restored completely to the original structure on rehydration.

The structure of **xst-cu-b4c-so4-topxtals** collapses on dehydration, and is partly restored on rehydration. The loss of water molecules coordinated to copper(II) may result in intra-layer rearrangements in covalent binding which prevent the complete restoration of the structure on rehydration. Although the dehydrated material heated to 95 °C is partly restored to the parent structure on rehydration, no guest-uptake was observed on exposure of this material to methanol.

References

- [1] **C. J. Pouchert.** *The Aldrich Library of Infrared Spectra*. 2nd ed. Aldrich Chemical Company, Milwaukee, Wisconsin, USA 1975.
- [2] **O. M. Yaghi, G. Li and H. Li.** “Selective binding and removal of guests in a microporous metal-organic framework”. *Nature* **378** (1995), 703–706. Cited in the Cambridge Structural Database, structure ZUWWET.
- [3] **J. L. C. Rowsell and O. M. Yaghi.** “Metal-organic frameworks: a new class of porous materials”. *Microporous and Mesoporous Mater.* **73** (2004), 3–14.
- [4] **C. N. Banwell.** *Fundamentals of Molecular Spectroscopy*. 2nd ed. McGRAW-HILL Book Company (UK) Limited, Maidenhead, Berkshire, England 1972.
- [5] **J. A. Dean** (editor). *Lange’s Handbook of Chemistry*. 15th ed. McGraw-Hill, Inc. 1999.
- [6] **A. L. Spek.** *PLATON: A Multipurpose Crystallographic Tool*. Utrecht University, Utrecht, The Netherlands 2001.
- [7] **D. A. Skoog, D. M. West and F. J. Holler.** *Fundamentals of Analytical Chemistry*. 7th ed. Saunders College Publishing 1996.
- [8] **G. M. Watkins.** *Ligand Isotope Vibrational Studies of Metal(II) Complexes*. Ph.D. thesis, University of Cape Town 1988.
- [9] **G. M. Watkins.** “Metal Organic Framework Compounds Involving 1,2,4,5-Benzenetetracarboxylic Acid”. Keynote Lecture, 38th Convention of the

- South African Chemical Institute, 3–8 December 2006, Durban, South Africa.
- [10] **K. Nakamoto and P. J. McCarthy** (editors). *Spectroscopy and Structure of Metal Chelate Compounds*. John Wiley & Sons, New York 1968.
- [11] **K. Nakamoto**. *Infrared and Raman Spectra of Inorganic and Coordination Compounds*. John Wiley & Sons, New York 1968.
- [12] **G. Varsányi and S. Szöke**. *Vibrational Spectra of Benzene Derivatives*. Academic Press, New York 1969.
- [13] **J. L. C. Rowsell and O. M. Yaghi**. “Effects, Functionalization, Catenation, and Variation of the Metal Oxide and Organic Linking Units on the Low-Pressure Hydrogen Absorption Properties of Metal-Organic Frameworks”. *J. Am. Chem. Soc.* **128** (2006), 1304–1315.
- [14] **C. Beevers and H. Lipson**. “The Crystal Structure of Copper Sulfate Pentahydrate $\text{CuSO}_4 (\text{H}_2\text{O})_5$ ”. *Proc. Royal Soc. Lond., Series A: Math. Phys. Sci.* **146** (1934), 570–582.
- [15] **M. Wojdyr and S. Krumm**. *Fityk 0.7.6 — User’s Manual*. <http://www.unipress.waw.pl/fityk/doc/fitykhhelp.html>. On-line manual has since been updated to cover later versions.
- [16] **I. C. Brock**. *Mn-Fit: A fitting and plotting package using MINUIT, Ver. 5.13*. http://www-zeus.physik.uni-bonn.de/~brock/mn_fit/manual/mn_fit.pdf, Physikalisches Institut der Universität Bonn, Germany 1995. Last accessed August 2007.

Part II

Copper(II) oxalate studies

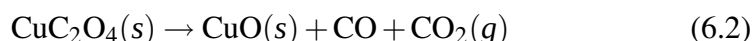
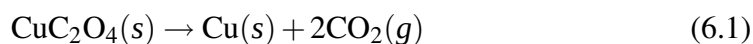
Chapter 6

Thermal behaviour of copper(II) oxalate

The thermal decomposition of copper(II) oxalate is normally reported as exothermic under non-oxidizing atmospheres. In the course of this research, it was found to be endothermic under argon, but exothermic under nitrogen. In this chapter the thermal behaviour of copper(II) oxalate under argon and nitrogen at various heating rates and purge-gas flow rates, and under oxygen, is examined, and an attempt is made to account for it.

6.1 INTRODUCTION

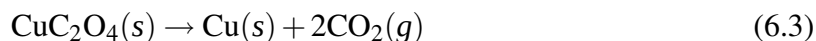
The thermal decomposition of copper(II) oxalate under nitrogen purge [1–3], in a self-generated atmosphere [4], and in various atmospheres including hydrogen and carbon dioxide [5], is reported to be exothermic, and it has been proposed that it takes place in a single step by two pathways [6, 7]:



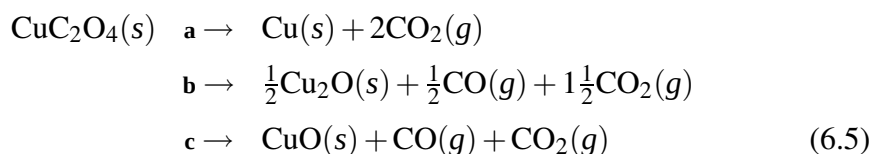
of which the first is said to predominate¹.

¹Dollimore, in [6], appears to have used, erroneously, the Ellingham diagram for the reaction, $4\text{Cu} + \text{O}_2 \rightleftharpoons 2\text{Cu}_2\text{O}$, in his thermodynamic argument to support this assertion.

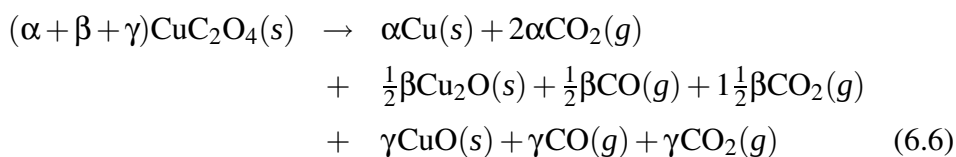
An alternative competitive decomposition mechanism, as a simplification of the mechanism proposed in the literature [4] for thermal decomposition under the self-generated atmosphere, may be devised which involves the formation of copper(I) oxide:



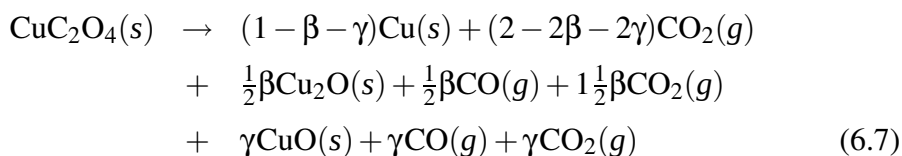
These equations may be combined into a set of three competing reactions:



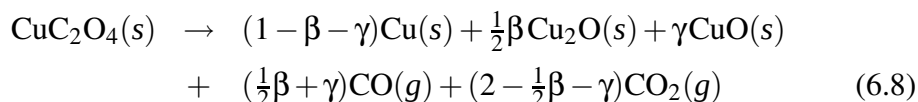
Equation 6.5 may be written as the overall chemical equation:



where $\alpha + \beta + \gamma = 1$. We may substitute for α using $\alpha = 1 - \beta - \gamma$ so that Equation 6.6 becomes:



This may be simplified to:



in which β is the fraction of the available copper(II) oxalate that undergoes de-

composition via process **b**, and γ is the fraction that undergoes decomposition via process **c**. Individually, $0 \leq \beta \leq 1$ and $0 \leq \gamma \leq 1$, and together $\beta + \gamma \leq 1$.

A thermochemical equation for this combined reaction may then be written as

$$\begin{aligned} \Delta H_r^\circ(\beta, \gamma) = & \frac{1}{2}\beta \Delta H_f^\circ \text{Cu}_2\text{O}(s) + \gamma \Delta H_f^\circ \text{CuO}(s) + (\frac{1}{2}\beta + \gamma) \Delta H_f^\circ \text{CO}(g) \\ & + (2 - \frac{1}{2}\beta - \gamma) \Delta H_f^\circ \text{CO}_2(g) - \Delta H_f^\circ \text{CuC}_2\text{O}_4(s) \end{aligned} \quad (6.9)$$

Using standard values for the enthalpies of formation of $\text{Cu}_2\text{O}(s)$, $\text{CuO}(s)$, $\text{CO}(g)$ and $\text{CO}_2(g)$ [8, p. D-38 *et seq.*], and a published value [9] of $-751.3 \text{ kJ mol}^{-1}$ for $\Delta H_f^\circ \text{CuC}_2\text{O}_4(s)$, this may be written numerically as:

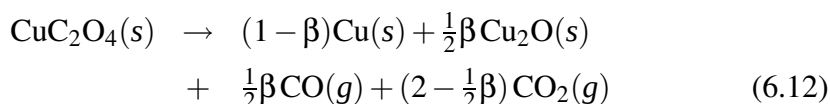
$$\Delta H_r^\circ(\beta, \gamma) / \text{kJ mol}^{-1} = 58.13\beta + 127.72\gamma - 35.56 \quad (6.10)$$

If it is assumed that only path **a** is followed, i.e., that no oxidation takes place via paths **b** and **c**, then $\Delta H_r^\circ(\beta = 0, \gamma = 0) / \text{kJ mol}^{-1} = -35.56$. If it assumed that complete oxidation takes place via paths **b** and **c**, then $\beta + \gamma = 1$, and so we may substitute using $\beta = 1 - \gamma$ in Equation 6.10 to give:

$$\begin{aligned} \Delta H_r^\circ(\gamma) / \text{kJ mol}^{-1} &= 58.13(1 - \gamma) + 127.72\gamma - 35.56 \\ &= 69.59\gamma + 22.57 \end{aligned} \quad (6.11)$$

Thus, if complete oxidation takes place via path **b** only (i.e., $\gamma = 0$), then $\Delta H_r^\circ(0) / \text{kJ mol}^{-1} = 22.57$ and if complete oxidation takes place via path **c** only (i.e., $\gamma = 1$), then $\Delta H_r^\circ(1) / \text{kJ mol}^{-1} = 92.16$. In other words, the DSC response for this reaction can be exothermic or endothermic, depending on β and γ . The most exothermic DSC response possible is $-35.56 \text{ kJ mol}^{-1}$, and the most endothermic response possible is $92.16 \text{ kJ mol}^{-1}$.

In the event that only process **a** and **b** take place (i.e., that $\gamma = 0$), then then Equation 6.8 becomes:



for which the thermochemical equation is:

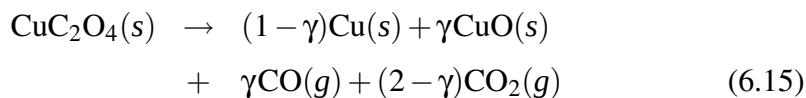
$$\begin{aligned}\Delta H_r^\circ(\beta) = & \frac{1}{2}\beta\Delta H_f^\circ \text{Cu}_2\text{O}(s) + \frac{1}{2}\beta\Delta H_f^\circ \text{CO}(g) + (2 - \frac{1}{2}\beta)\Delta H_f^\circ \text{CO}_2(g) \\ & - \Delta H_f^\circ \text{CuC}_2\text{O}_4(s)\end{aligned}\quad (6.13)$$

The corresponding numeric expression may be derived by setting $\gamma = 0$ in Equation 6.10 to give:

$$\Delta H_r^\circ(\beta)/\text{kJ mol}^{-1} = 58.13\beta - 35.56 \quad (6.14)$$

Clearly, in this case $-35.56 \leq \Delta H_r^\circ(\beta)/\text{kJ mol}^{-1} \leq +22.57$.

In the event that only processes **a** and **c** take place (i.e., that $\beta = 0$), then then Equation 6.8 becomes:



for which the thermochemical equation is:

$$\begin{aligned}\Delta H_r^\circ(\gamma) = & \gamma\Delta H_f^\circ \text{CuO}(s) + \gamma\Delta H_f^\circ \text{CO}(g) + (2 - \gamma)\Delta H_f^\circ \text{CO}_2(g) \\ & - \Delta H_f^\circ \text{CuC}_2\text{O}_4(s)\end{aligned}\quad (6.16)$$

The corresponding numeric expression may be derived by setting $\beta = 0$ in Equation 6.10 to give:

$$\Delta H_r^\circ(\gamma)/\text{kJ mol}^{-1} = 127.72\gamma - 35.56 \quad (6.17)$$

Clearly, in this case $-35.56 \leq \Delta H_r^\circ(\gamma)/\text{kJ mol}^{-1} \leq +92.16$ The equations given above provide possible explanations for the observed endothermic response under argon. It is the aim of this study to investigate how consistent the observed thermal analysis results are with the mechanisms traditionally associated with the thermal decomposition of copper(II) oxalate.

6.2 EXPERIMENTAL

6.2.1 Preparation

The copper(II) oxalate investigated here was from a stock sample which had been prepared by the method set forth in [2], i.e., by precipitation from dilute aqueous copper(II) sulfate (0.20 mol L^{-1}) and potassium oxalate (0.13 mol L^{-1}) solutions. The stock sample was dried in air at 120°C for five days prior to use.

6.2.2 Compositional analysis

Two portions of the undried and dried copper(II) oxalate were heated in the DSC under an oxygen atmosphere from 25°C to 350°C at $10^\circ\text{C min}^{-1}$, and the residues identified as CuO (tenorite) by X-ray powder diffraction. Figure 6.22 (p. 279) shows the DSC and derivative DSC curves, and Figure 6.23 (p. 280) shows a representative X-ray powder diffraction pattern of the residue. The experimental data are summarized in Table 6.1.

Table 6.1: Analytical data for undried and dried copper(II) oxalate. The expected molar mass of anhydrous copper(II) oxalate is $151.57 \text{ g mol}^{-1}$. The calculated formulae for the dried and undried material are $\text{CuC}_2\text{O}_4 \cdot 0.02\text{H}_2\text{O}$ and $\text{CuC}_2\text{O}_4 \cdot 0.1\text{H}_2\text{O}$, respectively.

Quantity	Undried		Dried	
Sample mass, m_s/mg	4.006	4.884	4.913	5.449
Residue mass, m_r/mg	2.082	2.526	2.582	2.843
% Cu	41.52	41.32	41.98	41.68
Ave. % Cu	41.42		41.83	
Ave. mol. mass/ g mol^{-1}	153.4		151.9	
Ave. % H_2O	1.2		0.2	
Ave. # H_2O	0.10		0.02	

6.2.3 X-ray powder diffraction

The undried and dried copper(II) oxalate samples, as well as representative samples of the residues from thermal analysis, were examined by means of X-ray

powder diffraction. A Philips vertical powder diffractometer, equipped with a Philips PW1965/40 proportional counter probe and a custom-built CR-RC-CR pulse-shaping amplifier/pulse-height discriminator/scaler/ratemeter/output filter unit, was used. The samples were mounted on glass slides using petroleum jelly, and a paper spacer was used to compensate for the thickness of the samples on the slides. Nickel-filtered Cu-K α radiation was used.

The X-ray powder diffraction patterns for the undried and dried copper(II) oxalate are shown in Figure 6.1 (p. 242). No observable structural changes occurred as a result of drying. The X-ray diffraction patterns obtained are similar to those reported in [10, p. 42].

6.2.4 Spectroscopy

The infrared spectra of both undried and dried copper(II) oxalate samples in KBr pellets were obtained. This matrix was chosen for easy comparison with the FTIR data for copper(II) oxalate reported in the literature [2]. The spectra are shown in Figure 6.2 (p. 243), and no change due to the drying process could be observed. Also, no trace of contamination by ionic sulfate (expected absorbance at about 1135–1075 cm $^{-1}$ [8, p. F-170]) could be detected.

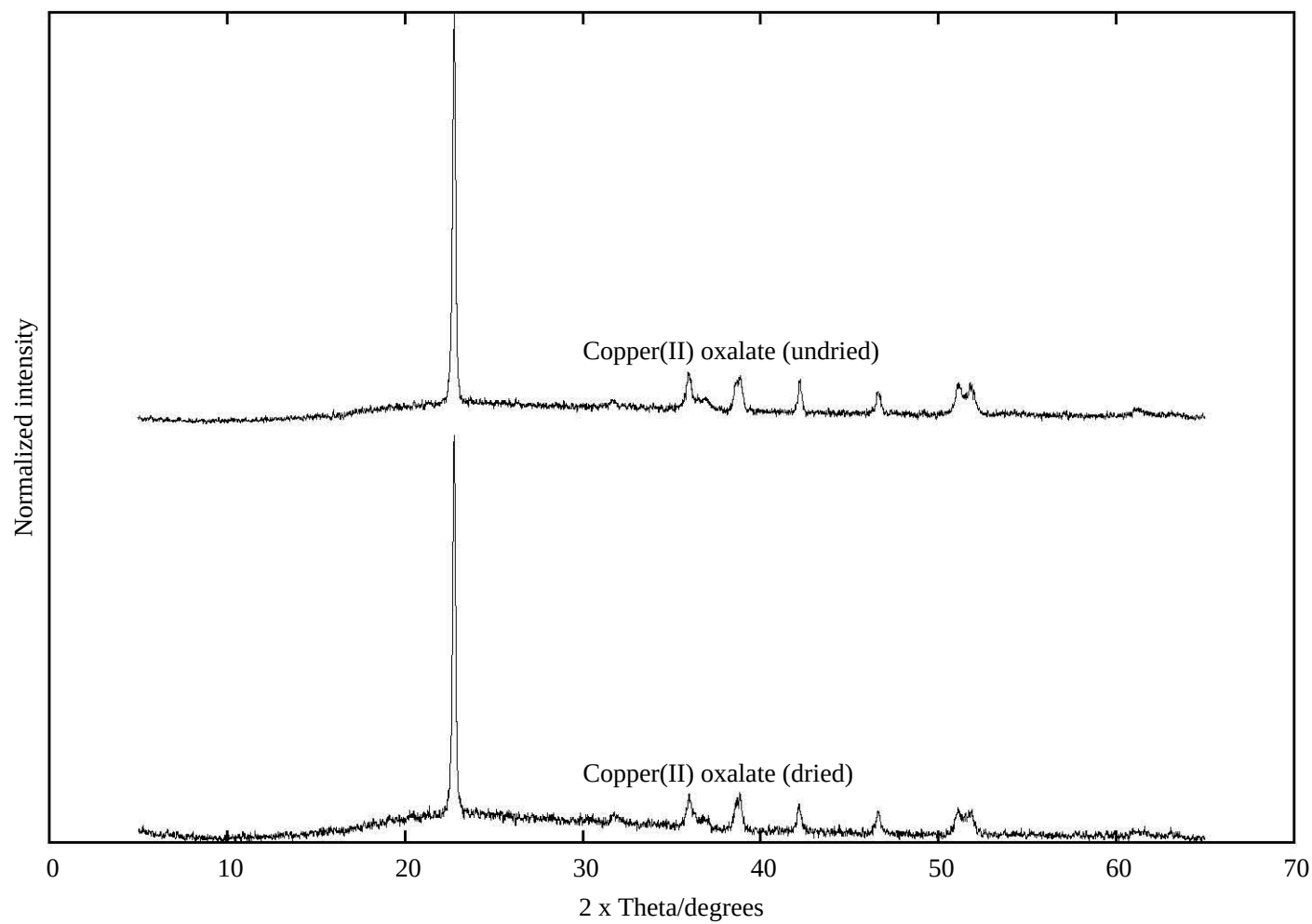


Figure 6.1: X-ray powder diffraction patterns (Cu-K_{α} radiation) for undried and dried copper(II) oxalate.

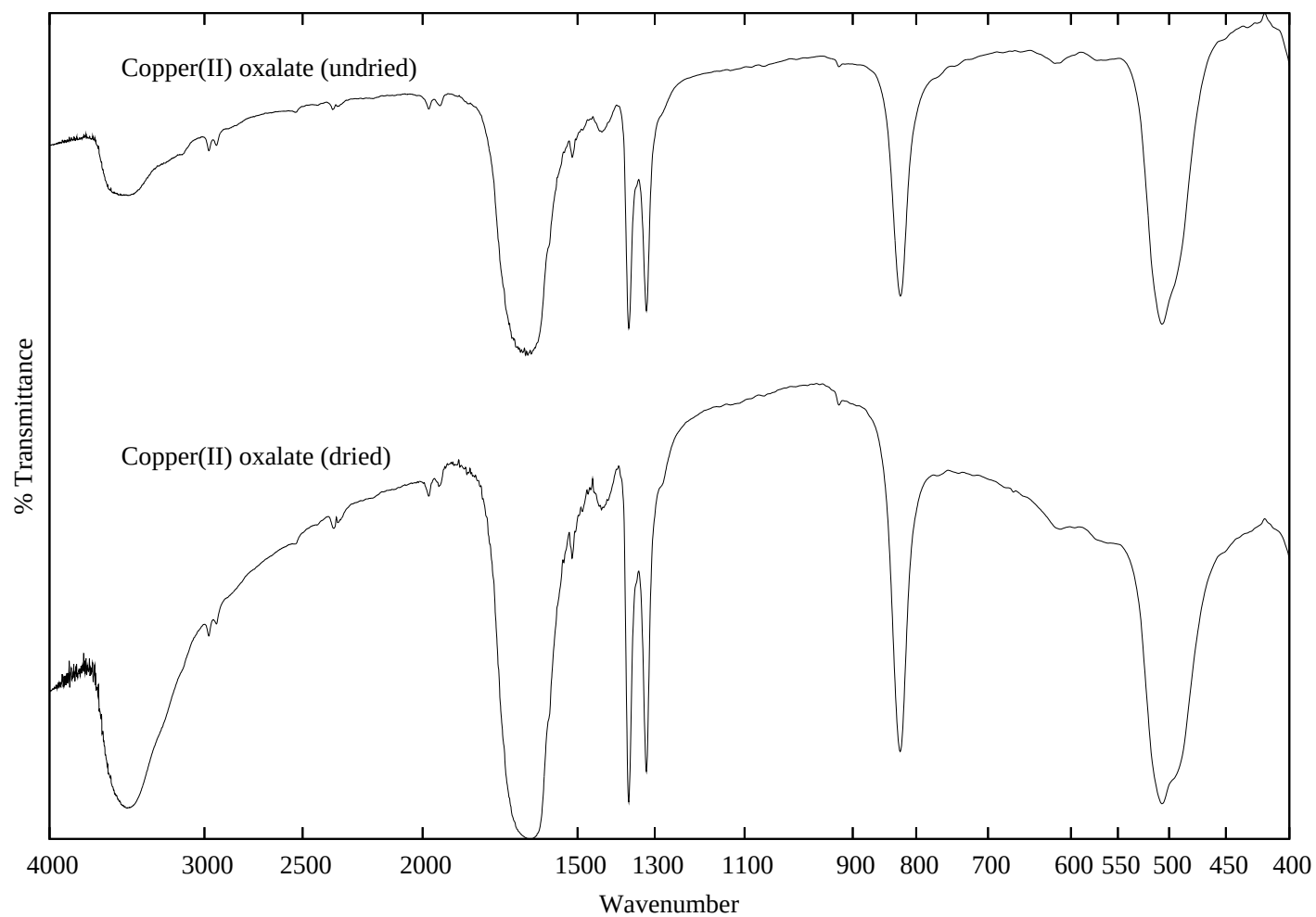


Figure 6.2: Infrared spectra of undried and dried copper(II) oxalate, obtained in KBr pellets. ***Logarithmic IR wavenumber scale.***

6.2.5 Thermal analysis

Copper(II) oxalate samples were examined by means of differential scanning calorimetry (DSC), and thermogravimetry (TG) coupled with evolved gas analysis (EGA) by FTIR. The differential scanning calorimeter and thermogravimetric analyzer were both Perkin-Elmer 7-Series instruments with Pyris Version 4.05 software.

The specifications of the purge gases used are given in Table 6.2. The pres-

Table 6.2: Specifications of the inert purge gases used. 1 vpm = 1 cm³ m⁻³ [11].

Gas	Manufacturer	Max. impurity/vpm				
		O ₂	H ₂ O	N ₂	CO ₂ + CO	C _n H _m
Nitrogen	AFROX	3	3	—	2	1
Argon	FEDGAS	2	2	6	2	1

ence of a non-indicating oxygen trap, specified to decrease the oxygen content to below 15 ppb, in tandem with an indicating trap, made no difference to the results obtained from preliminary runs, showing that the minor impurities in the cylinder gases do not interfere. Of the DSC data reported here, only the runs in cold-welded pans were performed with the oxygen trap in place.

Differential Scanning Calorimetry

The DSC was calibrated for temperature using the melting points of indium metal and zinc metal, and for heat-flow using the standard enthalpy of fusion of indium metal. These calibrations were performed under argon purge, and measurements with the same calibrants under nitrogen were practically unchanged.

DSC runs in various inert atmospheres Samples were heated from 25 °C to 350 °C at 10 °C min⁻¹ in argon, nitrogen, and mixed nitrogen-argon atmospheres. The samples were heated in crimped (but not sealed) aluminium pans. Some experiments were done under argon and nitrogen using sealed pans perforated by a single pin-prick. The solid residues were identified by means of X-ray powder diffraction.

Mixed atmospheres were generated by means of needle-valves. Each of the two components was controlled independently, and the two streams combined in a T-piece. The pressures ahead of the needle valves were set so that the minor component was at a slightly higher pressure than the major component. Gas compositions were determined by means of a common bubble-type flowmeter — the individual flow-rates were measured additively at the start of each set of runs in a given atmosphere, and subtractively after the set was complete. The average of the before and after flow rates is reported.

The DSC was purged for several hours at every change of atmosphere, and purged for at least 15 minutes after each sample change before applying the temperature programme.

DSC runs at various heating rates Samples were heated from 25 °C to 360 °C at heating rates of 10 °C min⁻¹, 5 °C min⁻¹ and 2 °C min⁻¹, under argon flowing at 25 ml min⁻¹ and under nitrogen flowing at 24 ml min⁻¹. The solid residues were identified by means of X-ray powder diffraction.

To minimize interference from residual air, the DSC was purged for at least an hour at every change of atmosphere, and for at least one hour after each sample change before applying the temperature programme.

DSC runs at various purge gas flow-rates In addition to the DSC runs above, samples were heated from 25 °C to 360 °C at 10 °C min⁻¹ under argon flowing at 17 ml min⁻¹ and under nitrogen flowing at 15 ml min⁻¹. The solid residues were identified by means of X-ray powder diffraction.

To minimize interference from residual air, the DSC was purged for at least an hour after each change of atmosphere at approximately 25 ml min⁻¹ with the atmosphere to be used, and for a further hour after placing the sample in the instrument. Thereafter, the flow was adjusted to the desired level (as measured by means of a bubble flow-meter) and the temperature programme applied.

DSC runs in oxygen Samples were heated from 25 °C to 350 °C at 10 °C min⁻¹ under oxygen flowing at 36 ml min⁻¹. The solid residues were identified by means of X-ray powder diffraction.

Thermogravimetry

The TG was calibrated for temperature under argon purge using the Curie points of Perkalloy and zinc, and for mass against a 20 mg standard mass. Furnace calibration was performed as recommended by the manufacturers.

Samples were heated from 25 °C to 315 °C at 10 °C min⁻¹, under nitrogen and under argon flowing at approximately 100 ml min⁻¹ (balance purge + sample purge). The solid residues were identified by means of X-ray powder diffraction.

To minimize the effect of residual air, the TG furnace was purged in the closed position for at least an hour at each change of atmosphere, and for at least fifteen minutes at each sample change. In addition, the furnace tube was kept at a positive pressure of the atmosphere in question whenever opened to insert a sample.

6.2.6 Evolved gas analysis

The TG exhaust line was interfaced to an FTIR gas cell fitted to a Perkin-Elmer FTIR-2000 spectrometer. To test whether the evolution of carbon monoxide could be detected in the purge gas in the presence of the exposed platinum parts of the furnace, a sample of nickel squarate dihydrate (NiC₄O₄ · 2H₂O) — whose gaseous decomposition products have been analyzed by mass spectrometry and shown to consist mainly of carbon monoxide and water with a small amount of carbon dioxide [12] — was decomposed in argon. A weak IR absorption was observed in the carbon monoxide region (doublet-envelope centred at 2143 cm⁻¹ [13]).

6.3 RESULTS AND DISCUSSION

6.3.1 TG-FTIR in inert atmospheres

TG curves

The TG curves for copper(II) oxalate heated from 25 °C to 315 °C at 10 °C min⁻¹ under argon and nitrogen atmospheres are given in Figure 6.3 (p. 248). The purge gases were purified by means of a 15 ppm oxygen/moisture/hydrocarbon trap in tandem with an oxygen indicator.

The TG curves are practically identical, showing a slow mass loss of approximately 0.8 % of the sample mass between 25 °C and 264 °C, followed by rapid decomposition between 264 °C and 310 °C. Residues heated beyond 320 °C showed a marked mass gain, probably due to oxidation by residual air in the furnace.

The residues under argon and nitrogen at 315 °C account, respectively, for 43.5 % and 43.2 % of the original sample masses. By comparison, the calculated mass percentage of copper in the dried copper(II) oxalate is 41.84 %.

It is clear, therefore, that some oxidation of the copper in the samples has taken place, by residual air in the TG, or by decomposition of carbon dioxide, or both. It can be seen from the X-ray powder diffraction patterns of the TG residues in Figure 6.3 (p. 248) that a substantial amount of oxidation takes place under both argon and nitrogen atmospheres.

It is reported [14], with particular reference to copper(II) oxalate as a diagnostic tool, that residual air in TG furnaces can be extremely difficult to remove effectively because of less-than-ideal design characteristics of their purging arrangements. This is particularly true of a Perkin-Elmer TG furnace which has been modified for interfacing to an FTIR gas cell. These modifications are mentioned in the manufacturer's on-line catalogue [15], and similar modifications are described in more detail in the open literature [16].

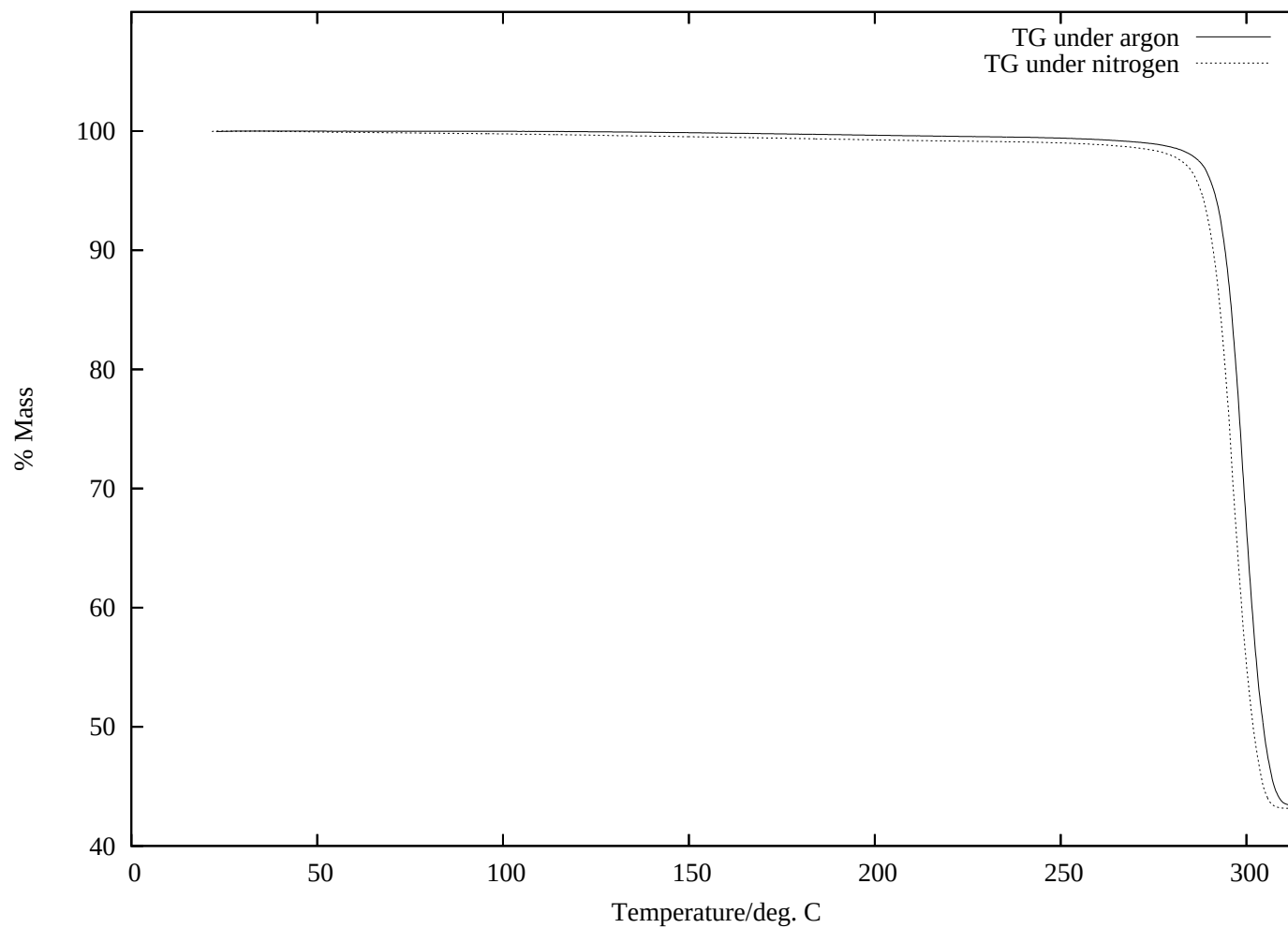


Figure 6.3: TG curves for copper(II) oxalate heated from 25 °C to 315 °C at 10 °C min⁻¹ in argon and in nitrogen at flow rates of approximately 100 ml min⁻¹. The purge gases were purified by means of a 15 ppb oxygen/moisture/hydrocarbon trap. Beyond 315 °C, the residues slowly gain mass because of residual oxygen in the TG furnace.

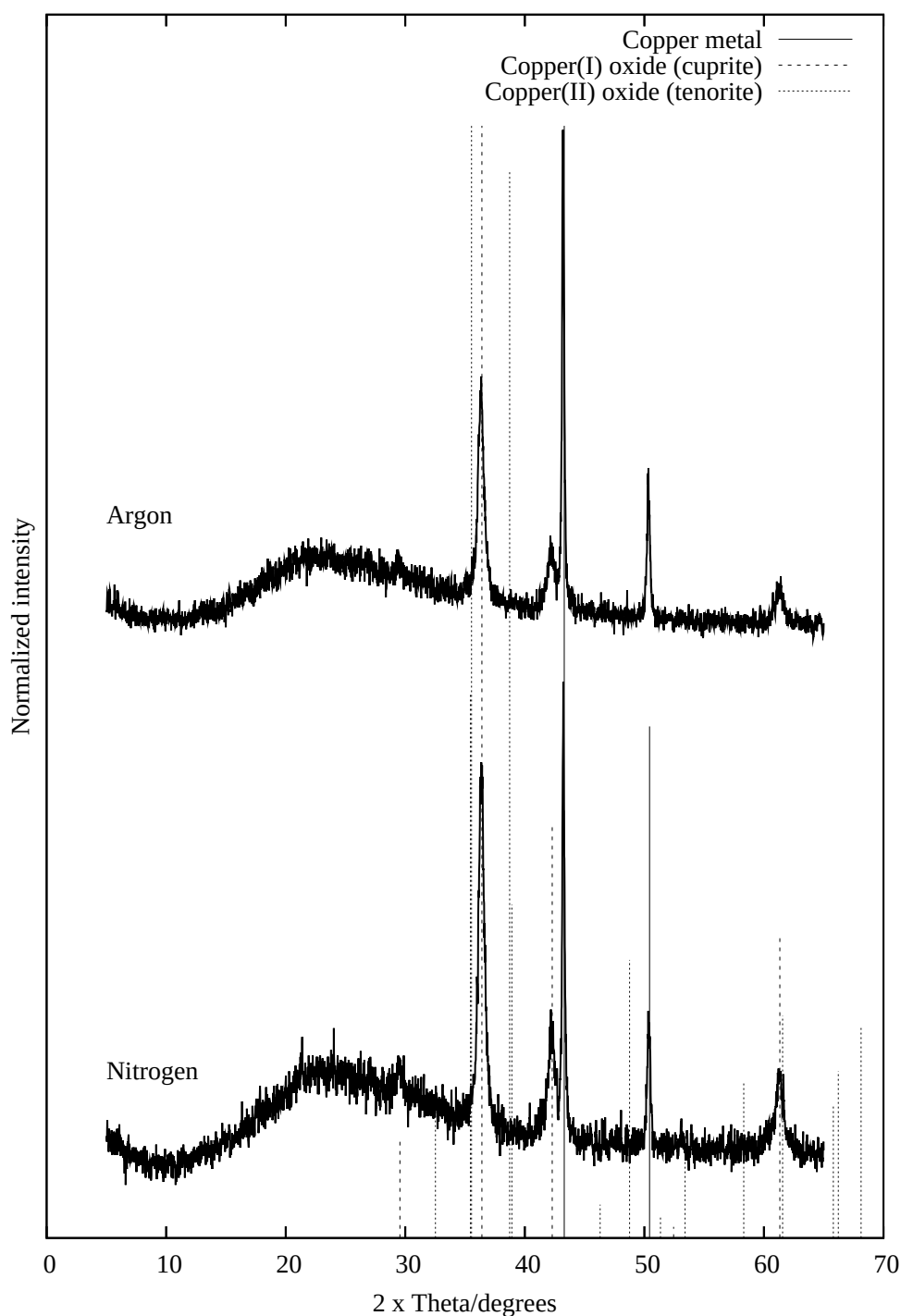


Figure 6.4: X-ray powder diffraction patterns ($\text{Cu-K}\alpha$ radiation) of the residues of copper(II) oxalate heated in a TG in open platinum pans, from 25 °C to 320 °C at 10 °C min^{-1} under argon and nitrogen atmospheres. The purge gases were purified by means of a 15 ppb oxygen/moisture/hydrocarbon trap. The vertical lines indicate the reflections for copper metal, copper(I) oxide (cuprite) and copper(II) oxide (tenorite) as calculated for $\lambda = 1.5404 \text{ \AA}$ [17, cards 4-0836, 5-0667 & 5-0661].

Evolved gas analysis

As explained above, the formation of copper(I) oxide through decomposition of carbon dioxide must result in the evolution of carbon monoxide. Three-dimensional plots of the evolved gas analysis data for TG runs under argon and nitrogen are shown in Figures 6.5 (p. 251) and 6.7 (p. 253), respectively. Individual spectra from the data-sets corresponding to argon and nitrogen are given in Figures 6.6 (p. 252) and 6.8 (p. 254), respectively.

In the three-dimensional plots, the Y-axes are labelled with the TG programme temperature as calculated from the run-time. It is clear that under both argon and nitrogen atmospheres, the main decomposition step (beginning at about 270 °C) is accompanied by the release of carbon dioxide (expected CO₂ antisymmetric stretch at 2349.3 cm⁻¹ and CO₂ bend at 667.3 cm⁻¹ [13]) and water (marked increase in the water symmetric stretch at 3651.7 cm⁻¹ [13]). In addition, a very slight disturbance in the baseplane at about (2200 cm⁻¹, 300 °C) is observable in the runs under both argon and nitrogen (Figures 6.5 and 6.7). The greatly magnified spectrum slices in this temperature region (Figures 6.6 and 6.8) exhibit the fundamental carbon monoxide absorption (doublet-envelope centred at 2143 cm⁻¹ [13]).

A considerable dead-volume exists between the TG furnace and the FTIR gas-cell, in the form of part of the furnace, part of the gas-cell's own volume, and the attendant stainless steel tubing, so a substantial broadening of the FTIR absorbance signals along the time-axis is to be expected, and a significant time-delay (approx. 1–3 min) is introduced between the appearance of a thermal event in the TG signal and the event being observed at the spectrometer. The large platinum surfaces in the TG furnace may also promote catalytic conversion of carbon monoxide to carbon dioxide in the presence of air.

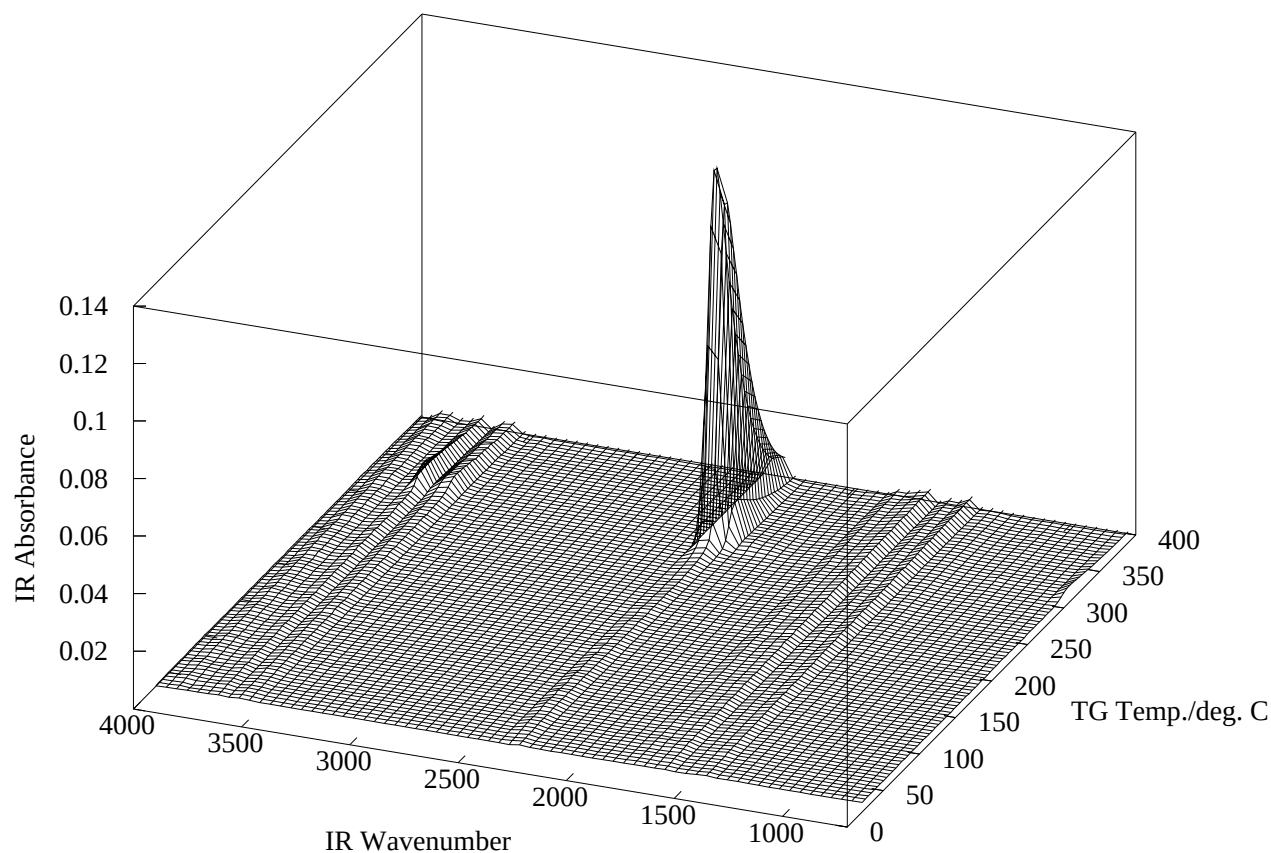


Figure 6.5: TG-FTIR evolved gas analysis results for copper(II) oxalate heated in argon. Absorbances for carbon dioxide gas and water are clearly visible beyond 280 °C, and a very slight disturbance in the baseplane at about (2200 cm⁻¹, 300 °C) suggests the evolution of a small amount of carbon monoxide (see detail in Figure 6.6 on p. 252). The samples were heated to 315 °C, the interval from 315 °C to 400 °C being plotted only because of a lag between the TG and IR responses, owing to the length of the connecting tube. **Linear IR wavenumber scale.**

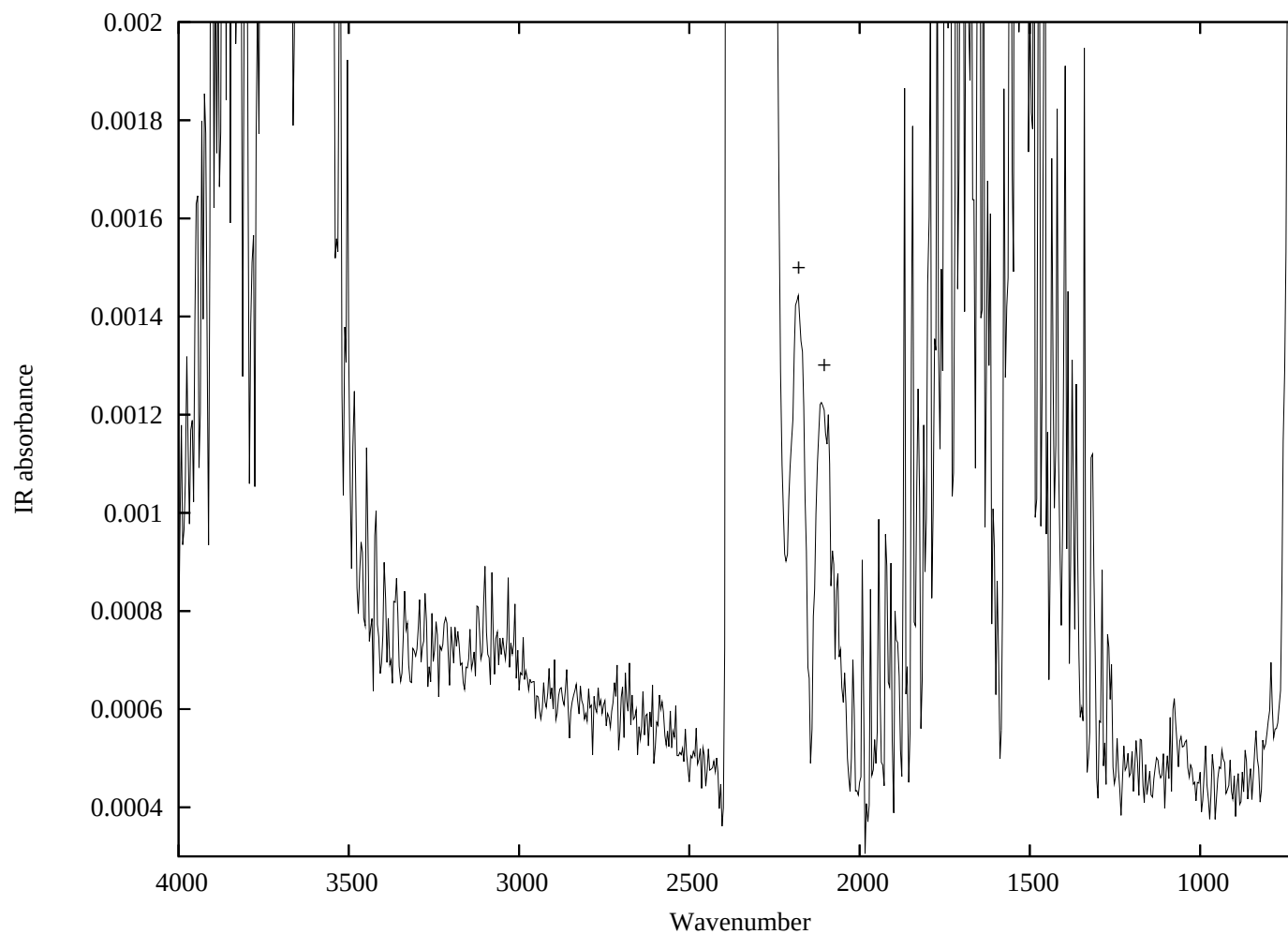


Figure 6.6: TG-FTIR evolved gas analysis results for copper(II) oxalate heated in argon: a greatly magnified spectrum slice at TG program temperature of 310.3 °C. The (+) symbols indicate peaks due to carbon monoxide gas (doublet-envelope centred at 2143 cm^{-1} [13]). Note the relative size of the water absorbances in the regions 4000–3500 cm^{-1} and 2000–1100 cm^{-1} , compared to Figure 6.5 (p. 251). **Linear IR wavenumber scale.**

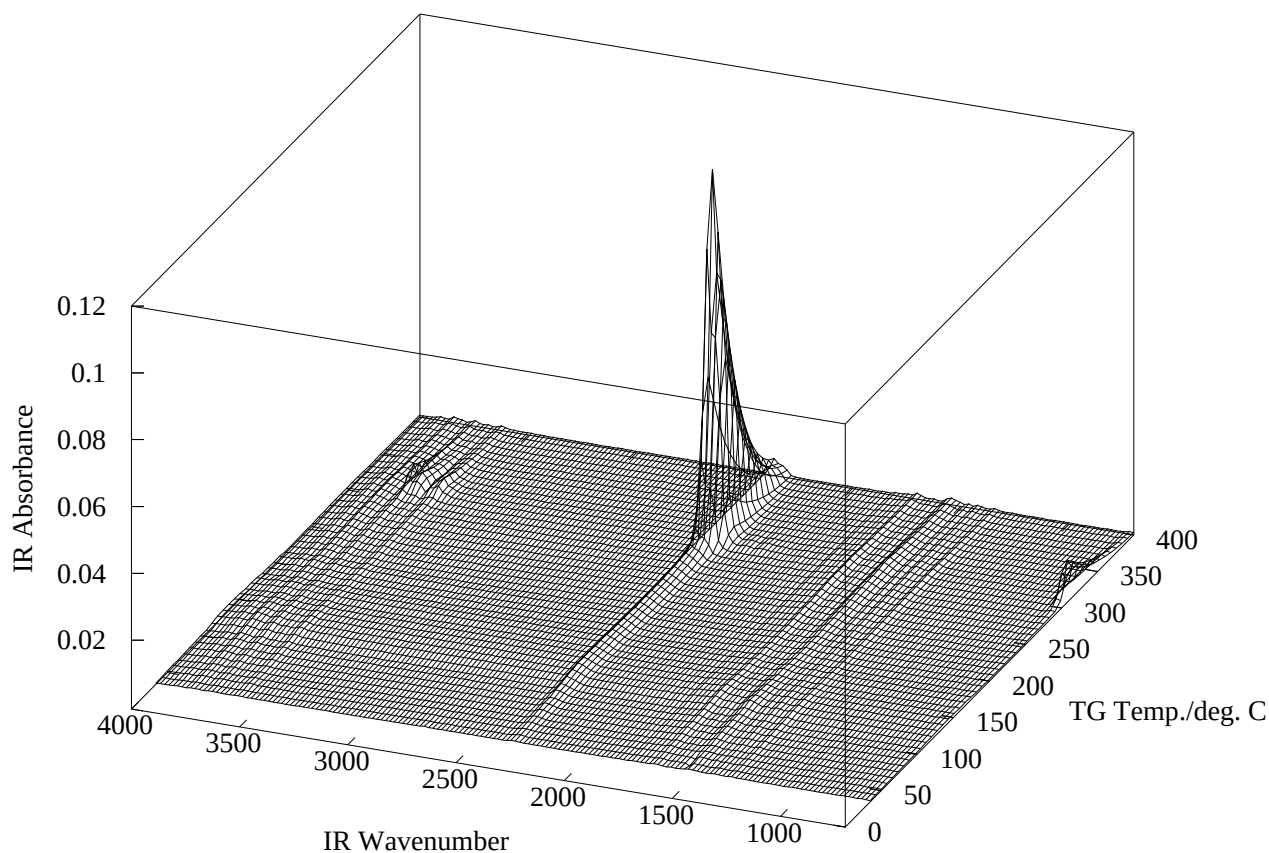


Figure 6.7: TG-FTIR evolved gas analysis results for copper(II) oxalate heated in nitrogen. Absorbances for carbon dioxide gas and water are clearly visible beyond 280 °C, and a very slight disturbance in the baseplane at about (2200 cm^{-1} , 300 °C) suggests the evolution of a small amount of carbon monoxide (compare Figure 6.6 on p. 252). The samples were heated to 315 °C, the interval from 315 °C to 400 °C being plotted only because of a lag between the TG and IR responses, owing to the length of the connecting tube. **Linear IR wavenumber scale.**

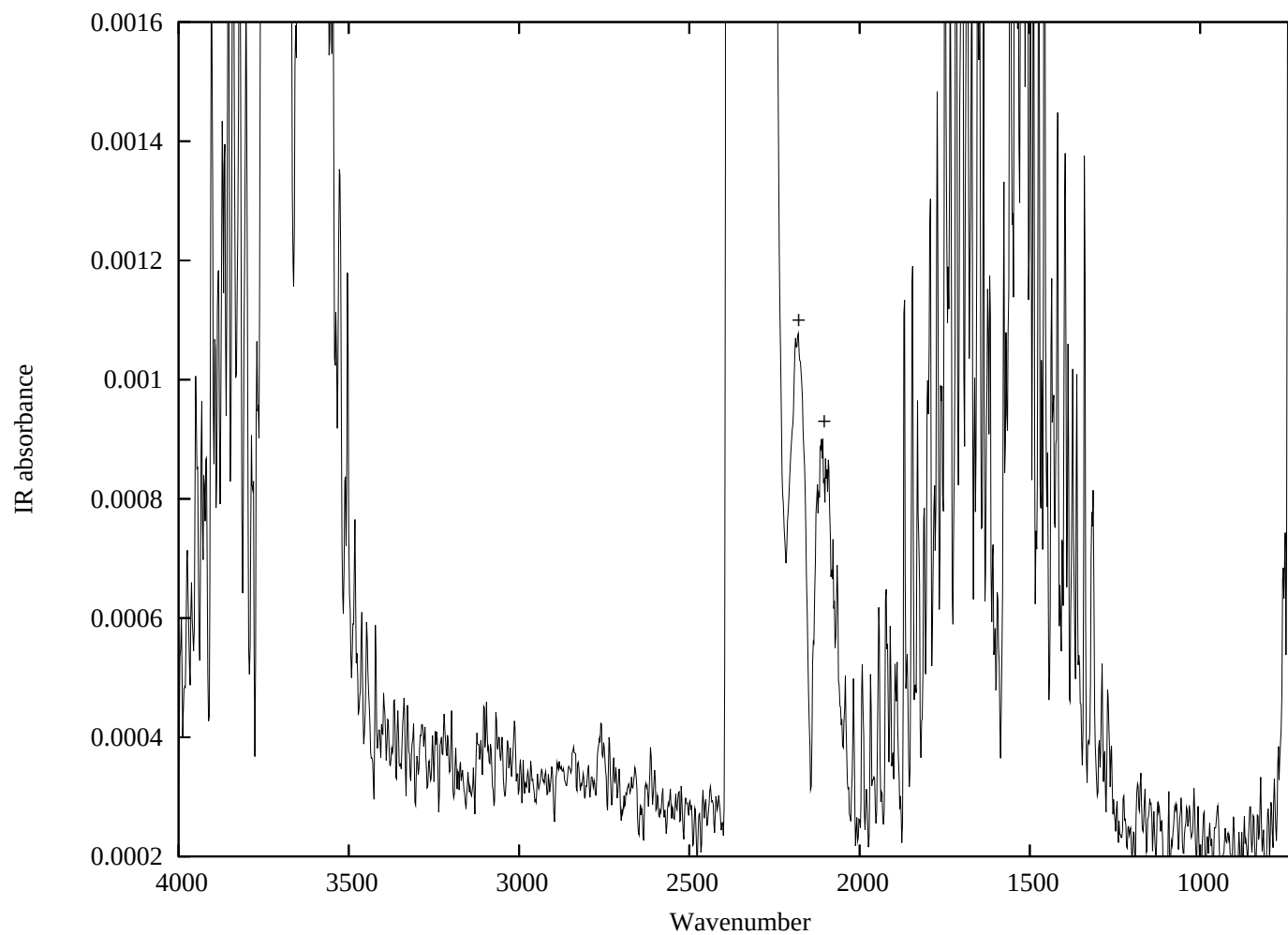


Figure 6.8: TG-FTIR evolved gas analysis results for copper(II) oxalate heated in nitrogen: a greatly magnified spectrum slice at TG program temperature of 309.8 °C. The (+) symbols indicate peaks due to carbon monoxide gas (doublet-envelope centred at 2143 cm^{-1} [13]). Note the relative size of the water absorbances in the regions 4000–3500 cm^{-1} and 2000–1100 cm^{-1} , compared to Figure 6.7 (p. 253). **Linear IR wavenumber scale.**

6.3.2 DSC in inert atmospheres

All the DSC responses for copper(II) oxalate heated under inert atmospheres consisted of a large, complex decomposition peak — endothermic under argon or an argon-rich argon-nitrogen mixture, and exothermic under nitrogen or a nitrogen-rich argon-nitrogen mixture — preceded by a small baseline disturbance or peak, typically appearing as shown in the DSC response under oxygen (Figure 6.22, p. 279). The small disturbances were sometimes obscured by noise or baseline-curvature. They also appear in the DSC curves, under nitrogen and oxygen, previously reported in [10, p. 47]. This section focuses on the main decomposition endo- and exotherms.

DSC in argon, nitrogen and mixed argon-nitrogen atmospheres

The DSC curves for copper(II) oxalate, run in argon, nitrogen and mixed argon-nitrogen atmospheres are shown in Figure 6.9 (p. 256). As the proportion of argon in the purge gas is decreased, the endothermic character of the decomposition decreases until, when nitrogen is the main component, the decomposition exhibits an exothermic character.

As shown by the endothermic peaks in Figure 6.9 (p. 256), and more clearly in the corresponding derivative DSC curves in Figure 6.10 (p. 257), the endothermic decompositions under pure argon and mainly argon atmospheres are complex, consisting of as many as four poorly-resolved stages. The exotherms share this complexity to some extent, showing two steps in the latter lobe of the derivative DSC curves. The complexity of the endotherms under argon suggests some contribution from an exothermic process which is dominant in the exothermic DSC peaks under mainly nitrogen and pure nitrogen atmospheres.

XRPD studies (Figure 6.11, p. 258) showed that, *regardless of the proportions of nitrogen and argon*, the DSC residues consisted mainly of copper metal with small amounts of copper(I) oxide (cuprite) and no discernable traces of copper(II) oxide (tenorite). The possibility that some oxidation of the residues took place during handling could not be excluded.

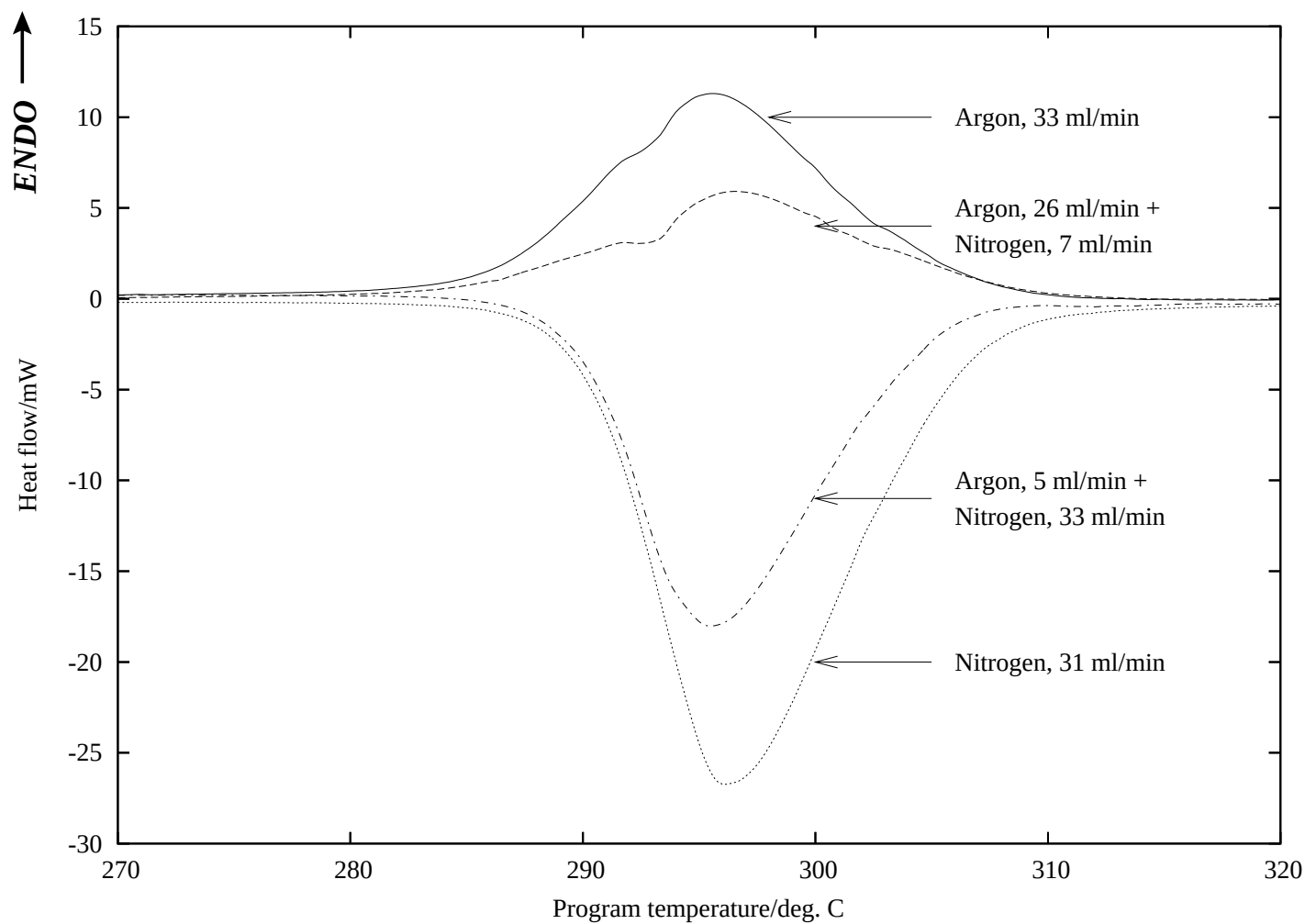


Figure 6.9: DSC curves of copper(II) oxalate, run in crimped aluminium pans, in various mixed argon-nitrogen atmospheres. Samples were heated in their specified atmospheres from 25 °C to 350 °C at 10 °C min⁻¹. Samples were of similar masses (4 mg). Baseline correction was performed by simple linear subtraction.

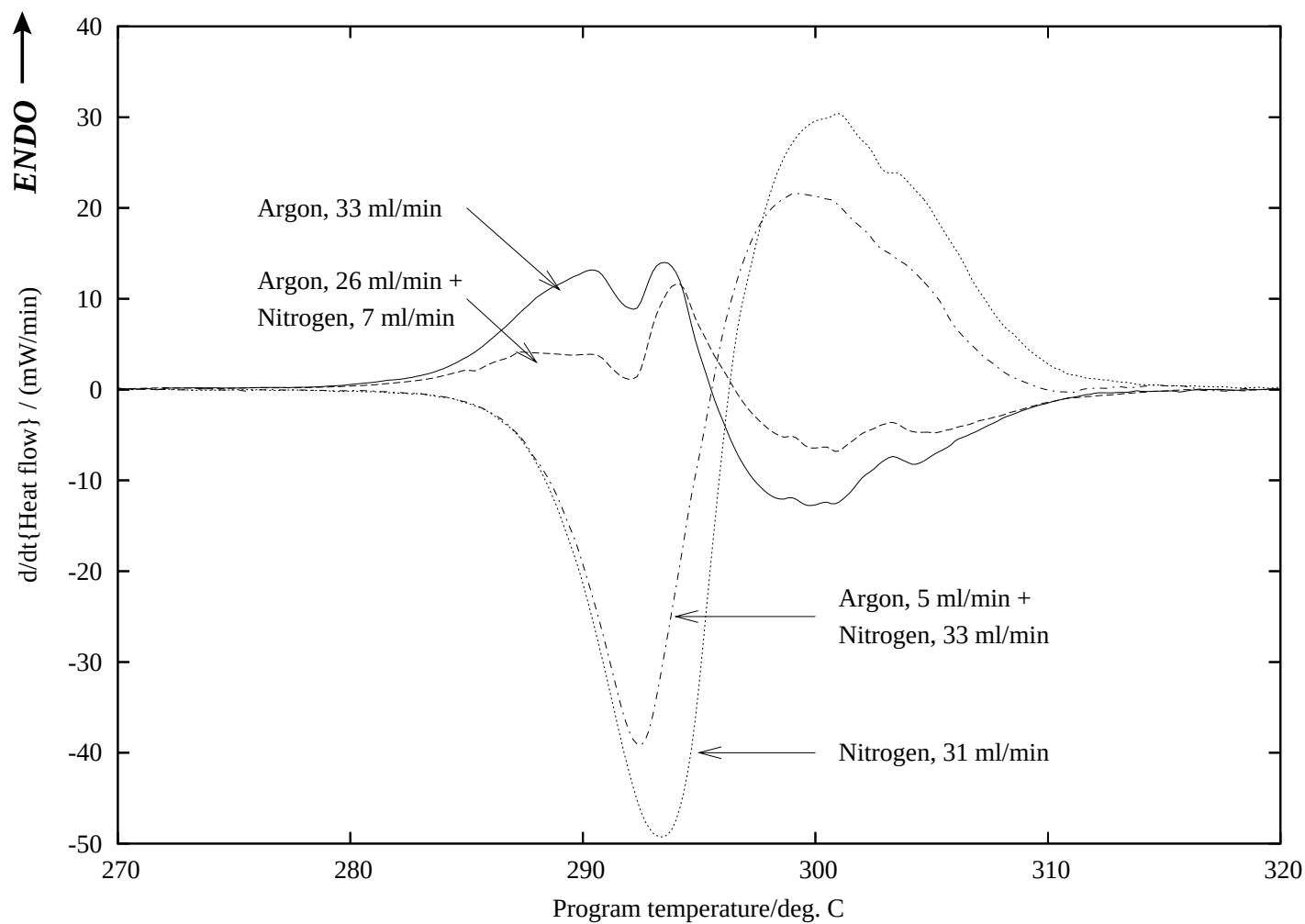


Figure 6.10: Derivative DSC curves of copper(II) oxalate, run in crimped aluminium pans, in various mixed argon-nitrogen atmospheres. Samples were heated in their specified atmospheres from 25 °C to 350 °C at 10 °C min⁻¹. Samples were of similar masses (4 mg). The derivatives were smoothed using a simple 11-point boxcar algorithm.

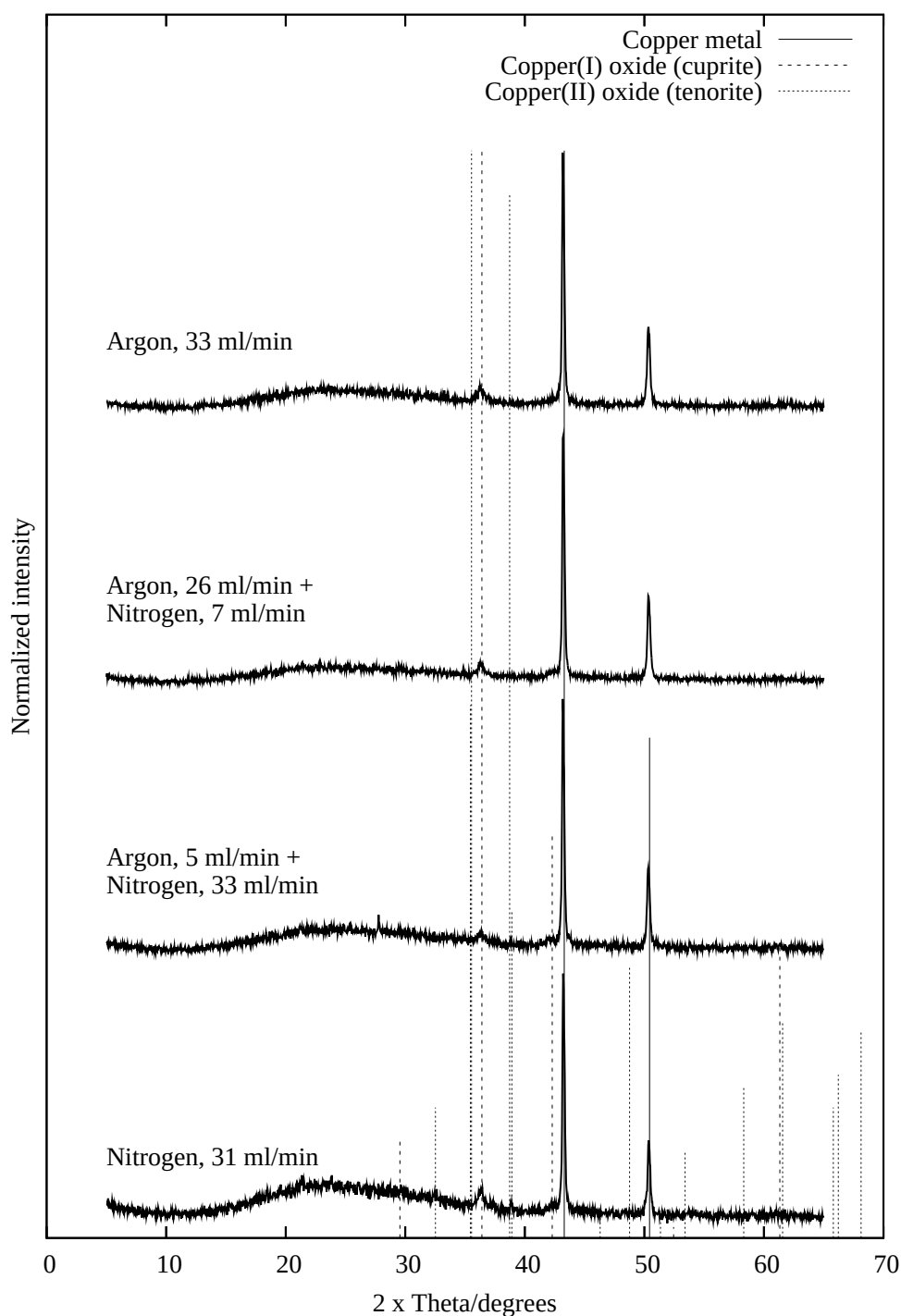


Figure 6.11: X-ray powder diffraction patterns ($\text{Cu-K}\alpha$ radiation) of the residues of copper(II) oxalate heated in a DSC in crimped aluminium pans, from 25 °C to 350 °C at 10 °C min⁻¹ under argon, mixed argon-nitrogen and nitrogen atmospheres. The vertical lines indicate the reflections for copper metal, copper(I) oxide (cuprite) and copper(II) oxide (tenorite) as calculated for $\lambda = 1.5404 \text{ \AA}$ [17, cards 4-0836, 5-0667 & 5-0661].

Tables 6.3 and 6.4 (pp. 259 and 260) summarize the mass and thermochemical data obtained from these DSC runs. The average percentages of the original sample masses that the residues constitute (i.e., the quantities $100m_r/m_s$) do not vary significantly from one inert atmosphere to the next. The calculated mass percentage of copper in the dried copper(II) oxalate (see analytical data in Table 6.1, p. 240) is 41.84%, which is very close to the experimental values of $100m_r/m_s$.

From the XRPD and mass data, there is no significant difference in the extent of oxidation to Cu_2O of the samples from one inert atmosphere to the next. There is thus no evidence from solid residues to suggest that different reactions are taking place under the four different inert atmospheres.

Table 6.3: DSC results of copper(II) oxalate heated in crimped aluminium pans, under 100% argon and 100% nitrogen atmospheres. The approximate flow-rates for argon and nitrogen were 33 and 31 ml min^{-1} , respectively. A representative sample from each triplet was found by XRPD to contain copper metal and a small amount of copper(I) oxide (cuprite).

Quantity	Argon			Nitrogen		
Sample mass, m_s/mg	4.031	4.060	4.099	3.978	4.311	4.981
Residue mass, m_r/mg	1.693	1.697	1.715	1.658	1.805	2.082
$100m_r/m_s$	41.99	41.80	41.84	41.68	41.87	41.80
Ave. $100m_r/m_s$	41.88			41.78		
Onset temp., $T_i/^\circ\text{C}$	289.1	288.4	289.3	290.1	289.7	288.9
End temp., $T_f/^\circ\text{C}$	304.7	303.8	304.4	305.9	305.5	305.2
Heat flow, $Q/\text{J g}^{-1}$	192.7	182.7	185.9	-393.6	-401.6	-397.2
Ave. $T_i/^\circ\text{C}$	288.9			289.6		
Ave. $T_f/^\circ\text{C}$	304.3			305.5		
Ave. $Q/\text{J g}^{-1}$	187.1			-397.5		
Ave. $\Delta H_r/\text{kJ mol}^{-1}$	28.42			-60.38		

To try to determine the origin of the endotherms, an attempt was made to study the thermal decomposition of copper(II) oxalate in its self-generated atmosphere. Preliminary experiments showed that cold-welded aluminium pans (sometimes used to study liquid samples) could not withstand the pressures of the evolved gaseous decomposition products, so in the experiments reported here, the samples were sealed in cold-welded pans which were then perforated by a single pin-prick.

Table 6.4: DSC results of copper(II) oxalate heated in crimped aluminium pans under mixed argon-nitrogen atmospheres. A representative sample from each triplet was found by XRPD to contain copper metal and a small amount of copper(I) oxide (cuprite).

Quantity	26 ml min ⁻¹ Argon 7 ml min ⁻¹ Nitrogen			5 ml min ⁻¹ Argon 33 ml min ⁻¹ Nitrogen		
Sample mass, m_s /mg	3.783	3.861	4.937	3.372	3.992	5.867
Residue mass, m_r /mg	1.584	1.621	2.069	1.404	1.668	2.454
$100m_r/m_s$	41.87	41.98	41.91	41.64	41.78	41.83
Ave. $100m_r/m_s$	41.92			41.75		
Onset temp., T_i /°C	291.4	291.6	289.9	289.4	289.9	288.5
End temp., T_f /°C	304.4	304.7	302.4	304.6	304.7	302.9
Heat flow, Q /J g ⁻¹	109.2	109.8	112.3	-248.1	-253.7	-267.7
Ave. T_i /°C	291.0			289.3		
Ave. T_f /°C	303.8			304.1		
Ave. Q /J g ⁻¹	110.4			-256.5		
Ave. ΔH_r /kJ mol ⁻¹	16.77			-38.96		

It was hoped that the tiny pin-hole would allow the evolved gases to escape slowly under pressure, thus surrounding the decomposing samples with their own self-generated atmosphere during decomposition. To maintain the calibration of the instrument, the furnace was purged with argon or nitrogen during the experiments.

The results are similar to those with crimped (unsealed) pans, as shown in Figures 6.12 (p. 262) and 6.13 (p. 263), but not as self-consistent. Under argon purge, an *endothermic* decomposition was observed, whereas under nitrogen an *exotherm* was obtained. While the DSC and derivative DSC curves are similar to those obtained with crimped pans under the same conditions (compare with Figures 6.9 and 6.10 on pp. 256 and 257), the more complex details of the peaks are not as clearly visible.

The mass and thermochemical data for duplicate runs under these conditions are given in Table 6.5 (p. 261). The residue mass percentages (i.e., $100m_r/m_s$) are a good match for the calculated mass-percentage of copper, 41.84%. The average thermochemical data for the runs under nitrogen are very close to those obtained using crimped pans (compare Table 6.3), but the average ΔH_r under argon is about

1.6 times as great.

Table 6.5: DSC results of copper(II) oxalate heated under 100% argon and 100% nitrogen atmospheres. The samples were run in sealed aluminium pans of the cold-welded type, which were perforated with a single pin-prick.

Quantity	Argon		Nitrogen	
Sample mass, m_s/mg	2.647	3.082	3.572	5.367
Residue mass, m_r/mg	1.104	1.277	1.486	2.237
$100m_r/m_s$	41.71	41.43	41.60	41.68
Ave. $100m_r/m_s$	41.57		41.64	
Onset temp., $T_i/^\circ\text{C}$	287.6	289.1	287.1	288.1
End temp., $T_f/^\circ\text{C}$	306.3	305.6	302.5	301.8
Heat flow, $Q/\text{J g}^{-1}$	331.4	283.1	-408.3	-421.1
Ave. $T_i/^\circ\text{C}$	288.4		287.6	
Ave. $T_f/^\circ\text{C}$	306.0		302.2	
Ave. $Q/\text{J g}^{-1}$	307.3		-414.7	
Ave. $\Delta H_r/\text{kJ mol}^{-1}$	46.68		-63.00	

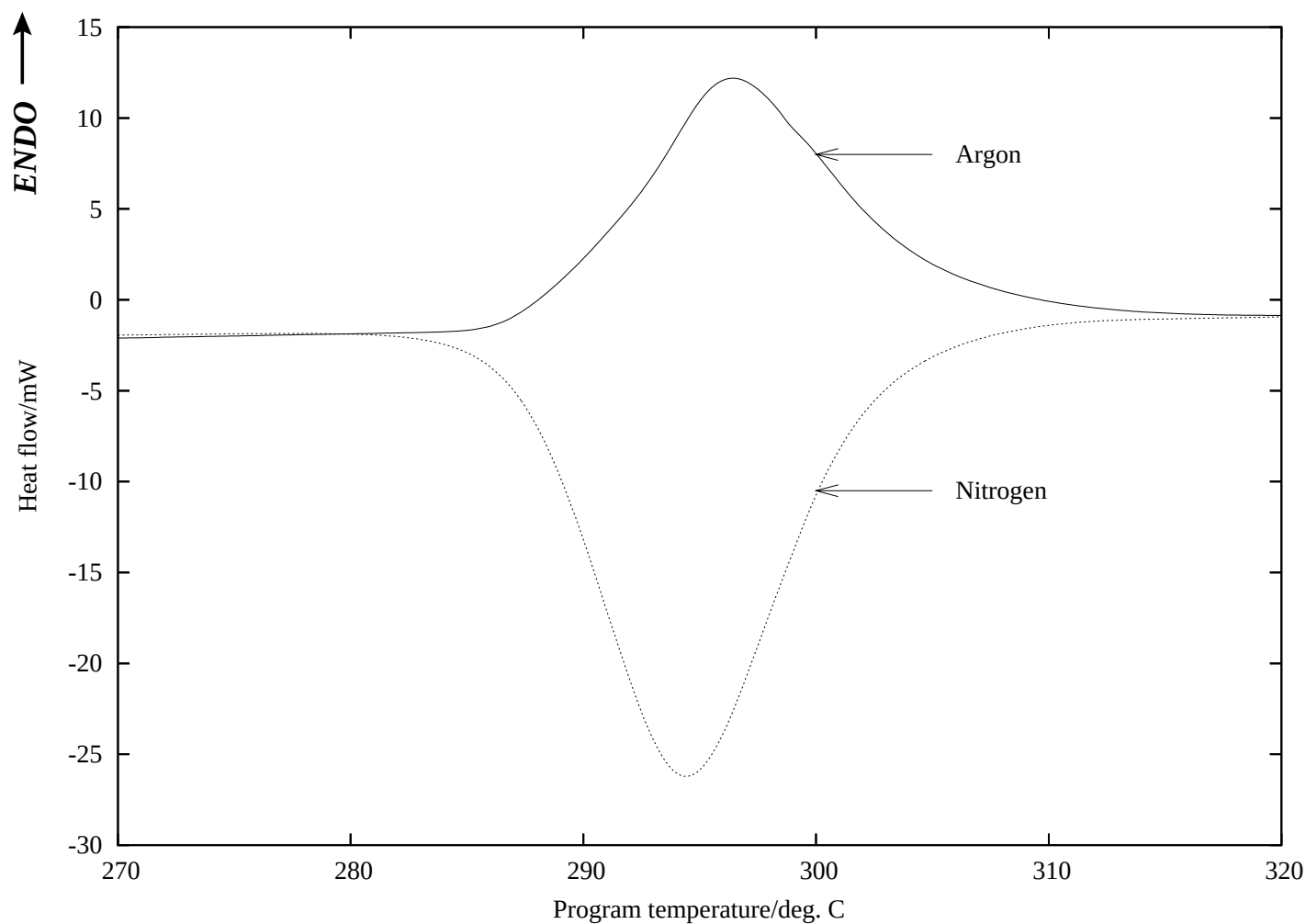


Figure 6.12: DSC curves of copper(II) oxalate in argon and nitrogen atmospheres. Samples were heated from 25 °C to 350 °C at 10 °C min⁻¹ in sealed, cold-welded pans perforated by a single pin-prick, in their specified atmospheres. The purge rates were approximately 40 ml min⁻¹. Samples were of similar masses (3 mg). Baseline corrections were performed by simple linear subtraction.

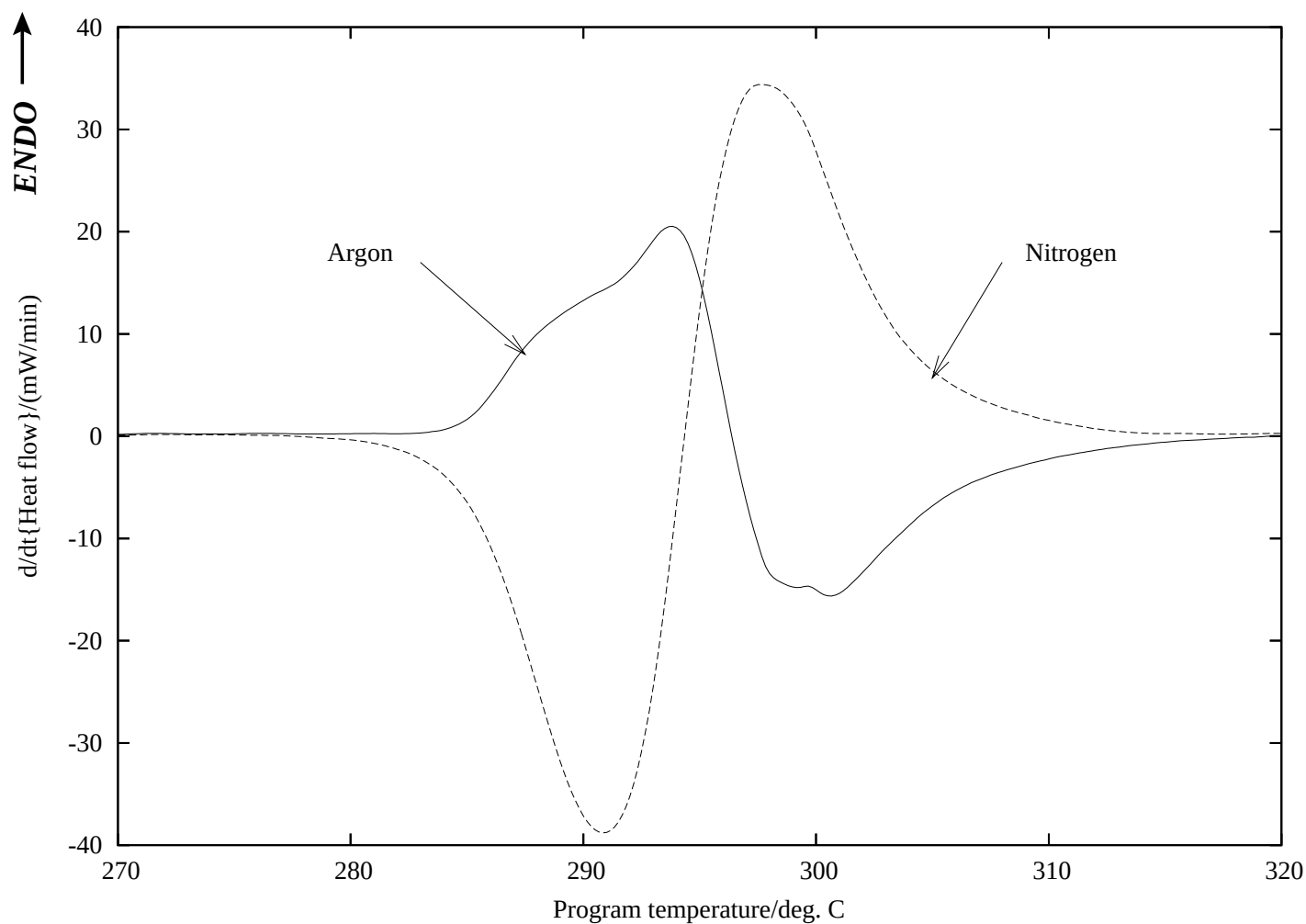


Figure 6.13: Derivative DSC curves of copper(II) oxalate in argon and nitrogen atmospheres. Samples were heated from 25 °C to 350 °C at 10 °C min⁻¹ in sealed, cold-welded pans perforated by a single pin-prick, in their specified atmospheres. The purge rates were approximately 40 ml min⁻¹. Samples were of similar masses (3 mg). The derivatives were smoothed using a simple 11-point boxcar algorithm.

DSC results at various heating rates

Figure 6.14 (p. 267) shows DSC curves for copper(II) oxalate heated under argon (25 ml min^{-1}) from 25°C to 360°C at $10^\circ\text{C min}^{-1}$, 5°C min^{-1} and 2°C min^{-1} .

Ignoring the expected shift towards lower temperatures in the onset, peak and end temperatures through the different heating rates, it is clear that as the heating rate is decreased, the DSC curves appear more complex. In graph **A** ($10^\circ\text{C min}^{-1}$), the left-hand lobe of the derivative DSC curve shows only one step, whereas the right-hand lobe shows two overlapping steps. In graph **B** (5°C min^{-1}), a similar derivative DSC curve is observed, with a shoulder on the left-hand lobe, and clearer resolution of the two steps in the right-hand lobe. Despite more intensive smoothing, the left-hand lobe derivative curve in graph **C** (2°C min^{-1}) shows two incompletely resolved steps, and the right-hand lobe shows further separation of the two steps observed in **A** and **B**.

The X-ray powder diffraction patterns of the DSC residues are given in Figure 6.15 (p. 268). The residue of the $10^\circ\text{C min}^{-1}$ run consists of a mixture of copper metal and copper(I) oxide (cuprite), with no detectable copper(II) oxide (tenorite). At the slower heating rates, some copper(II) oxide formation is observed: small copper(II) oxide peaks are visible at 5°C min^{-1} , and more pronounced peaks at 2°C min^{-1} .

Figure 6.16 (p. 269) shows DSC curves for copper(II) oxalate heated under nitrogen (24 ml min^{-1}) from 25°C to 360°C at $10^\circ\text{C min}^{-1}$, 5°C min^{-1} and 2°C min^{-1} .

The left-hand lobes of the derivative DSC curves in **A** ($10^\circ\text{C min}^{-1}$), **B** (5°C min^{-1}) and **C** (2°C min^{-1}) are all clearly single, but as under argon purge, the right-hand lobes show two steps becoming more clearly separated at lower heating rates.

The X-ray powder diffraction patterns of the DSC residues under nitrogen (Figure 6.17, p. 270) follow the same trend as those under argon: at $10^\circ\text{C min}^{-1}$ the residue consists of a mixture of copper metal and copper(I) oxide (cuprite) with no detectable copper(II) oxide (tenorite), but the magnitude of the tenorite peaks increases as the DSC heating rate decreases.

Table 6.6 (p. 271) gives a summary of the DSC results under argon and ni-

trogen. It is clear that slower heating rates give rise to greater oxidation of the residues under both argon and nitrogen. A few points must be noted:

- Although X-ray powder diffraction can be used to analyze multi-component mixtures [18], the data in this study should be regarded as qualitative. The data appear to suggest that more copper(I) oxide (cuprite) formation occurs at $2\text{ }^{\circ}\text{C min}^{-1}$ than at $5\text{ }^{\circ}\text{C min}^{-1}$, and also that more copper(II) oxide (tenorite) formation occurs at $2\text{ }^{\circ}\text{C min}^{-1}$ than at $5\text{ }^{\circ}\text{C min}^{-1}$, but even very small changes in intensity (due to sample preparation, for example) relative to the large Cu peaks could invalidate these conclusions. The extent to which the greater oxidation of the residues at $2\text{ }^{\circ}\text{C min}^{-1}$ than at $5\text{ }^{\circ}\text{C min}^{-1}$ can be attributed to copper(II) oxide (tenorite) formation, as opposed to copper(I) oxide (cuprite) formation, is limited.
- The greater relative masses of the residues (i.e., $100\text{ }m_r/m_s$) at $2\text{ }^{\circ}\text{C min}^{-1}$ under both argon and nitrogen cannot be explained by residual air in the DSC furnace. Great care was taken to remove residual air by extended purging, and purging over the longer run-times associated with slower heating rates should further decrease the effects of such contamination.
- The greater relative masses of the residues at $2\text{ }^{\circ}\text{C min}^{-1}$ under both argon and nitrogen are also not consistent with greater oxidation of the residues by oxygen impurity in the purge gas over a longer period.

Given that the maximum concentration of oxygen in the purge gases (flowing at about 30 ml min^{-1}) is 3 vpm, it may be calculated that in 50 minutes the volume of oxygen passing over the sample is $3 \times 10^{-6} \times 0.03\text{ L min}^{-1} \times 50\text{ min} = 4.5 \times 10^{-6}\text{ L}$. Taking the density of oxygen to be approximately 1.3 g L^{-1} at atmospheric pressure and room temperature (*cf.* [19, p. 2.16]), this means that approximately $6\text{ }\mu\text{g}$ of oxygen passes over the sample during and after decomposition at $2\text{ }^{\circ}\text{C min}^{-1}$. Even under the unreasonable assumption that *all* the oxygen in the purge gas reacts with the sample, this is not enough to account for the mass increase.

Therefore, the mass increase is probably because of secondary reaction of the sample material with carbon dioxide evolved during decomposition.

Mohamed, *et. al.*, report similar relative residue masses of around 44 % under nitrogen and carbon-dioxide atmospheres [5] at various heating rates.

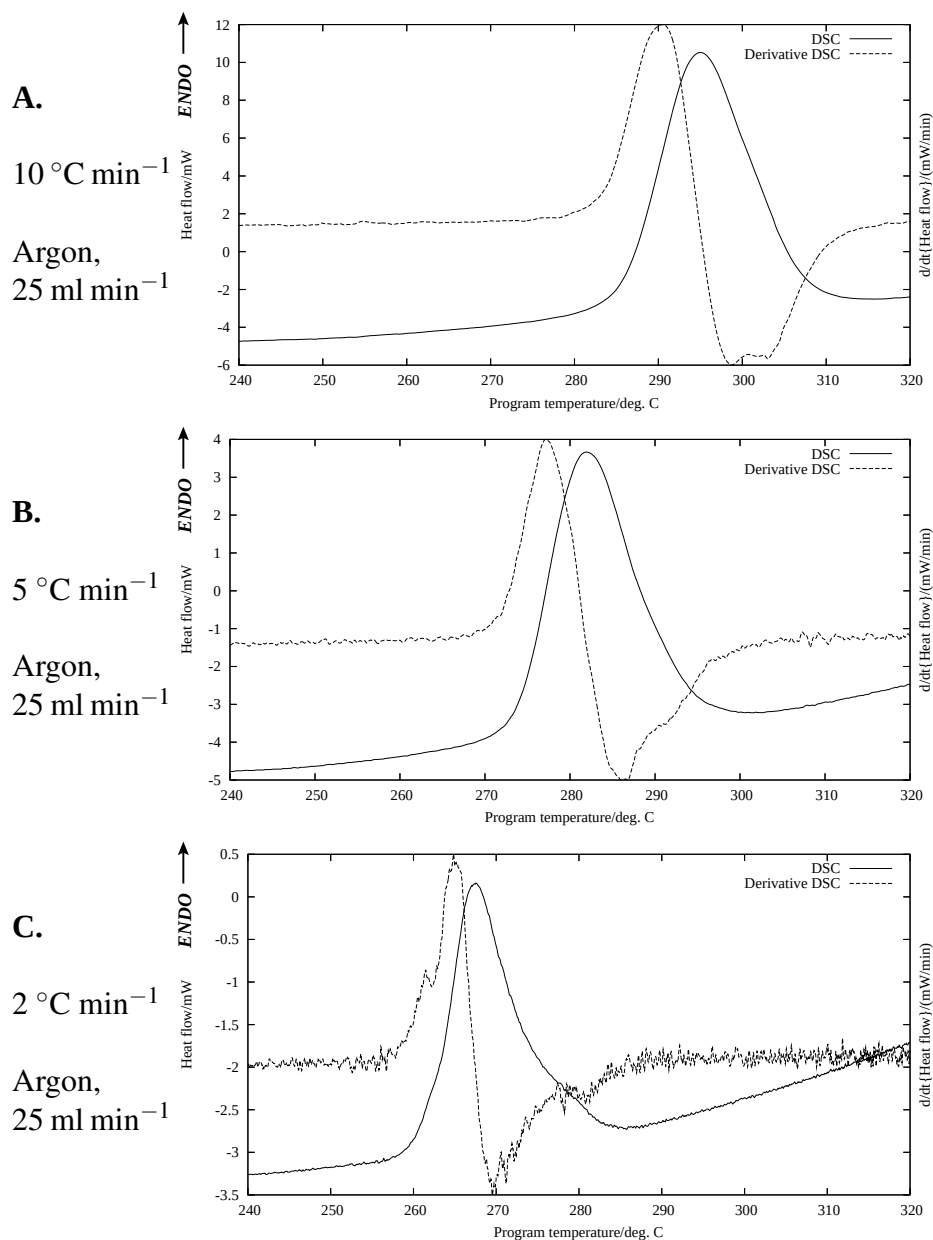


Figure 6.14: DSC curves of copper(II) oxalate under argon at different heating rates. The samples (4 mg) were heated in crimped aluminium pans from $25\text{ }^{\circ}\text{C}$ to $360\text{ }^{\circ}\text{C}$ at the specified heating rates. The derivatives were smoothed using a simple boxcar algorithm: an 11-point boxcar was used for **A** and **B**, and a 21-point boxcar for **C**.

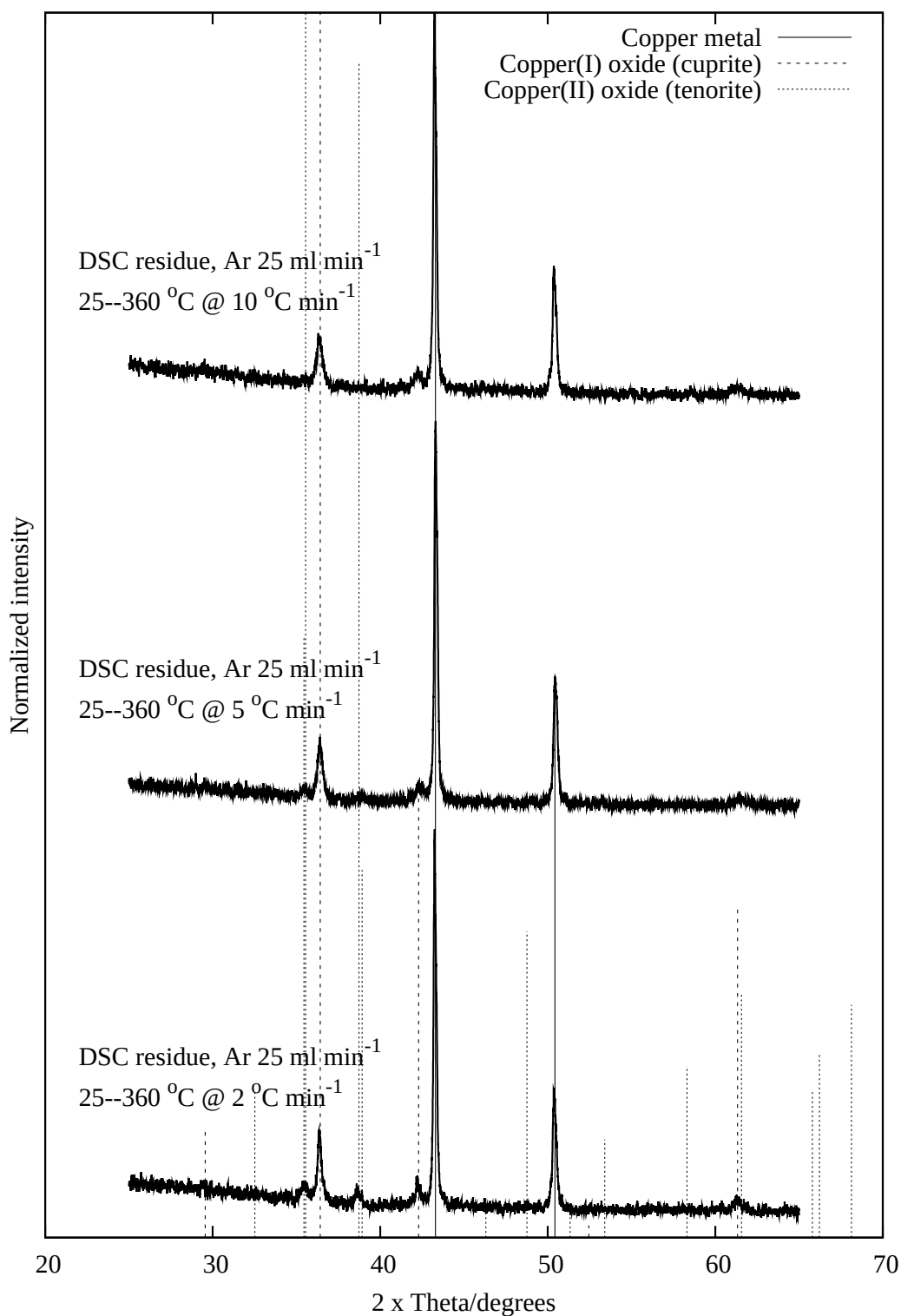


Figure 6.15: X-ray powder diffraction patterns of the residues of copper(II) oxalate heated under argon (25 ml min⁻¹) at different heating rates. The vertical lines indicate the reflections for copper metal, copper(I) oxide (cuprite) and copper(II) oxide (tenorite) as calculated for $\lambda = 1.5404 \text{ \AA}$ [17, cards 4-0836, 5-0667 & 5-0661].

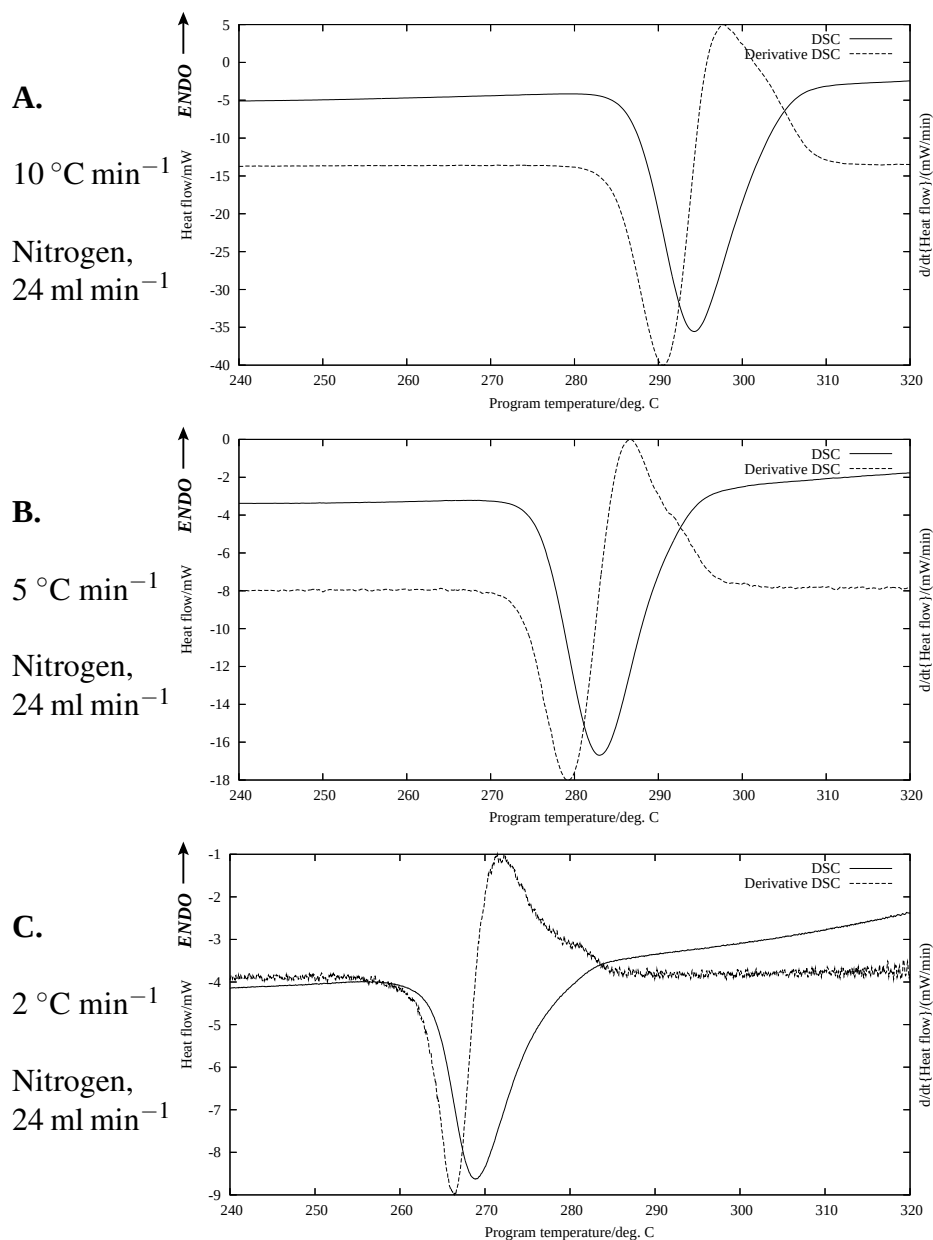


Figure 6.16: DSC curves of copper(II) oxalate under nitrogen at different heating rates. The samples (4 mg) were heated in crimped aluminium pans from $25\text{ }^{\circ}\text{C}$ to $360\text{ }^{\circ}\text{C}$ at the specified heating rates. The derivatives were smoothed using a simple boxcar algorithm: an 11-point boxcar was used for **A** and **B**, and a 21-point boxcar for **C**.

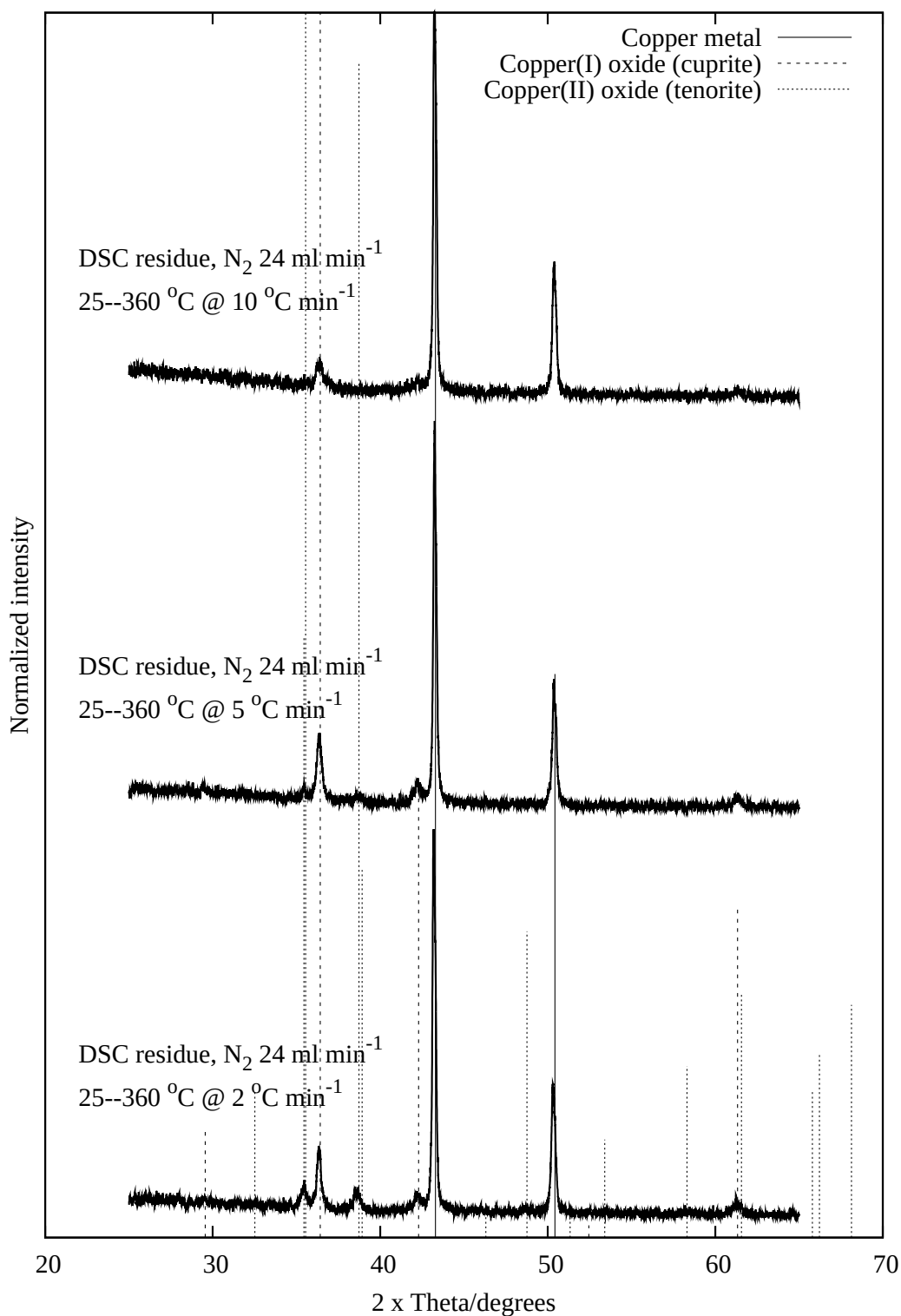


Figure 6.17: X-ray powder diffraction patterns of the residues of copper(II) oxalate heated under nitrogen (24 ml min^{-1}) at different heating rates. The vertical lines indicate the reflections for copper metal, copper(I) oxide (cuprite) and copper(II) oxide (tenorite) as calculated for $\lambda = 1.5404 \text{ \AA}$ [17, cards 4-0836, 5-0667 & 5-0661].

Table 6.6: DSC results for copper(II) oxalate heated under argon and nitrogen atmospheres at various heating rates. The samples were run in crimped aluminium pans.

Quantity	Argon, 25 ml min ⁻¹			Nitrogen, 24 ml min ⁻¹		
	10 °C min ⁻¹	5 °C min ⁻¹	2 °C min ⁻¹	10 °C min ⁻¹	5 °C min ⁻¹	2 °C min ⁻¹
Sample mass, m_s /mg	3.985	4.194	4.072	4.649	4.406	3.968
Residue mass, m_r /mg	1.689	1.790	1.795	1.962	1.878	1.748
$100m_r/m_s$	42.38	42.68	44.08	42.20	42.62	44.05
Onset temp., T_i /°C	285.8	274.0	262.4	287.0	275.8	263.9
End temp., T_f /°C	306.9	292.2	274.2	303.9	291.8	276.6
Heat flow, Q /J g ⁻¹	263.4	253.7	223.9	-435.1	-385.1	-330.9
ΔH_r /kJ mol ⁻¹	40.02	38.53	34.00	-66.09	-58.50	-50.27
Residue	Cu, Cu ₂ O	Cu, Cu ₂ O, CuO	Cu, Cu ₂ O, CuO	Cu, Cu ₂ O	Cu, Cu ₂ O, CuO	Cu, Cu ₂ O, CuO

DSC results at various purge gas flow-rates

Figures 6.18 (p. 273) and 6.20 (p. 275) show DSC curves of copper(II) oxalate heated as indicated at $10\text{ }^{\circ}\text{C min}^{-1}$ under argon and nitrogen, respectively, at various flow rates. Table 6.7 (p. 277) summarizes the DSC results.

It is clear, for runs under both argon and nitrogen, that decreasing the flow-rate of the purge gas results in peak-broadening and loss of resolution. Very small increases in relative residue mass are observed under both argon and nitrogen as the purge-rates are decreased. These increases are also inconsistent with oxidation by oxygen contamination in the purge gases. To avoid oxidation by residual air the DSC furnace was purged at a high flow-rate for more than an hour after each sample change before finally adjusting the flow-rate to its desired value and applying the temperature program.

The absolute values of ΔH_r under both argon and nitrogen, as estimated by integrating the DSC curves, appear to depend very much on the purge gas flow rate. Under both argon and nitrogen atmospheres, the absolute value of ΔH_r approximately doubles as the flow-rates are approximately halved. This behaviour does *not* agree with what is observed with the standard calibrant (indium metal).

The X-ray diffraction patterns under argon and nitrogen (Figures 6.19 and 6.21, pp. 274 and 276) show that all the DSC residues consist of mixtures of copper metal and copper(I) oxide (cuprite), with no copper(II) oxide (tenorite) observed. In agreement with the mass data, the X-ray diffraction patterns suggest that, under both argon and nitrogen atmospheres, the relative amount of copper(I) oxide in the DSC residues increases as the purge gas flow-rate is decreased.

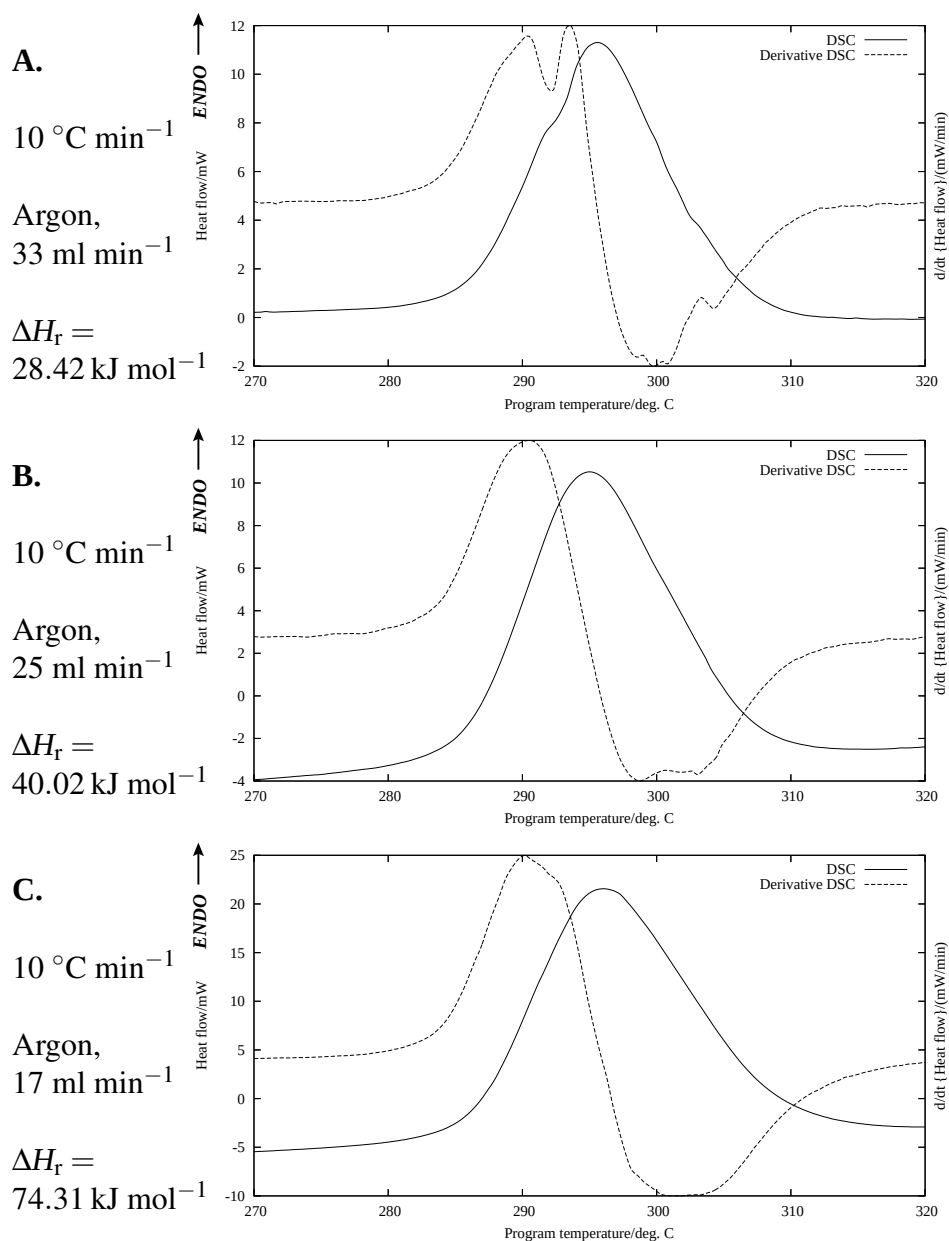


Figure 6.18: DSC curves of copper(II) oxalate samples (4 mg) heated in crimped aluminium pans at 10 °C min⁻¹ under argon purge at various flow rates. The values of ΔH_r were calculated assuming a molar mass of 151.9 g mol⁻¹. The ΔH_r for **A** is the average reported earlier.

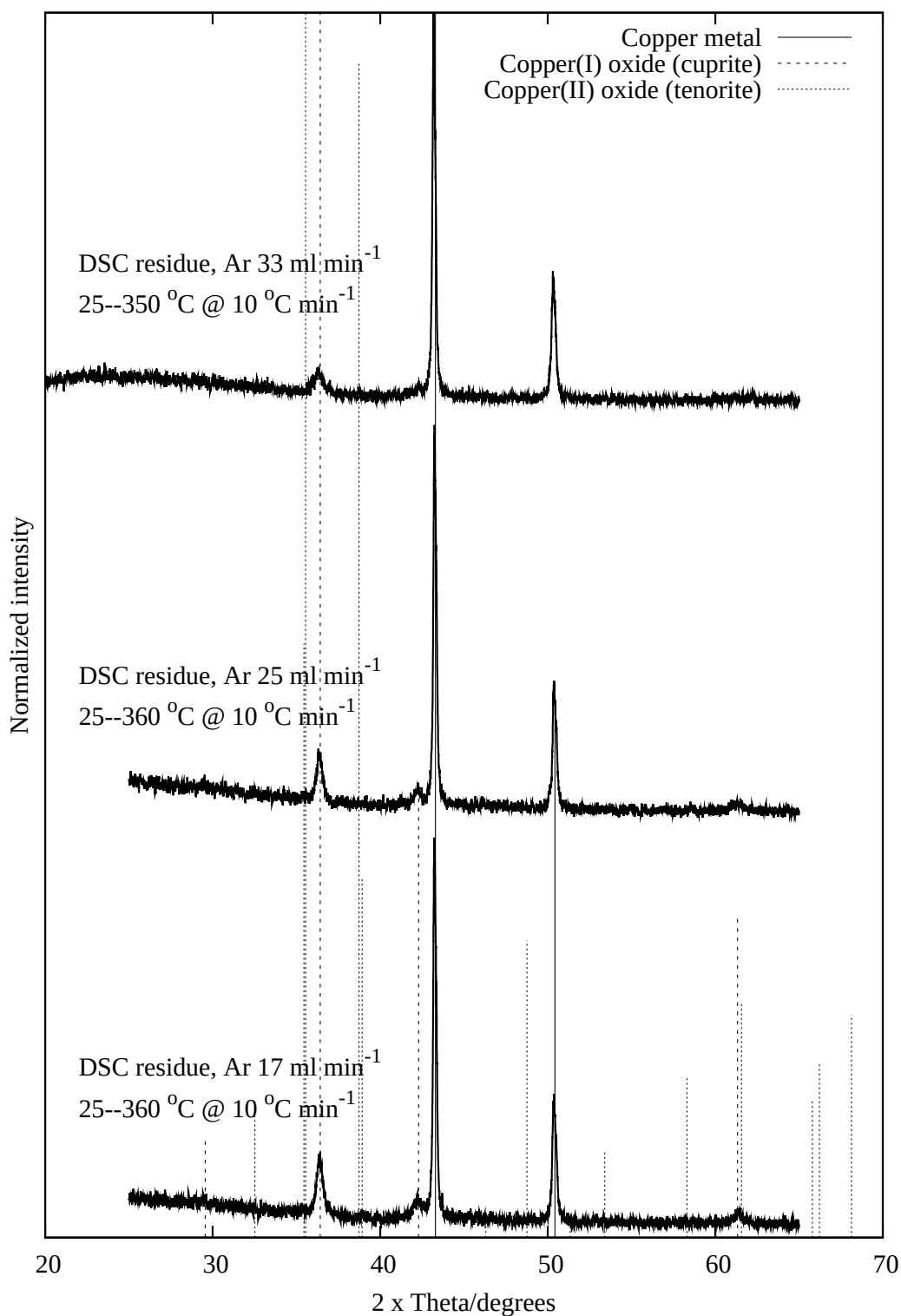


Figure 6.19: X-ray powder diffraction patterns of the residues of copper(II) oxalate heated as indicated under argon at various flow rates. The vertical lines indicate the reflections for copper metal, copper(I) oxide (cuprite) and copper(II) oxide (tenorite) as calculated for $\lambda = 1.5404 \text{ \AA}$ [17, cards 4-0836, 5-0667 & 5-0661].

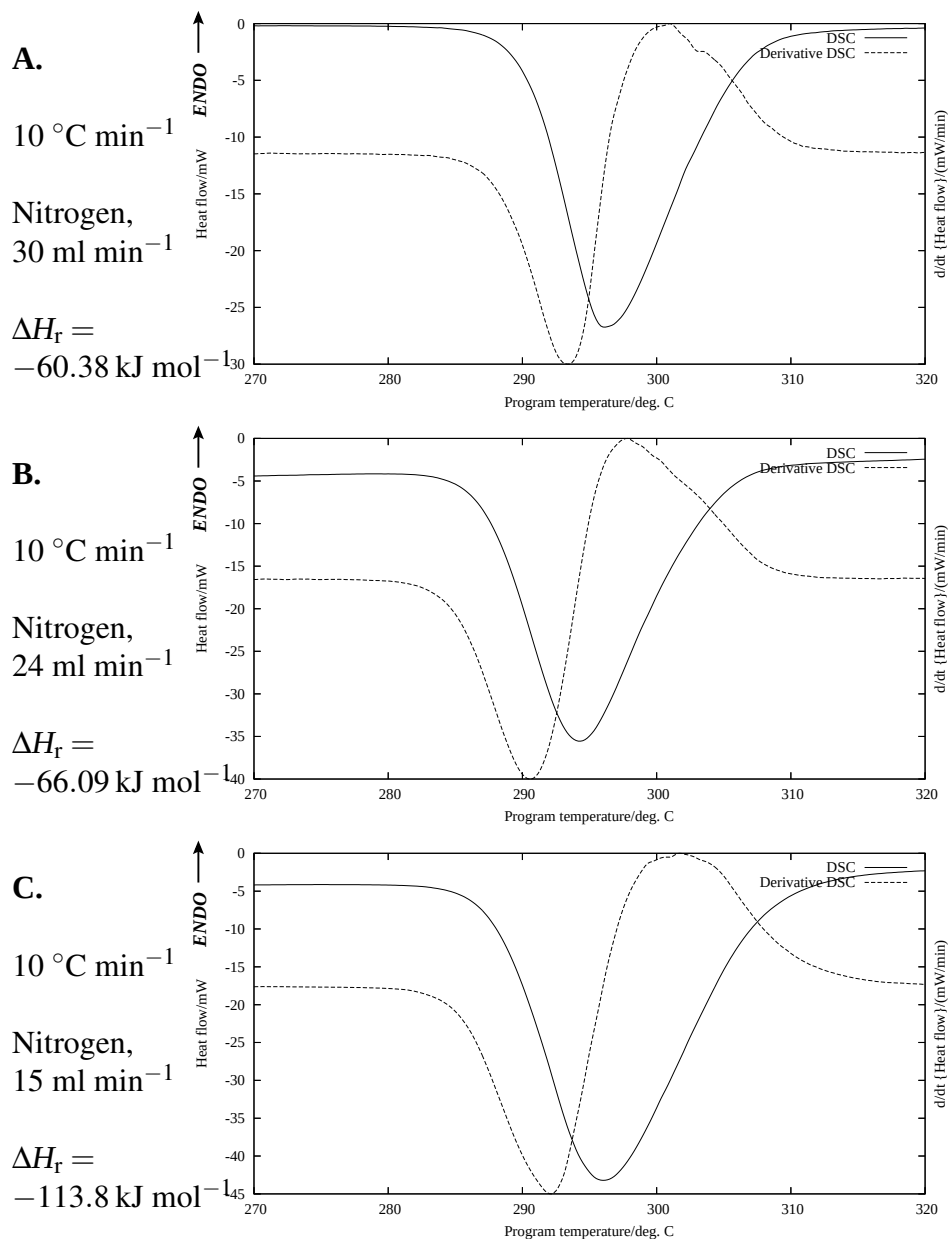


Figure 6.20: DSC curves of copper(II) oxalate samples (4 mg) heated in crimped aluminium pans at $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen purge at various flow rates. The values of ΔH_r were calculated assuming a molar mass of 151.9 g mol^{-1} . The ΔH_r for A is the average reported earlier.

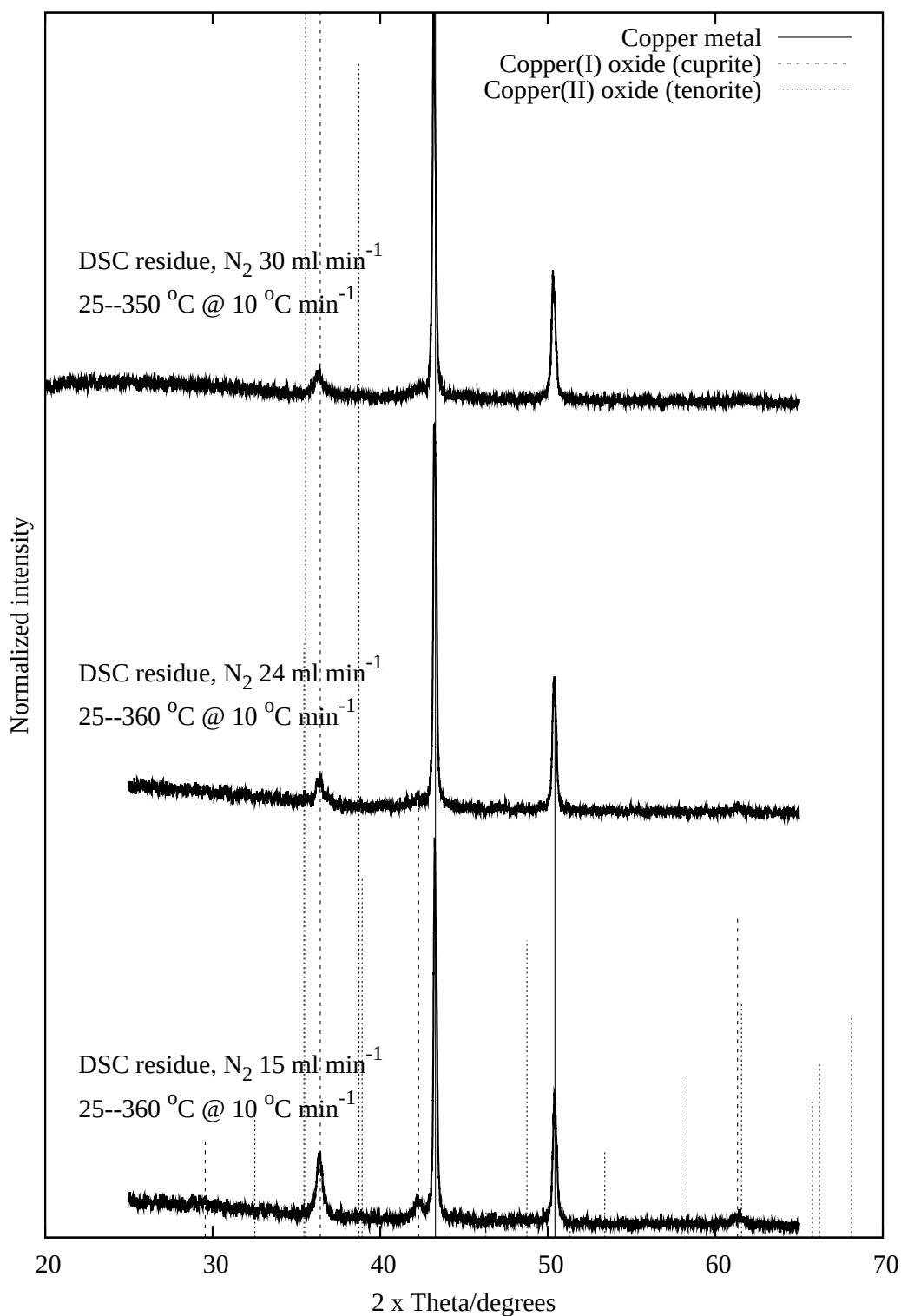


Figure 6.21: X-ray powder diffraction patterns of the residues of copper(II) oxalate heated as indicated under nitrogen at various flow rates. The vertical lines indicate the reflections for copper metal, copper(I) oxide (cuprite) and copper(II) oxide (tenorite) as calculated for $\lambda = 1.5404 \text{ \AA}$ [17, cards 4-0836, 5-0667 & 5-0661].

Table 6.7: DSC results for copper(II) oxalate heated at $10\text{ }^{\circ}\text{C min}^{-1}$ under argon and nitrogen atmospheres at various flow rates. The samples were run in crimped aluminium pans. Except where indicated, samples were heated from $25\text{ }^{\circ}\text{C}$ to $360\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$. Residues were identified by X-ray powder diffraction as mixtures of copper metal and copper(I) oxide (cuprite), with no detectable copper(II) oxide (tenorite).

Quantity	Argon, $10\text{ }^{\circ}\text{C min}^{-1}$			Nitrogen, $10\text{ }^{\circ}\text{C min}^{-1}$		
	*33 ml min^{-1}	25 ml min^{-1}	17 ml min^{-1}	*30 ml min^{-1}	24 ml min^{-1}	15 ml min^{-1}
Sample mass, m_s/mg	4.099	3.985	4.391	4.311	4.649	3.954
Residue mass, m_r/mg	1.715	1.689	1.865	1.805	1.962	1.677
$100m_r/m_s$	41.84	42.38	42.47	41.87	42.20	42.41
Onset temp., $T_i/^{\circ}\text{C}$	289.3	285.8	286.3	289.7	287.0	288.0
End temp., $T_f/^{\circ}\text{C}$	304.4	306.9	309.4	305.5	303.9	307.9
Heat flow, $Q/\text{J g}^{-1}$	187.1	263.4	489.2	-397.5	-435.1	-749.4
$\Delta H_f/\text{kJ mol}^{-1}$	28.42	40.02	74.31	-60.38	-66.09	-113.8

* Samples heated to $350\text{ }^{\circ}\text{C}$.

6.3.3 DSC results in oxygen

The DSC curve of copper(II) oxalate heated between 25 °C and 350 °C at 10 °C min⁻¹ in oxygen shows a large exothermic response preceded by a small peak or baseline disturbance, as shown in Figure 6.22 (p. 279), with the second peak much more strongly exothermic than the first. The large exothermic peak seems to be simpler than the exotherms under nitrogen. The residue was identified by XRPD as copper(II) oxide (tenorite) with no discernable trace of copper(I) oxide (cuprite) or copper metal.

The X-ray diffraction pattern (Figure 6.23, p. 280) is very weak, indicating poor crystallinity of the residue. The residue also displays a marked and reproducible tendency to gain mass rapidly after removal from the DSC furnace. Because care was taken to allow the residues to cool to room temperature in the furnace before being exposed to the atmosphere, and considering how much more oxidising oxygen is than air, the mass gain is believed to be due to adsorption of water vapour. This suggests that the residue has a very large surface area, and is finely divided, which would account for the weak XRPD signal.

Table 6.8 (p. 281) summarizes the DSC results in oxygen. Assuming the decomposition reaction:



the enthalpy of formation of copper(II) oxalate is given by:

$$\Delta H_f^\circ \text{CuC}_2\text{O}_4(\text{s}) = -\Delta H_r^\circ + \Delta H_f^\circ \text{CuO}(\text{s}) + 2\Delta H_f^\circ \text{CO}_2(\text{g}) \quad (6.19)$$

Taking the integrated exothermic DSC response as ΔH_r° and substituting standard values for $\Delta H_f^\circ \text{CuO}(\text{s})$ and $\Delta H_f^\circ \text{CO}_2(\text{g})$ [8, p. D-38 *et seq.*] gives $\Delta H_f^\circ \text{CuC}_2\text{O}_4(\text{g}) = -718.3 \text{ kJ mol}^{-1}$. This is approximately 5% below Le Van's published value of -751 kJ mol^{-1} [9].

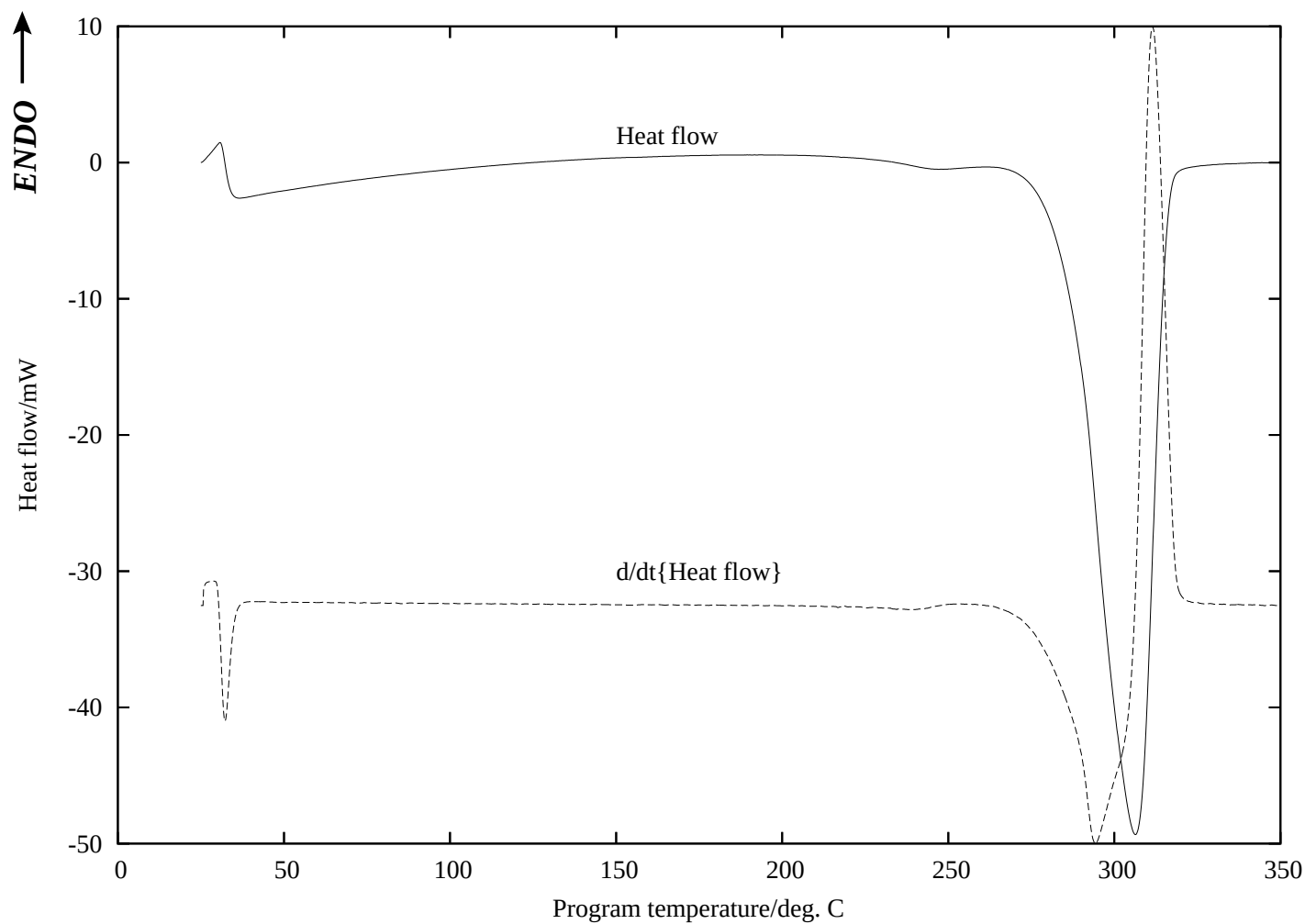


Figure 6.22: DSC and derivative DSC curves of copper(II) oxalate in oxygen. The sample (5 mg) was heated from 25 °C to 350 °C at 10 °C min⁻¹. Correction of the DSC curve baseline was performed by simple linear subtraction, and the derivative curve was smoothed by means of a simple 11-point boxcar algorithm.

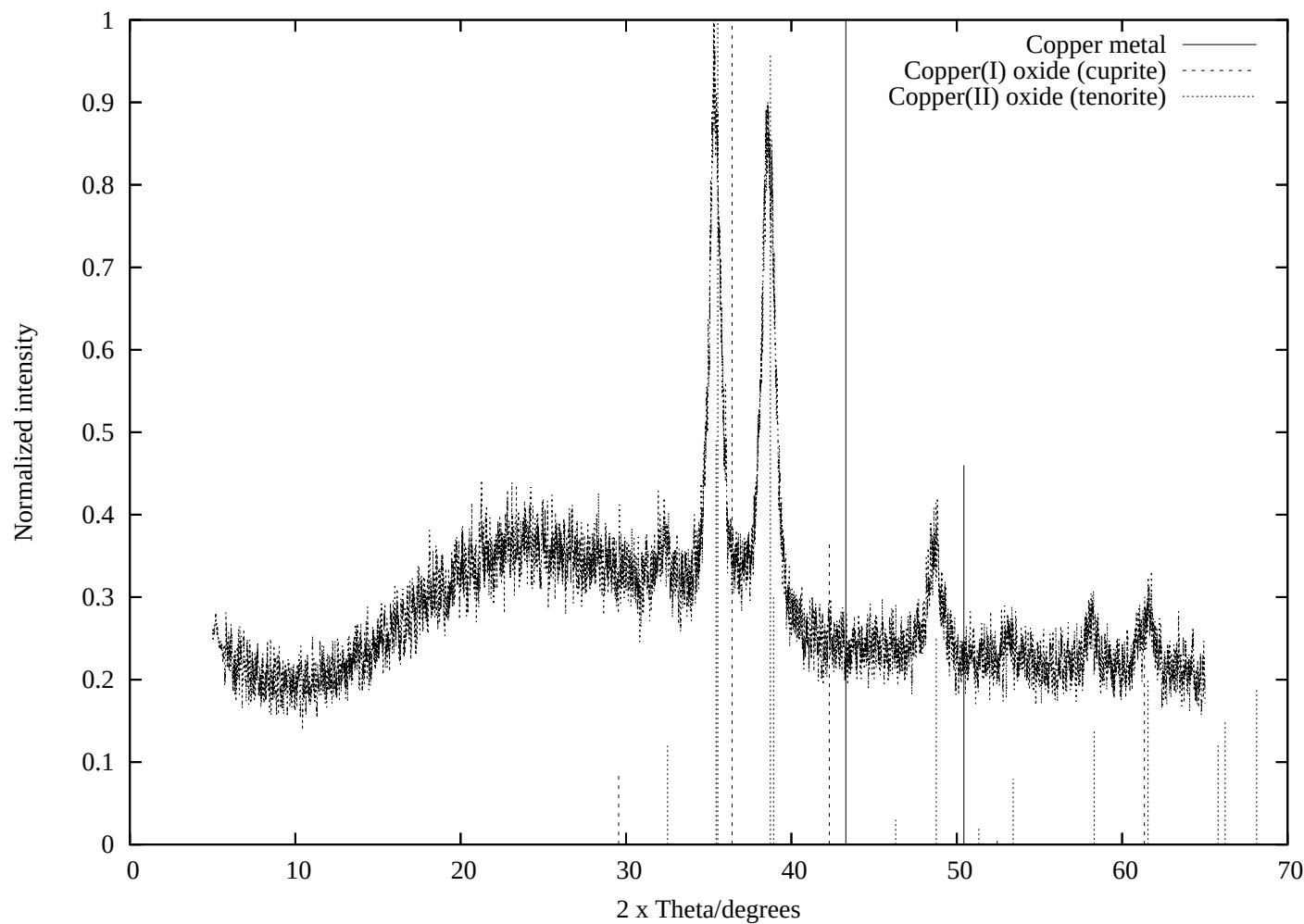


Figure 6.23: X-ray powder diffraction pattern ($\text{Cu-K}\alpha$ radiation) of the residue of copper(II) oxalate heated in the DSC from $25\text{ }^{\circ}\text{C}$ to $350\text{ }^{\circ}\text{C}$ at $10\text{ }^{\circ}\text{C min}^{-1}$ in oxygen. The signal is very weak (hence the noisy background) and shows significant peak-broadening, indicating poor crystallinity of the residue. The vertical lines indicate the reflections for copper metal, copper(I) oxide (cuprite) and copper(II) oxide (tenorite) as calculated for $\lambda = 1.5404\text{ \AA}$ [17, cards 4-0836, 5-0667 & 5-0661].

Table 6.8: DSC results of copper(II) oxalate heated in crimped aluminium pans under oxygen atmosphere. The flow rate of oxygen was 36 ml min^{-1} . The residue was identified by XRPD as copper(II) oxide (tenorite).

Quantity	Oxygen	
Sample mass, m_s/mg	4.913	5.449
Residue mass, m_r/mg	2.582	2.843
$100 m_r/m_s$	52.55	52.17
Ave. $100 m_r/m_s$	52.36	
Onset temp., $T_i/^\circ\text{C}$	286.2	286.0
End temp., $T_f/^\circ\text{C}$	315.8	315.4
Heat flow, $Q/\text{J g}^{-1}$	-1470.1	-1474.7
Ave. $T_i/^\circ\text{C}$	286.1	
Ave. $T_f/^\circ\text{C}$	315.6	
Ave. $Q/\text{J g}^{-1}$	-1472.4	
Ave. $\Delta H_r/\text{kJ mol}^{-1}$	-223.7	

6.3.4 Discussion

The fact the the decomposition of copper(II) oxalate is *exothermic* in atmospheres often regarded as inert, such as nitrogen and carbon dioxide, and in hydrogen, a reducing atmosphere, but appears to be *endothermic* in argon, suggests that a different reaction is taking place under argon. However, all other observations made in this study suggest that the reactions under nitrogen and under argon are the same.

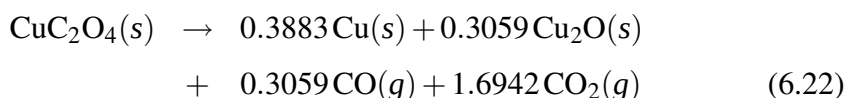
For all the DSC runs in which the sample was heated at $10^\circ\text{C min}^{-1}$, the residues were identified by X-ray powder diffraction as mainly copper metal with a small amount of copper(I) oxide (cuprite). Carbon monoxide gas was detected in the gas evolved during TG-experiments, so the DSC response may be described by Equation 6.13 (p. 239):

$$\begin{aligned} \Delta H_r^\circ(\beta) = & \frac{1}{2}\beta\Delta H_f^\circ \text{Cu}_2\text{O}(s) + \frac{1}{2}\beta\Delta H_f^\circ \text{CO}(g) + (2 - \frac{1}{2}\beta)\Delta H_f^\circ \text{CO}_2(g) \\ & - \Delta H_f^\circ \text{CuC}_2\text{O}_4(s) \end{aligned} \quad (6.20)$$

or, numerically:

$$\Delta H_r^\circ(\beta)/\text{kJ mol}^{-1} = 58.13\beta - 35.56 \quad (6.21)$$

For the overall DSC response to be endothermic, i.e., to satisfy the condition, $\Delta H_r^\circ(\beta)/\text{kJ mol}^{-1} > 0$, would require $\beta > 0.6117$. Assuming $\beta = 0.6117$, Equation 6.12 becomes:



Taking the formula mass of dried copper(II) oxalate as 151.9 g mol^{-1} , the residue mass would be expected to be 45.06 % of the original sample mass. This is significantly different to the experimental value of approximately 42 % obtained for the various DSC runs at $10^\circ\text{C min}^{-1}$.

The reasoning above may be re-inforced by removing its dependence on the value of $\Delta H_f^\circ \text{CuC}_2\text{O}_4(s)$. If we define β_{endo} as β at the experimental endothermic response of $46.68 \text{ kJ mol}^{-1}$ and β_{exo} as β at the experimental exothermic response of $-63.00 \text{ kJ mol}^{-1}$, we may write:

$$\begin{aligned} 46.48 - (-63.00) &= 58.13(\beta_{\text{endo}} - \beta_{\text{exo}}) \\ \therefore \beta_{\text{endo}} - \beta_{\text{exo}} &= 1.883 \end{aligned} \quad (6.23)$$

This is not possible, remembering that $0 \leq \beta \leq 1$. The mechanism is therefore not consistent with the observed experimental results, and cannot satisfactorily explain the endothermic DSC response under argon.

The DSC results at 5°C min^{-1} and 2°C min^{-1} are more difficult to interpret because of the additional formation of copper(II) oxide (tenorite) under both argon and nitrogen atmospheres at these heating rates. Everything else being unchanged, the effect of copper(II) oxide formation, at the expense of carbon dioxide formation, would be to render the DSC response more endothermic. Considering the mass data and the X-ray powder diffraction patterns of the residues at 2°C min^{-1} and 5°C min^{-1} , there is no reason to believe that the DSC residues under argon are different to those under nitrogen, and yet a large difference in the DSC response is observed when changing the purge gas from argon to nitrogen. It is

extremely unlikely that the change in the DSC response is due to changes in β and γ .

The absolute value of the observed ΔH_r values decrease slightly with decreasing heating-rate. This may be due to calibration effects — the DSC is calibrated at $10\text{ }^\circ\text{C min}^{-1}$, although heating rate does not enter into the calibration factor for DSC [20]. Further interpretation of this trend is not possible, because it is not possible to determine β and γ individually from the mass data and X-ray powder diffraction patterns.

The DSC runs at different purge rates show that the DSC responses are strongly dependent on the purge rate. Under both argon and nitrogen purge, small increases in residue mass percentage are observed as the purge rate is decreased, and X-ray powder diffraction studies of the residues show that only copper metal and copper(I) oxide are present. Again, oxidation of the solid residue at the expense of carbon dioxide production cannot satisfactorily explain the observed thermal behaviour.

It has been demonstrated that a mismatch in thermal conductivity between the evolved gaseous products and the DSC purge gas can lead to spurious results. Hallbrucker, *et. al.* [21], have shown that using helium (50 ml min^{-1}) as a purge gas in studying the thermal decomposition of large samples of copper(II) sulfate pentahydrate results in spurious *exotherms* accompanying the evolution of water vapour, owing to a large difference between the thermal conductivities of water vapour and of helium. They also reported similar behaviour under helium purge with samples known to evolve nitrogen gas. It would appear that the evolution of a gas with a significantly lower thermal conductivity than the instrument purge gas has the effect of blanketing the sample, thus reducing the heat flow from the sample furnace to the atmosphere compared to that of the reference furnace.

As reported in [19] for temperatures in the range $0\text{--}100\text{ }^\circ\text{C}$, and summarized in Table 6.10 (p. 291) at $20\text{ }^\circ\text{C}$, the thermal conductivity of argon is a slightly closer match to that of carbon dioxide, the expected major evolved gas component in this study, than is the thermal conductivity of nitrogen². The thermal

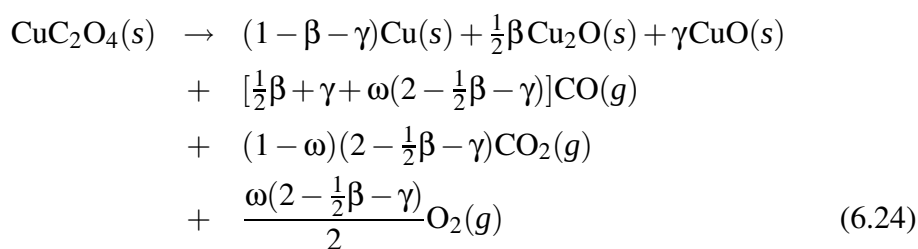
²To ensure that the DSC furnace was purging correctly, the reference furnace was blocked with a strip of adhesive tape and the flow rate through the sample furnace checked at the common exhaust line. The procedure was then repeated with the sample furnace blocked and the reference furnace open. The sample and reference furnaces were both found to be purging normally.

conductivities of helium and hydrogen are also an order of magnitude larger than that of nitrogen, whereas the thermal conductivities of argon and nitrogen are much closer together.

The DTA/DSC responses for the decomposition of cobalt(II) oxalate dihydrate are reported as endothermic under argon (66 ml min^{-1}) [22], nitrogen and carbon dioxide (both at 40 ml min^{-1}) [5], but exothermic under hydrogen (40 ml min^{-1}) [5]. However, because there are differences between the reported composition of the residue under hydrogen (Co [major] + Co_3O_4), under nitrogen (Co_3O_4 [major] + CoO) and argon (Co + CoO), and differences between the reactivity of the various gases, chemical factors may explain the differences in the DSC responses.

Other types of mechanisms have been proposed which may be useful here. Kinetic arguments have been used to propose that the decompositions of silver(I), nickel(II) and mercury(II) oxalate are accompanied by the evolution of $\text{CO}(g)$, $\text{CO}_2(g)$ and $\frac{1}{2}\text{O}(g)$ (or O), and that the oxalates of lead(II) and manganese(II) decompose to give $\text{CO}(g)$ and $\frac{1}{2}\text{O}(g)$ [23]. They are said to decompose by a mechanism of *dissociative evaporation*, i.e., by the congruent gasification³ of all reaction products irrespective of their saturated vapor pressure, and subsequent condensation of low-volatility species as described in various works, among others [24–27].

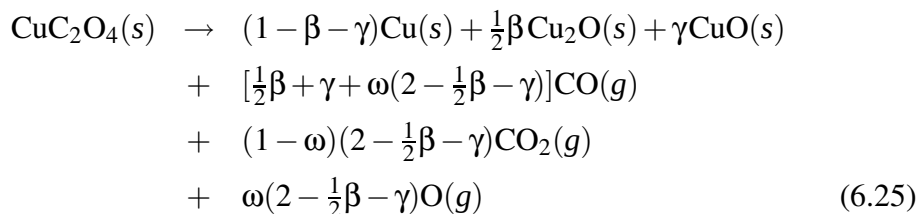
To take account of this possibility, Equation 6.8 may be rewritten as:



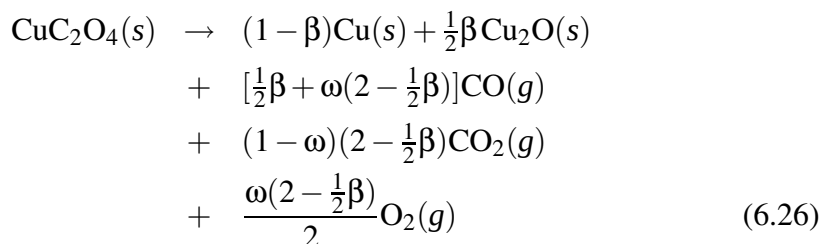
in which ω is the fraction of the available carbon dioxide which is released as $\text{CO}(g)$ and $\frac{1}{2}\text{O}_2(g)$ or $\text{O}(g)$ if it assumed that the oxygen is in the form of oxygen

³The author also refers to this as “congruent vaporization”.

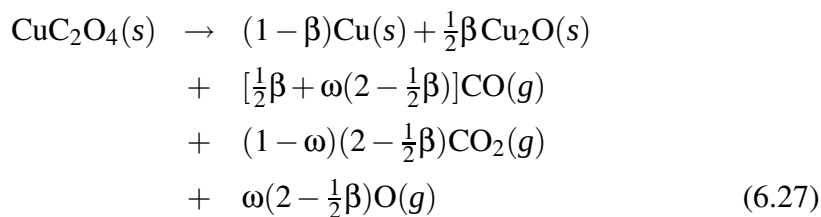
molecules, or as



if the oxygen is assumed to be monatomic. These equations contain too many variables to be useful in this study, and henceforth, for simplicity, only mechanisms which do *not* involve the formation of copper(II) oxide will be considered. The corresponding chemical equations can be obtained by setting $\gamma = 0$ in the above equations to give:



and



The corresponding thermochemical equations are:

$$\begin{aligned}
 \Delta H_r^\circ(\beta, \omega) = & \frac{1}{2}\beta\Delta H_f^\circ\text{Cu}_2\text{O}(s) + (\frac{1}{2}\beta + 2\omega - \frac{1}{2}\beta\omega)\Delta H_f^\circ\text{CO}(g) \\
 & + (1 - \omega)(2 - \frac{1}{2}\beta)\Delta H_f^\circ\text{CO}_2(g) - \Delta H_f^\circ\text{CuC}_2\text{O}_4(s)
 \end{aligned} \tag{6.28}$$

and

$$\begin{aligned}\Delta H_r^\circ(\beta, \omega) = & \frac{1}{2}\beta\Delta H_f^\circ \text{Cu}_2\text{O}(s) + (\frac{1}{2}\beta + 2\omega - \frac{1}{2}\beta\omega)\Delta H_f^\circ \text{CO}(g) \\ & + (1 - \omega)(2 - \frac{1}{2}\beta)\Delta H_f^\circ \text{CO}_2(g) + (2\omega - \frac{1}{2}\beta\omega)\Delta H_f^\circ \text{O}(g) \\ & - \Delta H_f^\circ \text{CuC}_2\text{O}_4(s)\end{aligned}\quad (6.29)$$

Substituting the standard enthalpies of formation of $\text{Cu}_2\text{O}(s)$, $\text{CO}_2(g)$, $\text{CO}(g)$ [8, p. D-38 *et seq.*] and $\text{CuC}_2\text{O}_4(s)$ [9], and a published (calculated) value of $249.15 \text{ kJ mol}^{-1}$ for $\Delta H_f^\circ \text{O}(g)$ [28], gives the numerical expressions:

$$\Delta H_r^\circ(\beta, \omega)/\text{kJ mol}^{-1} = 58.13\beta + 565.83\omega - 141.46\beta\omega - 35.56 \quad (6.30)$$

$$\Delta H_r^\circ(\beta, \omega)/\text{kJ mol}^{-1} = 58.13\beta + 1064.14\omega - 266.04\beta\omega - 35.56 \quad (6.31)$$

The sensitivity of these equations to the parameter, ω , is much greater than their sensitivity to β , so if a relatively small proportion of the available carbon dioxide were released as $\text{CO}(g)$ and $\text{O}_2(g)$, or as $\text{CO}(g)$ and $\text{O}(g)$ it would have a great effect on the observed heat flow, causing it to be more endothermic.

Figure 6.24 (p. 287) illustrates the dependence of $\Delta H_r^\circ(\beta, \omega)$ on β and ω for these mechanisms. The reactions can be either endothermic or exothermic, depending on β and ω , but changes in ω have a much greater effect than changes in β . It can be seen from the equations that the amounts (and hence the masses) of the solid residues are not functions of ω .

Such mechanisms appear to explain the endothermic DSC responses, but many of the exothermic DSC responses in this study (particularly those of DSC runs at $10^\circ\text{C min}^{-1}$ at the lower nitrogen flow rates) integrate to far more negative values than $-35.56 \text{ kJ mol}^{-1}$ (the minimum value of the functions above). The exothermic DSC responses under nitrogen reported in the literature in recent years are by no means uniform, as Table 6.9 (p. 288) shows. In addition, the range of the functions above is heavily dependent on the accuracy of the value for $\Delta H_f^\circ \text{CuC}_2\text{O}_4(g)$.

There is little agreement between the DSC results under oxidizing atmospheres, i.e., under air and oxygen. By writing the thermal decomposition of

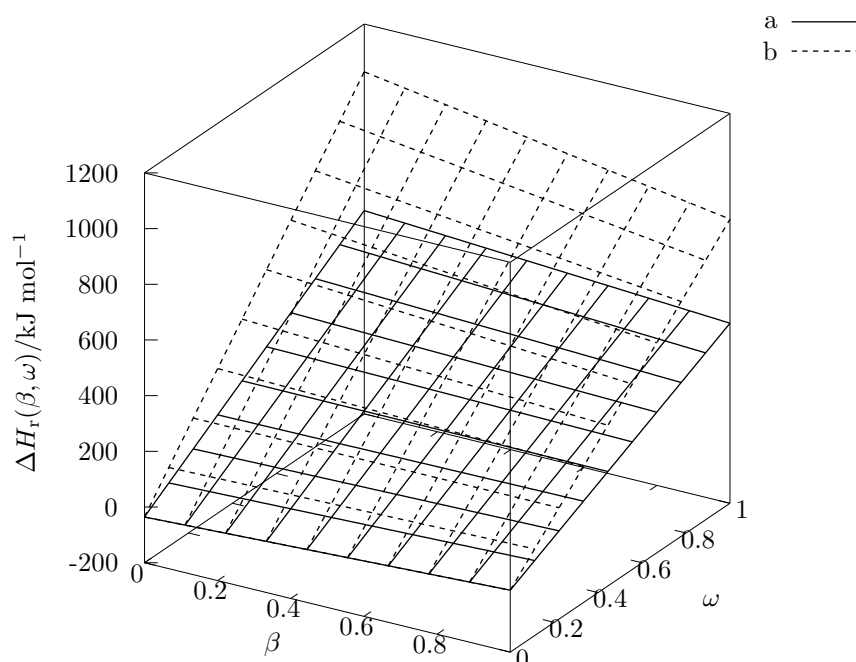
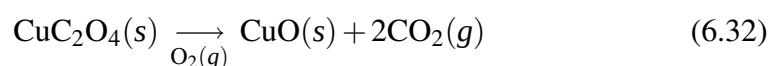


Figure 6.24: Three-dimensional plot of $\Delta H_r^\circ(\beta, \omega)$ for proposed mechanisms involving the loss of $\frac{1}{2}\text{O}_2(g)$ (surface **a**) and $\text{O}(g)$ (surface **b**), showing great sensitivity to ω , the fraction of available CO_2 that is given off as $\text{CO}(g)$ and $\frac{1}{2}\text{O}_2(g)$ (surface **a**) or $\text{O}(g)$ (surface **b**). Surface **a** corresponds to Equation 6.30 (p. 286), and surface **b** to Equation 6.31 (p. 286).

copper(II) oxalate under oxygen as:



for which ΔH_r is given by:

$$\Delta H_r^\circ = \Delta H_f^\circ \text{CuO}(s) + 2\Delta H_f^\circ \text{CO}_2(g) - \Delta H_f^\circ \text{CuC}_2\text{O}_4(s) \quad (6.33)$$

and substituting standard values for $\Delta H_f^\circ \text{CuO}(s)$ and $\Delta H_f^\circ \text{CO}_2(g)$ [8, p. D-38 *et seq.*] and a published value [9] of $-751.3 \text{ kJ mol}^{-1}$ for $\Delta H_f^\circ \text{CuC}_2\text{O}_4(s)$, a value of $-190.6 \text{ kJ mol}^{-1}$ is obtained for ΔH_r° . It can be seen from Table 6.9 that the experimental value closest to the calculated value is the one obtained in this study.

Table 6.9: DSC results of recent studies of the decomposition of copper(II) oxalate in different atmospheres and at various heating rates. Purge gas flow-rates are listed wherever possible.

Authors	Atmosphere	Sample mass/mg	dT/dt / $^{\circ}\text{C min}^{-1}$	$T_i/^{\circ}\text{C}$	$T_f/^{\circ}\text{C}$	$\Delta H_r/\text{kJ mol}^{-1}$
Broadbent, <i>et al.</i> [29]	Nitrogen, 30 ml min ⁻¹	4–10	5	—	—	-9±2
”	Air, 30 ml min ⁻¹	4–10	5	—	—	-134±5
Mohamed, Galwey & Halawy [5]	Nitrogen, 40 ml min ⁻¹	10–15	5	290	305	-11.9
”	Carbon dioxide, 40 ml min ⁻¹	”	5	300	318	-18.0
”	Hydrogen, 40 ml min ⁻¹	”	5 & 10	225	300	-21.1
”	Air, 40 ml min ⁻¹	”	5 & 10	—	—	-43.5
Gusev, Dalidovich, <i>et al</i> [4]	Argon/isochoric (sealed ampoules)	28–32	2	287	357	-29±2**
Coetzee, Eve & Brown [2]	Nitrogen	1–5*	20	291	—	-32.6±0.5
”	Oxygen	”	20	297	—	-138±4
<i>This study</i>	Nitrogen, 30 ml min ⁻¹	4	10	289.6	305.5	-60.38
”	Argon, 33 ml min ⁻¹	”	10	288.9	304.3	28.42
”	Oxygen, 36 ml min ⁻¹	”	10	286.1	315.6	-223.7

* This is implied, but not stated unequivocally, in the reference.

** ΔU

To attempt to justify the above proposals, the physical properties of argon and nitrogen were tabulated (Table 6.10, p. 291) and compared. The only quantities listed whose value for argon does not lie between the minimum and maximum values for H₂, CO₂ and N₂ is are the heat capacity and the collision frequency, which are both slightly lower for argon. No obvious explanation for the endothermic DSC results under argon is apparent from the physical data.

Other possibilities have been considered. Copper nitride, Cu₃N, exists [8, p. B-198] and is reported to decompose exothermically at temperatures greater than 327 °C under nitrogen [30], and at approximately 350 °C under argon [31]⁴. It has an X-ray diffraction pattern with peaks at $2\theta = 23.7^\circ$, 41.8° and 48.7° [32], which is distinguishable from those of copper metal and the copper oxides.

There is no evidence from XRPD patterns of the DSC residues, obtained in this study, of the presence of copper nitride, so any participation in the thermal decomposition of copper(II) oxalate by copper nitride would have to be temporary and thermochemical contributions to formation and subsequent decomposition of copper nitride as an intermediate would cancel out.

More importantly, exothermic decomposition occurs under CO₂ and H₂ atmospheres as well. This fact does not support the notion that a temporary interaction between nitrogen and the decomposing DSC sample, absent under argon, might somehow inhibit a process which would otherwise give an endothermic DSC response.

As reviewed in [3, p. 441, *et seq.*], the decompositions of copper(II) formate and copper(II) acetate take place by complex mechanisms involving the formation of volatile and unstable copper(I) intermediates, which cause copper to be deposited on the container walls. Copper(II) malonate, fumarate and maleate decompose via stepwise reduction of copper(II) to copper(I) to copper metal [3, p. 441, *et seq.*]. There is evidence for the decomposition of copper(II) oxalate proceeding via a copper(I) intermediate, with the overall decomposition (under vacuum) being [33]:



⁴The decomposition temperatures of copper nitride reported in the literature vary widely. The references cited here show DSC curves and specify the atmosphere.

Although the absence of copper oxides in the above chemical equation makes this inconsistent with the results obtained in this study, the complexity of the DSC responses seems to be consistent with a multi-step process. No evidence of copper deposition on the sample containers was observed.

Table 6.10: Physical properties of selected gases. The mean free paths were calculated as $\ell = \frac{m}{\sqrt{2}\pi\rho\sigma^2}$ [19, p. 5.171], where m is the mass of the gas molecule, ρ is the density and σ is the molecular diameter.

Property	Exo						Endo	Ratios	
	H ₂	CO ₂	N ₂	Min.	Max.	Min./Max.	Ar	N ₂ /Ar	Ar/N ₂
Mol. mass/g mol ⁻¹	2.016	44.01	28.01	H ₂	CO ₂	0.04581	39.95	0.7011	1.426
* C _p (@ 400 K)/J K ⁻¹ mol ⁻¹	29.2	41.3	29.2	H ₂ =N ₂	CO ₂	0.707	20.8	1.40	0.712
** Thermal conductivity (293 K)/mW m ⁻¹ K ⁻¹	182.8	16.0	25.6	CO ₂	H ₂	0.0875	17.6	1.45	0.688
† Density (293 K)/g m ⁻³	88	1975	1165	H ₂	CO ₂	0.045	1782.4	0.6536	1.530
‡ Mean free path (1 bar)/10 ⁻⁸ m	15	7.468	9.063	CO ₂	H ₂	0.50	10.10	0.8973	1.114
• Collision frequency (1 bar, 293 K)/10 ⁶ s ⁻¹	10060	6120	5070	N ₂	H ₂	0.5040	4000	1.2675	0.7890

* [19, p. 6.81 *et seq.*]
 ** [19, p. 5.148 *et seq.*]
 † [19, p. 3.13 *et seq.*]
 ‡ molecular diameters from [8, p. F-151]
 • [8, p. F-151]

6.4 CONCLUDING REMARKS

The evolution of oxygen gas or monatomic oxygen is a possible explanation for the thermal behaviour of copper(II) oxalate under argon. Further investigation is necessary:

1. to investigate the thermal behaviour of copper(II) oxalate under argon in DTA or heat-flux DSC instruments,
2. to determine the DSC response under various atmospheres, in the absence of potential catalytic surfaces, which have been shown to give spurious DSC results for the decomposition of zinc, nickel and iron(II) oxalates in air [34],
3. to determine whether O_2 or O can be detected experimentally, again with precautions against interference by potential catalytic surfaces,
4. to determine whether copper-bearing particles can be detected in the gas-phase,
5. to establish the reason for the greater extent of oxidation of the solid residues at lower heating rates,
6. to determine the nature of the flow-rate dependency of the DSC results, without which no robust interpretation of the DSC results is possible, and
7. to determine the nature of any solid-state rearrangements which may occur before or during the main decomposition.

In conclusion, the unexpected endothermic decomposition of copper(II) oxalate under argon cannot be explained unequivocally by the thermal, spectroscopic and X-ray methods employed in this study.

References

- [1] **D. Dollimore and D. L. Griffiths.** “Differential thermal analysis study of various oxalates in oxygen and nitrogen.” *J. Thermal Anal.* **2** (1970), 229–250.
- [2] **A. Coetzee, D. J. Eve and M. E. Brown.** “Thermal analysis of some mixed metal oxalates”. *J. Thermal Anal.* **39** (1993), 947–973.
- [3] **A. K. Galwey and M. E. Brown.** *Thermal Decomposition of Ionic Solids.* No. 86 in Studies in Physical and Theoretical Chemistry. Elsevier Science B. V., Amsterdam 1999.
- [4] **E. A. Gusev, S. V. Dalidovich, V. A. Shandakov and A. A. Veher.** “Thermal decomposition of copper(II), nickel(II), cobalt(II) and iron(II) oxalates in self-generated atmospheres”. *Thermochim. Acta* **89** (1985), 391–394.
- [5] **M. A. Mohamed, A. K. Galwey and S. A. Halawy.** “A comparative study of the thermal reactivities of transition metal oxalates in selected atmospheres”. *Thermochim. Acta* **429** (2004), 57–72.
- [6] **D. Dollimore, D. L. Griffiths and D. Nicholson.** “The thermal decomposition of oxalates. Part II. Thermogravimetric analysis of various oxalates in air and in nitrogen.” *J. Chem. Soc.* pp. 2617–2623.
- [7] **D. Dollimore.** “The thermal decomposition of oxalates. A review”. *Thermochim. Acta* **117** (1987), 331–363.
- [8] **R. C. Weast** (editor). *CRC Handbook of Chemistry and Physics.* 49th ed. The Chemical Rubber Co., Cleveland, Ohio, USA 1968–1969.

- [9] **M. L. Van.** “Standard enthalpies of formation of cobalt, nickel and copper oxalates, malonates, and succinates.” *Comptes Rendus des Seances de l’Academie des Sciences, Serie C: Sciences Chimiques* **272**(26) (1971), 2141–3. Abstract (CAN 76:7359).
- [10] **A. Coetzee.** *Thermal decomposition of mixed metal oxalates.* Master’s thesis, Rhodes University January 1993.
- [11] **Institute of Experimental Botany.** “SI Units and Symbols”. URL: <http://www.ueb.cas.cz/bp/notice-si.htm>. (last accessed Oct. 2005).
- [12] **A. K. Galwey and M. E. Brown.** “Thermal decomposition of nickel squarate dihydrate ($\text{NiC}_4\text{O}_4 \cdot 2\text{H}_2\text{O}$)”. *J. Chem. Soc., Faraday Trans. 1* **78**(2) (1982), 411–424. Main gaseous decomposition products also listed in abstract (CAN 96:169460).
- [13] **C. N. Banwell.** *Fundamentals of Molecular Spectroscopy.* 2nd ed. McGRAW-Hill Book Company (UK) Limited, Maidenhead, Birkshire, England 1972.
- [14] **J. Mullens, A. Vos, R. Carleer, J. Yperman and L. C. V. Poucke.** “The decomposition of copper oxalate to metallic copper is well suited for checking the inert working conditions of thermal analysis equipment”. *Thermochim. Acta* **207** (1992), 337–339.
- [15] **PerkinElmer Life and Analytical Sciences.** “TG/IR Interface”. URL: <http://las.perkinelmer.com>. Part no. L1200502/L1200503 (last accessed Jan. 2005).
- [16] **J. H. Slaghuis and P. M. Morgan.** “Evolved gas analysis using the Perkin-Elmer TGA7 HT—a novel method of gas sampling”. *Thermochim. Acta* **175**(2) (1991), 135–140.
- [17] **J. V. Smith** (editor). *Powder Diffraction File Sets 1–5.* American Society for Testing and Materials, Philadelphia, Pennsylvania, USA 1969.

- [18] **L. Alexander and H. P. Klug.** “Basic aspects of x-ray absorption in quantitative diffraction analysis of powder mixtures”. *Anal. Chem.* **20** (1948), 886–888.
- [19] **J. A. Dean** (editor). *Lange’s Handbook of Chemistry*. 15th ed. McGraw-Hill, Inc. 1999.
- [20] **M. E. Brown** (editor). *Introduction to Thermal Analysis*. 2nd ed. Kluwer Academic Publishers, Dordrecht 2001. Note: M. E. Brown is the author of this work, *not* the editor as stated erroneously by the publishers on the title page.
- [21] **A. Hallbrucker and E. Mayer.** “Gas evolution as an artefact in differential scanning calorimetry”. *J. Thermal Anal.* **35** (1989), 1733–1736.
- [22] **E. Ingier-Stocka and A. Grabowska.** “Thermal analysis of cobalt(II) salts with some carboxylic acids”. *Thermochim. Acta* **54** (1998), 115–123.
- [23] **B. V. L’vov.** “Kinetics and mechanism of thermal decomposition of nickel, manganese, silver, mercury and lead oxalates”. *Thermochim. Acta* **364** (2000), 99–109.
- [24] **B. V. L’vov.** “Mechanism of thermal decomposition of metal nitrates in graphite furnaces for atomic absorption analysis”. *Zh. Anal. Khim.* **45**(11) (1990), 2144–2153. Abstract (CAN 114:50400).
- [25] **B. V. L’vov.** “Mechanism of the thermal decomposition of nitrates from graphite furnace mass spectrometry studies”. *Mikrochim. Acta* **2**(1–6) (1991), 299–308. Abstract (CAN 115:288246).
- [26] **B. V. L’vov and A. V. Novichikhin.** “Mechanism of thermal decomposition of anhydrous metal nitrates”. *Spectrochim. Acta Part B* **50** (1995), 1427–1448.
- [27] **B. V. L’vov and A. V. Novichikhin.** “Mechanism of thermal decomposition of hydrated copper nitrate in vacuo”. *Spectrochim. Acta Part B* **50** (1995), 1459–1468.

- [28] **D. R. Stull and H. Prophet.** “JANAF Thermochemical Tables”. National Standard Reference Data System NSRDS—NBS 37, Office of Standard Reference Data, National Bureau of Standards, Washington, D.C., USA 1971.
- [29] **D. Broadbent, J. Dollimore, D. Dollimore and T. A. Evans.** “Kinetic study on the thermal decomposition of copper(II) oxalate”. *J. Chem. Soc. Faraday Trans. 1* **87** (1991), 161–166.
- [30] **A. Baiker and M. Maciejewski.** “Formation and thermal stability of copper and nickel nitrides”. *J. Chem. Soc. Faraday Trans. 1* **80** (1983), 2331–2341.
- [31] **T. Nosaka, M. Yoshitake, A. Okamoto, S. Ogawa and Y. Nakayama.** “Thermal decomposition of copper nitride films and dots formation by electron beam writing”. *Applied Surface Science* **169–170** (2001), 358–361.
- [32] **J. F. Pierson.** “Structure and properties of copper nitride films formed by reactive magnetron sputtering”. *Vacuum* **66** (2002), 59–64.
- [33] **M. A. Mohamed and A. K. Galwey.** “A kinetic and mechanistic study of the thermal decomposition of copper(II) oxalate”. *Thermochim. Acta* **217** (1993), 263–276.
- [34] **R. Majumdar, P. Sarkar, U. Ray and M. R. Mukhopadhyay.** “Secondary catalytic reactions during thermal decomposition of oxalates of zinc, nickel and iron(II)”. *Thermochim. Acta* **335** (1999), 43–53.

Part III

X-ray diffractometer data system

Chapter 7

The design and construction of an X-Ray detector circuit

7.1 INTRODUCTION

Owing to the repeated failure of the detector system in our Philips X-ray diffractometer, and to various difficulties encountered in attempting to replace the faulty modules with commercially available systems, it was decided to design and construct a custom-built system. This chapter provides a short overview of the earlier system, describes the design of the replacement system, discusses briefly the performance of the replacement system, and outlines various improvements that may be implemented which do not involve significant design changes.

7.2 A DESCRIPTION OF THE ORIGINAL PHILIPS POWDER DIFFRACTOMETER

The Philips powder diffractometer in use in the Department of Chemistry dates back to about 1970, although parts of the design date back to 1945 [1]. Figure 7.1 (p. 301) is a schematic representation of the system. The system comprises three basic parts, viz.,

Philips vertical goniometer: The vertical goniometer is equipped with a fixed

X-ray source, a movable arm with a mounting for the X-ray detector which pivots about the central specimen holder at a variable rate of 2θ degrees per minute, and a specimen stage that rotates about its central axis at θ degrees per minute. The goniometer is a purely electromechanical device, and will not be discussed any further, except to mention that it serves as a movable mounting for the sample and the proportional detector probe.

Philips PW1965/40 Proportional detector probe [2]: This consists of a small metal casing which contains a proportional counter tube, which constitutes the photon-counting element, and a transistor preamplifier mounted very close to the tube. Our system is equipped with a Philips PW1965/40-type probe (requiring, in addition to H.T., a +24 V DC supply), which contains a Philips 18511-type (Centronic ZP1610-type [3]) proportional counter tube. Other types include the later PW1965/50, whose preamplifier is a more compact design based on what appears to be a semi-integrated circuit, and the earlier PW1965/20 and PW1965/30, which require a -11 V DC supply instead of +24 V .

Philips PW4620 scintillation counter detector system [4]: This consists of a single metal cabinet, originally designed to interface with scintillation counters, but compatible with the PW1965/40 proportional detector probe. It contains the following functional units:

High-voltage power supply: This is a variable (0.2–2 kV, continuously) DC power supply, which supplies high voltage to the proportional counter tube. It is mounted in the same cabinet as the parts which follow, to make up a Philips PW4620 unit.

Regulated +24 V DC power supply: This powers the transistor circuitry of the preamplifier, and is used internally as well. Other regulated supplies are also provided, but are not relevant to this discussion.

Pulse-shaping amplifier: This conditions and amplifies the signal from the proportional detector probe. The nature of the conditioning required will be discussed later. An analogue output of the conditioned and amplified signal is provided.

Pulse-height discriminator: Also known as a *window discriminator* or *single-channel analyzer*, this module generates a single logical pulse for each input pulse whose amplitude passes between adjustable lower and upper thresholds. In practice, the lower threshold and the size of the discriminator window (i.e., the *difference* between the upper and lower thresholds) are set by means of a pair of front panel knobs. An analogue output of the pulse-height discriminator pulses is provided.

Ratemeter: This module provides a DC signal proportional to the number of logic pulses which arrive at its input per unit time. The output can be scaled to suit various count rate ranges, and smoothed to remove random fluctuations in the input count rate. Various output levels are provided (including a 0–10 mV range for chart-recorders), and a meter on the front panel provides a visual indication of the count rate.

The principles of operation of the relevant components are discussed in greater detail below.

7.2.1 Proportional counter probe (PW1965/40)

This consists of two subcomponents, viz., the proportional counter tube and the preamplifier.

Proportional counter tube

Detailed descriptions of proportional counter tubes are available in [5, Chapter 6] and in the manufacturers' literature [2, 6]. The Philips 18511 (Centronic ZP1610) proportional counter tube consists of a gas-tight metal jacket fitted with a mica side-window and a central metal electrode. The body of the tube contains a mixture of a xenon gas, the main component, plus a small quantity of an organic quencher gas, at a pressure of 40 kPa. The central metal electrode is electrically insulated from the rest of the counter. A DC potential difference of 1500–1800 V is applied between the central electrode (the anode) and the body of the tube (the cathode); the anode is held positive with respect to the cathode.

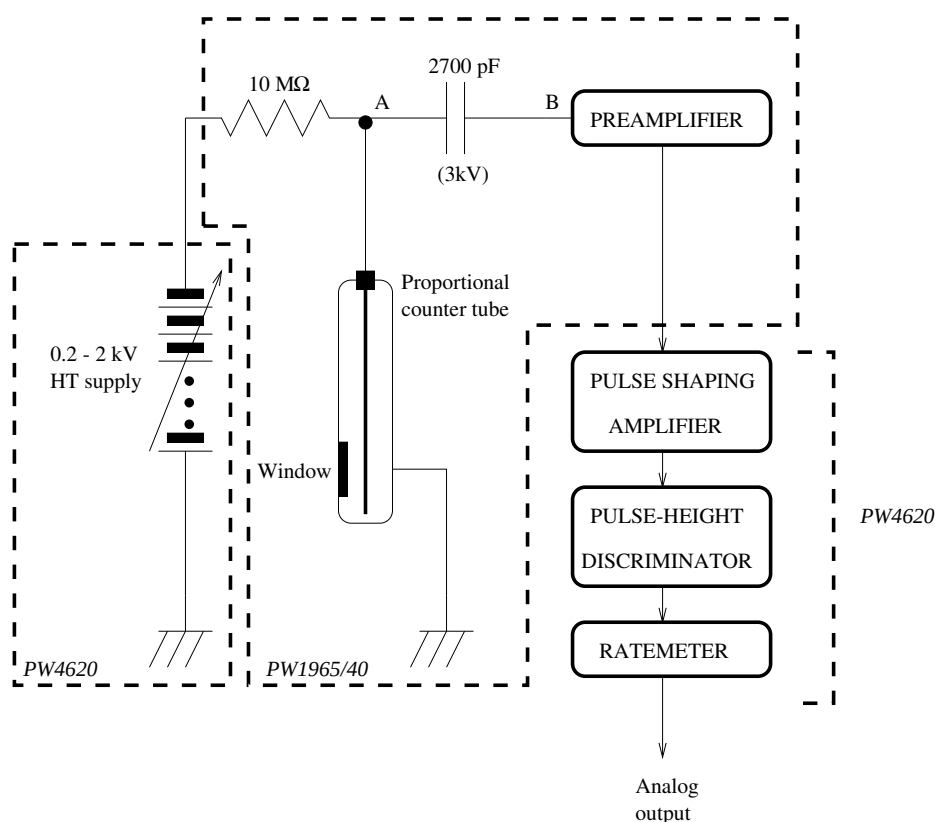


Figure 7.1: A simplified schematic diagram illustrating the various component parts of the original Philips X-ray detector, showing also in which unit each part resides. Parts of the HT supply section and low-voltage DC supplies are omitted for clarity.

In the steady state, and in the absence of any photons or other ionizing particles, no current flows through the proportional counter tube once its capacitance and the stray capacitance of its attendant wiring, etc., have been charged fully. Because no current is flowing, there is no voltage drop across the anode resistor ($10\text{ M}\Omega$), and hence point A is at the full HT supply potential¹. Point B, on the other side of a DC-blocking capacitor (2700 pF), is thus at 0 V with respect to ground.

When a sufficiently energetic ionizing particle, such as an X-ray photon, enters

¹If a standard multimeter were used to measure this voltage, it would under-read significantly, because the resistance of the power supply (mainly, the $10\text{ M}\Omega$ resistor) is comparable to that of a typical digital voltmeter.

the volume of the tube through the window, a number of noble gas atoms are ionized to give noble gas cations and free electrons as shown in Equation 7.1, in which X is a noble gas, for example argon or xenon.



The X^+ ions will be accelerated by the electric field towards the cathode, but because they have low mobility, they do not attain high kinetic energy between collisions. However, the electrons can, while being accelerated to the central anode, attain significant kinetic energy, and if they are accelerated such that their kinetic energy exceeds the ionization energy of the filler gas, secondary ionization of the filler gas atoms by the primary electrons occurs [7]. The secondary electrons, in turn, are sufficiently accelerated to give rise to further ionizations, and so on, in a cascading process called gas-amplification. In this way, each ionizing particle entering the volume of the proportional counter gives rise to an ionization event, the number of ions generated being approximately proportional to the energy of the ionizing particle [7]. The ionization gives rise to a momentary conduction, observable as a momentary voltage drop across the resistor in Figure 7.1 (p. 301), and hence as a short negative-going pulse at point B.

Collisions between accelerated electrons and filler gas molecules may generate excited uncharged species, without generating secondary electrons. While such collisions do not contribute directly to gas-amplification, the excited molecules may emit, in decaying to the ground state, ultraviolet or visible photons. These photons may, in turn, cause electrons to be emitted either by ionizing the filler gas or by photoelectric interaction with the walls of the counter. Such photon-induced ionizations form an integral part of the operation of Geiger-Müller tubes, but are undesirable in proportional counters because they may give rise to spurious pulses or loss of proportionality. The role of the organic component of the filler gas is to absorb the ultraviolet/visible photons in such a way as to suppress further ionizations [5, Chapter 6].

The specifications of the Philips 18511-type (Centronic ZP1610-type) proportional counter tube are given in Table 7.1 (p. 303).

Referring to Figure 7.1 (p. 301), the momentary conduction, caused by an

Table 7.1: Selected specifications of the Philips 18511 (Centronic ZP1610) proportional counter tube [6].

Property	Specification
Window thickness	2.0–2.5 mg/cm ²
Window dimensions	7 × 18 mm
Window material	mica
Cathode length (active)	67 mm
Cathode material	chrome iron
Filler gas	Xe/organic vapour
Filler gas pressure	40 kPa
Capacitance	2.0 pF
Weight	89 g
Supply voltage (rec.)	1550 V
Geiger threshold (min.)	1900 V
Op. voltage (1 mV pulse)	1460–1540 V
Op. voltage (10 mV pulse)	1690–1770 V
Absolute max. Voltage	1850 V

ionizing particle entering the volume of the proportional counter tube, causes a momentary voltage-drop at the anode of the tube, owing to the high resistance (10 M Ω) between the HT source and the anode. The charge that passed through the proportional counter is “integrated” onto the capacitor, and a small negative-going pulse therefore appears at point B, the input of the preamplifier.

Preamplifier circuit

The preamplifier circuit in the PW1965/40 proportional counter probe is a simple one, with a gain of approximately 10. It is a transistor circuit, comprising two stages: a bootstrapped emitter-follower DC-coupled to an inverting amplifier. A simple diode-clamp is provided at the input to protect the circuit against large negative transients (such as occur when the HT supply is switched on), and a small resistor (about 100 Ω) isolates the output of the amplifier from cabling capacitance, etc.

Each ionizing particle entering the volume of the proportional counter tube

gives rise to a preamplifier output pulse (positive-going) with a sharp rise time and a slow exponential decay. *The height of the pulse is proportional to the energy of the ionizing particle, and the exponential decay time constant is set mainly by the proportional detector probe circuitry.* Figure 7.2 shows an idealized preamplifier output pulse in terms of its exponential decay time constant, and the specifications of the preamplifier and output pulse characteristics are given in Table 7.2 (p. 305).

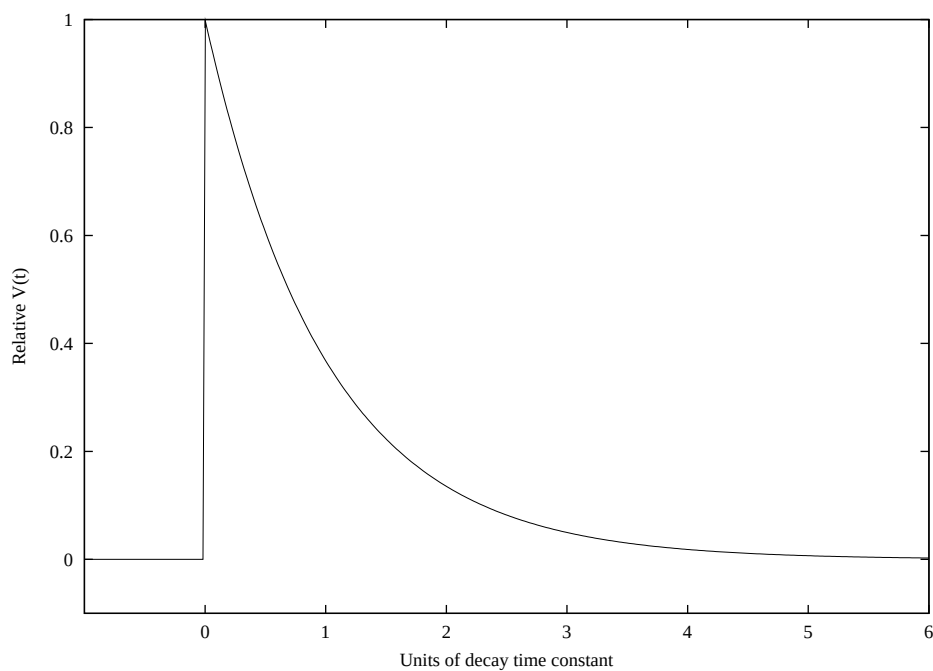


Figure 7.2: An idealized preamplifier output pulse, shown in terms of its exponential decay constant.

7.2.2 Pulse-shaping amplifier (in PW4620 unit)

Aside from the more conventional functions of an instrument amplifier, such as signal amplification with various gain settings and optional polarity inversion, this section has an interesting pulse-clipping feature.

With reference to the preamplifier output pulse-shape shown in Figure 7.2, all the relevant information carried by the pulse is contained in its rising edge

Table 7.2: Selected specifications of the preamplifier and pulse characteristics of the Philips PW1965/40 proportional detector probe [2].

Property	Specification
DC supply voltage	+24 V
Output impedance	100 Ω
Pulse polarity	Positive
Pulse rise-time (10 $\rightarrow$ 90%)	0.2 μ s
Pulse decay-time (90 $\rightarrow$ 10%)	60 μ s
Exponential decay time constant*	27 μ s
Typ. pulse amplitude	20–200 mV

* The exponential decay time constant, τ_d , is related to the 90 $\rightarrow$ 10%-pulse decay time, $\tau_{0.9\rightarrow 0.1}$ by $\tau_{0.9\rightarrow 0.1} = \tau_d \ln 9 \approx 2.2 \tau_d$ and hence $\tau_d \approx 0.46 \tau_{0.9\rightarrow 0.1}$

and peak-height. The long decay is merely a potential interference. If two identical ionizing particles were to arrive at the proportional counter within, say, one preamplifier decay time constant of each other, the second output pulse would ride on the tail of the first, thus having a peak height much higher than the first. This phenomenon is called pile-up, and if pulse-heights (read the energies of the ionizing particles) are of interest, it might be a significant source of error, especially at higher count rates.

Some pulse clipping must therefore be performed if the problem of pile-up is to be avoided. Various pulse-shaping methods exist:

Single delay-line (SDL) pulse-clipping

This is the pulse-clipping method used in the Philips PW4620 system [4]. The *characteristic impedance* of a coaxial transmission line is a property which depends on the dielectric spacer material and the diameters of the central conductor and shield, and is independent of the length of the cable [5, Chapter 16]. For example, coaxial cables often have a characteristic impedance of 50 Ω . Normally, transmission lines are terminated in resistances equal to their characteristic impedances: i.e., the central conductor is connected to the shield at the receiving end by means of a resistor whose value is equal to that of the characteristic impedance of the cable. Failure to do so would result in undesirable behaviour in

the context of signal transmission [8, §13.09].

A transmission line with a characteristic impedance of Z_0 , driven by a step function of amplitude A_i and terminated in a resistance R , will produce a reflected pulse of amplitude A_r such that [8, §13.09]

$$\frac{A_r}{A_i} = \frac{R - Z_0}{R + Z_0} \quad (7.2)$$

If $R = Z_0$, that is, the impedance of the load is matched to that of the transmission line, then the reflected pulse has a zero amplitude — i.e., no reflection takes place. Clearly, if R is a short (i.e., $R = 0$), then the reflected pulse amplitude is $-A_i$. The propagation speed of electrical pulses through coaxial cables is approximately $0.66 c$, which means that a pulse of duration $2L/0.66 c$ can be generated from a step-function by means of a shorted transmission line of length L . Figure 7.3 gives a schematic diagram of a shorted delay-line being driven by a step function. The voltage step propagates along the cable at a speed of $0.66 c$ until it encounters

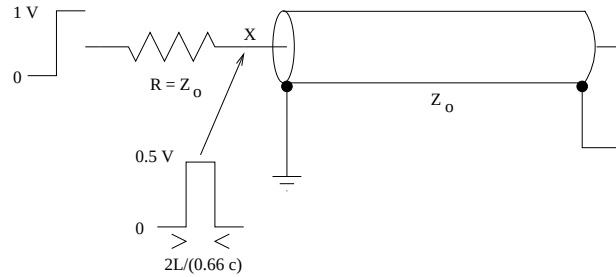


Figure 7.3: A shorted delay-line used to generate a short pulse from a step input.

the short at the far end. The short circuit forces the potential difference across the point of termination to be zero, and thus a negative-going step of equal amplitude but opposite polarity is produced. This so-called reflected step propagates along the cable in the opposite direction. When the reflected step meets the input step, it cancels it. However, because of the propagation delay, the voltage output at the point X in Figure 7.3 for a step function applied through the resistor is a short rectangular pulse. In this example, the output pulse amplitude is half the step height because the input resistor and the delay-line form a voltage divider at the frequencies of interest.

In practice, a line with a much reduced pulse propagation speed, called a

delay-line, is used — it is physically much smaller than an equivalent coaxial cable [4, 8, 9].

If a shorted delay-line were driven by a preamplifier pulse, the resultant output pulse would look as illustrated in Figure 7.4. The fact that the preamplifier pulse is not square causes the undershoot in the output pulse — it arises from the shifting of the reflected pulse tail relative to the input pulse tail. It may be dealt with by attenuating the reflected pulse slightly, by terminating the delay-line in a small resistance instead of a short circuit [5, Chapter 16].

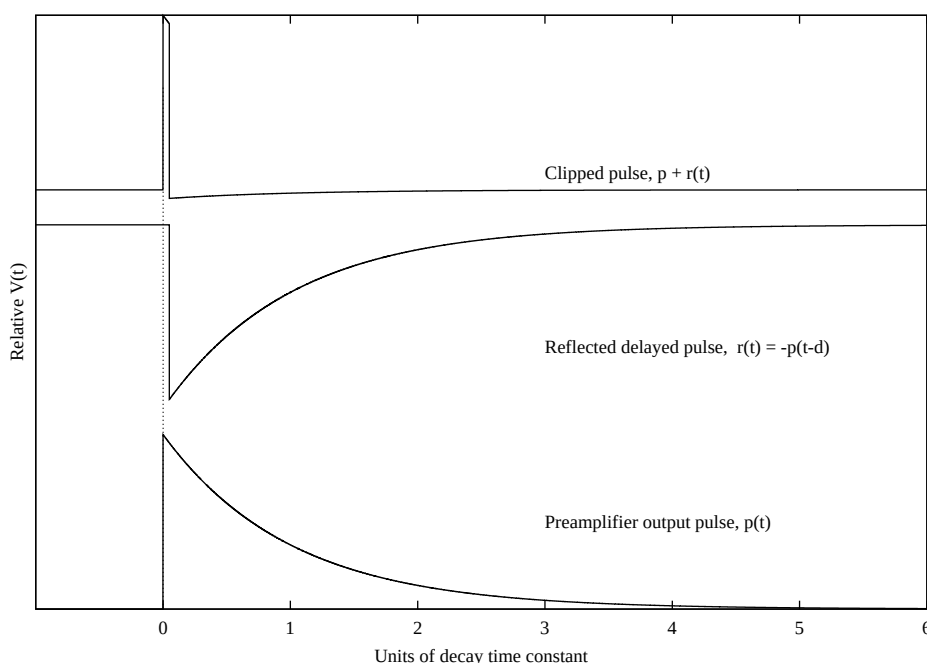


Figure 7.4: Illustrating the concept of single delay-line pulse-clipping. The lower trace shows a preamplifier pulse, $p(t)$, with a decay constant of τ_p . The middle trace shows the reflected pulse, $r(t) = -p(t - d)$, from the delay-line, lagging the original pulse by a delay, d , such that $d \ll \tau_p$. The sum of the preamplifier and reflected pulses is shown in the upper trace. The slight undershoot following the impulse may be removed by slightly attenuating the reflected pulse. (All amplitudes are as they appear the delay-line input.)

CR-RC pulse-shaping

Although this type of pulse-shaping was not available in the Philips PW4620 unit, it was provided as an option in more advanced Philips detector systems [9], and is employed in various nuclear detector systems manufactured by Canberra Industries [10]. Detailed descriptions may be found in [5, Chapter 16] and [11].

CR-RC pulse-shaping derives its name from the CR (capacitor-resistor) high-pass and RC (resistor-capacitor) low-pass filters² which it employs. Schematically, a CR-RC pulse shaper is nothing more than a cascaded high-pass filter and low-pass filter pair, separated by a unity gain buffer (or an amplifier, if the application requires it) to ensure that the filters work independently. Although other configurations are possible, the high- and low-pass filters most often have the same time-constant (and hence the same cut-off frequency). Figure 7.5 gives

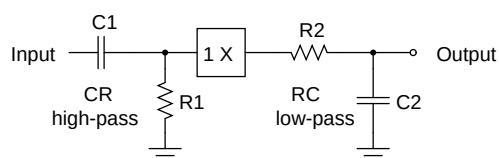


Figure 7.5: A simplified schematic of a CR-RC pulse-shaping amplifier [5, Chapter 16].

a simplified diagram of a CR-RC pulse-shaping circuit, while Figure 7.6 shows some pulse-shaping results. Trace **a** shows a raw preamplifier pulse with a decay constant of $27\ \mu\text{s}$ ($90 \rightarrow 10\%$ in $60\ \mu\text{s}$), and trace **b** shows the CR-filtered output (filter time constant of $1.5\ \mu\text{s}$). The CR-filtered output approximates a derivative: the sharp positive-going part is the derivative of the fast rise of the preamplifier pulse, the long undershoot or “tail” being approximately the derivative of the tail of the preamplifier pulse. The positive going part of the CR output peak is much shorter than the preamplifier pulse, but the “spike” is not well suited to operations like pulse-height discrimination or even pulse-counting.

Trace **d** (dotted line) shows the (amplified) output of the complete CR-RC circuit. The peak is slightly broader than the CR sub-circuit output, and more

²CR high-pass filtering approximates differentiation under certain conditions, and RC low-pass filtering approximates (leaky) integration: thus high- and low-pass filters are sometimes referred to as differentiators or integrators, respectively.

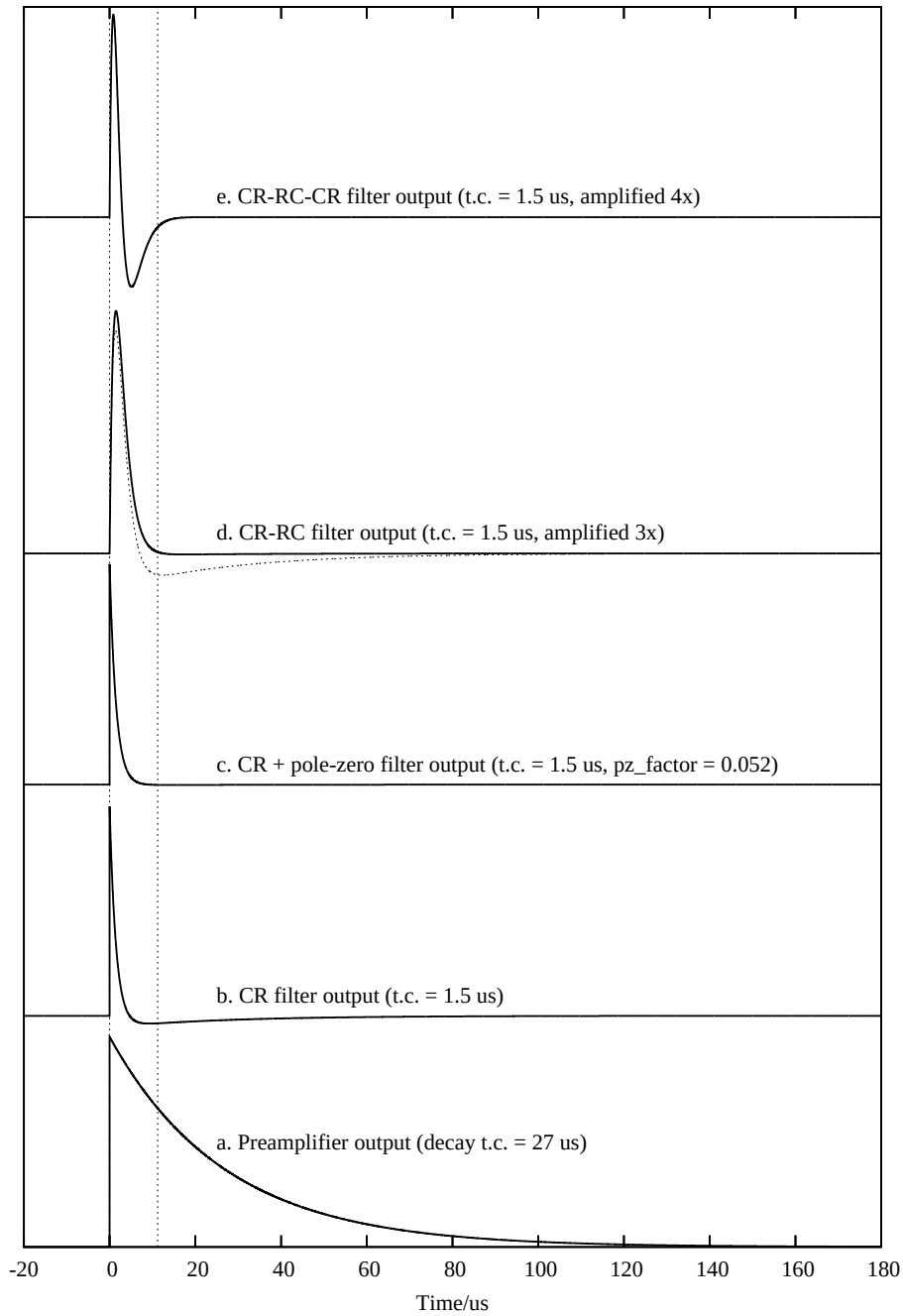


Figure 7.6: Traces at various stages of CR-RC-CR pulse shaping: **(a)** a typical preamplifier pulse (input to pulse-shaping system); **(b)** the output of a CR high-pass filter with undershoot (no pole-zero correction); **(c)** the output of a CR high-pass filter with undershoot removed by pole-zero correction ; **(d)** the output of of a CR-RC filter with pole-zero correction (dotted line shows output with no pole-zero) ; and **(e)** the output of a CR-RC-CR filter with pole-zero correction.

symmetrical, making it more suitable for further analysis. Two significant improvements may be achieved very simply at this stage:

1. The long undershoot in Trace **d** undermines pulse-height discrimination, particularly at higher count rates: a second preamplifier peak occurring at some time during this undershoot would sink into it somewhat, and appear smaller than it really is. This effect may be counteracted by adding a resistor across the capacitor C_1 (see Figure 7.5), with a resistance of

$$R_{pz} = \frac{\tau_p}{C_1}$$

in which τ_p is the decay constant of the preamplifier pulses. This resistor effects a correction termed *pole-zero cancellation*. Very simply, the resistor “leaks” some fraction of the input signal through to the output of the CR stage, thereby cancelling out the undershoot. Trace **d** (solid line) shows the output of a CR-RC pulse-shaping circuit with pole-zero cancellation. More rigorous descriptions are available in [5, Chapter 16] and [11].

2. The CR-RC output pulses are unipolar (with pole-zero cancellation, or else asymmetrically bipolar without), which may cause further problems with pulse-height discrimination. AC-coupling is inevitable in pulse-shaping amplifiers, and as such, unipolar pulse trains will undergo different zero-line shifts at different count rates, as shown in Figure 7.7 (p. 311). These shifts arise because the average voltage at the output of a blocking capacitor must be zero, because no DC current can flow through a capacitor. Zero-line shifts will introduce errors in pulse-height discrimination, and are therefore highly undesirable. Bipolar pulses, particularly those which integrate to zero, are immune to this problem, and so a simple way to avoid zero-line shifts is to add a second differentiating stage after the CR-RC circuit. In practice, the output pulses do not integrate exactly to zero, and thus the zero-line shifting is not entirely eliminated, but is greatly reduced [5, Chapter 16]. (Philips, and other manufacturers, solve the zero-line shifting problem by means of an electronic *gated baseline-restorer* circuit [4, 10].)

Figure 7.8 shows an improved CR-RC-CR circuit with pole-zero correction.

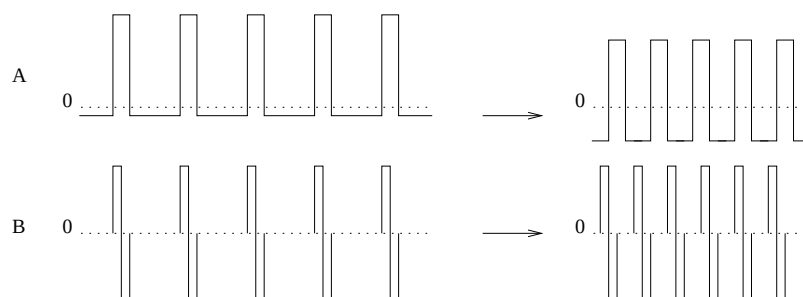


Figure 7.7: AC-coupled unipolar pulse trains (**A**) undergoing zero-line shifts with changing count-rate, because the average voltage on the blocking capacitor output must be zero. Bipolar pulse-trains (**B**) satisfy this condition, and are thus immune to zero-line shifts.

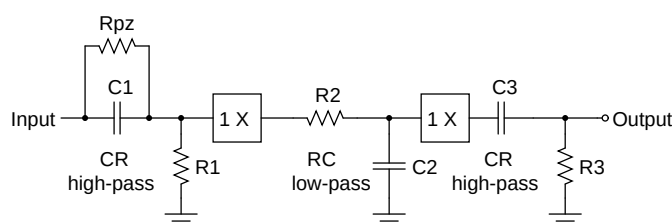


Figure 7.8: A simplified schematic of a CR-RC-CR pulse-shaper with pole-zero cancellation [5, Chapter 16].

Other methods

Double delay-line (DDL) pulse-shaping In this method, bipolar pulses are produced by using two delay lines instead of just one. This is an alternative to using SDL clipping with a gated baseline-restorer [5, Chapter 16].

Gaussian CR-(RC)ⁿ pulse-shaping Here, n cascaded RC low-pass filters are used instead of just one. With $n = 4$, the difference between the circuit output and a true Gaussian curve is negligible. The symmetrical unipolar peaks may then be passed through a gated baseline restorer; or they may be differentiated by a further CR stage (CR-(RC)ⁿ-CR pulse shaping), whose bipolar output pulses

would be more symmetrical than in plain CR-RC-CR shaping, due to the extra RC-stages, and hence more immune to zero-line shifts [5, Chapter 16].

7.2.3 Pulse-height discriminator (in Philips PW4620)

The purpose of a pulse-height discriminator or single-channel analyzer is to generate a single logic pulse for each pulse whose amplitude is between adjustable upper and lower thresholds. A pulse-height discriminator is often called a *window discriminator*, this nomenclature suggesting a common implementation in which the lower threshold and the *difference* between the upper and lower thresholds are the adjustable parameters. This implementation is convenient because it allows the window position to be adjusted without changing the window size. This section gives a generic technique for pulse-height discrimination, which is similar to the method adopted by Philips [4]. Figure 7.9 (p. 313) illustrates the basic concept of pulse-height discrimination.

Assume the availability of electronically generated lower and upper thresholds **LLT** and **ULT**, and the means of determining whether and when the input level crosses these thresholds. Assume further a single bit of memory, **FF**, which may be *set* to a value of 1 or *reset* to a value of 0. For an incoming pulse **IP**, shaped like trace **e** in Figure 7.6, the following operations have to be performed by the pulse-height discriminator:

1. if **IP** crosses **LLT** (rising edge), set **FF** to 1 .
2. if **IP** crosses **ULT** (rising edge), reset **FF** to 0 .
3. if **IP** crosses **LLT** (falling edge), generate a short pulse **GP**, the *gate pulse*.
4. output **GP** · **FF**, where · is the logical **AND** operator: thus, the gate pulse passes through to the output only if **FF** has the value 1 .

Note the following points:

- input pulses that do not cross the lower threshold at all simply disappear after the pulse-height discriminator,

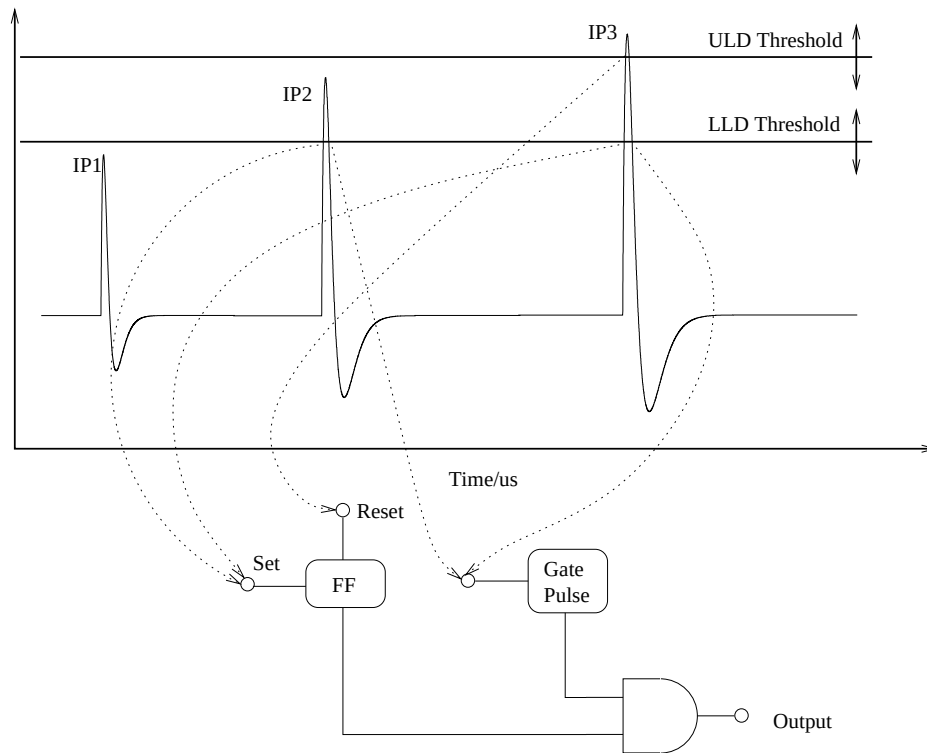


Figure 7.9: Diagrammatic representation of the various operations involved in pulse-height discrimination for three input pulses: **IP1**, which crosses neither the lower nor upper discriminator threshold and is thus *not* counted; **IP2**, which crosses the lower discriminator threshold but not the upper, and is thus counted; and **IP3** which crosses the upper discriminator threshold and is thus *not* counted. Leading edges crossing the lower threshold *set* the flip-flop, and leading edges crossing the upper threshold *reset* it. Trailing edges crossing the lower threshold generate a *gate pulse*, and the output is the logical **AND** of the flip-flop state and the gate pulse.

- the system is self-starting: no matter what the initial state of **FF**, it will be set to 0 by the rising edge of the first input pulse which crosses **LLT**, and
- the gate pulse, **GP** is generated only after the input pulse has completed, and so introduces additional dead-time into the system; depending on the specific pulse-shaping amplifier parameters and the width of the gate pulse, this may be less important with bipolar input pulses.

Depending on the system requirements, greater efforts may be required to ensure that:

- pulse-height discriminator pulses are of some minimum width as dictated by the counting system;
- the discriminator is not retriggerable, i.e., it is artificially rendered insensitive to input pulses from the moment an input pulse has entered the system until it has been processed completely: the more thoroughly this is observed, the more complex the discriminator will be.

7.2.4 Counting ratemeter (in Philips PW4620)

Ratemeter theory: analogue case

A ratemeter is a continuous output device which gives a varying DC voltage proportional to the input count rate. A simplified schematic diagram of an analog ratemeter is given in Figure 7.10 [12], and a detailed circuit diagram and analysis is available in [13]. Each pulse at the input causes the constant charge circuit

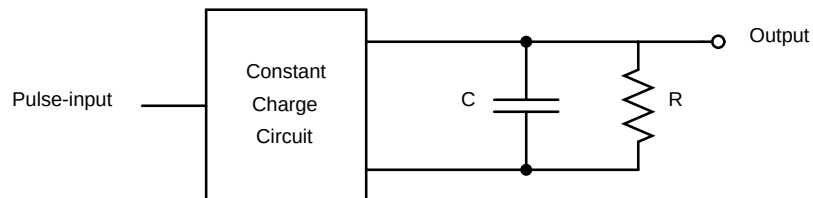


Figure 7.10: A simplified diagram of a ratemeter [12].

to inject a fixed charge, q , into the capacitor, C . The charge contained within the

capacitor is related to the voltage across it, V by the equation [8]:

$$Q = CV \quad (7.3)$$

The average current flowing into the capacitor is

$$\overline{I}_{\text{in}} = \left(\frac{dQ}{dt} \right)_{\text{in}} = rq \quad (7.4)$$

in which r is the number of pulses arriving at the input of the constant charge circuit per second. The average current flowing out of the capacitor is

$$\overline{I}_{\text{out}} = \left(\frac{dQ}{dt} \right)_{\text{out}} = \frac{V_C}{R} = \frac{Q(t)}{RC} \quad (7.5)$$

The net dQ/dt of the capacitor is obtained by combining Equations 7.4 and 7.5 to give the separable first-order differential equation

$$\frac{dQ}{dt} = rq - \frac{Q(t)}{RC} \quad (7.6)$$

Separating variables in Equation 7.6 and integrating on both sides gives:

$$\frac{dQ}{rq - Q(t)/RC} = dt \quad (7.7)$$

$$\int \frac{dQ}{rq - Q(t)/RC} = \int dt + K = t + K \quad (7.8)$$

where K is a constant of integration. Substituting

$$u = rq - Q(t)/RC$$

in the left hand side and integrating in terms of gives:

$$-RC \int \frac{du}{u} = -RC \ln u \quad (7.9)$$

Substituting back into this equation and recombining with Equation 7.8 gives:

$$-RC \ln \left(rq - \frac{Q(t)}{RC} \right) = t + K \quad (7.10)$$

$$\ln \left(rq - \frac{Q(t)}{RC} \right) = -\frac{t}{RC} + K' \quad (7.11)$$

$$rq - \frac{Q(t)}{RC} = e^{-t/RC + K'} \quad (7.12)$$

Given the initial condition that $Q(0) = 0$, it is clear from the equation above that

$$rq = e^{K'}$$

and hence that Equation 7.12 becomes

$$1 - \frac{Q(t)}{rqRC} = e^{-t/RC} \quad (7.13)$$

$$Q(t) = rqRC \left(1 - e^{-t/RC} \right) \quad (7.14)$$

Remembering Equation 7.3, an expression for $V(t)$ can now be written as

$$V(t) = rqR \left(1 - e^{-t/RC} \right) \quad (7.15)$$

The steady-state cases, $Q(\infty)$ and $V(\infty)$ for these results are

$$Q(\infty) = Q_{\infty}(r) = rqRC \quad (7.16)$$

$$V(\infty) = V_{\infty}(r) = rqR \quad (7.17)$$

The time constant of the ratemeter is defined as,

$$\tau_r = RC$$

If, instead of being a constant, r is a slowly-varying function of time (i.e., slowly within the time-frame of τ_r)

$$r = r(t)$$

then the term $-e^{-t/RC}$ may be disregarded, and

$$r(t) \approx \frac{Q(t)}{qRC} \quad (7.18)$$

$$r(t) \approx \frac{V(t)}{qR} \quad (7.19)$$

These equations, then, form the basis of an analogue ratemeter's filtering and scaling arrangements. The voltage-dependent results are most useful because voltage is very easy to measure, and it is clear that by varying the value of C , different time-constants may be obtained without affecting scaling. However, scaling cannot be changed internally (by changing R) without affecting the time constant.

Ratemeter theory: simplification leads to a digital case

By simplifying the relationships between the charge in the ratemeter capacitor and the input count rate, an equation for a digital ratemeter can be developed. It is relatively easy to count input pulses digitally, and it is similarly easy to keep track of "charge" in a register. The term q , signifying the charge-injection to the ratemeter capacitor in the analog case, loses all meaning in the digital context and may therefore be set to 1. The simplification:

$$k = \frac{1}{RC} = \frac{1}{\tau_r}$$

can also be made because resistance and capacitance as separate concepts have no place here. Then, Equation 7.6 becomes

$$\frac{dQ}{dt} = r - kQ(t) \quad (7.20)$$

The solution to this differential equation and the steady state equation are, respectively,

$$Q(t) = \frac{r}{k} (1 - e^{-k t}) \quad (7.21)$$

$$Q_{\infty}(r) = \frac{r}{k} = \tau_r r \quad (7.22)$$

Here, Q is the current value of a counter register, or some equivalent structure. Equation 7.22 can be arranged to give the basis of a digital ratemeter (for slowly varying r):

$$r(t) \approx kQ(t) = \frac{Q(t)}{\tau_r} \quad (7.23)$$

Assuming the existence of an asynchronous counter (i.e., one not clocked with the rest of the system) with an infinitely wide register, whose current count can be accessed by means of a subroutine `READ_CNTR_REG`, a suitable output device to which a number n may be written by means of the subroutine `OUTPUT(n)`, and a subroutine `PAUSE(n)` which suspends execution for n seconds, and taking for granted infinite precision in all numeric values, the basic execution sequence for a digital ratemeter is given in Table 7.3 (p. 320).

It is basically a continuously running (approximate) numerical simulation of the differential equation, Equation 7.22. Here, the time-constant is set by means of $k \cdot d$, the product of the fraction of Q to be removed *per unit time (not per loop iteration)* and the delay between successive counter samples *in the same time unit*. In Table 7.3, such scaling as may be required is relegated to the subroutine, `OUTPUT(n)`. A digital ratemeter would be most useful if it provided both numeric and analog voltage outputs.

More advanced configurations have been suggested. For example an auto-ranging digital ratemeter with selectable standard deviation is described in [14]. As explained in [15], a better approach might be to use a floating mean algorithm, which gives R_n , the current rate estimate, as

$$R_n = \frac{1}{mT} \sum_{i=q}^n N_i \quad (7.24)$$

where m is the number of measurements included in the mean, T is the time-interval for a single measurement, N_i is the number of pulses measured in the i th measurement, n is the total number of measurements acquired (so that the n th measurement is the most recent), and $q = 1$ when $n < m$ and $q = n - m + 1$ when $m \geq n$. A microprocessor-based implementation³ of a modification of this algorithm is given there. The coefficient of variation for the floating mean algorithm is said to be significantly better than the type of algorithm employed here. However, the algorithm chosen for the present implementation is based on the theoretical model which underlies the original ratemeter.

³Reference [15] states that there is a patent pending on the implementation it describes.

Table 7.3: Pseudo-code illustrating the basic digital ratemeter execution cycle.

```

.....
::: PSEUDOCODE FOR DIGITAL RATEMETER                                     :::
:::                                                                    :::
::: An illustration, assuming infinite precision                        :::
::: arithmetic and infinitely wide registers, of a digital            :::
::: ratemeter implementation. All scaling is relegated to             :::
::: the (non-existent) subroutine, OUTPUT.                            :::
:::                                                                    :::
::: Emmanuel Lamprecht (2004)                                         :::
.....

CONSTANTS:
    k,          ::: fraction of Q to remove per second
    d          ::: delay between cycles in seconds

VARIABLES:
    last_cnt,   ::: counter reading at last iteration
    current_cnt, ::: counter reading at curr. iteration
    cnt_change , ::: counter reading change
    Q

START: current_cnt := 0 ;      ::: initialization
      last_cnt := 0 ;         ::: initialization
      Q := 0 ;                ::: initialization

      LOOP FOREVER
      BEGIN
        current_cnt := READ_CNTR_REG ;
        cnt_change := current_cnt - last_cnt ;
        last_cnt := current_cnt ;
        Q := Q + cnt_change - k*d*Q ;
        OUTPUT(Q) ;
        PAUSE(d) ;
      END LOOP
STOP ::: program never gets here

```

7.3 DESIGN AND IMPLEMENTATION OF A REPLACEMENT DETECTOR SYSTEM

The aim was to produce a system that would serve as a plug-in replacement for all the functions of the Philips PW4620 unit except for the high-voltage power supply. It would take raw preamplifier pulse-input and produce scaled and smoothed ratemeter-type analog output. A prototype was designed with the following basic features:

1. a CR-RC-CR pulse-shaping amplifier, equipped with adjustable pole-zero cancellation and variable gain, with a time constant of $1.5 \mu\text{s}$ (allowing for a generous tolerance in the component values);
2. a simple pulse-height discriminator with adjustable upper and lower thresholds;
3. a digital ratemeter with both numeric (digital) and analog (voltage) outputs, and adjustable time constant and full scale; and
4. a +24 V regulated power-supply for the preamplifier.

The design was translated to a double-sided printed circuit board layout, and the solder-side layout was photo-etched onto a single-sided copper-coated fibre-glass board. The component side of the board was hand-wired. A single circuit-board contains all the necessary components except for the unregulated part of the power-supply (which occupies a separate board) and the +24 V power supply (which is built directly on a small back-pane, which distributes signals and power). The whole unit fits inside a 19-inch rack-mount cabinet.

User input is taken by means of three front-panel knobs — two to set the full-scale ratemeter output and one to set the ratemeter time-constant. In addition, potentiometers on the circuit board allow adjustment of the pole-zero resistor and the final pulse-shaping amplifier stage gain. Lastly, three jumpers are provided to allow the user to place the system in a state suitable for testing — setting the first and the third jumpers shorts the CR-differentiator capacitors (and effectively removes them from the circuit), while clearing the second disconnects the RC integrator capacitor from the circuit.

Two analog outputs are provided, viz., a pulse-shaping amplifier output (variable range) and a scaled ratemeter output (0–11 VDC). The ratemeter signal (in various raw and processed forms) is also given in numeric form as an RS-232 output. A front-panel meter monitors the analog ratemeter output signal.

7.4 CIRCUIT DESCRIPTION

A large number of books, articles and manufacturers' catalogs were consulted in the design of the circuit described here. For general information regarding the use of operational amplifiers in electronic circuits, see [8, 16, 17]. Active components used are the high-speed operational amplifier, AD817 [18]; the precision operational amplifier, OP177⁴ [19]; the voltage comparator, LM311 [22]; the monostable multivibrator, 74HC123 [23]; the high-speed NAND-gate, 74HC00 [24]; the 8-bit microcontroller, AT90S8535 [25, 26], the serial input digital-to-analog converter, AD7390 [27]; and the RS-232 line-driver/receiver, MAX233CPP [28].

7.4.1 Analog section and pulse-height discriminator

Figure 7.13 on p. 333 shows a diagram of the pulse-shaping amplifier and pulse-height discriminator. The individual functional units are discussed in detail below.

Pulse-shaping amplifier

AC-coupling and input protection: C_0 (0.1 μ F ceramic) AC-couples the previous stage (i.e., the PW1965/40 preamplifier) to the circuit. Power diodes D_1 and D_2 form an input protection clamp to absorb transients of either polarity, with R_0 (100 Ω) serving as a current-limiting resistor should the clamp ever be called on.

First high-pass filter + amplifier: C_1 (1500 pf) and R_1 (1 k Ω) form a high-pass filter, with variable pole-zero resistor R_{pz} (0–100 k Ω). The filter time constant, $R_1 C_1$, is 1.5 μ s, and with the values chosen, the pole-zero resistor

⁴The OP07 would be a low-cost, but equally suitable, alternative [20, 21].

will accommodate input waveform decay constants τ_p of up to 150 μs . A non-inverting amplifier of $10\times$ gain is embodied in operational amplifier **AD817/1** and resistors $\mathbf{R}_2$ (1 k Ω) and $\mathbf{R}_3$ (9.1 k Ω).

Low-pass active filter: The fragment comprising operational amplifier **AD817/2**, resistors $\mathbf{R}_4$ (10 k Ω), $\mathbf{R}_5$ (100 k Ω), $\mathbf{R}_{\text{gnd}}$ (9.1 k Ω) and capacitor $\mathbf{C}_2$ (15 pF) constitutes an active low-pass filter with a time-constant, $\mathbf{R}_5\mathbf{C}_2$, of 1.5 μs and an inverting $10\times$ DC gain.

Second high-pass filter + variable gain amplifier: The inverting amplifier, comprising operational amplifier **AD817/3** with associated resistors $\mathbf{R}_6$ (10 k Ω), $\mathbf{R}_7$ (10 k Ω) and $\mathbf{R}_8$ (variable, 0–100k Ω), has a variable gain of $1\text{--}11\times$. Following the amplifier is an RC high-pass filter, with a time-constant, $\mathbf{R}_{12}\mathbf{C}_3$, of 1.5 μs .

The output of the pulse-shaping amplifier is connected directly to the analog part of the pulse-height discriminator, and to a unity-gain buffer (**AD817/4**) which passes the signal to the outside world through a 50 Ω resistor ($\mathbf{R}_{10}$). Note the following:

1. All operational amplifiers operate on regulated dual 15 V supplies which are not shown on the diagram.
2. All resistors used in the construction of this part of the prototype were of the ordinary 5% tolerance type. This is probably sufficient for most purposes, and the present application certainly will not suffer from any reduction in accuracy that this may cause.
3. Strictly speaking, **AD817/3** should have a resistor to ground, as **AD817/2** does in $\mathbf{R}_{\text{gnd}}$. This was deemed unnecessary for the present application, since $\mathbf{C}_3$ would block any DC offset from passing through to the pulse-height discriminator.
4. The current set of parameters gives output pulses very close⁵ to those in the simulated curves shown in Figure 7.6 on p. 309: these were measured to

⁵For Cu-K α radiation at a detector potential difference of 1.6 kV.

have a width of approximately 10 μs at the baseline: very broad compared to the SDL-clipped pulses produced by the Philips PW4620 unit, which gives pulses approximately 1 μs wide at the equivalent point in the circuit. The current parameter set was chosen to allow very conservative design in the pulse-height discriminator, and can easily be adjusted by changing the filter capacitor values. *This would require some changes to the pulse-height discriminator section.*

Pulse-height discriminator

Lower-level Schmitt-trigger: The circuit illustrated in the diagram is a Schmitt-trigger with a variable threshold but a fixed hysteresis. The threshold is set by adjusting the potentiometer R_{13} (1 k Ω winding), whose output is then buffered by the operational amplifier **OP177/1** and applied to the Schmitt trigger formed by the comparator **LM311/1**, and associated resistors R_{14} (24 k Ω) and R_{15} (1 k Ω). The hysteresis is simply

$$\frac{R_{15}}{R_{14} + R_{15}} V$$

assuming a fixed (and comparatively insignificant) output impedance for the buffer. The open-collector output of the comparator is connected to a dedicated 5 V supply through R_{11} (1 k Ω).

Upper-level Schmitt-trigger: This section is identical to the lower-level Schmitt-trigger, and is built around **OP177/2** and **LM311/2**.

Logic section: The *falling edge* of the lower-level Schmitt-trigger (**LM311/1**) — i.e., the *rising edge* of the shaped bipolar pulse — generates a 470 ns downward-going pulse by means of the one-shot⁶ **O/S 1**, termed the *lower-level discriminator pulse (LLDP)*, indicating that the lower-level threshold has been crossed in the rising direction by the input pulse. This pulse is applied to the *set* input of a flip-flop⁷. *The inputs of the remaining gate*

⁶Half of a 74HC123 monostable multivibrator integrated circuit, configured with an RC time constant of 470 ns.

⁷The flip-flop itself is constructed of two *NAND* logic-gates. The flip-flop and the subsequent

are tied to ground. The upper-level discriminator output (i.e., the output of **LM311/2**) is connected directly to the *reset* input of the flip-flop.

Thus, if the rising edge of the input pulse crosses the upper threshold, **LLDP** will set the flip-flop. If the input pulse then goes on to cross the upper threshold *and stays above the threshold for a period longer than the duration of LLDP*, then the flip-flop will be left in the **reset** (i.e., 0) state just prior to the next step.

When the *falling edge* of the input pulse crosses the lower-level Schmitt-trigger threshold, the so-called gate pulse (**GP**, 470 ns, downward-going) is generated by the one-shot⁸ **O/S 2**.

GP and the flip-flop output are *NAND*-ed together, and the output of the *NAND* gate thus produces a downward-going logic pulse for each gate pulse generated while the flip-flop output was in the *set* (i.e., 1) state. This, then, is the logic output of the pulse-height discriminator, and is connected directly to the input of the counting system. Figures 7.11 (p. 328) and 7.12 (p. 329) show timing diagrams of the Schmitt-trigger outputs and logic levels at various parts of the circuit, against the backdrop of input pulses and discriminator thresholds.

Note the following points:

1. In the present simplified implementation, the thresholds **LLDT** and **ULDT** are generated independently, not in the preferred manner of providing an adjustable lower threshold and window-size. Thus, the pathological situation could arise in which **ULDT** is placed below **LLDT**. This condition is regarded as a user-error.
2. The 470 ns duration of the pulses **LLDP** and **GP** is a wider than the flip-flop, or indeed any component further along, demands. It was chosen conservatively because of some confusion regarding exactly what the performance limits are of the 74HC123-type monostable multivibrator — the

NAND gate to which it is connected together take up 3 out of the 4 *NAND*-gates available on a 74HC00 integrated circuit package.

⁸i.e., the other half of the 74HC123, also with a 470 ns time-constant.

pulse-generating element for both these pulses. National Semiconductor claim a 400 ns minimum pulse width, whereas Philips provide a somewhat more detailed specification giving a much smaller minimum for their version of the component: a value in close agreement with Horowitz and Hill's value of 40 ns for what they call "standard monostables". Because the more conservative value would still be adequate for our purposes, and because our particular component came from a second-source manufacturer other than National Semiconductor or Philips, 470 ns was accepted as a good starting point. The component could be obtained from Philips and the system configured for a narrower pulse.

3. Referring to Figure 7.11 (p. 328), it can be seen that as **LLDT** and **ULDT** are moved closer and closer to the peak of the input pulse, and closer and closer together, a certain minimum window-height will emerge in which the pulse **LLDP** (470 ns) cannot be trusted to end before the upper-threshold Schmitt-trigger output pulse ends. Thus, under these circumstances, pulses which have crossed the upper threshold by a narrow margin will not be excluded.

It must be emphasized that an arrangement such as this one will necessarily behave this way under some set of circumstances. One remedy would be to make this minimum window height as small as possible. This could be done by making **LLDP** narrow compared to the input pulses: say 1/10th of the pulse-width at the baseline for unipolar pulses, or 1/20 of the pulse-width for symmetrical bipolar pulses. To a crude first approximation, a 470 ns **LLDP** dictates a bipolar pulse width of 9.4 μ s: approximately what the pulse-shaping amplifier produces. (The approximation is cruder for the fact that the positive lobe of the bipolar peak is only about 1/3 as wide as the negative lobe.)

By narrowing **LLDP** as described, one could make it possible for the time constants of the pulse-shaping amplifiers to be made smaller, which would make the system more accurate at high count rates. A further improvement would be to generate the upper and lower thresholds in the preferred manner, i.e., to provide an adjustable lower threshold and window-

height, and then enforce electronically some minimum window height.

4. It is possible that a runt (i.e., narrower than specified) gate pulse could be generated from time to time under certain conditions. Gate pulses shorter than about $0.125\ \mu\text{s}$ cannot be detected reliably by the present counting system, but in the present embodiment, no runt gate pulse could cause a problem beyond the counting error that it would introduce by perhaps being ignored. This source of error is insignificant under normal circumstances.

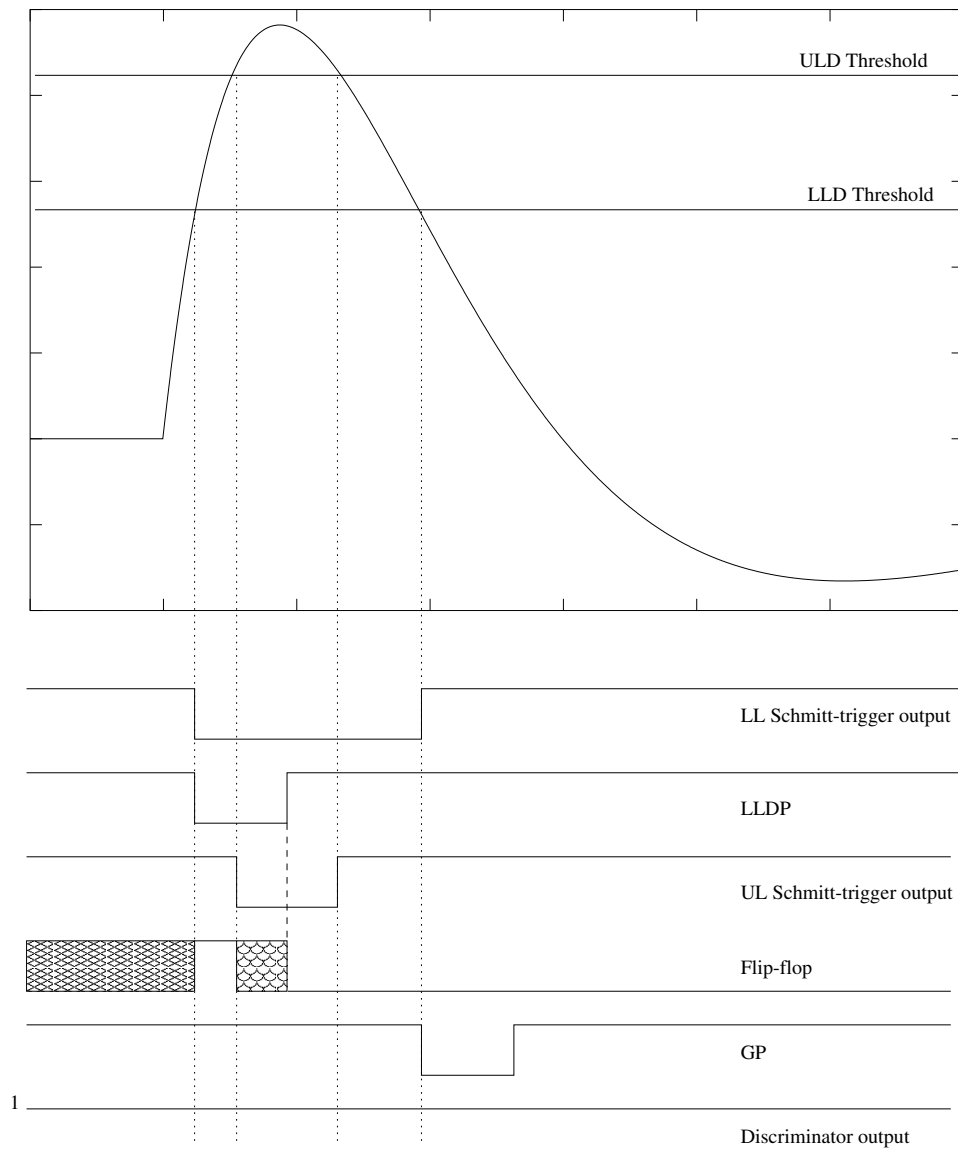


Figure 7.11: Pulse-height discriminator timing diagram of the outputs at the various stages of the circuit, for pulses which cross both the upper and lower discriminator thresholds. The cross-hatched area may be regarded as an undefined flip-flop state, whose logic value depends on the history of the output state. The “shingled” area is a logical no-man’s land in which both the *set* and *reset* inputs of the flip-flop are held low (i.e., applied): certain commercial flip-flops enforce a defined logic state when both their inputs are held low, so exactly which state the flip-flop settles in during this period depends on the implementation. This state should not persist until the gate-pulse **GP** is generated. The discriminator output is simply the logical *NAND* of **GP** and the flip-flop output. No logic output pulse is generated.

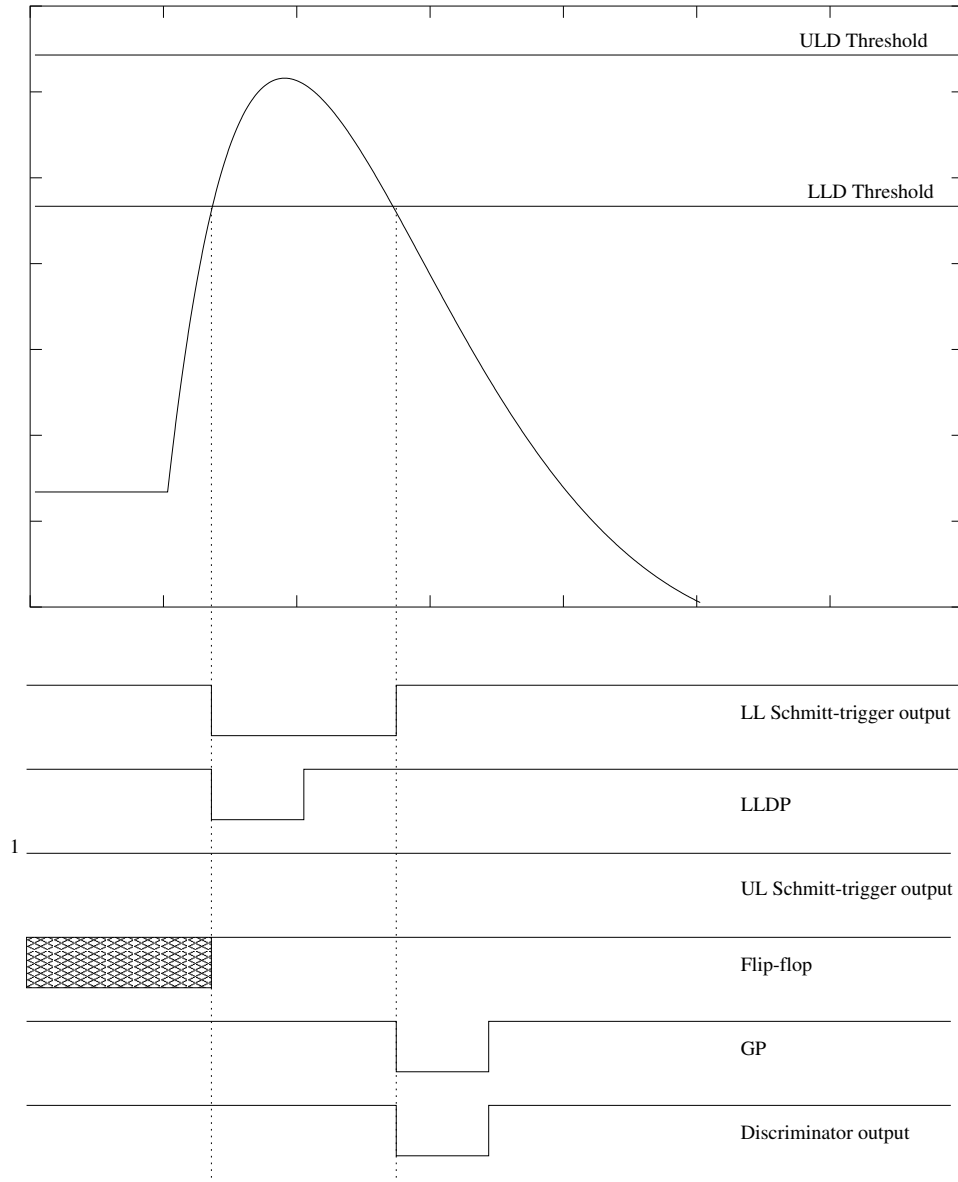


Figure 7.12: Pulse-height discriminator timing diagram of the outputs at the various stages of the circuit, for pulses which cross both only the lower discriminator threshold. The cross-hatched area may be regarded as an undefined flip-flop state, whose logic value depends on the history of the output state. The discriminator output is simply the logical *NAND* of **GP** and the flip-flop output. A negative-going logic output pulse is generated.

7.4.2 Digital and analog DC output section

Counting ratemeter

As described above, a ratemeter gives a DC voltage proportional to the input count rate. In the present implementation, this is achieved by means of a microcontroller-based counting, scaling and output system. An appropriately programmed microcontroller counts the number of pulse-height discriminator output pulses generated per second, runs a continual numeric simulation of an analog ratemeter, and provides very detailed numeric output, as well as an analog output signal — the latter by means of a digital-to-analog converter and differential amplifier.

The hardware part of the counting ratemeter is shown in Figure 7.14 on p. 334. The system may be described as follows in terms of its functional units:

Asynchronous counter: This is on-board the microcontroller, and allows the system to count pulses from an external source, in this case the pulse-height discriminator. The pulse-height discriminator signal is applied to the external counter pin, and the 16-bit counter register may then be accessed at any time by the microcontroller CPU.

Time-constant and range selectors: These are implemented as front-panel selectors connected to digital input lines, as shown on the diagram. Each selector grounds the selected pin on the microcontroller package. All the input pins have their optional internal pull-up resistors activated to hold them high otherwise. Time constants of 1, 4, and 8 seconds are available, while 15 full scale ranges $[x \times 10^y]$, $(\forall(x,y) : x \in \{1,2,4\}, y \in \{1,2,\dots,5\})$ are provided by means of two front panel switches. Eight times a second, before each data point is sent to output, the input lines connected to these selectors are sampled to determine how the data should be presented. Code is included to cause, when the selector switches are changed, the very next data point reported to be presented correctly according to the new scaling *and* time constant settings.

Serial port output: Each data point reported contains:

- the number of pulses that have been emitted by the pulse-height discriminator since the last data point was reported — this is raw data (i.e., it is a plain pulse count, independent of any computations by the microcontroller), and is provided so that external data treatment routines may be performed on the raw data if the user desires;
- the current value of the digital equivalent of the charge on the ratemeter capacitor, Q (cf. Equations 7.20 to 7.23 (p. 317) — this value is calculated based on the ratemeter time-constant, but is not affected by scaling;
- the current time-constant and full-scale settings; and
- the processed count rate, scaled between 0 and $(2^{10} - 1)$ in this case, i.e., the number fed to the DAC to generate the analog output signal — this value is computed by the microcontroller, based on the time constant and scaler settings.

A serial line-driver, the MAX233CPP (a convenient version, which requires only +5V and no external components to generate the nominal ± 12 V serial line levels) connects the microcontroller UART TxD (transmit) line to the outside world.

Digital-to-analog converter: The 10-bit AD7391-type digital-to-analog converter (DAC) takes a 10-bit digit (between 0 and $2^{10} - 1$) from the microcontroller and outputs a voltage between 0 and 5 VDC. Different DACs could be used, but a small change to the microcontroller program would have to be made.

Difference amplifier This takes the DAC signal (referred to digital ground) and outputs $2.2\times$ this signal, referred to analog ground. A small (optional) RC low-pass filter is placed at its output.

The following points should be noted:

1. All arithmetic calculations related to the ratemeter emulation are performed as integer operations rather than real-number computations. Because no floating-point arithmetic instructions are available on the ATMEL

AT90S8535 microcontroller, such operations would have to be performed by slow software routines. Test compilations with floating-point code in the appropriate sections generate executables which almost entirely fill the microcontroller program memory.

2. For greater accuracy at the final difference amplifier stage, the resistors should be of a precision type. In the prototype, ordinary 5% resistors were used for expediency, as great count-rate accuracy is not required. (This choice negates the accuracy of the OP177 precision operational amplifier — under present circumstances, nearly any operational amplifier would do, provided it is able to drive panel-meter of 1 k Ω impedance.)
3. All other factors aside, the asynchronous counter on-board the ATMEL AT90S8535 microcontroller imposes a minimum gate-pulse width (and related pulse-shaping parameters) on the components upstream. This minimum width is approximately 0.125 μ s, i.e., one microcontroller clock period. The asynchronous counter is, in fact, implemented in such a way that input state transitions must straddle the rising edge of the system clock. The counter is thus asynchronous only if the minimum pulse-width is observed.

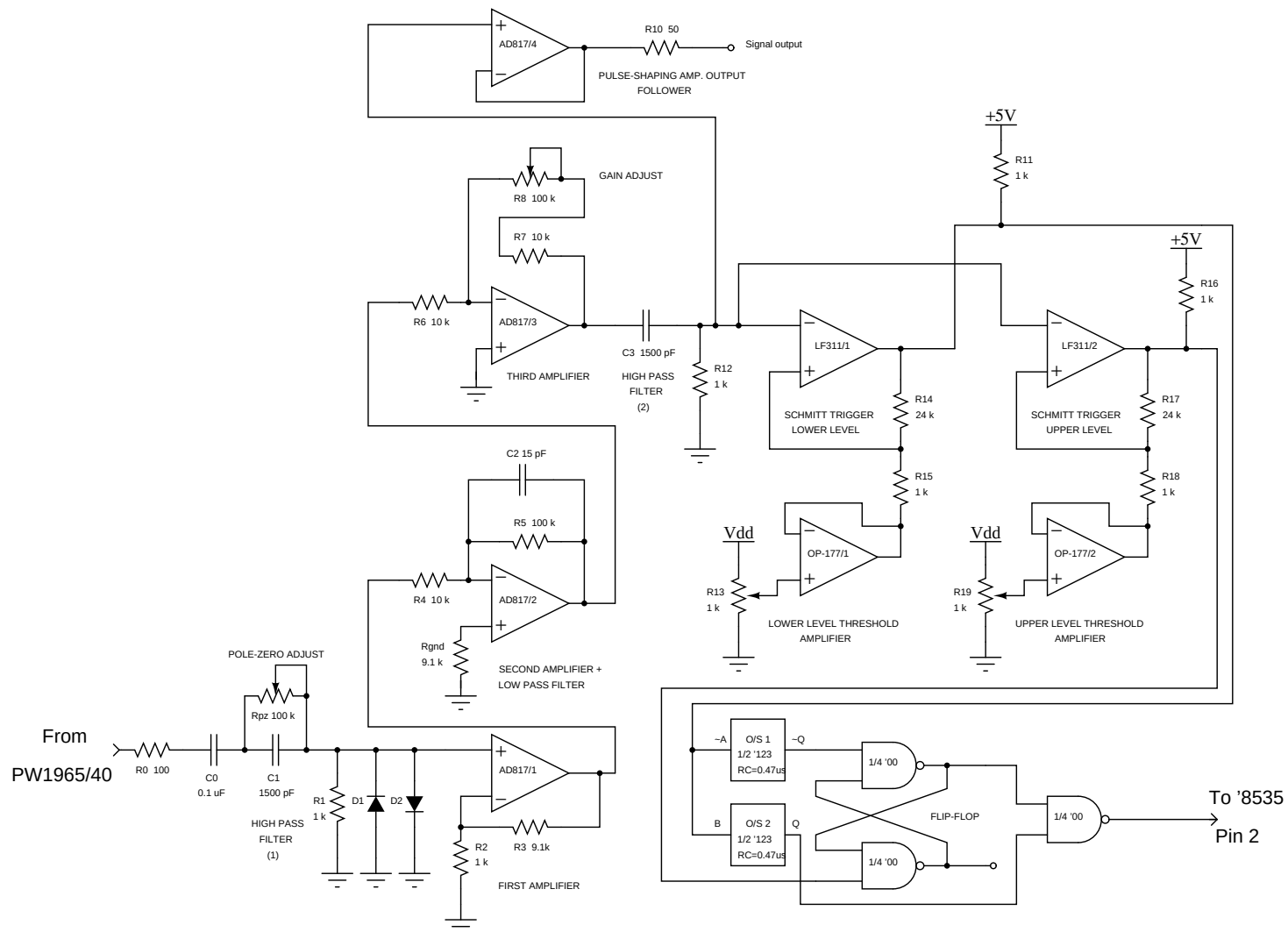


Figure 7.13: A schematic diagram of the new pulse-shaping amplifier and single-channel analyzer.

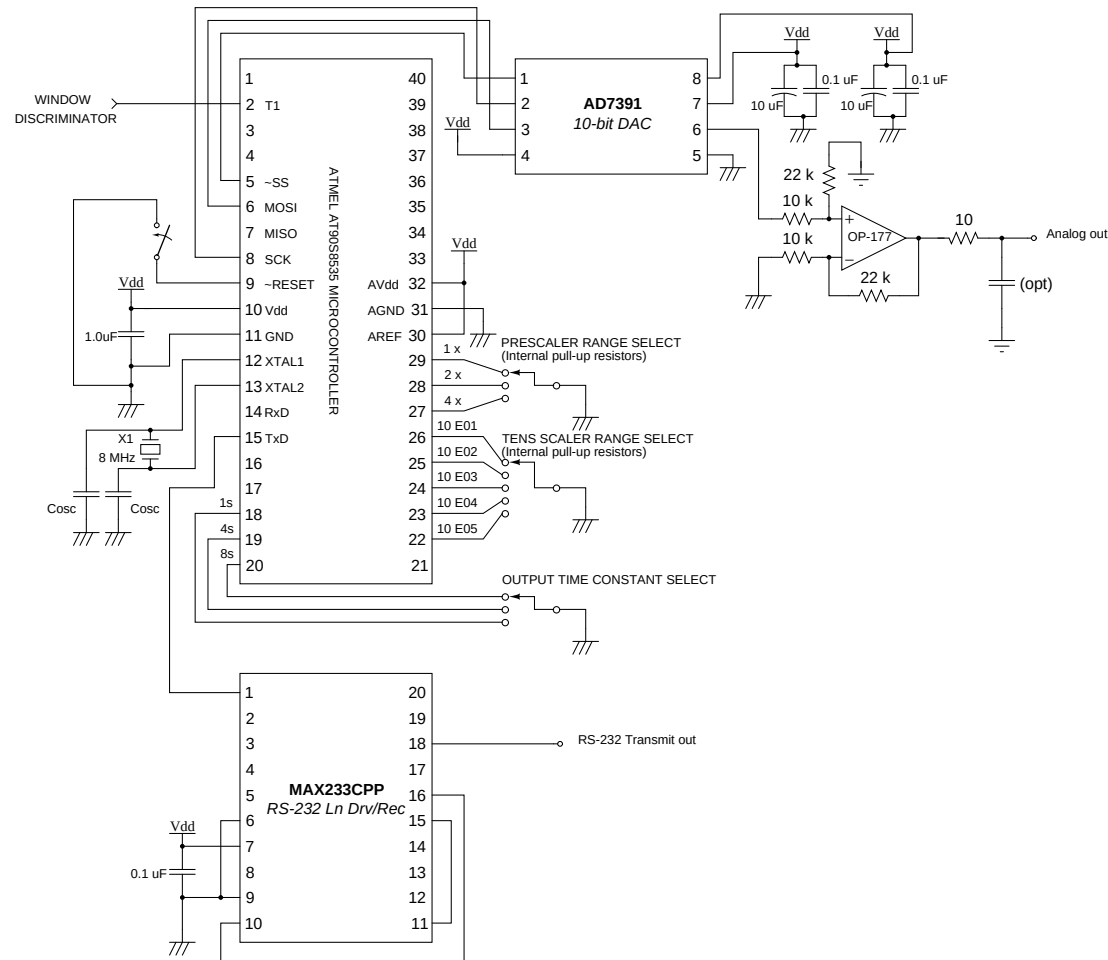


Figure 7.14: A schematic diagram of the new digital ratemeter/scaler and analog ratemeter output section.

7.5 CONCLUDING REMARKS

No serious attempt was made to discover the performance limits of the prototype. The final product fulfills its purpose in that it produces diffraction patterns which are indistinguishable from those provided by the original Philips system.

Bench-testing of the individual components (mainly with square-wave test inputs) revealed that the pulse-shaping amplifiers will deal with signals as fast as 1 MHz and beyond, with no observable drop-off in gain. The limiting factor in the present implementation is the wide **LLDP** pulse, which, in turn, imposes a minimum usable time-constant on the preceding pulse-shaping amplifier stage.

For a given *observed* count-rate, n_{obs} , measured by means of a counter tube with dead-time τ_d , the true count rate, n , is given by the following equation [29]:

$$n_{\text{obs}} = \frac{n}{1 + \tau_d n} \quad (7.25)$$

Thus, with its *overall* electronic dead-time of approximately 10 μs , the present system will under-read by about 1% at a true count-rate of 1000 c.p.s., and by about 10% at 10 000 c.p.s. By addressing the **LLDP**-problem as discussed in the circuit description, these thresholds could be raised to 10 000 and 100 000 c.p.s. respectively. This would put the system on a par with the Philips PW4620 system, with its pulse-clipping time of approximately 1 μs . The improvements suggested above were not put into practice because the maximum count-rate recorded by the prototype has been approximately 3000 c.p.s., which is well within the range of the current parameter set.

In the present implementation, a lower limit exists on the count rates that can be used. A small fixed baseline anomaly is introduced at count rates of the order of 10^2 c.p.s., and a much larger one at count rates of 10^1 . The anomaly takes the form of a threshold below which the count-rate display will not fall. It is not an offset — count-rates above this threshold are displayed accurately. The anomaly arises because of the fact that integer arithmetic is used in the ratemeter simulation rather than floating-point arithmetic. The error is present only in the analog output and the scaled/filtered numeric outputs — it is not present in the raw count-rates. Furthermore, it would not affect real XRPD results in the present system because

of the relatively high background count rate.

It was decided to halt development of the prototype at this point because its operation is entirely satisfactory for the present application. The object of the exercise was to restore the local XRPD facility to working order as quickly as possible, and the design and construction of the new detector system has achieved this. At the time of writing, the prototype has produced several hundred diffraction patterns over more than 1200 hours of operation, and it remains in use as the department's research diffractometer.

Further minor development of the source-code has led to the elimination of the above-mentioned low-rate counting anomaly. Using floating point arithmetic on the 8 MHz microcontroller was considered to be out of the question for performance reasons, so the ratemeter simulation was re-written using a simple form of binary fixed-point arithmetic, a digital signal processing technique discussed in some detail in [30, 31]. Preliminary test-simulations indicate that this approach is satisfactory. Any further examples of this system will include these improvements.

References

- [1] **W. Parrish, E. A. Hamacher and K. Lowitzsch.** “The “Norelco” X-ray diffractometer”. In **W. Parrish** (editor), *Advances in X-ray Diffractometry and X-ray Spectrography*. Centrex Publishing Company, Eindhoven 1962.
- [2] Philips Scientific Equipment. *PW1965/20/30/40: Proportional Detector Probe* (undated, c. 1970). Contains complete circuit diagrams.
- [3] **Centronic, Limited.** Private communication.
- [4] N. V. Philips Gloeilampenfabrieken, Eindhoven, The Netherlands. *PW4620: Channel, Rate Meter, H. V. Supply* 1971. Contains complete circuit diagrams.
- [5] **G. F. Knoll.** *Radiation Detection and Measurement*. John Wiley & Sons 1979.
- [6] Centronic, Limited. *Centronic Geiger-Müller Tubes Databook*. URL: <http://www.centronic.co.uk> .
- [7] **F. Daniels, J. H. Mathews, J. W. Williams, P. Bender and R. A. Alberty.** *Experimental Physical Chemistry*. 6th ed. McGraw-Hill Book Company, Inc., New York 1962. Chapter 23.
- [8] **P. Horowitz and W. Hill.** *The Art of Electronics*. 2nd ed. Cambridge University Press, Cambridge, UK 1989.
- [9] Philips. *Gamma Counting & Single Channel Spectroscopy: Operation Manual* (undated, c. 1970).

- [10] Canberra Industries. *Canberra Product Catalog*, 12th ed. URL: <http://www.canberra.com>.
- [11] **K. Kobayashi**. *Development of a Balloon-borne Hard X-ray Spectrometer for Solar Flare Observation*. Master's thesis, University of Tokyo February 2000. Chapter 2.
- [12] **T. Duncan**. *Electronics and Nuclear Physics*. John Murray, London 1969.
- [13] **United States Navy**. "Introduction to Wave-Generation and Wave-Shaping". In *Navy and Electronics and Electronics Training Series*, module 9, 1998. pp. 4–48 *et seq.* (NAVEDTRA 14181).
- [14] **G. White**. "An autoranging digital ratemeter". *Nuclear Instruments and Methods* **125**(2) (1975), 313–317. Abstract.
- [15] **R. K. Huffman**. "Microprocessor implementation of a time-variant floating mean counting algorithm". *Nuclear Instruments and Methods in Physics Research A* **431** (1999), 556–562. References therein.
- [16] **R. Mancini** (editor). *Op Amps for Everyone*. Design Reference. Texas Instruments, Dallas, Texas, USA August 2002. URL: <http://www.ti.com>.
- [17] "An applications guide for op amps". Application Note 20, National Semiconductor February 1969. URL: <http://www.national.com>.
- [18] "AD817: High speed, low power wide supply range amplifier". Datasheet, Analog Devices 1995. URL: <http://www.analog-devices.com>.
- [19] "OP177: Ultraprecision operational amplifier". Datasheet, Analog Devices 2002. URL: <http://www.analog-devices.com>.
- [20] "OP07C, OP07D: Precision operational amplifiers". Datasheet, Texas Instruments May 2004. URL: <http://www.ti.com>.
- [21] "OP07: Ultralow offset voltage operational amplifier". Datasheet, Analog Devices 2003. URL: <http://www.analog-devices.com>.

- [22] “LM111/LM211/LM311: Voltage comparator”. Datasheet, National Semiconductor January 2001. URL: <http://www.national.com> .
- [23] “MM74HC123A: Dual retriggerable monostable multivibrator”. Datasheet, Fairchild Semiconductor May 2001. URL: <http://www.fairchildsemi.com> .
- [24] “MM74HC00: Quad 2-input nand gate”. Datasheet, Fairchild Semiconductor February 1999. URL: <http://www.fairchildsemi.com> .
- [25] “8-bit AVR microcontroller with 4K/8K bytes in-system programmable flash: AT90S4434, AT90LS4434, AT90S8535, AT90LS8535”. Datasheet, Atmel Corporation, San Jose, CA, USA April 1999. URL: <http://www.atmel.com> .
- [26] “AVR instruction set”. Datasheet, Atmel Corporation, San Jose, CA, USA June 1999. URL: <http://www.atmel.com> .
- [27] “AD7390/AD7391: 3 V serial-input micropower 10-bit and 12-bit DACs”. Datasheet, Analog Devices 2002. URL: <http://www.analog-devices.com> .
- [28] “+5 V powered CMOS RS-232 drivers/receivers”. Datasheet, Analog Devices 1997. URL: <http://www.analog-devices.com> .
- [29] **W. Parrish**. “X-ray intensity measurements with counter tubes”. In **W. Parrish** (editor), *Advances in X-ray Diffractometry and X-ray Spectrography*. Centrex Publishing Company, Eindhoven 1962.
- [30] **R. Yates**. *Fixed-Point Arithmetic: An Introduction*. Digital Sound Labs March 2001. URL: <http://home.earthlink.net/yatescr/fp.pdf> (Last accessed February 2007).
- [31] **E. L. Oberstar**. *Fixed-Point Arithmetic and Fractional Math*. Oberstar Consulting 2005. URL: <http://www.superkits.net/whitepapers/Fixed Point Representation And Fractional Math.pdf> (Last accessed February 2007).

Part IV

Appendices

Appendix A

Copper determination by complexometric titration

The procedure for the determination of copper by EDTA titration given here is derived from the one given in [1, p.78]. A similar procedure is also given in [2].

A.1 REAGENTS AND SOLUTIONS

Murexide indicator : The indicator, in solid form, was taken from stock prepared by grinding murexide ¹ with sodium chloride in a 1:100 proportion.

Standard EDTA solution : Standard 0.001 *M* solutions were prepared using distilled water and pre-dried EDTA disodium salt. The EDTA disodium salt was dried in an oven for 24 hours to remove adsorbed water. The dried EDTA salt has the formula $\text{Na}_2\text{H}_2\text{C}_{10}\text{H}_{12}\text{O}_8\text{N}_2 \cdot 2\text{H}_2\text{O}$ (372.24 g mol⁻¹) [4]. No further standardization was performed.

pH 10 buffer : Ammonium chloride (70 g) was dissolved in conc. aqueous ammonia (570 ml) and the solution was diluted to 1 L using distilled deionized water.

¹Also known as *ammonium purpurate* and *purpuric acid ammonium salt* [3]. Solid murexide diluted by grinding with NaCl is more stable than the saturated aqueous solution also used as an indicator.

Sodium hydroxide solution : Sodium hydroxide solutions (1 *M* and 0.1 *M*) were prepared for pH adjustment.

A.2 PROCEDURE

The unknown substance (20 mg) was boiled in a small beaker with 20 ml conc. nitric acid plus a few drops of conc. sulfuric acid to decompose the organic material, until the volume was reduced to 2–5 ml. After cooling to room temperature, the solution was transferred to a volumetric flask and diluted to 100.0 ml² with distilled deionized water.

From this solution, 20 ml aliquots were taken for analysis. Each aliquot was placed in a conical flask and diluted to approx. 100 ml using distilled deionized water, after which the pH was adjusted to 7–10 by dropwise addition of aqueous sodium hydroxide³. After the addition of pH 10 buffer (1–2 ml) and a knife-tip of solid murexide indicator, the solution was titrated with standard EDTA solution to a colour change of green/yellow to violet.

Before the method was employed on the unknown copper(II) complexes, it was first tested on copper(II) acetate monohydrate. The test gave a copper content which was better than 99 % of the expected value.

²Where necessary, because of paucity of material, smaller samples were dissolved to a final volume of 50 ml.

³A too-high ammonia concentration causes partial decomposition of the copper(II)–murexide complex, making the end point difficult to determine.

References

- [1] **H. A. Flaschka.** *EDTA Titrations*. Pergamon Press, Inc., New York 1959.
- [2] **G. Schwartzbach.** *Complexometric Titrations*. Methuen, London 1960.
- [3] CAS registry number 3051-09-0.
- [4] **G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney.** *Vogel's Textbook of Quantitative Chemical Analysis*. 5th ed. Longman Scientific and Technical, UK 1989.

Appendix B

Analysis for chlorine, sodium and potassium

*The following tests were performed to determine whether chlorine, sodium or potassium were present in **xst-cu-b4c-no3-rhombi** and **xst-cu-b4c-cl-rhombi**.*

B.1 CHEMICAL ANALYSIS: SODIUM FUSION TEST

The chemical test employed for chloride detection is a simplification of the well-known Lassaigne test described in [1], [2]. In this procedure, an organic sample is fused with sodium metal, and in the process, any nitrogen, sulfur and halogens are converted to sodium cyanide, sodium sulfide and sodium halides, respectively. These are then dissolved in distilled water and detected by means of inorganic tests. Sodium halides are detected by precipitation with aqueous silver nitrate, but cyanide and sulfide interfere by also giving rise to precipitates unless precautions are taken.

The test was performed in duplicate for **xst-cu-b4c-cl-rhombi** and **xst-cu-b4c-no3-rhombi** (prepared in chloride-free media).

Procedure The sample (0.05 g) was placed in a small soda-glass test tube, held at an angle of about 30° to horizontal. Sodium metal (0.1 g) was placed immediately in front of the sample. The sample and the sodium metal were heated

together, so that the molten sodium ran downwards onto the sample. The mixture was then heated to a dull redness for about 2 minutes, after which the hot test tube was plunged into a mortar containing distilled water (20 ml). The shattered tube and sample were ground together.

The contents of the mortar were filtered to remove solid material, and the filtrate transferred to a boiling tube. The filtrate was rendered slightly acidic (as measured by pH paper) by the addition of dilute nitric acid. The filtrate was boiled for about 2 minutes to expel any HCN or H₂S, and then cooled under running water. About 1 ml silver nitrate solution (1 mol L⁻¹) was added.

Results For all the samples, extremely faint precipitates were observed which were thought to be due to slight contamination of the glassware or sodium during handling. To confirm this, one drop (approx. $\frac{1}{20}$ ml) of a very dilute sodium chloride solution (0.01 mol L⁻¹) was added to the acidified filtrate containing silver nitrate, and a visible precipitate was obtained.

It was therefore concluded that chloride was not present in the samples in any significant amount.

B.2 X-RAY FLUORESCENCE SPECTROMETRY

X-ray fluorescence spectroscopy was used to confirm the results of the above chemical test, and to determine whether sodium or potassium were present in significant quantities. The samples were compared to the following analyzed reference samples [3]:

KRF-13: Rhodes University in-house standard (basalt — Barkly East), containing less than 50 ppm chlorine, 1.89 % Na₂O and 0.39 % K₂O (equivalents).

NIM-L: International Reference Rock Standard (lujavrite — Pilanesberg) containing 1.2×10^3 ppm chlorine.

Semi-quantitative determinations were done for chlorine on the copper(II) complexes, **xst-cu-b4c-cl-rhombi** and **xst-cu-b4c-no3-rhombi**, and for sodium and potassium on **xst-cu-b4c-cl-rhombi**. A quantitative determination for sodium was later done on **xst-cu-b4c-no3-rhombi** by ICP-MS (see Chapter 4, p. 74 *et seq.*).

The analyses were performed on a Philips PW1480 wavelength-dispersive spectrometer. An X-ray tube with a rhodium target, operated at 40 kV and 70 mA, was used to excite the sample. X-ray fluorescence was detected by means of a gas-flow proportional counter (P10 gas), and for all the analyses the fine collimator was used. Parameters specific to each analysis are given below.

B.2.1 Test for chloride

Procedure To test, semi-quantitatively, whether chloride was present in significant quantities (i.e., $> 1\%$) in the copper(II) complexes **xst-cu-b4c-cl-rhombi** and **xst-cu-b4c-no3-rhombi**, X-ray fluorescence spectra were obtained for the complex in a known matrix (KRF-13) and compared to that of an analyzed standard (NIM-L).

Three samples were prepared:

1. a pellet consisting of KRF-13 only, for comparison purposes
2. a pellet consisting of **xst-cu-b4c-cl-rhombi**, backed with KRF-13, and
3. a pellet consisting of **xst-cu-b4c-no3-rhombi** (prepared in chloride-free media), backed with KRF-13.

The surfaces of the latter two pellets were about 70 % covered by their respective copper(II) complexes. The pellets were compressed in a die under 10 tons pressure.

A Philips PE-type analysing crystal ($2d = 8.7420 \text{ \AA}$)¹ was used. The corresponding expected 2θ values for chlorine are 60.49° (Cl- K_β , first-order) and 65.49° (Cl- K_α , first-order). X-ray spectra were obtained for these pellets, and for a reference sample, NIM-L, in the range $58 \leq 2\theta/^\circ \leq 68$.

Results As can be seen in Figure B.1, the spectra of the KRF-13 pellets containing the copper(II) complexes do not differ significantly from each other in the chlorine regions shown, nor do they differ significantly from that of the blank KRF-13 pellet. Therefore, the copper(II) complexes do not appear to differ from

¹Significant figures are reported as given by the manufacturer.

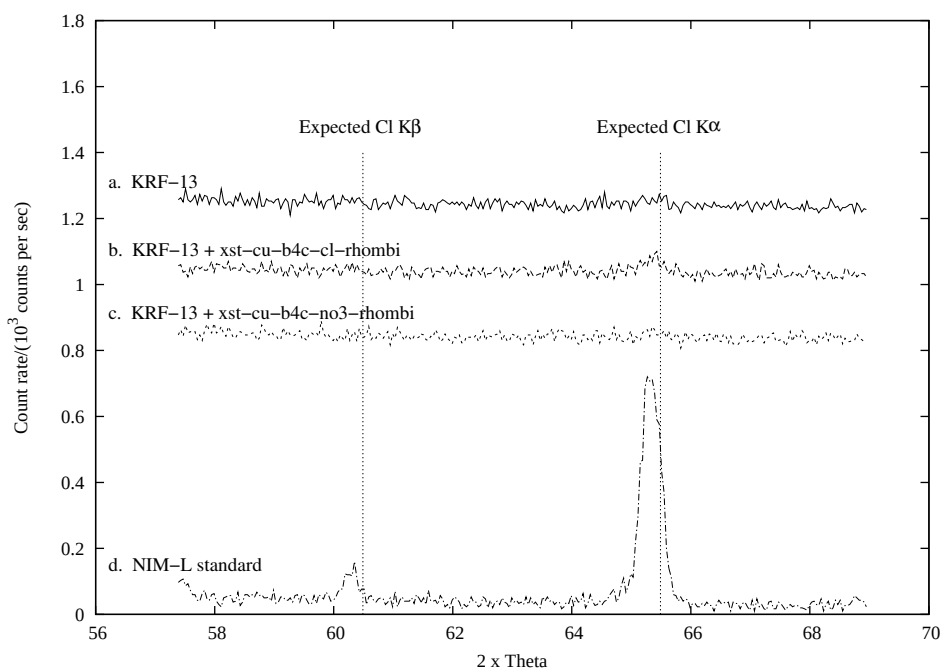


Figure B.1: X-ray fluorescence spectra for KRF-13 rock standard, KRF-13 with **xst-cu-b4c-cl-rhombi**, KRF-13 with **xst-cu-b4c-no3-rhombi** (prepared in chloride-free medium) and the NIM-L reference standard. The vertical lines show the expected lines for chlorine (Cl-K_β and Cl-K_α , PE analysing crystal) [4]. For clarity, the top three curves were shifted upwards from the baseline.

each other in terms of chlorine content, and do not appear to contain significantly more chlorine than the trivial amount present in KRF-13. Comparison of these spectra with the NIM-L spectrum shows that the copper(II) complexes contain very much less chlorine than NIM-L does, i.e., very much less than 0.12 %.

B.2.2 Test for sodium

Procedure To test, semi-quantitatively, whether sodium was present in significant quantities (i.e., $> 1\%$) in **xst-cu-b4c-cl-rhombi**, X-ray fluorescence spectra were obtained for the complex in a known matrix (boric acid) and compared to that of an analyzed standard (KRF-13). Two additional samples were prepared:

1. a pellet consisting of boric acid only, for comparison purposes, and
2. a pellet consisting of the **xst-cu-b4c-cl-rhombi** backed with boric acid.

The surface of the latter pellet was about 70 % covered by the copper(II) complex. The pellets were compressed in a die under 10 tons pressure. X-ray spectra were obtained for these pellets in the range $26 \leq 2\theta/^\circ \leq 29$. A Philips PX-1-type analyzing crystal ($2d = 50 \text{ \AA}$)² was used, and the corresponding expected 2θ value for sodium is 27.561° (Na- K_α , first-order).

Results As can be seen in Figure B.2, the boric acid pellet contains no significant amount of sodium compared to KRF-13. Also, it appears that the boric acid pellet surfaced with the copper(II) complex contains a greater amount of sodium than, or at least a significant amount of sodium compared to, the KRF-13 pellet (on the surfaces only).

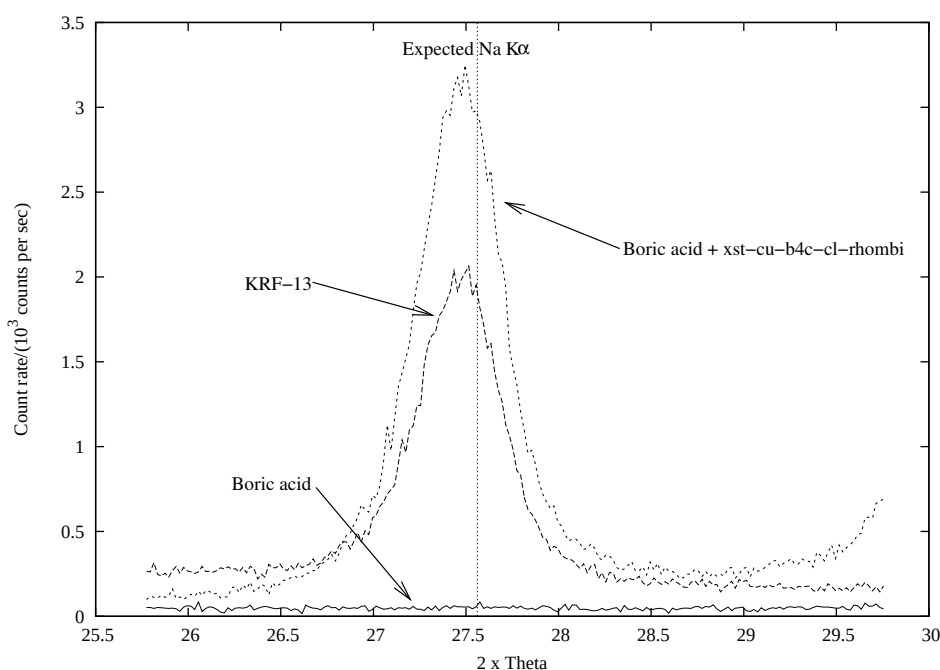


Figure B.2: X-ray fluorescence spectra for boric acid (binder), KRF-13 rock standard, and boric acid **xst-cu-b4c-cl-rhombi**. The vertical line shows the expected line for sodium (Na- K_α , PX-1 analysing crystal) [4].

²Attention is drawn to an erratum provided by the manufacturer indicating that this $2d$ value is written incorrectly as 50 nm in part of the manufacturer's documentation [4]

B.2.3 Test for potassium

Procedure To test, semi-quantitatively, whether potassium was present in significant quantities (i.e., $> 1\%$) in **xst-cu-b4c-cl-rhombi**, X-ray fluorescence spectra were obtained for the previously prepared blank KRF-13 and the copper(II) complex-on-KRF-13 pellets, in the range $135 \leq 2\theta/^\circ \leq 138.5$. A Philips LIF 200-type analysing crystal ($2d = 4.02760 \text{ \AA}$) was used, and the corresponding expected 2θ value for potassium is 136.70° ($K-K_\alpha$, first-order).

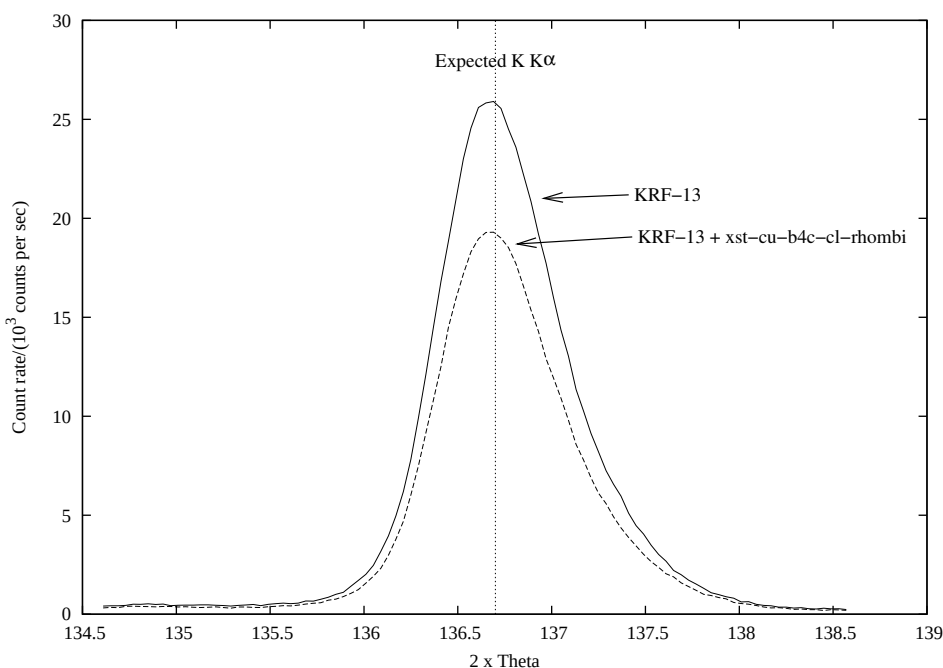


Figure B.3: X-ray fluorescence spectra for KRF-13 rock standard, and KRF-13 with **xst-cu-b4c-cl-rhombi**. The vertical line shows the expected line for potassium ($K-K_\alpha$, LIF 200 analysing crystal) [4].

Results In Figure B.3, the KRF-13 spectrum has a stronger peak than that of the copper(II) complex-on-KRF-13. KRF-13 contains only a small amount of potassium, and the addition of a significant amount of potassium in the copper(II) complex would result in an intense peak. It is therefore concluded that the copper(II) complex does not contain a significant amount of potassium. The lower peak intensity shown by the copper(II) complex-on-KRF-13 pellet is possibly due

to X-ray absorption by the copper(II) complex, which probably has a higher average atomic mass than KRF-13.

References

- [1] **B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell.** *Vogel's Textbook of Practical Organic Chemistry*. 5th ed. Addison Wesley Longman Limited, Harlow, England 1989.
- [2] **F. G. Mann and B. C. Saunders.** *Practical Organic Chemistry*. 3rd ed. Longmans, Green and Co., London 1952.
- [3] **G. S. Marsh.** Department of Geology, Rhodes University. Personal communication.
- [4] *Philips X-Ray Wavelengths and Two-theta Tables*. N. V. Philips Gloeilampenfabrieken, Eindhoven, the Netherlands 1989.

Appendix C

CD-ROM

The CD-ROM attached contains crystal structure data for **xut-cu-b4c-acet-xtals**, **xst-cu-b4c-cl-rhombi** and **xut-cu-pyr2-b4c-no3-xtals**, as well as the complete source code for the microcontroller component of the X-ray detector system described above. It also contains an example of the python scripts used to investigate decomposition stoichiometry in Part I. See the file README.txt in the root directory for details.

PLATON(V-201207)-Run for: c:xtal u u_kno~1knoR = 0.03

TIME: Jan 11 10:53:53 2008

(C) 1980-2007 A.L.Spek

Crystal Data

Input Cell (Lattice Type: P)		Temp = 113K	Reduced Cell		(Acta Cryst.(1976),A32,297-298)
a =	8.0742(1) Angstrom	alpha =	90 Degree	a =	8.074
b =	16.9044(3)	beta =	98.375(1)	b =	15.556
c =	15.5557(3)	gamma =	90	c =	16.904
V = 2100.55(6) Cubic-Angstrom		d(100) =	7.9881 Angstrom	Niggli Values	
Lambda(MoKa) = 0.71073 Angstrom		d(010) =	16.9044	65.193	241.980
		d(001) =	15.3898	0.000	0.000

Orthogonalization Matrices

(See e.g. J.D.Dunitz, Xray Analysis and Structure Determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

(X0) (8.07420 0 -2.26571) (X) , (X) (0.12385 0 0.01823) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 16.90440 0)*(Y) , (Y) = (0 0.05916 0)*(Y0) are defined as:
 (Z0) (0 0 15.38981) (Z) , (Z) (0 0 0.06498) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group P21/c No: 14, Laue: 2/m [Hall: -P 2ybc]

Lattice Type mP, Centric, Monoclinic, Order 4(2) [Schoenflies: C2h^5]

Nr ***** Symmetry Operation(s) *****

1	X ,	Y ,	Z
2	- X ,	1/2 + Y ,	1/2 - Z
3	- X ,	- Y ,	- Z
4	X ,	1/2 - Y ,	1/2 + Z

ADDSYM - CHECK (cf. MISSYM (C): Le Page, Y., J. Appl. Cryst. (1987), 20, 264-269; J. Appl. Cryst. (1988), 21, 983-984)

- ADDSYM Search on ALL NON-H Chemical Types [Max NonFit 20 Perc]
 - Number of Input Atoms Included in Search 38 (Unitcell 152)
 - Density based on Input Atom Set = 2.088 g.cm-3 - Vol / Non-H atom = 13.8 Ang+3
 - The Structure Implies the Following Symmetry Elements Subject to the Criteria:
 Criteria: 1.00 Deg (Metric), 0.25 Ang (Rot.), 0.45 Ang (Inv), 0.45 Ang (Transl)

Symm.	Input	Reduced	(Ang)	(Deg)	(%)	(Ang)	Input	Cell
Elem	Cell_Row	Cell_Row	d	Typ	Dot	Angle	Fit	MaxDev.
c	[0 1 0]	[0 0 1]	16.90	2	1	0.00	100	0
								Through
								Glide =
-1							100	0
								at

T.R.A.N.S.F.O.R.M.A.T.I.O.N M.A.T.R.I.X for CELL and HKL DATA

Reduced->Convent	Input->Reduced	T = Input->Convent:	a' = T a
(1 0 0)	(-1 0 0)	(-1 0 0)	Det(T)
(0 0 -1)	(0 0 -1)	(0 1 0)	=
(0 1 0)	(0 -1 0)	(0 0 -1)	1.000

Cell Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input mP	8.074	16.904	15.556	90.00	98.38	90.00	2101	Monoclinic	2/m
Reduced P	8.074	15.556	16.904	90.00	90.00	98.38	2101		
Convent mP	8.074	16.904	15.556	90.00	98.38	90.00	2101	Monoclinic	2/m

:: *** No Obvious Extra Crystallographic Symmetry was Detected ***

:: Note: Rerun in EQUAL Atom Type Mode for more Checks

(1:19-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

 Site = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
 ***** Move = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
 SYMBOLS: Type = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
 ***** El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
 ARU = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
 RESIDUE = collection of ARU's constituting an isolated unit (= molecule, ion).
 FLAGS : d = determined, c = calculated, R = riding G = group

Atom Types : C H Cu Na O
 Cov.Rad(Ang): 0.68 0.35 1.52 0.97 0.68
 Atom Volume : 13.87 5.08 26.90 26.00 11.39
 Atom Number : 6 1 29 11 8
 Atom Weight : 12.010 1.008 63.55 22.99 16.00
 Scat.Fact.f0: 5.999 1.000 28.986 10.992 7.999
 Scat.Fact.f': 0.003 0.000 0.320 0.036 0.011
 Scat.Fact.f": 0.002 0.000 1.265 0.025 0.006
 Mu/Rho(MoKa): 0.58 0.37 49.09 3.04 1.22
 Elem. Type : -- -- TR AK --

Sources - Cov. Radii : Manual Cambridge Crystallographic Data Base
 - Atom Volume: D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493
 - Atomic Wt. : SHELXL97
 - Scat. Fact.: SHELXL97 (International Tables)
 - mu/rho : International Tables C, table 4.2.4.2, p193-199

NOMOVE

 =====
 Residue = 1
 =====

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	Cu(1)	0.04108(4)	0.26508(2)	0.04931(2)	0.2200(3)	4.4810(3)	0.7589(3)	1	1	1	-	Met
d	Cu(2)	-0.33918(4)	0.24358(2)	-0.19199(2)	-2.3036(3)	4.1175(3)	-2.9547(3)	1	1	1	-	Met
d	Na(1)	-0.37130(13)	-0.15484(7)	-0.06681(7)	-2.8466(11)	-2.6175(12)	-1.0282(11)	1	1	1	-	Met
d	Na(2)	0.66950(13)	-0.13521(6)	-0.28886(7)	6.0601(11)	-2.2856(10)	-4.4455(11)	1	1	1	-	Met
d	O(1W)	0.9093(2)	-0.11348(12)	-0.35181(13)	8.1390(16)	-1.918(2)	-5.414(2)	1	1	1	-	D/A
d	O(3W)	0.6832(3)	0.00998(13)	-0.26961(18)	6.127(2)	0.169(2)	-4.149(3)	1	1	1	-	D/A
d	O(4W)	-0.6034(3)	-0.13127(15)	-0.00353(15)	-4.864(2)	-2.219(3)	-0.054(2)	1	1	1	-	D/A
d	O(5W)	-0.3417(4)	-0.01494(17)	-0.0611(2)	-2.621(3)	-0.253(3)	-0.940(3)	1	1	1	-	D/A
d	O(6W)	-0.3107(2)	0.18233(11)	-0.30069(12)	-1.8274(16)	3.0822(19)	-4.6276(18)	1	1	1	-	D/A
d	O(7W)	0.0147(2)	0.31534(11)	0.16348(12)	-0.2517(16)	5.3306(19)	2.5159(18)	1	1	1	-	D/A
d	O(11A)	0.1300(2)	0.19884(11)	-0.03592(12)	1.1310(16)	3.3613(19)	-0.5528(18)	1	1	1	-	D/A
d	O(11B)	-0.1881(2)	0.34295(12)	-0.01144(13)	-1.4928(16)	5.797(2)	-0.176(2)	1	1	1	-	D/A
d	O(12A)	-0.1160(2)	0.18213(11)	-0.12188(13)	-0.6605(16)	3.0788(19)	-1.876(2)	1	1	1	-	D/A
d	O(12B)	-0.4206(2)	0.31509(11)	-0.10649(12)	-3.1547(16)	5.3264(19)	-1.6389(18)	1	1	1	-	D/A

d	O(21A)	0.5064(2)	0.16066(11)	-0.16844(13)	4.4704(16)	2.7159(19)	-2.592(2)	1	1	1	-	D/A
d	O(21B)	-0.5717(2)	0.29498(11)	0.07349(13)	-4.7825(16)	4.9865(19)	1.131(2)	1	1	1	-	D/A
d	O(22A)	0.2691(2)	0.22636(11)	-0.21500(13)	2.6599(16)	3.8265(19)	-3.309(2)	1	1	1	-	D/A
d	O(22B)	-0.8169(2)	0.35198(11)	0.02233(12)	-6.6464(16)	5.9500(19)	0.3437(18)	1	1	1	-	D/A
d	O(41A)	0.4578(2)	-0.13806(11)	-0.20266(12)	4.1555(16)	-2.3338(19)	-3.1189(18)	1	1	1	-	D/A
d	O(42A)	0.2039(2)	-0.17085(11)	-0.26808(12)	2.2537(16)	-2.8881(19)	-4.1257(18)	1	1	1	-	D/A
d	O(51A)	0.0912(2)	-0.17665(11)	-0.08376(12)	0.9261(16)	-2.9862(19)	-1.2891(18)	1	1	1	-	D/A
d	O(52A)	-0.1540(2)	-0.13460(12)	-0.15299(13)	-0.8968(16)	-2.275(2)	-2.354(2)	1	1	1	-	D/A
d	C(1A)	0.1044(3)	0.09196(15)	-0.13415(17)	1.147(2)	1.555(3)	-2.065(3)	1	1	1	-	-
d	C(1B)	-0.4229(3)	0.42842(15)	-0.01846(17)	-3.373(2)	7.242(3)	-0.284(3)	1	1	1	-	-
d	C(2A)	0.2533(3)	0.09184(15)	-0.17076(17)	2.432(2)	1.553(3)	-2.628(3)	1	1	1	-	-
d	C(2B)	-0.5732(3)	0.42711(16)	0.01676(17)	-4.666(2)	7.220(3)	0.258(3)	1	1	1	-	-
d	C(3A)	0.3150(3)	0.01989(16)	-0.19732(17)	2.990(2)	0.336(3)	-3.037(3)	1	1	1	-	-
d	C(4A)	0.2326(3)	-0.05090(15)	-0.18754(17)	2.303(2)	-0.860(3)	-2.886(3)	1	1	1	-	-
d	C(5A)	0.0851(3)	-0.05085(15)	-0.15006(17)	1.027(2)	-0.860(3)	-2.309(3)	1	1	1	-	-
d	C(6A)	0.0224(3)	0.02055(16)	-0.12442(17)	0.463(2)	0.347(3)	-1.915(3)	1	1	1	-	-
d	C(6B)	-0.6483(3)	0.49853(16)	0.03422(17)	-5.312(2)	8.427(3)	0.527(3)	1	1	1	-	-
d	C(11A)	0.0315(3)	0.16424(15)	-0.09713(17)	0.474(2)	2.776(3)	-1.495(3)	1	1	1	-	-
d	C(11B)	-0.3349(3)	0.35506(15)	-0.04584(17)	-2.600(2)	6.002(3)	-0.705(3)	1	1	1	-	-
d	C(21A)	0.3471(3)	0.16631(15)	-0.18560(17)	3.223(2)	2.811(3)	-2.856(3)	1	1	1	-	-
d	C(21B)	-0.6563(3)	0.35120(15)	0.03919(17)	-5.388(2)	5.937(3)	0.603(3)	1	1	1	-	-
d	C(41A)	0.3049(3)	-0.12491(15)	-0.22010(17)	2.961(2)	-2.112(3)	-3.387(3)	1	1	1	-	-
d	C(51A)	-0.0016(3)	-0.12596(15)	-0.12961(17)	0.281(2)	-2.129(3)	-1.995(3)	1	1	1	-	-
cR	H(3A)	0.41530	0.01950	-0.22260	3.8576	0.3296	-3.4258	1	1	1	-	-
cR	H(6A)	-0.07850	0.02080	-0.09970	-0.4079	0.3516	-1.5344	1	1	1	-	-
cR	H(6B)	-0.75080	0.49750	0.05750	-6.1924	8.4099	0.8849	1	1	1	-	-
d	Cu(1)a	-0.95892(4)	0.26508(2)	0.04931(2)	-7.8542(3)	4.4810(3)	0.7589(3)	1	1	1	1.455	Met
d	Cu(2)a	-1.33918(4)	0.24358(2)	-0.19199(2)	-10.3778(3)	4.1175(3)	-2.9547(3)	1	1	1	1.455	Met
d	Na(1)a	-1.37130(13)	-0.15484(7)	-0.06681(7)	-10.9208(11)	-2.6175(12)	-1.0282(11)	1	1	1	1.455	Met
d	Na(2)a	-0.33050(13)	-0.13521(6)	-0.28886(7)	-2.0141(11)	-2.2856(10)	-4.4455(11)	1	1	1	1.455	Met
d	O(1W)a	-0.0907(2)	-0.11348(12)	-0.35181(13)	0.0648(16)	-1.918(2)	-5.414(2)	1	1	1	1.455	D/A
d	O(3W)a	-0.3168(3)	0.00998(13)	-0.26961(18)	-1.947(2)	0.169(2)	-4.149(3)	1	1	1	1.455	D/A
d	O(4W)a	-1.6034(3)	-0.13127(15)	-0.00353(15)	-12.938(2)	-2.219(3)	-0.054(2)	1	1	1	1.455	D/A
d	O(5W)a	-1.3417(4)	-0.01494(17)	-0.0611(2)	-10.695(3)	-0.253(3)	-0.940(3)	1	1	1	1.455	D/A
d	O(6W)a	-1.3107(2)	0.18233(11)	-0.30069(12)	-9.9016(16)	3.0822(19)	-4.6276(18)	1	1	1	1.455	D/A
d	O(7W)a	-0.9853(2)	0.31534(11)	0.16348(12)	-8.3259(16)	5.3306(19)	2.5159(18)	1	1	1	1.455	D/A
d	O(11A)a	-0.8700(2)	0.19884(11)	-0.03592(12)	-6.9432(16)	3.3613(19)	-0.5528(18)	1	1	1	1.455	D/A
d	O(11B)a	-1.1881(2)	0.34295(12)	-0.01144(13)	-9.5670(16)	5.797(2)	-0.176(2)	1	1	1	1.455	D/A
d	O(12A)a	-1.1160(2)	0.18213(11)	-0.12188(13)	-8.7347(16)	3.0788(19)	-1.876(2)	1	1	1	1.455	D/A
d	O(12B)a	-1.4206(2)	0.31509(11)	-0.10649(12)	-11.2289(16)	5.3264(19)	-1.6389(18)	1	1	1	1.455	D/A
d	O(21A)a	-0.4936(2)	0.16066(11)	-0.16844(13)	-3.6038(16)	2.7159(19)	-2.592(2)	1	1	1	1.455	D/A
d	O(21B)a	-1.5717(2)	0.29498(11)	0.07349(13)	-12.8567(16)	4.9865(19)	1.131(2)	1	1	1	1.455	D/A
d	O(22A)a	-0.7309(2)	0.22636(11)	-0.21500(13)	-5.4143(16)	3.8265(19)	-3.309(2)	1	1	1	1.455	D/A
d	O(22B)a	-1.8169(2)	0.35198(11)	0.02233(12)	-14.7206(16)	5.9500(19)	0.3437(18)	1	1	1	1.455	D/A
d	O(41A)a	-0.5422(2)	-0.13806(11)	-0.20266(12)	-3.9187(16)	-2.3338(19)	-3.1189(18)	1	1	1	1.455	D/A
d	O(42A)a	-0.7961(2)	-0.17085(11)	-0.26808(12)	-5.8205(16)	-2.8881(19)	-4.1257(18)	1	1	1	1.455	D/A

d	O(51A)a	-0.9088(2)	-0.17665(11)	-0.08376(12)	-7.1481(16)	-2.9862(19)	-1.2891(18)	1	1	1	1.455	D/A
d	O(52A)a	-1.1540(2)	-0.13460(12)	-0.15299(13)	-8.9710(16)	-2.275(2)	-2.354(2)	1	1	1	1.455	D/A
d	C(1A)a	-0.8956(3)	0.09196(15)	-0.13415(17)	-6.927(2)	1.555(3)	-2.065(3)	1	1	1	1.455	-
d	C(1B)a	-1.4229(3)	0.42842(15)	-0.01846(17)	-11.447(2)	7.242(3)	-0.284(3)	1	1	1	1.455	-
d	C(2A)a	-0.7467(3)	0.09184(15)	-0.17076(17)	-5.642(2)	1.553(3)	-2.628(3)	1	1	1	1.455	-
d	C(2B)a	-1.5732(3)	0.42711(16)	0.01676(17)	-12.740(2)	7.220(3)	0.258(3)	1	1	1	1.455	-
d	C(3A)a	-0.6850(3)	0.01989(16)	-0.19732(17)	-5.084(2)	0.336(3)	-3.037(3)	1	1	1	1.455	-
d	C(4A)a	-0.7674(3)	-0.05090(15)	-0.18754(17)	-5.771(2)	-0.860(3)	-2.886(3)	1	1	1	1.455	-
d	C(5A)a	-0.9149(3)	-0.05085(15)	-0.15006(17)	-7.047(2)	-0.860(3)	-2.309(3)	1	1	1	1.455	-
d	C(6A)a	-0.9776(3)	0.02055(16)	-0.12442(17)	-7.611(2)	0.347(3)	-1.915(3)	1	1	1	1.455	-
d	C(6B)a	-1.6483(3)	0.49853(16)	0.03422(17)	-13.386(2)	8.427(3)	0.527(3)	1	1	1	1.455	-
d	C(11A)a	-0.9685(3)	0.16424(15)	-0.09713(17)	-7.600(2)	2.776(3)	-1.495(3)	1	1	1	1.455	-
d	C(11B)a	-1.3349(3)	0.35506(15)	-0.04584(17)	-10.674(2)	6.002(3)	-0.705(3)	1	1	1	1.455	-
d	C(21A)a	-0.6529(3)	0.16631(15)	-0.18560(17)	-4.851(2)	2.811(3)	-2.856(3)	1	1	1	1.455	-
d	C(21B)a	-1.6563(3)	0.35120(15)	0.03919(17)	-13.462(2)	5.937(3)	0.603(3)	1	1	1	1.455	-
d	C(41A)a	-0.6951(3)	-0.12491(15)	-0.22010(17)	-5.114(2)	-2.112(3)	-3.387(3)	1	1	1	1.455	-
d	C(51A)a	-1.0016(3)	-0.12596(15)	-0.12961(17)	-7.793(2)	-2.129(3)	-1.995(3)	1	1	1	1.455	-
cR	H(3A)a	-0.58470	0.01950	-0.22260	-4.2166	0.3296	-3.4258	1	1	1	1.455	-
cR	H(6A)a	-1.07850	0.02080	-0.09970	-8.4821	0.3516	-1.5344	1	1	1	1.455	-
cR	H(6B)a	-1.75080	0.49750	0.05750	-14.2666	8.4099	0.8849	1	1	1	1.455	-
d	Cu(1)b	1.04108(4)	0.26508(2)	0.04931(2)	8.2942(3)	4.4810(3)	0.7589(3)	1	1	1	1.655	Met
d	Cu(2)b	0.66082(4)	0.24358(2)	-0.19199(2)	5.7706(3)	4.1175(3)	-2.9547(3)	1	1	1	1.655	Met
d	Na(1)b	0.62870(13)	-0.15484(7)	-0.06681(7)	5.2276(11)	-2.6175(12)	-1.0282(11)	1	1	1	1.655	Met
d	Na(2)b	1.66950(13)	-0.13521(6)	-0.28886(7)	14.1343(11)	-2.2856(10)	-4.4455(11)	1	1	1	1.655	Met
d	O(1W)b	1.9093(2)	-0.11348(12)	-0.35181(13)	16.2132(16)	-1.918(2)	-5.414(2)	1	1	1	1.655	D/A
d	O(3W)b	1.6832(3)	0.00998(13)	-0.26961(18)	14.201(2)	0.169(2)	-4.149(3)	1	1	1	1.655	D/A
d	O(4W)b	0.3966(3)	-0.13127(15)	-0.00353(15)	3.210(2)	-2.219(3)	-0.054(2)	1	1	1	1.655	D/A
d	O(5W)b	0.6583(4)	-0.01494(17)	-0.0611(2)	5.454(3)	-0.253(3)	-0.940(3)	1	1	1	1.655	D/A
d	O(6W)b	0.6893(2)	0.18233(11)	-0.30069(12)	6.2468(16)	3.0822(19)	-4.6276(18)	1	1	1	1.655	D/A
d	O(7W)b	1.0147(2)	0.31534(11)	0.16348(12)	7.8225(16)	5.3306(19)	2.5159(18)	1	1	1	1.655	D/A
d	O(11A)b	1.1300(2)	0.19884(11)	-0.03592(12)	9.2052(16)	3.3613(19)	-0.5528(18)	1	1	1	1.655	D/A
d	O(11B)b	0.8119(2)	0.34295(12)	-0.01144(13)	6.5814(16)	5.797(2)	-0.176(2)	1	1	1	1.655	D/A
d	O(12A)b	0.8840(2)	0.18213(11)	-0.12188(13)	7.4137(16)	3.0788(19)	-1.876(2)	1	1	1	1.655	D/A
d	O(12B)b	0.5794(2)	0.31509(11)	-0.10649(12)	4.9195(16)	5.3264(19)	-1.6389(18)	1	1	1	1.655	D/A
d	O(21A)b	1.5064(2)	0.16066(11)	-0.16844(13)	12.5446(16)	2.7159(19)	-2.592(2)	1	1	1	1.655	D/A
d	O(21B)b	0.4283(2)	0.29498(11)	0.07349(13)	3.2917(16)	4.9865(19)	1.131(2)	1	1	1	1.655	D/A
d	O(22A)b	1.2691(2)	0.22636(11)	-0.21500(13)	10.7341(16)	3.8265(19)	-3.309(2)	1	1	1	1.655	D/A
d	O(22B)b	0.1831(2)	0.35198(11)	0.02233(12)	1.4278(16)	5.9500(19)	0.3437(18)	1	1	1	1.655	D/A
d	O(41A)b	1.4578(2)	-0.13806(11)	-0.20266(12)	12.2297(16)	-2.3338(19)	-3.1189(18)	1	1	1	1.655	D/A
d	O(42A)b	1.2039(2)	-0.17085(11)	-0.26808(12)	10.3279(16)	-2.8881(19)	-4.1257(18)	1	1	1	1.655	D/A
d	O(51A)b	1.0912(2)	-0.17665(11)	-0.08376(12)	9.0003(16)	-2.9862(19)	-1.2891(18)	1	1	1	1.655	D/A
d	O(52A)b	0.8460(2)	-0.13460(12)	-0.15299(13)	7.1774(16)	-2.275(2)	-2.354(2)	1	1	1	1.655	D/A
d	C(1A)b	1.1044(3)	0.09196(15)	-0.13415(17)	9.221(2)	1.555(3)	-2.065(3)	1	1	1	1.655	-
d	C(1B)b	0.5771(3)	0.42842(15)	-0.01846(17)	4.701(2)	7.242(3)	-0.284(3)	1	1	1	1.655	-
d	C(2A)b	1.2533(3)	0.09184(15)	-0.17076(17)	10.506(2)	1.553(3)	-2.628(3)	1	1	1	1.655	-
d	C(2B)b	0.4268(3)	0.42711(16)	0.01676(17)	3.408(2)	7.220(3)	0.258(3)	1	1	1	1.655	-

d	C(3A)b	1.3150(3)	0.01989(16)	-0.19732(17)	11.065(2)	0.336(3)	-3.037(3)	1	1	1	1.655	-
d	C(4A)b	1.2326(3)	-0.05090(15)	-0.18754(17)	10.377(2)	-0.860(3)	-2.886(3)	1	1	1	1.655	-
d	C(5A)b	1.0851(3)	-0.05085(15)	-0.15006(17)	9.101(2)	-0.860(3)	-2.309(3)	1	1	1	1.655	-
d	C(6A)b	1.0224(3)	0.02055(16)	-0.12442(17)	8.537(2)	0.347(3)	-1.915(3)	1	1	1	1.655	-
d	C(6B)b	0.3517(3)	0.49853(16)	0.03422(17)	2.762(2)	8.427(3)	0.527(3)	1	1	1	1.655	-
d	C(11A)b	1.0315(3)	0.16424(15)	-0.09713(17)	8.549(2)	2.776(3)	-1.495(3)	1	1	1	1.655	-
d	C(11B)b	0.6651(3)	0.35506(15)	-0.04584(17)	5.474(2)	6.002(3)	-0.705(3)	1	1	1	1.655	-
d	C(21A)b	1.3471(3)	0.16631(15)	-0.18560(17)	11.297(2)	2.811(3)	-2.856(3)	1	1	1	1.655	-
d	C(21B)b	0.3437(3)	0.35120(15)	0.03919(17)	2.686(2)	5.937(3)	0.603(3)	1	1	1	1.655	-
d	C(41A)b	1.3049(3)	-0.12491(15)	-0.22010(17)	11.035(2)	-2.112(3)	-3.387(3)	1	1	1	1.655	-
d	C(51A)b	0.9984(3)	-0.12596(15)	-0.12961(17)	8.355(2)	-2.129(3)	-1.995(3)	1	1	1	1.655	-
cR	H(3A)b	1.41530	0.01950	-0.22260	11.9318	0.3296	-3.4258	1	1	1	1.655	-
cR	H(6A)b	0.92150	0.02080	-0.09970	7.6663	0.3516	-1.5344	1	1	1	1.655	-
cR	H(6B)b	0.24920	0.49750	0.05750	1.8818	8.4099	0.8849	1	1	1	1.655	-
d	Cu(1)c	-0.04108(4)	-0.23492(2)	-0.54931(2)	0.9129(3)	-3.9712(3)	-8.4538(3)	1	1	1	2.544	Met
d	Cu(2)c	0.33918(4)	-0.25642(2)	-0.30801(2)	3.4365(3)	-4.3347(3)	-4.7402(3)	1	1	1	2.544	Met
d	Na(1)c	0.37130(13)	-0.65484(7)	-0.43319(7)	3.9794(11)	-11.0697(12)	-6.6667(11)	1	1	1	2.544	Met
d	Na(2)c	-0.66950(13)	-0.63521(6)	-0.21114(7)	-4.9273(11)	-10.7378(10)	-3.2494(11)	1	1	1	2.544	Met
d	O(1W)c	-0.9093(2)	-0.61348(12)	-0.14819(13)	-7.0061(16)	-10.371(2)	-2.281(2)	1	1	1	2.544	D/A
d	O(3W)c	-0.6832(3)	-0.49002(13)	-0.23039(18)	-4.994(2)	-8.283(2)	-3.546(3)	1	1	1	2.544	D/A
d	O(4W)c	0.6034(3)	-0.63127(15)	-0.49647(15)	5.997(2)	-10.671(3)	-7.641(2)	1	1	1	2.544	D/A
d	O(5W)c	0.3417(4)	-0.51494(17)	-0.4389(2)	3.753(3)	-8.705(3)	-6.755(3)	1	1	1	2.544	D/A
d	O(6W)c	0.3107(2)	-0.31767(11)	-0.19931(12)	2.9602(16)	-5.3700(19)	-3.0673(18)	1	1	1	2.544	D/A
d	O(7W)c	-0.0147(2)	-0.18466(11)	-0.66348(12)	1.3846(16)	-3.1216(19)	-10.2108(18)	1	1	1	2.544	D/A
d	O(11A)c	-0.1300(2)	-0.30116(11)	-0.46408(12)	0.0018(16)	-5.0909(19)	-7.1421(18)	1	1	1	2.544	D/A
d	O(11B)c	0.1881(2)	-0.15705(12)	-0.48856(13)	2.6257(16)	-2.655(2)	-7.519(2)	1	1	1	2.544	D/A
d	O(12A)c	0.1160(2)	-0.31787(11)	-0.37812(13)	1.7933(16)	-5.3734(19)	-5.819(2)	1	1	1	2.544	D/A
d	O(12B)c	0.4206(2)	-0.18491(11)	-0.39351(12)	4.2876(16)	-3.1258(19)	-6.0560(18)	1	1	1	2.544	D/A
d	O(21A)c	-0.5064(2)	-0.33934(11)	-0.33156(13)	-3.3376(16)	-5.7363(19)	-5.103(2)	1	1	1	2.544	D/A
d	O(21B)c	0.5717(2)	-0.20502(11)	-0.57349(13)	5.9154(16)	-3.4657(19)	-8.826(2)	1	1	1	2.544	D/A
d	O(22A)c	-0.2691(2)	-0.27364(11)	-0.28500(13)	-1.5270(16)	-4.6257(19)	-4.386(2)	1	1	1	2.544	D/A
d	O(22B)c	0.8169(2)	-0.14802(11)	-0.52233(12)	7.7793(16)	-2.5022(19)	-8.0386(18)	1	1	1	2.544	D/A
d	O(41A)c	-0.4578(2)	-0.63806(11)	-0.29734(12)	-3.0227(16)	-10.7860(19)	-4.5760(18)	1	1	1	2.544	D/A
d	O(42A)c	-0.2039(2)	-0.67085(11)	-0.23192(12)	-1.1209(16)	-11.3403(19)	-3.5692(18)	1	1	1	2.544	D/A
d	O(51A)c	-0.0912(2)	-0.67665(11)	-0.41624(12)	0.2067(16)	-11.4384(19)	-6.4059(18)	1	1	1	2.544	D/A
d	O(52A)c	0.1540(2)	-0.63460(12)	-0.34701(13)	2.0297(16)	-10.728(2)	-5.340(2)	1	1	1	2.544	D/A
d	C(1A)c	-0.1044(3)	-0.40804(15)	-0.36585(17)	-0.014(2)	-6.898(3)	-5.630(3)	1	1	1	2.544	-
d	C(1B)c	0.4229(3)	-0.07158(15)	-0.48154(17)	4.506(2)	-1.210(3)	-7.411(3)	1	1	1	2.544	-
d	C(2A)c	-0.2533(3)	-0.40816(15)	-0.32924(17)	-1.299(2)	-6.900(3)	-5.067(3)	1	1	1	2.544	-
d	C(2B)c	0.5732(3)	-0.07289(16)	-0.51676(17)	5.799(2)	-1.232(3)	-7.953(3)	1	1	1	2.544	-
d	C(3A)c	-0.3150(3)	-0.48011(16)	-0.30268(17)	-1.858(2)	-8.116(3)	-4.658(3)	1	1	1	2.544	-
d	C(4A)c	-0.2326(3)	-0.55090(15)	-0.31246(17)	-1.170(2)	-9.313(3)	-4.809(3)	1	1	1	2.544	-
d	C(5A)c	-0.0851(3)	-0.55085(15)	-0.34994(17)	0.106(2)	-9.312(3)	-5.386(3)	1	1	1	2.544	-
d	C(6A)c	-0.0224(3)	-0.47945(16)	-0.37558(17)	0.670(2)	-8.105(3)	-5.780(3)	1	1	1	2.544	-
d	C(6B)c	0.6483(3)	-0.00147(16)	-0.53422(17)	6.445(2)	-0.025(3)	-8.222(3)	1	1	1	2.544	-
d	C(11A)c	-0.0315(3)	-0.33576(15)	-0.40287(17)	0.658(2)	-5.676(3)	-6.200(3)	1	1	1	2.544	-

d	C(11B)c	0.3349(3)	-0.14494(15)	-0.45416(17)	3.733(2)	-2.450(3)	-6.989(3)	1	1	1	2.544	-
d	C(21A)c	-0.3471(3)	-0.33369(15)	-0.31440(17)	-2.090(2)	-5.641(3)	-4.839(3)	1	1	1	2.544	-
d	C(21B)c	0.6563(3)	-0.14880(15)	-0.53919(17)	6.521(2)	-2.515(3)	-8.298(3)	1	1	1	2.544	-
d	C(41A)c	-0.3049(3)	-0.62491(15)	-0.27990(17)	-1.828(2)	-10.564(3)	-4.308(3)	1	1	1	2.544	-
d	C(51A)c	0.0016(3)	-0.62596(15)	-0.37039(17)	0.852(2)	-10.581(3)	-5.700(3)	1	1	1	2.544	-
cR	H(3A)c	-0.41530	-0.48050	-0.27740	-2.7247	-8.1226	-4.2691	1	1	1	2.544	-
cR	H(6A)c	0.07850	-0.47920	-0.40030	1.5408	-8.1006	-6.1605	1	1	1	2.544	-
cR	H(6B)c	0.75080	-0.00250	-0.55750	7.3252	-0.0423	-8.5798	1	1	1	2.544	-
d	Cu(1)d	-0.04108(4)	0.76508(2)	-0.54931(2)	0.9129(3)	12.9332(3)	-8.4538(3)	1	1	1	2.554	Met
d	Cu(2)d	0.33918(4)	0.74358(2)	-0.30801(2)	3.4365(3)	12.5697(3)	-4.7402(3)	1	1	1	2.554	Met
d	Na(1)d	0.37130(13)	0.34516(7)	-0.43319(7)	3.9794(11)	5.8347(12)	-6.6667(11)	1	1	1	2.554	Met
d	Na(2)d	-0.66950(13)	0.36479(6)	-0.21114(7)	-4.9273(11)	6.1666(10)	-3.2494(11)	1	1	1	2.554	Met
d	O(1W)d	-0.9093(2)	0.38652(12)	-0.14819(13)	-7.0061(16)	6.534(2)	-2.281(2)	1	1	1	2.554	D/A
d	O(3W)d	-0.6832(3)	0.50998(13)	-0.23039(18)	-4.994(2)	8.621(2)	-3.546(3)	1	1	1	2.554	D/A
d	O(4W)d	0.6034(3)	0.36873(15)	-0.49647(15)	5.997(2)	6.233(3)	-7.641(2)	1	1	1	2.554	D/A
d	O(5W)d	0.3417(4)	0.48506(17)	-0.4389(2)	3.753(3)	8.200(3)	-6.755(3)	1	1	1	2.554	D/A
d	O(6W)d	0.3107(2)	0.68233(11)	-0.19931(12)	2.9602(16)	11.5344(19)	-3.0673(18)	1	1	1	2.554	D/A
d	O(7W)d	-0.0147(2)	0.81534(11)	-0.66348(12)	1.3846(16)	13.7828(19)	-10.2108(18)	1	1	1	2.554	D/A
d	O(11A)d	-0.1300(2)	0.69884(11)	-0.46408(12)	0.0018(16)	11.8135(19)	-7.1421(18)	1	1	1	2.554	D/A
d	O(11B)d	0.1881(2)	0.84295(12)	-0.48856(13)	2.6257(16)	14.250(2)	-7.519(2)	1	1	1	2.554	D/A
d	O(12A)d	0.1160(2)	0.68213(11)	-0.37812(13)	1.7933(16)	11.5310(19)	-5.819(2)	1	1	1	2.554	D/A
d	O(12B)d	0.4206(2)	0.81509(11)	-0.39351(12)	4.2876(16)	13.7786(19)	-6.0560(18)	1	1	1	2.554	D/A
d	O(21A)d	-0.5064(2)	0.66066(11)	-0.33156(13)	-3.3376(16)	11.1681(19)	-5.103(2)	1	1	1	2.554	D/A
d	O(21B)d	0.5717(2)	0.79498(11)	-0.57349(13)	5.9154(16)	13.4387(19)	-8.826(2)	1	1	1	2.554	D/A
d	O(22A)d	-0.2691(2)	0.72636(11)	-0.28500(13)	-1.5270(16)	12.2787(19)	-4.386(2)	1	1	1	2.554	D/A
d	O(22B)d	0.8169(2)	0.85198(11)	-0.52233(12)	7.7793(16)	14.4022(19)	-8.0386(18)	1	1	1	2.554	D/A
d	O(41A)d	-0.4578(2)	0.36194(11)	-0.29734(12)	-3.0227(16)	6.1184(19)	-4.5760(18)	1	1	1	2.554	D/A
d	O(42A)d	-0.2039(2)	0.32915(11)	-0.23192(12)	-1.1209(16)	5.5641(19)	-3.5692(18)	1	1	1	2.554	D/A
d	O(51A)d	-0.0912(2)	0.32335(11)	-0.41624(12)	0.2067(16)	5.4660(19)	-6.4059(18)	1	1	1	2.554	D/A
d	O(52A)d	0.1540(2)	0.36540(12)	-0.34701(13)	2.0297(16)	6.177(2)	-5.340(2)	1	1	1	2.554	D/A
d	C(1A)d	-0.1044(3)	0.59196(15)	-0.36585(17)	-0.014(2)	10.007(3)	-5.630(3)	1	1	1	2.554	-
d	C(1B)d	0.4229(3)	0.92842(15)	-0.48154(17)	4.506(2)	15.694(3)	-7.411(3)	1	1	1	2.554	-
d	C(2A)d	-0.2533(3)	0.59184(15)	-0.32924(17)	-1.299(2)	10.005(3)	-5.067(3)	1	1	1	2.554	-
d	C(2B)d	0.5732(3)	0.92711(16)	-0.51676(17)	5.799(2)	15.672(3)	-7.953(3)	1	1	1	2.554	-
d	C(3A)d	-0.3150(3)	0.51989(16)	-0.30268(17)	-1.858(2)	8.788(3)	-4.658(3)	1	1	1	2.554	-
d	C(4A)d	-0.2326(3)	0.44910(15)	-0.31246(17)	-1.170(2)	7.592(3)	-4.809(3)	1	1	1	2.554	-
d	C(5A)d	-0.0851(3)	0.44915(15)	-0.34994(17)	0.106(2)	7.593(3)	-5.386(3)	1	1	1	2.554	-
d	C(6A)d	-0.0224(3)	0.52055(16)	-0.37558(17)	0.670(2)	8.800(3)	-5.780(3)	1	1	1	2.554	-
d	C(6B)d	0.6483(3)	0.99853(16)	-0.53422(17)	6.445(2)	16.880(3)	-8.222(3)	1	1	1	2.554	-
d	C(11A)d	-0.0315(3)	0.66424(15)	-0.40287(17)	0.658(2)	11.229(3)	-6.200(3)	1	1	1	2.554	-
d	C(11B)d	0.3349(3)	0.85506(15)	-0.45416(17)	3.733(2)	14.454(3)	-6.989(3)	1	1	1	2.554	-
d	C(21A)d	-0.3471(3)	0.66631(15)	-0.31440(17)	-2.090(2)	11.264(3)	-4.839(3)	1	1	1	2.554	-
d	C(21B)d	0.6563(3)	0.85120(15)	-0.53919(17)	6.521(2)	14.389(3)	-8.298(3)	1	1	1	2.554	-
d	C(41A)d	-0.3049(3)	0.37509(15)	-0.27990(17)	-1.828(2)	6.341(3)	-4.308(3)	1	1	1	2.554	-
d	C(51A)d	0.0016(3)	0.37404(15)	-0.37039(17)	0.852(2)	6.323(3)	-5.700(3)	1	1	1	2.554	-

cR	H(3A)d	-0.41530	0.51950	-0.27740	-2.7247	8.7818	-4.2691	1	1	1	2.554	-
cR	H(6A)d	0.07850	0.52080	-0.40030	1.5408	8.8038	-6.1605	1	1	1	2.554	-
cR	H(6B)d	0.75080	0.99750	-0.55750	7.3252	16.8621	-8.5798	1	1	1	2.554	-
d	Cu(1)e	0.95892(4)	-0.23492(2)	-0.54931(2)	8.9871(3)	-3.9712(3)	-8.4538(3)	1	1	1	2.644	Met
d	Cu(2)e	1.33918(4)	-0.25642(2)	-0.30801(2)	11.5107(3)	-4.3347(3)	-4.7402(3)	1	1	1	2.644	Met
d	Na(1)e	1.37130(13)	-0.65484(7)	-0.43319(7)	12.0536(11)	-11.0697(12)	-6.6667(11)	1	1	1	2.644	Met
d	Na(2)e	0.33050(13)	-0.63521(6)	-0.21114(7)	3.1469(11)	-10.7378(10)	-3.2494(11)	1	1	1	2.644	Met
d	O(1W)e	0.0907(2)	-0.61348(12)	-0.14819(13)	1.0681(16)	-10.371(2)	-2.281(2)	1	1	1	2.644	D/A
d	O(3W)e	0.3168(3)	-0.49002(13)	-0.23039(18)	3.080(2)	-8.283(2)	-3.546(3)	1	1	1	2.644	D/A
d	O(4W)e	1.6034(3)	-0.63127(15)	-0.49647(15)	14.071(2)	-10.671(3)	-7.641(2)	1	1	1	2.644	D/A
d	O(5W)e	1.3417(4)	-0.51494(17)	-0.4389(2)	11.828(3)	-8.705(3)	-6.755(3)	1	1	1	2.644	D/A
d	O(6W)e	1.3107(2)	-0.31767(11)	-0.19931(12)	11.0344(16)	-5.3700(19)	-3.0673(18)	1	1	1	2.644	D/A
d	O(7W)e	0.9853(2)	-0.18466(11)	-0.66348(12)	9.4588(16)	-3.1216(19)	-10.2108(18)	1	1	1	2.644	D/A
d	O(11A)e	0.8700(2)	-0.30116(11)	-0.46408(12)	8.0760(16)	-5.0909(19)	-7.1421(18)	1	1	1	2.644	D/A
d	O(11B)e	1.1881(2)	-0.15705(12)	-0.48856(13)	10.6999(16)	-2.655(2)	-7.519(2)	1	1	1	2.644	D/A
d	O(12A)e	1.1160(2)	-0.31787(11)	-0.37812(13)	9.8675(16)	-5.3734(19)	-5.819(2)	1	1	1	2.644	D/A
d	O(12B)e	1.4206(2)	-0.18491(11)	-0.39351(12)	12.3618(16)	-3.1258(19)	-6.0560(18)	1	1	1	2.644	D/A
d	O(21A)e	0.4936(2)	-0.33934(11)	-0.33156(13)	4.7366(16)	-5.7363(19)	-5.103(2)	1	1	1	2.644	D/A
d	O(21B)e	1.5717(2)	-0.20502(11)	-0.57349(13)	13.9896(16)	-3.4657(19)	-8.826(2)	1	1	1	2.644	D/A
d	O(22A)e	0.7309(2)	-0.27364(11)	-0.28500(13)	6.5472(16)	-4.6257(19)	-4.386(2)	1	1	1	2.644	D/A
d	O(22B)e	1.8169(2)	-0.14802(11)	-0.52233(12)	15.8535(16)	-2.5022(19)	-8.0386(18)	1	1	1	2.644	D/A
d	O(41A)e	0.5422(2)	-0.63806(11)	-0.29734(12)	5.0515(16)	-10.7860(19)	-4.5760(18)	1	1	1	2.644	D/A
d	O(42A)e	0.7961(2)	-0.67085(11)	-0.23192(12)	6.9533(16)	-11.3403(19)	-3.5692(18)	1	1	1	2.644	D/A
d	O(51A)e	0.9088(2)	-0.67665(11)	-0.41624(12)	8.2809(16)	-11.4384(19)	-6.4059(18)	1	1	1	2.644	D/A
d	O(52A)e	1.1540(2)	-0.63460(12)	-0.34701(13)	10.1039(16)	-10.728(2)	-5.340(2)	1	1	1	2.644	D/A
d	C(1A)e	0.8956(3)	-0.40804(15)	-0.36585(17)	8.060(2)	-6.898(3)	-5.630(3)	1	1	1	2.644	-
d	C(1B)e	1.4229(3)	-0.07158(15)	-0.48154(17)	12.580(2)	-1.210(3)	-7.411(3)	1	1	1	2.644	-
d	C(2A)e	0.7467(3)	-0.40816(15)	-0.32924(17)	6.775(2)	-6.900(3)	-5.067(3)	1	1	1	2.644	-
d	C(2B)e	1.5732(3)	-0.07289(16)	-0.51676(17)	13.873(2)	-1.232(3)	-7.953(3)	1	1	1	2.644	-
d	C(3A)e	0.6850(3)	-0.48011(16)	-0.30268(17)	6.217(2)	-8.116(3)	-4.658(3)	1	1	1	2.644	-
d	C(4A)e	0.7674(3)	-0.55090(15)	-0.31246(17)	6.904(2)	-9.313(3)	-4.809(3)	1	1	1	2.644	-
d	C(5A)e	0.9149(3)	-0.55085(15)	-0.34994(17)	8.180(2)	-9.312(3)	-5.386(3)	1	1	1	2.644	-
d	C(6A)e	0.9776(3)	-0.47945(16)	-0.37558(17)	8.744(2)	-8.105(3)	-5.780(3)	1	1	1	2.644	-
d	C(6B)e	1.6483(3)	-0.00147(16)	-0.53422(17)	14.519(2)	-0.025(3)	-8.222(3)	1	1	1	2.644	-
d	C(11A)e	0.9685(3)	-0.33576(15)	-0.40287(17)	8.733(2)	-5.676(3)	-6.200(3)	1	1	1	2.644	-
d	C(11B)e	1.3349(3)	-0.14494(15)	-0.45416(17)	11.807(2)	-2.450(3)	-6.989(3)	1	1	1	2.644	-
d	C(21A)e	0.6529(3)	-0.33369(15)	-0.31440(17)	5.984(2)	-5.641(3)	-4.839(3)	1	1	1	2.644	-
d	C(21B)e	1.6563(3)	-0.14880(15)	-0.53919(17)	14.595(2)	-2.515(3)	-8.298(3)	1	1	1	2.644	-
d	C(41A)e	0.6951(3)	-0.62491(15)	-0.27990(17)	6.247(2)	-10.564(3)	-4.308(3)	1	1	1	2.644	-
d	C(51A)e	1.0016(3)	-0.62596(15)	-0.37039(17)	8.926(2)	-10.581(3)	-5.700(3)	1	1	1	2.644	-
cR	H(3A)e	0.58470	-0.48050	-0.27740	5.3495	-8.1226	-4.2691	1	1	1	2.644	-
cR	H(6A)e	1.07850	-0.47920	-0.40030	9.6150	-8.1006	-6.1605	1	1	1	2.644	-
cR	H(6B)e	1.75080	-0.00250	-0.55750	15.3994	-0.0423	-8.5798	1	1	1	2.644	-
d	Cu(1)f	0.95892(4)	0.76508(2)	-0.54931(2)	8.9871(3)	12.9332(3)	-8.4538(3)	1	1	1	2.654	Met
d	Cu(2)f	1.33918(4)	0.74358(2)	-0.30801(2)	11.5107(3)	12.5697(3)	-4.7402(3)	1	1	1	2.654	Met

d	Na(1)f	1.37130(13)	0.34516(7)	-0.43319(7)	12.0536(11)	5.8347(12)	-6.6667(11)	1	1	1	2.654	Met
d	Na(2)f	0.33050(13)	0.36479(6)	-0.21114(7)	3.1469(11)	6.1666(10)	-3.2494(11)	1	1	1	2.654	Met
d	O(1W)f	0.0907(2)	0.38652(12)	-0.14819(13)	1.0681(16)	6.534(2)	-2.281(2)	1	1	1	2.654	D/A
d	O(3W)f	0.3168(3)	0.50998(13)	-0.23039(18)	3.080(2)	8.621(2)	-3.546(3)	1	1	1	2.654	D/A
d	O(4W)f	1.6034(3)	0.36873(15)	-0.49647(15)	14.071(2)	6.233(3)	-7.641(2)	1	1	1	2.654	D/A
d	O(5W)f	1.3417(4)	0.48506(17)	-0.4389(2)	11.828(3)	8.200(3)	-6.755(3)	1	1	1	2.654	D/A
d	O(6W)f	1.3107(2)	0.68233(11)	-0.19931(12)	11.0344(16)	11.5344(19)	-3.0673(18)	1	1	1	2.654	D/A
d	O(7W)f	0.9853(2)	0.81534(11)	-0.66348(12)	9.4588(16)	13.7828(19)	-10.2108(18)	1	1	1	2.654	D/A
d	O(11A)f	0.8700(2)	0.69884(11)	-0.46408(12)	8.0760(16)	11.8135(19)	-7.1421(18)	1	1	1	2.654	D/A
d	O(11B)f	1.1881(2)	0.84295(12)	-0.48856(13)	10.6999(16)	14.250(2)	-7.519(2)	1	1	1	2.654	D/A
d	O(12A)f	1.1160(2)	0.68213(11)	-0.37812(13)	9.8675(16)	11.5310(19)	-5.819(2)	1	1	1	2.654	D/A
d	O(12B)f	1.4206(2)	0.81509(11)	-0.39351(12)	12.3618(16)	13.7786(19)	-6.0560(18)	1	1	1	2.654	D/A
d	O(21A)f	0.4936(2)	0.66066(11)	-0.33156(13)	4.7366(16)	11.1681(19)	-5.103(2)	1	1	1	2.654	D/A
d	O(21B)f	1.5717(2)	0.79498(11)	-0.57349(13)	13.9896(16)	13.4387(19)	-8.826(2)	1	1	1	2.654	D/A
d	O(22A)f	0.7309(2)	0.72636(11)	-0.28500(13)	6.5472(16)	12.2787(19)	-4.386(2)	1	1	1	2.654	D/A
d	O(22B)f	1.8169(2)	0.85198(11)	-0.52233(12)	15.8535(16)	14.4022(19)	-8.0386(18)	1	1	1	2.654	D/A
d	O(41A)f	0.5422(2)	0.36194(11)	-0.29734(12)	5.0515(16)	6.1184(19)	-4.5760(18)	1	1	1	2.654	D/A
d	O(42A)f	0.7961(2)	0.32915(11)	-0.23192(12)	6.9533(16)	5.5641(19)	-3.5692(18)	1	1	1	2.654	D/A
d	O(51A)f	0.9088(2)	0.32335(11)	-0.41624(12)	8.2809(16)	5.4660(19)	-6.4059(18)	1	1	1	2.654	D/A
d	O(52A)f	1.1540(2)	0.36540(12)	-0.34701(13)	10.1039(16)	6.177(2)	-5.340(2)	1	1	1	2.654	D/A
d	C(1A)f	0.8956(3)	0.59196(15)	-0.36585(17)	8.060(2)	10.007(3)	-5.630(3)	1	1	1	2.654	-
d	C(1B)f	1.4229(3)	0.92842(15)	-0.48154(17)	12.580(2)	15.694(3)	-7.411(3)	1	1	1	2.654	-
d	C(2A)f	0.7467(3)	0.59184(15)	-0.32924(17)	6.775(2)	10.005(3)	-5.067(3)	1	1	1	2.654	-
d	C(2B)f	1.5732(3)	0.92711(16)	-0.51676(17)	13.873(2)	15.672(3)	-7.953(3)	1	1	1	2.654	-
d	C(3A)f	0.6850(3)	0.51989(16)	-0.30268(17)	6.217(2)	8.788(3)	-4.658(3)	1	1	1	2.654	-
d	C(4A)f	0.7674(3)	0.44910(15)	-0.31246(17)	6.904(2)	7.592(3)	-4.809(3)	1	1	1	2.654	-
d	C(5A)f	0.9149(3)	0.44915(15)	-0.34994(17)	8.180(2)	7.593(3)	-5.386(3)	1	1	1	2.654	-
d	C(6A)f	0.9776(3)	0.52055(16)	-0.37558(17)	8.744(2)	8.800(3)	-5.780(3)	1	1	1	2.654	-
d	C(6B)f	1.6483(3)	0.99853(16)	-0.53422(17)	14.519(2)	16.880(3)	-8.222(3)	1	1	1	2.654	-
d	C(11A)f	0.9685(3)	0.66424(15)	-0.40287(17)	8.733(2)	11.229(3)	-6.200(3)	1	1	1	2.654	-
d	C(11B)f	1.3349(3)	0.85506(15)	-0.45416(17)	11.807(2)	14.454(3)	-6.989(3)	1	1	1	2.654	-
d	C(21A)f	0.6529(3)	0.66631(15)	-0.31440(17)	5.984(2)	11.264(3)	-4.839(3)	1	1	1	2.654	-
d	C(21B)f	1.6563(3)	0.85120(15)	-0.53919(17)	14.595(2)	14.389(3)	-8.298(3)	1	1	1	2.654	-
d	C(41A)f	0.6951(3)	0.37509(15)	-0.27990(17)	6.247(2)	6.341(3)	-4.308(3)	1	1	1	2.654	-
d	C(51A)f	1.0016(3)	0.37404(15)	-0.37039(17)	8.926(2)	6.323(3)	-5.700(3)	1	1	1	2.654	-
cR	H(3A)f	0.58470	0.51950	-0.27740	5.3495	8.7818	-4.2691	1	1	1	2.654	-
cR	H(6A)f	1.07850	0.52080	-0.40030	9.6150	8.8038	-6.1605	1	1	1	2.654	-
cR	H(6B)f	1.75080	0.99750	-0.55750	15.3994	16.8621	-8.5798	1	1	1	2.654	-
d	Cu(1)g	-1.04108(4)	-0.26508(2)	-0.04931(2)	-8.2942(3)	-4.4810(3)	-0.7589(3)	1	1	1	3.455	Met
d	Cu(2)g	-0.66082(4)	-0.24358(2)	0.19199(2)	-5.7706(3)	-4.1175(3)	2.9547(3)	1	1	1	3.455	Met
d	Na(1)g	-0.62870(13)	0.15484(7)	0.06681(7)	-5.2276(11)	2.6175(12)	1.0282(11)	1	1	1	3.455	Met
d	Na(2)g	-1.66950(13)	0.13521(6)	0.28886(7)	-14.1343(11)	2.2856(10)	4.4455(11)	1	1	1	3.455	Met
d	O(1W)g	-1.9093(2)	0.11348(12)	0.35181(13)	-16.2132(16)	1.918(2)	5.414(2)	1	1	1	3.455	D/A
d	O(3W)g	-1.6832(3)	-0.00998(13)	0.26961(18)	-14.201(2)	-0.169(2)	4.149(3)	1	1	1	3.455	D/A
d	O(4W)g	-0.3966(3)	0.13127(15)	0.00353(15)	-3.210(2)	2.219(3)	0.054(2)	1	1	1	3.455	D/A
d	O(5W)g	-0.6583(4)	0.01494(17)	0.0611(2)	-5.454(3)	0.253(3)	0.940(3)	1	1	1	3.455	D/A

d	O(6W)g	-0.6893(2)	-0.18233(11)	0.30069(12)	-6.2468(16)	-3.0822(19)	4.6276(18)	1	1	1	3.455	D/A
d	O(7W)g	-1.0147(2)	-0.31534(11)	-0.16348(12)	-7.8225(16)	-5.3306(19)	-2.5159(18)	1	1	1	3.455	D/A
d	O(11A)g	-1.1300(2)	-0.19884(11)	0.03592(12)	-9.2052(16)	-3.3613(19)	0.5528(18)	1	1	1	3.455	D/A
d	O(11B)g	-0.8119(2)	-0.34295(12)	0.01144(13)	-6.5814(16)	-5.797(2)	0.176(2)	1	1	1	3.455	D/A
d	O(12A)g	-0.8840(2)	-0.18213(11)	0.12188(13)	-7.4137(16)	-3.0788(19)	1.876(2)	1	1	1	3.455	D/A
d	O(12B)g	-0.5794(2)	-0.31509(11)	0.10649(12)	-4.9195(16)	-5.3264(19)	1.6389(18)	1	1	1	3.455	D/A
d	O(21A)g	-1.5064(2)	-0.16066(11)	0.16844(13)	-12.5446(16)	-2.7159(19)	2.592(2)	1	1	1	3.455	D/A
d	O(21B)g	-0.4283(2)	-0.29498(11)	-0.07349(13)	-3.2917(16)	-4.9865(19)	-1.131(2)	1	1	1	3.455	D/A
d	O(22A)g	-1.2691(2)	-0.22636(11)	0.21500(13)	-10.7341(16)	-3.8265(19)	3.309(2)	1	1	1	3.455	D/A
d	O(22B)g	-0.1831(2)	-0.35198(11)	-0.02233(12)	-1.4278(16)	-5.9500(19)	-0.3437(18)	1	1	1	3.455	D/A
d	O(41A)g	-1.4578(2)	0.13806(11)	0.20266(12)	-12.2297(16)	2.3338(19)	3.1189(18)	1	1	1	3.455	D/A
d	O(42A)g	-1.2039(2)	0.17085(11)	0.26808(12)	-10.3279(16)	2.8881(19)	4.1257(18)	1	1	1	3.455	D/A
d	O(51A)g	-1.0912(2)	0.17665(11)	0.08376(12)	-9.0003(16)	2.9862(19)	1.2891(18)	1	1	1	3.455	D/A
d	O(52A)g	-0.8460(2)	0.13460(12)	0.15299(13)	-7.1774(16)	2.275(2)	2.354(2)	1	1	1	3.455	D/A
d	C(1A)g	-1.1044(3)	-0.09196(15)	0.13415(17)	-9.221(2)	-1.555(3)	2.065(3)	1	1	1	3.455	-
d	C(1B)g	-0.5771(3)	-0.42842(15)	0.01846(17)	-4.701(2)	-7.242(3)	0.284(3)	1	1	1	3.455	-
d	C(2A)g	-1.2533(3)	-0.09184(15)	0.17076(17)	-10.506(2)	-1.553(3)	2.628(3)	1	1	1	3.455	-
d	C(2B)g	-0.4268(3)	-0.42711(16)	-0.01676(17)	-3.408(2)	-7.220(3)	-0.258(3)	1	1	1	3.455	-
d	C(3A)g	-1.3150(3)	-0.01989(16)	0.19732(17)	-11.065(2)	-0.336(3)	3.037(3)	1	1	1	3.455	-
d	C(4A)g	-1.2326(3)	0.05090(15)	0.18754(17)	-10.377(2)	0.860(3)	2.886(3)	1	1	1	3.455	-
d	C(5A)g	-1.0851(3)	0.05085(15)	0.15006(17)	-9.101(2)	0.860(3)	2.309(3)	1	1	1	3.455	-
d	C(6A)g	-1.0224(3)	-0.02055(16)	0.12442(17)	-8.537(2)	-0.347(3)	1.915(3)	1	1	1	3.455	-
d	C(6B)g	-0.3517(3)	-0.49853(16)	-0.03422(17)	-2.762(2)	-8.427(3)	-0.527(3)	1	1	1	3.455	-
d	C(11A)g	-1.0315(3)	-0.16424(15)	0.09713(17)	-8.549(2)	-2.776(3)	1.495(3)	1	1	1	3.455	-
d	C(11B)g	-0.6651(3)	-0.35506(15)	0.04584(17)	-5.474(2)	-6.002(3)	0.705(3)	1	1	1	3.455	-
d	C(21A)g	-1.3471(3)	-0.16631(15)	0.18560(17)	-11.297(2)	-2.811(3)	2.856(3)	1	1	1	3.455	-
d	C(21B)g	-0.3437(3)	-0.35120(15)	-0.03919(17)	-2.686(2)	-5.937(3)	-0.603(3)	1	1	1	3.455	-
d	C(41A)g	-1.3049(3)	0.12491(15)	0.22010(17)	-11.035(2)	2.112(3)	3.387(3)	1	1	1	3.455	-
d	C(51A)g	-0.9984(3)	0.12596(15)	0.12961(17)	-8.355(2)	2.129(3)	1.995(3)	1	1	1	3.455	-
cR	H(3A)g	-1.41530	-0.01950	0.22260	-11.9318	-0.3296	3.4258	1	1	1	3.455	-
cR	H(6A)g	-0.92150	-0.02080	0.09970	-7.6663	-0.3516	1.5344	1	1	1	3.455	-
cR	H(6B)g	-0.24920	-0.49750	-0.05750	-1.8818	-8.4099	-0.8849	1	1	1	3.455	-
d	Cu(1)h	-1.04108(4)	0.73492(2)	-0.04931(2)	-8.2942(3)	12.4234(3)	-0.7589(3)	1	1	1	3.465	Met
d	Cu(2)h	-0.66082(4)	0.75642(2)	0.19199(2)	-5.7706(3)	12.7869(3)	2.9547(3)	1	1	1	3.465	Met
d	Na(1)h	-0.62870(13)	1.15484(7)	0.06681(7)	-5.2276(11)	19.5219(12)	1.0282(11)	1	1	1	3.465	Met
d	Na(2)h	-1.66950(13)	1.13521(6)	0.28886(7)	-14.1343(11)	19.1900(10)	4.4455(11)	1	1	1	3.465	Met
d	O(1W)h	-1.9093(2)	1.11348(12)	0.35181(13)	-16.2132(16)	18.823(2)	5.414(2)	1	1	1	3.465	D/A
d	O(3W)h	-1.6832(3)	0.99002(13)	0.26961(18)	-14.201(2)	16.736(2)	4.149(3)	1	1	1	3.465	D/A
d	O(4W)h	-0.3966(3)	1.13127(15)	0.00353(15)	-3.210(2)	19.123(3)	0.054(2)	1	1	1	3.465	D/A
d	O(5W)h	-0.6583(4)	1.01494(17)	0.0611(2)	-5.454(3)	17.157(3)	0.940(3)	1	1	1	3.465	D/A
d	O(6W)h	-0.6893(2)	0.81767(11)	0.30069(12)	-6.2468(16)	13.8222(19)	4.6276(18)	1	1	1	3.465	D/A
d	O(7W)h	-1.0147(2)	0.68466(11)	-0.16348(12)	-7.8225(16)	11.5738(19)	-2.5159(18)	1	1	1	3.465	D/A
d	O(11A)h	-1.1300(2)	0.80116(11)	0.03592(12)	-9.2052(16)	13.5431(19)	0.5528(18)	1	1	1	3.465	D/A
d	O(11B)h	-0.8119(2)	0.65705(12)	0.01144(13)	-6.5814(16)	11.107(2)	0.176(2)	1	1	1	3.465	D/A
d	O(12A)h	-0.8840(2)	0.81787(11)	0.12188(13)	-7.4137(16)	13.8256(19)	1.876(2)	1	1	1	3.465	D/A
d	O(12B)h	-0.5794(2)	0.68491(11)	0.10649(12)	-4.9195(16)	11.5780(19)	1.6389(18)	1	1	1	3.465	D/A

d	O(21A)h	-1.5064(2)	0.83934(11)	0.16844(13)	-12.5446(16)	14.1885(19)	2.592(2)	1	1	1	3.465	D/A
d	O(21B)h	-0.4283(2)	0.70502(11)	-0.07349(13)	-3.2917(16)	11.9179(19)	-1.131(2)	1	1	1	3.465	D/A
d	O(22A)h	-1.2691(2)	0.77364(11)	0.21500(13)	-10.7341(16)	13.0779(19)	3.309(2)	1	1	1	3.465	D/A
d	O(22B)h	-0.1831(2)	0.64802(11)	-0.02233(12)	-1.4278(16)	10.9544(19)	-0.3437(18)	1	1	1	3.465	D/A
d	O(41A)h	-1.4578(2)	1.13806(11)	0.20266(12)	-12.2297(16)	19.2382(19)	3.1189(18)	1	1	1	3.465	D/A
d	O(42A)h	-1.2039(2)	1.17085(11)	0.26808(12)	-10.3279(16)	19.7925(19)	4.1257(18)	1	1	1	3.465	D/A
d	O(51A)h	-1.0912(2)	1.17665(11)	0.08376(12)	-9.0003(16)	19.8906(19)	1.2891(18)	1	1	1	3.465	D/A
d	O(52A)h	-0.8460(2)	1.13460(12)	0.15299(13)	-7.1774(16)	19.180(2)	2.354(2)	1	1	1	3.465	D/A
d	C(1A)h	-1.1044(3)	0.90804(15)	0.13415(17)	-9.221(2)	15.350(3)	2.065(3)	1	1	1	3.465	-
d	C(1B)h	-0.5771(3)	0.57158(15)	0.01846(17)	-4.701(2)	9.662(3)	0.284(3)	1	1	1	3.465	-
d	C(2A)h	-1.2533(3)	0.90816(15)	0.17076(17)	-10.506(2)	15.352(3)	2.628(3)	1	1	1	3.465	-
d	C(2B)h	-0.4268(3)	0.57289(16)	-0.01676(17)	-3.408(2)	9.684(3)	-0.258(3)	1	1	1	3.465	-
d	C(3A)h	-1.3150(3)	0.98011(16)	0.19732(17)	-11.065(2)	16.568(3)	3.037(3)	1	1	1	3.465	-
d	C(4A)h	-1.2326(3)	1.05090(15)	0.18754(17)	-10.377(2)	17.765(3)	2.886(3)	1	1	1	3.465	-
d	C(5A)h	-1.0851(3)	1.05085(15)	0.15006(17)	-9.101(2)	17.764(3)	2.309(3)	1	1	1	3.465	-
d	C(6A)h	-1.0224(3)	0.97945(16)	0.12442(17)	-8.537(2)	16.557(3)	1.915(3)	1	1	1	3.465	-
d	C(6B)h	-0.3517(3)	0.50147(16)	-0.03422(17)	-2.762(2)	8.477(3)	-0.527(3)	1	1	1	3.465	-
d	C(11A)h	-1.0315(3)	0.83576(15)	0.09713(17)	-8.549(2)	14.128(3)	1.495(3)	1	1	1	3.465	-
d	C(11B)h	-0.6651(3)	0.64494(15)	0.04584(17)	-5.474(2)	10.902(3)	0.705(3)	1	1	1	3.465	-
d	C(21A)h	-1.3471(3)	0.83369(15)	0.18560(17)	-11.297(2)	14.093(3)	2.856(3)	1	1	1	3.465	-
d	C(21B)h	-0.3437(3)	0.64880(15)	-0.03919(17)	-2.686(2)	10.968(3)	-0.603(3)	1	1	1	3.465	-
d	C(41A)h	-1.3049(3)	1.12491(15)	0.22010(17)	-11.035(2)	19.016(3)	3.387(3)	1	1	1	3.465	-
d	C(51A)h	-0.9984(3)	1.12596(15)	0.12961(17)	-8.355(2)	19.034(3)	1.995(3)	1	1	1	3.465	-
cR	H(3A)h	-1.41530	0.98050	0.22260	-11.9318	16.5748	3.4258	1	1	1	3.465	-
cR	H(6A)h	-0.92150	0.97920	0.09970	-7.6663	16.5528	1.5344	1	1	1	3.465	-
cR	H(6B)h	-0.24920	0.50250	-0.05750	-1.8818	8.4945	-0.8849	1	1	1	3.465	-
d	Cu(1)i	-0.04108(4)	-0.26508(2)	-0.04931(2)	-0.2200(3)	-4.4810(3)	-0.7589(3)	1	1	1	3.555	Met
d	Cu(2)i	0.33918(4)	-0.24358(2)	0.19199(2)	2.3036(3)	-4.1175(3)	2.9547(3)	1	1	1	3.555	Met
d	Na(1)i	0.37130(13)	0.15484(7)	0.06681(7)	2.8466(11)	2.6175(12)	1.0282(11)	1	1	1	3.555	Met
d	Na(2)i	-0.66950(13)	0.13521(6)	0.28886(7)	-6.0601(11)	2.2856(10)	4.4455(11)	1	1	1	3.555	Met
d	O(1W)i	-0.9093(2)	0.11348(12)	0.35181(13)	-8.1390(16)	1.918(2)	5.414(2)	1	1	1	3.555	D/A
d	O(3W)i	-0.6832(3)	-0.00998(13)	0.26961(18)	-6.127(2)	-0.169(2)	4.149(3)	1	1	1	3.555	D/A
d	O(4W)i	0.6034(3)	0.13127(15)	0.00353(15)	4.864(2)	2.219(3)	0.054(2)	1	1	1	3.555	D/A
d	O(5W)i	0.3417(4)	0.01494(17)	0.0611(2)	2.621(3)	0.253(3)	0.940(3)	1	1	1	3.555	D/A
d	O(6W)i	0.3107(2)	-0.18233(11)	0.30069(12)	1.8274(16)	-3.0822(19)	4.6276(18)	1	1	1	3.555	D/A
d	O(7W)i	-0.0147(2)	-0.31534(11)	-0.16348(12)	0.2517(16)	-5.3306(19)	-2.5159(18)	1	1	1	3.555	D/A
d	O(11A)i	-0.1300(2)	-0.19884(11)	0.03592(12)	-1.1310(16)	-3.3613(19)	0.5528(18)	1	1	1	3.555	D/A
d	O(11B)i	0.1881(2)	-0.34295(12)	0.01144(13)	1.4928(16)	-5.797(2)	0.176(2)	1	1	1	3.555	D/A
d	O(12A)i	0.1160(2)	-0.18213(11)	0.12188(13)	0.6605(16)	-3.0788(19)	1.876(2)	1	1	1	3.555	D/A
d	O(12B)i	0.4206(2)	-0.31509(11)	0.10649(12)	3.1547(16)	-5.3264(19)	1.6389(18)	1	1	1	3.555	D/A
d	O(21A)i	-0.5064(2)	-0.16066(11)	0.16844(13)	-4.4704(16)	-2.7159(19)	2.592(2)	1	1	1	3.555	D/A
d	O(21B)i	0.5717(2)	-0.29498(11)	-0.07349(13)	4.7825(16)	-4.9865(19)	-1.131(2)	1	1	1	3.555	D/A
d	O(22A)i	-0.2691(2)	-0.22636(11)	0.21500(13)	-2.6599(16)	-3.8265(19)	3.309(2)	1	1	1	3.555	D/A
d	O(22B)i	0.8169(2)	-0.35198(11)	-0.02233(12)	6.6464(16)	-5.9500(19)	-0.3437(18)	1	1	1	3.555	D/A
d	O(41A)i	-0.4578(2)	0.13806(11)	0.20266(12)	-4.1555(16)	2.3338(19)	3.1189(18)	1	1	1	3.555	D/A
d	O(42A)i	-0.2039(2)	0.17085(11)	0.26808(12)	-2.2537(16)	2.8881(19)	4.1257(18)	1	1	1	3.555	D/A

d	O(51A)i	-0.0912(2)	0.17665(11)	0.08376(12)	-0.9261(16)	2.9862(19)	1.2891(18)	1	1	1	3.555	D/A
d	O(52A)i	0.1540(2)	0.13460(12)	0.15299(13)	0.8968(16)	2.275(2)	2.354(2)	1	1	1	3.555	D/A
d	C(1A)i	-0.1044(3)	-0.09196(15)	0.13415(17)	-1.147(2)	-1.555(3)	2.065(3)	1	1	1	3.555	-
d	C(1B)i	0.4229(3)	-0.42842(15)	0.01846(17)	3.373(2)	-7.242(3)	0.284(3)	1	1	1	3.555	-
d	C(2A)i	-0.2533(3)	-0.09184(15)	0.17076(17)	-2.432(2)	-1.553(3)	2.628(3)	1	1	1	3.555	-
d	C(2B)i	0.5732(3)	-0.42711(16)	-0.01676(17)	4.666(2)	-7.220(3)	-0.258(3)	1	1	1	3.555	-
d	C(3A)i	-0.3150(3)	-0.01989(16)	0.19732(17)	-2.990(2)	-0.336(3)	3.037(3)	1	1	1	3.555	-
d	C(4A)i	-0.2326(3)	0.05090(15)	0.18754(17)	-2.303(2)	0.860(3)	2.886(3)	1	1	1	3.555	-
d	C(5A)i	-0.0851(3)	0.05085(15)	0.15006(17)	-1.027(2)	0.860(3)	2.309(3)	1	1	1	3.555	-
d	C(6A)i	-0.0224(3)	-0.02055(16)	0.12442(17)	-0.463(2)	-0.347(3)	1.915(3)	1	1	1	3.555	-
d	C(6B)i	0.6483(3)	-0.49853(16)	-0.03422(17)	5.312(2)	-8.427(3)	-0.527(3)	1	1	1	3.555	-
d	C(11A)i	-0.0315(3)	-0.16424(15)	0.09713(17)	-0.474(2)	-2.776(3)	1.495(3)	1	1	1	3.555	-
d	C(11B)i	0.3349(3)	-0.35506(15)	0.04584(17)	2.600(2)	-6.002(3)	0.705(3)	1	1	1	3.555	-
d	C(21A)i	-0.3471(3)	-0.16631(15)	0.18560(17)	-3.223(2)	-2.811(3)	2.856(3)	1	1	1	3.555	-
d	C(21B)i	0.6563(3)	-0.35120(15)	-0.03919(17)	5.388(2)	-5.937(3)	-0.603(3)	1	1	1	3.555	-
d	C(41A)i	-0.3049(3)	0.12491(15)	0.22010(17)	-2.961(2)	2.112(3)	3.387(3)	1	1	1	3.555	-
d	C(51A)i	0.0016(3)	0.12596(15)	0.12961(17)	-0.281(2)	2.129(3)	1.995(3)	1	1	1	3.555	-
cR	H(3A)i	-0.41530	-0.01950	0.22260	-3.8576	-0.3296	3.4258	1	1	1	3.555	-
cR	H(6A)i	0.07850	-0.02080	0.09970	0.4079	-0.3516	1.5344	1	1	1	3.555	-
cR	H(6B)i	0.75080	-0.49750	-0.05750	6.1924	-8.4099	-0.8849	1	1	1	3.555	-
d	Cu(1)j	-0.95892(4)	-0.76508(2)	0.54931(2)	-8.9871(3)	-12.9332(3)	8.4538(3)	1	1	1	4.445	Met
d	Cu(2)j	-1.33918(4)	-0.74358(2)	0.30801(2)	-11.5107(3)	-12.5697(3)	4.7402(3)	1	1	1	4.445	Met
d	Na(1)j	-1.37130(13)	-0.34516(7)	0.43319(7)	-12.0536(11)	-5.8347(12)	6.6667(11)	1	1	1	4.445	Met
d	Na(2)j	-0.33050(13)	-0.36479(6)	0.21114(7)	-3.1469(11)	-6.1666(10)	3.2494(11)	1	1	1	4.445	Met
d	O(1W)j	-0.0907(2)	-0.38652(12)	0.14819(13)	-1.0681(16)	-6.534(2)	2.281(2)	1	1	1	4.445	D/A
d	O(3W)j	-0.3168(3)	-0.50998(13)	0.23039(18)	-3.080(2)	-8.621(2)	3.546(3)	1	1	1	4.445	D/A
d	O(4W)j	-1.6034(3)	-0.36873(15)	0.49647(15)	-14.071(2)	-6.233(3)	7.641(2)	1	1	1	4.445	D/A
d	O(5W)j	-1.3417(4)	-0.48506(17)	0.4389(2)	-11.828(3)	-8.200(3)	6.755(3)	1	1	1	4.445	D/A
d	O(6W)j	-1.3107(2)	-0.68233(11)	0.19931(12)	-11.0344(16)	-11.5344(19)	3.0673(18)	1	1	1	4.445	D/A
d	O(7W)j	-0.9853(2)	-0.81534(11)	0.66348(12)	-9.4588(16)	-13.7828(19)	10.2108(18)	1	1	1	4.445	D/A
d	O(11A)j	-0.8700(2)	-0.69884(11)	0.46408(12)	-8.0760(16)	-11.8135(19)	7.1421(18)	1	1	1	4.445	D/A
d	O(11B)j	-1.1881(2)	-0.84295(12)	0.48856(13)	-10.6999(16)	-14.250(2)	7.519(2)	1	1	1	4.445	D/A
d	O(12A)j	-1.1160(2)	-0.68213(11)	0.37812(13)	-9.8675(16)	-11.5310(19)	5.819(2)	1	1	1	4.445	D/A
d	O(12B)j	-1.4206(2)	-0.81509(11)	0.39351(12)	-12.3618(16)	-13.7786(19)	6.0560(18)	1	1	1	4.445	D/A
d	O(21A)j	-0.4936(2)	-0.66066(11)	0.33156(13)	-4.7366(16)	-11.1681(19)	5.103(2)	1	1	1	4.445	D/A
d	O(21B)j	-1.5717(2)	-0.79498(11)	0.57349(13)	-13.9896(16)	-13.4387(19)	8.826(2)	1	1	1	4.445	D/A
d	O(22A)j	-0.7309(2)	-0.72636(11)	0.28500(13)	-6.5472(16)	-12.2787(19)	4.386(2)	1	1	1	4.445	D/A
d	O(22B)j	-1.8169(2)	-0.85198(11)	0.52233(12)	-15.8535(16)	-14.4022(19)	8.0386(18)	1	1	1	4.445	D/A
d	O(41A)j	-0.5422(2)	-0.36194(11)	0.29734(12)	-5.0515(16)	-6.1184(19)	4.5760(18)	1	1	1	4.445	D/A
d	O(42A)j	-0.7961(2)	-0.32915(11)	0.23192(12)	-6.9533(16)	-5.5641(19)	3.5692(18)	1	1	1	4.445	D/A
d	O(51A)j	-0.9088(2)	-0.32335(11)	0.41624(12)	-8.2809(16)	-5.4660(19)	6.4059(18)	1	1	1	4.445	D/A
d	O(52A)j	-1.1540(2)	-0.36540(12)	0.34701(13)	-10.1039(16)	-6.177(2)	5.340(2)	1	1	1	4.445	D/A
d	C(1A)j	-0.8956(3)	-0.59196(15)	0.36585(17)	-8.060(2)	-10.007(3)	5.630(3)	1	1	1	4.445	-
d	C(1B)j	-1.4229(3)	-0.92842(15)	0.48154(17)	-12.580(2)	-15.694(3)	7.411(3)	1	1	1	4.445	-
d	C(2A)j	-0.7467(3)	-0.59184(15)	0.32924(17)	-6.775(2)	-10.005(3)	5.067(3)	1	1	1	4.445	-
d	C(2B)j	-1.5732(3)	-0.92711(16)	0.51676(17)	-13.873(2)	-15.672(3)	7.953(3)	1	1	1	4.445	-

d	C(3A)j	-0.6850(3)	-0.51989(16)	0.30268(17)	-6.217(2)	-8.788(3)	4.658(3)	1	1	1	4.445	-
d	C(4A)j	-0.7674(3)	-0.44910(15)	0.31246(17)	-6.904(2)	-7.592(3)	4.809(3)	1	1	1	4.445	-
d	C(5A)j	-0.9149(3)	-0.44915(15)	0.34994(17)	-8.180(2)	-7.593(3)	5.386(3)	1	1	1	4.445	-
d	C(6A)j	-0.9776(3)	-0.52055(16)	0.37558(17)	-8.744(2)	-8.800(3)	5.780(3)	1	1	1	4.445	-
d	C(6B)j	-1.6483(3)	-0.99853(16)	0.53422(17)	-14.519(2)	-16.880(3)	8.222(3)	1	1	1	4.445	-
d	C(11A)j	-0.9685(3)	-0.66424(15)	0.40287(17)	-8.733(2)	-11.229(3)	6.200(3)	1	1	1	4.445	-
d	C(11B)j	-1.3349(3)	-0.85506(15)	0.45416(17)	-11.807(2)	-14.454(3)	6.989(3)	1	1	1	4.445	-
d	C(21A)j	-0.6529(3)	-0.66631(15)	0.31440(17)	-5.984(2)	-11.264(3)	4.839(3)	1	1	1	4.445	-
d	C(21B)j	-1.6563(3)	-0.85120(15)	0.53919(17)	-14.595(2)	-14.389(3)	8.298(3)	1	1	1	4.445	-
d	C(41A)j	-0.6951(3)	-0.37509(15)	0.27990(17)	-6.247(2)	-6.341(3)	4.308(3)	1	1	1	4.445	-
d	C(51A)j	-1.0016(3)	-0.37404(15)	0.37039(17)	-8.926(2)	-6.323(3)	5.700(3)	1	1	1	4.445	-
cR	H(3A)j	-0.58470	-0.51950	0.27740	-5.3495	-8.7818	4.2691	1	1	1	4.445	-
cR	H(6A)j	-1.07850	-0.52080	0.40030	-9.6150	-8.8038	6.1605	1	1	1	4.445	-
cR	H(6B)j	-1.75080	-0.99750	0.55750	-15.3994	-16.8621	8.5798	1	1	1	4.445	-

 =====
 ***** Residue = 2 *****
 =====

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site SSN*SSOF =		S.O.F	Move	Type
d	O(2W)	-0.0156(3)	0.46199(13)	0.11565(15)	-0.388(2)	7.810(2)	1.780(2)	1	1	1	-	D/A

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)	
a =[1455.01]	= -1+x, y, z	= [	1	-1	0	0	1	-1	0	0
b =[1655.01]	= 1+x, y, z	= [	1	1	0	0	1	1	0	0
c =[2544.01]	= -x, -1/2+y, -1/2-z	= [	2	0	-1	-1	1	0	-1/2	-1/2
d =[2554.01]	= -x, 1/2+y, -1/2-z	= [	2	0	0	-1	1	0	1/2	-1/2
e =[2644.01]	= 1-x, -1/2+y, -1/2-z	= [	2	1	-1	-1	1	1	-1/2	-1/2
f =[2654.01]	= 1-x, 1/2+y, -1/2-z	= [	2	1	0	-1	1	1	1/2	-1/2
g =[3455.01]	= -1-x, -y, -z	= [	3	-1	0	0	1	-1	0	0
h =[3465.01]	= -1-x, 1-y, -z	= [	3	-1	1	0	1	-1	1	0
i =[3555.01]	= -x, -y, -z	= [	3	0	0	0	1	0	0	0
j =[4445.01]	= -1+x, -1/2-y, 1/2+z	= [	4	-1	-1	0	1	-1	-1/2	1/2

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

$X(J) = X(sym) + TX$, $Y(J) = Y(sym) + TY$, $Z(J) = Z(sym) + TZ$,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

:: Starred ARUs belong (chemically) to the previous ARU

:: Analysis of Polymeric Structure(s)

:: Resd # 1 - Infinite Three-Dimensional Framework :: Det = 1, Base Vectors: #1 = [0 1 0], #2 = [1 0 0], #3 = [0 0 1],

Ordered Structure							Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)					
Resd Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	H	Cu	Na	O	
1	1	-0.495	-0.244	0.002	644.25	1	4	15	3	2	2	18
2	1	-0.016	0.462	0.116	16.00	1	4	-	-	-	-	1

Unit Cell Weight = 2641.02 60 12 8 8 76

Calculated Analysis (Percent) = 27.3 0.5 19.3 7.0 46.0

Moiety_Formula = C15 H3 Cu2 Na2 O18, 0

Sum_Formula = C15 H3 Cu2 Na2 O19

Formula_Weight = 660.25 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 4

SpaceGroup_Z = 4 ==> Z' = 4 / 4 = 1.000

Calculated Density = 2.0878(1) g cm-3 [= Mg m-3]

F(000) = 1300.0 [1303.63]

mu(MoKa) = 21.68 cm-1 = 2.168 mm-1

Resonant Scattering = 4.15 Percent - (E. Girard et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 2182.0[2143.7] Ang**3, 298[113]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)

** WARNING **

Please Check the Derived Crystal Data.
They may be Incorrect for Disordered,
Incomplete or Polymeric Structures.

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f, f' & f''

=====

(An)isotropic, Equivalent and Main Axes Displacement Parameters - Unusual Values Marked with a # - [Optional Coordinate Split-up]

=====

Residue = 1

=====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Cu1	0.00545(15)	0.00382(16)	0.00751(17)	-0.00060(12)	0.00243(12)	-0.00138(11)	0.00545(9)	0.0030	0.0050	0.0084	2.82
		[0.0450	0.2647	0.0508]	[0.0371	0.2654	0.0478]					
2	Cu2	0.00407(15)	0.00371(16)	0.00815(17)	-0.00013(12)	0.00145(11)	-0.00085(11)	0.00525(9)	0.0030	0.0046	0.0082	2.76
		[-0.3369	0.2435	-0.1898]	[-0.3415	0.2437	-0.1941]					
3	Na1	0.0081(5)	0.0144(6)	0.0137(6)	0.0005(5)	0.0005(4)	0.0006(4)	0.0122(3)	0.0080	0.0139	0.0147	1.84
		[-0.3708	-0.1533	-0.0657]	[-0.3718	-0.1564	-0.0680]					
4	Na2	0.0076(5)	0.0111(5)	0.0136(6)	0.0011(4)	0.0028(4)	0.0004(4)	0.0106(3)	0.0071	0.0107	0.0141	1.98
		[0.6720	-0.1346	-0.2870]	[0.6670	-0.1358	-0.2908]					
5	O1W	0.0098(9)	0.0144(10)	0.0128(10)	0.0006(8)	0.0020(8)	-0.0002(7)	0.0123(6)	0.0097	0.0126	0.0146	1.51
		[0.9094	-0.1122	-0.3513]	[0.9092	-0.1147	-0.3523]					
6	O3W	0.0152(11)	0.0146(11)	0.0475(16)	-0.0002(11)	0.0084(10)	0.0041(9)	0.0254(7)	0.0101	0.0185	0.0476	4.71
		[0.6902	0.0100	-0.2624]	[0.6762	0.0100	-0.2768]					
7	O4W	0.0116(10)	0.0430(15)	0.0168(11)	0.0042(10)	0.0022(9)	0.0004(10)	0.0238(7)	0.0115	0.0162	0.0437	3.78
		[-0.6027	-0.1254	-0.0024]	[-0.6041	-0.1372	-0.0046]					
8	O5W	0.0408(17)	0.0317(15)	0.0474(18)	-0.0009(13)	0.0039(14)	-0.0023(12)	0.0402(10)	0.0311	0.0409	0.0487	1.57
		[-0.3436	-0.0149	-0.0586]	[-0.3398	-0.0149	-0.0636]					
9	O6W	0.0094(4)						0.0094(4)				
10	O7W	0.0091(4)						0.0091(4)				
11	O11A	0.0075(8)	0.0070(9)	0.0092(9)	-0.0035(7)	0.0012(7)	-0.0009(7)	0.0079(5)	0.0044	0.0076	0.0118	2.69
		[0.1321	0.1975	-0.0337]	[0.1279	0.2002	-0.0381]					
12	O11B	0.0070(9)	0.0105(9)	0.0161(10)	-0.0022(8)	-0.0018(7)	0.0029(7)	0.0116(5)	0.0052	0.0102	0.0192	3.67
		[-0.1915	0.3417	-0.0081]	[-0.1847	0.3442	-0.0148]					
13	O12A	0.0077(9)	0.0112(9)	0.0148(10)	0.0000(8)	-0.0018(7)	0.0042(7)	0.0116(5)	0.0045	0.0127	0.0175	3.90
		[-0.1207	0.1810	-0.1190]	[-0.1113	0.1832	-0.1247]					
14	O12B	0.0074(9)	0.0068(9)	0.0098(9)	-0.0027(7)	0.0006(7)	-0.0017(7)	0.0081(5)	0.0044	0.0084	0.0114	2.57
		[-0.4189	0.3140	-0.1042]	[-0.4223	0.3162	-0.1087]					
15	O21A	0.0061(9)	0.0061(9)	0.0139(10)	0.0000(7)	0.0026(7)	-0.0018(7)	0.0086(5)	0.0041	0.0077	0.0139	3.41
		[0.5099	0.1606	-0.1652]	[0.5029	0.1607	-0.1717]					
16	O21B	0.0094(9)	0.0070(9)	0.0132(10)	0.0017(8)	-0.0010(7)	-0.0006(7)	0.0101(5)	0.0066	0.0084	0.0154	2.35
		[-0.5746	0.2954	0.0756]	[-0.5688	0.2945	0.0714]					
17	O22A	0.0097(9)	0.0055(9)	0.0122(10)	0.0016(7)	-0.0006(7)	-0.0001(7)	0.0094(5)	0.0051	0.0088	0.0141	2.75
		[0.2657	0.2267	-0.2128]	[0.2725	0.2260	-0.2172]					
18	O22B	0.0048(8)	0.0058(9)	0.0136(10)	0.0005(7)	0.0015(7)	-0.0015(7)	0.0081(5)	0.0036	0.0069	0.0137	3.80
		[-0.8148	0.3522	0.0260]	[-0.8190	0.3517	0.0187]					
19	O41A	0.0056(9)	0.0097(9)	0.0114(10)	-0.0002(7)	0.0013(7)	0.0018(7)	0.0089(5)	0.0049	0.0103	0.0115	2.37
		[0.4585	-0.1386	-0.2003]	[0.4571	-0.1376	-0.2050]					

20	O42A	0.0064(8)	0.0048(9)	0.0103(9)	-0.0016(7)	0.0014(7)	0.0007(7)	0.0072(5)	0.0040	0.0067	0.0108	2.67
		[0.2052	-0.1714	-0.2656]	[0.2026	-0.1703	-0.2706]					
21	O51A	0.0086(9)	0.0052(9)	0.0113(10)	0.0019(7)	0.0024(7)	-0.0006(7)	0.0083(5)	0.0044	0.0085	0.0119	2.73
		[0.0944	-0.1761	-0.0814]	[0.0880	-0.1772	-0.0861]					
22	O52A	0.0070(9)	0.0112(10)	0.0164(10)	0.0007(8)	-0.0005(8)	-0.0036(7)	0.0118(6)	0.0049	0.0125	0.0178	3.65
		[-0.1564	-0.1336	-0.1494]	[-0.1516	-0.1356	-0.1566]					
23	C1A	0.0057(11)	0.0056(12)	0.0068(12)	-0.0001(10)	-0.0007(9)	0.0004(9)	0.0062(7)	0.0047	0.0056	0.0083	1.77
		[0.1024	0.0918	-0.1333]	[0.1064	0.0921	-0.1350]					
24	C1B	0.0058(11)	0.0073(12)	0.0067(12)	-0.0004(10)	0.0008(9)	0.0004(9)	0.0066(7)	0.0057	0.0065	0.0076	1.34
		[-0.4224	0.4290	-0.0188]	[-0.4234	0.4278	-0.0181]					
25	C2A	0.0064(11)	0.0061(12)	0.0086(12)	0.0008(10)	-0.0005(9)	-0.0015(9)	0.0072(7)	0.0047	0.0065	0.0103	2.18
		[0.2507	0.0924	-0.1694]	[0.2559	0.0913	-0.1721]					
26	C2B	0.0056(11)	0.0077(12)	0.0068(12)	-0.0008(10)	-0.0009(9)	-0.0015(9)	0.0069(7)	0.0039	0.0081	0.0087	2.24
		[-0.5763	0.4279	0.0174]	[-0.5701	0.4263	0.0161]					
27	C3A	0.0055(11)	0.0089(13)	0.0082(12)	-0.0002(10)	0.0014(9)	-0.0003(9)	0.0075(7)	0.0053	0.0082	0.0090	1.68
		[0.3142	0.0211	-0.1977]	[0.3158	0.0187	-0.1969]					
28	C4A	0.0058(11)	0.0059(12)	0.0067(12)	-0.0008(10)	-0.0011(9)	0.0003(9)	0.0063(7)	0.0044	0.0057	0.0089	2.02
		[0.2301	-0.0512	-0.1865]	[0.2351	-0.0506	-0.1886]					
29	C5A	0.0059(11)	0.0065(12)	0.0057(12)	0.0007(10)	0.0000(9)	-0.0018(9)	0.0061(7)	0.0044	0.0053	0.0087	1.98
		[0.0824	-0.0501	-0.1496]	[0.0878	-0.0516	-0.1505]					
30	C6A	0.0059(11)	0.0088(13)	0.0091(12)	0.0002(10)	0.0014(10)	-0.0003(9)	0.0079(7)	0.0058	0.0087	0.0092	1.60
		[0.0232	0.0210	-0.1233]	[0.0216	0.0201	-0.1256]					
31	C6B	0.0053(11)	0.0089(12)	0.0064(12)	-0.0005(10)	-0.0002(9)	0.0004(9)	0.0070(7)	0.0048	0.0070	0.0091	1.91
		[-0.6473	0.4999	0.0338]	[-0.6493	0.4971	0.0347]					
32	C11A	0.0071(11)	0.0037(11)	0.0075(12)	0.0015(9)	0.0024(9)	-0.0013(9)	0.0060(7)	0.0023	0.0070	0.0085	3.63
		[0.0365	0.1644	-0.0956]	[0.0265	0.1641	-0.0987]					
33	C11B	0.0070(12)	0.0053(12)	0.0082(12)	0.0020(10)	0.0028(9)	-0.0010(9)	0.0067(7)	0.0032	0.0073	0.0095	3.02
		[-0.3308	0.3556	-0.0440]	[-0.3390	0.3545	-0.0477]					
34	C21A	0.0068(11)	0.0068(12)	0.0051(12)	-0.0018(9)	0.0014(9)	-0.0023(9)	0.0062(7)	0.0038	0.0052	0.0095	2.50
		[0.3431	0.1673	-0.1862]	[0.3511	0.1654	-0.1850]					
35	C21B	0.0062(11)	0.0065(12)	0.0078(12)	-0.0026(10)	0.0010(9)	-0.0011(9)	0.0068(7)	0.0042	0.0064	0.0099	2.32
		[-0.6542	0.3501	0.0408]	[-0.6584	0.3523	0.0375]					
36	C41A	0.0085(12)	0.0055(12)	0.0060(12)	0.0008(9)	0.0028(9)	-0.0003(9)	0.0065(7)	0.0042	0.0061	0.0092	2.19
		[0.3088	-0.1249	-0.2195]	[0.3010	-0.1249	-0.2207]					
37	C51A	0.0075(12)	0.0062(12)	0.0072(12)	-0.0019(10)	0.0026(9)	-0.0017(9)	0.0068(7)	0.0047	0.0056	0.0101	2.15
		[0.0020	-0.1266	-0.1287]	[-0.0052	-0.1254	-0.1305]					
38	H3A	0.00900						0.00900				
39	H6A	0.01000						0.01000				
40	H6B	0.00800						0.00800				
U(i,j)-Average		0.0081	0.0093	0.0122	-0.0001	0.0012	-0.0003	0.0099	0.0080	0.0094	0.0123	1.52

 =====
 ***** Residue = 2 *****
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	O2W	0.0252(12)	0.0131(11)	0.0250(12)	-0.0001(9)	-0.0010(10)	0.0039(9)	0.0216(7)	0.0119	0.0217	0.0311	2.61
		[-0.0086	0.4624	0.1138]	[-0.0226	0.4616	0.1175]					
U(i,j)-Average		0.0252	0.0131	0.0250	-0.0001	-0.0010	0.0039	0.0216	0.0119	0.0217	0.0311	2.61

=====
 The Displacement Factor has the Form of $\text{Exp}(-T)$

where

$T = 8 * (\pi^2) * U_{iso} * \sin(\theta / \lambda)^2$, for Isotropic Atoms,

$T = 2 * (\pi^2) * (U_{11} * (h^2) + U_{22} * (k^2) + U_{33} * (l^2) + 2 * U_{23} * k * l + 2 * U_{13} * h * l + 2 * U_{12} * h * k)$, for Anisotr. Atoms

$U_{eq} = 1/3 \text{ Sum}(i,j) (U_{ij} * a(i) * a(j) * \sin(\theta_{ij}))$

U1, U2, U3 are the three Main Axes Components of U_{ij}

Reference U(eq): R.X. Fischer & E. Tillmanns, Acta Cryst. (1988). C44, 775-776

Ueq [or U(iso)] Averages per Element

	Non-H	C	H	Cu	Na	O
Average	0.0102	0.0067	0.0090	0.0054	0.0114	0.0133
Minimum	0.0052	0.0060	0.0080	0.0052	0.0106	0.0072
Maximum	0.0402	0.0079	0.0100	0.0055	0.0122	0.0402
Ratio	7.6571	1.3167	1.2500	1.0381	1.1509	5.5833
Number	38	15	3	2	2	19

 =====
 ***** Residue = 1 *****
 =====

:: No TLS-Analysis for Polymeric or Disordered Structures

Rigid-Body Model Libration Corrections for Bond Distances and "Hirshfeld Rigid-Bond" Test (Acta Cryst, (1976), A32, 239-244)

Bond		Bond Distance		Components of the Correction			Vibration Along the Interatomic Bond				Angle with Lib. Axes		
Atom(I)	Atom(J)	Obsd	Calcd	Del(L)	Del(M)	Del(N)	I to J	J to I	Difference	Sqrt(Diff)	L(1)	L(2)	L(3)
Cu(1)	- O(11A)	1.9505	0	0	0	0	0.0051(2)	0.0057(9)	0.0006(9)	0.0238	0.00	0.00	0.00
Cu(1)	- O(11B)	2.3539	0	0	0	0	0.0071(2)	0.0060(9)	0.0012(9)	0.0340	0.00	0.00	0.00
Cu(1)	- O(22B)b	1.9466	0	0	0	0	0.0031(2)	0.0042(9)	0.0012(9)	0.0343	0.00	0.00	0.00
Cu(1)	- O(51A)i	1.9568	0	0	0	0	0.0031(2)	0.0049(9)	0.0017(9)	0.0418	0.00	0.00	0.00
Cu(2)	- O(12A)	2.2233	0	0	0	0	0.0057(2)	0.0049(9)	0.0008(9)	0.0282	0.00	0.00	0.00
Cu(2)	- O(12B)	1.9792	0	0	0	0	0.0059(2)	0.0073(9)	0.0014(9)	0.0369	0.00	0.00	0.00
Cu(2)	- O(21A)a	1.9459	0	0	0	0	0.0031(2)	0.0043(9)	0.0012(9)	0.0348	0.00	0.00	0.00
Cu(2)	- O(42A)d	1.9670	0	0	0	0	0.0034(2)	0.0044(9)	0.0009(9)	0.0306	0.00	0.00	0.00
O(11A)	- C(11A)	1.2887	0	0	0	0	0.0057(9)	0.0078(11)	0.0021(14)	0.0456	0.00	0.00	0.00
O(11B)	- C(11B)	1.2444	0	0	0	0	0.0057(9)	0.0081(12)	0.0024(15)	0.0486	0.00	0.00	0.00
O(12A)	- C(11A)	1.2347	0	0	0	0	0.0053(9)	0.0078(11)	0.0025(15)	0.0504	0.00	0.00	0.00
O(12B)	- C(11B)	1.2788	0	0	0	0	0.0053(9)	0.0090(12)	0.0037(15)	0.0609	0.00	0.00	0.00
O(21A)	- C(21A)	1.2786	0	0	0	0	0.0066(9)	0.0072(12)	0.0006(15)	0.0243	0.00	0.00	0.00
O(21B)	- C(21B)	1.2443	0	0	0	0	0.0072(9)	0.0088(12)	0.0016(15)	0.0406	0.00	0.00	0.00
O(22A)	- C(21A)	1.2459	0	0	0	0	0.0059(9)	0.0093(12)	0.0035(15)	0.0588	0.00	0.00	0.00
O(22B)	- C(21B)	1.2851	0	0	0	0	0.0050(9)	0.0062(12)	0.0013(15)	0.0359	0.00	0.00	0.00
O(41A)	- C(41A)	1.2448	0	0	0	0	0.0052(9)	0.0087(12)	0.0035(15)	0.0590	0.00	0.00	0.00
O(42A)	- C(41A)	1.2837	0	0	0	0	0.0065(9)	0.0079(12)	0.0014(15)	0.0373	0.00	0.00	0.00
O(51A)	- C(51A)	1.2840	0	0	0	0	0.0075(9)	0.0099(12)	0.0025(15)	0.0499	0.00	0.00	0.00
O(52A)	- C(51A)	1.2399	0	0	0	0	0.0060(10)	0.0075(12)	0.0014(15)	0.0376	0.00	0.00	0.00
C(1A)	- C(2A)	1.4033	0	0	0	0	0.0075(12)	0.0085(12)	0.0009(16)	0.0304	0.00	0.00	0.00
C(1A)	- C(6A)	1.3956	0	0	0	0	0.0063(12)	0.0078(12)	0.0015(17)	0.0381	0.00	0.00	0.00
C(1A)	- C(11A)	1.5066	0	0	0	0	0.0061(12)	0.0064(11)	0.0003(16)	0.0181	0.00	0.00	0.00
C(1B)	- C(2B)	1.4025	0	0	0	0	0.0061(12)	0.0076(12)	0.0015(16)	0.0382	0.00	0.00	0.00
C(1B)	- C(11B)	1.5206	0	0	0	0	0.0064(12)	0.0074(12)	0.0010(17)	0.0316	0.00	0.00	0.00
C(1B)	- C(6B)h	1.3988	0	0	0	0	0.0075(12)	0.0089(12)	0.0014(16)	0.0372	0.00	0.00	0.00
C(2A)	- C(3A)	1.3993	0	0	0	0	0.0084(12)	0.0083(12)	0.0001(17)	0.0083	0.00	0.00	0.00
C(2A)	- C(21A)	1.5042	0	0	0	0	0.0050(12)	0.0053(12)	0.0002(16)	0.0156	0.00	0.00	0.00
C(2B)	- C(6B)	1.3954	0	0	0	0	0.0085(12)	0.0078(12)	0.0008(16)	0.0277	0.00	0.00	0.00
C(2B)	- C(21B)	1.5122	0	0	0	0	0.0069(12)	0.0069(12)	0.0001(16)	0.0075	0.00	0.00	0.00
C(3A)	- C(4A)	1.3883	0	0	0	0	0.0078(12)	0.0068(12)	0.0010(17)	0.0323	0.00	0.00	0.00
C(4A)	- C(5A)	1.4002	0	0	0	0	0.0080(12)	0.0067(12)	0.0013(16)	0.0363	0.00	0.00	0.00
C(4A)	- C(41A)	1.4996	0	0	0	0	0.0059(12)	0.0062(12)	0.0003(17)	0.0164	0.00	0.00	0.00
C(5A)	- C(6A)	1.3896	0	0	0	0	0.0083(12)	0.0086(12)	0.0004(17)	0.0193	0.00	0.00	0.00
C(5A)	- C(51A)	1.5061	0	0	0	0	0.0047(12)	0.0056(12)	0.0009(17)	0.0299	0.00	0.00	0.00
C(6B)	- C(1B)h	1.3988	0	0	0	0	0.0089(12)	0.0075(12)	0.0014(16)	0.0372	0.00	0.00	0.00

$$\text{Sqrt}(\text{Sum}(\text{DelIJ}^2)/\text{Nrb}) = 0.0017$$

- Indicates bonds exceeding the 5.0 sigma test level

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Analysis of Bond Distance and Angle Values - Identification of Chiral Center(s) and Their (R/S)-Configuration (Cahn-Ingold-Prelog)

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The Following Tests are done. Faults are Marked Under Note

- V : Valency Check Fault for H, C
- S : Bond Too Short
- A : Unusual Bond Angle Values (PLEASE CHECK)

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*** PLEASE NOTE: R/S ASSIGNMENTS ARE TENTATIVE *** (CIP Special rules NOT Implemented)

*** See Angew.Chem.Intern. Ed. Eng., (1966), 5, 385 & (1982), 21, 567 for Authoritative Details for Special Cases

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 ***** Residue = 1 *****
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Flag Label - Connected to (May be Incomplete for Polymeric Structures)										=A.N.G.L.E.S=				=B.O.N.D.S=							
										nra	min	max	Aver	min	max	nrb	tnr	Hyb	RS	Note	
d	Cu(1)	- O(7W)	O(11A)	O(11B)	O(22B)b	O(51A)i	O(52A)i	-----	-----	-----	15	52	176	104.3	1.947	2.805	6	522			
d	Cu(2)	- O(6W)	O(12A)	O(12B)	O(21A)a	O(41A)d	O(42A)d	-----	-----	-----	15	55	172	104.3	1.946	2.674	6	523			
d	Na(1)	- O(4W)	O(5W)	O(52A)	O(41A)a	O(21B)g	O(11A)i	-----	-----	-----	15	78	175	105.1	2.275	2.449	6	507			
d	Na(2)	- O(1W)	O(3W)	O(41A)	O(52A)b	O(12B)c	O(22A)e	-----	-----	-----	15	77	167	104.4	2.322	2.538	6	505			
d	O(1W)	- Na(2)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	391	sp2		
d	O(3W)	- Na(2)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	391	sp2		
d	O(4W)	- Na(1)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	396	sp2		
d	O(5W)	- Na(1)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	396	sp2		
d	O(6W)	- Cu(2)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	457	sp2		
d	O(7W)	- Cu(1)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	451	sp2		
d	O(11A)	- Cu(1)	C(11A)	Na(1)i	-----	-----	-----	-----	-----	-----	3	94	134	116.2	1.289	2.449	3	456			
d	O(11B)	- Cu(1)	C(11B)	-----	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	454	sp3		
d	O(12A)	- Cu(2)	C(11A)	-----	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	459	sp3		
d	O(12B)	- Cu(2)	C(11B)	Na(2)d	-----	-----	-----	-----	-----	-----	3	95	128	116.4	1.279	2.538	3	461			
d	O(21A)	- C(21A)	Cu(2)b	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.0	1.279	1.946	2	464	sp3		
d	O(21B)	- C(21B)	Na(1)g	-----	-----	-----	-----	-----	-----	-----	1	130	130	130.0	1.244	2.413	2	387	sp3		
d	O(22A)	- C(21A)	Na(2)f	-----	-----	-----	-----	-----	-----	-----	1	134	134	134.1	1.246	2.391	2	383	sp3		
d	O(22B)	- C(21B)	Cu(1)a	-----	-----	-----	-----	-----	-----	-----	1	124	124	123.8	1.285	1.947	2	470	sp3		
d	O(41A)	- Na(2)	C(41A)	Na(1)b	Cu(2)c	-----	-----	-----	-----	-----	6	75	131	107.2	1.245	2.674	4	480			
d	O(42A)	- C(41A)	Cu(2)c	-----	-----	-----	-----	-----	-----	-----	1	107	107	107.1	1.284	1.967	2	478	sp3		
d	O(51A)	- C(51A)	Cu(1)i	-----	-----	-----	-----	-----	-----	-----	1	111	111	111.4	1.284	1.957	2	484	sp3		
d	O(52A)	- Na(1)	C(51A)	Na(2)a	Cu(1)i	-----	-----	-----	-----	-----	6	72	135	106.1	1.240	2.805	4	486			
d	C(1A)	- C(2A)	C(6A)	C(11A)	-----	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	186	sp2		
d	C(1B)	- C(2B)	C(11B)	C(6B)h	-----	-----	-----	-----	-----	-----	3	117	124	120.0	1.399	1.521	3	187	sp2		
d	C(2A)	- C(1A)	C(3A)	C(21A)	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	189	sp2		
d	C(2B)	- C(1B)	C(6B)	C(21B)	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	193	sp2		
d	C(3A)	- C(2A)	C(4A)	H(3A)	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	133	sp2		
d	C(4A)	- C(3A)	C(5A)	C(41A)	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	200	sp2		
d	C(5A)	- C(4A)	C(6A)	C(51A)	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	204	sp2		
d	C(6A)	- C(1A)	C(5A)	H(6A)	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	138	sp2		
d	C(6B)	- C(2B)	H(6B)	C(1B)h	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.951	1.399	3	123	sp2		
d	C(11A)	- O(11A)	O(12A)	C(1A)	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	280	sp2		
d	C(11B)	- O(11B)	O(12B)	C(1B)	-----	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	282	sp2		
d	C(21A)	- O(21A)	O(22A)	C(2A)	-----	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	283	sp2		
d	C(21B)	- O(21B)	O(22B)	C(2B)	-----	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	287	sp2		
d	C(41A)	- O(41A)	O(42A)	C(4A)	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	294	sp2		
d	C(51A)	- O(51A)	O(52A)	C(5A)	-----	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	298	sp2		
cR	H(3A)	- C(3A)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	30			
cR	H(6A)	- C(6A)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	33			

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cR	H(6B)	- C(6B)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	25	
d	Cu(1)a	- O(22B)	O(7W)a	O(11A)a	O(11B)a	O(51A)g	O(52A)g	-----	-----	-----	15	52	176	104.3	1.947	2.805	6	525	
d	Cu(2)a	- O(6W)a	O(12A)a	O(12B)a	-----	-----	-----	-----	-----	-----	3	89	164	120.0	1.979	2.223	3	514	
d	Na(1)a	- O(4W)a	O(5W)a	O(52A)a	O(11A)g	-----	-----	-----	-----	-----	6	78	160	103.0	2.275	2.449	4	496	
d	Na(2)a	- O(52A)	O(1W)a	O(3W)a	O(41A)a	O(22A)c	-----	-----	-----	-----	10	82	167	102.6	2.322	2.473	5	506	
d	O(1W)a	- Na(2)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	394	
d	O(3W)a	- Na(2)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	394	
d	O(4W)a	- Na(1)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	374	
d	O(5W)a	- Na(1)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	374	
d	O(6W)a	- Cu(2)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	417	
d	O(7W)a	- Cu(1)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	469	
d	O(11A)a	- Cu(1)a	C(11A)a	Na(1)g	-----	-----	-----	-----	-----	-----	3	94	134	116.2	1.289	2.449	3	473	
d	O(11B)a	- Cu(1)a	C(11B)a	-----	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	471	
d	O(12A)a	- Cu(2)a	C(11A)a	-----	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	419	
d	O(12B)a	- Cu(2)a	C(11B)a	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.4	1.279	1.979	2	418	
d	O(21A)a	- Cu(2)	C(21A)a	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.0	1.279	1.946	2	458	
d	O(21B)a	- C(21B)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.244	1.244	1	307	
d	O(22A)a	- C(21A)a	Na(2)d	-----	-----	-----	-----	-----	-----	-----	1	134	134	134.1	1.246	2.391	2	380	
d	O(22B)a	- C(21B)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	307	
d	O(41A)a	- Na(1)	Na(2)a	C(41A)a	-----	-----	-----	-----	-----	-----	3	98	131	119.8	1.245	2.367	3	398	
d	O(42A)a	- C(41A)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	349	
d	O(51A)a	- C(51A)a	Cu(1)g	-----	-----	-----	-----	-----	-----	-----	1	111	111	111.4	1.284	1.957	2	441	
d	O(52A)a	- Na(1)a	C(51A)a	Cu(1)g	-----	-----	-----	-----	-----	-----	3	72	129	92.8	1.240	2.805	3	443	
d	C(1A)a	- C(2A)a	C(6A)a	C(11A)a	-----	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	195	
d	C(1B)a	- C(2B)a	C(11B)a	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.2	1.403	1.521	2	194	?
d	C(2A)a	- C(1A)a	C(3A)a	C(21A)a	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	185	
d	C(2B)a	- C(1B)a	C(6B)a	C(21B)a	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	142	
d	C(3A)a	- C(2A)a	C(4A)a	H(3A)a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	111	
d	C(4A)a	- C(3A)a	C(5A)a	C(41A)a	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	163	
d	C(5A)a	- C(4A)a	C(6A)a	C(51A)a	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	178	
d	C(6A)a	- C(1A)a	C(5A)a	H(6A)a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	125	
d	C(6B)a	- C(2B)a	H(6B)a	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.0	0.951	1.395	2	60	?
d	C(11A)a	- O(11A)a	O(12A)a	C(1A)a	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	289	
d	C(11B)a	- O(11B)a	O(12B)a	C(1B)a	-----	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	288	
d	C(21A)a	- O(21A)a	O(22A)a	C(2A)a	-----	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	279	
d	C(21B)a	- O(21B)a	O(22B)a	C(2B)a	-----	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	210	
d	C(41A)a	- O(41A)a	O(42A)a	C(4A)a	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	257	
d	C(51A)a	- O(51A)a	O(52A)a	C(5A)a	-----	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	272	
cR	H(3A)a	- C(3A)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	20	
cR	H(6A)a	- C(6A)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	26	
cR	H(6B)a	- C(6B)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	4	
d	Cu(1)b	- O(7W)b	O(11A)b	O(11B)b	-----	-----	-----	-----	-----	-----	3	87	160	120.0	1.950	2.354	3	512	
d	Cu(2)b	- O(21A)	O(6W)b	O(12A)b	O(12B)b	O(41A)f	O(42A)f	-----	-----	-----	15	55	172	104.3	1.946	2.674	6	524	
d	Na(1)b	- O(41A)	O(4W)b	O(5W)b	O(52A)b	O(21B)i	-----	-----	-----	-----	10	78	175	104.1	2.275	2.413	5	504	
d	Na(2)b	- O(1W)b	O(3W)b	O(41A)b	O(12B)e	-----	-----	-----	-----	-----	6	77	167	107.5	2.322	2.538	4	495	

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d	O(1W)b - Na(2)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	373								
d	O(3W)b - Na(2)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	373								
d	O(4W)b - Na(1)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	389								
d	O(5W)b - Na(1)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	389								
d	O(6W)b - Cu(2)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	463								
d	O(7W)b - Cu(1)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	411								
d	O(11A)b- Cu(1)b	C(11A)b	-----	-----	-----	-----	-----	-----	-----	1	121	121	120.9	1.289	1.950	2	412								
d	O(11B)b- Cu(1)b	C(11B)b	-----	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	413								
d	O(12A)b- Cu(2)b	C(11A)b	-----	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	465								
d	O(12B)b- Cu(2)b	C(11B)b	Na(2)f	-----	-----	-----	-----	-----	-----	3	95	128	116.4	1.279	2.538	3	467								
d	O(21A)b- C(21A)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.279	1.279	1	317								
d	O(21B)b- C(21B)b	Na(1)i	-----	-----	-----	-----	-----	-----	-----	1	130	130	130.0	1.244	2.413	2	378								
d	O(22A)b- C(21A)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.246	1.246	1	317								
d	O(22B)b- Cu(1)	C(21B)b	-----	-----	-----	-----	-----	-----	-----	1	124	124	123.8	1.285	1.947	2	452								
d	O(41A)b- Na(2)b	C(41A)b	Cu(2)e	-----	-----	-----	-----	-----	-----	3	75	131	96.7	1.245	2.674	3	439								
d	O(42A)b- C(41A)b	Cu(2)e	-----	-----	-----	-----	-----	-----	-----	1	107	107	107.1	1.284	1.967	2	437								
d	O(51A)b- C(51A)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	345								
d	O(52A)b- Na(2)	Na(1)b	C(51A)b	-----	-----	-----	-----	-----	-----	3	96	135	120.0	1.240	2.383	3	393								
d	C(1A)b - C(2A)b	C(6A)b	C(11A)b	-----	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	190								
d	C(1B)b - C(2B)b	C(11B)b	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.2	1.403	1.521	2	191								?
d	C(2A)b - C(1A)b	C(3A)b	C(21A)b	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	147								
d	C(2B)b - C(1B)b	C(6B)b	C(21B)b	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	183								
d	C(3A)b - C(2A)b	C(4A)b	H(3A)b	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	101								
d	C(4A)b - C(3A)b	C(5A)b	C(41A)b	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	177								
d	C(5A)b - C(4A)b	C(6A)b	C(51A)b	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	161								
d	C(6A)b - C(1A)b	C(5A)b	H(6A)b	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	119								
d	C(6B)b - C(2B)b	H(6B)b	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.0	0.951	1.395	2	108								?
d	C(11A)b- O(11A)b	O(12A)b	C(1A)b	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	284								
d	C(11B)b- O(11B)b	O(12B)b	C(1B)b	-----	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	285								
d	C(21A)b- O(21A)b	O(22A)b	C(2A)b	-----	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	220								
d	C(21B)b- O(21B)b	O(22B)b	C(2B)b	-----	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	277								
d	C(41A)b- O(41A)b	O(42A)b	C(4A)b	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	271								
d	C(51A)b- O(51A)b	O(52A)b	C(5A)b	-----	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	255								
cR	H(3A)b - C(3A)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	16								
cR	H(6A)b - C(6A)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	23								
cR	H(6B)b - C(6B)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	19								
d	Cu(1)c - O(7W)c	O(11A)c	O(11B)c	-----	-----	-----	-----	-----	-----	3	87	160	120.0	1.950	2.354	3	513								
d	Cu(2)c - O(41A)c	O(42A)c	O(6W)c	O(12A)c	O(12B)c	O(21A)e	-----	-----	-----	15	55	172	104.3	1.946	2.674	6	526								
d	Na(1)c - O(4W)c	O(5W)c	O(52A)c	O(41A)e	-----	-----	-----	-----	-----	6	78	160	96.5	2.275	2.383	4	494								
d	Na(2)c - O(1W)c	O(3W)c	O(41A)c	-----	-----	-----	-----	-----	-----	3	82	167	112.8	2.322	2.473	3	490								
d	O(1W)c - Na(2)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	366								
d	O(3W)c - Na(2)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	366								
d	O(4W)c - Na(1)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	370								
d	O(5W)c - Na(1)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	370								
d	O(6W)c - Cu(2)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	475								
d	O(7W)c - Cu(1)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	414								

d	O(11A)c-	Cu(1)c	C(11A)c	-----	-----	-----	-----	-----	-----	-----	1	121	121	120.9	1.289	1.950	2	415	
d	O(11B)c-	Cu(1)c	C(11B)c	-----	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	416	
d	O(12A)c-	Cu(2)c	C(11A)c	-----	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	477	
d	O(12B)c-	Na(2)	Cu(2)c	C(11B)c	-----	-----	-----	-----	-----	-----	3	95	128	116.4	1.279	2.538	3	479	
d	O(21A)c-	C(21A)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.279	1.279	1	347	
d	O(21B)c-	C(21B)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.244	1.244	1	355	
d	O(22A)c-	Na(2)a	C(21A)c	-----	-----	-----	-----	-----	-----	-----	1	134	134	134.1	1.246	2.391	2	395	
d	O(22B)c-	C(21B)c	Cu(1)e	-----	-----	-----	-----	-----	-----	-----	1	124	124	123.8	1.285	1.947	2	432	
d	O(41A)c-	Na(2)c	C(41A)c	-----	-----	-----	-----	-----	-----	-----	1	131	131	131.4	1.245	2.322	2	367	
d	O(42A)c-	C(41A)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	331	
d	O(51A)c-	C(51A)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	337	
d	O(52A)c-	Na(1)c	C(51A)c	Na(2)e	-----	-----	-----	-----	-----	-----	3	96	135	120.0	1.240	2.383	3	372	
d	C(1A)c -	C(2A)c	C(6A)c	C(11A)c	-----	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	198	
d	C(1B)c -	C(2B)c	C(11B)c	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.2	1.403	1.521	2	199	?
d	C(2A)c -	C(1A)c	C(3A)c	C(21A)c	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	162	
d	C(2B)c -	C(1B)c	C(6B)c	C(21B)c	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	174	
d	C(3A)c -	C(2A)c	C(4A)c	H(3A)c	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	83	
d	C(4A)c -	C(3A)c	C(5A)c	C(41A)c	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	154	
d	C(5A)c -	C(4A)c	C(6A)c	C(51A)c	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	157	
d	C(6A)c -	C(1A)c	C(5A)c	H(6A)c	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	131	
d	C(6B)c -	C(2B)c	H(6B)c	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.0	0.951	1.395	2	97	?
d	C(11A)c-	O(11A)c	O(12A)c	C(1A)c	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	292	
d	C(11B)c-	O(11B)c	O(12B)c	C(1B)c	-----	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	293	
d	C(21A)c-	O(21A)c	O(22A)c	C(2A)c	-----	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	256	
d	C(21B)c-	O(21B)c	O(22B)c	C(2B)c	-----	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	268	
d	C(41A)c-	O(41A)c	O(42A)c	C(4A)c	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	246	
d	C(51A)c-	O(51A)c	O(52A)c	C(5A)c	-----	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	250	
cR	H(3A)c -	C(3A)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	8	
cR	H(6A)c -	C(6A)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	29	
cR	H(6B)c -	C(6B)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	14	
d	Cu(1)d -	O(7W)d	O(11A)d	O(11B)d	-----	-----	-----	-----	-----	-----	3	87	160	120.0	1.950	2.354	3	510	
d	Cu(2)d -	O(6W)d	O(12A)d	O(12B)d	O(21A)f	-----	-----	-----	-----	-----	6	87	164	105.4	1.946	2.223	4	517	
d	Na(1)d -	O(4W)d	O(5W)d	O(52A)d	O(41A)f	-----	-----	-----	-----	-----	6	78	160	96.5	2.275	2.383	4	500	
d	Na(2)d -	O(12B)	O(22A)a	O(1W)d	O(3W)d	O(41A)d	-----	-----	-----	-----	10	77	167	107.7	2.322	2.538	5	499	
d	O(1W)d -	Na(2)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	379	
d	O(3W)d -	Na(2)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	379	
d	O(4W)d -	Na(1)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	381	
d	O(5W)d -	Na(1)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	381	
d	O(6W)d -	Cu(2)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	427	
d	O(7W)d -	Cu(1)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	405	
d	O(11A)d-	Cu(1)d	C(11A)d	-----	-----	-----	-----	-----	-----	-----	1	121	121	120.9	1.289	1.950	2	407	
d	O(11B)d-	Cu(1)d	C(11B)d	-----	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	406	
d	O(12A)d-	Cu(2)d	C(11A)d	-----	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	430	
d	O(12B)d-	Cu(2)d	C(11B)d	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.4	1.279	1.979	2	429	
d	O(21A)d-	C(21A)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.279	1.279	1	315	
d	O(21B)d-	C(21B)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.244	1.244	1	351	

d	O(22A)d-	C(21A)d	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.246	1.246	1	315	
d	O(22B)d-	C(21B)d	Cu(1)f	-----	-----	-----	-----	-----	-----	1	124	124	123.8	1.285	1.947	2	424	
d	O(41A)d-	Cu(2)	Na(2)d	C(41A)d	-----	-----	-----	-----	-----	3	75	131	96.7	1.245	2.674	3	462	
d	O(42A)d-	Cu(2)	C(41A)d	-----	-----	-----	-----	-----	-----	1	107	107	107.1	1.284	1.967	2	460	
d	O(51A)d-	C(51A)d	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	339	
d	O(52A)d-	Na(1)d	C(51A)d	Na(2)f	-----	-----	-----	-----	-----	3	96	135	120.0	1.240	2.383	3	384	
d	C(1A)d -	C(2A)d	C(6A)d	C(11A)d	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	173	
d	C(1B)d -	C(2B)d	C(11B)d	-----	-----	-----	-----	-----	-----	1	124	124	124.2	1.403	1.521	2	172	?
d	C(2A)d -	C(1A)d	C(3A)d	C(21A)d	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	146	
d	C(2B)d -	C(1B)d	C(6B)d	C(21B)d	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	168	
d	C(3A)d -	C(2A)d	C(4A)d	H(3A)d	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	114	
d	C(4A)d -	C(3A)d	C(5A)d	C(41A)d	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	188	
d	C(5A)d -	C(4A)d	C(6A)d	C(51A)d	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	158	
d	C(6A)d -	C(1A)d	C(5A)d	H(6A)d	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	95	
d	C(6B)d -	C(2B)d	H(6B)d	-----	-----	-----	-----	-----	-----	1	119	119	119.0	0.951	1.395	2	93	?
d	C(11A)d-	O(11A)d	O(12A)d	C(1A)d	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	266	
d	C(11B)d-	O(11B)d	O(12B)d	C(1B)d	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	265	
d	C(21A)d-	O(21A)d	O(22A)d	C(2A)d	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	218	
d	C(21B)d-	O(21B)d	O(22B)d	C(2B)d	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	264	
d	C(41A)d-	O(41A)d	O(42A)d	C(4A)d	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	281	
d	C(51A)d-	O(51A)d	O(52A)d	C(5A)d	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	252	
cR	H(3A)d -	C(3A)d	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	22	
cR	H(6A)d -	C(6A)d	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	13	
cR	H(6B)d -	C(6B)d	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	11	
d	Cu(1)e -	O(22B)c	O(7W)e	O(11A)e	O(11B)e	-----	-----	-----	-----	6	87	160	104.6	1.947	2.354	4	518	
d	Cu(2)e -	O(41A)b	O(42A)b	O(6W)e	O(12A)e	O(12B)e	-----	-----	-----	10	55	164	100.2	1.967	2.674	5	519	
d	Na(1)e -	O(4W)e	O(5W)e	O(52A)e	-----	-----	-----	-----	-----	3	78	160	107.4	2.275	2.383	3	489	
d	Na(2)e -	O(52A)c	O(1W)e	O(3W)e	O(41A)e	-----	-----	-----	-----	6	82	167	98.6	2.322	2.473	4	494	
d	O(1W)e -	Na(2)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	370	
d	O(3W)e -	Na(2)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	370	
d	O(4W)e -	Na(1)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	368	
d	O(5W)e -	Na(1)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	368	
d	O(6W)e -	Cu(2)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	435	
d	O(7W)e -	Cu(1)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	431	
d	O(11A)e-	Cu(1)e	C(11A)e	-----	-----	-----	-----	-----	-----	1	121	121	120.9	1.289	1.950	2	433	
d	O(11B)e-	Cu(1)e	C(11B)e	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	434	
d	O(12A)e-	Cu(2)e	C(11A)e	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	436	
d	O(12B)e-	Na(2)b	Cu(2)e	C(11B)e	-----	-----	-----	-----	-----	3	95	128	116.4	1.279	2.538	3	438	
d	O(21A)e-	Cu(2)c	C(21A)e	-----	-----	-----	-----	-----	-----	1	124	124	124.0	1.279	1.946	2	476	
d	O(21B)e-	C(21B)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.244	1.244	1	305	
d	O(22A)e-	Na(2)	C(21A)e	-----	-----	-----	-----	-----	-----	1	134	134	134.1	1.246	2.391	2	392	
d	O(22B)e-	C(21B)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	305	
d	O(41A)e-	Na(1)c	Na(2)e	C(41A)e	-----	-----	-----	-----	-----	3	98	131	119.8	1.245	2.367	3	371	
d	O(42A)e-	C(41A)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	335	
d	O(51A)e-	C(51A)e	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	333	
d	O(52A)e-	Na(1)e	C(51A)e	-----	-----	-----	-----	-----	-----	1	129	129	129.2	1.240	2.383	2	369	

d	C(1A)e - C(2A)e	C(6A)e	C(11A)e	-----	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	175	
d	C(1B)e - C(2B)e	C(11B)e	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.2	1.403	1.521	2	176	?
d	C(2A)e - C(1A)e	C(3A)e	C(21A)e	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	197	
d	C(2B)e - C(1B)e	C(6B)e	C(21B)e	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	141	
d	C(3A)e - C(2A)e	C(4A)e	H(3A)e	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	129	
d	C(4A)e - C(3A)e	C(5A)e	C(41A)e	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	156	
d	C(5A)e - C(4A)e	C(6A)e	C(51A)e	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	155	
d	C(6A)e - C(1A)e	C(5A)e	H(6A)e	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	99	
d	C(6B)e - C(2B)e	H(6B)e	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.0	0.951	1.395	2	61	?
d	C(11A)e- O(11A)e	O(12A)e	C(1A)e	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	269	
d	C(11B)e- O(11B)e	O(12B)e	C(1B)e	-----	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	270	
d	C(21A)e- O(21A)e	O(22A)e	C(2A)e	-----	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	291	
d	C(21B)e- O(21B)e	O(22B)e	C(2B)e	-----	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	212	
d	C(41A)e- O(41A)e	O(42A)e	C(4A)e	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	251	
d	C(51A)e- O(51A)e	O(52A)e	C(5A)e	-----	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	245	
cR	H(3A)e - C(3A)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	28	
cR	H(6A)e - C(6A)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	15	
cR	H(6B)e - C(6B)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	3	
d	Cu(1)f - O(22B)d	O(7W)f	O(11A)f	O(11B)f	-----	-----	-----	-----	-----	6	87	160	104.6	1.947	2.354	4	516	
d	Cu(2)f - O(6W)f	O(12A)f	O(12B)f	-----	-----	-----	-----	-----	-----	3	89	164	120.0	1.979	2.223	3	511	
d	Na(1)f - O(4W)f	O(5W)f	O(52A)f	-----	-----	-----	-----	-----	-----	3	78	160	107.4	2.275	2.383	3	492	
d	Na(2)f - O(22A)	O(12B)b	O(52A)d	O(1W)f	O(3W)f	O(41A)f	-----	-----	-----	15	77	167	104.4	2.322	2.538	6	501	
d	O(1W)f - Na(2)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	382	
d	O(3W)f - Na(2)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	382	
d	O(4W)f - Na(1)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	360	
d	O(5W)f - Na(1)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	360	
d	O(6W)f - Cu(2)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	402	
d	O(7W)f - Cu(1)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	423	
d	O(11A)f- Cu(1)f	C(11A)f	-----	-----	-----	-----	-----	-----	-----	1	121	121	120.9	1.289	1.950	2	426	
d	O(11B)f- Cu(1)f	C(11B)f	-----	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	425	
d	O(12A)f- Cu(2)f	C(11A)f	-----	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	404	
d	O(12B)f- Cu(2)f	C(11B)f	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.4	1.279	1.979	2	403	
d	O(21A)f- Cu(2)d	C(21A)f	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.0	1.279	1.946	2	428	
d	O(21B)f- C(21B)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.244	1.244	1	303	
d	O(22A)f- C(21A)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.246	1.246	1	353	
d	O(22B)f- C(21B)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	303	
d	O(41A)f- Cu(2)b	Na(1)d	Na(2)f	C(41A)f	-----	-----	-----	-----	-----	6	75	131	107.2	1.245	2.674	4	468	
d	O(42A)f- Cu(2)b	C(41A)f	-----	-----	-----	-----	-----	-----	-----	1	107	107	107.1	1.284	1.967	2	466	
d	O(51A)f- C(51A)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	325	
d	O(52A)f- Na(1)f	C(51A)f	-----	-----	-----	-----	-----	-----	-----	1	129	129	129.2	1.240	2.383	2	361	
d	C(1A)f - C(2A)f	C(6A)f	C(11A)f	-----	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	170	
d	C(1B)f - C(2B)f	C(11B)f	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.2	1.403	1.521	2	169	?
d	C(2A)f - C(1A)f	C(3A)f	C(21A)f	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	171	
d	C(2B)f - C(1B)f	C(6B)f	C(21B)f	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	140	
d	C(3A)f - C(2A)f	C(4A)f	H(3A)f	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	121	
d	C(4A)f - C(3A)f	C(5A)f	C(41A)f	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	192	

d	C(5A)f - C(4A)f	C(6A)f	C(51A)f	-----	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	151	
d	C(6A)f - C(1A)f	C(5A)f	H(6A)f	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	92	
d	C(6B)f - C(2B)f	H(6B)f	-----	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.0	0.951	1.395	2	59	?
d	C(11A)f- O(11A)f	O(12A)f	C(1A)f	-----	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	263	
d	C(11B)f- O(11B)f	O(12B)f	C(1B)f	-----	-----	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	262	
d	C(21A)f- O(21A)f	O(22A)f	C(2A)f	-----	-----	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	267	
d	C(21B)f- O(21B)f	O(22B)f	C(2B)f	-----	-----	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	208	
d	C(41A)f- O(41A)f	O(42A)f	C(4A)f	-----	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	286	
d	C(51A)f- O(51A)f	O(52A)f	C(5A)f	-----	-----	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	248	
cR	H(3A)f - C(3A)f	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	24	
cR	H(6A)f - C(6A)f	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	12	
cR	H(6B)f - C(6B)f	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	2	
d	Cu(1)g - O(51A)a	O(52A)a	O(7W)g	O(11A)g	O(11B)g	-----	-----	-----	-----	-----	-10	52	160	99.7	1.950	2.805	5	520	
d	Cu(2)g - O(6W)g	O(12A)g	O(12B)g	O(21A)i	O(41A)j	O(42A)j	-----	-----	-----	-----	-15	55	172	104.3	1.946	2.674	6	521	
d	Na(1)g - O(21B)	O(11A)a	O(4W)g	O(5W)g	O(52A)g	O(41A)i	-----	-----	-----	-----	-15	78	175	105.1	2.275	2.449	6	503	
d	Na(2)g - O(1W)g	O(3W)g	O(41A)g	-----	-----	-----	-----	-----	-----	-----	3	82	167	112.8	2.322	2.473	3	493	
d	O(1W)g - Na(2)g	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	358	
d	O(3W)g - Na(2)g	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	358	
d	O(4W)g - Na(1)g	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	386	
d	O(5W)g - Na(1)g	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	386	
d	O(6W)g - Cu(2)g	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	445	
d	O(7W)g - Cu(1)g	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	440	
d	O(11A)g- Na(1)a	Cu(1)g	C(11A)g	-----	-----	-----	-----	-----	-----	-----	3	94	134	116.2	1.289	2.449	3	444	
d	O(11B)g- Cu(1)g	C(11B)g	-----	-----	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	442	
d	O(12A)g- Cu(2)g	C(11A)g	-----	-----	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	447	
d	O(12B)g- Cu(2)g	C(11B)g	Na(2)j	-----	-----	-----	-----	-----	-----	-----	3	95	128	116.4	1.279	2.538	3	449	
d	O(21A)g- C(21A)g	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.279	1.279	1	319	
d	O(21B)g- Na(1)	C(21B)g	-----	-----	-----	-----	-----	-----	-----	-----	1	130	130	130.0	1.244	2.413	2	397	
d	O(22A)g- C(21A)g	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.246	1.246	1	319	
d	O(22B)g- C(21B)g	Cu(1)i	-----	-----	-----	-----	-----	-----	-----	-----	1	124	124	123.8	1.285	1.947	2	482	
d	O(41A)g- Na(2)g	C(41A)g	-----	-----	-----	-----	-----	-----	-----	-----	1	131	131	131.4	1.245	2.322	2	359	
d	O(42A)g- C(41A)g	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	323	
d	O(51A)g- Cu(1)a	C(51A)g	-----	-----	-----	-----	-----	-----	-----	-----	1	111	111	111.4	1.284	1.957	2	472	
d	O(52A)g- Cu(1)a	Na(1)g	C(51A)g	Na(2)i	-----	-----	-----	-----	-----	-----	6	72	135	106.1	1.240	2.805	4	474	
d	C(1A)g - C(2A)g	C(6A)g	C(11A)g	-----	-----	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	180	
d	C(1B)g - C(2B)g	C(11B)g	-----	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.2	1.403	1.521	2	181	?
d	C(2A)g - C(1A)g	C(3A)g	C(21A)g	-----	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	148	
d	C(2B)g - C(1B)g	C(6B)g	C(21B)g	-----	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	201	
d	C(3A)g - C(2A)g	C(4A)g	H(3A)g	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	76	
d	C(4A)g - C(3A)g	C(5A)g	C(41A)g	-----	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	150	
d	C(5A)g - C(4A)g	C(6A)g	C(51A)g	-----	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	196	
d	C(6A)g - C(1A)g	C(5A)g	H(6A)g	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	127	
d	C(6B)g - C(2B)g	H(6B)g	-----	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.0	0.951	1.395	2	134	?
d	C(11A)g- O(11A)g	O(12A)g	C(1A)g	-----	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	274	
d	C(11B)g- O(11B)g	O(12B)g	C(1B)g	-----	-----	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	275	
d	C(21A)g- O(21A)g	O(22A)g	C(2A)g	-----	-----	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	224	

d	C(21B)g-	O(21B)g	O(22B)g	C(2B)g	-----	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	295
d	C(41A)g-	O(41A)g	O(42A)g	C(4A)g	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	249
d	C(51A)g-	O(51A)g	O(52A)g	C(5A)g	-----	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	290
cR	H(3A)g -	C(3A)g	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	5
cR	H(6A)g -	C(6A)g	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	27
cR	H(6B)g -	C(6B)g	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	31
d	Cu(1)h -	O(7W)h	O(11A)h	O(11B)h	-----	-----	-----	-----	-----	-----	3	87	160	120.0	1.950	2.354	3	509
d	Cu(2)h -	O(6W)h	O(12A)h	O(12B)h	-----	-----	-----	-----	-----	-----	3	89	164	120.0	1.979	2.223	3	509
d	Na(1)h -	O(4W)h	O(5W)h	O(52A)h	-----	-----	-----	-----	-----	-----	3	78	160	107.4	2.275	2.383	3	487
d	Na(2)h -	O(1W)h	O(3W)h	O(41A)h	-----	-----	-----	-----	-----	-----	3	82	167	112.8	2.322	2.473	3	488
d	O(1W)h -	Na(2)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	362
d	O(3W)h -	Na(2)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	362
d	O(4W)h -	Na(1)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	364
d	O(5W)h -	Na(1)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	364
d	O(6W)h -	Cu(2)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	408
d	O(7W)h -	Cu(1)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	408
d	O(11A)h-	Cu(1)h	C(11A)h	-----	-----	-----	-----	-----	-----	-----	1	121	121	120.9	1.289	1.950	2	410
d	O(11B)h-	Cu(1)h	C(11B)h	-----	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	409
d	O(12A)h-	Cu(2)h	C(11A)h	-----	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	410
d	O(12B)h-	Cu(2)h	C(11B)h	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.4	1.279	1.979	2	409
d	O(21A)h-	C(21A)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.279	1.279	1	311
d	O(21B)h-	C(21B)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.244	1.244	1	309
d	O(22A)h-	C(21A)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.246	1.246	1	311
d	O(22B)h-	C(21B)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	309
d	O(41A)h-	Na(2)h	C(41A)h	-----	-----	-----	-----	-----	-----	-----	1	131	131	131.4	1.245	2.322	2	363
d	O(42A)h-	C(41A)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	327
d	O(51A)h-	C(51A)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	329
d	O(52A)h-	Na(1)h	C(51A)h	-----	-----	-----	-----	-----	-----	-----	1	129	129	129.2	1.240	2.383	2	365
d	C(1A)h -	C(2A)h	C(6A)h	C(11A)h	-----	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	167
d	C(1B)h -	C(6B)	C(2B)h	C(11B)h	-----	-----	-----	-----	-----	-----	3	117	124	120.0	1.399	1.521	3	166
d	C(2A)h -	C(1A)h	C(3A)h	C(21A)h	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	144
d	C(2B)h -	C(1B)h	C(6B)h	C(21B)h	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	143
d	C(3A)h -	C(2A)h	C(4A)h	H(3A)h	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	70
d	C(4A)h -	C(3A)h	C(5A)h	C(41A)h	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	152
d	C(5A)h -	C(4A)h	C(6A)h	C(51A)h	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	153
d	C(6A)h -	C(1A)h	C(5A)h	H(6A)h	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	90
d	C(6B)h -	C(1B)	C(2B)h	H(6B)h	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.951	1.399	3	116
d	C(11A)h-	O(11A)h	O(12A)h	C(1A)h	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	261
d	C(11B)h-	O(11B)h	O(12B)h	C(1B)h	-----	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	260
d	C(21A)h-	O(21A)h	O(22A)h	C(2A)h	-----	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	222
d	C(21B)h-	O(21B)h	O(22B)h	C(2B)h	-----	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	216
d	C(41A)h-	O(41A)h	O(42A)h	C(4A)h	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	244
d	C(51A)h-	O(51A)h	O(52A)h	C(5A)h	-----	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	243
cR	H(3A)h -	C(3A)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	6
cR	H(6A)h -	C(6A)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	10

=====																				=====				
cR	H(6B)h	- C(6B)h	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	21						
d	Cu(1)i	- O(51A)	O(52A)	O(22B)g	O(7W)i	O(11A)i	O(11B)i	-----	-----	-----	-15	52	176	104.3	1.947	2.805	6	527						
d	Cu(2)i	- O(6W)i	O(12A)i	O(12B)i	-----	-----	-----	-----	-----	-----	3	89	164	120.0	1.979	2.223	3	515						
d	Na(1)i	- O(11A)	O(21B)b	O(4W)i	O(5W)i	O(52A)i	-----	-----	-----	-----	-10	78	175	107.2	2.275	2.449	5	498						
d	Na(2)i	- O(52A)g	O(1W)i	O(3W)i	O(41A)i	-----	-----	-----	-----	-----	6	82	167	98.6	2.322	2.473	4	502						
d	O(1W)i	- Na(2)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	385						
d	O(3W)i	- Na(2)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	385						
d	O(4W)i	- Na(1)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	377						
d	O(5W)i	- Na(1)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	377						
d	O(6W)i	- Cu(2)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	420						
d	O(7W)i	- Cu(1)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	481						
d	O(11A)i-	Na(1)	Cu(1)i	C(11A)i	-----	-----	-----	-----	-----	-----	3	94	134	116.2	1.289	2.449	3	485						
d	O(11B)i-	Cu(1)i	C(11B)i	-----	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	483						
d	O(12A)i-	Cu(2)i	C(11A)i	-----	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	422						
d	O(12B)i-	Cu(2)i	C(11B)i	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.4	1.279	1.979	2	421						
d	O(21A)i-	Cu(2)g	C(21A)i	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.0	1.279	1.946	2	446						
d	O(21B)i-	Na(1)b	C(21B)i	-----	-----	-----	-----	-----	-----	-----	1	130	130	130.0	1.244	2.413	2	390						
d	O(22A)i-	C(21A)i	Na(2)j	-----	-----	-----	-----	-----	-----	-----	1	134	134	134.1	1.246	2.391	2	376						
d	O(22B)i-	C(21B)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	343						
d	O(41A)i-	Na(1)g	Na(2)i	C(41A)i	-----	-----	-----	-----	-----	-----	3	98	131	119.8	1.245	2.367	3	388						
d	O(42A)i-	C(41A)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	341						
d	O(51A)i-	Cu(1)	C(51A)i	-----	-----	-----	-----	-----	-----	-----	1	111	111	111.4	1.284	1.957	2	453						
d	O(52A)i-	Cu(1)	Na(1)i	C(51A)i	-----	-----	-----	-----	-----	-----	3	72	129	92.8	1.240	2.805	3	455						
d	C(1A)i	- C(2A)i	C(6A)i	C(11A)i	-----	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	203						
d	C(1B)i	- C(2B)i	C(11B)i	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.2	1.403	1.521	2	202	?					
d	C(2A)i	- C(1A)i	C(3A)i	C(21A)i	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	179						
d	C(2B)i	- C(1B)i	C(6B)i	C(21B)i	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	160						
d	C(3A)i	- C(2A)i	C(4A)i	H(3A)i	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	104						
d	C(4A)i	- C(3A)i	C(5A)i	C(41A)i	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	159						
d	C(5A)i	- C(4A)i	C(6A)i	C(51A)i	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	184						
d	C(6A)i	- C(1A)i	C(5A)i	H(6A)i	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	136						
d	C(6B)i	- C(2B)i	H(6B)i	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.0	0.951	1.395	2	81	?					
d	C(11A)i-	O(11A)i	O(12A)i	C(1A)i	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	297						
d	C(11B)i-	O(11B)i	O(12B)i	C(1B)i	-----	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	296						
d	C(21A)i-	O(21A)i	O(22A)i	C(2A)i	-----	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	273						
d	C(21B)i-	O(21B)i	O(22B)i	C(2B)i	-----	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	254						
d	C(41A)i-	O(41A)i	O(42A)i	C(4A)i	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	253						
d	C(51A)i-	O(51A)i	O(52A)i	C(5A)i	-----	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	278						
cR	H(3A)i	- C(3A)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	17						
cR	H(6A)i	- C(6A)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	32						
cR	H(6B)i	- C(6B)i	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	7						
d	Cu(1)j	- O(7W)j	O(11A)j	O(11B)j	-----	-----	-----	-----	-----	-----	3	87	160	120.0	1.950	2.354	3	508						
d	Cu(2)j	- O(6W)j	O(12A)j	O(12B)j	-----	-----	-----	-----	-----	-----	3	89	164	120.0	1.979	2.223	3	508						
d	Na(1)j	- O(4W)j	O(5W)j	O(52A)j	-----	-----	-----	-----	-----	-----	3	78	160	107.4	2.275	2.383	3	491						
d	Na(2)j	- O(12B)g	O(22A)i	O(1W)j	O(3W)j	O(41A)j	-----	-----	-----	-----	-10	77	167	107.7	2.322	2.538	5	497						

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d	O(1W)j	- Na(2)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.323	2.323	1	375								
d	O(3W)j	- Na(2)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.473	2.473	1	375								
d	O(4W)j	- Na(1)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.275	2.275	1	356								
d	O(5W)j	- Na(1)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.377	2.377	1	356								
d	O(6W)j	- Cu(2)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.024	2.024	1	399								
d	O(7W)j	- Cu(1)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.008	2.008	1	399								
d	O(11A)j	- Cu(1)j	C(11A)j	-----	-----	-----	-----	-----	-----	1	121	121	120.9	1.289	1.950	2	401								
d	O(11B)j	- Cu(1)j	C(11B)j	-----	-----	-----	-----	-----	-----	1	155	155	155.3	1.244	2.354	2	400								
d	O(12A)j	- Cu(2)j	C(11A)j	-----	-----	-----	-----	-----	-----	1	161	161	160.6	1.235	2.223	2	401								
d	O(12B)j	- Cu(2)j	C(11B)j	-----	-----	-----	-----	-----	-----	1	128	128	128.4	1.279	1.979	2	400								
d	O(21A)j	- C(21A)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.279	1.279	1	313								
d	O(21B)j	- C(21B)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.244	1.244	1	301								
d	O(22A)j	- C(21A)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.246	1.246	1	313								
d	O(22B)j	- C(21B)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	301								
d	O(41A)j	- Cu(2)g	Na(2)j	C(41A)j	-----	-----	-----	-----	-----	3	75	131	96.7	1.245	2.674	3	450								
d	O(42A)j	- Cu(2)g	C(41A)j	-----	-----	-----	-----	-----	-----	1	107	107	107.1	1.284	1.967	2	448								
d	O(51A)j	- C(51A)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.284	1.284	1	321								
d	O(52A)j	- Na(1)j	C(51A)j	-----	-----	-----	-----	-----	-----	1	129	129	129.2	1.240	2.383	2	357								
d	C(1A)j	- C(2A)j	C(6A)j	C(11A)j	-----	-----	-----	-----	-----	3	116	124	119.9	1.396	1.507	3	165								
d	C(1B)j	- C(2B)j	C(11B)j	-----	-----	-----	-----	-----	-----	1	124	124	124.2	1.403	1.521	2	164								?
d	C(2A)j	- C(1A)j	C(3A)j	C(21A)j	-----	-----	-----	-----	-----	3	118	123	120.0	1.399	1.504	3	145								
d	C(2B)j	- C(1B)j	C(6B)j	C(21B)j	-----	-----	-----	-----	-----	3	118	123	120.0	1.395	1.512	3	139								
d	C(3A)j	- C(2A)j	C(4A)j	H(3A)j	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.399	3	107								
d	C(4A)j	- C(3A)j	C(5A)j	C(41A)j	-----	-----	-----	-----	-----	3	118	123	120.0	1.388	1.500	3	182								
d	C(5A)j	- C(4A)j	C(6A)j	C(51A)j	-----	-----	-----	-----	-----	3	118	122	119.9	1.390	1.506	3	149								
d	C(6A)j	- C(1A)j	C(5A)j	H(6A)j	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.396	3	87								
d	C(6B)j	- C(2B)j	H(6B)j	-----	-----	-----	-----	-----	-----	1	119	119	119.0	0.951	1.395	2	58								?
d	C(11A)j	- O(11A)j	O(12A)j	C(1A)j	-----	-----	-----	-----	-----	3	115	126	119.9	1.235	1.507	3	259								
d	C(11B)j	- O(11B)j	O(12B)j	C(1B)j	-----	-----	-----	-----	-----	3	114	128	120.0	1.244	1.521	3	258								
d	C(21A)j	- O(21A)j	O(22A)j	C(2A)j	-----	-----	-----	-----	-----	3	115	125	120.0	1.246	1.504	3	214								
d	C(21B)j	- O(21B)j	O(22B)j	C(2B)j	-----	-----	-----	-----	-----	3	114	125	120.0	1.244	1.512	3	206								
d	C(41A)j	- O(41A)j	O(42A)j	C(4A)j	-----	-----	-----	-----	-----	3	117	123	120.0	1.245	1.500	3	276								
d	C(51A)j	- O(51A)j	O(52A)j	C(5A)j	-----	-----	-----	-----	-----	3	115	124	120.0	1.240	1.506	3	247								
cR	H(3A)j	- C(3A)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	18								
cR	H(6A)j	- C(6A)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	9								
cR	H(6B)j	- C(6B)j	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	1								


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***** Residue = 2 *****
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Flag Label - Connected to (May be Incomplete for Polymeric Structures)
-----
d 0(2W) - ----- 0 0 0 0.0 0.000 0.000 0 299 V

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Asymmetric Residue Unit (= ARU) Code List
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ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)	
a =[1455.01]	= -1+x, y, z	= [	1	-1	0	0	1	-1.495	-0.244	0.002
b =[1655.01]	= 1+x, y, z	= [	1	1	0	0	1	0.505	-0.244	0.002
c =[2544.01]	= -x, -1/2+y, -1/2-z	= [	2	0	-1	-1	1	0.495	-0.744	-0.502
d =[2554.01]	= -x, 1/2+y, -1/2-z	= [	2	0	0	-1	1	0.495	0.256	-0.502
e =[2644.01]	= 1-x, -1/2+y, -1/2-z	= [	2	1	-1	-1	1	1.495	-0.744	-0.502
f =[2654.01]	= 1-x, 1/2+y, -1/2-z	= [	2	1	0	-1	1	1.495	0.256	-0.502
g =[3455.01]	= -1-x, -y, -z	= [	3	-1	0	0	1	-0.505	0.244	-0.002
h =[3465.01]	= -1-x, 1-y, -z	= [	3	-1	1	0	1	-0.505	1.244	-0.002
i =[3555.01]	= -x, -y, -z	= [	3	0	0	0	1	0.495	0.244	-0.002
j =[4445.01]	= -1+x, -1/2-y, 1/2+z	= [	4	-1	-1	0	1	-1.495	-0.256	0.502

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

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Analysis of the IntraMolecular Geometry in Terms of Unique Molecule(s)/Ions, with Bond Criterium: $d(i-j) < R(i) + R(j) + \text{Tol}$

-- Tol = 0.40 Ang. for Normal Bonds + 0.70 for (Earth)alkali-NonMetal Contacts and adjusted by -.40 Ang. for Metal-Metal Distances

-- The Bond Distance and Angle su's have been Incremented to Include the Effect of the Unit-cell su.
(Rel.Error in Dist. 0.0000 Ang. , Abs. Angle Error 0.001 Deg.)

-- Bonds below with '>' or '<' Substituted for '-' have Distances that Deviate from Expected Values(Based on the hybridisations).

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Residue = 1

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Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

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Cu(1) - O(7W)	2.0079(19)	Cu(1) - O(11A)	1.9505(18)	Cu(1) - O(11B)	2.3539(19)	Cu(1) - O(22B)b	1.9466(18)
Cu(1) - O(51A)i	1.9568(18)	Cu(1) - O(52A)i	2.805(2)	Cu(2) - O(6W)	2.0242(19)	Cu(2) - O(12A)	2.2233(18)
Cu(2) - O(12B)	1.9792(18)	Cu(2) - O(21A)a	1.9459(18)	Cu(2) - O(41A)d	2.6738(19)	Cu(2) - O(42A)d	1.9670(18)
Na(1) - O(4W)	2.275(3)	Na(1) - O(5W)	2.377(3)	Na(1) - O(52A)	2.383(2)	Na(1) - O(41A)a	2.367(2)
Na(1) - O(21B)g	2.413(2)	Na(1) - O(11A)i	2.449(2)	Na(2) - O(1W)	2.323(2)	Na(2) - O(3W)	2.473(2)
Na(2) - O(41A)	2.322(2)	Na(2) - O(52A)b	2.371(2)	Na(2) - O(12B)c	2.538(2)	Na(2) - O(22A)e	2.391(2)
O(11A) - C(11A)	1.289(3)	O(11B) - C(11B)	1.244(3)	O(12A) - C(11A)	1.235(3)	O(12B) - C(11B)	1.279(3)
O(21A) - C(21A)	1.279(3)	O(21B) - C(21B)	1.244(3)	O(22A) - C(21A)	1.246(3)	O(22B) - C(21B)	1.285(3)
O(41A) - C(41A)	1.245(3)	O(42A) - C(41A)	1.284(3)	O(51A) - C(51A)	1.284(3)	O(52A) - C(51A)	1.240(3)
C(1A) - C(2A)	1.403(4)	C(1A) - C(6A)	1.396(4)	C(1A) > C(11A)	1.507(4)	C(1B) - C(2B)	1.403(4)
C(1B) > C(11B)	1.521(4)	C(1B) - C(6B)h	1.399(4)	C(2A) - C(3A)	1.399(4)	C(2A) > C(21A)	1.504(4)
C(2B) - C(6B)	1.395(4)	C(2B) > C(21B)	1.512(4)	C(3A) - C(4A)	1.388(4)	C(4A) - C(5A)	1.400(4)
C(4A) > C(41A)	1.500(4)	C(5A) - C(6A)	1.390(4)	C(5A) > C(51A)	1.506(4)		

C(3A) - H(3A)	0.95	C(6A) - H(6A)	0.95	C(6B) - H(6B)	0.95

Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().

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O(7W) - Cu(1) - O(11A)	160.24(7)	O(7W) - Cu(1) - O(11B)	86.56(7)	O(7W) - Cu(1) - O(22B)b	90.75(8)
O(7W) - Cu(1) - O(51A)i	87.05(8)	O(7W) - Cu(1) - O(52A)i	83.78(7)	O(11A) - Cu(1) - O(11B)	113.19(7)
O(11A) - Cu(1) - O(22B)b	90.00(8)	O(11A) - Cu(1) - O(51A)i	90.99(8)	O(11A) - Cu(1) - O(52A)i	79.54(7)
O(11B) - Cu(1) - O(22B)b	86.83(7)	O(11B) - Cu(1) - O(51A)i	96.24(7)	O(11B) - Cu(1) - O(52A)i	147.27(6)
O(22B)b - Cu(1) - O(51A)i	176.11(8)	O(22B)b - Cu(1) - O(52A)i	124.40(6)	O(51A)i - Cu(1) - O(52A)i	52.16(6)
O(6W) - Cu(2) - O(12A)	89.33(7)	O(6W) - Cu(2) - O(12B)	164.37(7)	O(6W) - Cu(2) - O(21A)a	86.72(8)
O(6W) - Cu(2) - O(41A)d	86.84(7)	O(6W) - Cu(2) - O(42A)d	88.65(7)	O(12A) - Cu(2) - O(12B)	106.29(7)
O(12A) - Cu(2) - O(21A)a	93.84(7)	O(12A) - Cu(2) - O(41A)d	147.42(6)	O(12A) - Cu(2) - O(42A)d	92.91(7)
O(12B) - Cu(2) - O(21A)a	91.65(8)	O(12B) - Cu(2) - O(41A)d	80.24(7)	O(12B) - Cu(2) - O(42A)d	90.98(7)
O(21A)a - Cu(2) - O(41A)d	118.18(7)	O(21A)a - Cu(2) - O(42A)d	171.77(8)	O(41A)d - Cu(2) - O(42A)d	54.69(6)
O(4W) - Na(1) - O(5W)	83.93(11)	O(4W) - Na(1) - O(52A)	159.82(10)	O(4W) - Na(1) - O(41A)a	87.45(8)
O(4W) - Na(1) - O(21B)g	91.53(9)	O(4W) - Na(1) - O(11A)i	113.46(8)	O(5W) - Na(1) - O(52A)	78.46(10)
O(5W) - Na(1) - O(41A)a	87.51(10)	O(5W) - Na(1) - O(21B)g	174.81(10)	O(5W) - Na(1) - O(11A)i	102.22(10)
O(52A) - Na(1) - O(41A)a	82.05(7)	O(52A) - Na(1) - O(21B)g	105.56(8)	O(52A) - Na(1) - O(11A)i	80.20(7)
O(41A)a - Na(1) - O(21B)g	89.80(7)	O(41A)a - Na(1) - O(11A)i	157.54(8)	O(21B)g - Na(1) - O(11A)i	81.87(7)
O(1W) - Na(2) - O(3W)	82.46(8)	O(1W) - Na(2) - O(41A)	167.39(8)	O(1W) - Na(2) - O(52A)b	86.87(7)

O(1W) - Na(2) - O(12B)c	114.38(8)	O(1W) - Na(2) - O(22A)e	89.02(7)	O(3W) - Na(2) - O(41A)	88.53(8)
O(3W) - Na(2) - O(52A)b	82.95(9)	O(3W) - Na(2) - O(12B)c	115.05(8)	O(3W) - Na(2) - O(22A)e	164.33(9)
O(41A) - Na(2) - O(52A)b	83.27(7)	O(41A) - Na(2) - O(12B)c	77.45(7)	O(41A) - Na(2) - O(22A)e	97.62(7)
O(52A)b- Na(2) - O(12B)c	152.90(8)	O(52A)b- Na(2) - O(22A)e	83.47(8)	O(12B)c- Na(2) - O(22A)e	80.45(7)
Cu(1) - O(11A) - C(11A)	120.94(15)	Cu(1) - O(11A) - Na(1)i	93.87(8)	C(11A) - O(11A) - Na(1)i	133.72(16)
Cu(1) - O(11B) - C(11B)	155.30(18)	Cu(2) - O(12A) - C(11A)	160.64(18)	Cu(2) - O(12B) - C(11B)	128.43(16)
Cu(2) - O(12B) - Na(2)d	94.63(7)	C(11B) - O(12B) - Na(2)d	126.24(16)	C(21A) - O(21A) - Cu(2)b	124.03(17)
C(21B) - O(21B) - Na(1)g	129.95(16)	C(21A) - O(22A) - Na(2)f	134.13(16)	C(21B) - O(22B) - Cu(1)a	123.84(17)
Na(2) - O(41A) - C(41A)	131.35(17)	Na(2) - O(41A) - Na(1)b	97.80(7)	Na(2) - O(41A) - Cu(2)c	83.67(6)
C(41A) - O(41A) - Na(1)b	130.30(17)	C(41A) - O(41A) - Cu(2)c	75.21(14)	Na(1)b - O(41A) - Cu(2)c	124.60(8)
C(41A) - O(42A) - Cu(2)c	107.07(15)	C(51A) - O(51A) - Cu(1)i	111.36(15)	Na(1) - O(52A) - C(51A)	129.23(18)
Na(1) - O(52A) - Na(2)a	96.01(7)	Na(1) - O(52A) - Cu(1)i	76.58(6)	C(51A) - O(52A) - Na(2)a	134.75(18)
C(51A) - O(52A) - Cu(1)i	72.45(15)	Na(2)a - O(52A) - Cu(1)i	127.73(8)	C(2A) - C(1A) - C(6A)	119.4(2)
C(2A) - C(1A) - C(11A)	124.2(2)	C(6A) - C(1A) - C(11A)	116.2(2)	C(2B) - C(1B) - C(11B)	124.3(2)
C(2B) - C(1B) - C(6B)h	118.9(2)	C(11B) - C(1B) - C(6B)h	116.8(2)	C(1A) - C(2A) - C(3A)	119.0(2)
C(1A) - C(2A) - C(21A)	122.8(2)	C(3A) - C(2A) - C(21A)	118.3(2)	C(1B) - C(2B) - C(6B)	119.2(2)
C(1B) - C(2B) - C(21B)	122.8(2)	C(6B) - C(2B) - C(21B)	118.0(2)	C(2A) - C(3A) - C(4A)	121.3(2)
C(3A) - C(4A) - C(5A)	119.7(2)	C(3A) - C(4A) - C(41A)	117.8(2)	C(5A) - C(4A) - C(41A)	122.5(2)
C(4A) - C(5A) - C(6A)	119.2(2)	C(4A) - C(5A) - C(51A)	122.5(2)	C(6A) - C(5A) - C(51A)	118.1(2)
C(1A) - C(6A) - C(5A)	121.5(2)	C(2B) - C(6B) - C(1B)h	121.9(2)	O(11A) - C(11A) - O(12A)	125.6(2)
O(11A) - C(11A) - C(1A)	114.7(2)	O(12A) - C(11A) - C(1A)	119.5(2)	O(11B) - C(11B) - O(12B)	127.6(2)
O(11B) - C(11B) - C(1B)	117.9(2)	O(12B) - C(11B) - C(1B)	114.4(2)	O(21A) - C(21A) - O(22A)	125.2(2)
O(21A) - C(21A) - C(2A)	114.8(2)	O(22A) - C(21A) - C(2A)	120.0(2)	O(21B) - C(21B) - O(22B)	124.8(2)
O(21B) - C(21B) - C(2B)	120.9(2)	O(22B) - C(21B) - C(2B)	114.4(2)	O(41A) - C(41A) - O(42A)	123.0(2)
O(41A) - C(41A) - C(4A)	119.9(2)	O(42A) - C(41A) - C(4A)	117.1(2)	O(51A) - C(51A) - O(52A)	123.9(2)
O(51A) - C(51A) - C(5A)	115.4(2)	O(52A) - C(51A) - C(5A)	120.6(2)		
C(2A) - C(3A) - H(3A)	119	C(4A) - C(3A) - H(3A)	119	C(1A) - C(6A) - H(6A)	119
C(5A) - C(6A) - H(6A)	119	C(2B) - C(6B) - H(6B)	119	H(6B) - C(6B) - C(1B)h	119

Torsion/Dihedral Angles (Deg.) - Klyne & Prelog Convention (Dunitz, p241) - (Excl. Minor Disorder & Embedded Bond Angl. > 160. Deg.)

O(11B) Cu(1) O(11A) C(11A)	-39.3(2)	O(11B) Cu(1) O(11A) Na(1)i	172.66(6)	O(22B)bCu(1) O(11A) C(11A)	-125.89(19)
O(22B)bCu(1) O(11A) Na(1)i	86.11(7)	O(51A)iCu(1) O(11A) C(11A)	57.88(19)	O(51A)iCu(1) O(11A) Na(1)i	-90.13(7)
O(52A)iCu(1) O(11A) C(11A)	109.05(19)	O(52A)iCu(1) O(11A) Na(1)i	-38.96(6)	O(7W) Cu(1) O(11B) C(11B)	-110.8(4)
O(11A) Cu(1) O(11B) C(11B)	69.6(4)	O(22B)bCu(1) O(11B) C(11B)	158.3(4)	O(51A)iCu(1) O(11B) C(11B)	-24.2(4)
O(52A)iCu(1) O(11B) C(11B)	-37.9(5)	O(7W) Cu(1) O(22B)bC(21B)b	93.5(2)	O(11A) Cu(1) O(22B)bC(21B)b	-66.8(2)
O(11B) Cu(1) O(22B)bC(21B)b	180.0(2)	O(7W) Cu(1) O(51A)iC(51A)i	-86.20(17)	O(11A) Cu(1) O(51A)iC(51A)i	74.13(17)
O(11B) Cu(1) O(51A)iC(51A)i	-172.41(17)	O(7W) Cu(1) O(52A)iNa(1)i	-127.85(7)	O(7W) Cu(1) O(52A)iC(51A)i	92.90(16)
O(11A) Cu(1) O(52A)iNa(1)i	41.51(7)	O(11A) Cu(1) O(52A)iC(51A)i	-97.73(16)	O(11B) Cu(1) O(52A)iNa(1)i	158.48(10)
O(11B) Cu(1) O(52A)iC(51A)i	19.2(2)	O(12A) Cu(2) O(12B) C(11B)	36.8(2)	O(12A) Cu(2) O(12B) Na(2)d	-178.01(6)
O(21A)aCu(2) O(12B) C(11B)	131.3(2)	O(21A)aCu(2) O(12B) Na(2)d	-83.53(8)	O(41A)dCu(2) O(12B) C(11B)	-110.4(2)
O(41A)dCu(2) O(12B) Na(2)d	34.80(6)	O(42A)dCu(2) O(12B) C(11B)	-56.5(2)	O(42A)dCu(2) O(12B) Na(2)d	88.67(7)
O(6W) Cu(2) O(21A)aC(21A)a	-99.0(2)	O(12A) Cu(2) O(21A)aC(21A)a	171.9(2)	O(12B) Cu(2) O(21A)aC(21A)a	65.5(2)
O(6W) Cu(2) O(41A)dNa(2)d	132.45(7)	O(6W) Cu(2) O(41A)dC(41A)d	-91.76(15)	O(12A) Cu(2) O(41A)dNa(2)d	-143.76(11)
O(12A) Cu(2) O(41A)dC(41A)d	-8.0(2)	O(12B) Cu(2) O(41A)dNa(2)d	-38.73(7)	O(12B) Cu(2) O(41A)dC(41A)d	97.06(15)
O(6W) Cu(2) O(42A)dC(41A)d	88.23(17)	O(12A) Cu(2) O(42A)dC(41A)d	177.49(16)	O(12B) Cu(2) O(42A)dC(41A)d	-76.15(17)
O(4W) Na(1) O(52A) C(51A)	112.8(3)	O(4W) Na(1) O(52A) Na(2)a	-66.3(3)	O(4W) Na(1) O(52A) Cu(1)i	166.3(3)

O(5W)	Na(1)	O(52A)	C(51A)	83.1(2)	O(5W)	Na(1)	O(52A)	Na(2)a	-96.05(10)	O(5W)	Na(1)	O(52A)	Cu(1)i	136.54(9)
O(41A)aNa(1)	O(52A)	C(51A)		172.1(2)	O(41A)aNa(1)	O(52A)	Na(2)a		-6.99(8)	O(41A)aNa(1)	O(52A)	Cu(1)i		-134.39(7)
O(21B)gNa(1)	O(52A)	C(51A)		-100.3(2)	O(21B)gNa(1)	O(52A)	Na(2)a		80.58(9)	O(21B)gNa(1)	O(52A)	Cu(1)i		-46.83(7)
O(11A)iNa(1)	O(52A)	C(51A)		-21.7(2)	O(11A)iNa(1)	O(52A)	Na(2)a		159.20(8)	O(11A)iNa(1)	O(52A)	Cu(1)i		31.80(5)
O(4W)	Na(1)	O(41A)aNa(2)a		169.88(9)	O(4W)	Na(1)	O(41A)aC(41A)a		-2.2(2)	O(5W)	Na(1)	O(41A)aNa(2)a		85.85(10)
O(5W)	Na(1)	O(41A)aC(41A)a		-86.2(2)	O(52A)	Na(1)	O(41A)aNa(2)a		7.16(8)	O(52A)	Na(1)	O(41A)aC(41A)a		-164.9(2)
O(4W)	Na(1)	O(21B)gC(21B)g		-118.6(2)	O(52A)	Na(1)	O(21B)gC(21B)g		72.3(2)	O(4W)	Na(1)	O(11A)iCu(1)i		147.94(9)
O(4W)	Na(1)	O(11A)iC(11A)i		-71.0(2)	O(5W)	Na(1)	O(11A)iCu(1)i		-123.43(10)	O(5W)	Na(1)	O(11A)iC(11A)i		17.6(2)
O(52A)	Na(1)	O(11A)iCu(1)i		-47.63(8)	O(52A)	Na(1)	O(11A)iC(11A)i		93.4(2)	O(3W)	Na(2)	O(41A)	C(41A)	81.7(2)
O(3W)	Na(2)	O(41A)	Na(1)b	-90.25(9)	O(3W)	Na(2)	O(41A)	Cu(2)c	145.60(8)	O(52A)bNa(2)	O(41A)	C(41A)		164.8(2)
O(52A)bNa(2)	O(41A)	Na(1)b		-7.18(8)	O(52A)bNa(2)	O(41A)	Cu(2)c		-131.33(7)	O(12B)cNa(2)	O(41A)	C(41A)		-34.4(2)
O(12B)cNa(2)	O(41A)	Na(1)b		153.67(8)	O(12B)cNa(2)	O(41A)	Cu(2)c		29.51(5)	O(22A)eNa(2)	O(41A)	C(41A)		-112.8(2)
O(22A)eNa(2)	O(41A)	Na(1)b		75.28(8)	O(22A)eNa(2)	O(41A)	Cu(2)c		-48.87(7)	O(1W)	Na(2)	O(52A)bNa(1)b		179.23(8)
O(1W)	Na(2)	O(52A)bC(51A)b		0.2(3)	O(3W)	Na(2)	O(52A)bNa(1)b		96.45(9)	O(3W)	Na(2)	O(52A)bC(51A)b		-82.6(3)
O(41A)	Na(2)	O(52A)bNa(1)b		7.10(8)	O(41A)	Na(2)	O(52A)bC(51A)b		-171.9(3)	O(1W)	Na(2)	O(12B)cCu(2)c		143.04(8)
O(1W)	Na(2)	O(12B)cC(11B)c		-70.6(2)	O(3W)	Na(2)	O(12B)cCu(2)c		-123.93(9)	O(3W)	Na(2)	O(12B)cC(11B)c		22.4(2)
O(41A)	Na(2)	O(12B)cCu(2)c		-41.58(7)	O(41A)	Na(2)	O(12B)cC(11B)c		104.8(2)	O(1W)	Na(2)	O(22A)eC(21A)e		-123.3(2)
O(41A)	Na(2)	O(22A)eC(21A)e		67.5(2)	C(6A)	C(1A)	C(2A)	C(3A)	0.6(4)	C(6A)	C(1A)	C(2A)	C(21A)	178.4(2)
C(11A)	C(1A)	C(2A)	C(3A)	175.4(2)	C(11A)	C(1A)	C(2A)	C(21A)	-6.7(4)	C(2A)	C(1A)	C(6A)	C(5A)	0.1(4)
C(11A)	C(1A)	C(6A)	C(5A)	-175.1(2)	C(2A)	C(1A)	C(11A)	O(11A)	-57.2(3)	C(2A)	C(1A)	C(11A)	O(12A)	127.8(3)
C(6A)	C(1A)	C(11A)	O(11A)	117.8(3)	C(6A)	C(1A)	C(11A)	O(12A)	-57.2(3)	C(11B)	C(1B)	C(2B)	C(6B)	-175.8(2)
C(11B)	C(1B)	C(2B)	C(21B)	5.9(4)	C(6B)h	C(1B)	C(2B)	C(6B)	0.7(4)	C(6B)h	C(1B)	C(2B)	C(21B)	-177.7(2)
C(2B)	C(1B)	C(11B)	O(11B)	-122.3(3)	C(2B)	C(1B)	C(11B)	O(12B)	61.6(3)	C(6B)h	C(1B)	C(11B)	O(11B)	61.2(3)
C(6B)h	C(1B)	C(11B)	O(12B)	-115.0(3)	C(2B)	C(1B)	C(6B)h	C(2B)h	-0.7(4)	C(11B)	C(1B)	C(6B)h	C(2B)h	176.1(2)
C(1A)	C(2A)	C(3A)	C(4A)	-0.5(4)	C(21A)	C(2A)	C(3A)	C(4A)	-178.4(2)	C(1A)	C(2A)	C(21A)	O(21A)	139.9(3)
C(1A)	C(2A)	C(21A)	O(22A)	-42.2(4)	C(3A)	C(2A)	C(21A)	O(21A)	-42.2(3)	C(3A)	C(2A)	C(21A)	O(22A)	135.7(3)
C(1B)	C(2B)	C(6B)	C(1B)h	-0.7(4)	C(21B)	C(2B)	C(6B)	C(1B)h	177.7(2)	C(1B)	C(2B)	C(21B)	O(21B)	40.3(4)
C(1B)	C(2B)	C(21B)	O(22B)	-141.8(3)	C(6B)	C(2B)	C(21B)	O(21B)	-138.0(3)	C(6B)	C(2B)	C(21B)	O(22B)	39.9(3)
C(2A)	C(3A)	C(4A)	C(5A)	-0.3(4)	C(2A)	C(3A)	C(4A)	C(41A)	178.3(2)	C(3A)	C(4A)	C(5A)	C(6A)	0.9(4)
C(3A)	C(4A)	C(5A)	C(51A)	-174.0(2)	C(41A)	C(4A)	C(5A)	C(6A)	-177.6(2)	C(41A)	C(4A)	C(5A)	C(51A)	7.5(4)
C(3A)	C(4A)	C(41A)	O(41A)	46.3(4)	C(3A)	C(4A)	C(41A)	O(42A)	-131.3(3)	C(5A)	C(4A)	C(41A)	O(41A)	-135.1(3)
C(5A)	C(4A)	C(41A)	O(42A)	47.3(4)	C(4A)	C(5A)	C(6A)	C(1A)	-0.9(4)	C(51A)	C(5A)	C(6A)	C(1A)	174.3(2)
C(4A)	C(5A)	C(51A)	O(51A)	52.7(3)	C(4A)	C(5A)	C(51A)	O(52A)	-130.6(3)	C(6A)	C(5A)	C(51A)	O(51A)	-122.3(3)
C(6A)	C(5A)	C(51A)	O(52A)	54.5(4)	O(12A)	C(11A)	O(11A)	Cu(1)	18.2(4)	O(12A)	C(11A)	O(11A)	Na(1)i	151.2(2)
C(1A)	C(11A)	O(11A)	Cu(1)	-156.33(17)	C(1A)	C(11A)	O(11A)	Na(1)i	-23.3(3)	O(12B)	C(11B)	O(11B)	Cu(1)	-42.6(6)
C(1B)	C(11B)	O(11B)	Cu(1)	141.8(3)	O(11B)	C(11B)	O(12B)	Cu(2)	-21.2(4)	O(11B)	C(11B)	O(12B)	Na(2)d	-156.3(2)
C(1B)	C(11B)	O(12B)	Cu(2)	154.54(17)	C(1B)	C(11B)	O(12B)	Na(2)d	19.4(3)	O(22A)	C(21A)	O(21A)	Cu(2)b	-4.1(4)
C(2A)	C(21A)	O(21A)	Cu(2)b	173.72(17)	O(21A)	C(21A)	O(22A)	Na(2)f	-24.8(4)	C(2A)	C(21A)	O(22A)	Na(2)f	157.56(18)
O(22B)	C(21B)	O(21B)	Na(1)g	30.1(4)	C(2B)	C(21B)	O(21B)	Na(1)g	-152.22(18)	O(21B)	C(21B)	O(22B)	Cu(1)a	1.0(4)
C(2B)	C(21B)	O(22B)	Cu(1)a	-176.84(16)	O(42A)	C(41A)	O(41A)	Na(2)	69.1(3)	O(42A)	C(41A)	O(41A)	Na(1)b	-121.4(2)
O(42A)	C(41A)	O(41A)	Cu(2)c	1.7(2)	C(4A)	C(41A)	O(41A)	Na(2)	-108.3(3)	C(4A)	C(41A)	O(41A)	Na(1)b	61.2(3)
C(4A)	C(41A)	O(41A)	Cu(2)c	-175.7(2)	O(41A)	C(41A)	O(42A)	Cu(2)c	-2.4(3)	C(4A)	C(41A)	O(42A)	Cu(2)c	175.11(18)
O(52A)	C(51A)	O(51A)	Cu(1)i	-3.9(3)	C(5A)	C(51A)	O(51A)	Cu(1)i	172.78(17)	O(51A)	C(51A)	O(52A)	Na(1)	57.7(3)
O(51A)	C(51A)	O(52A)	Na(2)a	-123.6(3)	O(51A)	C(51A)	O(52A)	Cu(1)i	2.6(2)	C(5A)	C(51A)	O(52A)	Na(1)	-118.8(2)
C(5A)	C(51A)	O(52A)	Na(2)a	60.0(3)	C(5A)	C(51A)	O(52A)	Cu(1)i	-173.8(3)					
C(2A)	C(1A)	C(6A)	H(6A)	-180	C(11A)	C(1A)	C(6A)	H(6A)	5	C(2B)	C(1B)	C(6B)h	H(6B)h	179
C(11B)	C(1B)	C(6B)h	H(6B)h	-4	C(1A)	C(2A)	C(3A)	H(3A)	179	C(21A)	C(2A)	C(3A)	H(3A)	2

C(1B)	C(2B)	C(6B)	H(6B)	179	C(21B)	C(2B)	C(6B)	H(6B)	-2	H(3A)	C(3A)	C(4A)	C(5A)	180
H(3A)	C(3A)	C(4A)	C(41A)	-2	C(4A)	C(5A)	C(6A)	H(6A)	179	C(51A)	C(5A)	C(6A)	H(6A)	-6

[illegible]

Selected Bond Lengths (Angstrom) - see M.F.C. Ladd & R.A. Palmer, Structure Determination by X-Ray Crystallography (1985)

Formal single bonds

C4-C4	1.54	C4-C3	1.52	C4-C2	1.46	C4-N3	1.47	C4-N2	1.47	C4-O2	1.43	C3-C3	1.46	C3-C2	1.45	C3-N3	1.40	C3-N2	1.40
C3-O2	1.36	C2-C2	1.38	C2-N3	1.33	C2-N2	1.33	C2-O2	1.36	N3-N3	1.45	N3-N2	1.45	N3-O2	1.36	N2-N2	1.45	N2-O2	1.41

Formal double bonds

C3-C3 1.34 C3-C2 1.31 C3-N2 1.32 C3-O1 1.22 C2-C2 1.28 C2-N2 1.32 C2-O1 1.16 N3-O1 1.24 N2-N2 1.25 N2-O1 1.21

Formal triple bonds

Aromatic bonds

C2-C2 1.20 C2-N1 1.16 C3-C3 1.40 C2-N2 1.34 N2-N2 1.35

The notation in the table indicates the connectivity of the atoms

For more detailed standard bond distance tabulations see: J. Chem. Soc. Perkin II, (1987), S1-S19; J. Chem. Soc. Dalton Trans. (1989), S1 - S83 or International Tables C, (1992), 707-791.

Automatic Search for Rings (3 to 6-Membered) and Planes Determined by 4 or More Connected Atoms (with Deviation < 0.10 Ang.)

Least-Squares Planes - $P \cdot X + Q \cdot Y + R \cdot Z = S$:: First Line Orthogonal(X0,Y0,Z0), Second Line Fractional(X,Y,Z)
 Ring/Plan/Resd/Lspl N Indicates that the Ring/Plane/Residue Involves N Atoms
 Sigref - R.M.S-Error of the Contributing Atoms
 Sigpln - $\text{Sqrt}(\text{Sum}(j=1:N)(D(j)**2)/(N-3))$
 Chisq - Chi-Squared = $\text{Sum}(j=1:N)(D(j)**2)/\text{Sigref}**2$
 Pl.Hyp. - Result of the Chi.Sq. Test for Planarity (See Stout & Jensen, p424)

Calculated via Substitution in

$D = P \cdot X + Q \cdot Y + R \cdot Z - S$ (2nd Line)

**** - Atoms Deviating by More Than 1.5 Angstrom and Hydrogen Atoms are NOT Listed
 Note - Weights : UNIT
 **** - Maximum Metal Containing Ring Size: 6
 - Maximum Number of Bonds to Ring Metal: 6
 - Deviations from planes are in Angstrom Units
 - The Plane determining Atoms have been Marked #

Nr	1	P	Q	R	S	Sigref	0.002	Sigpln	0.027	Chisq	211.9	Pl.Hyp.	P<5
Ring		-0.2871(13)	0.4970(6)	0.8189(5)	2.791(2)	#Cu(1)	-0.006(1)	#O(51A)	0.015(2)	#O(52A)	0.010(2)	#C(51A)	-0.019(3)
A	4	-2.318(11)	8.402(10)	13.253(8)	2.791(2)	O(11B)	0.375(2)	O(12B)	-0.580(2)	C(11B)	0.361(3)	Cu(2)a	-0.185(1)
						O(4W)a	-0.224(2)	O(5W)a	-0.616(3)	O(11A)	0.420(2)	O(12A)	-0.289(2)
						C(11A)	-0.453(3)	O(7W)b	-0.328(2)	O(21B)	-0.332(2)	O(22B)	0.038(2)
						C(1B)b	-0.774(3)	C(2B)b	0.030(3)	C(6B)b	1.036(3)	C(21B)	-0.118(3)
						Cu(2)d	-1.412(1)	Na(2)d	-0.972(1)	O(1W)d	0.600(2)	O(3W)d	0.024(3)
						O(6W)d	-0.420(2)	O(21A)	-0.460(2)	O(22A)	0.159(2)	C(21A)	-0.555(3)
						Cu(2)g	-0.761(1)	Na(1)g	0.853(1)	O(4W)g	-0.722(2)	O(5W)g	-0.330(3)
						O(6W)g	1.260(2)	O(11A)	-1.366(2)	O(12A)	-0.657(2)	O(22A)	1.098(2)
						C(1A)g	0.774(3)	C(6A)g	1.055(3)	C(11A)	-0.493(3)	C(21A)	1.394(3)
						Na(1)i	-1.466(1)	O(6W)i	-1.059(2)	O(21A)	-0.735(2)	O(22A)	-1.220(2)
						C(2A)i	-0.713(3)	C(3A)i	0.387(3)	C(4A)i	0.661(3)	C(5A)i	-0.178(3)
						C(6A)i	-1.263(3)	C(21A)	-0.924(3)	Cu(1)j	0.283(1)	O(7W)j	1.435(2)
						O(11A)	-0.496(2)	O(11B)	-0.645(2)	O(12A)	-0.924(2)	O(12B)	-1.131(2)
						O(22B)	1.185(2)	O(41A)	-0.635(2)	O(42A)	-0.638(2)	O(52A)	1.413(2)
						C(1A)j	-0.840(3)	C(1B)j	-0.912(3)	C(2B)j	-0.085(3)	C(4A)j	-0.645(3)
						C(5A)j	0.194(3)	C(6A)j	0.079(3)	C(6B)j	-0.280(3)	C(11A)	-0.788(3)
						C(11B)	-0.862(3)	C(21B)	1.042(3)	C(41A)	-0.622(3)	C(51A)	1.297(3)

Nr	2	P	Q	R	S	Sigref	0.002	Sigpln	0.017	Chisq	95.0	Pl.Hyp.	P<5
Ring		-0.2639(12)	0.5448(6)	0.7960(5)	0.495(5)	#Cu(2)	0.004(1)	#O(41A)	-0.007(2)	#O(42A)	-0.009(2)	#C(41A)	0.012(3)
A	4	-2.130(10)	9.209(10)	12.848(8)	0.495(5)	O(4W)	-0.464(2)	O(5W)	-0.690(3)	O(11A)	0.598(2)	O(12A)	-0.137(2)
						C(11A)	-0.298(3)	Na(1)a	0.142(1)	O(5W)a	1.441(3)	O(6W)a	0.113(2)
						O(21A)	-0.128(2)	O(22A)	0.384(2)	O(51A)	-1.262(2)	O(52A)	-1.242(2)
						C(1A)a	0.536(3)	C(2A)a	-0.253(3)	C(3A)a	-1.388(3)	C(5A)a	-0.942(3)
						C(6A)a	0.178(3)	C(21A)	0.043(3)	C(51A)	-1.186(3)	Cu(1)b	0.362(1)
						O(11B)	0.787(2)	O(12B)	-0.196(2)	C(11B)	0.769(3)	Cu(1)d	-0.420(1)

						O(7W)d	-1.480(2)	O(11A)	0.255(2)	O(11B)	0.590(2)	O(12A)	0.681(2)
						O(12B)	1.059(2)	O(22B)	-1.101(2)	C(1A)d	0.478(3)	C(1B)d	0.967(3)
						C(2A)d	1.265(3)	C(2B)d	0.182(3)	C(3A)d	1.075(3)	C(4A)d	0.122(3)
						C(5A)d	-0.674(3)	C(6A)d	-0.479(3)	C(6B)d	0.455(3)	C(11A)	0.513(3)
						C(11B)	0.830(3)	C(21B)	-0.982(3)	Cu(2)f	-0.458(1)	Na(2)f	-0.553(1)
						O(1W)f	0.967(2)	O(3W)f	0.566(3)	O(6W)f	0.435(2)	O(12A)	-1.449(2)
						O(12B)	-1.071(2)	O(21A)	0.277(2)	O(22A)	0.975(2)	C(1B)f	-1.164(3)
						C(2A)f	-0.866(3)	C(3A)f	-1.056(3)	C(11B)	-1.300(3)	C(21A)	0.210(3)
						Cu(1)g	-1.352(1)	Cu(2)g	1.137(1)	O(11A)	0.543(2)	O(12A)	1.277(2)
						O(12B)	-0.794(2)	C(11A)	1.438(3)	Cu(2)i	-0.994(1)	Na(1)i	0.998(1)
						O(4W)i	-0.526(2)	O(5W)i	-0.300(3)	O(6W)i	1.027(2)	O(12A)	-0.853(2)
						O(21A)	1.269(2)	O(22A)	0.756(2)	C(1A)i	0.604(3)	C(2A)i	1.393(3)
						C(6A)i	0.962(3)	C(11A)	-0.692(3)	C(21A)	1.098(3)	Cu(2)j	-0.532(1)
						Na(2)j	-0.437(1)	O(6W)j	-1.425(2)	O(11A)	0.886(2)	O(11B)	0.551(2)
						O(12A)	0.459(2)	O(12B)	0.081(2)	O(21A)	-1.267(2)	O(41A)	1.147(2)
						O(42A)	1.150(2)	C(1A)j	0.662(3)	C(1B)j	0.174(3)	C(2A)j	-0.124(3)
						C(2B)j	0.959(3)	C(3A)j	0.066(3)	C(4A)j	1.019(3)	C(6B)j	0.685(3)
						C(11A)	0.628(3)	C(11B)	0.310(3)	C(21A)	-1.200(3)	C(41A)	1.128(3)
Nr	3	P	Q	R	S	Sigref	0.002	Sigpln	0.017	Chisq	94.9	Pl.Hyp.	P<5
Ring	-0.2639(12)	-0.5448(6)	0.7960(5)	-2.315(5)	#O(41A)	0.007(2)	#O(42A)	0.009(2)	#C(41A)	-0.012(3)	#Cu(2)c	-0.004(1)	
A	4	-2.130(10)	-9.209(10)	12.848(8)	-2.315(5)	Cu(1)	0.420(1)	O(7W)	1.480(2)	O(11A)	-0.255(2)	O(11B)	-0.590(2)
						O(12A)	-0.681(2)	O(12B)	-1.059(2)	O(22B)	1.101(2)	C(1A)	-0.478(3)
						C(1B)	-0.967(3)	C(2A)	-1.265(3)	C(2B)	-0.182(3)	C(3A)	-1.075(3)
						C(4A)	-0.122(3)	C(5A)	0.674(3)	C(6A)	0.479(3)	C(6B)	-0.455(3)
						C(11A)	-0.513(3)	C(11B)	-0.830(3)	C(21B)	0.982(3)	Cu(2)a	0.458(1)
						Na(2)a	0.553(1)	O(1W)a	-0.967(2)	O(3W)a	-0.566(3)	O(6W)a	-0.435(2)
						O(12A)	1.449(2)	O(12B)	1.071(2)	O(21A)	-0.277(2)	O(22A)	-0.975(2)
						C(1B)a	1.164(3)	C(2A)a	0.866(3)	C(3A)a	1.056(3)	C(11B)	1.300(3)
						C(21A)	-0.210(3)	O(5W)b	0.265(3)	O(7W)b	-0.650(2)	O(21B)	-0.370(2)
						O(22B)	-1.030(2)	O(51A)	0.541(2)	O(52A)	-0.214(2)	C(5A)b	-1.457(3)
						C(21B)	-1.148(3)	C(51A)	-0.318(3)	O(4W)c	0.464(2)	O(5W)c	0.690(3)
						O(11A)	-0.598(2)	O(12A)	0.137(2)	C(11A)	0.298(3)	O(1W)d	-1.211(2)
						Na(1)e	-0.142(1)	O(5W)e	-1.441(3)	O(6W)e	-0.113(2)	O(21A)	0.128(2)
						O(22A)	-0.384(2)	O(51A)	1.262(2)	O(52A)	1.242(2)	C(1A)e	-0.536(3)
						C(2A)e	0.253(3)	C(3A)e	1.388(3)	C(5A)e	0.942(3)	C(6A)e	-0.178(3)
						C(21A)	-0.043(3)	C(51A)	1.186(3)	Cu(2)h	-0.776(1)	Na(2)h	-0.871(1)
						O(1W)h	0.649(2)	O(3W)h	0.248(3)	O(6W)h	0.117(2)	O(12B)	-1.390(2)
						O(21A)	-0.041(2)	O(22A)	0.657(2)	C(1B)h	-1.482(3)	C(2A)h	-1.184(3)
						C(3A)h	-1.374(3)	C(21A)	-0.108(3)	Na(1)i	0.956(1)	O(4W)i	-0.134(2)
Nr	4	P	Q	R	S	Sigref	0.002	Sigpln	0.027	Chisq	211.9	Pl.Hyp.	P<5
Ring	-0.2871(13)	0.4970(6)	0.8189(5)	-2.791(2)	#O(51A)	-0.015(2)	#O(52A)	-0.010(2)	#C(51A)	0.019(3)	#Cu(1)i	0.006(1)	
A	4	-2.318(11)	8.402(10)	13.253(8)	-2.791(2)	Na(1)	1.466(1)	O(6W)	1.059(2)	O(21A)	0.735(2)	O(22A)	1.220(2)
						C(2A)	0.713(3)	C(3A)	-0.387(3)	C(4A)	-0.661(3)	C(5A)	0.178(3)
						C(6A)	1.263(3)	C(21A)	0.924(3)	Na(2)a	-1.407(1)	O(3W)a	0.037(3)

=====													
						O(41A)	0.202(2)	O(42A)	-0.352(2)	C(41A)	0.436(3)	Cu(2)b	0.761(1)
						Na(1)b	-0.853(1)	O(4W)b	0.722(2)	O(5W)b	0.330(3)	O(6W)b	-1.260(2)
						O(11A)	1.366(2)	O(12A)	0.657(2)	O(22A)	-1.098(2)	C(1A)b	-0.774(3)
						C(6A)b	-1.055(3)	C(11A)	0.493(3)	C(21A)	-1.394(3)	Na(1)d	-0.910(1)
						O(5W)d	0.258(3)	O(7W)d	0.883(2)	O(21B)	0.545(2)	O(22B)	1.134(2)
						O(51A)	0.203(2)	O(52A)	0.906(2)	C(21B)	1.276(3)	C(51A)	1.022(3)
						Cu(1)f	-0.283(1)	O(7W)f	-1.435(2)	O(11A)	0.496(2)	O(11B)	0.645(2)
						O(12A)	0.924(2)	O(12B)	1.131(2)	O(22B)	-1.185(2)	O(41A)	0.635(2)
						O(42A)	0.638(2)	O(52A)	-1.413(2)	C(1A)f	0.840(3)	C(1B)f	0.912(3)
						C(2B)f	0.085(3)	C(4A)f	0.645(3)	C(5A)f	-0.194(3)	C(6A)f	-0.079(3)
						C(6B)f	0.280(3)	C(11A)	0.788(3)	C(11B)	0.862(3)	C(21B)	-1.042(3)
						C(41A)	0.622(3)	C(51A)	-1.297(3)	O(7W)g	0.328(2)	O(21B)	0.332(2)
						O(22B)	-0.038(2)	C(1B)g	0.774(3)	C(2B)g	-0.030(3)	C(6B)g	-1.036(3)
						C(21B)	0.118(3)	O(11B)	-0.375(2)	O(12B)	0.580(2)	C(11B)	-0.361(3)

Nr	5	P	Q	R	S	Sigref	0.003	Sigpln	0.005	Chisq	12.3	Pl.Hyp.	P<5

Ring		0.4030(10)	-0.1154(11)	0.9079(5)	-1.589(3)	#C(1A)	-0.002(3)	#C(2A)	0.004(3)	#C(3A)	-0.001(3)	#C(4A)	-0.004(3)
A	6	3.254(8)	-1.951(18)	13.059(7)	-1.589(3)	#C(5A)	0.006(3)	#C(6A)	-0.003(3)	Na(1)	-0.189(1)	Na(2)	0.259(1)
						O(1W)	0.175(2)	O(3W)	0.272(3)	O(4W)	-0.164(2)	O(5W)	-0.291(3)
						O(11A)	1.155(2)	O(11B)	0.159(2)	O(12A)	-0.735(2)	O(21A)	0.724(2)
						O(21B)	0.113(2)	O(22A)	-0.784(2)	O(22B)	-1.464(2)	O(41A)	0.702(2)
						O(42A)	-0.915(2)	O(51A)	1.137(2)	O(52A)	-0.647(2)	C(1B)	-0.864(3)
						C(2B)	-0.890(3)	C(6B)	-1.046(3)	C(11A)	0.103(3)	C(11B)	-0.792(3)
						C(21A)	-0.030(3)	C(21B)	-0.720(3)	C(41A)	-0.049(3)	C(51A)	0.137(3)
						Cu(1)a	-1.404(1)	O(7W)a	-0.097(2)	Cu(2)b	0.757(1)	O(6W)b	-0.450(2)
						O(12B)	1.469(2)	Cu(2)c	-0.829(1)	O(6W)c	0.617(2)	O(42A)	-0.794(2)
						O(52A)	-1.203(2)	O(6W)d	-1.334(2)	Na(2)e	1.147(1)	O(1W)e	1.146(2)
						O(3W)e	0.567(3)	O(5W)e	1.228(3)	O(11A)	-1.053(2)	O(11B)	-0.619(2)
						O(12A)	0.903(2)	O(12B)	1.434(2)	O(21A)	-0.472(2)	O(21B)	-0.386(2)
						O(22A)	0.780(2)	O(22B)	0.969(2)	O(41A)	0.715(2)	O(51A)	0.431(2)
						C(1A)e	0.522(3)	C(1B)e	0.071(3)	C(2A)e	0.516(3)	C(2B)e	0.102(3)
						C(3A)e	0.802(3)	C(4A)e	1.081(3)	C(5A)e	1.071(3)	C(6A)e	0.801(3)
						C(6B)e	-0.021(3)	C(11A)	0.135(3)	C(11B)	0.285(3)	C(21A)	0.259(3)
						C(21B)	0.228(3)	C(41A)	1.415(3)	C(51A)	1.233(3)	Cu(2)f	0.474(1)
						Na(1)f	-0.279(1)	Na(2)f	-0.804(1)	O(1W)f	-0.805(2)	O(3W)f	-1.384(3)
						O(4W)f	-0.396(2)	O(5W)f	-0.723(3)	O(12A)	-1.048(2)	O(12B)	-0.517(2)
						O(22A)	-1.171(2)	O(22B)	-0.982(2)	O(41A)	-1.236(2)	O(42A)	0.509(2)
						O(52A)	0.100(2)	C(1A)f	-1.429(3)	C(2A)f	-1.435(3)	C(3A)f	-1.149(3)
						C(4A)f	-0.870(3)	C(5A)f	-0.880(3)	C(6A)f	-1.150(3)	C(41A)	-0.536(3)
						C(51A)	-0.718(3)	Na(1)g	0.114(1)	Na(2)g	-0.335(1)	O(1W)g	-0.251(2)
						O(3W)g	-0.348(3)	O(4W)g	0.089(2)	O(5W)g	0.216(3)	O(11A)	-1.231(2)
						O(11B)	-0.234(2)	O(12A)	0.660(2)	O(21A)	-0.799(2)	O(21B)	-0.189(2)
						O(22A)	0.709(2)	O(22B)	1.389(2)	O(41A)	-0.777(2)	O(42A)	0.839(2)
						O(51A)	-1.212(2)	O(52A)	0.572(2)	C(1A)g	-0.073(3)	C(1B)g	0.788(3)
						C(2A)g	-0.080(3)	C(2B)g	0.815(3)	C(3A)g	-0.074(3)	C(4A)g	-0.072(3)
						C(5A)g	-0.081(3)	C(6A)g	-0.073(3)	C(6B)g	0.971(3)	C(11A)	-0.178(3)
						C(11B)	0.716(3)	C(21A)	-0.046(3)	C(21B)	0.644(3)	C(41A)	-0.026(3)

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						C(51A)	-0.213(3)	Cu(2)h	0.471(1)	O(12A)	-1.291(2)	O(12B)	-0.242(2)
						O(22A)	-1.242(2)	O(22B)	-0.562(2)	O(42A)	-1.112(2)	O(52A)	-1.379(2)
						C(1B)h	-1.163(3)	C(2B)h	-1.136(3)	C(6B)h	-0.980(3)	C(11B)	-1.235(3)
						C(21B)	-1.307(3)	Cu(1)i	1.329(1)	O(7W)i	0.022(2)	O(6W)j	1.258(2)

Nr	6	P	Q	R	S	Sigref	0.003	Sigpln	0.003	Chisq	5.3	Pl.Hyp.	

Ring	0.3835(10)	-0.0044(11)	0.9236(4)	-1.585(10)	#C(1B)	-0.002(3)	#C(2B)	0.002(3)	#C(6B)	-0.002(3)	#C(1B)h	0.002(3)	
A 6	3.096(8)	-0.074(18)	13.344(7)	-1.585(10)	#C(2B)h	-0.002(3)	#C(6B)h	0.002(3)	Na(1)	-0.445(1)	Na(2)	-0.187(1)	
					O(1W)	-0.286(2)	O(3W)	0.102(3)	O(4W)	-0.321(2)	O(5W)	-0.287(3)	
					O(11A)	1.493(2)	O(11B)	0.825(2)	O(12A)	-0.414(2)	O(12B)	-1.162(2)	
					O(21A)	0.893(2)	O(21B)	0.774(2)	O(22A)	-0.468(2)	O(22B)	-0.672(2)	
					O(41A)	0.308(2)	O(42A)	-1.349(2)	O(51A)	0.762(2)	O(52A)	-0.924(2)	
					C(1A)	0.111(3)	C(2A)	0.084(3)	C(3A)	-0.075(3)	C(4A)	-0.194(3)	
					C(5A)	-0.150(3)	C(6A)	-0.008(3)	C(11A)	0.374(3)	C(11B)	-0.090(3)	
					C(21A)	0.171(3)	C(21B)	0.050(3)	C(41A)	-0.399(3)	C(51A)	-0.140(3)	
					Cu(1)a	-0.746(1)	O(7W)a	0.693(2)	Cu(2)b	1.051(1)	O(6W)b	-0.307(2)	
					Cu(2)c	-1.456(1)	O(6W)c	-0.090(2)	O(6W)d	-0.163(2)	Na(1)e	0.098(1)	
					Na(2)e	-0.163(1)	O(1W)e	-0.067(2)	O(3W)e	-0.473(3)	O(4W)e	-0.030(2)	
					O(5W)e	-0.080(3)	O(11B)	-1.245(2)	O(12A)	0.018(2)	O(12B)	0.746(2)	
					O(21A)	-1.286(2)	O(21B)	-1.187(2)	O(22A)	0.065(2)	O(22B)	0.251(2)	
					O(41A)	-0.657(2)	O(42A)	1.004(2)	O(51A)	-1.106(2)	O(52A)	0.574(2)	
					C(1A)e	-0.494(3)	C(1B)e	-0.430(3)	C(2A)e	-0.467(3)	C(2B)e	-0.435(3)	
					C(3A)e	-0.298(3)	C(4A)e	-0.168(3)	C(5A)e	-0.212(3)	C(6A)e	-0.365(3)	
					C(6B)e	-0.441(3)	C(11A)	-0.768(3)	C(11B)	-0.332(3)	C(21A)	-0.565(3)	
					C(21B)	-0.471(3)	C(41A)	0.048(3)	C(51A)	-0.211(3)	Na(1)f	0.025(1)	
					Na(2)f	-0.236(1)	O(1W)f	-0.140(2)	O(3W)f	-0.546(3)	O(4W)f	-0.103(2)	
					O(5W)f	-0.154(3)	O(11B)	-1.318(2)	O(12A)	-0.056(2)	O(12B)	0.672(2)	
					O(21A)	-1.360(2)	O(21B)	-1.260(2)	O(22A)	-0.009(2)	O(22B)	0.177(2)	
					O(41A)	-0.731(2)	O(42A)	0.931(2)	O(51A)	-1.180(2)	O(52A)	0.500(2)	
					C(1A)f	-0.568(3)	C(1B)f	-0.504(3)	C(2A)f	-0.540(3)	C(2B)f	-0.508(3)	
					C(3A)f	-0.372(3)	C(4A)f	-0.242(3)	C(5A)f	-0.285(3)	C(6A)f	-0.439(3)	
					C(6B)f	-0.514(3)	C(11A)	-0.841(3)	C(11B)	-0.406(3)	C(21A)	-0.638(3)	
					C(21B)	-0.545(3)	C(41A)	-0.026(3)	C(51A)	-0.284(3)	Na(1)g	0.518(1)	
					Na(2)g	0.261(1)	O(1W)g	0.360(2)	O(3W)g	-0.028(3)	O(4W)g	0.394(2)	
					O(5W)g	0.361(3)	O(11A)	-1.420(2)	O(11B)	-0.751(2)	O(12A)	0.488(2)	
					O(12B)	1.235(2)	O(21A)	-0.820(2)	O(21B)	-0.700(2)	O(22A)	0.541(2)	
					O(22B)	0.746(2)	O(41A)	-0.235(2)	O(42A)	1.422(2)	O(51A)	-0.689(2)	
					O(52A)	0.997(2)	C(1A)g	-0.038(3)	C(1B)g	0.076(3)	C(2A)g	-0.010(3)	
					C(2B)g	0.071(3)	C(3A)g	0.148(3)	C(4A)g	0.267(3)	C(5A)g	0.224(3)	
					C(6A)g	0.081(3)	C(6B)g	0.076(3)	C(11A)	-0.301(3)	C(11B)	0.163(3)	
					C(21A)	-0.097(3)	C(21B)	0.024(3)	C(41A)	0.473(3)	C(51A)	0.214(3)	
					Na(1)h	0.445(1)	Na(2)h	0.187(1)	O(1W)h	0.286(2)	O(3W)h	-0.102(3)	
					O(4W)h	0.321(2)	O(5W)h	0.287(3)	O(11A)	-1.493(2)	O(11B)	-0.825(2)	
					O(12A)	0.414(2)	O(12B)	1.162(2)	O(21A)	-0.893(2)	O(21B)	-0.774(2)	
					O(22A)	0.468(2)	O(22B)	0.672(2)	O(41A)	-0.308(2)	O(42A)	1.349(2)	
					O(51A)	-0.762(2)	O(52A)	0.924(2)	C(1A)h	-0.111(3)	C(2A)h	-0.084(3)	
					C(3A)h	0.075(3)	C(4A)h	0.194(3)	C(5A)h	0.150(3)	C(6A)h	0.008(3)	

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						C(11A)	-0.374(3)	C(11B)	0.090(3)	C(21A)	-0.171(3)	C(21B)	-0.050(3)
						C(41A)	0.399(3)	C(51A)	0.140(3)	Cu(1)i	0.819(1)	O(7W)i	-0.619(2)
						O(6W)j	0.237(2)						

Nr	7	P	Q	R	S	Sigref	0.002	Sigpln	2.625	Chisq	999999.9	Pl.Hyp.	

Resd	0.4131	0.0771	0.9074	-1.5513	#Cu(1)	2.676(1)	#Cu(2)	-1.764(1)	#Na(1)	-0.759(1)	#Na(2)	-0.156(1)	
A407	3.3352	1.3026	13.0293	-1.5513	#O(1W)	-0.148(2)	#O(3W)	0.330(3)	#O(4W)	-0.678(2)	#O(5W)	-0.404(3)	
					#O(6W)	-3.165(2)	#O(7W)	4.141(2)	#O(11A)	1.776(2)	#O(11B)	1.222(2)	
					#O(12A)	-0.186(2)	#O(12B)	-0.829(2)	#O(21A)	1.255(2)	#O(21B)	0.986(2)	
					#O(22A)	-0.058(2)	#O(22B)	-0.424(2)	#O(41A)	0.258(2)	#O(42A)	-1.484(2)	
					#O(51A)	0.534(2)	#O(52A)	-1.131(2)	#C(1A)	0.271(3)	#C(1B)	0.458(3)	
					#C(2A)	0.291(3)	#C(2B)	0.414(3)	#C(3A)	0.057(3)	#C(4A)	-0.183(3)	
					#C(5A)	-0.186(3)	#C(6A)	0.032(3)	#C(6B)	0.484(3)	#C(11A)	0.605(3)	
					#C(11B)	0.300(3)	#C(21A)	0.507(3)	#C(21B)	0.330(3)	#C(41A)	-0.462(3)	
					#C(51A)	-0.307(3)	#Cu(1)a	-0.659(1)	#Cu(2)a	-5.099(1)	#Na(1)a	-4.095(1)	
					#Na(2)a	-3.491(1)	#O(1W)a	-3.483(2)	#O(3W)a	-3.005(3)	#O(4W)a	-4.013(2)	
					#O(5W)a	-3.739(3)	#O(6W)a	-6.501(2)	#O(7W)a	0.806(2)	#O(11A)	-1.559(2)	
					#O(11B)	-2.114(2)	#O(12A)	-3.522(2)	#O(12B)	-4.164(2)	#O(21A)	-2.080(2)	
					#O(21B)	-2.349(2)	#O(22A)	-3.393(2)	#O(22B)	-3.759(2)	#O(41A)	-3.078(2)	
					#O(42A)	-4.819(2)	#O(51A)	-2.801(2)	#O(52A)	-4.466(2)	#C(1A)a	-3.064(3)	
					#C(1B)a	-2.877(3)	#C(2A)a	-3.044(3)	#C(2B)a	-2.921(3)	#C(3A)a	-3.278(3)	
					#C(4A)a	-3.518(3)	#C(5A)a	-3.522(3)	#C(6A)a	-3.304(3)	#C(6B)a	-2.851(3)	
					#C(11A)	-2.731(3)	#C(11B)	-3.036(3)	#C(21A)	-2.828(3)	#C(21B)	-3.005(3)	
					#C(41A)	-3.798(3)	#C(51A)	-3.642(3)	#Cu(1)b	6.011(1)	#Cu(2)b	1.571(1)	
					#Na(1)b	2.576(1)	#Na(2)b	3.180(1)	#O(1W)b	3.188(2)	#O(3W)b	3.665(3)	
					#O(4W)b	2.657(2)	#O(5W)b	2.931(3)	#O(6W)b	0.170(2)	#O(7W)b	7.476(2)	
					#O(11A)	5.111(2)	#O(11B)	4.557(2)	#O(12A)	3.149(2)	#O(12B)	2.507(2)	
					#O(21A)	4.590(2)	#O(21B)	4.322(2)	#O(22A)	3.278(2)	#O(22B)	2.911(2)	
					#O(41A)	3.593(2)	#O(42A)	1.851(2)	#O(51A)	3.869(2)	#O(52A)	2.204(2)	
					#C(1A)b	3.607(3)	#C(1B)b	3.794(3)	#C(2A)b	3.626(3)	#C(2B)b	3.750(3)	
					#C(3A)b	3.392(3)	#C(4A)b	3.153(3)	#C(5A)b	3.149(3)	#C(6A)b	3.367(3)	
					#C(6B)b	3.820(3)	#C(11A)	3.940(3)	#C(11B)	3.635(3)	#C(21A)	3.843(3)	
					#C(21B)	3.666(3)	#C(41A)	2.873(3)	#C(51A)	3.028(3)	#Cu(1)c	-6.049(1)	
					#Cu(2)c	-1.665(1)	#Na(1)c	-3.708(1)	#Na(2)c	-4.260(1)	#O(1W)c	-4.211(2)	
					#O(3W)c	-4.368(3)	#O(4W)c	-3.727(2)	#O(5W)c	-3.698(3)	#O(6W)c	-0.423(2)	
					#O(7W)c	-7.383(2)	#O(11A)	-5.321(2)	#O(11B)	-4.392(2)	#O(12A)	-3.403(2)	
					#O(12B)	-2.414(2)	#O(21A)	-4.900(2)	#O(21B)	-4.281(2)	#O(22A)	-3.416(2)	
					#O(22B)	-2.723(2)	#O(41A)	-4.681(2)	#O(42A)	-3.024(2)	#O(51A)	-5.058(2)	
					#O(52A)	-3.283(2)	#C(1A)c	-4.095(3)	#C(1B)c	-3.406(3)	#C(2A)c	-4.115(3)	
					#C(2B)c	-3.365(3)	#C(3A)c	-4.068(3)	#C(4A)c	-4.013(3)	#C(5A)c	-4.010(3)	
					#C(6A)c	-4.042(3)	#C(6B)c	-3.249(3)	#C(11A)	-4.240(3)	#C(11B)	-3.438(3)	
					#C(21A)	-4.138(3)	#C(21B)	-3.479(3)	#C(41A)	-3.927(3)	#C(51A)	-4.085(3)	
					#Cu(1)d	-4.746(1)	#Cu(2)d	-0.362(1)	#Na(1)d	-2.405(1)	#Na(2)d	-2.958(1)	
					#O(1W)d	-2.909(2)	#O(3W)d	-3.065(3)	#O(4W)d	-2.425(2)	#O(5W)d	-2.396(3)	
					#O(6W)d	0.880(2)	#O(7W)d	-6.080(2)	#O(11A)	-4.019(2)	#O(11B)	-3.089(2)	
					#O(12A)	-2.100(2)	#O(12B)	-1.111(2)	#O(21A)	-3.597(2)	#O(21B)	-2.979(2)	
					#O(22A)	-2.113(2)	#O(22B)	-1.420(2)	#O(41A)	-3.378(2)	#O(42A)	-1.722(2)	

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#O(51A) -3.755(2) #O(52A) -1.980(2) #C(1A)d -2.793(3) #C(1B)d -2.103(3)
#C(2A)d -2.812(3) #C(2B)d -2.062(3) #C(3A)d -2.766(3) #C(4A)d -2.711(3)
#C(5A)d -2.707(3) #C(6A)d -2.739(3) #C(6B)d -1.946(3) #C(11A) -2.938(3)
#C(11B) -2.135(3) #C(21A) -2.835(3) #C(21B) -2.176(3) #C(41A) -2.624(3)
#C(51A) -2.782(3) #Cu(1)e -2.714(1) #Cu(2)e 1.671(1) #Na(1)e -0.372(1)
#Na(2)e -0.925(1) #O(1W)e -0.876(2) #O(3W)e -1.032(3) #O(4W)e -0.392(2)
#O(5W)e -0.363(3) #O(6W)e 2.912(2) #O(7W)e -4.048(2) #O(11A) -1.986(2)
#O(11B) -1.056(2) #O(12A) -0.067(2) #O(12B) 0.921(2) #O(21A) -1.565(2)
#O(21B) -0.946(2) #O(22A) -0.081(2) #O(22B) 0.613(2) #O(41A) -1.346(2)
#O(42A) 0.311(2) #O(51A) -1.722(2) #O(52A) 0.052(2) #C(1A)e -0.760(3)
#C(1B)e -0.070(3) #C(2A)e -0.780(3) #C(2B)e -0.030(3) #C(3A)e -0.733(3)
#C(4A)e -0.678(3) #C(5A)e -0.674(3) #C(6A)e -0.706(3) #C(6B)e 0.086(3)
#C(11A) -0.905(3) #C(11B) -0.103(3) #C(21A) -0.802(3) #C(21B) -0.144(3)
#C(41A) -0.591(3) #C(51A) -0.749(3) #Cu(1)f -1.411(1) #Cu(2)f 2.973(1)
#Na(1)f 0.930(1) #Na(2)f 0.378(1) #O(1W)f 0.426(2) #O(3W)f 0.270(3)
#O(4W)f 0.911(2) #O(5W)f 0.939(3) #O(6W)f 4.215(2) #O(7W)f -2.745(2)
#O(11A) -0.683(2) #O(11B) 0.246(2) #O(12A) 1.235(2) #O(12B) 2.224(2)
#O(21A) -0.262(2) #O(21B) 0.357(2) #O(22A) 1.222(2) #O(22B) 1.915(2)
#O(41A) -0.043(2) #O(42A) 1.613(2) #O(51A) -0.420(2) #O(52A) 1.355(2)
#C(1A)f 0.543(3) #C(1B)f 1.232(3) #C(2A)f 0.523(3) #C(2B)f 1.273(3)
#C(3A)f 0.569(3) #C(4A)f 0.625(3) #C(5A)f 0.628(3) #C(6A)f 0.596(3)
#C(6B)f 1.389(3) #C(11A) 0.398(3) #C(11B) 1.200(3) #C(21A) 0.500(3)
#C(21B) 1.159(3) #C(41A) 0.711(3) #C(51A) 0.553(3) #Cu(1)g -2.909(1)
#Cu(2)g 1.532(1) #Na(1)g 0.527(1) #Na(2)g -0.077(1) #O(1W)g -0.085(2)
#O(3W)g -0.563(3) #O(4W)g 0.446(2) #O(5W)g 0.171(3) #O(6W)g 2.933(2)
#O(7W)g -4.374(2) #O(11A) -2.009(2) #O(11B) -1.454(2) #O(12A) -0.046(2)
#O(12B) 0.596(2) #O(21A) -1.488(2) #O(21B) -1.219(2) #O(22A) -0.175(2)
#O(22B) 0.191(2) #O(41A) -0.491(2) #O(42A) 1.251(2) #O(51A) -0.767(2)
#O(52A) 0.898(2) #C(1A)g -0.504(3) #C(1B)g -0.691(3) #C(2A)g -0.524(3)
#C(2B)g -0.647(3) #C(3A)g -0.290(3) #C(4A)g -0.050(3) #C(5A)g -0.046(3)
#C(6A)g -0.264(3) #C(6B)g -0.717(3) #C(11A) -0.837(3) #C(11B) -0.532(3)
#C(21A) -0.740(3) #C(21B) -0.563(3) #C(41A) 0.230(3) #C(51A) 0.074(3)
#Cu(1)h -1.606(1) #Cu(2)h 2.834(1) #Na(1)h 1.829(1) #Na(2)h 1.225(1)
#O(1W)h 1.218(2) #O(3W)h 0.740(3) #O(4W)h 1.748(2) #O(5W)h 1.474(3)
#O(6W)h 4.235(2) #O(7W)h -3.071(2) #O(11A) -0.706(2) #O(11B) -0.152(2)
#O(12A) 1.256(2) #O(12B) 1.899(2) #O(21A) -0.185(2) #O(21B) 0.084(2)
#O(22A) 1.128(2) #O(22B) 1.494(2) #O(41A) 0.812(2) #O(42A) 2.554(2)
#O(51A) 0.536(2) #O(52A) 2.201(2) #C(1A)h 0.799(3) #C(1B)h 0.612(3)
#C(2A)h 0.779(3) #C(2B)h 0.656(3) #C(3A)h 1.013(3) #C(4A)h 1.253(3)
#C(5A)h 1.256(3) #C(6A)h 1.038(3) #C(6B)h 0.586(3) #C(11A) 0.465(3)
#C(11B) 0.770(3) #C(21A) 0.563(3) #C(21B) 0.740(3) #C(41A) 1.532(3)
#C(51A) 1.377(3) #Cu(1)i 0.427(1) #Cu(2)i 4.867(1) #Na(1)i 3.862(1)
#Na(2)i 3.258(1) #O(1W)i 3.250(2) #O(3W)i 2.773(3) #O(4W)i 3.781(2)
#O(5W)i 3.507(3) #O(6W)i 6.268(2) #O(7W)i -1.039(2) #O(11A) 1.327(2)
#O(11B) 1.881(2) #O(12A) 3.289(2) #O(12B) 3.931(2) #O(21A) 1.848(2)
#O(21B) 2.116(2) #O(22A) 3.160(2) #O(22B) 3.526(2) #O(41A) 2.845(2)
#O(42A) 4.587(2) #O(51A) 2.569(2) #O(52A) 4.234(2) #C(1A)i 2.831(3)
#C(1B)i 2.644(3) #C(2A)i 2.812(3) #C(2B)i 2.688(3) #C(3A)i 3.046(3)
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					#C(4A)i	3.285(3)	#C(5A)i	3.289(3)	#C(6A)i	3.071(3)	#C(6B)i	2.618(3)	
					#C(11A)	2.498(3)	#C(11B)	2.803(3)	#C(21A)	2.595(3)	#C(21B)	2.772(3)	
					#C(41A)	3.565(3)	#C(51A)	3.409(3)	#Cu(1)j	4.514(1)	#Cu(2)j	0.129(1)	
					#Na(1)j	2.172(1)	#Na(2)j	2.725(1)	#O(1W)j	2.676(2)	#O(3W)j	2.832(3)	
					#O(4W)j	2.192(2)	#O(5W)j	2.163(3)	#O(6W)j	-1.112(2)	#O(7W)j	5.848(2)	
					#O(11A)	3.786(2)	#O(11B)	2.856(2)	#O(12A)	1.867(2)	#O(12B)	0.879(2)	
					#O(21A)	3.364(2)	#O(21B)	2.746(2)	#O(22A)	1.881(2)	#O(22B)	1.187(2)	
					#O(41A)	3.146(2)	#O(42A)	1.489(2)	#O(51A)	3.522(2)	#O(52A)	1.748(2)	
					#C(1A)j	2.560(3)	#C(1B)j	1.870(3)	#C(2A)j	2.580(3)	#C(2B)j	1.830(3)	
					#C(3A)j	2.533(3)	#C(4A)j	2.478(3)	#C(5A)j	2.474(3)	#C(6A)j	2.506(3)	
					#C(6B)j	1.714(3)	#C(11A)	2.705(3)	#C(11B)	1.903(3)	#C(21A)	2.602(3)	
					#C(21B)	1.944(3)	#C(41A)	2.391(3)	#C(51A)	2.549(3)			

Nr	8	P	Q	R	S	Sigref	0.002	Sigpln	0.005	Chisq	10.9	Pl.Hyp.	P<5

Plan		0.6566(6)	0.7337(5)	-0.1751(8)	3.303(2)	#Cu(1)	-0.004(1)	#O(7W)	0.002(2)	#O(11A)	0.002(2)	#O(11B)	0.001(2)
A 4		5.301(5)	12.402(8)	-4.182(12)	3.303(2)	Cu(2)	-1.278(1)	Na(2)	-0.223(1)	O(6W)	-1.432(2)	O(12A)	-1.150(2)
						O(12B)	-1.180(2)	C(1A)	-1.049(3)	C(1B)	-0.155(2)	C(2A)	-0.108(3)
						C(2B)	-1.115(3)	C(3A)	-0.562(3)	C(6B)	-0.701(3)	C(11A)	-0.693(3)
						C(11B)	-0.484(3)	C(21A)	1.375(2)	O(5W)b	0.257(3)	O(51A)	0.641(2)
						O(52A)	0.152(2)	C(51A)	0.969(3)	O(21B)	-0.417(2)	O(22B)	1.376(2)
						C(1B)c	0.064(3)	C(2B)c	0.992(3)	C(11B)	-1.427(2)	C(21B)	0.585(3)
						Na(2)d	-1.446(1)	O(3W)d	0.363(2)	O(41A)	0.002(2)	O(42A)	0.668(2)
						C(41A)	0.903(3)	Cu(1)e	1.164(1)	O(4W)e	-0.556(2)	O(5W)e	-0.742(3)
						O(6W)e	0.539(2)	O(11A)	-0.486(2)	O(12A)	0.252(2)	C(11A)	-0.649(3)
						Cu(1)h	0.498(1)	Na(2)h	0.717(1)	O(1W)h	-1.087(2)	O(3W)h	-1.076(2)
						O(7W)h	0.492(2)	O(11A)	0.492(2)	O(11B)	0.494(2)	O(22A)	-1.336(2)
						C(1B)h	0.649(3)	C(2A)h	0.602(3)	C(3A)h	1.056(3)	C(6B)h	1.195(3)
						C(11A)	1.187(3)	C(11B)	0.978(3)	C(21A)	-0.881(3)	Na(1)i	0.306(1)
						O(52A)	-1.458(2)						

Nr	9	P	Q	R	S	Sigref	0.002	Sigpln	0.025	Chisq	495.1	Pl.Hyp.	P<5

Plan		-0.1838(5)	0.3787(8)	0.9071(4)	2.318(4)	#Cu(1)	0.027(1)	#O(11B)	-0.008(2)	#O(21B)	-0.009(2)	#O(22B)	-0.016(2)
A 6		-1.484(4)	6.401(14)	14.377(6)	2.318(4)	#C(2B)b	0.023(3)	#C(21B)	-0.017(3)	O(12B)	-1.208(2)	O(21B)	1.475(2)
						O(22B)	1.469(2)	C(1B)	0.787(3)	C(11B)	-0.207(3)	C(21B)	1.468(3)
						O(4W)a	-0.829(2)	O(5W)a	-1.301(3)	O(11A)	-0.270(2)	O(11B)	1.476(2)
						O(12A)	-1.248(2)	O(12B)	0.276(2)	C(11A)	-1.226(3)	C(11B)	1.277(3)
						Cu(1)b	-1.458(1)	O(7W)b	0.545(2)	O(11B)	-1.492(2)	C(1B)b	-0.698(3)
						C(6B)b	0.843(3)	O(1W)d	-0.625(2)	O(3W)d	-1.352(3)	O(6W)d	-1.277(2)
						O(22A)	-1.367(2)	Cu(2)g	-0.136(1)	Na(1)g	0.567(1)	O(4W)g	-0.838(2)
						O(5W)g	-0.367(3)	O(11A)	-1.397(2)	O(12A)	-0.420(2)	O(21A)	1.311(2)
						O(22A)	1.208(2)	C(1A)g	0.661(3)	C(2A)g	1.409(3)	C(6A)g	0.857(3)
						C(11A)	-0.442(3)	C(21A)	1.285(3)	O(7W)h	1.220(2)	C(6B)h	0.922(3)
						Na(1)i	-0.918(1)	O(6W)i	0.377(2)	O(21A)	-0.173(2)	O(22A)	-0.277(2)
						O(51A)	0.152(2)	O(52A)	0.514(2)	C(1A)i	-0.823(3)	C(2A)i	-0.075(3)
						C(3A)i	0.859(3)	C(4A)i	1.049(3)	C(5A)i	0.291(3)	C(6A)i	-0.628(3)
						C(21A)	-0.199(3)	C(51A)	0.349(3)	Cu(2)j	-0.662(1)	Na(2)j	-1.127(1)

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					O(11A)	1.172(2)	O(11B)	1.074(2)	O(12A)	0.408(2)	O(12B)	0.231(2)
					O(21A)	-1.048(2)	O(41A)	0.445(2)	O(42A)	0.091(2)	C(1A)j	0.482(3)
					C(1B)j	0.774(3)	C(2A)j	-0.265(3)	C(3A)j	-0.278(3)	C(4A)j	0.438(3)
					C(5A)j	1.196(3)	C(6A)j	1.201(3)	C(6B)j	1.417(3)	C(11A)	0.660(3)
					C(11B)	0.719(3)	C(21A)	-1.094(3)	C(41A)	0.337(3)		

Nr 10	P	Q	R	S	Sigref	0.002	Sigpln	0.024	Chisq	531.5	Pl.Hyp.	P<5

Plan	-0.1741(5)	0.4203(6)	0.8905(3)	2.546(3)	#Cu(1)	-0.025(1)	#O(11B)	-0.006(2)	#O(21B)	-0.016(2)	#O(22B)	0.012(2)
A 6	-1.406(4)	7.106(11)	14.099(5)	2.546(3)	#C(21B)	0.018(3)	#O(51A)	0.018(2)	O(12B)	-1.218(2)	O(21B)	1.390(2)
					O(22B)	1.418(2)	C(1B)	0.832(3)	C(11B)	-0.199(3)	C(21B)	1.424(3)
					Cu(1)a	1.381(1)	O(4W)a	-1.275(2)	O(11A)	-0.417(2)	O(11B)	1.400(2)
					O(12A)	-1.402(2)	O(12B)	0.188(2)	C(11A)	-1.387(3)	C(11B)	1.207(3)
					Cu(1)b	-1.431(1)	O(7W)b	0.573(2)	O(11B)	-1.412(2)	C(1B)b	-0.574(3)
					C(2B)b	0.125(3)	C(6B)b	0.984(3)	O(1W)d	-0.611(2)	O(3W)d	-1.211(3)
					O(6W)d	-0.945(2)	O(22A)	-1.025(2)	Cu(2)g	-0.641(1)	Na(1)g	0.380(1)
					O(4W)g	-1.006(2)	O(5W)g	-0.653(3)	O(6W)g	1.367(2)	O(12A)	-0.879(2)
					O(21A)	0.805(2)	O(22A)	0.661(2)	O(51A)	1.424(2)	C(1A)g	0.244(3)
					C(2A)g	0.971(3)	C(5A)g	1.456(3)	C(6A)g	0.499(3)	C(11A)	-0.894(3)
					C(21A)	0.783(3)	O(7W)h	1.440(2)	C(6B)h	1.029(3)	Na(1)i	-1.026(1)
					O(6W)i	-0.039(2)	O(21A)	-0.601(2)	O(22A)	-0.745(2)	O(52A)	0.351(2)
					C(1A)i	-1.162(3)	C(2A)i	-0.435(3)	C(3A)i	0.537(3)	C(4A)i	0.787(3)
					C(5A)i	0.050(3)	C(6A)i	-0.907(3)	C(21A)	-0.623(3)	C(51A)	0.174(3)
					Cu(1)j	1.110(1)	O(11A)	0.254(2)	O(11B)	0.023(2)	O(12A)	-0.493(2)
					O(12B)	-0.793(2)	O(22B)	1.319(2)	O(41A)	-0.164(2)	O(42A)	-0.496(2)
					O(52A)	1.372(2)	C(1A)j	-0.335(3)	C(1B)j	-0.353(3)	C(2A)j	-1.060(3)
					C(2B)j	0.364(3)	C(3A)j	-1.010(3)	C(4A)j	-0.253(3)	C(5A)j	0.482(3)
					C(6A)j	0.425(3)	C(6B)j	0.208(3)	C(11A)	-0.224(3)	C(11B)	-0.342(3)
					C(21B)	1.336(3)	C(41A)	-0.288(3)	C(51A)	1.426(3)		

Nr 11	P	Q	R	S	Sigref	0.002	Sigpln	0.022	Chisq	298.3	Pl.Hyp.	P<5

Plan	-0.2938(11)	0.4913(5)	0.8200(5)	2.7778(18)	#Cu(1)	-0.019(1)	#O(22B)	0.007(2)	#O(51A)	0.018(2)	#O(52A)	0.007(2)
A 5	-2.372(9)	8.304(8)	13.285(8)	2.7778(18)	#C(51A)	-0.014(3)	O(11B)	0.364(2)	O(12B)	-0.578(2)	C(11B)	0.356(3)
					Cu(2)a	-0.129(1)	O(4W)a	-0.111(2)	O(5W)a	-0.531(3)	O(11A)	0.460(2)
					O(12A)	-0.237(2)	C(11A)	-0.407(3)	O(7W)b	-0.395(2)	O(21B)	-0.368(2)
					C(1B)b	-0.834(3)	C(2B)b	-0.021(3)	C(6B)b	0.982(3)	C(21B)	-0.156(3)
					Cu(2)d	-1.499(1)	Na(2)d	-0.965(1)	O(1W)d	0.621(2)	O(3W)d	0.017(3)
					O(6W)d	-0.496(2)	O(21A)	-0.495(2)	O(22A)	0.106(2)	C(21A)	-0.598(3)
					Cu(2)g	-0.682(1)	Na(1)g	0.887(1)	O(4W)g	-0.700(2)	O(5W)g	-0.280(3)
					O(6W)g	1.338(2)	O(11A)	-1.271(2)	O(12A)	-0.574(2)	O(22A)	1.209(2)
					C(1A)g	0.861(3)	C(6A)g	1.130(3)	C(11A)	-0.404(3)	Na(1)i	-1.485(1)
					O(6W)i	-1.034(2)	O(21A)	-0.673(2)	O(22A)	-1.163(2)	C(2A)i	-0.671(3)
					C(3A)i	0.426(3)	C(4A)i	0.688(3)	C(5A)i	-0.160(3)	C(6A)i	-1.242(3)
					C(21A)	-0.870(3)	Cu(1)j	0.441(1)	O(11A)	-0.352(2)	O(11B)	-0.469(2)
					O(12A)	-0.772(2)	O(12B)	-0.949(2)	O(22B)	1.396(2)	O(41A)	-0.547(2)
					O(42A)	-0.542(2)	C(1A)j	-0.709(3)	C(1B)j	-0.715(3)	C(2B)j	0.120(3)
					C(3A)j	-1.449(3)	C(4A)j	-0.536(3)	C(5A)j	0.312(3)	C(6A)j	0.208(3)

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						C(6B)j	-0.063(3)	C(11A)	-0.644(3)	C(11B)	-0.678(3)	C(21B)	1.246(3)
						C(41A)	-0.525(3)	C(51A)	1.413(3)				

Nr 12	P	Q	R	S	Sigref	0.001	Sigpln	0.029	Chisq	784.2	Pl.Hyp.	P<5	

Plan	0.6198(3)	0.7360(3)	-0.2723(7)	2.391(3)	#Cu(2)	0.017(1)	#O(6W)	0.006(2)	#O(12A)	-0.023(2)	#O(12B)	0.021(2)	
A 5	5.004(2)	12.442(5)	-5.595(10)	2.391(3)	#Na(2)d	-0.021(1)	Cu(1)	0.837(1)	Na(2)	0.893(1)	O(7W)	0.692(2)	
					O(11A)	0.935(2)	O(11B)	0.999(2)	O(41A)	-0.684(2)	C(1A)	0.027(3)	
					C(1B)	0.927(3)	C(2A)	0.975(3)	C(2B)	-0.038(3)	C(3A)	0.537(3)	
					C(4A)	-0.811(3)	C(6A)	-1.327(3)	C(6B)	0.377(3)	C(11A)	0.354(3)	
					C(11B)	0.608(3)	C(41A)	-1.188(3)	Na(1)b	-0.797(1)	O(5W)b	1.060(3)	
					O(51A)	1.341(2)	O(52A)	1.024(2)	O(7W)c	-1.050(2)	O(11B)	-0.670(2)	
					O(12B)	-0.385(2)	O(21B)	1.128(2)	C(11B)	0.023(3)	O(1W)d	-1.302(2)	
					O(41A)	1.486(2)	Na(1)e	-1.253(1)	O(4W)e	0.556(2)	O(5W)e	0.372(3)	
					O(6W)e	1.331(2)	O(11A)	0.812(2)	O(12A)	1.354(2)	O(22A)	-0.543(2)	
					C(1A)e	-0.939(3)	C(6A)e	-1.363(3)	C(11A)	0.532(3)	O(1W)h	-0.059(2)	
					O(3W)h	-0.004(2)	O(21A)	-0.428(2)	O(22A)	-0.318(2)	C(21A)	0.203(3)	
					Na(1)i	1.020(1)	O(5W)i	-0.837(3)	O(51A)	-1.118(2)	O(52A)	-0.801(2)	

Nr 13	P	Q	R	S	Sigref	0.002	Sigpln	0.019	Chisq	108.5	Pl.Hyp.	P<5	

Plan	-0.1248(15)	0.6006(10)	0.7898(6)	0.436(4)	#Cu(2)	-0.009(1)	#O(12A)	0.015(2)	#C(11A)	-0.008(3)	#O(41A)	0.002(2)	
A 4	-1.008(12)	10.153(17)	12.437(9)	0.436(4)	O(4W)	-1.204(2)	O(5W)	-1.003(3)	O(11A)	1.005(2)	O(21A)	-1.410(2)	
					O(22A)	-1.083(2)	C(1A)	-1.276(3)	C(21A)	-1.405(3)	Cu(2)a	0.999(1)	
					Na(1)a	-1.457(1)	O(4W)a	-0.197(2)	O(5W)a	0.005(3)	O(6W)a	-1.003(2)	
					O(12A)	1.022(2)	O(21A)	-0.402(2)	O(22A)	-0.075(2)	C(1A)a	-0.268(3)	
					C(2A)a	-0.875(3)	C(6A)a	-0.789(3)	C(11A)	1.000(3)	C(21A)	-0.398(3)	
					Cu(2)b	-1.017(1)	O(11A)	-0.002(2)	O(12A)	-0.993(2)	O(12B)	0.855(2)	
					C(11A)	-1.016(3)	Cu(1)d	0.542(1)	Na(2)d	1.317(1)	O(5W)d	-1.314(3)	
					O(7W)d	-0.395(2)	O(11A)	1.019(2)	O(21B)	-0.073(2)	O(22B)	0.895(2)	
					O(42A)	0.227(2)	O(52A)	-1.197(2)	C(1A)d	1.129(3)	C(3A)d	1.396(3)	
					C(4A)d	0.472(3)	C(5A)d	-0.142(3)	C(6A)d	0.201(3)	C(11A)	1.329(3)	
					C(21B)	0.839(3)	C(41A)	0.199(3)	C(51A)	-1.246(3)	Cu(1)f	-0.466(1)	
					Na(2)f	0.309(1)	O(7W)f	-1.403(2)	O(11A)	0.011(2)	O(11B)	0.849(2)	
					O(12A)	0.662(2)	O(21B)	-1.081(2)	O(22B)	-0.113(2)	O(41A)	-1.006(2)	
					O(42A)	-0.781(2)	C(1A)f	0.122(3)	C(2A)f	0.726(3)	C(2B)f	0.965(3)	
					C(3A)f	0.388(3)	C(4A)f	-0.536(3)	C(5A)f	-1.150(3)	C(6A)f	-0.807(3)	
					C(6B)f	1.397(3)	C(11A)	0.322(3)	C(11B)	1.252(3)	C(21B)	-0.169(3)	
					C(41A)	-0.809(3)	Cu(2)g	0.145(1)	O(4W)g	1.341(2)	O(5W)g	1.139(3)	
					O(11A)	-0.869(2)	O(12A)	0.122(2)	O(22A)	1.219(2)	C(1A)g	1.412(3)	
					C(11A)	0.144(3)	Cu(2)i	-0.863(1)	O(4W)i	0.333(2)	O(5W)i	0.132(3)	
					O(6W)i	1.140(2)	O(12A)	-0.886(2)	O(21A)	0.538(2)	O(22A)	0.211(2)	
					C(1A)i	0.404(3)	C(2A)i	1.011(3)	C(6A)i	0.926(3)	C(11A)	-0.863(3)	
					C(21A)	0.534(3)	Cu(1)j	-0.405(1)	Na(2)j	-1.180(1)	O(5W)j	1.450(3)	
					O(7W)j	0.531(2)	O(11A)	-0.882(2)	O(21B)	0.210(2)	O(22B)	-0.758(2)	
					O(41A)	0.134(2)	O(42A)	-0.091(2)	O(52A)	1.333(2)	C(1A)j	-0.993(3)	
					C(3A)j	-1.259(3)	C(4A)j	-0.336(3)	C(5A)j	0.278(3)	C(6A)j	-0.064(3)	
					C(11A)	-1.193(3)	C(21B)	-0.703(3)	C(41A)	-0.062(3)	C(51A)	1.383(3)	

Nr 14	P	Q	R	S	Sigref	0.002	Sigpln	0.044	Chisq	977.3	Pl.Hyp.	P<5
Plan	-0.1830(9)	0.5334(6)	0.8258(3)	0.187(3)	#Cu(2)	-0.009(1)	#O(12A)	0.027(2)	#C(11A)	-0.028(3)	#O(42A)	0.038(2)
A 5	-1.478(7)	9.017(10)	13.124(5)	0.187(3)	#C(41A)	-0.028(3)	O(4W)	-0.525(2)	O(5W)	-0.619(3)	O(11A)	0.942(2)
					O(22A)	-1.366(2)	C(1A)	-1.273(3)	Cu(2)a	1.468(1)	Na(1)a	-0.434(1)
					O(4W)a	0.952(2)	O(5W)a	0.859(3)	O(6W)a	-0.553(2)	O(21A)	-0.220(2)
					O(22A)	0.112(2)	C(1A)a	0.205(3)	C(2A)a	-0.497(3)	C(5A)a	-1.263(3)
					C(6A)a	-0.190(3)	C(11A)	1.450(3)	C(21A)	-0.159(3)	Cu(1)b	1.312(1)
					Cu(2)b	-1.487(1)	O(11A)	-0.536(2)	O(12A)	-1.451(2)	O(12B)	0.400(2)
					C(11B)	1.430(3)	Cu(1)d	-0.437(1)	Na(2)d	1.320(1)	O(11A)	0.215(2)
					O(11B)	0.723(2)	O(12A)	0.829(2)	O(12B)	1.376(2)	O(21B)	-1.391(2)
					O(22B)	-0.568(2)	O(41A)	-0.150(2)	C(1A)d	0.503(3)	C(1B)d	1.239(3)
					C(2A)d	1.203(3)	C(2B)d	0.543(3)	C(3A)d	0.994(3)	C(4A)d	0.105(3)
					C(5A)d	-0.604(3)	C(6A)d	-0.390(3)	C(6B)d	0.847(3)	C(11A)	0.561(3)
					C(11B)	1.067(3)	C(21B)	-0.559(3)	Cu(2)f	0.496(1)	Na(2)f	-0.158(1)
					O(1W)f	1.219(2)	O(3W)f	0.919(3)	O(6W)f	1.412(2)	O(11A)	-1.262(2)
					O(11B)	-0.754(2)	O(12A)	-0.649(2)	O(12B)	-0.102(2)	O(21A)	0.689(2)
					O(42A)	-1.440(2)	C(1A)f	-0.975(3)	C(1B)f	-0.239(3)	C(2A)f	-0.275(3)
					C(2B)f	-0.935(3)	C(3A)f	-0.484(3)	C(4A)f	-1.373(3)	C(6B)f	-0.631(3)
					C(11A)	-0.917(3)	C(11B)	-0.411(3)	C(21A)	0.730(3)	Cu(2)g	1.113(1)
					O(11A)	0.161(2)	O(12A)	1.077(2)	O(12B)	-0.774(2)	C(11A)	1.131(3)
					Cu(2)i	-0.365(1)	O(4W)i	0.151(2)	O(5W)i	0.245(3)	O(11A)	-1.317(2)
					O(12A)	-0.401(2)	O(21A)	1.323(2)	O(22A)	0.991(2)	C(1A)i	0.899(3)
					C(6A)i	1.294(3)	C(11A)	-0.347(3)	C(21A)	1.262(3)	Cu(2)j	-0.870(1)
					Na(2)j	-0.217(1)	O(3W)j	-1.294(3)	O(11A)	0.888(2)	O(11B)	0.380(2)
					O(12A)	0.274(2)	O(12B)	-0.273(2)	O(21A)	-1.063(2)	O(41A)	1.253(2)
					O(42A)	1.065(2)	C(1A)j	0.600(3)	C(1B)j	-0.136(3)	C(2A)j	-0.099(3)
					C(2B)j	0.561(3)	C(3A)j	0.110(3)	C(4A)j	0.998(3)	C(6A)j	1.493(3)
					C(6B)j	0.257(3)	C(11A)	0.542(3)	C(11B)	0.036(3)	C(21A)	-1.104(3)
					C(41A)	1.132(3)						
Nr 15	P	Q	R	S	Sigref	0.002	Sigpln	0.043	Chisq	1466.1	Pl.Hyp.	P<5
Plan	-0.2906(10)	0.5191(4)	0.8038(5)	0.384(5)	#Cu(2)	0.048(1)	#O(21A)	-0.011(2)	#O(41A)	-0.007(2)	#O(42A)	-0.039(2)
A 6	-2.346(8)	8.776(7)	13.028(8)	0.384(5)	#C(4A)d	0.032(3)	#C(41A)	-0.024(3)	O(4W)	-0.166(2)	O(5W)	-0.509(3)
					O(11A)	0.588(2)	O(12A)	-0.101(2)	C(11A)	-0.282(3)	Na(1)a	0.604(1)
					O(6W)a	0.374(2)	O(22A)	0.516(2)	O(51A)	-0.893(2)	O(52A)	-0.851(2)
					C(1A)a	0.777(3)	C(2A)a	-0.051(3)	C(3A)a	-1.173(3)	C(4A)a	-1.474(3)
					C(5A)a	-0.639(3)	C(6A)a	0.469(3)	C(21A)	0.189(3)	C(51A)	-0.828(3)
					Cu(1)b	0.142(1)	O(11B)	0.572(2)	O(12B)	-0.366(2)	C(11B)	0.574(3)
					Cu(1)d	-0.730(1)	Cu(2)d	1.333(1)	O(11A)	0.008(2)	O(11B)	0.207(2)
					O(12A)	0.404(2)	O(12B)	0.655(2)	C(1A)d	0.289(3)	C(1B)d	0.498(3)
					C(2A)d	1.115(3)	C(2B)d	-0.325(3)	C(3A)d	0.974(3)	C(5A)d	-0.802(3)
					C(6A)d	-0.657(3)	C(6B)d	-0.102(3)	C(11A)	0.270(3)	C(11B)	0.417(3)
					C(21B)	-1.479(3)	Cu(2)f	-1.014(1)	Na(2)f	-0.709(1)	O(1W)f	0.865(2)
					O(3W)f	0.347(3)	O(6W)f	-0.068(2)	O(21A)	-0.064(2)	O(22A)	0.562(2)
					C(2A)f	-1.232(3)	C(3A)f	-1.372(3)	C(21A)	-0.165(3)	Cu(1)g	-0.910(1)

=====													
						O(11A)	0.990(2)	O(11B)	-1.340(2)	O(12B)	-0.402(2)	C(11B)	-1.342(3)
						Cu(2)i	-0.816(1)	Na(1)i	0.974(1)	O(4W)i	-0.602(2)	O(5W)i	-0.259(3)
						O(6W)i	1.204(2)	O(11A)	-1.356(2)	O(12A)	-0.667(2)	O(22A)	1.062(2)
						C(1A)i	0.802(3)	C(6A)i	1.109(3)	C(11A)	-0.486(3)	C(21A)	1.389(3)
						Cu(2)j	0.246(1)	Na(2)j	-0.059(1)	O(3W)j	-1.115(3)	O(6W)j	-0.700(2)
						O(11B)	1.371(2)	O(12A)	1.175(2)	O(12B)	0.923(2)	O(21A)	-0.704(2)
						O(22A)	-1.330(2)	C(1A)j	1.289(3)	C(1B)j	1.081(3)	C(2A)j	0.464(3)
						C(3A)j	0.604(3)	C(11A)	1.308(3)	C(11B)	1.161(3)	C(21A)	-0.603(3)

Nr 16	P	Q	R	S	Sigref	0.002	Sigpln	0.019	Chisq	90.3	Pl.Hyp.	P<5	

Plan	0.1978(11)	0.9800(2)	0.0212(9)	-3.142(3)	#Na(1)	-0.008(1)	#O(4W)	0.004(3)	#O(41A)	0.014(2)	#C(41A)	-0.010(3)	
A 4	1.597(9)	16.567(4)	-0.122(13)	-3.142(3)	O(42A)	0.670(2)	O(51A)	0.372(2)	O(52A)	0.685(2)	C(51A)	1.069(3)	
					Na(2)a	0.410(1)	O(1W)a	1.160(2)	O(5W)a	0.759(3)	O(42A)	-0.927(2)	
					O(51A)	-1.226(2)	O(52A)	-0.912(2)	C(4A)a	1.096(3)	C(5A)a	0.857(3)	
					C(51A)	-0.528(3)	Cu(1)c	-0.748(1)	Cu(2)c	-0.527(1)	O(7W)c	0.140(2)	
					O(11B)	0.900(2)	O(12B)	0.799(2)	O(21B)	0.729(2)	C(11B)	1.331(3)	
					Cu(1)e	0.849(1)	Cu(2)e	1.071(1)	O(6W)e	-0.003(2)	O(11A)	-0.401(2)	
					O(12A)	-0.295(2)	O(22A)	-0.189(2)	C(11A)	-0.824(3)	C(21A)	-1.305(3)	
					O(3W)g	0.256(2)	O(6W)g	-1.016(2)	O(12A)	-1.302(2)	C(1A)g	-0.161(3)	
					C(2A)g	-0.402(3)	C(3A)g	0.689(3)	C(6A)g	1.154(3)	C(11A)	-1.238(3)	
					Cu(1)i	-1.309(1)	Cu(2)i	-0.374(1)	O(6W)i	0.582(2)	O(11A)	-0.364(2)	
					O(12A)	0.296(2)	O(12B)	-1.419(2)	O(21A)	-0.349(2)	O(21B)	-0.822(2)	
					O(22A)	-1.064(2)	O(22B)	-1.381(2)	C(1A)i	1.436(3)	C(2A)i	1.196(3)	
					C(11A)	0.359(3)	C(21A)	-0.190(3)					

Nr 17	P	Q	R	S	Sigref	0.002	Sigpln	0.040	Chisq	676.1	Pl.Hyp.	P<5	

Plan	-0.6476(6)	0.0577(6)	0.7598(6)	0.952(3)	#Na(1)	-0.041(1)	#O(5W)	0.016(3)	#O(21B)	0.032(2)	#C(21B)	-0.013(3)	
A 5	-5.229(5)	0.975(11)	13.161(9)	0.952(3)	#O(11A)	0.006(2)	Cu(1)	-0.260(1)	Cu(2)	-1.468(1)	O(7W)	1.430(2)	
					O(11B)	0.215(2)	O(12B)	0.153(2)	C(1B)	1.434(3)	C(11B)	0.542(3)	
					O(21A)	-0.432(2)	O(22A)	0.261(2)	O(41A)	-0.919(2)	O(42A)	-0.485(2)	
					C(2A)a	0.794(3)	C(3A)a	0.052(3)	C(4A)a	0.542(3)	C(21A)	0.181(3)	
					C(41A)	-0.336(3)	O(22B)	-1.272(2)	Na(2)c	-0.850(1)	O(1W)c	1.254(2)	
					O(3W)c	-0.890(3)	Na(2)d	0.125(1)	O(3W)d	0.085(3)	O(4W)g	1.296(2)	
					O(22B)	-0.632(2)	C(2B)g	0.642(3)	C(6B)g	-0.050(3)	O(21B)	1.008(2)	
					O(22B)	0.343(2)	C(6B)h	0.925(3)	C(21B)	0.962(3)	Cu(2)i	-0.436(1)	
					O(6W)i	1.203(2)	O(12A)	-0.132(2)	O(51A)	0.799(2)	O(52A)	0.387(2)	
					C(1A)i	1.270(3)	C(6A)i	0.782(3)	C(11A)	0.331(3)	C(51A)	0.868(3)	
					O(1W)j	1.095(2)							

Nr 18	P	Q	R	S	Sigref	0.002	Sigpln	0.011	Chisq	77.2	Pl.Hyp.	P<5	

Plan	-0.1362(7)	0.9884(1)	0.0671(5)	-3.376(4)	#Na(2)	-0.007(1)	#O(1W)	0.008(2)	#Na(1)b	0.008(1)	#O(52A)	-0.009(2)	
A 5	-1.099(6)	16.7085(15)	1.341(9)	-3.376(4)	#C(51A)	0.000(3)	Na(1)	1.107(1)	O(41A)	0.294(2)	O(42A)	-0.063(2)	
					O(51A)	0.212(2)	O(52A)	1.091(2)	C(41A)	0.658(3)	C(51A)	1.099(3)	
					Na(2)a	1.092(1)	O(1W)a	1.107(2)	O(41A)	1.393(2)	O(42A)	1.037(2)	
					O(51A)	1.311(2)	Na(2)b	-1.106(1)	O(1W)b	-1.091(2)	O(3W)b	1.330(2)	

						0(4W)b	0.742(3)	0(41A)	-0.806(2)	0(42A)	-1.162(2)	0(51A)	-0.888(2)
						C(4A)b	0.919(3)	C(5A)b	1.132(3)	C(41A)	-0.441(3)	Cu(1)c	-1.241(1)
						O(7W)c	-0.584(2)	O(11B)	-0.111(2)	O(12B)	-0.704(2)	O(21B)	-1.448(2)
						O(22A)	-1.283(2)	O(22B)	-0.696(2)	C(1B)c	1.069(3)	C(2B)c	0.835(3)
						C(11B)	-0.023(3)	C(21B)	-0.555(3)	O(11B)	-1.210(2)	C(1B)e	-0.031(3)
						C(2B)e	-0.265(3)	C(6B)e	0.823(3)	C(11B)	-1.123(3)	Cu(1)g	0.025(1)
						Cu(2)g	0.290(1)	O(6W)g	1.490(2)	O(7W)g	-0.997(2)	O(11A)	1.344(2)
						O(11B)	-1.447(2)	O(12A)	1.468(2)	O(12B)	-1.109(2)	O(21B)	-1.181(2)
						O(22A)	1.277(2)	Cu(1)i	-1.074(1)	Cu(2)i	-0.810(1)	O(6W)i	0.391(2)
						O(11A)	0.245(2)	O(12A)	0.369(2)	O(21A)	1.474(2)	O(22A)	0.178(2)
						C(11A)	0.796(3)	C(21A)	1.227(3)	Na(1)j	-0.303(1)	O(4W)j	-0.357(3)
						O(42A)	-0.938(2)	O(51A)	-0.470(2)	O(52A)	-0.996(2)	C(51A)	-1.276(3)
Nr 19	P	Q	R	S	Sigref	0.002	Sigpln	0.002	Chisq	0.8	Pl.Hyp.		
Plan	-0.523(4)	-0.0877(5)	0.848(2)	-6.739(13)	#Na(2)	-0.001(1)	#O(3W)	0.000(3)	#O(22A)	0.000(2)	#C(21A)	0.000(3)	
A 4	-4.23(3)	-1.482(9)	14.23(3)	-6.739(13)	Cu(2)b	0.853(1)	O(6W)b	-0.723(2)	O(11A)	1.158(2)	O(12A)	0.999(2)	
					O(51A)	1.197(2)	O(52A)	1.186(2)	C(1A)b	0.026(3)	C(2A)b	-1.124(3)	
					C(4A)b	-1.063(3)	C(5A)b	0.093(3)	C(6A)b	0.617(3)	C(11A)	0.754(3)	
					C(51A)	0.862(3)	Cu(1)c	-0.556(1)	Cu(2)c	1.303(1)	Na(1)c	-0.024(1)	
					O(5W)c	-0.188(3)	O(11A)	1.131(2)	O(11B)	-0.776(2)	O(12A)	1.339(2)	
					O(12B)	-0.364(2)	C(11B)	-0.924(3)	Cu(2)d	-0.179(1)	O(11A)	-0.351(2)	
					O(12A)	-0.143(2)	O(51A)	0.722(2)	O(52A)	0.609(2)	C(1A)d	1.097(3)	
					C(5A)d	1.453(3)	C(6A)d	0.718(3)	C(11A)	0.155(3)	C(51A)	0.907(3)	
					O(6W)e	-1.166(2)	O(21A)	0.438(2)	O(41A)	1.162(2)	O(42A)	1.068(2)	
					C(2A)e	-0.497(3)	C(3A)e	0.248(3)	C(4A)e	-0.134(3)	C(5A)e	-1.291(3)	
					C(41A)	0.744(3)	O(3W)f	1.366(3)	O(21A)	-1.044(2)	O(22A)	-1.482(2)	
					O(41A)	-0.320(2)	O(42A)	-0.413(2)	C(3A)f	-1.233(3)	C(21A)	-1.482(3)	
					C(41A)	-0.737(3)							
Nr 20	P	Q	R	S	Sigref	0.002	Sigpln	0.051	Chisq	1296.5	Pl.Hyp.	P<5	
Plan	-0.6376(6)	-0.0820(6)	0.7660(5)	-7.102(2)	#Na(2)	0.021(1)	#O(3W)	0.004(3)	#O(12B)	-0.014(2)	#O(22A)	-0.053(2)	
A 5	-5.148(5)	-1.386(9)	13.234(8)	-7.102(2)	#C(21A)	0.043(3)	Cu(2)b	0.822(1)	O(6W)b	-0.678(2)	O(11A)	0.534(2)	
					O(12A)	0.686(2)	O(51A)	0.621(2)	O(52A)	0.909(2)	C(1A)b	-0.486(3)	
					C(5A)b	-0.399(3)	C(6A)b	0.164(3)	C(11A)	0.279(3)	C(51A)	0.422(3)	
					Cu(1)c	0.370(1)	Na(1)c	0.366(1)	O(5W)c	0.249(3)	O(7W)c	-1.347(2)	
					O(11B)	-0.114(2)	C(1B)c	-1.348(3)	C(11B)	-0.431(3)	Cu(1)d	-1.016(1)	
					Cu(2)d	0.250(1)	Na(1)d	-1.020(1)	O(5W)d	-1.137(3)	O(11A)	0.661(2)	
					O(11B)	-1.500(2)	O(12A)	0.556(2)	O(12B)	-1.400(2)	O(52A)	1.211(2)	
					C(11A)	1.012(3)	O(21A)	0.644(2)	O(41A)	1.260(2)	O(42A)	0.865(2)	
					C(2A)e	-0.533(3)	C(3A)e	0.236(3)	C(4A)e	-0.220(3)	C(5A)e	-1.475(3)	
					C(41A)	0.686(3)	O(21A)	-0.742(2)	O(22A)	-1.439(2)	O(41A)	-0.125(2)	
					O(42A)	-0.521(2)	C(3A)f	-1.150(3)	C(21A)	-1.343(3)	C(41A)	-0.700(3)	
Nr 21	P	Q	R	S	Sigref	0.001	Sigpln	0.028	Chisq	406.9	Pl.Hyp.	P<5	
Plan	0.5731(4)	0.7826(3)	-0.2431(8)	3.4269(16)	#Cu(1)	0.022(1)	#O(7W)	-0.011(2)	#O(11A)	-0.014(2)	#Na(1)i	0.003(1)	

A	4	4.627(3)	13.230(4)	-5.039(12)	3.4269(16)	Cu(2)	-0.806(1)	Na(2)	-0.662(1)	O(1W)	1.052(2)	O(3W)	1.225(2)
						O(6W)	-0.937(2)	O(11B)	0.298(2)	O(12A)	-0.940(2)	O(12B)	-0.668(2)
						C(1A)	-1.051(3)	C(1B)	0.377(3)	C(2A)	-0.179(3)	C(2B)	-0.513(3)
						C(3A)	-0.712(3)	C(6B)	-0.004(3)	C(11A)	-0.619(3)	C(11B)	-0.048(3)
						C(21A)	1.315(3)	O(5W)b	-0.271(3)	O(42A)	1.234(2)	O(51A)	-0.293(2)
						O(52A)	-0.522(2)	C(51A)	0.180(3)	O(21B)	-0.604(2)	O(22B)	1.027(2)
						C(1B)c	0.010(3)	C(2B)c	0.865(3)	C(21B)	0.359(3)	Na(2)d	-0.635(1)
						O(3W)d	1.320(2)	O(41A)	0.742(2)	O(42A)	1.153(2)	Cu(1)e	0.670(1)
						Cu(2)e	0.930(1)	O(6W)e	-0.560(2)	O(11A)	-1.047(2)	O(12A)	-0.563(2)
						C(11A)	-1.357(3)	O(1W)h	0.697(2)	O(3W)h	0.524(2)	O(11B)	1.451(2)
						O(21A)	-0.142(2)	O(22A)	-0.148(2)	C(1B)h	1.372(3)	C(21A)	0.434(3)
						O(4W)i	1.084(2)						

Nr	22	P	Q	R	S	Sigref	0.002	Sigpln	0.024	Chisq	179.0	Pl.Hyp.	P<5
Plan		-0.1428(7)	0.3573(14)	0.9230(6)	-2.075(6)	#O(21A)	0.014(2)	#O(22A)	0.008(2)	#C(21A)	-0.017(3)	#Cu(2)b	-0.005(1)
A	4	-1.153(5)	6.04(2)	14.529(9)	-2.075(6)	Cu(2)	1.148(1)	Na(1)	0.597(1)	O(5W)	1.491(3)	O(6W)	-0.834(2)
						O(51A)	-0.314(2)	O(52A)	-0.783(2)	C(1A)	0.561(3)	C(2A)	-0.143(3)
						C(3A)	-1.035(3)	C(4A)	-1.225(3)	C(5A)	-0.510(3)	C(6A)	0.366(3)
						C(51A)	-0.567(3)	O(3W)a	-1.417(3)	O(6W)a	0.319(2)	O(21A)	1.167(2)
						O(22A)	1.161(2)	O(41A)	-1.078(2)	O(51A)	0.839(2)	O(52A)	0.370(2)
						C(2A)a	1.010(3)	C(3A)a	0.118(3)	C(4A)a	-0.072(3)	C(5A)a	0.643(3)
						C(21A)	1.136(3)	C(41A)	-1.076(3)	C(51A)	0.586(3)	Na(1)b	-0.556(1)
						O(4W)b	0.774(2)	O(5W)b	0.338(3)	O(11A)	1.451(2)	O(12A)	0.385(2)
						O(21A)	-1.139(2)	O(22A)	-1.145(2)	O(51A)	-1.467(2)	C(1A)b	-0.592(3)
						C(2A)b	-1.296(3)	C(6A)b	-0.787(3)	C(11A)	0.466(3)	C(21A)	-1.170(3)
						Cu(1)d	-1.237(1)	O(11A)	-0.297(2)	O(11B)	-0.149(2)	O(12A)	0.568(2)
						O(12B)	0.796(2)	O(22B)	-1.310(2)	O(41A)	0.469(2)	O(42A)	0.929(2)
						O(52A)	-0.937(2)	C(1A)d	0.455(3)	C(1B)d	0.199(3)	C(2A)d	1.158(3)
						C(2B)d	-0.494(3)	C(3A)d	1.181(3)	C(4A)d	0.516(3)	C(5A)d	-0.198(3)
						C(6A)d	-0.212(3)	C(6B)d	-0.403(3)	C(11A)	0.270(3)	C(11B)	0.255(3)
						C(21B)	-1.374(3)	C(41A)	0.626(3)	C(51A)	-1.049(3)	Cu(2)f	0.547(1)
						Na(2)f	0.830(1)	O(3W)f	1.443(3)	O(11A)	-1.450(2)	O(11B)	-1.302(2)
						O(12A)	-0.586(2)	O(12B)	-0.357(2)	O(21A)	0.679(2)	O(22A)	1.479(2)
						O(41A)	-0.684(2)	O(42A)	-0.225(2)	C(1A)f	-0.698(3)	C(1B)f	-0.954(3)
						C(2A)f	0.005(3)	C(3A)f	0.028(3)	C(4A)f	-0.637(3)	C(5A)f	-1.351(3)
						C(6A)f	-1.365(3)	C(11A)	-0.883(3)	C(11B)	-0.898(3)	C(21A)	0.779(3)
						C(41A)	-0.528(3)	Cu(1)g	0.958(1)	O(7W)g	-1.035(2)	O(11B)	1.106(2)
						O(21B)	-0.280(2)	O(22B)	-0.164(2)	C(1B)g	0.421(3)	C(2B)g	-0.256(3)
						C(6B)g	-1.028(3)	C(11B)	1.363(3)	C(21B)	-0.219(3)	Cu(1)i	-0.195(1)
						O(11B)	-0.047(2)	O(12B)	1.234(2)	O(21B)	-1.434(2)	O(22B)	-1.317(2)
						C(1B)i	-0.732(3)	C(2B)i	-1.409(3)	C(11B)	0.210(3)	C(21B)	-1.372(3)

Nr	23	P	Q	R	S	Sigref	0.002	Sigpln	0.001	Chisq	0.2	Pl.Hyp.	
Plan		-0.523(4)	0.0877(5)	0.848(2)	-3.861(5)	#O(22A)	0.000(2)	#C(21A)	0.000(3)	#Na(2)f	0.001(1)	#O(3W)f	0.000(3)
A	4	-4.23(3)	1.482(9)	14.23(3)	-3.861(5)	O(6W)	1.166(2)	O(21A)	-0.438(2)	O(41A)	-1.162(2)	O(42A)	-1.068(2)
						C(2A)	0.497(3)	C(3A)	-0.248(3)	C(4A)	0.134(3)	C(5A)	1.291(3)

=====												
						C(41A)	-0.744(3)	Na(2)a	0.947(1)	O(1W)a	-0.930(2)	O(3W)a 1.378(3)
						Cu(1)b	0.556(1)	Cu(2)b	-1.303(1)	Na(1)b	0.024(1)	O(5W)b 0.188(3)
						O(11A)	-1.131(2)	O(11B)	0.776(2)	O(12A)	-1.339(2)	O(12B) 0.364(2)
						C(11B)	0.924(3)	O(6W)c	-0.759(2)	O(21A)	0.781(2)	O(22A) 0.538(2)
						O(41A)	0.619(2)	O(42A)	0.429(2)	C(2A)c	-0.358(3)	C(3A)c 0.174(3)
						C(4A)c	-0.418(3)	C(21A)	0.360(3)	C(41A)	0.241(3)	Cu(2)d -0.853(1)
						O(6W)d	0.723(2)	O(11A)	-1.158(2)	O(12A)	-0.999(2)	O(51A) -1.197(2)
						O(52A)	-1.186(2)	C(1A)d	-0.026(3)	C(2A)d	1.124(3)	C(4A)d 1.063(3)
						C(5A)d	-0.093(3)	C(6A)d	-0.617(3)	C(11A)	-0.754(3)	C(51A) -0.862(3)
						Na(2)e	-1.481(1)	O(1W)e	0.460(2)	O(3W)e	-1.482(3)	O(7W)i 1.130(2)
						O(21B)	-0.038(2)	O(22B)	-0.430(2)	C(2B)i	0.568(3)	C(6B)i -0.104(3)
						C(21B)	0.010(3)					

Nr 24	P	Q	R	S	Sigref	0.002		Sigpln	0.025	Chisq	495.1	Pl.Hyp. P<5

Plan	-0.1838(5)	0.3787(8)	0.9071(4)	3.802(6)	#O(21B)	-0.009(2)	#O(22B)	-0.016(2)	#C(2B)	0.023(3)	#C(21B)	-0.017(3)
A 6	-1.484(4)	6.401(14)	14.377(6)	3.802(6)	#Cu(1)a	0.027(1)	#O(11B)	-0.008(2)	Cu(1)	-1.458(1)	O(7W)	0.545(2)
					O(11B)	-1.492(2)	C(1B)	-0.698(3)	C(6B)	0.843(3)	O(12B)	-1.208(2)
					O(21B)	1.475(2)	O(22B)	1.469(2)	C(1B)a	0.787(3)	C(11B)	-0.207(3)
					C(21B)	1.468(3)	O(7W)b	-0.940(2)	O(21B)	-1.493(2)	O(22B)	-1.500(2)
					C(2B)b	-1.461(3)	C(6B)b	-0.641(3)	Na(1)g	-0.918(1)	O(6W)g	0.377(2)
					O(21A)	-0.173(2)	O(22A)	-0.277(2)	O(51A)	0.152(2)	O(52A)	0.514(2)
					C(1A)g	-0.823(3)	C(2A)g	-0.075(3)	C(3A)g	0.859(3)	C(4A)g	1.049(3)
					C(5A)g	0.291(3)	C(6A)g	-0.628(3)	C(21A)	-0.199(3)	C(51A)	0.349(3)
					O(7W)h	-0.264(2)	O(21B)	0.290(2)	O(22B)	0.296(2)	C(1B)h	0.978(3)
					C(2B)h	0.257(3)	C(6B)h	-0.562(3)	C(21B)	0.297(3)	O(3W)i	1.024(3)
					O(6W)i	-1.108(2)	O(41A)	0.674(2)	O(42A)	1.448(2)	O(51A)	-1.332(2)
					O(52A)	-0.970(2)	C(3A)i	-0.625(3)	C(4A)i	-0.435(3)	C(5A)i	-1.193(3)
					C(41A)	0.614(3)	C(51A)	-1.135(3)	Cu(1)j	0.621(1)	O(5W)j	1.394(3)
					O(11A)	-0.312(2)	O(11B)	-0.411(2)	O(12A)	-1.076(2)	O(12B)	-1.254(2)
					O(22B)	0.950(2)	O(41A)	-1.040(2)	O(42A)	-1.393(2)	O(51A)	1.461(2)
					O(52A)	0.560(2)	C(1A)j	-1.002(3)	C(1B)j	-0.710(3)	C(2B)j	0.028(3)
					C(4A)j	-1.046(3)	C(5A)j	-0.288(3)	C(6A)j	-0.284(3)	C(6B)j	-0.067(3)
					C(11A)	-0.825(3)	C(11B)	-0.765(3)	C(21B)	0.959(3)	C(41A)	-1.148(3)
					C(51A)	0.615(3)						

Nr 25	P	Q	R	S	Sigref	0.001		Sigpln	0.036	Chisq	666.3	Pl.Hyp. P<5

Plan	-0.4282(4)	0.6543(4)	-0.6234(6)	-1.350(6)	#Na(2)	0.031(1)	#O(1W)	-0.015(2)	#O(41A)	-0.012(2)	#Cu(2)c	-0.003(1)
A 4	-3.457(3)	11.060(7)	-8.624(10)	-1.350(6)	Na(1)	1.497(1)	O(3W)	1.423(2)	O(42A)	1.067(2)	O(51A)	-0.197(2)
					C(41A)	0.812(3)	C(51A)	1.080(3)	Cu(1)b	0.257(1)	O(4W)b	-1.443(2)
					O(5W)b	-0.565(3)	O(7W)b	-0.081(2)	O(11A)	-0.048(2)	O(12A)	1.359(2)
					O(21A)	-0.629(2)	O(22A)	1.320(2)	C(1A)b	-0.295(3)	C(2A)b	-0.495(3)
					C(3A)b	-1.275(3)	C(6A)b	-0.885(3)	C(11A)	0.437(3)	C(21A)	0.132(3)
					O(1W)c	-1.014(2)	O(3W)c	0.279(2)	O(12A)	0.694(2)	O(12B)	1.244(2)
					O(22B)	1.393(2)	C(1A)c	0.353(3)	C(2A)c	0.550(3)	C(3A)c	-0.261(3)
					C(4A)c	-1.245(3)	C(5A)c	-1.431(3)	C(6A)c	-0.637(3)	C(11A)	1.219(3)
					Cu(1)e	0.173(1)	O(11A)	-0.987(2)	O(11B)	-0.282(2)	O(21A)	-1.251(2)

=====												
						O(21B)	-1.406(2)	C(1B)e	-0.209(3)	C(2B)e	-0.439(3)	C(6B)e 0.242(3)
						C(11B)	-0.952(3)	C(21B)	-1.373(3)	Cu(2)g	-0.715(1)	O(6W)g -0.877(2)
						O(11B)	0.265(2)	O(12A)	1.340(2)	O(12B)	-1.051(2)	O(21B) 0.202(2)
						O(22A)	1.380(2)	C(11B)	-0.673(3)	C(21B)	-1.008(3)	Cu(1)i -1.015(1)
						Na(1)i	1.202(1)	O(3W)i	1.276(2)	O(4W)i	0.685(2)	O(5W)i -0.194(3)
						O(7W)i	-0.677(2)	O(11A)	-0.710(2)	O(21A)	-0.129(2)	O(52A) 0.986(2)
						C(1A)i	-0.464(3)	C(2A)i	-0.263(3)	C(3A)i	0.517(3)	C(4A)i 1.099(3)
						C(5A)i	0.912(3)	C(6A)i	0.127(3)	C(11A)	-1.196(3)	C(21A) -0.890(3)
						Na(1)j	-1.463(1)	O(4W)j	-1.467(2)			

Nr 26	P	Q	R	S	Sigref	0.002	Sigpln	0.019	Chisq	90.3	Pl.Hyp.	P<5

Plan	0.1978(11)	0.9800(2)	0.0212(9)	-1.545(6)	#O(41A)	0.014(2)	#C(41A)	-0.010(3)	#Na(1)b	-0.008(1)	#O(4W)b	0.004(3)
A 4	1.597(9)	16.567(4)	-0.122(13)	-1.545(6)	Na(2)	0.410(1)	O(1W)	1.160(2)	O(5W)	0.759(3)	O(42A)	-0.927(2)
					O(51A)	-1.226(2)	O(52A)	-0.912(2)	C(4A)	1.096(3)	C(5A)	0.857(3)
					C(51A)	-0.528(3)	Na(2)a	-1.188(1)	O(1W)a	-0.437(2)	O(3W)a	1.237(2)
					O(5W)a	-0.838(3)	C(3A)a	0.805(3)	C(4A)a	-0.501(3)	C(5A)a	-0.740(3)
					C(6A)a	0.339(3)	O(42A)	0.670(2)	O(51A)	0.372(2)	O(52A)	0.685(2)
					C(51A)	1.069(3)	O(7W)c	-1.457(2)	O(11B)	-0.697(2)	O(12B)	-0.799(2)
					O(21B)	-0.869(2)	O(22B)	0.461(2)	C(1B)c	1.093(3)	C(2B)c	1.316(3)
					C(11B)	-0.266(3)	C(21B)	0.194(3)	Cu(1)e	-0.748(1)	Cu(2)e	-0.527(1)
					O(7W)e	0.140(2)	O(11B)	0.900(2)	O(12B)	0.799(2)	O(21B)	0.729(2)
					C(11B)	1.331(3)	Na(2)g	1.084(1)	O(1W)g	0.333(2)	O(3W)g	-1.341(2)
					O(5W)g	0.734(3)	O(41A)	1.479(2)	C(3A)g	-0.909(3)	C(4A)g	0.397(3)
					C(5A)g	0.636(3)	C(6A)g	-0.443(3)	O(3W)i	0.256(2)	O(6W)i	-1.016(2)
					O(12A)	-1.302(2)	C(1A)i	-0.161(3)	C(2A)i	-0.402(3)	C(3A)i	0.689(3)
					C(6A)i	1.154(3)	C(11A)	-1.238(3)				

Nr 27	P	Q	R	S	Sigref	0.002	Sigpln	0.022	Chisq	298.3	Pl.Hyp.	P<5

Plan	-0.2938(11)	0.4913(5)	0.8200(5)	-2.7778(18)	#O(51A)	-0.018(2)	#O(52A)	-0.007(2)	#C(51A)	0.014(3)	#O(22B)	-0.007(2)
A 5	-2.372(8)	8.304(8)	13.285(8)	-2.7778(18)	#Cu(1)i	0.019(1)	Na(1)	1.485(1)	O(6W)	1.034(2)	O(21A)	0.673(2)
					O(22A)	1.163(2)	C(2A)	0.671(3)	C(3A)	-0.426(3)	C(4A)	-0.688(3)
					C(5A)	0.160(3)	C(6A)	1.242(3)	C(21A)	0.870(3)	Na(2)a	-1.398(1)
					O(3W)a	0.031(3)	O(41A)	0.225(2)	O(42A)	-0.314(2)	C(41A)	0.466(3)
					Cu(2)b	0.682(1)	Na(1)b	-0.887(1)	O(4W)b	0.700(2)	O(5W)b	0.280(3)
					O(6W)b	-1.338(2)	O(11A)	1.271(2)	O(12A)	0.574(2)	O(22A)	-1.209(2)
					C(1A)b	-0.861(3)	C(6A)b	-1.130(3)	C(11A)	0.404(3)	Na(1)d	-0.992(1)
					O(5W)d	0.165(3)	O(7W)d	0.769(2)	O(21B)	0.405(2)	O(22B)	0.976(2)
					O(51A)	0.150(2)	O(52A)	0.837(2)	C(21B)	1.127(3)	C(51A)	0.960(3)
					Cu(1)f	-0.441(1)	O(11A)	0.352(2)	O(11B)	0.469(2)	O(12A)	0.772(2)
					O(12B)	0.949(2)	O(22B)	-1.396(2)	O(41A)	0.547(2)	O(42A)	0.542(2)
					C(1A)f	0.709(3)	C(1B)f	0.715(3)	C(2B)f	-0.120(3)	C(3A)f	1.449(3)
					C(4A)f	0.536(3)	C(5A)f	-0.312(3)	C(6A)f	-0.208(3)	C(6B)f	0.063(3)
					C(11A)	0.644(3)	C(11B)	0.678(3)	C(21B)	-1.246(3)	C(41A)	0.525(3)
					C(51A)	-1.413(3)	O(7W)g	0.395(2)	O(21B)	0.368(2)	C(1B)g	0.834(3)
					C(2B)g	0.021(3)	C(6B)g	-0.982(3)	C(21B)	0.156(3)	O(11B)	-0.364(2)
					O(12B)	0.578(2)	C(11B)	-0.356(3)				

Nr 28	P	Q	R	S	Sigref	0.002	Sigpln	0.011	Chisq	77.3	Pl.Hyp.	P<5
Plan	-0.1362(7)	0.9884(1)	0.0671(5)	-2.276(3)	#Na(1)	0.008(1)	#O(52A)	-0.009(2)	#C(51A)	0.000(3)	#Na(2)a	-0.007(1)
A 5	-1.099(6)	16.7085(15)	1.341(9)	-2.276(3)	#O(1W)a	0.008(2)	Na(2)	-1.106(1)	O(1W)	-1.091(2)	O(3W)	1.330(2)
					O(4W)	0.742(3)	O(41A)	-0.806(2)	O(42A)	-1.162(2)	O(51A)	-0.888(2)
					C(4A)	0.919(3)	C(5A)	1.132(3)	C(41A)	-0.441(3)	Na(1)a	1.107(1)
					O(41A)	0.294(2)	O(42A)	-0.063(2)	O(51A)	0.212(2)	O(52A)	1.091(2)
					C(41A)	0.658(3)	C(51A)	1.099(3)	Na(1)b	-1.092(1)	O(3W)b	0.231(2)
					O(4W)b	-0.358(3)	O(5W)b	1.221(3)	O(52A)	-1.108(2)	C(3A)b	0.898(3)
					C(4A)b	-0.181(3)	C(5A)b	0.033(3)	C(6A)b	1.329(3)	C(51A)	-1.100(3)
					O(11B)	-1.210(2)	C(1B)c	-0.031(3)	C(2B)c	-0.265(3)	C(6B)c	0.823(3)
					C(11B)	-1.123(3)	C(1B)e	-1.130(3)	C(2B)e	-1.364(3)	C(6B)e	-0.277(3)
					Cu(1)g	-1.074(1)	Cu(2)g	-0.810(1)	O(6W)g	0.391(2)	O(11A)	0.245(2)
					O(12A)	0.369(2)	O(21A)	1.474(2)	O(22A)	0.178(2)	C(11A)	0.796(3)
					C(21A)	1.227(3)	O(6W)i	-0.708(2)	O(11A)	-0.855(2)	O(12A)	-0.731(2)
					O(21A)	0.375(2)	O(22A)	-0.922(2)	C(1A)i	1.035(3)	C(2A)i	1.249(3)
					C(11A)	-0.303(3)	C(21A)	0.128(3)	Na(1)j	-1.402(1)	O(4W)j	-1.456(3)
Nr 29	P	Q	R	S	Sigref	0.003	Sigpln	0.031	Chisq	879.8	Pl.Hyp.	P<5
Plan	0.4203(7)	-0.1244(5)	0.8988(3)	-1.537(2)	#C(1A)	-0.030(3)	#C(2A)	0.004(3)	#C(3A)	0.022(3)	#C(4A)	0.018(3)
A 9	3.394(6)	-2.104(9)	12.880(5)	-1.537(2)	#C(5A)	0.000(3)	#C(6A)	-0.033(3)	#C(11A)	0.047(3)	#C(21A)	-0.026(3)
					#C(41A)	-0.001(3)	Na(1)	-0.258(1)	Na(2)	0.373(1)	O(1W)	0.330(2)
					O(3W)	0.362(3)	O(4W)	-0.281(2)	O(5W)	-0.379(3)	O(11A)	1.097(2)
					O(11B)	0.029(2)	O(12A)	-0.810(2)	O(21A)	0.748(2)	O(21B)	-0.078(2)
					O(22A)	-0.796(2)	O(41A)	0.770(2)	O(42A)	-0.865(2)	O(51A)	1.139(2)
					O(52A)	-0.674(2)	C(1B)	-1.038(3)	C(2B)	-1.091(3)	C(6B)	-1.272(3)
					C(11B)	-0.937(3)	C(21B)	-0.925(3)	C(51A)	0.127(3)	O(7W)a	-0.365(2)
					Cu(2)b	0.794(1)	O(6W)b	-0.380(2)	O(12B)	1.469(2)	Cu(2)c	-0.740(1)
					Na(1)c	-1.405(1)	O(4W)c	-1.482(2)	O(6W)c	0.692(2)	O(42A)	-0.731(2)
					O(52A)	-1.075(2)	O(6W)d	-1.411(2)	Na(2)e	1.275(1)	O(1W)e	1.226(2)
					O(3W)e	0.675(3)	O(11A)	-0.855(2)	O(11B)	-0.394(2)	O(12A)	1.123(2)
					O(21A)	-0.345(2)	O(21B)	-0.085(2)	O(22A)	0.922(2)	O(22B)	1.287(2)
					O(41A)	0.889(2)	O(51A)	0.683(2)	C(1A)e	0.722(3)	C(1B)e	0.314(3)
					C(2A)e	0.689(3)	C(2B)e	0.373(3)	C(3A)e	0.973(3)	C(4A)e	1.275(3)
					C(5A)e	1.293(3)	C(6A)e	1.026(3)	C(6B)e	0.253(3)	C(11A)	0.341(3)
					C(11B)	0.522(3)	C(21A)	0.405(3)	C(21B)	0.526(3)	C(51A)	1.482(3)
					Cu(2)f	0.550(1)	Na(1)f	-0.115(1)	Na(2)f	-0.829(1)	O(1W)f	-0.877(2)
					O(3W)f	-1.428(3)	O(4W)f	-0.192(2)	O(5W)f	-0.583(3)	O(12A)	-0.981(2)
					O(12B)	-0.425(2)	O(22A)	-1.182(2)	O(22B)	-0.817(2)	O(41A)	-1.214(2)
					O(42A)	0.559(2)	O(51A)	-1.420(2)	O(52A)	0.215(2)	C(1A)f	-1.381(3)
					C(2A)f	-1.415(3)	C(3A)f	-1.131(3)	C(4A)f	-0.828(3)	C(5A)f	-0.810(3)
					C(6A)f	-1.078(3)	C(41A)	-0.499(3)	C(51A)	-0.622(3)	Na(1)g	-0.062(1)
					Na(2)g	-0.693(1)	O(1W)g	-0.651(2)	O(3W)g	-0.682(3)	O(4W)g	-0.040(2)
					O(5W)g	0.058(3)	O(11A)	-1.418(2)	O(11B)	-0.350(2)	O(12A)	0.489(2)
					O(21A)	-1.069(2)	O(21B)	-0.243(2)	O(22A)	0.475(2)	O(22B)	1.368(2)
					O(41A)	-1.091(2)	O(42A)	0.544(2)	O(51A)	-1.460(2)	O(52A)	0.353(2)

=====												
					C(1A)g	-0.290(3)	C(1B)g	0.717(3)	C(2A)g	-0.324(3)	C(2B)g	0.771(3)
					C(3A)g	-0.343(3)	C(4A)g	-0.338(3)	C(5A)g	-0.320(3)	C(6A)g	-0.288(3)
					C(6B)g	0.951(3)	C(11A)	-0.368(3)	C(11B)	0.617(3)	C(21A)	-0.295(3)
					C(21B)	0.604(3)	C(41A)	-0.320(3)	C(51A)	-0.448(3)	Cu(2)h	0.176(1)
					O(6W)h	1.350(2)	O(12B)	-0.499(2)	O(22B)	-0.736(2)	C(1B)h	-1.387(3)
					C(2B)h	-1.333(3)	C(6B)h	-1.153(3)	C(11B)	-1.487(3)	C(21B)	-1.499(3)
					Cu(1)i	1.320(1)	O(7W)i	0.044(2)	O(6W)j	1.091(2)		

Nr 30	P	Q	R	S	Sigref	0.003	Sigpln	0.033	Chisq	1182.5	Pl.Hyp.	P<5

Plan	0.4095(6)	-0.0102(5)	0.9123(3)	-1.739(5)	#C(1B)	0.025(3)	#C(2B)	-0.010(3)	#C(6B)	-0.041(3)	#C(11B)	-0.030(3)
A 10	3.306(5)	-0.172(8)	13.112(4)	-1.739(5)	#C(21B)	0.023(3)	#C(1B)h	-0.025(3)	#C(2B)h	0.010(3)	#C(6B)h	0.041(3)
					#C(11B)	0.030(3)	#C(21B)	-0.023(3)	Na(1)	-0.338(1)	Na(2)	0.188(1)
					O(1W)	0.152(2)	O(3W)	0.461(3)	O(4W)	-0.280(2)	O(5W)	-0.189(3)
					O(11B)	0.908(2)	O(12A)	-0.274(2)	O(12B)	-1.102(2)	O(21A)	1.177(2)
					O(21B)	0.762(2)	O(22A)	-0.229(2)	O(22B)	-0.730(2)	O(41A)	0.619(2)
					O(42A)	-1.073(2)	O(51A)	0.973(2)	O(52A)	-0.753(2)	C(1A)	0.310(3)
					C(2A)	0.322(3)	C(3A)	0.190(3)	C(4A)	0.058(3)	C(5A)	0.062(3)
					C(6A)	0.178(3)	C(11A)	0.541(3)	C(21A)	0.425(3)	C(41A)	-0.117(3)
					C(51A)	0.056(3)	Cu(1)a	-0.831(1)	O(7W)a	0.571(2)	Cu(2)b	1.365(1)
					O(6W)b	0.044(2)	Cu(2)c	-1.134(1)	O(6W)c	0.208(2)	Cu(2)d	-1.306(1)
					O(6W)d	0.036(2)	Na(1)e	0.706(1)	Na(2)e	0.172(1)	O(1W)e	0.201(2)
					O(3W)e	-0.150(3)	O(4W)e	0.639(2)	O(5W)e	0.509(3)	O(11A)	-1.418(2)
					O(11B)	-0.712(2)	O(12A)	0.526(2)	O(12B)	1.308(2)	O(21A)	-0.918(2)
					O(21B)	-0.549(2)	O(22A)	0.466(2)	O(22B)	0.923(2)	O(41A)	-0.257(2)
					O(42A)	1.445(2)	O(51A)	-0.598(2)	O(52A)	1.114(2)	C(1A)e	-0.027(3)
					C(1B)e	0.142(3)	C(2A)e	-0.039(3)	C(2B)e	0.177(3)	C(3A)e	0.118(3)
					C(4A)e	0.274(3)	C(5A)e	0.270(3)	C(6A)e	0.129(3)	C(6B)e	0.185(3)
					C(11A)	-0.284(3)	C(11B)	0.223(3)	C(21A)	-0.167(3)	C(21B)	0.171(3)
					C(41A)	0.475(3)	C(51A)	0.302(3)	Na(1)f	0.534(1)	Na(2)f	0.001(1)
					O(1W)f	0.030(2)	O(3W)f	-0.322(3)	O(4W)f	0.468(2)	O(5W)f	0.337(3)
					O(11B)	-0.883(2)	O(12A)	0.354(2)	O(12B)	1.137(2)	O(21A)	-1.090(2)
					O(21B)	-0.720(2)	O(22A)	0.294(2)	O(22B)	0.751(2)	O(41A)	-0.429(2)
					O(42A)	1.274(2)	O(51A)	-0.769(2)	O(52A)	0.942(2)	C(1A)f	-0.198(3)
					C(1B)f	-0.030(3)	C(2A)f	-0.211(3)	C(2B)f	0.006(3)	C(3A)f	-0.054(3)
					C(4A)f	0.102(3)	C(5A)f	0.099(3)	C(6A)f	-0.043(3)	C(6B)f	0.013(3)
					C(11A)	-0.455(3)	C(11B)	0.051(3)	C(21A)	-0.339(3)	C(21B)	-0.001(3)
					C(41A)	0.303(3)	C(51A)	0.130(3)	Na(1)g	0.510(1)	Na(2)g	-0.017(1)
					O(1W)g	0.020(2)	O(3W)g	-0.290(3)	O(4W)g	0.451(2)	O(5W)g	0.361(3)
					O(11A)	-1.492(2)	O(11B)	-0.737(2)	O(12A)	0.446(2)	O(12B)	1.274(2)
					O(21A)	-1.006(2)	O(21B)	-0.590(2)	O(22A)	0.401(2)	O(22B)	0.901(2)
					O(41A)	-0.448(2)	O(42A)	1.244(2)	O(51A)	-0.801(2)	O(52A)	0.925(2)
					C(1A)g	-0.138(3)	C(1B)g	0.147(3)	C(2A)g	-0.150(3)	C(2B)g	0.181(3)
					C(3A)g	-0.018(3)	C(4A)g	0.114(3)	C(5A)g	0.110(3)	C(6A)g	-0.007(3)
					C(6B)g	0.213(3)	C(11A)	-0.370(3)	C(11B)	0.202(3)	C(21A)	-0.253(3)
					C(21B)	0.149(3)	C(41A)	0.289(3)	C(51A)	0.116(3)	Na(1)h	0.338(1)
					Na(2)h	-0.188(1)	O(1W)h	-0.152(2)	O(3W)h	-0.461(3)	O(4W)h	0.280(2)
					O(5W)h	0.189(3)	O(11B)	-0.908(2)	O(12A)	0.274(2)	O(12B)	1.102(2)

=====												
					O(21A)	-1.177(2)	O(21B)	-0.762(2)	O(22A)	0.229(2)	O(22B)	0.730(2)
					O(41A)	-0.619(2)	O(42A)	1.073(2)	O(51A)	-0.973(2)	O(52A)	0.753(2)
					C(1A)h	-0.310(3)	C(2A)h	-0.322(3)	C(3A)h	-0.190(3)	C(4A)h	-0.058(3)
					C(5A)h	-0.062(3)	C(6A)h	-0.178(3)	C(11A)	-0.541(3)	C(21A)	-0.425(3)
					C(41A)	0.117(3)	C(51A)	-0.056(3)	Cu(1)i	1.002(1)	O(7W)i	-0.399(2)
					Cu(2)j	1.477(1)	O(6W)j	0.136(2)				

Nr 31	P	Q	R	S	Sigref	0.002	Sigpln	0.031	Chisq	198.9	Pl.Hyp.	P<5

Plan	0.4212(11)	0.5836(11)	-0.6943(9)	2.831(2)	#O(11A)	-0.009(2)	#O(12A)	-0.010(2)	#C(1A)	-0.007(3)	#C(11A)	0.027(3)
A 4	3.400(9)	9.865(19)	-11.639(14)	2.831(2)	Cu(1)	-0.650(1)	Cu(2)	0.653(1)	Na(2)	1.474(1)	O(6W)	1.411(2)
					O(11B)	0.046(2)	O(12B)	0.087(2)	O(41A)	-0.278(2)	O(42A)	-0.703(2)
					C(1B)	0.172(3)	C(2A)	0.924(3)	C(2B)	-0.762(3)	C(3A)	0.733(3)
					C(4A)	-0.359(3)	C(5A)	-1.297(3)	C(6A)	-1.104(3)	C(6B)	-0.516(3)
					C(11B)	0.067(3)	C(41A)	-0.465(3)	O(1W)a	-0.164(2)	O(3W)a	-0.672(3)
					O(21A)	-0.964(2)	O(22A)	-0.581(2)	C(21A)	-1.250(3)	Na(1)b	-1.443(1)
					O(5W)b	-0.029(3)	O(21B)	0.680(2)	O(22B)	1.004(2)	O(51A)	0.112(2)
					O(52A)	0.499(2)	C(21B)	1.346(3)	C(51A)	0.830(3)	Cu(1)c	1.105(1)
					Cu(2)c	-0.622(1)	O(4W)c	-1.228(2)	O(11A)	-0.843(2)	O(12A)	-1.171(2)
					O(12B)	1.355(2)	Na(2)d	0.949(1)	O(1W)d	-0.385(2)	Na(1)e	0.414(1)
					O(6W)e	0.812(2)	O(21A)	-0.641(2)	O(22A)	0.272(2)	O(52A)	-1.129(2)
					C(1A)e	0.447(3)	C(2A)e	-0.486(3)	C(5A)e	-1.081(3)	C(6A)e	0.135(3)
					C(21A)	-0.244(3)	C(51A)	-1.289(3)	Cu(1)h	1.453(1)	Cu(2)h	0.150(1)
					Na(2)h	-0.671(1)	O(6W)h	-0.608(2)	O(11A)	0.812(2)	O(11B)	0.757(2)
					O(12A)	0.813(2)	O(12B)	0.716(2)	O(41A)	1.080(2)	C(1A)h	0.810(3)
					C(1B)h	0.631(3)	C(2A)h	-0.121(3)	C(3A)h	0.070(3)	C(4A)h	1.162(3)
					C(6B)h	1.319(3)	C(11A)	0.776(3)	C(11B)	0.736(3)	C(21A)	-1.347(3)
					C(41A)	1.268(3)	Na(1)i	-0.819(1)	O(4W)i	0.475(2)		

Nr 32	P	Q	R	S	Sigref	0.002	Sigpln	0.024	Chisq	117.3	Pl.Hyp.	P<5

Plan	0.4611(11)	0.5461(12)	-0.6994(9)	2.593(8)	#O(11B)	0.008(2)	#O(12B)	0.007(2)	#C(1B)	0.006(3)	#C(11B)	-0.021(3)
A 4	3.723(9)	9.23(2)	-11.808(13)	2.593(8)	Cu(1)	-0.575(1)	Cu(2)	0.660(1)	O(6W)	1.484(2)	O(11A)	0.151(2)
					O(12A)	0.096(2)	O(41A)	0.230(2)	O(42A)	-0.246(2)	C(1A)	0.229(3)
					C(2A)	1.214(3)	C(2B)	-0.982(3)	C(3A)	1.093(3)	C(4A)	0.018(3)
					C(5A)	-0.974(3)	C(6A)	-0.851(3)	C(6B)	-0.808(3)	C(11A)	0.187(3)
					C(41A)	-0.012(3)	O(1W)a	0.176(2)	O(3W)a	-0.497(3)	O(21A)	-0.959(2)
					O(22A)	-0.686(2)	C(21A)	-1.297(3)	Na(1)b	-0.893(1)	O(5W)b	0.442(3)
					O(21B)	0.857(2)	O(22B)	1.074(2)	O(51A)	0.828(2)	O(52A)	1.121(2)
					C(21B)	1.466(3)	C(51A)	1.492(3)	Cu(2)c	-0.060(1)	O(4W)c	-0.312(2)
					O(5W)c	-0.892(3)	O(11A)	-0.377(2)	O(12A)	-0.631(2)	C(11A)	-1.053(3)
					Na(2)d	0.775(1)	O(1W)d	-0.660(2)	O(21A)	0.027(2)	O(22A)	0.967(2)
					O(51A)	-0.541(2)	O(52A)	-0.057(2)	C(1A)e	1.295(3)	C(2A)e	0.307(3)
					C(3A)e	-0.901(3)	C(4A)e	-1.132(3)	C(5A)e	-0.140(3)	C(6A)e	1.056(3)
					C(21A)	0.470(3)	C(51A)	-0.269(3)	Cu(1)h	0.898(1)	Cu(2)h	-0.337(1)
					O(6W)h	-1.161(2)	O(11A)	0.172(2)	O(11B)	0.315(2)	O(12A)	0.227(2)
					O(12B)	0.315(2)	O(41A)	0.093(2)	O(42A)	0.568(2)	C(1A)h	0.094(3)
					C(1B)h	0.317(3)	C(2A)h	-0.892(3)	C(2B)h	1.305(3)	C(3A)h	-0.771(3)

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					C(4A)h	0.305(3)	C(5A)h	1.296(3)	C(6A)h	1.173(3)	C(6B)h	1.131(3)
					C(11A)	0.135(3)	C(11B)	0.343(3)	C(41A)	0.335(3)	Na(1)i	-0.570(1)
					O(4W)i	0.824(2)						

Nr 33	P	Q	R	S	Sigref	0.002	Sigpln	0.013	Chisq	32.8	Pl.Hyp.	P<5

Plan	-0.1871(13)	0.2985(13)	0.9359(4)	-2.448(7)	#O(21A)	-0.004(2)	#O(22A)	-0.004(2)	#C(2A)	-0.003(3)	#C(21A)	0.011(3)
A 4	-1.511(10)	5.05(2)	14.827(8)	-2.448(7)	Cu(2)	1.343(1)	Na(1)	1.237(1)	O(6W)	-0.621(2)	O(51A)	0.177(2)
					O(52A)	-0.267(2)	C(1A)	0.765(3)	C(3A)	-0.853(3)	C(4A)	-0.941(3)
					C(5A)	-0.162(3)	C(6A)	0.673(3)	C(51A)	-0.107(3)	O(3W)a	-1.020(3)
					O(6W)a	0.890(2)	O(41A)	-0.434(2)	O(42A)	-1.186(2)	O(52A)	1.244(2)
					C(3A)a	0.658(3)	C(4A)a	0.570(3)	C(5A)a	1.349(3)	C(41A)	-0.395(3)
					C(51A)	1.404(3)	Cu(2)b	-0.168(1)	Na(1)b	-0.274(1)	O(4W)b	1.134(2)
					O(5W)b	0.472(3)	O(11A)	1.212(2)	O(12A)	0.224(2)	O(51A)	-1.334(2)
					C(1A)b	-0.746(3)	C(6A)b	-0.838(3)	C(11A)	0.278(3)	C(21A)	-1.500(3)
					O(1W)c	-1.471(2)	Cu(2)d	1.121(1)	O(11A)	-0.710(2)	O(11B)	-0.827(2)
					O(12A)	0.108(2)	O(12B)	0.091(2)	O(41A)	0.558(2)	O(42A)	0.978(2)
					O(52A)	-1.086(2)	C(1A)d	0.168(3)	C(1B)d	-0.646(3)	C(2A)d	0.936(3)
					C(2B)d	-1.402(3)	C(3A)d	1.060(3)	C(4A)d	0.433(3)	C(5A)d	-0.346(3)
					C(6A)d	-0.460(3)	C(6B)d	-1.414(3)	C(11A)	-0.126(3)	C(11B)	-0.477(3)
					C(41A)	0.651(3)	C(51A)	-1.159(3)	Cu(2)f	-0.390(1)	Na(2)f	0.659(1)
					O(3W)f	1.127(3)	O(6W)f	0.956(2)	O(12A)	-1.403(2)	O(12B)	-1.420(2)
					O(21A)	0.120(2)	O(22A)	0.783(2)	O(41A)	-0.954(2)	O(42A)	-0.533(2)
					C(1A)f	-1.343(3)	C(2A)f	-0.575(3)	C(3A)f	-0.451(3)	C(4A)f	-1.078(3)
					C(21A)	0.162(3)	C(41A)	-0.860(3)	O(7W)g	-0.034(2)	O(21B)	0.517(2)
					O(22B)	0.618(2)	C(1B)g	1.432(3)	C(2B)g	0.689(3)	C(6B)g	-0.043(3)
					C(21B)	0.614(3)	Cu(1)i	0.442(1)	O(11B)	0.603(2)	O(21B)	-0.994(2)
					O(22B)	-0.893(2)	C(1B)i	-0.079(3)	C(2B)i	-0.822(3)	C(11B)	0.830(3)
					C(21B)	-0.897(3)						

Nr 34	P	Q	R	S	Sigref	0.002	Sigpln	0.014	Chisq	43.3	Pl.Hyp.	P<5

Plan	-0.2902(12)	-0.4937(12)	0.8198(7)	-2.606(6)	#O(41A)	-0.005(2)	#O(42A)	-0.004(2)	#C(4A)	-0.004(3)	#C(41A)	0.013(3)
A 4	-2.343(9)	-8.35(2)	13.274(11)	-2.606(6)	Cu(1)	0.952(1)	Cu(2)	-1.180(1)	O(11A)	0.165(2)	O(11B)	0.033(2)
					O(12A)	-0.260(2)	O(12B)	-0.452(2)	C(1A)	-0.187(3)	C(1B)	-0.224(3)
					C(2A)	-1.021(3)	C(2B)	0.607(3)	C(3A)	-0.917(3)	C(5A)	0.839(3)
					C(6A)	0.731(3)	C(6B)	0.419(3)	C(11A)	-0.128(3)	C(11B)	-0.181(3)
					Cu(2)a	1.163(1)	Na(2)a	0.675(1)	O(1W)a	-0.904(2)	O(3W)a	-0.314(3)
					O(6W)a	0.164(2)	O(21A)	0.186(2)	O(22A)	-0.424(2)	C(2A)a	1.323(3)
					C(3A)a	1.426(3)	C(21A)	0.284(3)	Cu(1)b	-1.391(1)	O(5W)b	0.377(3)
					O(7W)b	-0.234(2)	O(21B)	0.116(2)	O(22B)	-0.464(2)	O(51A)	0.412(2)
					O(52A)	-0.284(2)	C(21B)	-0.610(3)	C(51A)	-0.403(3)	Cu(2)c	-0.137(1)
					Na(1)c	1.451(1)	O(4W)c	-0.130(2)	O(5W)c	0.277(3)	O(11A)	-0.736(2)
					O(12A)	-0.032(2)	C(1A)c	1.400(3)	C(11A)	0.134(3)	O(1W)d	-0.456(2)
					Na(1)e	-0.892(1)	O(6W)e	-0.460(2)	O(21A)	-0.120(2)	O(22A)	-0.606(2)
					O(51A)	0.599(2)	O(52A)	0.592(2)	C(1A)e	-0.943(3)	C(2A)e	-0.108(3)
					C(3A)e	0.990(3)	C(4A)e	1.258(3)	C(5A)e	0.414(3)	C(6A)e	-0.669(3)
					C(21A)	-0.312(3)	C(51A)	0.567(3)	Cu(2)h	0.390(1)	Na(2)h	0.878(1)

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						O(6W)h	1.389(2)	O(11A)	-0.956(2)	O(11B)	-0.823(2)	O(12A)	-0.530(2)
						O(12B)	-0.339(2)	O(21A)	1.367(2)	O(41A)	-0.786(2)	O(42A)	-0.786(2)
						C(1A)h	-0.604(3)	C(1B)h	-0.567(3)	C(2A)h	0.230(3)	C(2B)h	-1.398(3)
						C(3A)h	0.127(3)	C(4A)h	-0.787(3)	C(6B)h	-1.209(3)	C(11A)	-0.663(3)
						C(11B)	-0.610(3)	C(21A)	1.269(3)	C(41A)	-0.803(3)	Na(1)i	1.331(1)
						O(4W)i	0.143(2)						

Nr 35	P	Q	R	S	Sigref	0.002		Sigpln	0.020	Chisq	78.1	Pl.Hyp.	P<5

Plan	-0.3301(12)	0.4206(12)	0.8450(7)	-2.657(2)	#O(51A)	0.0006(2)	#O(52A)	0.0006(2)	#C(5A)	0.0005(3)	#C(51A)	-0.017(3)	
A 4	-2.666(10)	7.11(2)	13.753(11)	-2.657(2)	O(6W)	0.646(2)	O(21A)	0.133(2)	O(22A)	0.592(2)	C(1A)	1.188(3)	
					C(2A)	0.286(3)	C(3A)	-0.755(3)	C(4A)	-0.904(3)	C(6A)	1.032(3)	
					C(21A)	0.362(3)	Na(2)a	-1.396(1)	O(3W)a	-0.136(3)	O(41A)	0.333(2)	
					O(42A)	-0.123(2)	C(41A)	0.595(3)	Cu(2)b	-0.013(1)	Na(1)b	-1.039(1)	
					O(4W)b	0.618(2)	O(5W)b	-0.044(3)	O(11A)	0.565(2)	O(12A)	-0.081(2)	
					C(1A)b	-1.478(3)	C(11A)	-0.261(3)	O(1W)c	-1.319(2)	Cu(1)d	0.652(1)	
					O(5W)d	-0.841(3)	O(7W)d	-0.631(2)	O(11B)	1.430(2)	O(21B)	-1.101(2)	
					O(22B)	-0.646(2)	O(51A)	-0.525(2)	O(52A)	0.072(2)	C(2B)d	0.614(3)	
					C(5A)d	1.265(3)	C(6A)d	1.253(3)	C(6B)d	0.682(3)	C(21B)	-0.455(3)	
					C(51A)	0.218(3)	Cu(2)f	0.138(1)	Na(2)f	1.466(1)	O(6W)f	1.274(2)	
					O(11A)	-1.075(2)	O(11B)	-1.235(2)	O(12A)	-0.668(2)	O(12B)	-0.746(2)	
					O(21A)	1.479(2)	O(41A)	-0.304(2)	O(42A)	-0.314(2)	C(1A)f	-0.553(3)	
					C(1B)f	-1.157(3)	C(2A)f	0.347(3)	C(3A)f	0.365(3)	C(4A)f	-0.493(3)	
					C(5A)f	-1.401(3)	C(6A)f	-1.413(3)	C(11A)	-0.742(3)	C(11B)	-1.067(3)	
					C(21A)	1.331(3)	C(41A)	-0.378(3)	O(7W)g	0.871(2)	O(21B)	0.691(2)	
					O(22B)	0.335(2)	C(1B)g	1.403(3)	C(2B)g	0.527(3)	C(6B)g	-0.421(3)	
					C(21B)	0.537(3)	Cu(1)i	0.203(1)	O(11B)	-0.126(2)	O(12B)	0.760(2)	
					C(1B)i	-1.263(3)	C(11B)	-0.130(3)					

(Acute) Angles (Degrees) Between Planes (Numbers I,J from List Above)

1, 2=	3.31(12)	1, 3=	62.82(12)	1, 4=	0.00(12)	1, 5=	55.23(12)	1, 6=	49.91(12)	1, 7=	48.49(9)	1, 8=	88.12(11)
1, 9=	10.34(10)	1, 10=	8.85(10)	1, 11=	0.51(11)	1, 12=	87.99(10)	1, 13=	11.17(14)	1, 14=	6.33(11)	1, 15=	1.55(11)
1, 16=	63.41(12)	1, 17=	33.20(11)	1, 18=	54.17(10)	1, 19=	36.8(3)	1, 20=	39.68(10)	1, 21=	88.54(10)	1, 22=	12.99(13)
1, 23=	27.4(3)	1, 24=	10.34(10)	1, 25=	86.43(10)	1, 26=	63.41(12)	1, 27=	0.51(11)	1, 28=	54.17(10)	1, 29=	56.40(10)
1, 30=	51.36(10)	1, 31=	66.46(14)	1, 32=	64.30(14)	1, 33=	14.43(14)	1, 34=	59.39(13)	1, 35=	5.24(14)	2, 3=	66.02(12)
2, 4=	3.31(12)	2, 5=	56.39(12)	2, 6=	50.83(12)	2, 7=	49.06(8)	2, 8=	85.00(10)	2, 9=	12.36(10)	2, 10=	10.34(10)
2, 11=	3.77(11)	2, 12=	88.82(9)	2, 13=	8.60(14)	2, 14=	4.98(10)	2, 15=	2.17(11)	2, 16=	60.10(11)	2, 17=	36.19(10)
2, 18=	51.11(10)	2, 19=	40.1(3)	2, 20=	42.83(10)	2, 21=	85.32(10)	2, 22=	14.75(13)	2, 23=	30.6(3)	2, 24=	12.36(10)
2, 25=	88.46(10)	2, 26=	60.10(11)	2, 27=	3.77(11)	2, 28=	51.11(10)	2, 29=	57.54(10)	2, 30=	52.22(9)	2, 31=	69.77(13)
2, 32=	67.61(13)	2, 33=	16.87(14)	2, 34=	62.60(13)	2, 35=	8.55(13)	3, 4=	62.82(12)	3, 5=	47.22(12)	3, 6=	50.48(12)
3, 7=	55.16(8)	3, 8=	44.58(10)	3, 9=	55.65(10)	3, 10=	58.28(10)	3, 11=	62.44(11)	3, 12=	38.63(9)	3, 13=	70.46(14)
3, 14=	65.47(10)	3, 15=	64.30(11)	3, 16=	55.31(11)	3, 17=	41.90(10)	3, 18=	63.32(10)	3, 19=	30.6(3)	3, 20=	34.65(10)
3, 21=	39.55(10)	3, 22=	54.71(13)	3, 23=	40.1(3)	3, 24=	55.65(10)	3, 25=	42.30(10)	3, 26=	55.31(11)	3, 27=	62.44(11)
3, 28=	63.32(10)	3, 29=	47.75(10)	3, 30=	51.42(9)	3, 31=	10.98(13)	3, 32=	12.61(13)	3, 33=	50.82(14)	3, 34=	3.56(13)
3, 35=	57.95(13)	4, 5=	55.23(12)	4, 6=	49.91(12)	4, 7=	48.49(9)	4, 8=	88.12(11)	4, 9=	10.34(10)	4, 10=	8.85(10)
4, 11=	0.51(11)	4, 12=	87.99(10)	4, 13=	11.17(14)	4, 14=	6.33(11)	4, 15=	1.55(11)	4, 16=	63.41(12)	4, 17=	33.20(11)
4, 18=	54.17(10)	4, 19=	36.8(3)	4, 20=	39.68(10)	4, 21=	88.54(10)	4, 22=	12.99(13)	4, 23=	27.4(3)	4, 24=	10.34(10)

4, 25=	86.43(10)	4, 26=	63.41(12)	4, 27=	0.51(11)	4, 28=	54.17(10)	4, 29=	56.40(10)	4, 30=	51.36(10)	4, 31=	66.46(14)
4, 32=	64.30(14)	4, 33=	14.43(14)	4, 34=	59.39(13)	4, 35=	5.24(14)	5, 6=	6.53(12)	5, 7=	11.06(9)	5, 8=	88.80(11)
5, 9=	45.11(11)	5, 10=	46.39(10)	5, 11=	55.30(11)	5, 12=	85.27(10)	5, 13=	53.32(14)	5, 14=	52.09(11)	5, 15=	56.45(11)
5, 16=	89.19(12)	5, 17=	65.03(11)	5, 18=	83.80(10)	5, 19=	55.3(3)	5, 20=	63.38(10)	5, 21=	85.41(10)	5, 22=	42.34(13)
5, 23=	56.7(3)	5, 24=	45.11(11)	5, 25=	35.51(10)	5, 26=	89.19(12)	5, 27=	55.30(11)	5, 28=	83.80(10)	5, 29=	1.24(10)
5, 30=	6.05(10)	5, 31=	58.13(14)	5, 32=	59.19(14)	5, 33=	42.28(14)	5, 34=	46.82(14)	5, 35=	54.16(14)	6, 7=	5.05(9)
6, 8=	85.01(11)	6, 9=	40.04(11)	6, 10=	41.08(10)	6, 11=	50.02(11)	6, 12=	89.03(10)	6, 13=	47.24(14)	6, 14=	46.36(11)
6, 15=	51.05(11)	6, 16=	84.77(12)	6, 17=	63.05(11)	6, 18=	89.69(10)	6, 19=	54.4(3)	6, 20=	62.40(10)	6, 21=	89.53(10)
6, 22=	37.24(13)	6, 23=	54.4(3)	6, 24=	40.04(11)	6, 25=	42.03(10)	6, 26=	84.77(12)	6, 27=	50.02(11)	6, 28=	89.69(10)
6, 29=	7.34(10)	6, 30=	1.66(10)	6, 31=	61.17(14)	6, 32=	61.87(14)	6, 33=	37.70(14)	6, 34=	49.61(14)	6, 35=	49.31(14)
7, 8=	80.28(6)	7, 9=	39.07(6)	7, 10=	39.78(5)	7, 11=	48.66(7)	7, 12=	86.24(5)	7, 13=	44.65(11)	7, 14=	44.37(6)
7, 15=	49.51(7)	7, 16=	79.83(8)	7, 17=	64.76(6)	7, 18=	85.36(5)	7, 19=	56.9(2)	7, 20=	64.82(6)	7, 21=	85.62(5)
7, 22=	36.28(9)	7, 23=	56.0(2)	7, 24=	39.07(6)	7, 25=	46.20(5)	7, 26=	79.83(8)	7, 27=	48.66(7)	7, 28=	85.36(5)
7, 29=	11.58(5)	7, 30=	5.01(5)	7, 31=	65.73(10)	7, 32=	66.29(10)	7, 33=	37.35(11)	7, 34=	54.13(10)	7, 35=	48.48(11)
8, 9=	89.90(8)	8, 10=	87.81(8)	8, 11=	88.63(9)	8, 12=	5.96(8)	8, 13=	77.27(13)	8, 14=	82.73(9)	8, 15=	87.17(9)
8, 16=	32.31(10)	8, 17=	58.95(9)	8, 18=	51.39(8)	8, 19=	56.2(2)	8, 20=	52.21(8)	8, 21=	6.78(8)	8, 22=	89.61(11)
8, 23=	64.7(2)	8, 24=	89.90(8)	8, 25=	72.06(8)	8, 26=	32.31(10)	8, 27=	88.63(9)	8, 28=	51.39(8)	8, 29=	88.43(8)
8, 30=	84.16(8)	8, 31=	34.29(12)	8, 32=	34.33(12)	8, 33=	86.12(12)	8, 34=	45.87(12)	8, 35=	86.79(12)	9, 10=	2.63(8)
9, 11=	10.32(9)	9, 12=	85.28(7)	9, 13=	14.82(13)	9, 14=	10.03(9)	9, 15=	11.74(9)	9, 16=	69.27(10)	9, 17=	33.89(9)
9, 18=	62.60(8)	9, 19=	33.7(2)	9, 20=	38.65(8)	9, 21=	88.31(8)	9, 22=	2.80(11)	9, 23=	26.1(2)	9, 24=	0.00(8)
9, 25=	76.17(8)	9, 26=	69.27(10)	9, 27=	10.32(9)	9, 28=	62.60(8)	9, 29=	46.30(8)	9, 30=	41.55(8)	9, 31=	60.91(12)
9, 32=	59.18(12)	9, 33=	4.89(12)	9, 34=	52.41(12)	9, 35=	9.43(12)	10, 11=	8.95(9)	10, 12=	87.65(7)	10, 13=	12.19(12)
10, 14=	7.49(8)	10, 15=	10.08(8)	10, 16=	66.65(9)	10, 17=	35.55(8)	10, 18=	60.07(7)	10, 19=	36.0(2)	10, 20=	40.65(7)
10, 21=	89.27(7)	10, 22=	4.44(11)	10, 23=	28.0(2)	10, 24=	2.63(8)	10, 25=	78.14(7)	10, 26=	66.65(9)	10, 27=	8.95(9)
10, 28=	60.07(7)	10, 29=	47.56(7)	10, 30=	42.54(7)	10, 31=	63.49(12)	10, 32=	61.74(12)	10, 33=	7.49(12)	10, 34=	55.04(11)
10, 35=	9.32(12)	11, 12=	87.49(8)	11, 13=	11.68(13)	11, 14=	6.80(10)	11, 15=	1.86(10)	11, 16=	63.85(11)	11, 17=	32.69(9)
11, 18=	54.51(9)	11, 19=	36.3(3)	11, 20=	39.18(9)	11, 21=	89.04(9)	11, 22=	13.01(12)	11, 23=	26.9(3)	11, 24=	10.32(9)
11, 25=	86.33(9)	11, 26=	63.85(11)	11, 27=	0.00(10)	11, 28=	54.51(9)	11, 29=	56.47(9)	11, 30=	51.49(9)	11, 31=	66.02(13)
11, 32=	63.85(13)	11, 33=	14.30(13)	11, 34=	59.01(13)	11, 35=	4.77(13)	12, 13=	81.39(12)	12, 14=	86.89(8)	12, 15=	89.03(8)
12, 16=	33.06(9)	12, 17=	55.55(8)	12, 18=	51.33(7)	12, 19=	51.7(2)	12, 20=	48.39(7)	12, 21=	4.13(7)	12, 22=	85.59(10)
12, 23=	60.6(2)	12, 24=	85.28(7)	12, 25=	67.30(7)	12, 26=	33.06(9)	12, 27=	87.49(8)	12, 28=	51.33(7)	12, 29=	85.65(7)
12, 30=	89.88(6)	12, 31=	28.40(11)	12, 32=	28.58(11)	12, 33=	81.31(12)	12, 34=	39.96(11)	12, 35=	82.81(11)	13, 14=	5.50(13)
13, 15=	10.63(13)	13, 16=	54.50(14)	13, 17=	44.31(13)	13, 18=	48.42(12)	13, 19=	47.0(3)	13, 20=	50.56(12)	13, 21=	78.08(12)
13, 22=	15.98(15)	13, 23=	38.1(3)	13, 24=	14.82(13)	13, 25=	87.37(12)	13, 26=	54.50(14)	13, 27=	11.68(13)	13, 28=	48.42(12)
13, 29=	54.36(12)	13, 30=	48.45(12)	13, 31=	75.50(15)	13, 32=	73.63(15)	13, 33=	19.65(15)	13, 34=	67.22(15)	13, 35=	16.01(15)
14, 15=	6.35(9)	14, 16=	59.73(10)	14, 17=	39.03(9)	14, 18=	52.59(8)	14, 19=	41.5(2)	14, 20=	45.12(8)	14, 21=	83.58(8)
14, 22=	11.77(11)	14, 23=	32.6(2)	14, 24=	10.03(9)	14, 25=	84.98(8)	14, 26=	59.73(10)	14, 27=	6.80(10)	14, 28=	52.59(8)
14, 29=	53.21(8)	14, 30=	47.70(8)	14, 31=	70.17(12)	14, 32=	68.24(12)	14, 33=	14.91(13)	14, 34=	62.17(12)	14, 35=	10.69(12)
15, 16=	62.07(10)	15, 17=	34.02(9)	15, 18=	52.65(8)	15, 19=	38.0(2)	15, 20=	40.67(9)	15, 21=	87.46(8)	15, 22=	14.33(12)
15, 23=	28.5(2)	15, 24=	11.74(9)	15, 25=	87.88(8)	15, 26=	62.07(10)	15, 27=	1.86(10)	15, 28=	52.65(8)	15, 29=	57.61(9)
15, 30=	52.49(8)	15, 31=	67.82(12)	15, 32=	65.63(12)	15, 33=	15.93(13)	15, 34=	60.86(12)	15, 35=	6.53(12)	16, 17=	86.82(10)
16, 18=	19.41(10)	16, 19=	80.1(3)	16, 20=	79.04(10)	16, 21=	28.93(10)	16, 22=	70.03(12)	16, 23=	90.0(3)	16, 24=	69.27(10)
16, 25=	57.10(9)	16, 26=	0.00(11)	16, 27=	63.85(11)	16, 28=	19.41(10)	16, 29=	88.87(10)	16, 30=	84.81(9)	16, 31=	50.17(13)
16, 32=	52.30(13)	16, 33=	74.02(13)	16, 34=	58.41(13)	16, 35=	68.60(13)	17, 18=	78.69(8)	17, 19=	12.1(2)	17, 20=	8.04(8)
17, 21=	59.29(8)	17, 22=	35.47(11)	17, 23=	8.9(2)	17, 24=	33.89(9)	17, 25=	80.87(8)	17, 26=	86.82(10)	17, 27=	32.69(9)
17, 28=	78.69(8)	17, 29=	66.20(8)	17, 30=	64.70(8)	17, 31=	39.95(12)	17, 32=	37.01(12)	17, 33=	31.84(12)	17, 34=	38.53(12)
17, 35=	28.34(12)	18, 19=	87.6(2)	18, 20=	86.72(8)	18, 21=	47.22(7)	18, 22=	64.24(11)	18, 23=	77.6(2)	18, 24=	62.60(8)
18, 25=	48.46(7)	18, 26=	19.41(10)	18, 27=	54.51(9)	18, 28=	0.00(8)	18, 29=	83.11(8)	18, 30=	89.74(7)	18, 31=	61.78(12)

18,32=	64.53(12)	18,33=	67.46(12)	18,34=	66.83(12)	18,35=	58.84(12)	19,20=	8.1(2)	19,21=	54.9(2)	19,22=	34.3(3)
19,23=	10.1(3)	19,24=	33.7(2)	19,25=	68.8(2)	19,26=	80.1(3)	19,27=	36.3(3)	19,28=	87.6(2)	19,29=	56.5(2)
19,30=	56.0(2)	19,31=	30.7(3)	19,32=	28.1(3)	19,33=	30.1(3)	19,34=	27.1(3)	19,35=	31.6(3)	20,21=	52.00(8)
20,22=	39.75(11)	20,23=	12.6(2)	20,24=	38.65(8)	20,25=	75.04(7)	20,26=	79.04(10)	20,27=	39.18(9)	20,28=	86.72(8)
20,29=	64.49(8)	20,30=	63.99(7)	20,31=	31.98(12)	20,32=	29.01(12)	20,33=	35.73(12)	20,34=	31.41(12)	20,35=	34.58(12)
21,22=	88.48(11)	21,23=	64.1(2)	21,24=	88.31(8)	21,25=	65.28(7)	21,26=	28.93(10)	21,27=	89.04(9)	21,28=	47.22(7)
21,29=	85.70(8)	21,30=	89.71(7)	21,31=	29.91(12)	21,32=	30.50(12)	21,33=	84.20(12)	21,34=	41.24(12)	21,35=	86.25(12)
22,23=	27.3(3)	22,24=	2.80(11)	22,25=	73.71(11)	22,26=	70.03(12)	22,27=	13.01(12)	22,28=	64.24(11)	22,29=	43.52(11)
22,30=	38.75(11)	22,31=	60.50(14)	22,32=	58.92(14)	22,33=	4.28(14)	22,34=	51.56(14)	22,35=	12.20(14)	23,24=	26.1(2)
23,25=	75.7(2)	23,26=	90.0(3)	23,27=	26.9(3)	23,28=	77.6(2)	23,29=	57.9(2)	23,30=	56.1(2)	23,31=	40.7(3)
23,32=	38.2(3)	23,33=	23.5(3)	23,34=	36.5(3)	23,35=	22.2(3)	24,25=	76.17(8)	24,26=	69.27(10)	24,27=	10.32(9)
24,28=	62.60(8)	24,29=	46.30(8)	24,30=	41.55(8)	24,31=	60.91(12)	24,32=	59.18(12)	24,33=	4.89(12)	24,34=	52.41(12)
24,35=	9.43(12)	25,26=	57.10(9)	25,27=	86.33(9)	25,28=	48.46(7)	25,29=	34.75(7)	25,30=	41.35(7)	25,31=	50.63(12)
25,32=	53.43(12)	25,33=	72.06(12)	25,34=	44.78(11)	25,35=	83.67(12)	26,27=	63.85(11)	26,28=	19.41(10)	26,29=	88.87(10)
26,30=	84.81(9)	26,31=	50.17(13)	26,32=	52.30(13)	26,33=	74.02(13)	26,34=	58.41(13)	26,35=	68.60(13)	27,28=	54.51(9)
27,29=	56.47(9)	27,30=	51.49(9)	27,31=	66.02(13)	27,32=	63.85(13)	27,33=	14.30(13)	27,34=	59.01(13)	27,35=	4.77(13)
28,29=	83.11(8)	28,30=	89.74(7)	28,31=	61.78(12)	28,32=	64.53(12)	28,33=	67.46(12)	28,34=	66.83(12)	28,35=	58.84(12)
29,30=	6.63(7)	29,31=	58.69(12)	29,32=	59.82(12)	29,33=	43.50(12)	29,34=	47.45(12)	29,35=	55.36(12)	30,31=	62.17(11)
30,32=	62.95(11)	30,33=	39.28(12)	30,34=	50.65(11)	30,35=	50.85(12)	31,32=	3.15(15)	31,33=	56.33(15)	31,34=	11.62(15)
31,35=	61.30(15)	32,33=	54.70(15)	32,34=	12.37(15)	32,35=	59.10(15)	33,34=	47.61(15)	33,35=	11.99(15)	34,35=	54.49(15)

(Acute) Angles (Degrees) Between Axes, Lines, Bonds and L.S.-Plane

Bond / Plane	NM --> M	1	2	3	4	5	6	7	8	9	10
Axes 0 --->a	/ OM =	16.69(9),	15.30(8),	15.30(8),	16.69(9),	23.77(9),	22.55(9),	24.40,	41.04(6),	10.59(6),	10.03(5),
	1M =	17.09(7),	38.30(5),	7.17(11),	10.55(6),	16.89(7),	11.41(8),	40.36(6),	7.83(5),	31.6(2),	39.61(6),
	2M =	34.97(5),	8.21(9),	31.6(2),	10.59(6),	25.35(5),	11.41(8),	17.09(7),	7.83(5),	24.86(5),	24.17(5),
	3M =	24.91(10),	27.46(10),	10.79(11),	16.87(10),	19.28(11),					
b	/ OM =	29.80(9),	33.01(8),	33.01(8),	29.80(9),	6.63(9),	0.25(9),	4.42,	47.20(6),	22.25(6),	24.86(5),
	1M =	29.42(7),	47.40(5),	36.91(11),	32.23(6),	31.27(7),	78.53(8),	3.31(6),	81.27(5),	5.0(2),	4.70(6),
	2M =	51.50(5),	20.93(9),	5.0(2),	22.25(6),	40.86(5),	78.53(8),	29.42(7),	81.27(5),	7.15(5),	0.58(5),
	3M =	35.70(10),	33.10(10),	17.37(11),	29.58(10),	24.88(11),					
c	/ OM =	58.42(9),	55.69(8),	55.69(8),	58.42(9),	57.09(9),	59.08(9),	56.89,	15.59(6),	67.55(6),	65.01(5),
	1M =	58.65(7),	21.08(5),	53.08(11),	57.53(6),	56.88(7),	0.45(8),	57.78(6),	4.95(5),	66.2(2),	58.29(6),
	2M =	18.90(5),	69.06(9),	66.2(2),	67.55(6),	33.67(5),	0.45(8),	58.65(7),	4.95(5),	55.89(5),	57.45(5),
	3M =	48.44(10),	49.38(10),	72.39(11),	58.57(10),	62.14(11),					
a*	/ OM =	9.49(9),	8.34(8),	8.34(8),	9.49(9),	32.07(9),	30.92(9),	32.74,	38.61(6),	2.85(6),	2.44(5),
	1M =	9.86(7),	34.99(5),	0.48(11),	3.49(6),	9.81(7),	11.47(8),	32.01(6),	7.18(5),	23.2(2),	31.28(6),
	2M =	32.11(5),	0.39(9),	23.2(2),	2.85(6),	30.96(5),	11.47(8),	9.86(7),	7.18(5),	33.15(5),	32.55(5),
	3M =	18.39(10),	20.75(10),	2.80(11),	9.66(10),	11.74(11),					
b*	/ OM =	29.80(9),	33.01(8),	33.01(8),	29.80(9),	6.63(9),	0.25(9),	4.42,	47.20(6),	22.25(6),	24.86(5),
	1M =	29.42(7),	47.40(5),	36.91(11),	32.23(6),	31.27(7),	78.53(8),	3.31(6),	81.27(5),	5.0(2),	4.70(6),
	2M =	51.50(5),	20.93(9),	5.0(2),	22.25(6),	40.86(5),	78.53(8),	29.42(7),	81.27(5),	7.15(5),	0.58(5),
	3M =	35.70(10),	33.10(10),	17.37(11),	29.58(10),	24.88(11),					
c*	/ OM =	54.97(9),	52.75(8),	52.75(8),	54.97(9),	65.22(9),	67.45(9),	65.15,	10.08(6),	65.11(6),	62.94(5),

Cu(1)	-0(7W)	1M =	55.08(7),	15.80(5),	52.16(11),	55.67(6),	53.49(7),	1.22(8),	49.45(6),	3.85(5),	58.0(2),	50.00(6),	
		2M =	14.07(5),	67.37(9),	58.0(2),	65.11(6),	38.56(5),	1.22(8),	55.08(7),	3.85(5),	64.00(5),	65.82(5),	
		3M =	43.97(10),	44.38(10),	69.37(11),	55.06(10),	57.68(11),						
	/ 0M =	83.90(10),	81.52(10),	31.87(10),	83.90(10),	40.62(10),	45.75(10),	46.86(5),	0.17(8),	85.71(8),	86.40(7),		
		1M =	83.95(9),	4.15(7),	77.05(12),	82.47(8),	82.44(9),	22.76(10),	57.29(8),	30.60(8),	55.9(2),	51.76(8),	
		2M =	0.93(8),	82.95(11),	64.4(2),	85.71(8),	9.68(7),	22.76(10),	83.95(9),	30.60(8),	39.43(8),	44.25(7),	
	3M =	27.36(12),	29.29(12),	81.59(12),	35.21(12),	84.27(12),							
		-0(11A)	/ 0M =	75.96(10),	76.24(10),	20.23(10),	75.96(10),	20.86(10),	26.07(10),	27.49(5),	0.19(8),	65.96(8),	67.15(7),
		1M =	76.09(9),	2.87(7),	69.10(12),	71.27(8),	76.98(8),	28.98(10),	57.84(8),	42.54(7),	49.8(2),	49.99(8),	
	2M =	1.04(7),	63.19(11),	59.9(2),	65.96(8),	9.00(7),	28.98(10),	76.09(9),	42.54(7),	19.67(8),	24.61(7),		
		3M =	19.18(12),	21.85(12),	62.64(12),	23.79(12),	74.57(12),						
		-0(11B)	/ 0M =	9.30(10),	10.40(9),	25.39(9),	9.30(10),	45.92(10),	40.41(10),	38.16(5),	0.12(8),	0.85(8),	0.46(7),
	1M =	9.37(9),	3.95(6),	6.49(12),	5.94(8),	10.52(8),	23.31(9),	11.64(8),	38.70(7),	0.3(2),	6.54(7),		
		2M =	6.73(7),	3.61(11),	5.4(2),	0.85(8),	67.68(7),	23.31(9),	9.37(9),	38.70(7),	47.09(7),	41.76(7),	
		3M =	17.20(11),	14.34(11),	3.94(12),	22.99(11),	8.04(12),						
	-0(22B)	/ 0M =	1.28(10),	4.45(10),	48.13(10),	1.28(10),	1.76(10),	2.16(10),	6.94(5),	86.76(8),	1.25(8),	1.10(7),	
		1M =	0.78(9),	86.46(7),	11.97(12),	6.48(8),	2.29(8),	59.07(10),	31.36(8),	40.33(8),	34.9(2),	38.38(8),	
		2M =	86.42(7),	0.91(11),	26.1(2),	1.25(8),	21.16(7),	59.07(10),	0.78(9),	40.33(8),	1.42(8),	2.97(7),	
	3M =	58.19(12),	57.93(12),	5.19(12),	46.68(12),	3.88(12),							
		-0(51A)	/ 0M =	0.59(10),	2.63(10),	51.85(10),	0.59(10),	5.63(10),	1.66(10),	3.15(5),	82.95(8),	3.68(8),	1.27(7),
		1M =	1.09(9),	87.48(7),	9.89(12),	4.39(8),	0.49(8),	59.18(10),	32.76(8),	41.08(7),	37.1(2),	40.06(8),	
	2M =	87.95(7),	3.49(11),	28.0(2),	3.68(8),	24.70(7),	59.18(10),	1.09(9),	41.08(7),	5.30(8),	0.86(7),		
		3M =	61.71(12),	61.25(12),	7.77(12),	50.29(12),	5.80(12),						
		-0(52A)	/ 0M =	0.33(10),	2.25(9),	54.83(9),	0.33(10),	44.78(10),	38.41(10),	33.73(4),	31.20(7),	10.01(7),	7.70(6),
	1M =	0.53(8),	35.74(6),	3.05(12),	0.36(8),	1.21(8),	45.30(9),	13.33(7),	50.52(7),	25.1(2),	20.27(7),		
		2M =	37.98(7),	12.10(10),	16.7(2),	10.01(7),	76.49(6),	45.30(9),	0.53(8),	50.52(7),	45.28(7),	38.73(6),	
3M =		48.78(11),	45.72(11),	14.63(12),	51.67(11),	4.03(11),							
Cu(2)	-0(6W)	/ 0M =	86.89(10),	86.94(10),	26.19(10),	86.89(10),	36.62(10),	42.13(10),	43.80(5),	4.37(8),	80.61(8),	82.71(7),	
		1M =	86.43(9),	0.32(7),	81.59(12),	86.75(8),	86.55(9),	28.18(10),	54.08(8),	36.37(8),	51.2(2),	47.83(8),	
		2M =	3.70(8),	78.29(11),	60.3(2),	80.61(8),	4.58(7),	28.18(10),	86.43(9),	36.37(8),	35.47(8),	40.72(7),	
	3M =	21.99(12),	24.03(12),	75.97(12),	29.56(12),	82.39(12),							
		-0(12A)	/ 0M =	2.70(10),	3.62(9),	26.48(9),	2.70(10),	52.41(10),	47.19(10),	45.21(5),	3.30(8),	7.32(8),	6.15(7),
		1M =	2.79(9),	1.03(6),	0.60(12),	0.94(8),	3.86(8),	17.54(9),	7.86(8),	31.99(7),	3.8(2),	3.50(7),	
	2M =	3.44(7),	10.11(11),	0.9(2),	7.32(8),	67.62(7),	17.54(9),	2.79(9),	31.99(7),	53.61(7),	48.60(7),		
		3M =	17.36(11),	14.70(11),	10.16(12),	24.46(11),	1.74(12),						
		-0(12B)	/ 0M =	76.28(10),	77.27(10),	18.06(10),	76.28(10),	21.09(10),	26.52(10),	28.21(5),	2.83(8),	65.98(8),	67.47(7),
	1M =	76.30(9),	0.12(7),	71.01(12),	72.47(8),	77.53(8),	31.85(9),	54.97(8),	44.98(7),	47.3(2),	47.17(8),		
		2M =	4.01(7),	63.29(11),	57.4(2),	65.98(8),	9.75(7),	31.85(9),	76.30(9),	44.98(7),	19.93(7),	25.10(7),	
		3M =	16.63(12),	19.25(12),	62.25(12),	21.61(12),	73.88(12),						
	-0(21A)	/ 0M =	0.78(10),	3.89(10),	45.80(10),	0.78(10),	0.98(10),	4.65(10),	9.35(5),	88.80(8),	1.09(8),	1.18(7),	
		1M =	0.28(9),	84.27(7),	11.66(12),	6.21(8),	1.72(8),	56.53(10),	32.19(8),	37.48(8),	34.8(2),	38.88(8),	
		2M =	82.71(7),	0.57(11),	26.4(2),	1.09(8),	17.53(7),	56.53(10),	0.28(9),	37.48(8),	1.37(8),	5.53(7),	
	3M =	56.21(12),	56.28(12),	4.84(12),	44.61(12),	4.30(12),							
		-0(41A)	/ 0M =	2.72(10),	0.23(9),	55.02(9),	2.72(10),	48.18(10),	41.79(10),	37.13(4),	28.59(7),	12.55(7),	10.29(6),
		1M =	2.90(8),	33.32(6),	0.24(12),	3.00(8),	1.19(8),	41.86(9),	14.09(7),	47.36(7),	26.0(2),	20.76(7),	
	2M =	35.38(7),	14.71(10),	17.9(2),	12.55(7),	79.34(6),	41.86(9),	2.90(8),	47.36(7),	48.69(7),	42.14(6),		
		3M =	48.11(11),	45.13(11),	17.09(12),	52.04(11),	6.25(11),						
		-0(42A)	/ 0M =	3.61(10),	0.39(10),	53.90(10),	3.61(10),	7.25(10),	3.51(10),	1.24(5),	81.51(8),	6.63(8),	4.23(7),

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Na(1)	1M =	4.10(9),	87.47(7),	6.89(12),	1.39(8),	2.53(8),	56.41(10),	35.76(8),	38.61(7),	40.1(2),	43.08(8),
	2M =	84.93(7),	6.40(11),	31.0(2),	6.63(8),	24.74(7),	56.41(10),	4.10(9),	38.61(7),	6.87(7),	2.65(7),
	3M =	64.07(12),	63.82(12),	10.68(12),	52.53(12),	8.81(12),					
	-0(4W) / 0M =	43.80(11),	42.07(11),	28.64(11),	43.80(11),	0.63(12),	3.13(12),	2.04(8),	31.91(10),	38.14(10),	37.53(9),
	1M =	44.23(10),	32.49(9),	33.63(13),	37.53(10),	43.84(10),	0.30(11),	65.43(10),	18.82(9),	54.2(3),	61.50(9),
	2M =	28.37(9),	35.75(12),	57.4(3),	38.14(10),	13.14(9),	0.30(11),	44.23(10),	18.82(9),	0.56(9),	1.47(9),
	3M =	34.64(13),	37.77(13),	38.23(13),	31.45(13),	46.72(13),					
	-0(5W) / 0M =	29.83(11),	33.11(11),	32.52(11),	29.83(11),	2.46(11),	3.80(11),	8.60(7),	51.80(9),	23.12(9),	25.75(9),
	1M =	29.41(10),	51.36(9),	37.94(13),	32.94(10),	31.23(10),	83.98(11),	1.37(9),	76.60(9),	6.1(3),	6.54(9),
	2M =	55.49(9),	22.08(12),	3.9(3),	23.12(9),	35.95(9),	83.98(11),	29.41(10),	76.60(9),	2.90(9),	3.59(9),
	3M =	36.51(13),	34.14(13),	18.29(13),	29.24(13),	24.73(13),					
	-0(52A) / 0M =	38.27(10),	35.50(10),	47.49(10),	38.27(10),	11.08(10),	11.59(10),	8.98(5),	47.74(8),	36.94(8),	35.30(7),
Na(2)	1M =	38.78(9),	49.85(7),	27.10(12),	32.20(8),	37.64(8),	16.90(9),	70.83(8),	0.39(7),	65.9(2),	73.71(7),
	2M =	45.78(7),	35.40(11),	62.6(2),	36.94(8),	5.20(7),	16.90(9),	38.78(9),	0.39(7),	10.03(7),	10.03(7),
	3M =	54.57(11),	57.67(11),	39.14(12),	49.88(11),	42.85(12),					
	-0(41A) / 0M =	32.26(10),	31.22(10),	40.46(10),	32.26(10),	86.80(10),	81.93(10),	78.39(5),	3.14(8),	42.28(8),	41.10(7),
	1M =	32.17(9),	2.75(7),	34.69(12),	35.64(8),	31.08(8),	0.52(9),	21.78(8),	6.94(7),	31.5(2),	23.44(7),
	2M =	2.80(7),	45.06(11),	30.1(2),	42.28(8),	55.40(7),	0.52(9),	32.17(9),	6.94(7),	87.91(7),	83.04(7),
	3M =	29.51(11),	28.32(12),	44.93(12),	40.69(11),	33.13(12),					
	-0(21B) / 0M =	28.03(10),	31.34(9),	33.34(9),	28.03(10),	0.02(10),	6.08(10),	10.98(5),	56.52(8),	22.12(8),	24.74(7),
	1M =	27.59(9),	55.64(7),	36.90(12),	31.68(8),	29.37(8),	88.55(9),	1.75(8),	71.49(7),	8.4(2),	9.53(7),
	2M =	59.75(7),	21.33(11),	1.5(2),	22.12(8),	32.47(7),	88.55(9),	27.59(9),	71.49(7),	0.36(7),	6.00(7),
	3M =	38.40(11),	36.26(11),	17.37(12),	30.22(11),	22.84(12),					
	-0(11A) / 0M =	10.17(10),	9.42(9),	29.64(9),	10.17(10),	64.64(10),	60.03(10),	58.42(5),	7.13(8),	19.99(8),	18.98(7),
Na(2)	1M =	10.04(9),	2.00(6),	13.89(12),	14.06(8),	9.07(8),	8.36(9),	1.11(8),	20.63(7),	12.0(2),	4.18(7),
	2M =	0.39(7),	22.79(11),	8.9(2),	19.99(8),	64.32(7),	8.36(9),	10.04(9),	20.63(7),	65.87(7),	61.52(7),
	3M =	19.30(11),	17.12(11),	22.49(12),	28.42(11),	10.75(12),					
	-0(1W) / 0M =	31.33(10),	28.82(10),	40.87(10),	31.33(10),	2.08(10),	2.45(10),	0.20(5),	50.96(8),	28.88(8),	27.44(7),
	1M =	31.82(9),	51.69(7),	20.25(12),	25.08(8),	30.88(8),	18.86(9),	62.54(8),	0.37(7),	56.7(2),	64.57(7),
	2M =	47.57(7),	27.15(11),	53.9(2),	28.88(8),	1.13(7),	18.86(9),	31.82(9),	0.37(7),	1.05(7),	0.89(7),
	3M =	49.36(12),	52.26(12),	30.71(12),	42.82(11),	35.55(12),					
	-0(3W) / 0M =	35.70(10),	38.96(9),	26.90(9),	35.70(10),	0.30(10),	6.70(10),	11.33(5),	46.46(8),	28.65(8),	31.27(7),
	1M =	35.30(9),	45.61(6),	43.41(12),	38.56(8),	37.13(8),	78.66(9),	7.51(8),	80.16(7),	0.0(2),	0.39(7),
	2M =	49.74(7),	27.47(11),	10.0(2),	28.65(8),	34.27(7),	78.66(9),	35.30(9),	80.16(7),	0.25(7),	6.33(7),
	3M =	30.49(11),	28.08(11),	23.78(12),	23.56(11),	30.65(12),					
	-0(41A) / 0M =	43.88(10),	41.30(10),	43.05(10),	43.88(10),	10.99(10),	12.31(10),	10.26(5),	40.84(8),	41.40(8),	40.02(7),
Na(2)	1M =	44.38(9),	42.79(7),	32.77(12),	37.66(8),	43.39(8),	9.82(9),	74.63(8),	7.44(7),	66.3(2),	74.25(7),
	2M =	38.70(7),	39.58(11),	65.8(2),	41.40(8),	1.06(7),	9.82(9),	44.38(9),	7.44(7),	9.87(7),	10.69(7),
	3M =	48.97(12),	52.12(12),	43.01(12),	45.79(11),	48.16(12),					
	-0(52A) / 0M =	36.09(10),	35.46(10),	35.13(10),	36.09(10),	81.96(10),	84.41(10),	84.47(5),	9.10(8),	45.65(8),	44.84(7),
	1M =	35.94(9),	3.16(7),	39.82(12),	40.12(8),	35.05(8),	6.67(9),	21.42(8),	0.04(7),	30.0(2),	22.01(7),
	2M =	3.39(7),	48.45(11),	30.1(2),	45.65(8),	48.48(7),	6.67(9),	35.94(9),	0.04(7),	82.00(7),	85.97(7),
	3M =	24.29(11),	23.40(12),	47.61(12),	35.74(11),	36.27(12),					
	-0(12B) / 0M =	28.92(10),	30.08(9),	8.08(9),	28.92(10),	55.02(10),	58.48(10),	62.85(5),	36.18(8),	34.93(7),	35.63(7),
	1M =	28.54(8),	30.25(6),	37.79(12),	34.94(8),	28.62(8),	28.43(9),	2.81(8),	15.94(7),	8.2(2),	0.79(7),
	2M =	30.34(7),	37.17(10),	11.6(2),	34.93(7),	28.56(7),	28.43(9),	28.54(8),	15.94(7),	55.36(7),	59.49(6),
	3M =	2.68(11),	3.38(11),	34.19(12),	8.86(11),	26.42(11),					
	-0(22A) / 0M =	31.64(10),	34.55(10),	29.95(10),	31.64(10),	12.57(10),	6.05(10),	1.79(5),	36.06(8),	22.68(8),	25.13(7),

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O(11A)-C(11A) /	1M =	31.35(9),	36.94(7),	36.41(12),	32.60(8),	33.18(8),	66.68(9),	9.76(8),	83.44(7),	0.0(2),	1.75(7),
	2M =	40.94(7),	20.85(11),	9.9(2),	22.68(8),	47.99(7),	66.68(9),	31.35(9),	83.44(7),	13.28(7),	6.66(7),
	3M =	30.18(11),	27.26(11),	17.88(12),	26.39(11),	27.25(12),					
	0M =	42.68(16),	44.00(16),	11.55(16),	42.68(16),	54.75(16),	60.29(16),	65.34(13),	32.66(15),	47.84(15),	48.85(14),
O(11B)-C(11B) /	1M =	42.27(15),	26.80(14),	51.84(17),	48.81(15),	42.46(15),	34.13(16),	14.58(15),	25.36(14),	18.3(3),	11.42(14),
	2M =	28.00(14),	49.83(16),	23.1(3),	47.84(15),	22.14(14),	34.13(16),	42.27(15),	25.36(14),	54.56(14),	60.56(14),
	3M =	1.61(17),	1.63(17),	46.41(17),	13.14(17),	39.82(17),					
	0M =	0.64(16),	0.82(16),	11.16(16),	0.64(16),	49.81(16),	47.30(16),	47.82(14),	22.90(15),	9.21(15),	8.90(15),
O(12A)-C(11A) /	1M =	0.38(16),	18.34(15),	7.25(18),	5.78(15),	0.12(15),	1.37(16),	15.22(15),	14.79(15),	5.2(3),	13.18(15),
	2M =	16.13(15),	11.94(17),	6.9(3),	9.21(15),	48.93(15),	1.37(16),	0.38(16),	14.79(15),	50.98(15),	48.96(15),
	3M =	0.95(17),	1.32(17),	10.52(18),	9.89(17),	0.20(17),					
	0M =	7.65(16),	7.49(16),	7.84(16),	7.65(16),	42.75(16),	39.68(16),	39.85(14),	21.70(15),	1.04(15),	0.67(15),
O(12B)-C(11B) /	1M =	7.90(16),	17.78(15),	1.04(18),	2.53(15),	8.41(15),	2.96(16),	22.02(15),	20.28(15),	11.4(3),	19.25(15),
	2M =	15.07(15),	3.78(17),	14.0(3),	1.04(15),	48.26(15),	2.96(16),	7.90(16),	20.28(15),	43.96(15),	41.32(15),
	3M =	1.72(17),	4.26(17),	2.50(18),	6.15(17),	8.38(17),					
	0M =	47.38(16),	48.98(16),	10.30(16),	47.38(16),	50.94(16),	56.94(16),	61.91(13),	33.00(15),	51.49(15),	52.80(14),
O(21A)-C(21A) /	1M =	46.94(15),	27.32(14),	57.10(17),	53.63(15),	47.30(15),	38.25(16),	17.71(15),	30.81(14),	20.2(3),	13.85(15),
	2M =	28.99(14),	53.18(16),	26.0(3),	51.49(15),	17.16(14),	38.25(16),	46.94(15),	30.81(14),	50.59(14),	56.94(14),
	3M =	0.91(17),	1.26(17),	49.44(17),	12.22(17),	44.10(17),					
	0M =	8.52(16),	7.68(16),	3.00(16),	8.52(16),	36.11(16),	34.42(16),	35.78(13),	33.34(15),	1.16(15),	0.99(14),
O(21B)-C(21B) /	1M =	8.86(15),	29.56(14),	0.20(17),	2.74(15),	8.99(15),	7.13(16),	28.63(15),	11.12(14),	19.2(3),	27.23(15),
	2M =	26.77(14),	1.41(16),	20.0(3),	1.16(15),	36.54(14),	7.13(16),	8.86(15),	11.12(14),	37.23(14),	36.06(14),
	3M =	12.94(17),	15.34(17),	0.66(17),	4.41(17),	10.31(17),					
	0M =	9.90(16),	11.93(16),	38.71(16),	9.90(16),	42.02(16),	35.57(16),	31.81(14),	18.37(15),	0.35(15),	1.60(15),
O(22A)-C(21A) /	1M =	9.81(16),	22.10(15),	10.63(18),	8.40(15),	11.36(15),	40.04(16),	2.11(15),	52.44(15),	9.9(3),	4.44(15),
	2M =	24.96(15),	2.82(17),	2.2(3),	0.35(15),	76.52(15),	40.04(16),	9.81(16),	52.44(15),	42.91(15),	36.44(15),
	3M =	32.37(17),	29.31(17),	4.47(18),	35.71(17),	7.09(17),					
	0M =	13.73(16),	15.90(16),	37.85(16),	13.73(16),	37.29(16),	30.81(16),	26.97(14),	21.38(15),	3.57(15),	5.61(15),
O(22B)-C(21B) /	1M =	13.61(16),	24.74(15),	15.01(18),	12.56(15),	15.21(15),	44.53(16),	3.66(15),	57.40(15),	8.2(3),	3.26(15),
	2M =	27.83(15),	1.17(17),	0.0(3),	3.57(15),	72.36(15),	44.53(16),	13.61(16),	57.40(15),	38.15(15),	31.65(15),
	3M =	32.50(17),	29.37(17),	0.69(18),	34.66(17),	10.67(17),					
	0M =	6.95(16),	5.93(16),	5.28(16),	6.95(16),	35.39(16),	34.20(16),	35.94(13),	36.88(15),	0.04(15),	0.28(14),
O(41A)-C(41A) /	1M =	7.31(15),	32.99(14),	1.78(17),	1.03(15),	7.33(15),	10.83(16),	28.77(15),	7.47(14),	19.9(3),	27.96(14),
	2M =	30.27(14),	2.46(16),	20.0(3),	0.04(15),	33.50(14),	10.83(16),	7.31(15),	7.47(14),	36.47(14),	35.83(14),
	3M =	15.44(17),	17.74(17),	0.15(17),	6.53(17),	9.03(17),					
	0M =	10.83(16),	10.31(16),	0.89(16),	10.83(16),	37.10(16),	34.61(16),	35.34(14),	27.49(15),	2.78(15),	2.88(15),
O(42A)-C(41A) /	1M =	11.13(16),	23.88(15),	3.26(18),	5.33(15),	11.44(15),	1.12(16),	27.91(15),	17.02(15),	17.7(3),	25.61(15),
	2M =	20.98(15),	0.11(17),	19.6(3),	2.78(15),	41.48(15),	1.12(16),	11.13(16),	17.02(15),	38.28(15),	36.27(15),
	3M =	8.65(17),	11.21(17),	1.79(18),	0.79(17),	12.11(17),					
	0M =	37.85(16),	39.95(16),	0.97(16),	37.85(16),	42.40(16),	47.71(16),	52.75(13),	44.80(15),	40.51(15),	42.12(14),
O(51A)-C(51A) /	1M =	37.38(15),	39.04(14),	48.50(17),	44.18(15),	38.05(15),	45.56(16),	6.63(15),	34.17(14),	8.4(3),	2.29(15),
	2M =	40.48(14),	41.95(16),	14.6(3),	40.51(15),	11.45(14),	45.56(16),	37.38(15),	34.17(14),	42.31(14),	48.08(14),
	3M =	10.69(17),	10.48(17),	38.02(17),	0.75(17),	33.97(17),					
	0M =	1.49(16),	3.37(16),	41.94(16),	1.49(16),	51.13(16),	44.68(16),	40.91(13),	14.82(15),	8.82(15),	6.97(14),
O(52A)-C(51A) /	1M =	1.43(15),	19.23(14),	1.69(17),	0.34(15),	2.91(15),	32.88(16),	3.07(15),	43.72(14),	15.1(3),	8.93(15),
	2M =	21.58(14),	11.36(16),	8.3(3),	8.82(15),	83.94(14),	32.88(16),	1.43(15),	43.72(14),	52.02(14),	45.56(14),
	3M =	34.01(17),	31.13(17),	12.77(17),	39.35(17),	1.02(17),					
	0M =	1.35(16),	2.56(16),	4.80(16),	1.35(16),	39.24(16),	39.17(16),	41.66(14),	41.24(15),	7.66(15),	8.20(15),

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C(1A) -C(2A) /	1M =	0.96(16),	36.60(15),	10.45(18),	7.39(15),	1.06(15),	18.03(16),	22.81(15),	0.38(15),	15.2(3),	23.13(15),	
	2M =	34.47(15),	10.04(17),	13.9(3),	7.66(15),	30.70(15),	18.03(16),	0.96(16),	0.38(15),	40.19(15),	40.73(15),	
	3M =	15.50(17),	17.41(17),	7.41(18),	5.50(17),	1.08(17),						
	0M =	36.33(18),	34.20(18),	34.09(18),	36.33(18),	0.27(18),	1.12(18),	0.80(16),	42.11(17),	32.22(17),	31.17(17),	
	1M =	36.80(18),	42.52(17),	25.6(2),	30.00(18),	36.13(18),	9.86(18),	63.93(17),	8.81(17),	55.0(3),	63.04(17),	
	2M =	38.41(17),	30.13(19),	55.1(3),	32.22(17),	8.21(17),	9.86(18),	36.80(18),	8.81(17),	1.39(17),	0.50(17),	
	3M =	41.58(19),	44.61(19),	33.2(2),	36.46(19),	39.96(19),						
	-C(6A) /	0M =	11.61(19),	14.86(18),	43.31(18),	11.61(19),	0.02(19),	4.88(19),	9.89(16),	77.23(17),	8.05(17),	10.53(17),
	1M =	11.12(18),	75.86(17),	21.9(2),	16.44(18),	12.73(18),	70.45(18),	20.43(18),	51.35(17),	25.1(3),	27.75(17),	
	2M =	79.72(17),	8.05(19),	15.8(3),	8.05(17),	25.02(17),	70.45(18),	11.12(18),	51.35(17),	0.11(17),	5.40(17),	
	3M =	51.79(19),	50.67(19),	3.8(2),	41.09(19),	6.4(2),						
	-C(11A) /	0M =	57.24(17),	59.38(17),	1.32(17),	57.24(17),	4.01(18),	10.05(18),	12.78(15),	13.64(16),	47.07(16),	49.06(16),
C(1B) -C(2B) /	1M =	57.10(17),	12.55(16),	57.29(19),	55.75(16),	58.73(17),	45.61(17),	38.55(16),	62.60(16),	28.9(3),	30.52(16),	
	2M =	16.68(16),	44.63(18),	38.7(3),	47.07(16),	29.08(16),	45.61(17),	57.10(17),	62.60(16),	2.94(16),	8.86(16),	
	3M =	1.30(18),	1.57(18),	42.81(19),	2.24(18),	53.91(19),						
	0M =	34.99(18),	32.84(18),	34.03(18),	34.99(18),	1.09(18),	0.19(18),	1.80(16),	43.21(17),	30.94(17),	29.87(17),	
	1M =	35.46(18),	43.50(17),	24.3(2),	28.65(18),	34.78(18),	10.93(18),	62.86(17),	7.81(17),	54.3(3),	62.29(17),	
	2M =	39.40(17),	28.87(19),	54.0(3),	30.94(17),	8.26(17),	10.93(18),	35.46(18),	7.81(17),	2.20(17),	1.43(17),	
	3M =	41.75(19),	44.76(19),	32.0(2),	36.32(19),	38.64(19),						
	-C(11B) /	0M =	51.09(17),	53.02(17),	5.14(17),	51.09(17),	2.71(17),	3.30(17),	5.99(15),	12.49(16),	40.81(16),	42.69(16),
	1M =	51.00(17),	12.12(16),	50.54(19),	49.19(16),	52.54(16),	44.80(17),	35.92(16),	63.36(16),	25.4(3),	27.99(16),	
	2M =	16.24(16),	38.30(18),	34.9(3),	40.81(16),	35.34(16),	44.80(17),	51.00(17),	63.36(16),	3.78(16),	2.09(16),	
	3M =	3.99(18),	0.99(18),	36.72(19),	1.61(18),	48.15(18),						
	-C(6B)h /	0M =	9.87(19),	13.16(18),	47.23(18),	9.87(19),	4.78(19),	0.20(19),	5.22(16),	74.72(17),	5.55(17),	8.09(17),
C(2A) -C(3A) /	1M =	9.40(18),	75.36(17),	19.8(2),	14.35(18),	11.07(18),	71.41(18),	21.32(17),	53.28(17),	26.9(3),	28.92(17),	
	2M =	79.49(17),	5.34(19),	17.3(3),	5.55(17),	29.92(17),	71.41(18),	9.40(18),	53.28(17),	4.72(17),	0.67(17),	
	3M =	55.03(19),	53.58(19),	1.1(2),	44.80(19),	4.6(2),						
	0M =	51.79(19),	54.22(18),	7.80(18),	51.79(19),	0.23(19),	6.49(19),	9.63(16),	18.94(17),	41.87(17),	44.02(17),	
	1M =	51.60(18),	18.24(17),	53.4(2),	51.07(18),	53.32(18),	51.18(18),	32.04(17),	68.91(17),	22.4(3),	24.01(17),	
	2M =	22.37(17),	39.58(19),	32.2(3),	41.87(17),	33.88(17),	51.18(18),	51.60(18),	68.91(17),	0.76(17),	5.41(17),	
	3M =	7.84(19),	4.96(19),	37.4(2),	4.24(19),	48.1(2),						
	-C(21A) /	0M =	8.09(17),	11.32(17),	45.69(17),	8.09(17),	1.29(18),	3.31(18),	8.28(15),	80.35(16),	4.73(16),	7.18(16),
	1M =	7.59(17),	79.50(16),	18.49(19),	12.99(17),	9.19(17),	67.07(17),	24.06(16),	48.20(16),	28.5(3),	31.34(16),	
	2M =	83.34(16),	4.81(18),	19.3(3),	4.73(16),	24.65(16),	67.07(17),	7.59(17),	48.20(16),	1.12(16),	3.92(16),	
	3M =	54.62(18),	53.68(18),	0.53(19),	43.65(18),	2.87(19),						
	-C(21B) /	0M =	46.11(19),	48.31(18),	11.30(18),	46.11(19),	6.41(19),	0.20(19),	2.88(16),	17.29(18),	35.97(17),	38.01(17),
C(2B) -C(6B) /	1M =	45.97(18),	17.31(17),	46.9(2),	44.85(18),	47.60(18),	49.50(18),	29.74(18),	68.62(17),	19.3(3),	21.82(17),	
	2M =	21.41(17),	33.57(19),	28.8(3),	35.97(17),	40.11(17),	49.50(18),	45.97(18),	68.62(17),	7.42(17),	1.30(17),	
	3M =	10.15(19),	7.15(19),	31.7(2),	7.76(19),	42.8(2),						
	0M =	5.61(17),	8.89(17),	50.35(17),	5.61(17),	6.48(17),	1.80(17),	3.18(15),	77.40(16),	1.52(16),	4.03(16),	
	1M =	5.13(17),	79.28(16),	15.65(19),	10.18(16),	6.80(17),	67.10(17),	25.70(16),	49.33(16),	31.2(3),	33.28(16),	
	2M =	83.28(16),	1.39(18),	21.7(3),	1.52(16),	29.55(16),	67.10(17),	5.13(17),	49.33(16),	6.32(16),	1.23(16),	
	3M =	58.73(18),	57.48(18),	2.85(19),	48.12(18),	0.37(18),						
	-C(3A) -C(4A) /	0M =	11.39(19),	14.63(18),	43.36(18),	11.39(19),	0.10(19),	4.93(19),	9.94(17),	77.56(18),	7.88(18),	10.34(17),
	1M =	10.90(18),	76.14(17),	21.7(2),	16.24(18),	12.50(18),	70.12(18),	20.69(18),	51.01(17),	25.3(3),	28.00(17),	
	2M =	79.98(17),	7.89(19),	16.0(3),	7.88(18),	24.80(17),	70.12(18),	10.90(18),	51.01(17),	0.20(17),	5.46(17),	
	3M =	51.9(2),	50.8(2),	3.6(2),	41.2(2),	6.2(2),						
	-C(4A) -C(5A) /	0M =	36.82(18),	34.66(18),	34.61(18),	36.82(18),	0.39(19),	1.78(19),	0.15(16),	42.06(17),	32.78(17),	31.72(17),

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	1M =	37.29(18),	42.57(17),	26.1(2),	30.48(18),	36.60(18),	9.84(18),	64.57(17),	8.76(17),	55.7(3),	63.70(17),
	2M =	38.45(17),	30.70(19),	55.7(3),	32.78(17),	7.69(17),	9.84(18),	37.29(18),	8.76(17),	0.74(17),	0.15(17),
	3M =	42.02(19),	45.07(19),	33.8(2),	37.00(19),	40.48(19),					
-C(41A) /	0M =	54.51(18),	56.74(17),	4.18(17),	54.51(18),	1.74(18),	7.87(18),	10.74(15),	15.41(16),	44.40(16),	46.44(16),
	1M =	54.36(17),	14.56(16),	55.06(19),	53.25(17),	56.01(17),	47.56(17),	35.87(16),	65.06(16),	26.1(3),	27.85(16),
	2M =	18.69(16),	42.00(18),	35.9(3),	44.40(16),	31.69(16),	47.56(17),	54.36(17),	65.06(16),	0.70(16),	6.71(16),
	3M =	4.03(18),	1.13(19),	40.08(19),	0.61(18),	51.09(19),					
C(5A) -C(6A) /	0M =	51.34(19),	53.74(18),	8.05(18),	51.34(19),	0.35(19),	5.90(19),	9.02(16),	18.72(18),	41.39(18),	43.53(17),
	1M =	51.16(18),	18.08(17),	52.8(2),	50.55(18),	52.86(18),	50.98(18),	31.93(18),	68.89(17),	22.2(3),	23.91(17),
	2M =	22.21(17),	39.08(19),	32.0(3),	41.39(18),	34.41(17),	50.98(18),	51.16(18),	68.89(17),	1.35(17),	4.81(17),
	3M =	8.0(2),	5.1(2),	36.9(2),	4.48(19),	47.7(2),					
-C(51A) /	0M =	6.06(17),	9.33(17),	49.14(17),	6.06(17),	5.01(18),	0.38(18),	4.59(15),	78.66(16),	2.21(16),	4.70(16),
	1M =	5.58(17),	79.92(16),	16.23(19),	10.74(16),	7.22(17),	66.90(17),	25.54(16),	48.75(16),	30.7(3),	33.04(16),
	2M =	84.04(16),	2.15(18),	21.3(3),	2.21(16),	28.01(16),	66.90(17),	5.58(17),	48.75(16),	4.84(16),	0.21(16),
	3M =	57.76(18),	56.62(18),	2.10(19),	47.00(18),	0.83(19),					
Cu(1)a-0(22B) /	0M =	1.28(10),	4.45(10),	48.13(10),	1.28(10),	1.76(10),	2.16(10),	6.94(5),	86.76(8),	1.25(8),	1.10(7),
	1M =	0.78(9),	86.46(7),	11.97(12),	6.48(8),	2.29(8),	59.07(10),	31.36(8),	40.33(8),	34.9(2),	38.38(8),
	2M =	86.42(7),	0.91(11),	26.1(2),	1.25(8),	21.16(7),	59.07(10),	0.78(9),	40.33(8),	1.42(8),	2.97(7),
	3M =	58.19(12),	57.93(12),	5.19(12),	46.68(12),	3.88(12),					
-0(7W)a /	0M =	83.90(10),	81.52(10),	31.87(10),	83.90(10),	40.62(10),	45.75(10),	46.86(5),	0.17(8),	85.71(8),	86.40(7),
	1M =	83.95(9),	4.15(7),	77.05(12),	82.47(8),	82.44(9),	22.76(10),	57.29(8),	30.60(8),	55.9(2),	51.76(8),
	2M =	0.93(8),	82.95(11),	64.4(2),	85.71(8),	9.68(7),	22.76(10),	83.95(9),	30.60(8),	39.43(8),	44.25(7),
	3M =	27.36(12),	29.29(12),	81.59(12),	35.21(12),	84.27(12),					
-0(11A) /	0M =	75.96(10),	76.24(10),	20.23(10),	75.96(10),	20.86(10),	26.07(10),	27.49(5),	0.19(8),	65.96(8),	67.15(7),
	1M =	76.09(9),	2.87(7),	69.10(12),	71.27(8),	76.98(8),	28.98(10),	57.84(8),	42.54(7),	49.8(2),	49.99(8),
	2M =	1.04(7),	63.19(11),	59.9(2),	65.96(8),	9.00(7),	28.98(10),	76.09(9),	42.54(7),	19.67(8),	24.61(7),
	3M =	19.18(12),	21.85(12),	62.64(12),	23.79(12),	74.57(12),					
-0(11B) /	0M =	9.30(10),	10.40(9),	25.39(9),	9.30(10),	45.92(10),	40.41(10),	38.16(5),	0.12(8),	0.85(8),	0.46(7),
	1M =	9.37(9),	3.95(6),	6.49(12),	5.94(8),	10.52(8),	23.31(9),	11.64(8),	38.70(7),	0.3(2),	6.54(7),
	2M =	6.73(7),	3.61(11),	5.4(2),	0.85(8),	67.68(7),	23.31(9),	9.37(9),	38.70(7),	47.09(7),	41.76(7),
	3M =	17.20(11),	14.34(11),	3.94(12),	22.99(11),	8.04(12),					
-0(51A) /	0M =	0.59(10),	2.63(10),	51.85(10),	0.59(10),	5.63(10),	1.66(10),	3.15(5),	82.95(8),	3.68(8),	1.27(7),
	1M =	1.09(9),	87.48(7),	9.89(12),	4.39(8),	0.49(8),	59.18(10),	32.76(8),	41.08(7),	37.1(2),	40.06(8),
	2M =	87.95(7),	3.49(11),	28.0(2),	3.68(8),	24.70(7),	59.18(10),	1.09(9),	41.08(7),	5.30(8),	0.86(7),
	3M =	61.71(12),	61.25(12),	7.77(12),	50.29(12),	5.80(12),					
-0(52A) /	0M =	0.33(10),	2.25(9),	54.83(9),	0.33(10),	44.78(10),	38.41(10),	33.73(4),	31.20(7),	10.01(7),	7.70(6),
	1M =	0.53(8),	35.74(6),	3.05(12),	0.36(8),	1.21(8),	45.30(9),	13.33(7),	50.52(7),	25.1(2),	20.27(7),
	2M =	37.98(7),	12.10(10),	16.7(2),	10.01(7),	76.49(6),	45.30(9),	0.53(8),	50.52(7),	45.28(7),	38.73(6),
	3M =	48.78(11),	45.72(11),	14.63(12),	51.67(11),	4.03(11),					
Cu(2)a-0(6W)a /	0M =	86.89(10),	86.94(10),	26.19(10),	86.89(10),	36.62(10),	42.13(10),	43.80(5),	4.37(8),	80.61(8),	82.71(7),
	1M =	86.43(9),	0.32(7),	81.59(12),	86.75(8),	86.55(9),	28.18(10),	54.08(8),	36.37(8),	51.2(2),	47.83(8),
	2M =	3.70(8),	78.29(11),	60.3(2),	80.61(8),	4.58(7),	28.18(10),	86.43(9),	36.37(8),	35.47(8),	40.72(7),
	3M =	21.99(12),	24.03(12),	75.97(12),	29.56(12),	82.39(12),					
-0(12A) /	0M =	2.70(10),	3.62(9),	26.48(9),	2.70(10),	52.41(10),	47.19(10),	45.21(5),	3.30(8),	7.32(8),	6.15(7),
	1M =	2.79(9),	1.03(6),	0.60(12),	0.94(8),	3.86(8),	17.54(9),	7.86(8),	31.99(7),	3.8(2),	3.50(7),
	2M =	3.44(7),	10.11(11),	0.9(2),	7.32(8),	67.62(7),	17.54(9),	2.79(9),	31.99(7),	53.61(7),	48.60(7),
	3M =	17.36(11),	14.70(11),	10.16(12),	24.46(11),	1.74(12),					
-0(12B) /	0M =	76.28(10),	77.27(10),	18.06(10),	76.28(10),	21.09(10),	26.52(10),	28.21(5),	2.83(8),	65.98(8),	67.47(7),

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Na(1)a-O(4W)a /	1M =	76.30(9),	0.12(7),	71.01(12),	72.47(8),	77.53(8),	31.85(9),	54.97(8),	44.98(7),	47.3(2),	47.17(8),
	2M =	4.01(7),	63.29(11),	57.4(2),	65.98(8),	9.75(7),	31.85(9),	76.30(9),	44.98(7),	19.93(7),	25.10(7),
	3M =	16.63(12),	19.25(12),	62.25(12),	21.61(12),	73.88(12),					
	0M =	43.80(11),	42.07(11),	28.64(11),	43.80(11),	0.63(12),	3.13(12),	2.04(8),	31.91(10),	38.14(10),	37.53(9),
	1M =	44.23(10),	32.49(9),	33.63(13),	37.53(10),	43.84(10),	0.30(11),	65.43(10),	18.82(9),	54.2(3),	61.50(9),
	2M =	28.37(9),	35.75(12),	57.4(3),	38.14(10),	13.14(9),	0.30(11),	44.23(10),	18.82(9),	0.56(9),	1.47(9),
	3M =	34.64(13),	37.77(13),	38.23(13),	31.45(13),	46.72(13),					
	-O(5W)a /	0M =	29.83(11),	33.11(11),	32.52(11),	29.83(11),	2.46(11),	3.80(11),	8.60(7),	51.80(9),	23.12(9),
	1M =	29.41(10),	51.36(9),	37.94(13),	32.94(10),	31.23(10),	83.98(11),	1.37(9),	76.60(9),	6.1(3),	6.54(9),
	2M =	55.49(9),	22.08(12),	3.9(3),	23.12(9),	35.95(9),	83.98(11),	29.41(10),	76.60(9),	2.90(9),	3.59(9),
	3M =	36.51(13),	34.14(13),	18.29(13),	29.24(13),	24.73(13),					
	-O(52A) /	0M =	38.27(10),	35.50(10),	47.49(10),	38.27(10),	11.08(10),	11.59(10),	8.98(5),	47.74(8),	36.94(8),
Na(2)a-O(52A) /	1M =	38.78(9),	49.85(7),	27.10(12),	32.20(8),	37.64(8),	16.90(9),	70.83(8),	0.39(7),	65.9(2),	73.71(7),
	2M =	45.78(7),	35.40(11),	62.6(2),	36.94(8),	5.20(7),	16.90(9),	38.78(9),	0.39(7),	10.03(7),	10.03(7),
	3M =	54.57(11),	57.67(11),	39.14(12),	49.88(11),	42.85(12),					
	-O(11A) /	0M =	10.17(10),	9.42(9),	29.64(9),	10.17(10),	64.64(10),	60.03(10),	58.42(5),	7.13(8),	19.99(8),
	1M =	10.04(9),	2.00(6),	13.89(12),	14.06(8),	9.07(8),	8.36(9),	1.11(8),	20.63(7),	12.0(2),	4.18(7),
	2M =	0.39(7),	22.79(11),	8.9(2),	19.99(8),	64.32(7),	8.36(9),	10.04(9),	20.63(7),	65.87(7),	61.52(7),
	3M =	19.30(11),	17.12(11),	22.49(12),	28.42(11),	10.75(12),					
	-O(1W)a /	0M =	36.09(10),	35.46(10),	35.13(10),	36.09(10),	81.96(10),	84.41(10),	84.47(5),	9.10(8),	45.65(8),
	1M =	35.94(9),	3.16(7),	39.82(12),	40.12(8),	35.05(8),	6.67(9),	21.42(8),	0.04(7),	30.0(2),	22.01(7),
	2M =	3.39(7),	48.45(11),	30.1(2),	45.65(8),	48.48(7),	6.67(9),	35.94(9),	0.04(7),	82.00(7),	85.97(7),
	3M =	24.29(11),	23.40(12),	47.61(12),	35.74(11),	36.27(12),					
	-O(3W)a /	0M =	31.33(10),	28.82(10),	40.87(10),	31.33(10),	2.08(10),	2.45(10),	0.20(5),	50.96(8),	28.88(8),
O(11A)-C(11A) /	1M =	31.82(9),	51.69(7),	20.25(12),	25.08(8),	30.88(8),	18.86(9),	62.54(8),	0.37(7),	56.7(2),	64.57(7),
	2M =	47.57(7),	27.15(11),	53.9(2),	28.88(8),	1.13(7),	18.86(9),	31.82(9),	0.37(7),	1.05(7),	0.89(7),
	3M =	49.36(12),	52.26(12),	30.71(12),	42.82(11),	35.55(12),					
	-O(41A) /	0M =	35.70(10),	38.96(9),	26.90(9),	35.70(10),	0.30(10),	6.70(10),	11.33(5),	46.46(8),	28.65(8),
	1M =	35.30(9),	45.61(6),	43.41(12),	38.56(8),	37.13(8),	78.66(9),	7.51(8),	80.16(7),	0.0(2),	0.39(7),
	2M =	49.74(7),	27.47(11),	10.0(2),	28.65(8),	34.27(7),	78.66(9),	35.30(9),	80.16(7),	0.25(7),	6.33(7),
	3M =	30.49(11),	28.08(11),	23.78(12),	23.56(11),	30.65(12),					
	-O(22A) /	0M =	43.88(10),	41.30(10),	43.05(10),	43.88(10),	10.99(10),	12.31(10),	10.26(5),	40.84(8),	41.40(8),
	1M =	44.38(9),	42.79(7),	32.77(12),	37.66(8),	43.39(8),	9.82(9),	74.63(8),	7.44(7),	66.3(2),	74.25(7),
	2M =	38.70(7),	39.58(11),	65.8(2),	41.40(8),	1.06(7),	9.82(9),	44.38(9),	7.44(7),	9.87(7),	10.69(7),
	3M =	48.97(12),	52.12(12),	43.01(12),	45.79(11),	48.16(12),					
	-O(11B)-C(11B) /	0M =	31.64(10),	34.55(10),	29.95(10),	31.64(10),	12.57(10),	6.05(10),	1.79(5),	36.06(8),	22.68(8),
O(12A)-C(11A) /	1M =	31.35(9),	36.94(7),	36.41(12),	32.60(8),	33.18(8),	66.68(9),	9.76(8),	83.44(7),	0.0(2),	1.75(7),
	2M =	40.94(7),	20.85(11),	9.9(2),	22.68(8),	47.99(7),	66.68(9),	31.35(9),	83.44(7),	13.28(7),	6.66(7),
	3M =	30.18(11),	27.26(11),	17.88(12),	26.39(11),	27.25(12),					
	0M =	42.68(16),	44.00(16),	11.55(16),	42.68(16),	54.75(16),	60.29(16),	65.34(13),	32.66(15),	47.84(15),	48.85(14),
	1M =	42.27(15),	26.80(14),	51.84(17),	48.81(15),	42.46(15),	34.13(16),	14.58(15),	25.36(14),	18.3(3),	11.42(14),
	2M =	28.00(14),	49.83(16),	23.1(3),	47.84(15),	22.14(14),	34.13(16),	42.27(15),	25.36(14),	54.56(14),	60.56(14),
	3M =	1.61(17),	1.63(17),	46.41(17),	13.14(17),	39.82(17),					
	0M =	0.64(16),	0.82(16),	11.16(16),	0.64(16),	49.81(16),	47.30(16),	47.82(14),	22.90(15),	9.21(15),	8.90(15),
	1M =	0.38(16),	18.34(15),	7.25(18),	5.78(15),	0.12(15),	1.37(16),	15.22(15),	14.79(15),	5.2(3),	13.18(15),
	2M =	16.13(15),	11.94(17),	6.9(3),	9.21(15),	48.93(15),	1.37(16),	0.38(16),	14.79(15),	50.98(15),	48.96(15),
	3M =	0.95(17),	1.32(17),	10.52(18),	9.89(17),	0.20(17),					
	0M =	7.65(16),	7.49(16),	7.84(16),	7.65(16),	42.75(16),	39.68(16),	39.85(14),	21.70(15),	1.04(15),	0.67(15),

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O(12B)-C(11B) /	1M =	7.90(16),	17.78(15),	1.04(18),	2.53(15),	8.41(15),	2.96(16),	22.02(15),	20.28(15),	11.4(3),	19.25(15),
	2M =	15.07(15),	3.78(17),	14.0(3),	1.04(15),	48.26(15),	2.96(16),	7.90(16),	20.28(15),	43.96(15),	41.32(15),
	3M =	1.72(17),	4.26(17),	2.50(18),	6.15(17),	8.38(17),					
	0M =	47.38(16),	48.98(16),	10.30(16),	47.38(16),	50.94(16),	56.94(16),	61.91(13),	33.00(15),	51.49(15),	52.80(14),
O(21A)-C(21A) /	1M =	46.94(15),	27.32(14),	57.11(17),	53.63(15),	47.30(15),	38.25(16),	17.71(15),	30.81(14),	20.2(3),	13.85(15),
	2M =	28.99(14),	53.18(16),	26.0(3),	51.49(15),	17.16(14),	38.25(16),	46.94(15),	30.81(14),	50.59(14),	56.94(14),
	3M =	0.91(17),	1.26(17),	49.44(17),	12.22(17),	44.10(17),					
	0M =	8.52(16),	7.68(16),	3.00(16),	8.52(16),	36.11(16),	34.42(16),	35.78(13),	33.34(15),	1.16(15),	0.99(14),
O(21B)-C(21B) /	1M =	8.86(15),	29.56(14),	0.20(17),	2.74(15),	8.99(15),	7.13(16),	28.63(15),	11.12(14),	19.2(3),	27.23(15),
	2M =	26.77(14),	1.41(16),	20.0(3),	1.16(15),	36.54(14),	7.13(16),	8.86(15),	11.12(14),	37.23(14),	36.06(14),
	3M =	12.94(17),	15.34(17),	0.66(17),	4.41(17),	10.31(17),					
	0M =	9.90(16),	11.93(16),	38.71(16),	9.90(16),	42.02(16),	35.57(16),	31.81(14),	18.37(15),	0.35(15),	1.60(15),
O(22A)-C(21A) /	1M =	9.81(16),	22.10(15),	10.63(18),	8.40(15),	11.36(15),	40.04(16),	2.11(15),	52.44(15),	9.9(3),	4.44(15),
	2M =	24.96(15),	2.82(17),	2.2(3),	0.35(15),	76.52(15),	40.04(16),	9.81(16),	52.44(15),	42.91(15),	36.44(15),
	3M =	32.37(17),	29.31(17),	4.47(18),	35.71(17),	7.09(17),					
	0M =	13.73(16),	15.90(16),	37.85(16),	13.73(16),	37.29(16),	30.81(16),	26.97(14),	21.38(15),	3.57(15),	5.61(15),
O(22B)-C(21B) /	1M =	13.61(16),	24.74(15),	15.01(18),	12.56(15),	15.21(15),	44.53(16),	3.66(15),	57.40(15),	8.2(3),	3.26(15),
	2M =	27.83(15),	1.17(17),	0.0(3),	3.57(15),	72.36(15),	44.53(16),	13.61(16),	57.40(15),	38.15(15),	31.65(15),
	3M =	32.50(17),	29.37(17),	0.69(18),	34.66(17),	10.67(17),					
	0M =	6.95(16),	5.93(16),	5.28(16),	6.95(16),	35.39(16),	34.20(16),	35.94(13),	36.88(15),	0.04(15),	0.28(14),
O(41A)-C(41A) /	1M =	7.31(15),	32.99(14),	1.78(17),	1.03(15),	7.33(15),	10.83(16),	28.77(15),	7.47(14),	19.9(3),	27.96(14),
	2M =	30.27(14),	2.46(16),	20.0(3),	0.04(15),	33.50(14),	10.83(16),	7.31(15),	7.47(14),	36.47(14),	35.83(14),
	3M =	15.44(17),	17.74(17),	0.15(17),	6.53(17),	9.03(17),					
	0M =	10.83(16),	10.31(16),	0.89(16),	10.83(16),	37.10(16),	34.61(16),	35.34(14),	27.49(15),	2.78(15),	2.88(15),
O(42A)-C(41A) /	1M =	11.13(16),	23.88(15),	3.26(18),	5.33(15),	11.44(15),	1.12(16),	27.91(15),	17.02(15),	17.7(3),	25.61(15),
	2M =	20.98(15),	0.11(17),	19.6(3),	2.78(15),	41.48(15),	1.12(16),	11.13(16),	17.02(15),	38.28(15),	36.27(15),
	3M =	8.65(17),	11.21(17),	1.79(18),	0.79(17),	12.11(17),					
	0M =	37.85(16),	39.95(16),	0.97(16),	37.85(16),	42.40(16),	47.71(16),	52.75(13),	44.80(15),	40.51(15),	42.12(14),
O(51A)-C(51A) /	1M =	37.38(15),	39.04(14),	48.50(17),	44.18(15),	38.05(15),	45.56(16),	6.63(15),	34.17(14),	8.4(3),	2.29(15),
	2M =	40.48(14),	41.95(16),	14.6(3),	40.51(15),	11.45(14),	45.56(16),	37.38(15),	34.17(14),	42.31(14),	48.08(14),
	3M =	10.69(17),	10.48(17),	38.02(17),	0.75(17),	33.97(17),					
	0M =	1.49(16),	3.37(16),	41.94(16),	1.49(16),	51.13(16),	44.68(16),	40.91(13),	14.82(15),	8.82(15),	6.97(14),
O(52A)-C(51A) /	1M =	1.43(15),	19.23(14),	1.69(17),	0.34(15),	2.91(15),	32.88(16),	3.07(15),	43.72(14),	15.1(3),	8.93(15),
	2M =	21.58(14),	11.36(16),	8.3(3),	8.82(15),	83.94(14),	32.88(16),	1.43(15),	43.72(14),	52.02(14),	45.56(14),
	3M =	34.01(17),	31.13(17),	12.77(17),	39.35(17),	1.02(17),					
	0M =	1.35(16),	2.56(16),	4.80(16),	1.35(16),	39.24(16),	39.17(16),	41.66(14),	41.24(15),	7.66(15),	8.20(15),
C(1A)a-C(2A)a /	1M =	0.96(16),	36.60(15),	10.45(18),	7.39(15),	1.06(15),	18.03(16),	22.81(15),	0.38(15),	15.2(3),	23.13(15),
	2M =	34.47(15),	10.04(17),	13.9(3),	7.66(15),	30.70(15),	18.03(16),	0.96(16),	0.38(15),	40.19(15),	40.73(15),
	3M =	15.50(17),	17.41(17),	7.41(18),	5.50(17),	1.08(17),					
	0M =	36.33(18),	34.20(18),	34.09(18),	36.33(18),	0.27(18),	1.12(18),	0.80(16),	42.11(17),	32.22(17),	31.17(17),
-C(6A)a /	1M =	36.80(18),	42.52(17),	25.6(2),	30.00(18),	36.13(18),	9.86(18),	63.93(17),	8.81(17),	55.0(3),	63.04(17),
	2M =	38.41(17),	30.13(19),	55.1(3),	32.22(17),	8.21(17),	9.86(18),	36.80(18),	8.81(17),	1.39(17),	0.50(17),
	3M =	41.58(19),	44.61(19),	33.2(2),	36.46(19),	39.96(19),					
	0M =	11.61(19),	14.86(18),	43.31(18),	11.61(19),	0.02(19),	4.88(19),	9.89(16),	77.23(17),	8.05(17),	10.53(17),
-C(11A) /	1M =	11.12(18),	75.86(17),	21.9(2),	16.44(18),	12.73(18),	70.45(18),	20.43(18),	51.35(17),	25.1(3),	27.75(17),
	2M =	79.72(17),	8.05(19),	15.8(3),	8.05(17),	25.02(17),	70.45(18),	11.12(18),	51.35(17),	0.11(17),	5.40(17),
	3M =	51.79(19),	50.67(19),	3.8(2),	41.09(19),	6.4(2),					
	0M =	57.24(17),	59.38(17),	1.32(17),	57.24(17),	4.01(18),	10.05(18),	12.78(15),	13.64(16),	47.07(16),	49.06(16),

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	1M =	57.10(17),	12.55(16),	57.29(19),	55.75(16),	58.73(17),	45.61(17),	38.55(16),	62.60(16),	28.9(3),	30.52(16),
	2M =	16.68(16),	44.63(18),	38.7(3),	47.07(16),	29.08(16),	45.61(17),	57.10(17),	62.60(16),	2.94(16),	8.86(16),
	3M =	1.30(18),	1.57(18),	42.81(19),	2.24(18),	53.91(19),					
C(1B)a-C(2B)a /	0M =	34.99(18),	32.84(18),	34.03(18),	34.99(18),	1.09(18),	0.19(18),	1.80(16),	43.21(17),	30.94(17),	29.87(17),
	1M =	35.46(18),	43.50(17),	24.3(2),	28.65(18),	34.78(18),	10.93(18),	62.86(17),	7.81(17),	54.3(3),	62.29(17),
	2M =	39.40(17),	28.87(19),	54.0(3),	30.94(17),	8.26(17),	10.93(18),	35.46(18),	7.81(17),	2.20(17),	1.43(17),
	3M =	41.75(19),	44.76(19),	32.0(2),	36.32(19),	38.64(19),					
-C(11B) /	0M =	51.09(17),	53.02(17),	5.14(17),	51.09(17),	2.71(17),	3.30(17),	5.99(15),	12.49(16),	40.81(16),	42.69(16),
	1M =	51.00(17),	12.12(16),	50.54(19),	49.19(16),	52.54(16),	44.80(17),	35.92(16),	63.36(16),	25.4(3),	27.99(16),
	2M =	16.24(16),	38.30(18),	34.9(3),	40.81(16),	35.34(16),	44.80(17),	51.00(17),	63.36(16),	3.78(16),	2.09(16),
	3M =	3.99(18),	0.99(18),	36.72(19),	1.61(18),	48.15(18),					
C(2A)a-C(3A)a /	0M =	51.79(19),	54.22(18),	7.80(18),	51.79(19),	0.23(19),	6.49(19),	9.63(16),	18.94(17),	41.87(17),	44.02(17),
	1M =	51.60(18),	18.24(17),	53.4(2),	51.07(18),	53.32(18),	51.18(18),	32.04(17),	68.91(17),	22.4(3),	24.01(17),
	2M =	22.37(17),	39.58(19),	32.2(3),	41.87(17),	33.88(17),	51.18(18),	51.60(18),	68.91(17),	0.76(17),	5.41(17),
	3M =	7.84(19),	4.96(19),	37.4(2),	4.24(19),	48.1(2),					
-C(21A) /	0M =	8.09(17),	11.32(17),	45.69(17),	8.09(17),	1.29(18),	3.31(18),	8.28(15),	80.35(16),	4.73(16),	7.18(16),
	1M =	7.59(17),	79.50(16),	18.49(19),	12.99(17),	9.19(17),	67.07(17),	24.06(16),	48.20(16),	28.5(3),	31.34(16),
	2M =	83.34(16),	4.81(18),	19.3(3),	4.73(16),	24.65(16),	67.07(17),	7.59(17),	48.20(16),	1.12(16),	3.92(16),
	3M =	54.62(18),	53.68(18),	0.53(19),	43.65(18),	2.87(19),					
C(2B)a-C(6B)a /	0M =	46.11(19),	48.31(18),	11.30(18),	46.11(19),	6.41(19),	0.20(19),	2.88(16),	17.29(18),	35.97(17),	38.01(17),
	1M =	45.97(18),	17.31(17),	46.9(2),	44.85(18),	47.60(18),	49.50(18),	29.74(18),	68.62(17),	19.3(3),	21.82(17),
	2M =	21.41(17),	33.57(19),	28.8(3),	35.97(17),	40.11(17),	49.50(18),	45.97(18),	68.62(17),	7.42(17),	1.30(17),
	3M =	10.15(19),	7.15(19),	31.7(2),	7.76(19),	42.8(2),					
-C(21B) /	0M =	5.61(17),	8.89(17),	50.35(17),	5.61(17),	6.48(17),	1.80(17),	3.18(15),	77.40(16),	1.52(16),	4.03(16),
	1M =	5.13(17),	79.28(16),	15.65(19),	10.18(16),	6.80(17),	67.10(17),	25.70(16),	49.33(16),	31.2(3),	33.28(16),
	2M =	83.28(16),	1.39(18),	21.7(3),	1.52(16),	29.55(16),	67.10(17),	5.13(17),	49.33(16),	6.32(16),	1.23(16),
	3M =	58.73(18),	57.48(18),	2.85(19),	48.12(18),	0.37(18),					
C(3A)a-C(4A)a /	0M =	11.39(19),	14.63(18),	43.36(18),	11.39(19),	0.10(19),	4.93(19),	9.94(17),	77.56(18),	7.88(18),	10.34(17),
	1M =	10.90(18),	76.14(17),	21.7(2),	16.24(18),	12.50(18),	70.12(18),	20.69(18),	51.01(17),	25.3(3),	28.00(17),
	2M =	79.98(17),	7.89(19),	16.0(3),	7.88(18),	24.80(17),	70.12(18),	10.90(18),	51.01(17),	0.20(17),	5.46(17),
	3M =	51.9(2),	50.8(2),	3.6(2),	41.2(2),	6.2(2),					
C(4A)a-C(5A)a /	0M =	36.82(18),	34.66(18),	34.61(18),	36.82(18),	0.39(19),	1.78(19),	0.15(16),	42.06(17),	32.78(17),	31.72(17),
	1M =	37.29(18),	42.57(17),	26.1(2),	30.48(18),	36.60(18),	9.84(18),	64.57(17),	8.76(17),	55.7(3),	63.70(17),
	2M =	38.45(17),	30.70(19),	55.7(3),	32.78(17),	7.69(17),	9.84(18),	37.29(18),	8.76(17),	0.74(17),	0.15(17),
	3M =	42.02(19),	45.07(19),	33.8(2),	37.00(19),	40.48(19),					
-C(41A) /	0M =	54.51(18),	56.74(17),	4.18(17),	54.51(18),	1.74(18),	7.87(18),	10.74(15),	15.41(16),	44.40(16),	46.44(16),
	1M =	54.36(17),	14.56(16),	55.06(19),	53.25(17),	56.01(17),	47.56(17),	35.87(16),	65.06(16),	26.1(3),	27.85(16),
	2M =	18.69(16),	42.00(18),	35.9(3),	44.40(16),	31.69(16),	47.56(17),	54.36(17),	65.06(16),	0.70(16),	6.71(16),
	3M =	4.03(18),	1.13(19),	40.08(19),	0.61(18),	51.09(19),					
C(5A)a-C(6A)a /	0M =	51.34(19),	53.74(18),	8.05(18),	51.34(19),	0.35(19),	5.90(19),	9.02(16),	18.72(18),	41.39(18),	43.53(17),
	1M =	51.16(18),	18.08(17),	52.8(2),	50.55(18),	52.86(18),	50.98(18),	31.93(18),	68.89(17),	22.2(3),	23.91(17),
	2M =	22.21(17),	39.08(19),	32.0(3),	41.39(18),	34.41(17),	50.98(18),	51.16(18),	68.89(17),	1.35(17),	4.81(17),
	3M =	8.0(2),	5.1(2),	36.9(2),	4.48(19),	47.7(2),					
-C(51A) /	0M =	6.06(17),	9.33(17),	49.14(17),	6.06(17),	5.01(18),	0.38(18),	4.59(15),	78.66(16),	2.21(16),	4.70(16),
	1M =	5.58(17),	79.92(16),	16.23(19),	10.74(16),	7.22(17),	66.90(17),	25.54(16),	48.75(16),	30.7(3),	33.04(16),
	2M =	84.04(16),	2.15(18),	21.3(3),	2.21(16),	28.01(16),	66.90(17),	5.58(17),	48.75(16),	4.84(16),	0.21(16),
	3M =	57.76(18),	56.62(18),	2.10(19),	47.00(18),	0.83(19),					
Cu(1)b-O(7W)b /	0M =	83.90(10),	81.52(10),	31.87(10),	83.90(10),	40.62(10),	45.75(10),	46.86(5),	0.17(8),	85.71(8),	86.40(7),

	1M =	83.95(9),	4.15(7),	77.05(12),	82.47(8),	82.44(9),	22.76(10),	57.29(8),	30.60(8),	55.9(2),	51.76(8),
	2M =	0.93(8),	82.95(11),	64.4(2),	85.71(8),	9.68(7),	22.76(10),	83.95(9),	30.60(8),	39.43(8),	44.25(7),
	3M =	27.36(12),	29.29(12),	81.59(12),	35.21(12),	84.27(12),					
-O(11A) /	0M =	75.96(10),	76.24(10),	20.23(10),	75.96(10),	20.86(10),	26.07(10),	27.49(5),	0.19(8),	65.96(8),	67.15(7),
	1M =	76.09(9),	2.87(7),	69.10(12),	71.27(8),	76.98(8),	28.98(10),	57.84(8),	42.54(7),	49.8(2),	49.99(8),
	2M =	1.04(7),	63.19(11),	59.9(2),	65.96(8),	9.00(7),	28.98(10),	76.09(9),	42.54(7),	19.67(8),	24.61(7),
	3M =	19.18(12),	21.85(12),	62.64(12),	23.79(12),	74.57(12),					
-O(11B) /	0M =	9.30(10),	10.40(9),	25.39(9),	9.30(10),	45.92(10),	40.41(10),	38.16(5),	0.12(8),	0.85(8),	0.46(7),
	1M =	9.37(9),	3.95(6),	6.49(12),	5.94(8),	10.52(8),	23.31(9),	11.64(8),	38.70(7),	0.3(2),	6.54(7),
	2M =	6.73(7),	3.61(11),	5.4(2),	0.85(8),	67.68(7),	23.31(9),	9.37(9),	38.70(7),	47.09(7),	41.76(7),
	3M =	17.20(11),	14.34(11),	3.94(12),	22.99(11),	8.04(12),					
Cu(2)b-O(21A) /	0M =	0.78(10),	3.89(10),	45.80(10),	0.78(10),	0.98(10),	4.65(10),	9.35(5),	88.80(8),	1.09(8),	1.18(7),
	1M =	0.28(9),	84.27(7),	11.66(12),	6.21(8),	1.72(8),	56.53(10),	32.19(8),	37.48(8),	34.8(2),	38.88(8),
	2M =	82.71(7),	0.57(11),	26.4(2),	1.09(8),	17.53(7),	56.53(10),	0.28(9),	37.48(8),	1.37(8),	5.53(7),
	3M =	56.21(12),	56.28(12),	4.84(12),	44.61(12),	4.30(12),					
-O(6W)b /	0M =	86.89(10),	86.94(10),	26.19(10),	86.89(10),	36.62(10),	42.13(10),	43.80(5),	4.37(8),	80.61(8),	82.71(7),
	1M =	86.43(9),	0.32(7),	81.59(12),	86.75(8),	86.55(9),	28.18(10),	54.08(8),	36.37(8),	51.2(2),	47.83(8),
	2M =	3.70(8),	78.29(11),	60.3(2),	80.61(8),	4.58(7),	28.18(10),	86.43(9),	36.37(8),	35.47(8),	40.72(7),
	3M =	21.99(12),	24.03(12),	75.97(12),	29.56(12),	82.39(12),					
-O(12A) /	0M =	2.70(10),	3.62(9),	26.48(9),	2.70(10),	52.41(10),	47.19(10),	45.21(5),	3.30(8),	7.32(8),	6.15(7),
	1M =	2.79(9),	1.03(6),	0.60(12),	0.94(8),	3.86(8),	17.54(9),	7.86(8),	31.99(7),	3.8(2),	3.50(7),
	2M =	3.44(7),	10.11(11),	0.9(2),	7.32(8),	67.62(7),	17.54(9),	2.79(9),	31.99(7),	53.61(7),	48.60(7),
	3M =	17.36(11),	14.70(11),	10.16(12),	24.46(11),	1.74(12),					
-O(12B) /	0M =	76.28(10),	77.27(10),	18.06(10),	76.28(10),	21.09(10),	26.52(10),	28.21(5),	2.83(8),	65.98(8),	67.47(7),
	1M =	76.30(9),	0.12(7),	71.01(12),	72.47(8),	77.53(8),	31.85(9),	54.97(8),	44.98(7),	47.3(2),	47.17(8),
	2M =	4.01(7),	63.29(11),	57.4(2),	65.98(8),	9.75(7),	31.85(9),	76.30(9),	44.98(7),	19.93(7),	25.10(7),
	3M =	16.63(12),	19.25(12),	62.25(12),	21.61(12),	73.88(12),					
-O(41A) /	0M =	2.72(10),	0.23(9),	55.02(9),	2.72(10),	48.18(10),	41.79(10),	37.13(4),	28.59(7),	12.55(7),	10.29(6),
	1M =	2.90(8),	33.32(6),	0.24(12),	3.00(8),	1.19(8),	41.86(9),	14.09(7),	47.36(7),	26.0(2),	20.76(7),
	2M =	35.38(7),	14.71(10),	17.9(2),	12.55(7),	79.34(6),	41.86(9),	2.90(8),	47.36(7),	48.69(7),	42.14(6),
	3M =	48.11(11),	45.13(11),	17.09(12),	52.04(11),	6.25(11),					
-O(42A) /	0M =	3.61(10),	0.39(10),	53.90(10),	3.61(10),	7.25(10),	3.51(10),	1.24(5),	81.51(8),	6.63(8),	4.23(7),
	1M =	4.10(9),	87.47(7),	6.89(12),	1.39(8),	2.53(8),	56.41(10),	35.76(8),	38.61(7),	40.1(2),	43.08(8),
	2M =	84.93(7),	6.40(11),	31.0(2),	6.63(8),	24.74(7),	56.41(10),	4.10(9),	38.61(7),	6.87(7),	2.65(7),
	3M =	64.07(12),	63.82(12),	10.68(12),	52.53(12),	8.81(12),					
Na(1)b-O(41A) /	0M =	32.26(10),	31.22(10),	40.46(10),	32.26(10),	86.80(10),	81.93(10),	78.39(5),	3.14(8),	42.28(8),	41.10(7),
	1M =	32.17(9),	2.75(7),	34.69(12),	35.64(8),	31.08(8),	0.52(9),	21.78(8),	6.94(7),	31.5(2),	23.44(7),
	2M =	2.80(7),	45.06(11),	30.1(2),	42.28(8),	55.40(7),	0.52(9),	32.17(9),	6.94(7),	87.91(7),	83.04(7),
	3M =	29.51(11),	28.32(12),	44.93(12),	40.69(11),	33.13(12),					
-O(4W)b /	0M =	43.80(11),	42.07(11),	28.64(11),	43.80(11),	0.63(12),	3.13(12),	2.04(8),	31.91(10),	38.14(10),	37.53(9),
	1M =	44.23(10),	32.49(9),	33.63(13),	37.53(10),	43.84(10),	0.30(11),	65.43(10),	18.82(9),	54.2(3),	61.50(9),
	2M =	28.37(9),	35.75(12),	57.4(3),	38.14(10),	13.14(9),	0.30(11),	44.23(10),	18.82(9),	0.56(9),	1.47(9),
	3M =	34.64(13),	37.77(13),	38.23(13),	31.45(13),	46.72(13),					
-O(5W)b /	0M =	29.83(11),	33.11(11),	32.52(11),	29.83(11),	2.46(11),	3.80(11),	8.60(7),	51.80(9),	23.12(9),	25.75(9),
	1M =	29.41(10),	51.36(9),	37.94(13),	32.94(10),	31.23(10),	83.98(11),	1.37(9),	76.60(9),	6.1(3),	6.54(9),
	2M =	55.49(9),	22.08(12),	3.9(3),	23.12(9),	35.95(9),	83.98(11),	29.41(10),	76.60(9),	2.90(9),	3.59(9),
	3M =	36.51(13),	34.14(13),	18.29(13),	29.24(13),	24.73(13),					
-O(52A) /	0M =	38.27(10),	35.50(10),	47.49(10),	38.27(10),	11.08(10),	11.59(10),	8.98(5),	47.74(8),	36.94(8),	35.30(7),

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	1M =	38.78(9),	49.85(7),	27.10(12),	32.20(8),	37.64(8),	16.90(9),	70.83(8),	0.39(7),	65.9(2),	73.71(7),
	2M =	45.78(7),	35.40(11),	62.6(2),	36.94(8),	5.20(7),	16.90(9),	38.78(9),	0.39(7),	10.03(7),	10.03(7),
	3M =	54.57(11),	57.67(11),	39.14(12),	49.88(11),	42.85(12),					
-O(21B) /	0M =	28.03(10),	31.34(9),	33.34(9),	28.03(10),	0.02(10),	6.08(10),	10.98(5),	56.52(8),	22.12(8),	24.74(7),
	1M =	27.59(9),	55.64(7),	36.90(12),	31.68(8),	29.37(8),	88.55(9),	1.75(8),	71.49(7),	8.4(2),	9.53(7),
	2M =	59.75(7),	21.33(11),	1.5(2),	22.12(8),	32.47(7),	88.55(9),	27.59(9),	71.49(7),	0.36(7),	6.00(7),
	3M =	38.40(11),	36.26(11),	17.37(12),	30.22(11),	22.84(12),					
Na(2)b-O(1W)b /	0M =	31.33(10),	28.82(10),	40.87(10),	31.33(10),	2.08(10),	2.45(10),	0.20(5),	50.96(8),	28.88(8),	27.44(7),
	1M =	31.82(9),	51.69(7),	20.25(12),	25.08(8),	30.88(8),	18.86(9),	62.54(8),	0.37(7),	56.7(2),	64.57(7),
	2M =	47.57(7),	27.15(11),	53.9(2),	28.88(8),	1.13(7),	18.86(9),	31.82(9),	0.37(7),	1.05(7),	0.89(7),
	3M =	49.36(12),	52.26(12),	30.71(12),	42.82(11),	35.55(12),					
-O(3W)b /	0M =	35.70(10),	38.96(9),	26.90(9),	35.70(10),	0.30(10),	6.70(10),	11.33(5),	46.46(8),	28.65(8),	31.27(7),
	1M =	35.30(9),	45.61(6),	43.41(12),	38.56(8),	37.13(8),	78.66(9),	7.51(8),	80.16(7),	0.0(2),	0.39(7),
	2M =	49.74(7),	27.47(11),	10.0(2),	28.65(8),	34.27(7),	78.66(9),	35.30(9),	80.16(7),	0.25(7),	6.33(7),
	3M =	30.49(11),	28.08(11),	23.78(12),	23.56(11),	30.65(12),					
-O(41A) /	0M =	43.88(10),	41.30(10),	43.05(10),	43.88(10),	10.99(10),	12.31(10),	10.26(5),	40.84(8),	41.40(8),	40.02(7),
	1M =	44.38(9),	42.79(7),	32.77(12),	37.66(8),	43.39(8),	9.82(9),	74.63(8),	7.44(7),	66.3(2),	74.25(7),
	2M =	38.70(7),	39.58(11),	65.8(2),	41.40(8),	1.06(7),	9.82(9),	44.38(9),	7.44(7),	9.87(7),	10.69(7),
	3M =	48.97(12),	52.12(12),	43.01(12),	45.79(11),	48.16(12),					
-O(12B) /	0M =	28.92(10),	30.08(9),	8.08(9),	28.92(10),	55.02(10),	58.48(10),	62.85(5),	36.18(8),	34.93(7),	35.63(7),
	1M =	28.54(8),	30.25(6),	37.79(12),	34.94(8),	28.62(8),	28.43(9),	2.81(8),	15.94(7),	8.2(2),	0.79(7),
	2M =	30.34(7),	37.17(10),	11.6(2),	34.93(7),	28.56(7),	28.43(9),	28.54(8),	15.94(7),	55.36(7),	59.49(6),
	3M =	2.68(11),	3.38(11),	34.19(12),	8.86(11),	26.42(11),					
O(11A)-C(11A) /	0M =	42.68(16),	44.00(16),	11.55(16),	42.68(16),	54.75(16),	60.29(16),	65.34(13),	32.66(15),	47.84(15),	48.85(14),
	1M =	42.27(15),	26.80(14),	51.84(17),	48.81(15),	42.46(15),	34.13(16),	14.58(15),	25.36(14),	18.3(3),	11.42(14),
	2M =	28.00(14),	49.83(16),	23.1(3),	47.84(15),	22.14(14),	34.13(16),	42.27(15),	25.36(14),	54.56(14),	60.56(14),
	3M =	1.61(17),	1.63(17),	46.41(17),	13.14(17),	39.82(17),					
O(11B)-C(11B) /	0M =	0.64(16),	0.82(16),	11.16(16),	0.64(16),	49.81(16),	47.30(16),	47.82(14),	22.90(15),	9.21(15),	8.90(15),
	1M =	0.38(16),	18.34(15),	7.25(18),	5.78(15),	0.12(15),	1.37(16),	15.22(15),	14.79(15),	5.2(3),	13.18(15),
	2M =	16.13(15),	11.94(17),	6.9(3),	9.21(15),	48.93(15),	1.37(16),	0.38(16),	14.79(15),	50.98(15),	48.96(15),
	3M =	0.95(17),	1.32(17),	10.52(18),	9.89(17),	0.20(17),					
O(12A)-C(11A) /	0M =	7.65(16),	7.49(16),	7.84(16),	7.65(16),	42.75(16),	39.68(16),	39.85(14),	21.70(15),	1.04(15),	0.67(15),
	1M =	7.90(16),	17.78(15),	1.04(18),	2.53(15),	8.41(15),	2.96(16),	22.02(15),	20.28(15),	11.4(3),	19.25(15),
	2M =	15.07(15),	3.78(17),	14.0(3),	1.04(15),	48.26(15),	2.96(16),	7.90(16),	20.28(15),	43.96(15),	41.32(15),
	3M =	1.72(17),	4.26(17),	2.50(18),	6.15(17),	8.38(17),					
O(12B)-C(11B) /	0M =	47.38(16),	48.98(16),	10.30(16),	47.38(16),	50.94(16),	56.94(16),	61.91(13),	33.00(15),	51.49(15),	52.80(14),
	1M =	46.94(15),	27.32(14),	57.10(17),	53.63(15),	47.30(15),	38.25(16),	17.71(15),	30.81(14),	20.2(3),	13.85(15),
	2M =	28.99(14),	53.18(16),	26.0(3),	51.49(15),	17.16(14),	38.25(16),	46.94(15),	30.81(14),	50.59(14),	56.94(14),
	3M =	0.91(17),	1.26(17),	49.44(17),	12.22(17),	44.10(17),					
O(21A)-C(21A) /	0M =	8.52(16),	7.68(16),	3.00(16),	8.52(16),	36.11(16),	34.42(16),	35.78(13),	33.34(15),	1.16(15),	0.99(14),
	1M =	8.86(15),	29.56(14),	0.20(17),	2.74(15),	8.99(15),	7.13(16),	28.63(15),	11.12(14),	19.2(3),	27.23(15),
	2M =	26.77(14),	1.41(16),	20.0(3),	1.16(15),	36.54(14),	7.13(16),	8.86(15),	11.12(14),	37.23(14),	36.06(14),
	3M =	12.94(17),	15.34(17),	0.66(17),	4.41(17),	10.31(17),					
O(21B)-C(21B) /	0M =	9.90(16),	11.93(16),	38.71(16),	9.90(16),	42.02(16),	35.57(16),	31.81(14),	18.37(15),	0.35(15),	1.60(15),
	1M =	9.81(16),	22.10(15),	10.63(18),	8.40(15),	11.36(15),	40.04(16),	2.11(15),	52.44(15),	9.9(3),	4.44(15),
	2M =	24.96(15),	2.82(17),	2.2(3),	0.35(15),	76.52(15),	40.04(16),	9.81(16),	52.44(15),	42.91(15),	36.44(15),
	3M =	32.37(17),	29.31(17),	4.47(18),	35.71(17),	7.09(17),					
O(22A)-C(21A) /	0M =	13.73(16),	15.90(16),	37.85(16),	13.73(16),	37.29(16),	30.81(16),	26.97(14),	21.38(15),	3.57(15),	5.61(15),

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O(22B)-C(21B) /	1M =	13.61(16),	24.74(15),	15.01(18),	12.56(15),	15.21(15),	44.53(16),	3.66(15),	57.40(15),	8.2(3),	3.26(15),
	2M =	27.83(15),	1.17(17),	0.0(3),	3.57(15),	72.36(15),	44.53(16),	13.61(16),	57.40(15),	38.15(15),	31.65(15),
	3M =	32.50(17),	29.37(17),	0.69(18),	34.66(17),	10.67(17),					
	0M =	6.95(16),	5.93(16),	5.28(16),	6.95(16),	35.39(16),	34.20(16),	35.94(13),	36.88(15),	0.04(15),	0.28(14),
O(41A)-C(41A) /	1M =	7.31(15),	32.99(14),	1.78(17),	1.03(15),	7.33(15),	10.83(16),	28.77(15),	7.47(14),	19.9(3),	27.96(14),
	2M =	30.27(14),	2.46(16),	20.0(3),	0.04(15),	33.50(14),	10.83(16),	7.31(15),	7.47(14),	36.47(14),	35.83(14),
	3M =	15.44(17),	17.74(17),	0.15(17),	6.53(17),	9.03(17),					
	0M =	10.83(16),	10.31(16),	0.89(16),	10.83(16),	37.10(16),	34.61(16),	35.34(14),	27.49(15),	2.78(15),	2.88(15),
O(42A)-C(41A) /	1M =	11.13(16),	23.88(15),	3.26(18),	5.33(15),	11.44(15),	1.12(16),	27.91(15),	17.02(15),	17.7(3),	25.61(15),
	2M =	20.98(15),	0.11(17),	19.6(3),	2.78(15),	41.48(15),	1.12(16),	11.13(16),	17.02(15),	38.28(15),	36.27(15),
	3M =	8.65(17),	11.21(17),	1.79(18),	0.79(17),	12.11(17),					
	0M =	37.85(16),	39.95(16),	0.97(16),	37.85(16),	42.40(16),	47.71(16),	52.75(13),	44.80(15),	40.51(15),	42.12(14),
O(51A)-C(51A) /	1M =	37.38(15),	39.04(14),	48.50(17),	44.18(15),	38.05(15),	45.56(16),	6.63(15),	34.17(14),	8.4(3),	2.29(15),
	2M =	40.48(14),	41.95(16),	14.6(3),	40.51(15),	11.45(14),	45.56(16),	37.38(15),	34.17(14),	42.31(14),	48.08(14),
	3M =	10.69(17),	10.48(17),	38.02(17),	0.75(17),	33.97(17),					
	0M =	1.49(16),	3.37(16),	41.94(16),	1.49(16),	51.13(16),	44.68(16),	40.91(13),	14.82(15),	8.82(15),	6.97(14),
O(52A)-C(51A) /	1M =	1.43(15),	19.23(14),	1.69(17),	0.34(15),	2.91(15),	32.88(16),	3.07(15),	43.72(14),	15.1(3),	8.93(15),
	2M =	21.58(14),	11.36(16),	8.3(3),	8.82(15),	83.94(14),	32.88(16),	1.43(15),	43.72(14),	52.02(14),	45.56(14),
	3M =	34.01(17),	31.13(17),	12.77(17),	39.35(17),	1.02(17),					
	0M =	1.35(16),	2.56(16),	4.80(16),	1.35(16),	39.24(16),	39.17(16),	41.66(14),	41.24(15),	7.66(15),	8.20(15),
C(1A)b-C(2A)b /	1M =	0.96(16),	36.60(15),	10.45(18),	7.39(15),	1.06(15),	18.03(16),	22.81(15),	0.38(15),	15.2(3),	23.13(15),
	2M =	34.47(15),	10.04(17),	13.9(3),	7.66(15),	30.70(15),	18.03(16),	0.96(16),	0.38(15),	40.19(15),	40.73(15),
	3M =	15.50(17),	17.41(17),	7.41(18),	5.50(17),	1.08(17),					
	0M =	36.33(18),	34.20(18),	34.09(18),	36.33(18),	0.27(18),	1.12(18),	0.79(16),	42.11(17),	32.22(17),	31.17(17),
-C(6A)b /	1M =	36.80(18),	42.52(17),	25.6(2),	30.00(18),	36.13(18),	9.86(18),	63.93(17),	8.81(17),	55.0(3),	63.04(17),
	2M =	38.41(17),	30.13(19),	55.1(3),	32.22(17),	8.21(17),	9.86(18),	36.80(18),	8.81(17),	1.39(17),	0.50(17),
	3M =	41.58(19),	44.61(19),	33.2(2),	36.46(19),	39.96(19),					
	0M =	11.61(19),	14.86(18),	43.31(18),	11.61(19),	0.02(19),	4.88(19),	9.89(16),	77.23(17),	8.05(17),	10.53(17),
-C(11A) /	1M =	11.12(18),	75.86(17),	21.9(2),	16.44(18),	12.73(18),	70.45(18),	20.43(18),	51.35(17),	25.1(3),	27.75(17),
	2M =	79.72(17),	8.05(19),	15.8(3),	8.05(17),	25.02(17),	70.45(18),	11.12(18),	51.35(17),	0.11(17),	5.40(17),
	3M =	51.79(19),	50.67(19),	3.8(2),	41.09(19),	6.4(2),					
	0M =	57.24(17),	59.38(17),	1.32(17),	57.24(17),	4.01(18),	10.05(18),	12.78(15),	13.64(16),	47.07(16),	49.06(16),
C(1B)b-C(2B)b /	1M =	57.10(17),	12.55(16),	57.29(19),	55.75(16),	58.73(17),	45.61(17),	38.55(16),	62.60(16),	28.9(3),	30.52(16),
	2M =	16.68(16),	44.63(18),	38.7(3),	47.07(16),	29.08(16),	45.61(17),	57.10(17),	62.60(16),	2.94(16),	8.86(16),
	3M =	1.30(18),	1.57(18),	42.81(19),	2.24(18),	53.91(19),					
	0M =	34.99(18),	32.84(18),	34.03(18),	34.99(18),	1.09(18),	0.19(18),	1.80(16),	43.21(17),	30.94(17),	29.87(17),
-C(11B) /	1M =	35.46(18),	43.50(17),	24.3(2),	28.65(18),	34.78(18),	10.93(18),	62.86(17),	7.81(17),	54.3(3),	62.29(17),
	2M =	39.40(17),	28.87(19),	54.0(3),	30.94(17),	8.26(17),	10.93(18),	35.46(18),	7.81(17),	2.20(17),	1.43(17),
	3M =	41.75(19),	44.76(19),	32.0(2),	36.32(19),	38.64(19),					
	0M =	51.09(17),	53.02(17),	5.14(17),	51.09(17),	2.71(17),	3.30(17),	5.99(15),	12.49(16),	40.81(16),	42.69(16),
C(2A)b-C(3A)b /	1M =	51.00(17),	12.12(16),	50.54(19),	49.19(16),	52.54(16),	44.80(17),	35.92(16),	63.36(16),	25.4(3),	27.99(16),
	2M =	16.24(16),	38.30(18),	34.9(3),	40.81(16),	35.34(16),	44.80(17),	51.00(17),	63.36(16),	3.78(16),	2.09(16),
	3M =	3.99(18),	0.99(18),	36.72(19),	1.61(18),	48.15(18),					
	0M =	51.79(19),	54.22(18),	7.80(18),	51.79(19),	0.23(19),	6.49(19),	9.63(16),	18.94(17),	41.87(17),	44.02(17),
-C(21A) /	1M =	51.60(18),	18.24(17),	53.4(2),	51.07(18),	53.32(18),	51.18(18),	32.04(17),	68.91(17),	22.4(3),	24.01(17),
	2M =	22.37(17),	39.58(19),	32.2(3),	41.87(17),	33.88(17),	51.18(18),	51.60(18),	68.91(17),	0.76(17),	5.41(17),
	3M =	7.84(19),	4.96(19),	37.4(2),	4.24(19),	48.1(2),					
	0M =	8.09(17),	11.32(17),	45.69(17),	8.09(17),	1.29(18),	3.31(18),	8.28(15),	80.35(16),	4.73(16),	7.18(16),

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C(2B)b-C(6B)b /	1M =	7.59(17),	79.50(16),	18.49(19),	12.99(17),	9.19(17),	67.07(17),	24.06(16),	48.20(16),	28.5(3),	31.34(16),
	2M =	83.34(16),	4.81(18),	19.3(3),	4.73(16),	24.65(16),	67.07(17),	7.59(17),	48.20(16),	1.12(16),	3.92(16),
	3M =	54.62(18),	53.68(18),	0.53(19),	43.65(18),	2.87(19),					
	0M =	46.11(19),	48.31(18),	11.30(18),	46.11(19),	6.41(19),	0.20(19),	2.88(16),	17.29(18),	35.97(17),	38.01(17),
	1M =	45.97(18),	17.31(17),	46.9(2),	44.85(18),	47.60(18),	49.50(18),	29.74(18),	68.62(17),	19.3(3),	21.82(17),
-C(21B) /	2M =	21.41(17),	33.57(19),	28.8(3),	35.97(17),	40.11(17),	49.50(18),	45.97(18),	68.62(17),	7.42(17),	1.30(17),
	3M =	10.15(19),	7.15(19),	31.7(2),	7.76(19),	42.8(2),					
	0M =	5.61(17),	8.89(17),	50.35(17),	5.61(17),	6.48(17),	1.80(17),	3.18(15),	77.40(16),	1.52(16),	4.03(16),
	1M =	5.13(17),	79.28(16),	15.65(19),	10.18(16),	6.80(17),	67.10(17),	25.70(16),	49.33(16),	31.2(3),	33.28(16),
	2M =	83.28(16),	1.39(18),	21.7(3),	1.52(16),	29.55(16),	67.10(17),	5.13(17),	49.33(16),	6.32(16),	1.23(16),
C(3A)b-C(4A)b /	3M =	58.73(18),	57.48(18),	2.85(19),	48.12(18),	0.37(18),					
	0M =	11.39(19),	14.63(18),	43.36(18),	11.39(19),	0.10(19),	4.93(19),	9.94(17),	77.56(18),	7.88(18),	10.34(17),
	1M =	10.90(18),	76.14(17),	21.7(2),	16.24(18),	12.50(18),	70.12(18),	20.69(18),	51.01(17),	25.3(3),	28.00(17),
	2M =	79.98(17),	7.89(19),	16.0(3),	7.88(18),	24.80(17),	70.12(18),	10.90(18),	51.01(17),	0.20(17),	5.46(17),
	3M =	51.9(2),	50.8(2),	3.6(2),	41.2(2),	6.2(2),					
C(4A)b-C(5A)b /	0M =	36.82(18),	34.66(18),	34.61(18),	36.82(18),	0.39(19),	1.78(19),	0.15(16),	42.06(17),	32.78(17),	31.72(17),
	1M =	37.29(18),	42.57(17),	26.1(2),	30.48(18),	36.60(18),	9.84(18),	64.57(17),	8.76(17),	55.7(3),	63.70(17),
	2M =	38.45(17),	30.70(19),	55.7(3),	32.78(17),	7.69(17),	9.84(18),	37.29(18),	8.76(17),	0.74(17),	0.15(17),
	3M =	42.02(19),	45.07(19),	33.8(2),	37.00(19),	40.48(19),					
	0M =	54.51(18),	56.74(17),	4.18(17),	54.51(18),	1.74(18),	7.87(18),	10.74(15),	15.41(16),	44.40(16),	46.44(16),
-C(41A) /	1M =	54.36(17),	14.56(16),	55.06(19),	53.25(17),	56.01(17),	47.56(17),	35.87(16),	65.06(16),	26.1(3),	27.85(16),
	2M =	18.69(16),	42.00(18),	35.9(3),	44.40(16),	31.69(16),	47.56(17),	54.36(17),	65.06(16),	0.70(16),	6.71(16),
	3M =	4.03(18),	1.13(19),	40.08(19),	0.61(18),	51.09(19),					
	0M =	51.34(19),	53.74(18),	8.05(18),	51.34(19),	0.35(19),	5.90(19),	9.02(16),	18.72(18),	41.39(18),	43.53(17),
	1M =	51.16(18),	18.08(17),	52.8(2),	50.55(18),	52.86(18),	50.98(18),	31.93(18),	68.89(17),	22.2(3),	23.91(17),
C(5A)b-C(6A)b /	2M =	22.21(17),	39.08(19),	32.0(3),	41.39(18),	34.41(17),	50.98(18),	51.16(18),	68.89(17),	1.35(17),	4.81(17),
	3M =	8.0(2),	5.1(2),	36.9(2),	4.48(19),	47.7(2),					
	0M =	6.06(17),	9.33(17),	49.14(17),	6.06(17),	5.01(18),	0.38(18),	4.59(15),	78.66(16),	2.21(16),	4.70(16),
	1M =	5.58(17),	79.92(16),	16.23(19),	10.74(16),	7.22(17),	66.90(17),	25.54(16),	48.75(16),	30.7(3),	33.04(16),
	2M =	84.04(16),	2.15(18),	21.3(3),	2.21(16),	28.01(16),	66.90(17),	5.58(17),	48.75(16),	4.84(16),	0.21(16),
Cu(1)c-O(7W)c /	3M =	57.76(18),	56.62(18),	2.10(19),	47.00(18),	0.83(19),					
	0M =	35.01(10),	31.87(10),	81.52(10),	35.01(10),	48.47(10),	46.05(10),	41.64(5),	38.16(8),	42.59(8),	39.96(7),
	1M =	35.36(9),	44.05(7),	27.79(12),	32.68(8),	33.50(9),	26.27(10),	52.43(8),	19.12(8),	64.4(2),	58.74(8),
	2M =	42.73(8),	43.64(11),	55.9(2),	42.59(8),	46.20(7),	26.27(10),	35.36(9),	19.12(8),	47.77(8),	44.94(7),
	3M =	72.45(12),	72.07(12),	47.44(12),	83.96(12),	39.72(12),					
-O(11A) /	0M =	23.54(10),	20.23(10),	76.24(10),	23.54(10),	29.25(10),	26.39(10),	21.90(5),	57.74(8),	28.59(8),	26.03(7),
	1M =	23.99(9),	63.53(7),	14.16(12),	19.55(8),	22.23(8),	39.85(10),	51.29(8),	27.30(7),	59.9(2),	59.32(8),
	2M =	61.70(7),	28.84(11),	49.8(2),	28.59(8),	36.50(7),	39.85(10),	23.99(9),	27.30(7),	28.66(8),	25.34(7),
	3M =	87.04(12),	87.75(12),	33.05(12),	76.00(12),	28.75(12),					
	0M =	23.22(10),	25.39(9),	10.40(9),	23.22(10),	36.11(10),	40.05(10),	44.76(5),	54.94(8),	26.00(8),	27.52(7),
-O(11B) /	1M =	22.74(9),	48.98(6),	33.97(12),	29.55(8),	23.46(8),	44.46(9),	7.88(8),	28.71(7),	5.4(2),	11.86(7),
	2M =	49.30(7),	27.55(11),	0.3(2),	26.00(8),	11.15(7),	44.46(9),	22.74(9),	28.71(7),	36.39(7),	40.89(7),
	3M =	20.92(11),	21.29(11),	23.73(12),	9.30(11),	19.31(12),					
	0M =	52.30(10),	55.02(9),	0.23(9),	52.30(10),	34.93(10),	41.29(10),	45.97(4),	38.28(7),	51.62(7),	53.87(6),
	1M =	51.80(8),	33.53(6),	63.48(12),	58.29(8),	52.91(8),	53.08(9),	19.25(7),	48.05(7),	17.9(2),	13.40(7),
Cu(2)c-O(41A) /	2M =	36.33(7),	52.06(10),	26.0(2),	51.62(7),	0.21(6),	53.08(9),	51.80(8),	48.05(7),	34.40(7),	40.97(6),
	3M =	7.41(11),	6.23(11),	47.78(12),	2.84(11),	47.59(11),					
	0M =	52.56(10),	53.90(10),	0.39(10),	52.56(10),	2.50(10),	3.14(10),	5.27(5),	5.17(8),	42.25(8),	43.79(7),

	1M =	52.57(9),	4.79(7),	49.77(12),	49.49(8),	53.87(8),	37.48(10),	42.00(8),	56.07(7),	31.0(2),	34.22(8),
	2M =	8.92(7),	39.57(11),	40.1(2),	42.25(8),	32.95(7),	37.48(10),	52.57(9),	56.07(7),	3.64(7),	1.79(7),
	3M =	2.35(12),	5.40(12),	38.64(12),	3.87(12),	50.52(12),					
-O(6W)c /	0M =	29.35(10),	26.19(10),	86.94(10),	29.35(10),	45.61(10),	42.48(10),	37.83(5),	42.41(8),	36.82(8),	34.19(7),
	1M =	29.70(9),	48.36(7),	22.02(12),	26.92(8),	27.85(9),	32.02(10),	48.66(8),	24.71(8),	60.3(2),	55.59(8),
	2M =	47.39(8),	37.86(11),	51.2(2),	36.82(8),	48.51(7),	32.02(10),	29.70(9),	24.71(8),	45.04(8),	41.51(7),
	3M =	76.26(12),	74.98(12),	41.67(12),	86.67(12),	34.12(12),					
-O(12A) /	0M =	24.67(10),	26.48(9),	3.62(9),	24.67(10),	43.20(10),	46.85(10),	51.41(5),	47.99(8),	28.77(8),	29.99(7),
	1M =	24.22(9),	42.05(6),	34.86(12),	30.98(8),	24.70(8),	37.91(9),	4.76(8),	23.19(7),	0.9(2),	7.92(7),
	2M =	42.16(7),	30.62(11),	3.8(2),	28.77(8),	18.26(7),	37.91(9),	24.22(9),	23.19(7),	43.53(7),	47.78(7),
	3M =	14.30(11),	14.86(11),	27.09(12),	2.71(11),	21.26(12),					
-O(12B) /	0M =	21.36(10),	18.06(10),	77.27(10),	21.36(10),	30.05(10),	26.86(10),	22.25(5),	57.87(8),	26.80(8),	24.22(7),
	1M =	21.80(9),	63.78(7),	12.23(12),	17.58(8),	20.01(8),	42.03(9),	48.45(8),	30.04(7),	57.4(2),	56.46(8),
	2M =	62.38(7),	27.18(11),	47.3(2),	26.80(8),	39.05(7),	42.03(9),	21.80(9),	30.04(7),	29.52(7),	25.89(7),
	3M =	87.65(12),	85.44(12),	31.36(12),	76.26(12),	26.54(12),					
-O(21A) /	0M =	44.62(10),	45.80(10),	3.89(10),	44.62(10),	10.56(10),	5.01(10),	2.95(5),	3.28(8),	34.37(8),	35.80(7),
	1M =	44.66(9),	3.75(7),	41.54(12),	41.32(8),	45.88(8),	35.29(10),	38.01(8),	54.63(8),	26.4(2),	30.64(8),
	2M =	7.79(7),	31.65(11),	34.8(2),	34.37(8),	39.89(7),	35.29(10),	44.66(9),	54.63(8),	11.72(8),	6.37(7),
	3M =	0.55(12),	2.58(12),	30.96(12),	0.52(12),	42.92(12),					
Na(1)c-O(4W)c /	0M =	31.20(11),	28.64(11),	42.07(11),	31.20(11),	2.95(12),	3.21(12),	0.50(8),	51.77(10),	29.01(10),	27.51(9),
	1M =	31.70(10),	52.65(9),	20.09(13),	24.98(10),	30.72(10),	19.75(11),	62.78(10),	1.35(9),	57.4(3),	65.16(9),
	2M =	48.52(9),	27.33(12),	54.2(3),	29.01(10),	0.10(9),	19.75(11),	31.70(10),	1.35(9),	1.94(9),	1.67(9),
	3M =	50.60(13),	53.50(13),	30.95(13),	44.00(13),	35.50(13),					
-O(5W)c /	0M =	29.44(11),	32.52(11),	33.11(11),	29.44(11),	10.76(11),	4.30(11),	0.22(7),	42.37(9),	21.14(9),	23.69(9),
	1M =	29.10(10),	43.11(9),	35.46(13),	31.16(10),	30.95(10),	72.81(11),	5.21(9),	83.58(9),	3.9(3),	2.82(9),
	2M =	47.14(9),	19.57(12),	6.1(3),	21.14(9),	45.61(9),	72.81(11),	29.10(10),	83.58(9),	11.36(9),	4.75(9),
	3M =	34.48(13),	31.69(13),	16.27(13),	29.59(13),	24.75(13),					
-O(52A) /	0M =	49.65(10),	47.49(10),	35.50(10),	49.65(10),	9.15(10),	11.52(10),	10.26(5),	31.96(8),	45.21(8),	44.31(7),
	1M =	50.12(9),	33.57(7),	38.90(12),	43.32(8),	49.44(8),	0.54(9),	73.97(8),	16.90(7),	62.6(2),	69.44(7),
	2M =	29.46(7),	42.99(11),	65.9(2),	45.21(8),	5.59(7),	0.54(9),	50.12(9),	16.90(7),	7.96(7),	9.86(7),
	3M =	40.34(11),	43.49(11),	45.80(12),	38.53(11),	53.22(12),					
-O(41A) /	0M =	40.76(10),	40.46(10),	31.22(10),	40.76(10),	76.11(10),	81.52(10),	86.37(5),	13.34(8),	49.77(8),	49.31(7),
	1M =	40.55(9),	7.38(7),	45.49(12),	45.28(8),	39.84(8),	13.05(9),	22.63(8),	6.67(7),	30.1(2),	22.22(7),
	2M =	7.97(7),	52.52(11),	31.5(2),	49.77(8),	41.78(7),	13.05(9),	40.55(9),	6.67(7),	75.82(7),	81.97(7),
	3M =	20.65(11),	20.09(12),	51.06(12),	32.25(11),	40.34(12),					
Na(2)c-O(1W)c /	0M =	42.62(10),	40.87(10),	28.82(10),	42.62(10),	0.02(10),	2.37(10),	1.20(5),	33.00(8),	37.07(8),	36.42(7),
	1M =	43.05(9),	33.49(7),	32.42(12),	36.34(8),	42.64(8),	0.76(9),	64.91(8),	17.83(7),	53.9(2),	61.30(7),
	2M =	29.38(7),	34.70(11),	56.7(2),	37.07(8),	13.10(7),	0.76(9),	43.05(9),	17.83(7),	1.20(7),	0.71(7),
	3M =	35.05(12),	38.17(12),	37.23(12),	31.57(11),	45.60(12),					
-O(3W)c /	0M =	23.76(10),	26.90(9),	38.96(9),	23.76(10),	13.55(10),	7.20(10),	2.49(5),	47.00(8),	15.79(8),	18.37(7),
	1M =	23.41(9),	48.27(6),	30.32(12),	25.81(8),	25.26(8),	74.73(9),	0.93(8),	77.58(7),	10.0(2),	8.97(7),
	2M =	52.21(7),	14.35(11),	0.0(2),	15.79(8),	47.36(7),	74.73(9),	23.41(9),	77.58(7),	14.04(7),	7.50(7),
	3M =	40.61(11),	37.83(11),	10.91(12),	35.47(11),	18.98(12),					
-O(41A) /	0M =	45.54(10),	43.05(10),	41.30(10),	45.54(10),	10.71(10),	12.30(10),	10.44(5),	38.57(8),	42.61(8),	41.33(7),
	1M =	46.04(9),	40.45(7),	34.48(12),	39.28(8),	45.11(8),	7.46(9),	75.16(8),	9.82(7),	65.8(2),	73.55(7),
	2M =	36.36(7),	40.69(11),	66.3(2),	42.61(8),	0.50(7),	7.46(9),	46.04(9),	9.82(7),	9.57(7),	10.67(7),
	3M =	46.90(12),	50.05(12),	43.99(12),	44.13(11),	49.68(12),					
O(11A)-C(11A) /	0M =	13.10(16),	11.55(16),	44.00(16),	13.10(16),	67.13(16),	60.75(16),	57.02(13),	7.26(15),	23.43(15),	21.81(14),

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O(11B)-C(11B) /	1M =	13.10(15),	12.55(14),	13.95(17),	15.57(15),	11.76(15),	19.18(16),	11.50(15),	27.97(14),	23.1(3),	15.80(14),
	2M =	13.94(14),	26.09(16),	18.3(3),	23.43(15),	76.13(14),	19.18(16),	13.10(15),	27.97(14),	68.08(14),	61.66(14),
	3M =	33.91(17),	31.61(17),	26.96(17),	42.49(17),	14.99(17),					
	0M =	10.06(16),	11.16(16),	0.82(16),	10.06(16),	46.55(16),	47.18(16),	50.03(14),	39.09(15),	16.54(15),	17.04(15),
O(12A)-C(11A) /	1M =	9.68(16),	33.83(15),	18.89(18),	16.04(15),	9.72(15),	20.26(16),	14.09(15),	4.01(15),	6.9(3),	14.77(15),
	2M =	32.37(15),	18.93(17),	5.2(3),	16.54(15),	32.59(15),	20.26(16),	9.68(16),	4.01(15),	47.39(15),	48.67(15),
	3M =	10.10(17),	11.69(17),	16.31(18),	0.53(17),	7.75(17),					
	0M =	6.34(16),	7.84(16),	7.49(16),	6.34(16),	38.48(16),	39.52(16),	42.73(14),	46.82(15),	11.75(15),	12.57(15),
O(12B)-C(11B) /	1M =	5.92(16),	41.75(15),	16.02(18),	12.54(15),	6.20(15),	25.37(16),	20.28(15),	7.91(15),	14.0(3),	21.70(15),
	2M =	40.05(15),	13.95(17),	11.4(3),	11.75(15),	25.19(15),	25.37(16),	5.92(16),	7.91(15),	39.28(15),	40.95(15),
	3M =	18.41(17),	19.99(17),	10.94(18),	7.75(17),	3.46(17),					
	0M =	12.16(16),	10.30(16),	48.98(16),	12.16(16),	63.95(16),	57.43(16),	53.20(13),	13.34(15),	22.48(15),	20.63(14),
O(21A)-C(21A) /	1M =	12.21(15),	18.60(14),	11.83(17),	13.98(15),	10.74(15),	24.62(16),	14.08(15),	32.16(14),	26.0(3),	19.03(15),
	2M =	20.02(14),	25.03(16),	20.2(3),	22.48(15),	80.54(14),	24.62(16),	12.21(15),	32.16(14),	64.70(14),	58.08(14),
	3M =	39.24(17),	36.80(17),	26.38(17),	47.17(17),	14.56(17),					
	0M =	4.24(16),	3.00(16),	7.68(16),	4.24(16),	34.90(16),	34.37(16),	36.60(13),	41.24(15),	2.08(15),	2.61(14),
O(21B)-C(21B) /	1M =	4.62(15),	37.11(14),	4.95(17),	1.83(15),	4.51(15),	15.70(16),	28.07(15),	2.59(14),	20.0(3),	28.03(15),
	2M =	34.57(14),	4.48(16),	19.2(3),	2.08(15),	29.84(14),	15.70(16),	4.62(15),	2.59(14),	35.90(14),	35.96(14),
	3M =	18.12(17),	20.25(17),	1.89(17),	8.67(17),	6.67(17),					
	0M =	35.97(16),	38.71(16),	11.93(16),	35.97(16),	29.54(16),	35.10(16),	40.15(14),	53.66(15),	35.77(15),	37.89(15),
O(22A)-C(21A) /	1M =	35.46(16),	48.43(15),	47.14(18),	41.97(15),	36.59(15),	58.62(16),	2.94(15),	45.82(15),	2.2(3),	2.74(15),
	2M =	50.66(15),	36.51(17),	9.9(3),	35.77(15),	1.54(15),	58.62(16),	35.46(16),	45.82(15),	29.39(15),	35.34(15),
	3M =	20.86(17),	20.17(17),	32.27(18),	9.82(17),	31.27(17),					
	0M =	34.93(16),	37.85(16),	15.90(16),	34.93(16),	24.70(16),	30.34(16),	35.38(14),	56.20(15),	33.70(15),	35.96(15),
O(22B)-C(21B) /	1M =	34.42(16),	51.35(15),	46.03(18),	40.67(15),	35.70(15),	63.58(16),	1.73(15),	50.19(15),	0.0(3),	4.40(15),
	2M =	53.94(15),	34.18(17),	8.2(3),	33.70(15),	6.50(15),	63.58(16),	34.42(16),	50.19(15),	24.52(15),	30.54(15),
	3M =	24.44(17),	23.54(17),	29.90(18),	13.63(17),	30.02(17),					
	0M =	6.36(16),	5.28(16),	5.93(16),	6.36(16),	35.23(16),	34.19(16),	36.06(13),	37.97(15),	0.40(15),	0.78(14),
O(41A)-C(41A) /	1M =	6.73(15),	34.02(14),	2.49(17),	0.40(15),	6.72(15),	12.01(16),	28.70(15),	6.30(14),	20.0(3),	28.07(14),
	2M =	31.35(14),	2.88(16),	19.9(3),	0.40(15),	32.58(14),	12.01(16),	6.73(15),	6.30(14),	36.29(14),	35.81(14),
	3M =	16.16(17),	18.42(17),	0.50(17),	7.11(17),	8.53(17),					
	0M =	0.59(16),	0.89(16),	10.31(16),	0.59(16),	34.20(16),	34.51(16),	37.30(14),	46.35(15),	4.98(15),	5.73(15),
O(42A)-C(41A) /	1M =	1.01(16),	41.89(15),	9.07(18),	5.60(15),	0.74(15),	21.68(16),	26.59(15),	3.46(15),	19.6(3),	27.49(15),
	2M =	39.61(15),	7.22(17),	17.7(3),	4.98(15),	25.38(15),	21.68(16),	1.01(16),	3.46(15),	35.11(15),	36.02(15),
	3M =	21.03(17),	22.92(17),	4.33(18),	10.95(17),	3.42(17),					
	0M =	0.70(16),	0.97(16),	39.95(16),	0.70(16),	54.48(16),	48.16(16),	44.65(13),	10.55(15),	11.04(15),	9.33(14),
O(51A)-C(51A) /	1M =	0.73(15),	15.11(14),	1.27(17),	2.96(15),	0.67(15),	28.15(16),	2.62(15),	39.37(14),	14.6(3),	8.00(15),
	2M =	17.32(14),	13.66(16),	8.4(3),	11.04(15),	81.95(14),	28.15(16),	0.73(15),	39.37(14),	55.46(14),	49.14(14),
	3M =	31.37(17),	28.61(17),	14.76(17),	37.62(17),	2.86(17),					
	0M =	39.60(16),	41.94(16),	3.37(16),	39.60(16),	38.64(16),	44.22(16),	49.26(13),	46.34(15),	41.21(15),	43.03(14),
O(52A)-C(51A) /	1M =	39.11(15),	40.77(14),	50.54(17),	45.87(15),	39.95(15),	49.92(16),	7.50(15),	38.91(14),	8.3(3),	2.63(15),
	2M =	42.59(14),	42.37(16),	15.1(3),	41.21(15),	6.96(14),	49.92(16),	39.11(15),	38.91(14),	38.47(14),	44.46(14),
	3M =	12.69(17),	12.23(17),	38.28(17),	1.42(17),	35.39(17),					
	0M =	5.37(16),	4.80(16),	2.56(16),	5.37(16),	41.28(16),	39.25(16),	40.28(14),	29.10(15),	2.53(15),	2.50(15),
C(1A)c-C(2A)c /	1M =	5.68(16),	25.02(15),	2.29(18),	0.17(15),	5.96(15),	4.51(16),	23.66(15),	13.08(15),	13.9(3),	21.93(15),
	2M =	22.43(15),	5.17(17),	15.2(3),	2.53(15),	41.65(15),	4.51(16),	5.68(16),	13.08(15),	42.43(15),	40.91(15),
	3M =	7.45(17),	9.82(17),	3.37(18),	1.17(17),	6.77(17),					
	0M =	36.23(18),	34.09(18),	34.20(18),	36.23(18),	0.25(18),	1.12(18),	0.81(16),	42.27(17),	32.14(17),	31.09(17),

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	1M =	36.70(18),	42.69(17),	25.5(2),	29.90(18),	36.02(18),	10.02(18),	63.91(17),	8.64(17),	55.1(3),	63.07(17),
	2M =	38.58(17),	30.06(19),	55.0(3),	32.14(17),	8.10(17),	10.02(18),	36.70(18),	8.64(17),	1.37(17),	0.50(17),
	3M =	41.71(19),	44.74(19),	33.1(2),	36.56(19),	39.87(19),					
-C(6A)c /	0M =	41.19(19),	43.31(18),	14.86(18),	41.19(19),	11.54(19),	5.32(19),	2.21(16),	17.10(17),	31.00(17),	32.99(17),
	1M =	41.07(18),	17.68(17),	41.7(2),	39.77(18),	42.67(18),	48.85(18),	26.67(18),	68.26(17),	15.8(3),	18.89(17),
	2M =	21.71(17),	28.56(19),	25.1(3),	31.00(17),	45.15(17),	48.85(18),	41.07(18),	68.26(17),	12.55(17),	6.41(17),
	3M =	12.94(19),	9.86(19),	26.8(2),	11.35(19),	38.1(2),					
-C(11A) /	0M =	1.99(17),	1.32(17),	59.38(17),	1.99(17),	14.89(18),	10.46(18),	5.53(15),	72.61(16),	6.78(16),	4.22(16),
	1M =	2.45(17),	77.57(16),	7.63(19),	2.21(16),	0.73(17),	61.05(17),	31.98(16),	45.68(16),	38.7(3),	39.85(16),
	2M =	79.25(16),	7.07(18),	28.9(3),	6.78(16),	35.12(16),	61.05(17),	2.45(17),	45.68(16),	14.67(16),	9.81(16),
	3M =	67.50(18),	65.95(18),	11.27(19),	57.14(18),	7.23(19),					
C(1B)c-C(2B)c /	0M =	36.09(18),	34.03(18),	32.84(18),	36.09(18),	1.29(18),	0.19(18),	1.66(16),	41.42(17),	31.74(17),	30.76(17),
	1M =	36.56(18),	41.69(17),	25.5(2),	29.76(18),	35.93(18),	9.13(18),	63.09(17),	9.62(17),	54.0(3),	61.97(17),
	2M =	37.59(17),	29.61(19),	54.3(3),	31.74(17),	9.45(17),	9.13(18),	36.56(18),	9.62(17),	2.42(17),	1.45(17),
	3M =	40.35(19),	43.38(19),	32.6(2),	35.22(19),	39.62(19),					
-C(11B) /	0M =	1.87(17),	5.14(17),	53.02(17),	1.87(17),	8.10(17),	3.71(17),	1.22(15),	78.64(16),	2.06(16),	0.43(16),
	1M =	1.38(17),	82.13(16),	11.98(19),	6.50(16),	3.04(16),	63.36(17),	29.51(16),	45.92(16),	34.9(3),	37.09(16),
	2M =	85.39(16),	2.12(18),	25.4(3),	2.06(16),	29.26(16),	63.36(17),	1.38(17),	45.92(16),	7.87(16),	3.04(16),
	3M =	61.92(18),	60.86(18),	6.37(19),	51.01(18),	3.37(18),					
C(2A)c-C(3A)c /	0M =	4.49(19),	7.80(18),	54.22(18),	4.49(19),	11.81(19),	6.92(19),	1.91(16),	71.95(17),	0.53(17),	2.05(17),
	1M =	4.03(18),	75.15(17),	14.0(2),	8.59(18),	5.77(18),	67.60(18),	25.48(17),	51.74(17),	32.2(3),	33.33(17),
	2M =	78.49(17),	0.92(19),	22.4(3),	0.53(17),	35.44(17),	67.60(18),	4.03(18),	51.74(17),	11.71(17),	6.43(17),
	3M =	61.41(19),	59.65(19),	5.1(2),	51.66(19),	0.7(2),					
-C(21A) /	0M =	43.73(17),	45.69(17),	11.32(17),	43.73(17),	9.83(18),	3.73(18),	0.86(15),	14.02(16),	33.46(16),	35.35(16),
	1M =	43.64(17),	14.40(16),	43.49(19),	41.92(17),	45.18(17),	46.00(17),	30.28(16),	65.37(16),	19.3(3),	22.52(16),
	2M =	18.47(16),	30.95(18),	28.5(3),	33.46(16),	42.69(16),	46.00(17),	43.64(17),	65.37(16),	10.88(16),	4.89(16),
	3M =	9.30(18),	6.22(18),	29.36(19),	7.82(18),	40.84(19),					
C(2B)c-C(6B)c /	0M =	8.02(19),	11.30(18),	48.31(18),	8.02(19),	5.06(19),	0.24(19),	4.77(16),	76.52(18),	3.89(17),	6.41(17),
	1M =	7.54(18),	77.47(17),	18.1(2),	12.58(18),	9.20(18),	69.30(18),	23.34(18),	51.19(17),	28.8(3),	30.90(17),
	2M =	81.59(17),	3.74(19),	19.3(3),	3.89(17),	29.20(17),	69.30(18),	7.54(18),	51.19(17),	4.94(17),	0.29(17),
	3M =	56.47(19),	55.15(19),	0.5(2),	46.00(19),	2.8(2),					
-C(21B) /	0M =	48.22(17),	50.35(17),	8.89(17),	48.22(17),	4.76(17),	1.38(17),	4.32(15),	15.62(16),	38.03(16),	40.02(16),
	1M =	48.10(17),	15.46(16),	48.55(19),	46.76(16),	49.70(17),	47.91(17),	32.11(16),	66.79(16),	21.7(3),	24.18(16),
	2M =	19.58(16),	35.60(18),	31.2(3),	38.03(16),	38.12(16),	47.91(17),	48.10(17),	66.79(16),	5.80(16),	0.24(16),
	3M =	7.80(18),	4.80(18),	33.80(19),	5.35(18),	45.03(18),					
C(3A)c-C(4A)c /	0M =	41.25(19),	43.36(18),	14.63(18),	41.25(19),	11.57(19),	5.37(19),	2.28(17),	16.76(18),	31.05(18),	33.03(17),
	1M =	41.14(18),	17.34(17),	41.7(2),	39.79(18),	42.73(18),	48.51(18),	26.92(18),	67.93(17),	16.0(3),	19.15(17),
	2M =	21.37(17),	28.61(19),	25.3(3),	31.05(18),	45.11(17),	48.51(18),	41.14(18),	67.93(17),	12.59(17),	6.47(17),
	3M =	12.7(2),	9.6(2),	26.8(2),	11.1(2),	38.2(2),					
C(4A)c-C(5A)c /	0M =	36.77(18),	34.61(18),	34.66(18),	36.77(18),	0.39(19),	1.78(19),	0.15(16),	42.13(17),	32.75(17),	31.69(17),
	1M =	37.25(18),	42.64(17),	26.0(2),	30.44(18),	36.56(18),	9.91(18),	64.56(17),	8.69(17),	55.7(3),	63.71(17),
	2M =	38.52(17),	30.67(19),	55.7(3),	32.75(17),	7.64(17),	9.91(18),	37.25(18),	8.69(17),	0.73(17),	0.15(17),
	3M =	42.08(19),	45.12(19),	33.8(2),	37.05(19),	40.44(19),					
-C(41A) /	0M =	0.87(18),	4.18(17),	56.74(17),	0.87(18),	12.88(18),	8.29(18),	3.31(15),	73.44(16),	3.89(16),	1.33(16),
	1M =	0.40(17),	77.64(16),	10.51(19),	5.09(17),	2.13(17),	63.80(17),	29.32(16),	47.95(16),	35.9(3),	37.15(16),
	2M =	80.22(16),	4.18(18),	26.1(3),	3.89(16),	34.50(16),	63.80(17),	0.40(17),	47.95(16),	12.70(16),	7.69(16),
	3M =	64.63(18),	63.07(19),	8.38(19),	54.40(18),	4.37(19),					
C(5A)c-C(6A)c /	0M =	4.74(19),	8.05(18),	53.74(18),	4.74(19),	11.21(19),	6.33(19),	1.32(16),	72.48(18),	0.19(18),	2.38(17),

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	1M =	4.27(18),	75.54(17),	14.3(2),	8.89(18),	6.01(18),	67.75(18),	25.38(18),	51.64(17),	32.0(3),	33.21(17),
	2M =	78.97(17),	0.56(19),	22.2(3),	0.19(18),	34.85(17),	67.75(18),	4.27(18),	51.64(17),	11.11(17),	5.83(17),
	3M =	61.1(2),	59.3(2),	4.7(2),	51.21(19),	0.5(2),					
-C(51A) /	0M =	47.09(17),	49.14(17),	9.33(17),	47.09(17),	6.16(18),	0.04(18),	2.86(15),	14.87(16),	36.86(16),	38.81(16),
	1M =	46.98(17),	14.86(16),	47.16(19),	45.48(16),	48.56(17),	47.11(17),	31.89(16),	66.18(16),	21.3(3),	24.01(16),
	2M =	18.97(16),	34.39(18),	30.7(3),	36.86(16),	39.31(16),	47.11(17),	46.98(17),	66.18(16),	7.20(16),	1.20(16),
	3M =	7.94(18),	4.92(18),	32.68(19),	5.80(18),	44.01(19),					
Cu(1)d-O(7W)d /	0M =	35.01(10),	31.87(10),	81.52(10),	35.01(10),	48.47(10),	46.05(10),	41.64(5),	38.16(8),	42.59(8),	39.96(7),
	1M =	35.36(9),	44.05(7),	27.79(12),	32.68(8),	33.50(9),	26.27(10),	52.43(8),	19.12(8),	64.4(2),	58.74(8),
	2M =	42.73(8),	43.64(11),	55.9(2),	42.59(8),	46.20(7),	26.27(10),	35.36(9),	19.12(8),	47.77(8),	44.94(7),
	3M =	72.45(12),	72.07(12),	47.44(12),	83.96(12),	39.72(12),					
-O(11A) /	0M =	23.54(10),	20.23(10),	76.24(10),	23.54(10),	29.25(10),	26.39(10),	21.90(5),	57.74(8),	28.59(8),	26.03(7),
	1M =	23.99(9),	63.53(7),	14.16(12),	19.55(8),	22.23(8),	39.85(10),	51.29(8),	27.30(7),	59.9(2),	59.32(8),
	2M =	61.70(7),	28.84(11),	49.8(2),	28.59(8),	36.50(7),	39.85(10),	23.99(9),	27.30(7),	28.66(8),	25.34(7),
	3M =	87.04(12),	87.75(12),	33.05(12),	76.00(12),	28.75(12),					
-O(11B) /	0M =	23.22(10),	25.39(9),	10.40(9),	23.22(10),	36.11(10),	40.05(10),	44.76(5),	54.94(8),	26.00(8),	27.52(7),
	1M =	22.74(9),	48.98(6),	33.97(12),	29.55(8),	23.46(8),	44.46(9),	7.88(8),	28.71(7),	5.4(2),	11.86(7),
	2M =	49.30(7),	27.55(11),	0.3(2),	26.00(8),	11.15(7),	44.46(9),	22.74(9),	28.71(7),	36.39(7),	40.89(7),
	3M =	20.92(11),	21.29(11),	23.73(12),	9.30(11),	19.31(12),					
Cu(2)d-O(6W)d /	0M =	29.35(10),	26.19(10),	86.94(10),	29.35(10),	45.61(10),	42.48(10),	37.83(5),	42.41(8),	36.82(8),	34.19(7),
	1M =	29.70(9),	48.36(7),	22.02(12),	26.92(8),	27.85(9),	32.02(10),	48.66(8),	24.71(8),	60.3(2),	55.59(8),
	2M =	47.39(8),	37.86(11),	51.2(2),	36.82(8),	48.51(7),	32.02(10),	29.70(9),	24.71(8),	45.04(8),	41.51(7),
	3M =	76.26(12),	74.98(12),	41.67(12),	86.67(12),	34.12(12),					
-O(12A) /	0M =	24.67(10),	26.48(9),	3.62(9),	24.67(10),	43.20(10),	46.85(10),	51.41(5),	47.99(8),	28.77(8),	29.99(7),
	1M =	24.22(9),	42.05(6),	34.86(12),	30.98(8),	24.70(8),	37.91(9),	4.76(8),	23.19(7),	0.9(2),	7.92(7),
	2M =	42.16(7),	30.62(11),	3.8(2),	28.77(8),	18.26(7),	37.91(9),	24.22(9),	23.19(7),	43.53(7),	47.78(7),
	3M =	14.30(11),	14.86(11),	27.09(12),	2.71(11),	21.26(12),					
-O(12B) /	0M =	21.36(10),	18.06(10),	77.27(10),	21.36(10),	30.05(10),	26.86(10),	22.25(5),	57.87(8),	26.80(8),	24.22(7),
	1M =	21.80(9),	63.78(7),	12.23(12),	17.58(8),	20.01(8),	42.03(9),	48.45(8),	30.04(7),	57.4(2),	56.46(8),
	2M =	62.38(7),	27.18(11),	47.3(2),	26.80(8),	39.05(7),	42.03(9),	21.80(9),	30.04(7),	29.52(7),	25.89(7),
	3M =	87.65(12),	85.44(12),	31.36(12),	76.26(12),	26.54(12),					
-O(21A) /	0M =	44.62(10),	45.80(10),	3.89(10),	44.62(10),	10.56(10),	5.01(10),	2.95(5),	3.28(8),	34.37(8),	35.80(7),
	1M =	44.66(9),	3.75(7),	41.54(12),	41.32(8),	45.88(8),	35.29(10),	38.01(8),	54.63(8),	26.4(2),	30.64(8),
	2M =	7.79(7),	31.65(11),	34.8(2),	34.37(8),	39.89(7),	35.29(10),	44.66(9),	54.63(8),	11.72(8),	6.37(7),
	3M =	0.55(12),	2.58(12),	30.96(12),	0.52(12),	42.92(12),					
Na(1)d-O(4W)d /	0M =	31.20(11),	28.64(11),	42.07(11),	31.20(11),	2.95(12),	3.21(12),	0.50(8),	51.77(10),	29.01(10),	27.51(9),
	1M =	31.70(10),	52.65(9),	20.09(13),	24.98(10),	30.72(10),	19.75(11),	62.78(10),	1.35(9),	57.4(3),	65.16(9),
	2M =	48.52(9),	27.33(12),	54.2(3),	29.01(10),	0.10(9),	19.75(11),	31.70(10),	1.36(9),	1.94(9),	1.67(9),
	3M =	50.60(13),	53.50(13),	30.95(13),	44.00(13),	35.50(13),					
-O(5W)d /	0M =	29.44(11),	32.52(11),	33.11(11),	29.44(11),	10.76(11),	4.30(11),	0.22(7),	42.37(9),	21.14(9),	23.69(9),
	1M =	29.10(10),	43.11(9),	35.46(13),	31.16(10),	30.95(10),	72.81(11),	5.21(9),	83.58(9),	3.9(3),	2.82(9),
	2M =	47.14(9),	19.57(12),	6.1(3),	21.14(9),	45.61(9),	72.81(11),	29.10(10),	83.58(9),	11.36(9),	4.75(9),
	3M =	34.48(13),	31.69(13),	16.27(13),	29.59(13),	24.75(13),					
-O(52A) /	0M =	49.65(10),	47.49(10),	35.50(10),	49.65(10),	9.15(10),	11.52(10),	10.26(5),	31.96(8),	45.21(8),	44.31(7),
	1M =	50.12(9),	33.57(7),	38.90(12),	43.32(8),	49.44(8),	0.54(9),	73.97(8),	16.90(7),	62.6(2),	69.44(7),
	2M =	29.46(7),	42.99(11),	65.9(2),	45.21(8),	5.59(7),	0.54(9),	50.12(9),	16.90(7),	7.96(7),	9.86(7),
	3M =	40.34(11),	43.49(11),	45.80(12),	38.53(11),	53.22(12),					
-O(41A) /	0M =	40.76(10),	40.46(10),	31.22(10),	40.76(10),	76.11(10),	81.52(10),	86.37(5),	13.34(8),	49.77(8),	49.31(7),

Na(2)d-O(12B) /	1M =	40.55(9),	7.38(7),	45.49(12),	45.28(8),	39.84(8),	13.05(9),	22.63(8),	6.67(7),	30.1(2),	22.22(7),	
	2M =	7.97(7),	52.52(11),	31.5(2),	49.77(8),	41.78(7),	13.05(9),	40.55(9),	6.67(7),	75.82(7),	81.97(7),	
	3M =	20.65(11),	20.09(12),	51.06(12),	32.25(11),	40.34(12),						
	0M =	8.89(10),	8.08(9),	30.08(9),	8.89(10),	63.61(10),	58.79(10),	57.01(5),	6.00(8),	18.78(7),	17.72(7),	
	1M =	8.77(8),	0.94(6),	12.43(12),	12.69(8),	7.77(8),	9.95(9),	0.62(8),	22.31(7),	11.6(2),	3.90(7),	
	2M =	0.75(7),	21.57(10),	8.2(2),	18.78(7),	65.67(7),	9.95(9),	8.77(8),	22.31(7),	64.84(7),	60.25(6),	
	3M =	19.85(11),	17.61(11),	21.37(12),	28.75(11),	9.58(11),						
	-O(22A) /	0M =	26.64(10),	29.95(10),	34.55(10),	26.64(10),	0.48(10),	5.56(10),	10.49(5),	57.94(8),	20.84(8),	23.46(7),
	1M =	26.19(9),	57.13(7),	35.59(12),	30.35(8),	27.96(8),	89.60(9),	3.24(8),	70.27(7),	9.9(2),	11.02(7),	
	2M =	61.24(7),	20.09(11),	0.0(2),	20.84(8),	32.52(7),	89.60(9),	26.19(9),	70.27(7),	0.79(7),	5.52(7),	
	3M =	39.77(11),	37.66(11),	16.10(12),	31.46(11),	21.43(12),						
	-O(1W)d /	0M =	42.62(10),	40.87(10),	28.82(10),	42.62(10),	0.02(10),	2.37(10),	1.20(5),	33.00(8),	37.07(8),	36.42(7),
1M =	43.05(9),	33.49(7),	32.42(12),	36.34(8),	42.64(8),	0.76(9),	64.91(8),	17.83(7),	53.9(2),	61.30(7),		
2M =	29.38(7),	34.70(11),	56.7(2),	37.07(8),	13.10(7),	0.76(9),	43.05(9),	17.83(7),	1.20(7),	0.71(7),		
3M =	35.05(12),	38.17(12),	37.23(12),	31.57(11),	45.60(12),							
-O(3W)d /	0M =	23.76(10),	26.90(9),	38.96(9),	23.76(10),	13.55(10),	7.20(10),	2.49(5),	47.00(8),	15.79(8),	18.37(7),	
1M =	23.41(9),	48.27(6),	30.32(12),	25.81(8),	25.26(8),	74.73(9),	0.93(8),	77.58(7),	10.0(2),	8.97(7),		
2M =	52.21(7),	14.35(11),	0.0(2),	15.79(8),	47.36(7),	74.73(9),	23.41(9),	77.58(7),	14.04(7),	7.50(7),		
3M =	40.61(11),	37.83(11),	10.91(12),	35.47(11),	18.98(12),							
-O(41A) /	0M =	45.54(10),	43.05(10),	41.30(10),	45.54(10),	10.71(10),	12.30(10),	10.44(5),	38.57(8),	42.61(8),	41.33(7),	
1M =	46.04(9),	40.45(7),	34.48(12),	39.28(8),	45.11(8),	7.46(9),	75.16(8),	9.82(7),	65.8(2),	73.55(7),		
2M =	36.36(7),	40.69(11),	66.3(2),	42.61(8),	0.50(7),	7.46(9),	46.04(9),	9.82(7),	9.57(7),	10.67(7),		
3M =	46.90(12),	50.05(12),	43.99(12),	44.13(11),	49.68(12),							
O(11A)-C(11A) /	0M =	13.10(16),	11.55(16),	44.00(16),	13.10(16),	67.13(16),	60.75(16),	57.02(13),	7.26(15),	23.43(15),	21.81(14),	
1M =	13.10(15),	12.55(14),	13.95(17),	15.57(15),	11.76(15),	19.18(16),	11.50(15),	27.97(14),	23.1(3),	15.80(14),		
2M =	13.94(14),	26.09(16),	18.3(3),	23.43(15),	76.13(14),	19.18(16),	13.10(15),	27.97(14),	68.08(14),	61.66(14),		
3M =	33.91(17),	31.61(17),	26.96(17),	42.49(17),	14.99(17),							
O(11B)-C(11B) /	0M =	10.06(16),	11.16(16),	0.82(16),	10.06(16),	46.55(16),	47.18(16),	50.03(14),	39.09(15),	16.54(15),	17.04(15),	
1M =	9.68(16),	33.83(15),	18.89(18),	16.04(15),	9.72(15),	20.26(16),	14.09(15),	4.01(15),	6.9(3),	14.77(15),		
2M =	32.37(15),	18.93(17),	5.2(3),	16.54(15),	32.59(15),	20.26(16),	9.68(16),	4.01(15),	47.39(15),	48.67(15),		
3M =	10.10(17),	11.69(17),	16.31(18),	0.53(17),	7.75(17),							
O(12A)-C(11A) /	0M =	6.34(16),	7.84(16),	7.49(16),	6.34(16),	38.48(16),	39.52(16),	42.73(14),	46.82(15),	11.75(15),	12.57(15),	
1M =	5.92(16),	41.75(15),	16.02(18),	12.54(15),	6.20(15),	25.37(16),	20.28(15),	7.91(15),	14.0(3),	21.70(15),		
2M =	40.05(15),	13.95(17),	11.4(3),	11.75(15),	25.19(15),	25.37(16),	5.92(16),	7.91(15),	39.28(15),	40.95(15),		
3M =	18.41(17),	19.99(17),	10.94(18),	7.75(17),	3.46(17),							
O(12B)-C(11B) /	0M =	12.16(16),	10.30(16),	48.98(16),	12.16(16),	63.95(16),	57.43(16),	53.20(13),	13.34(15),	22.48(15),	20.63(14),	
1M =	12.21(15),	18.60(14),	11.83(17),	13.98(15),	10.74(15),	24.62(16),	14.08(15),	32.16(14),	26.0(3),	19.03(15),		
2M =	20.02(14),	25.03(16),	20.2(3),	22.48(15),	80.54(14),	24.62(16),	12.21(15),	32.16(14),	64.70(14),	58.08(14),		
3M =	39.24(17),	36.80(17),	26.38(17),	47.17(17),	14.56(17),							
O(21A)-C(21A) /	0M =	4.24(16),	3.00(16),	7.68(16),	4.24(16),	34.90(16),	34.37(16),	36.60(13),	41.24(15),	2.08(15),	2.61(14),	
1M =	4.62(15),	37.11(14),	4.95(17),	1.83(15),	4.51(15),	15.70(16),	28.07(15),	2.59(14),	20.0(3),	28.03(15),		
2M =	34.57(14),	4.48(16),	19.2(3),	2.08(15),	29.84(14),	15.70(16),	4.62(15),	2.59(14),	35.90(14),	35.96(14),		
3M =	18.12(17),	20.25(17),	1.89(17),	8.67(17),	6.67(17),							
O(21B)-C(21B) /	0M =	35.97(16),	38.71(16),	11.93(16),	35.97(16),	29.54(16),	35.10(16),	40.15(14),	53.66(15),	35.77(15),	37.89(15),	
1M =	35.46(16),	48.43(15),	47.14(18),	41.97(15),	36.59(15),	58.62(16),	2.94(15),	45.82(15),	2.2(3),	2.74(15),		
2M =	50.66(15),	36.51(17),	9.9(3),	35.77(15),	1.54(15),	58.62(16),	35.46(16),	45.82(15),	29.39(15),	35.34(15),		
3M =	20.86(17),	20.17(17),	32.27(18),	9.82(17),	31.27(17),							
O(22A)-C(21A) /	0M =	34.93(16),	37.85(16),	15.90(16),	34.93(16),	24.70(16),	30.34(16),	35.38(14),	56.20(15),	33.70(15),	35.96(15),	

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O(22B)-C(21B) /	1M =	34.42(16),	51.35(15),	46.03(18),	40.67(15),	35.70(15),	63.58(16),	1.73(15),	50.19(15),	0.0(3),	4.40(15),
	2M =	53.94(15),	34.18(17),	8.2(3),	33.70(15),	6.50(15),	63.58(16),	34.42(16),	50.19(15),	24.52(15),	30.54(15),
	3M =	24.44(17),	23.54(17),	29.90(18),	13.63(17),	30.02(17),					
	0M =	6.36(16),	5.28(16),	5.93(16),	6.36(16),	35.23(16),	34.19(16),	36.06(13),	37.97(15),	0.40(15),	0.78(14),
O(41A)-C(41A) /	1M =	6.73(15),	34.02(14),	2.49(17),	0.40(15),	6.72(15),	12.01(16),	28.70(15),	6.30(14),	20.0(3),	28.07(14),
	2M =	31.35(14),	2.88(16),	19.9(3),	0.40(15),	32.58(14),	12.01(16),	6.73(15),	6.30(14),	36.29(14),	35.81(14),
	3M =	16.16(17),	18.42(17),	0.50(17),	7.11(17),	8.53(17),					
	0M =	0.59(16),	0.89(16),	10.31(16),	0.59(16),	34.20(16),	34.51(16),	37.30(14),	46.35(15),	4.98(15),	5.73(15),
O(42A)-C(41A) /	1M =	1.01(16),	41.89(15),	9.07(18),	5.60(15),	0.74(15),	21.68(16),	26.59(15),	3.46(15),	19.6(3),	27.49(15),
	2M =	39.61(15),	7.22(17),	17.7(3),	4.98(15),	25.38(15),	21.68(16),	1.01(16),	3.46(15),	35.11(15),	36.02(15),
	3M =	21.03(17),	22.92(17),	4.33(18),	10.95(17),	3.42(17),					
	0M =	0.70(16),	0.97(16),	39.95(16),	0.70(16),	54.48(16),	48.16(16),	44.65(13),	10.55(15),	11.04(15),	9.33(14),
O(51A)-C(51A) /	1M =	0.73(15),	15.11(14),	1.27(17),	2.96(15),	0.67(15),	28.15(16),	2.62(15),	39.37(14),	14.6(3),	8.00(15),
	2M =	17.32(14),	13.66(16),	8.4(3),	11.04(15),	81.95(14),	28.15(16),	0.73(15),	39.37(14),	55.46(14),	49.14(14),
	3M =	31.37(17),	28.61(17),	14.76(17),	37.62(17),	2.86(17),					
	0M =	39.60(16),	41.94(16),	3.37(16),	39.60(16),	38.64(16),	44.22(16),	49.26(13),	46.34(15),	41.21(15),	43.03(14),
O(52A)-C(51A) /	1M =	39.11(15),	40.77(14),	50.54(17),	45.87(15),	39.95(15),	49.92(16),	7.50(15),	38.91(14),	8.3(3),	2.63(15),
	2M =	42.59(14),	42.37(16),	15.1(3),	41.21(15),	6.96(14),	49.92(16),	39.11(15),	38.91(14),	38.47(14),	44.46(14),
	3M =	12.69(17),	12.23(17),	38.28(17),	1.42(17),	35.39(17),					
	0M =	5.37(16),	4.80(16),	2.56(16),	5.37(16),	41.28(16),	39.25(16),	40.28(14),	29.10(15),	2.53(15),	2.50(15),
C(1A)d-C(2A)d /	1M =	5.68(16),	25.02(15),	2.29(18),	0.17(15),	5.96(15),	4.51(16),	23.66(15),	13.08(15),	13.9(3),	21.93(15),
	2M =	22.43(15),	5.17(17),	15.2(3),	2.53(15),	41.65(15),	4.51(16),	5.68(16),	13.08(15),	42.43(15),	40.91(15),
	3M =	7.45(17),	9.82(17),	3.37(18),	1.17(17),	6.77(17),					
	0M =	36.23(18),	34.09(18),	34.20(18),	36.23(18),	0.25(18),	1.12(18),	0.81(16),	42.27(17),	32.14(17),	31.09(17),
-C(6A)d /	1M =	36.70(18),	42.69(17),	25.5(2),	29.90(18),	36.02(18),	10.02(18),	63.91(17),	8.64(17),	55.1(3),	63.07(17),
	2M =	38.58(17),	30.06(19),	55.0(3),	32.14(17),	8.10(17),	10.02(18),	36.70(18),	8.64(17),	1.37(17),	0.50(17),
	3M =	41.71(19),	44.74(19),	33.1(2),	36.56(19),	39.87(19),					
	0M =	41.19(19),	43.31(18),	14.86(18),	41.19(19),	11.54(19),	5.32(19),	2.21(16),	17.10(17),	31.00(17),	32.99(17),
-C(11A) /	1M =	41.07(18),	17.68(17),	41.7(2),	39.77(18),	42.67(18),	48.85(18),	26.67(18),	68.26(17),	15.8(3),	18.89(17),
	2M =	21.71(17),	28.56(19),	25.1(3),	31.00(17),	45.15(17),	48.85(18),	41.07(18),	68.26(17),	12.55(17),	6.41(17),
	3M =	12.94(19),	9.86(19),	26.8(2),	11.35(19),	38.1(2),					
	0M =	1.99(17),	1.32(17),	59.38(17),	1.99(17),	14.89(18),	10.46(18),	5.53(15),	72.61(16),	6.78(16),	4.22(16),
C(1B)d-C(2B)d /	1M =	2.45(17),	77.57(16),	7.63(19),	2.21(16),	0.73(17),	61.05(17),	31.98(16),	45.68(16),	38.7(3),	39.85(16),
	2M =	79.25(16),	7.07(18),	28.9(3),	6.78(16),	35.12(16),	61.05(17),	2.45(17),	45.68(16),	14.67(16),	9.81(16),
	3M =	67.50(18),	65.95(18),	11.27(19),	57.14(18),	7.23(19),					
	0M =	36.09(18),	34.03(18),	32.84(18),	36.09(18),	1.29(18),	0.19(18),	1.66(16),	41.42(17),	31.74(17),	30.76(17),
-C(11B) /	1M =	36.56(18),	41.69(17),	25.5(2),	29.76(18),	35.93(18),	9.13(18),	63.09(17),	9.62(17),	54.0(3),	61.97(17),
	2M =	37.59(17),	29.61(19),	54.3(3),	31.74(17),	9.45(17),	9.13(18),	36.56(18),	9.62(17),	2.42(17),	1.45(17),
	3M =	40.35(19),	43.38(19),	32.6(2),	35.22(19),	39.62(19),					
	0M =	1.87(17),	5.14(17),	53.02(17),	1.87(17),	8.10(17),	3.71(17),	1.22(15),	78.64(16),	2.06(16),	0.43(16),
C(2A)d-C(3A)d /	1M =	1.38(17),	82.13(16),	11.98(19),	6.50(16),	3.04(16),	63.36(17),	29.51(16),	45.92(16),	34.9(3),	37.09(16),
	2M =	85.39(16),	2.12(18),	25.4(3),	2.06(16),	29.26(16),	63.36(17),	1.38(17),	45.92(16),	7.87(16),	3.04(16),
	3M =	61.92(18),	60.86(18),	6.37(19),	51.01(18),	3.37(18),					
	0M =	4.49(19),	7.80(18),	54.22(18),	4.49(19),	11.81(19),	6.92(19),	1.91(16),	71.95(17),	0.53(17),	2.05(17),
-C(21A) /	1M =	4.03(18),	75.15(17),	14.0(2),	8.59(18),	5.77(18),	67.60(18),	25.48(17),	51.74(17),	32.2(3),	33.33(17),
	2M =	78.49(17),	0.92(19),	22.4(3),	0.53(17),	35.44(17),	67.60(18),	4.03(18),	51.74(17),	11.71(17),	6.43(17),
	3M =	61.41(19),	59.65(19),	5.1(2),	51.66(19),	0.7(2),					
	0M =	43.73(17),	45.69(17),	11.32(17),	43.73(17),	9.83(18),	3.73(18),	0.86(15),	14.02(16),	33.46(16),	35.35(16),

C(2B)d-C(6B)d /	1M =	43.64(17),	14.40(16),	43.49(19),	41.92(17),	45.18(17),	46.00(17),	30.28(16),	65.37(16),	19.3(3),	22.52(16),	
	2M =	18.47(16),	30.95(18),	28.5(3),	33.46(16),	42.69(16),	46.00(17),	43.64(17),	65.37(16),	10.88(16),	4.89(16),	
	3M =	9.30(18),	6.22(18),	29.36(19),	7.82(18),	40.84(19),						
	0M =	8.02(19),	11.30(18),	48.31(18),	8.02(19),	5.06(19),	0.24(19),	4.77(16),	76.52(18),	3.89(17),	6.41(17),	
	1M =	7.54(18),	77.47(17),	18.1(2),	12.58(18),	9.20(18),	69.30(18),	23.34(18),	51.19(17),	28.8(3),	30.90(17),	
	2M =	81.59(17),	3.74(19),	19.3(3),	3.89(17),	29.20(17),	69.30(18),	7.54(18),	51.19(17),	4.94(17),	0.29(17),	
	3M =	56.47(19),	55.15(19),	0.5(2),	46.00(19),	2.8(2),						
	-C(21B) /	0M =	48.22(17),	50.35(17),	8.89(17),	48.22(17),	4.76(17),	1.38(17),	4.32(15),	15.62(16),	38.03(16),	40.02(16),
	1M =	48.10(17),	15.46(16),	48.55(19),	46.76(16),	49.70(17),	47.91(17),	32.11(16),	66.79(16),	21.7(3),	24.18(16),	
	2M =	19.58(16),	35.60(18),	31.2(3),	38.03(16),	38.12(16),	47.91(17),	48.10(17),	66.79(16),	5.80(16),	0.24(16),	
	3M =	7.80(18),	4.80(18),	33.80(19),	5.35(18),	45.03(18),						
	C(3A)d-C(4A)d /	0M =	41.25(19),	43.36(18),	14.63(18),	41.25(19),	11.57(19),	5.37(19),	2.28(17),	16.76(18),	31.05(18),	33.03(17),
1M =	41.14(18),	17.34(17),	41.7(2),	39.79(18),	42.73(18),	48.51(18),	26.92(18),	67.93(17),	16.0(3),	19.15(17),		
2M =	21.37(17),	28.61(19),	25.3(3),	31.05(18),	45.11(17),	48.51(18),	41.14(18),	67.93(17),	12.59(17),	6.47(17),		
3M =	12.7(2),	9.6(2),	26.8(2),	11.1(2),	38.2(2),							
C(4A)d-C(5A)d /	0M =	36.77(18),	34.61(18),	34.66(18),	36.77(18),	0.39(19),	1.78(19),	0.15(16),	42.13(17),	32.75(17),	31.69(17),	
1M =	37.25(18),	42.64(17),	26.0(2),	30.44(18),	36.56(18),	9.91(18),	64.56(17),	8.69(17),	55.7(3),	63.71(17),		
2M =	38.52(17),	30.67(19),	55.7(3),	32.75(17),	7.64(17),	9.91(18),	37.25(18),	8.69(17),	0.73(17),	0.15(17),		
3M =	42.08(19),	45.12(19),	33.8(2),	37.05(19),	40.44(19),							
-C(41A) /	0M =	0.87(18),	4.18(17),	56.74(17),	0.87(18),	12.88(18),	8.29(18),	3.31(15),	73.44(16),	3.89(16),	1.33(16),	
1M =	0.40(17),	77.64(16),	10.51(19),	5.09(17),	2.13(17),	63.80(17),	29.32(16),	47.95(16),	35.9(3),	37.15(16),		
2M =	80.22(16),	4.18(18),	26.1(3),	3.89(16),	34.50(16),	63.80(17),	0.40(17),	47.95(16),	12.70(16),	7.69(16),		
3M =	64.63(18),	63.07(19),	8.38(19),	54.40(18),	4.37(19),							
C(5A)d-C(6A)d /	0M =	4.74(19),	8.05(18),	53.74(18),	4.74(19),	11.21(19),	6.33(19),	1.32(16),	72.48(18),	0.19(18),	2.38(17),	
1M =	4.27(18),	75.54(17),	14.3(2),	8.89(18),	6.01(18),	67.75(18),	25.38(18),	51.64(17),	32.0(3),	33.21(17),		
2M =	78.97(17),	0.56(19),	22.2(3),	0.19(18),	34.85(17),	67.75(18),	4.27(18),	51.64(17),	11.11(17),	5.83(17),		
3M =	61.1(2),	59.3(2),	4.7(2),	51.21(19),	0.5(2),							
-C(51A) /	0M =	47.09(17),	49.14(17),	9.33(17),	47.09(17),	6.16(18),	0.04(18),	2.86(15),	14.87(16),	36.86(16),	38.81(16),	
1M =	46.98(17),	14.86(16),	47.16(19),	45.48(16),	48.56(17),	47.11(17),	31.89(16),	66.18(16),	21.3(3),	24.01(16),		
2M =	18.97(16),	34.39(18),	30.7(3),	36.86(16),	39.31(16),	47.11(17),	46.98(17),	66.18(16),	7.20(16),	1.20(16),		
3M =	7.94(18),	4.92(18),	32.68(19),	5.80(18),	44.01(19),							
Cu(1)e-O(22B) /	0M =	46.71(10),	48.13(10),	4.45(10),	46.71(10),	8.25(10),	2.53(10),	0.26(5),	6.25(8),	36.39(8),	37.97(7),	
1M =	46.71(9),	6.48(7),	44.36(12),	43.81(8),	48.03(8),	38.42(10),	37.40(8),	57.64(8),	26.1(2),	29.81(8),		
2M =	10.56(7),	33.72(11),	34.9(2),	36.39(8),	38.79(7),	38.42(10),	46.71(9),	57.64(8),	9.38(8),	3.85(7),		
3M =	1.78(12),	1.33(12),	32.75(12),	1.01(12),	44.63(12),							
-O(7W)e /	0M =	35.01(10),	31.87(10),	81.52(10),	35.01(10),	48.47(10),	46.05(10),	41.64(5),	38.16(8),	42.59(8),	39.96(7),	
1M =	35.36(9),	44.05(7),	27.79(12),	32.68(8),	33.50(9),	26.27(10),	52.43(8),	19.12(8),	64.4(2),	58.74(8),		
2M =	42.73(8),	43.64(11),	55.9(2),	42.59(8),	46.20(7),	26.27(10),	35.36(9),	19.12(8),	47.77(8),	44.94(7),		
3M =	72.45(12),	72.07(12),	47.44(12),	83.96(12),	39.72(12),							
-O(11A) /	0M =	23.54(10),	20.23(10),	76.24(10),	23.54(10),	29.25(10),	26.39(10),	21.90(5),	57.74(8),	28.59(8),	26.03(7),	
1M =	23.99(9),	63.53(7),	14.16(12),	19.55(8),	22.23(8),	39.85(10),	51.29(8),	27.30(7),	59.9(2),	59.32(8),		
2M =	61.70(7),	28.84(11),	49.8(2),	28.59(8),	36.50(7),	39.85(10),	23.99(9),	27.30(7),	28.66(8),	25.34(7),		
3M =	87.04(12),	87.75(12),	33.05(12),	76.00(12),	28.75(12),							
-O(11B) /	0M =	23.22(10),	25.39(9),	10.40(9),	23.22(10),	36.11(10),	40.05(10),	44.76(5),	54.94(8),	26.00(8),	27.52(7),	
1M =	22.74(9),	48.98(6),	33.97(12),	29.55(8),	23.46(8),	44.46(9),	7.88(8),	28.71(7),	5.4(2),	11.86(7),		
2M =	49.30(7),	27.55(11),	0.3(2),	26.00(8),	11.15(7),	44.46(9),	22.74(9),	28.71(7),	36.39(7),	40.89(7),		
3M =	20.92(11),	21.29(11),	23.73(12),	9.30(11),	19.31(12),							
Cu(2)e-O(41A) /	0M =	52.30(10),	55.02(9),	0.23(9),	52.30(10),	34.93(10),	41.29(10),	45.97(4),	38.28(7),	51.62(7),	53.87(6),	

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	1M =	51.80(8),	33.53(6),	63.48(12),	58.29(8),	52.91(8),	53.08(9),	19.25(7),	48.05(7),	17.9(2),	13.40(7),
	2M =	36.33(7),	52.06(10),	26.0(2),	51.62(7),	0.21(6),	53.08(9),	51.80(8),	48.05(7),	34.40(7),	40.97(6),
	3M =	7.41(11),	6.23(11),	47.78(12),	2.84(11),	47.59(11),					
-O(42A) /	OM =	52.56(10),	53.90(10),	0.39(10),	52.56(10),	2.50(10),	3.14(10),	5.27(5),	5.17(8),	42.25(8),	43.79(7),
	1M =	52.57(9),	4.79(7),	49.77(12),	49.49(8),	53.87(8),	37.48(10),	42.00(8),	56.07(7),	31.0(2),	34.22(8),
	2M =	8.92(7),	39.57(11),	40.1(2),	42.25(8),	32.95(7),	37.48(10),	52.57(9),	56.07(7),	3.64(7),	1.79(7),
	3M =	2.35(12),	5.40(12),	38.64(12),	3.87(12),	50.52(12),					
-O(6W)e /	OM =	29.35(10),	26.19(10),	86.94(10),	29.35(10),	45.61(10),	42.48(10),	37.83(5),	42.41(8),	36.82(8),	34.19(7),
	1M =	29.70(9),	48.36(7),	22.02(12),	26.92(8),	27.85(9),	32.02(10),	48.66(8),	24.71(8),	60.3(2),	55.59(8),
	2M =	47.39(8),	37.86(11),	51.2(2),	36.82(8),	48.51(7),	32.02(10),	29.70(9),	24.71(8),	45.04(8),	41.51(7),
	3M =	76.26(12),	74.98(12),	41.67(12),	86.67(12),	34.12(12),					
-O(12A) /	OM =	24.67(10),	26.48(9),	3.62(9),	24.67(10),	43.20(10),	46.85(10),	51.41(5),	47.99(8),	28.77(8),	29.99(7),
	1M =	24.22(9),	42.05(6),	34.86(12),	30.98(8),	24.70(8),	37.91(9),	4.76(8),	23.19(7),	0.9(2),	7.92(7),
	2M =	42.16(7),	30.62(11),	3.8(2),	28.77(8),	18.26(7),	37.91(9),	24.22(9),	23.19(7),	43.53(7),	47.78(7),
	3M =	14.30(11),	14.86(11),	27.09(12),	2.71(11),	21.26(12),					
-O(12B) /	OM =	21.36(10),	18.06(10),	77.27(10),	21.36(10),	30.05(10),	26.86(10),	22.25(5),	57.87(8),	26.80(8),	24.22(7),
	1M =	21.80(9),	63.78(7),	12.23(12),	17.58(8),	20.01(8),	42.03(9),	48.45(8),	30.04(7),	57.4(2),	56.46(8),
	2M =	62.38(7),	27.18(11),	47.3(2),	26.80(8),	39.05(7),	42.03(9),	21.80(9),	30.04(7),	29.52(7),	25.89(7),
	3M =	87.65(12),	85.44(12),	31.36(12),	76.26(12),	26.54(12),					
Na(1)e-O(4W)e /	OM =	31.20(11),	28.64(11),	42.07(11),	31.20(11),	2.95(12),	3.21(12),	0.50(8),	51.77(10),	29.01(10),	27.51(9),
	1M =	31.70(10),	52.65(9),	20.09(13),	24.98(10),	30.72(10),	19.75(11),	62.78(10),	1.35(9),	57.4(3),	65.16(9),
	2M =	48.52(9),	27.33(12),	54.2(3),	29.01(10),	0.10(9),	19.75(11),	31.70(10),	1.35(9),	1.94(9),	1.67(9),
	3M =	50.60(13),	53.50(13),	30.95(13),	44.00(13),	35.50(13),					
-O(5W)e /	OM =	29.44(11),	32.52(11),	33.11(11),	29.44(11),	10.76(11),	4.30(11),	0.22(7),	42.37(9),	21.14(9),	23.69(9),
	1M =	29.10(10),	43.11(9),	35.46(13),	31.16(10),	30.95(10),	72.81(11),	5.21(9),	83.58(9),	3.9(3),	2.82(9),
	2M =	47.14(9),	19.57(12),	6.1(3),	21.14(9),	45.61(9),	72.81(11),	29.10(10),	83.58(9),	11.36(9),	4.75(9),
	3M =	34.48(13),	31.69(13),	16.27(13),	29.59(13),	24.75(13),					
-O(52A) /	OM =	49.65(10),	47.49(10),	35.50(10),	49.65(10),	9.15(10),	11.52(10),	10.26(5),	31.96(8),	45.21(8),	44.31(7),
	1M =	50.12(9),	33.57(7),	38.90(12),	43.32(8),	49.44(8),	0.54(9),	73.97(8),	16.90(7),	62.6(2),	69.44(7),
	2M =	29.46(7),	42.99(11),	65.9(2),	45.21(8),	5.59(7),	0.54(9),	50.12(9),	16.90(7),	7.96(7),	9.86(7),
	3M =	40.34(11),	43.49(11),	45.80(12),	38.53(11),	53.22(12),					
Na(2)e-O(52A) /	OM =	35.79(10),	35.13(10),	35.46(10),	35.79(10),	82.38(10),	84.43(10),	84.08(5),	8.73(8),	45.38(8),	44.55(7),
	1M =	35.63(9),	2.79(7),	39.43(12),	39.78(8),	34.73(8),	6.18(9),	21.39(8),	0.53(7),	30.1(2),	22.06(7),
	2M =	3.00(7),	48.18(11),	30.0(2),	45.38(8),	48.98(7),	6.18(9),	35.63(9),	0.53(7),	82.46(7),	86.04(7),
	3M =	24.61(11),	23.70(12),	47.39(12),	36.04(11),	36.01(12),					
-O(1W)e /	OM =	42.62(10),	40.87(10),	28.82(10),	42.62(10),	0.02(10),	2.37(10),	1.20(5),	33.00(8),	37.07(8),	36.42(7),
	1M =	43.05(9),	33.49(7),	32.42(12),	36.34(8),	42.64(8),	0.76(9),	64.91(8),	17.83(7),	53.9(2),	61.30(7),
	2M =	29.38(7),	34.70(11),	56.7(2),	37.07(8),	13.10(7),	0.76(9),	43.05(9),	17.83(7),	1.20(7),	0.71(7),
	3M =	35.05(12),	38.17(12),	37.23(12),	31.57(11),	45.60(12),					
-O(3W)e /	OM =	23.76(10),	26.90(9),	38.96(9),	23.76(10),	13.55(10),	7.20(10),	2.49(5),	47.00(8),	15.79(8),	18.37(7),
	1M =	23.41(9),	48.27(6),	30.32(12),	25.81(8),	25.26(8),	74.73(9),	0.93(8),	77.58(7),	10.0(2),	8.97(7),
	2M =	52.21(7),	14.35(11),	0.0(2),	15.79(8),	47.36(7),	74.73(9),	23.41(9),	77.58(7),	14.04(7),	7.50(7),
	3M =	40.61(11),	37.83(11),	10.91(12),	35.47(11),	18.98(12),					
-O(41A) /	OM =	45.54(10),	43.05(10),	41.30(10),	45.54(10),	10.71(10),	12.30(10),	10.44(5),	38.57(8),	42.61(8),	41.33(7),
	1M =	46.04(9),	40.45(7),	34.48(12),	39.28(8),	45.11(8),	7.46(9),	75.16(8),	9.82(7),	65.8(2),	73.55(7),
	2M =	36.36(7),	40.69(11),	66.3(2),	42.61(8),	0.50(7),	7.46(9),	46.04(9),	9.82(7),	9.57(7),	10.67(7),
	3M =	46.90(12),	50.05(12),	43.99(12),	44.13(11),	49.68(12),					
O(11A)-C(11A) /	OM =	13.10(16),	11.55(16),	44.00(16),	13.10(16),	67.13(16),	60.75(16),	57.02(13),	7.26(15),	23.43(15),	21.81(14),

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O(11B)-C(11B) /	1M =	13.10(15),	12.55(14),	13.95(17),	15.57(15),	11.76(15),	19.18(16),	11.50(15),	27.97(14),	23.1(3),	15.80(14),
	2M =	13.94(14),	26.09(16),	18.3(3),	23.43(15),	76.13(14),	19.18(16),	13.10(15),	27.97(14),	68.08(14),	61.66(14),
	3M =	33.91(17),	31.61(17),	26.96(17),	42.49(17),	14.99(17),					
	0M =	10.06(16),	11.16(16),	0.82(16),	10.06(16),	46.55(16),	47.18(16),	50.03(14),	39.09(15),	16.54(15),	17.04(15),
O(12A)-C(11A) /	1M =	9.68(16),	33.83(15),	18.89(18),	16.04(15),	9.72(15),	20.26(16),	14.09(15),	4.01(15),	6.9(3),	14.77(15),
	2M =	32.37(15),	18.93(17),	5.2(3),	16.54(15),	32.59(15),	20.26(16),	9.68(16),	4.01(15),	47.39(15),	48.67(15),
	3M =	10.10(17),	11.69(17),	16.31(18),	0.53(17),	7.75(17),					
	0M =	6.34(16),	7.84(16),	7.49(16),	6.34(16),	38.48(16),	39.52(16),	42.73(14),	46.82(15),	11.75(15),	12.57(15),
O(12B)-C(11B) /	1M =	5.92(16),	41.75(15),	16.02(18),	12.54(15),	6.20(15),	25.37(16),	20.28(15),	7.91(15),	14.0(3),	21.70(15),
	2M =	40.05(15),	13.95(17),	11.4(3),	11.75(15),	25.19(15),	25.37(16),	5.93(16),	7.91(15),	39.28(15),	40.95(15),
	3M =	18.41(17),	19.99(17),	10.94(18),	7.75(17),	3.46(17),					
	0M =	12.16(16),	10.30(16),	48.98(16),	12.16(16),	63.95(16),	57.43(16),	53.20(13),	13.34(15),	22.48(15),	20.63(14),
O(21A)-C(21A) /	1M =	12.21(15),	18.60(14),	11.83(17),	13.98(15),	10.74(15),	24.62(16),	14.08(15),	32.16(14),	26.0(3),	19.03(15),
	2M =	20.02(14),	25.03(16),	20.2(3),	22.48(15),	80.54(14),	24.62(16),	12.21(15),	32.16(14),	64.70(14),	58.08(14),
	3M =	39.24(17),	36.80(17),	26.38(17),	47.17(17),	14.56(17),					
	0M =	4.24(16),	3.00(16),	7.68(16),	4.24(16),	34.90(16),	34.37(16),	36.60(13),	41.24(15),	2.08(15),	2.61(14),
O(21B)-C(21B) /	1M =	4.62(15),	37.11(14),	4.95(17),	1.83(15),	4.51(15),	15.70(16),	28.07(15),	2.59(14),	20.0(3),	28.03(15),
	2M =	34.57(14),	4.48(16),	19.2(3),	2.08(15),	29.84(14),	15.70(16),	4.62(15),	2.59(14),	35.90(14),	35.96(14),
	3M =	18.12(17),	20.25(17),	1.89(17),	8.67(17),	6.67(17),					
	0M =	35.97(16),	38.71(16),	11.93(16),	35.97(16),	29.54(16),	35.10(16),	40.15(14),	53.66(15),	35.77(15),	37.89(15),
O(22A)-C(21A) /	1M =	35.46(16),	48.43(15),	47.14(18),	41.97(15),	36.59(15),	58.62(16),	2.94(15),	45.82(15),	2.2(3),	2.74(15),
	2M =	50.66(15),	36.51(17),	9.9(3),	35.77(15),	1.54(15),	58.62(16),	35.46(16),	45.82(15),	29.39(15),	35.34(15),
	3M =	20.86(17),	20.17(17),	32.27(18),	9.82(17),	31.27(17),					
	0M =	34.93(16),	37.85(16),	15.90(16),	34.93(16),	24.70(16),	30.34(16),	35.38(14),	56.20(15),	33.70(15),	35.96(15),
O(22B)-C(21B) /	1M =	34.42(16),	51.35(15),	46.03(18),	40.67(15),	35.70(15),	63.58(16),	1.73(15),	50.19(15),	0.0(3),	4.40(15),
	2M =	53.94(15),	34.18(17),	8.2(3),	33.70(15),	6.50(15),	63.58(16),	34.42(16),	50.19(15),	24.52(15),	30.54(15),
	3M =	24.44(17),	23.54(17),	29.90(18),	13.63(17),	30.02(17),					
	0M =	6.36(16),	5.28(16),	5.93(16),	6.36(16),	35.23(16),	34.19(16),	36.06(13),	37.97(15),	0.40(15),	0.78(14),
O(41A)-C(41A) /	1M =	6.73(15),	34.02(14),	2.49(17),	0.40(15),	6.72(15),	12.01(16),	28.70(15),	6.30(14),	20.0(3),	28.07(14),
	2M =	31.35(14),	2.88(16),	19.9(3),	0.40(15),	32.58(14),	12.01(16),	6.73(15),	6.30(14),	36.29(14),	35.81(14),
	3M =	16.16(17),	18.42(17),	0.50(17),	7.11(17),	8.53(17),					
	0M =	0.59(16),	0.89(16),	10.31(16),	0.59(16),	34.20(16),	34.51(16),	37.30(14),	46.35(15),	4.98(15),	5.73(15),
O(42A)-C(41A) /	1M =	1.01(16),	41.89(15),	9.07(18),	5.60(15),	0.74(15),	21.68(16),	26.59(15),	3.46(15),	19.6(3),	27.49(15),
	2M =	39.61(15),	7.22(17),	17.7(3),	4.98(15),	25.38(15),	21.68(16),	1.01(16),	3.46(15),	35.11(15),	36.02(15),
	3M =	21.03(17),	22.92(17),	4.33(18),	10.95(17),	3.42(17),					
	0M =	0.70(16),	0.97(16),	39.95(16),	0.70(16),	54.48(16),	48.16(16),	44.65(13),	10.55(15),	11.04(15),	9.33(14),
O(51A)-C(51A) /	1M =	0.73(15),	15.11(14),	1.27(17),	2.96(15),	0.67(15),	28.15(16),	2.62(15),	39.37(14),	14.6(3),	8.00(15),
	2M =	17.32(14),	13.66(16),	8.4(3),	11.04(15),	81.95(14),	28.15(16),	0.73(15),	39.37(14),	55.46(14),	49.14(14),
	3M =	31.37(17),	28.61(17),	14.76(17),	37.62(17),	2.86(17),					
	0M =	39.60(16),	41.94(16),	3.37(16),	39.60(16),	38.64(16),	44.22(16),	49.26(13),	46.34(15),	41.21(15),	43.03(14),
O(52A)-C(51A) /	1M =	39.11(15),	40.77(14),	50.54(17),	45.87(15),	39.95(15),	49.92(16),	7.50(15),	38.91(14),	8.3(3),	2.63(15),
	2M =	42.59(14),	42.37(16),	15.1(3),	41.21(15),	6.96(14),	49.92(16),	39.11(15),	38.91(14),	38.47(14),	44.46(14),
	3M =	12.69(17),	12.23(17),	38.28(17),	1.42(17),	35.39(17),					
	0M =	5.37(16),	4.80(16),	2.56(16),	5.37(16),	41.28(16),	39.25(16),	40.28(14),	29.10(15),	2.53(15),	2.50(15),
C(1A)e-C(2A)e /	1M =	5.68(16),	25.02(15),	2.29(18),	0.17(15),	5.96(15),	4.51(16),	23.66(15),	13.08(15),	13.9(3),	21.93(15),
	2M =	22.43(15),	5.17(17),	15.2(3),	2.53(15),	41.65(15),	4.51(16),	5.68(16),	13.08(15),	42.43(15),	40.91(15),
	3M =	7.45(17),	9.82(17),	3.37(18),	1.17(17),	6.77(17),					
	0M =	36.23(18),	34.09(18),	34.20(18),	36.23(18),	0.25(18),	1.12(18),	0.81(16),	42.27(17),	32.14(17),	31.09(17),

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	1M =	36.70(18),	42.69(17),	25.5(2),	29.90(18),	36.02(18),	10.02(18),	63.91(17),	8.64(17),	55.1(3),	63.07(17),
	2M =	38.58(17),	30.06(19),	55.0(3),	32.14(17),	8.10(17),	10.02(18),	36.70(18),	8.64(17),	1.37(17),	0.50(17),
	3M =	41.71(19),	44.74(19),	33.1(2),	36.56(19),	39.87(19),					
-C(6A)e /	0M =	41.19(19),	43.31(18),	14.86(18),	41.19(19),	11.54(19),	5.32(19),	2.21(16),	17.10(17),	31.00(17),	32.99(17),
	1M =	41.07(18),	17.68(17),	41.7(2),	39.77(18),	42.67(18),	48.85(18),	26.67(18),	68.26(17),	15.8(3),	18.89(17),
	2M =	21.71(17),	28.56(19),	25.1(3),	31.00(17),	45.15(17),	48.85(18),	41.07(18),	68.26(17),	12.55(17),	6.41(17),
	3M =	12.94(19),	9.86(19),	26.8(2),	11.35(19),	38.1(2),					
-C(11A) /	0M =	1.99(17),	1.32(17),	59.38(17),	1.99(17),	14.89(18),	10.46(18),	5.53(15),	72.61(16),	6.78(16),	4.22(16),
	1M =	2.45(17),	77.57(16),	7.63(19),	2.21(16),	0.73(17),	61.05(17),	31.98(16),	45.68(16),	38.7(3),	39.85(16),
	2M =	79.25(16),	7.07(18),	28.9(3),	6.78(16),	35.12(16),	61.05(17),	2.45(17),	45.68(16),	14.67(16),	9.81(16),
	3M =	67.50(18),	65.95(18),	11.27(19),	57.14(18),	7.23(19),					
C(1B)e-C(2B)e /	0M =	36.09(18),	34.03(18),	32.84(18),	36.09(18),	1.29(18),	0.19(18),	1.66(16),	41.42(17),	31.74(17),	30.76(17),
	1M =	36.56(18),	41.69(17),	25.5(2),	29.76(18),	35.93(18),	9.13(18),	63.09(17),	9.62(17),	54.0(3),	61.97(17),
	2M =	37.59(17),	29.61(19),	54.3(3),	31.74(17),	9.45(17),	9.13(18),	36.56(18),	9.62(17),	2.42(17),	1.45(17),
	3M =	40.35(19),	43.38(19),	32.6(2),	35.22(19),	39.62(19),					
-C(11B) /	0M =	1.87(17),	5.14(17),	53.02(17),	1.87(17),	8.10(17),	3.71(17),	1.22(15),	78.64(16),	2.06(16),	0.43(16),
	1M =	1.38(17),	82.13(16),	11.98(19),	6.50(16),	3.04(16),	63.36(17),	29.51(16),	45.92(16),	34.9(3),	37.09(16),
	2M =	85.39(16),	2.12(18),	25.4(3),	2.06(16),	29.26(16),	63.36(17),	1.38(17),	45.92(16),	7.87(16),	3.04(16),
	3M =	61.92(18),	60.86(18),	6.37(19),	51.01(18),	3.37(18),					
C(2A)e-C(3A)e /	0M =	4.49(19),	7.80(18),	54.22(18),	4.49(19),	11.81(19),	6.92(19),	1.91(16),	71.95(17),	0.53(17),	2.05(17),
	1M =	4.03(18),	75.15(17),	14.0(2),	8.59(18),	5.77(18),	67.60(18),	25.48(17),	51.74(17),	32.2(3),	33.33(17),
	2M =	78.49(17),	0.92(19),	22.4(3),	0.53(17),	35.44(17),	67.60(18),	4.03(18),	51.74(17),	11.71(17),	6.43(17),
	3M =	61.41(19),	59.65(19),	5.1(2),	51.66(19),	0.7(2),					
-C(21A) /	0M =	43.73(17),	45.69(17),	11.32(17),	43.73(17),	9.83(18),	3.73(18),	0.86(15),	14.02(16),	33.46(16),	35.35(16),
	1M =	43.64(17),	14.40(16),	43.49(19),	41.92(17),	45.18(17),	46.00(17),	30.28(16),	65.37(16),	19.3(3),	22.52(16),
	2M =	18.47(16),	30.95(18),	28.5(3),	33.46(16),	42.69(16),	46.00(17),	43.64(17),	65.37(16),	10.88(16),	4.89(16),
	3M =	9.30(18),	6.22(18),	29.36(19),	7.82(18),	40.84(19),					
C(2B)e-C(6B)e /	0M =	8.02(19),	11.30(18),	48.31(18),	8.02(19),	5.06(19),	0.24(19),	4.77(16),	76.52(18),	3.89(17),	6.41(17),
	1M =	7.54(18),	77.47(17),	18.1(2),	12.58(18),	9.20(18),	69.30(18),	23.34(18),	51.19(17),	28.8(3),	30.90(17),
	2M =	81.59(17),	3.74(19),	19.3(3),	3.89(17),	29.20(17),	69.30(18),	7.54(18),	51.19(17),	4.94(17),	0.29(17),
	3M =	56.47(19),	55.15(19),	0.5(2),	46.00(19),	2.8(2),					
-C(21B) /	0M =	48.22(17),	50.35(17),	8.89(17),	48.22(17),	4.76(17),	1.38(17),	4.32(15),	15.62(16),	38.03(16),	40.02(16),
	1M =	48.10(17),	15.46(16),	48.55(19),	46.76(16),	49.70(17),	47.91(17),	32.11(16),	66.79(16),	21.7(3),	24.18(16),
	2M =	19.58(16),	35.60(18),	31.2(3),	38.03(16),	38.12(16),	47.91(17),	48.10(17),	66.79(16),	5.80(16),	0.24(16),
	3M =	7.80(18),	4.80(18),	33.80(19),	5.35(18),	45.03(18),					
C(3A)e-C(4A)e /	0M =	41.25(19),	43.36(18),	14.63(18),	41.25(19),	11.57(19),	5.37(19),	2.28(17),	16.76(18),	31.05(18),	33.03(17),
	1M =	41.14(18),	17.34(17),	41.7(2),	39.79(18),	42.73(18),	48.51(18),	26.92(18),	67.93(17),	16.0(3),	19.15(17),
	2M =	21.37(17),	28.61(19),	25.3(3),	31.05(18),	45.11(17),	48.51(18),	41.14(18),	67.93(17),	12.59(17),	6.47(17),
	3M =	12.7(2),	9.6(2),	26.8(2),	11.1(2),	38.2(2),					
C(4A)e-C(5A)e /	0M =	36.77(18),	34.61(18),	34.66(18),	36.77(18),	0.39(19),	1.78(19),	0.15(16),	42.13(17),	32.75(17),	31.69(17),
	1M =	37.25(18),	42.64(17),	26.0(2),	30.44(18),	36.56(18),	9.91(18),	64.56(17),	8.69(17),	55.7(3),	63.71(17),
	2M =	38.52(17),	30.67(19),	55.7(3),	32.75(17),	7.64(17),	9.91(18),	37.25(18),	8.69(17),	0.73(17),	0.15(17),
	3M =	42.08(19),	45.12(19),	33.8(2),	37.05(19),	40.44(19),					
-C(41A) /	0M =	0.87(18),	4.18(17),	56.74(17),	0.87(18),	12.88(18),	8.29(18),	3.31(15),	73.44(16),	3.89(16),	1.33(16),
	1M =	0.40(17),	77.64(16),	10.51(19),	5.09(17),	2.13(17),	63.80(17),	29.32(16),	47.95(16),	35.9(3),	37.15(16),
	2M =	80.22(16),	4.18(18),	26.1(3),	3.89(16),	34.50(16),	63.80(17),	0.40(17),	47.95(16),	12.70(16),	7.69(16),
	3M =	64.63(18),	63.07(19),	8.38(19),	54.40(18),	4.37(19),					
C(5A)e-C(6A)e /	0M =	4.74(19),	8.05(18),	53.74(18),	4.74(19),	11.21(19),	6.33(19),	1.32(16),	72.48(18),	0.19(18),	2.38(17),

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	1M =	4.27(18),	75.54(17),	14.3(2),	8.89(18),	6.01(18),	67.75(18),	25.38(18),	51.64(17),	32.0(3),	33.21(17),
	2M =	78.97(17),	0.56(19),	22.2(3),	0.19(18),	34.85(17),	67.75(18),	4.27(18),	51.64(17),	11.11(17),	5.83(17),
	3M =	61.1(2),	59.3(2),	4.7(2),	51.21(19),	0.5(2),					
-C(51A) /	0M =	47.09(17),	49.14(17),	9.33(17),	47.09(17),	6.16(18),	0.04(18),	2.86(15),	14.87(16),	36.86(16),	38.81(16),
	1M =	46.98(17),	14.86(16),	47.16(19),	45.48(16),	48.56(17),	47.11(17),	31.89(16),	66.18(16),	21.3(3),	24.01(16),
	2M =	18.97(16),	34.39(18),	30.7(3),	36.86(16),	39.31(16),	47.11(17),	46.98(17),	66.18(16),	7.20(16),	1.20(16),
	3M =	7.94(18),	4.92(18),	32.68(19),	5.80(18),	44.01(19),					
Cu(1)f-O(22B) /	0M =	46.71(10),	48.13(10),	4.45(10),	46.71(10),	8.25(10),	2.53(10),	0.26(5),	6.25(8),	36.39(8),	37.97(7),
	1M =	46.71(9),	6.48(7),	44.36(12),	43.81(8),	48.03(8),	38.42(10),	37.40(8),	57.64(8),	26.1(2),	29.81(8),
	2M =	10.56(7),	33.72(11),	34.9(2),	36.39(8),	38.79(7),	38.42(10),	46.71(9),	57.64(8),	9.38(8),	3.85(7),
	3M =	1.78(12),	1.33(12),	32.75(12),	1.01(12),	44.63(12),					
-O(7W)f /	0M =	35.01(10),	31.87(10),	81.52(10),	35.01(10),	48.47(10),	46.05(10),	41.64(5),	38.16(8),	42.59(8),	39.96(7),
	1M =	35.36(9),	44.05(7),	27.79(12),	32.68(8),	33.50(9),	26.27(10),	52.43(8),	19.12(8),	64.4(2),	58.74(8),
	2M =	42.73(8),	43.64(11),	55.9(2),	42.59(8),	46.20(7),	26.27(10),	35.36(9),	19.12(8),	47.77(8),	44.94(7),
	3M =	72.45(12),	72.07(12),	47.44(12),	83.96(12),	39.72(12),					
-O(11A) /	0M =	23.54(10),	20.23(10),	76.24(10),	23.54(10),	29.25(10),	26.39(10),	21.90(5),	57.74(8),	28.59(8),	26.03(7),
	1M =	23.99(9),	63.53(7),	14.16(12),	19.55(8),	22.23(8),	39.85(10),	51.29(8),	27.30(7),	59.9(2),	59.32(8),
	2M =	61.70(7),	28.84(11),	49.8(2),	28.59(8),	36.50(7),	39.85(10),	23.99(9),	27.30(7),	28.66(8),	25.34(7),
	3M =	87.04(12),	87.75(12),	33.05(12),	76.00(12),	28.75(12),					
-O(11B) /	0M =	23.22(10),	25.39(9),	10.40(9),	23.22(10),	36.11(10),	40.05(10),	44.76(5),	54.94(8),	26.00(8),	27.52(7),
	1M =	22.74(9),	48.98(6),	33.97(12),	29.55(8),	23.46(8),	44.46(9),	7.88(8),	28.71(7),	5.4(2),	11.86(7),
	2M =	49.30(7),	27.55(11),	0.3(2),	26.00(8),	11.15(7),	44.46(9),	22.74(9),	28.71(7),	36.39(7),	40.89(7),
	3M =	20.92(11),	21.29(11),	23.73(12),	9.30(11),	19.31(12),					
Cu(2)f-O(6W)f /	0M =	29.35(10),	26.19(10),	86.94(10),	29.35(10),	45.61(10),	42.48(10),	37.83(5),	42.41(8),	36.82(8),	34.19(7),
	1M =	29.70(9),	48.36(7),	22.02(12),	26.92(8),	27.85(9),	32.02(10),	48.66(8),	24.71(8),	60.3(2),	55.59(8),
	2M =	47.39(8),	37.86(11),	51.2(2),	36.82(8),	48.51(7),	32.02(10),	29.70(9),	24.71(8),	45.04(8),	41.51(7),
	3M =	76.26(12),	74.98(12),	41.67(12),	86.67(12),	34.12(12),					
-O(12A) /	0M =	24.67(10),	26.48(9),	3.62(9),	24.67(10),	43.20(10),	46.85(10),	51.41(5),	47.99(8),	28.77(8),	29.99(7),
	1M =	24.22(9),	42.05(6),	34.86(12),	30.98(8),	24.70(8),	37.91(9),	4.76(8),	23.19(7),	0.9(2),	7.92(7),
	2M =	42.16(7),	30.62(11),	3.8(2),	28.77(8),	18.26(7),	37.91(9),	24.22(9),	23.19(7),	43.53(7),	47.78(7),
	3M =	14.30(11),	14.86(11),	27.09(12),	2.71(11),	21.26(12),					
-O(12B) /	0M =	21.36(10),	18.06(10),	77.27(10),	21.36(10),	30.05(10),	26.86(10),	22.25(5),	57.87(8),	26.80(8),	24.22(7),
	1M =	21.80(9),	63.78(7),	12.23(12),	17.58(8),	20.01(8),	42.03(9),	48.45(8),	30.04(7),	57.4(2),	56.46(8),
	2M =	62.38(7),	27.18(11),	47.3(2),	26.80(8),	39.05(7),	42.03(9),	21.80(9),	30.04(7),	29.52(7),	25.89(7),
	3M =	87.65(12),	85.44(12),	31.36(12),	76.26(12),	26.54(12),					
Na(1)f-O(4W)f /	0M =	31.20(11),	28.64(11),	42.07(11),	31.20(11),	2.95(12),	3.21(12),	0.50(8),	51.77(10),	29.01(10),	27.51(9),
	1M =	31.70(10),	52.65(9),	20.09(13),	24.98(10),	30.72(10),	19.75(11),	62.78(10),	1.35(9),	57.4(3),	65.16(9),
	2M =	48.52(9),	27.33(12),	54.2(3),	29.01(10),	0.10(9),	19.75(11),	31.70(10),	1.35(9),	1.94(9),	1.67(9),
	3M =	50.60(13),	53.50(13),	30.95(13),	44.00(13),	35.50(13),					
-O(5W)f /	0M =	29.44(11),	32.52(11),	33.11(11),	29.44(11),	10.76(11),	4.30(11),	0.22(7),	42.37(9),	21.14(9),	23.69(9),
	1M =	29.10(10),	43.11(9),	35.46(13),	31.16(10),	30.95(10),	72.81(11),	5.21(9),	83.58(9),	3.9(3),	2.82(9),
	2M =	47.14(9),	19.57(12),	6.1(3),	21.14(9),	45.61(9),	72.81(11),	29.10(10),	83.58(9),	11.36(9),	4.75(9),
	3M =	34.48(13),	31.69(13),	16.27(13),	29.59(13),	24.75(13),					
-O(52A) /	0M =	49.65(10),	47.49(10),	35.50(10),	49.65(10),	9.15(10),	11.52(10),	10.26(5),	31.96(8),	45.21(8),	44.31(7),
	1M =	50.12(9),	33.57(7),	38.90(12),	43.32(8),	49.44(8),	0.54(9),	73.97(8),	16.90(7),	62.6(2),	69.44(7),
	2M =	29.46(7),	42.99(11),	65.9(2),	45.21(8),	5.59(7),	0.54(9),	50.12(9),	16.90(7),	7.96(7),	9.86(7),
	3M =	40.34(11),	43.49(11),	45.80(12),	38.53(11),	53.22(12),					
Na(2)f-O(22A) /	0M =	26.64(10),	29.95(10),	34.55(10),	26.64(10),	0.48(10),	5.56(10),	10.49(5),	57.94(8),	20.84(8),	23.46(7),

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	1M =	26.19(9),	57.13(7),	35.59(12),	30.35(8),	27.96(8),	89.60(9),	3.24(8),	70.27(7),	9.9(2),	11.02(7),
	2M =	61.24(7),	20.09(11),	0.0(2),	20.84(8),	32.52(7),	89.60(9),	26.19(9),	70.27(7),	0.79(7),	5.52(7),
	3M =	39.77(11),	37.66(11),	16.10(12),	31.46(11),	21.43(12),					
-O(12B) /	0M =	8.89(10),	8.08(9),	30.08(9),	8.89(10),	63.61(10),	58.79(10),	57.01(5),	6.00(8),	18.78(7),	17.72(7),
	1M =	8.77(8),	0.94(6),	12.43(12),	12.69(8),	7.77(8),	9.95(9),	0.62(8),	22.31(7),	11.6(2),	3.90(7),
	2M =	0.75(7),	21.57(10),	8.2(2),	18.78(7),	65.67(7),	9.95(9),	8.77(8),	22.31(7),	64.84(7),	60.25(6),
	3M =	19.85(11),	17.61(11),	21.37(12),	28.75(11),	9.58(11),					
-O(52A) /	0M =	35.79(10),	35.13(10),	35.46(10),	35.79(10),	82.38(10),	84.43(10),	84.08(5),	8.73(8),	45.38(8),	44.55(7),
	1M =	35.63(9),	2.79(7),	39.43(12),	39.78(8),	34.73(8),	6.18(9),	21.39(8),	0.53(7),	30.1(2),	22.06(7),
	2M =	3.00(7),	48.18(11),	30.0(2),	45.38(8),	48.98(7),	6.18(9),	35.63(9),	0.53(7),	82.46(7),	86.04(7),
	3M =	24.61(11),	23.70(12),	47.39(12),	36.04(11),	36.01(12),					
-O(1W)f /	0M =	42.62(10),	40.87(10),	28.82(10),	42.62(10),	0.02(10),	2.37(10),	1.20(5),	33.00(8),	37.07(8),	36.42(7),
	1M =	43.05(9),	33.49(7),	32.42(12),	36.34(8),	42.64(8),	0.76(9),	64.91(8),	17.83(7),	53.9(2),	61.30(7),
	2M =	29.38(7),	34.70(11),	56.7(2),	37.07(8),	13.10(7),	0.76(9),	43.05(9),	17.83(7),	1.20(7),	0.71(7),
	3M =	35.05(12),	38.17(12),	37.23(12),	31.57(11),	45.60(12),					
-O(3W)f /	0M =	23.76(10),	26.90(9),	38.96(9),	23.76(10),	13.55(10),	7.20(10),	2.49(5),	47.00(8),	15.79(8),	18.37(7),
	1M =	23.41(9),	48.27(6),	30.32(12),	25.81(8),	25.26(8),	74.73(9),	0.93(8),	77.58(7),	10.0(2),	8.97(7),
	2M =	52.21(7),	14.35(11),	0.0(2),	15.79(8),	47.36(7),	74.73(9),	23.41(9),	77.58(7),	14.04(7),	7.50(7),
	3M =	40.61(11),	37.83(11),	10.91(12),	35.47(11),	18.98(12),					
-O(41A) /	0M =	45.54(10),	43.05(10),	41.30(10),	45.54(10),	10.71(10),	12.30(10),	10.44(5),	38.57(8),	42.61(8),	41.33(7),
	1M =	46.04(9),	40.45(7),	34.48(12),	39.28(8),	45.11(8),	7.46(9),	75.16(8),	9.82(7),	65.8(2),	73.55(7),
	2M =	36.36(7),	40.69(11),	66.3(2),	42.61(8),	0.50(7),	7.46(9),	46.04(9),	9.82(7),	9.57(7),	10.67(7),
	3M =	46.90(12),	50.05(12),	43.99(12),	44.13(11),	49.68(12),					
O(11A)-C(11A) /	0M =	13.10(16),	11.55(16),	44.00(16),	13.10(16),	67.13(16),	60.75(16),	57.02(13),	7.26(15),	23.43(15),	21.81(14),
	1M =	13.10(15),	12.55(14),	13.95(17),	15.57(15),	11.76(15),	19.18(16),	11.50(15),	27.97(14),	23.1(3),	15.80(14),
	2M =	13.94(14),	26.09(16),	18.3(3),	23.43(15),	76.13(14),	19.18(16),	13.10(15),	27.97(14),	68.08(14),	61.66(14),
	3M =	33.91(17),	31.61(17),	26.96(17),	42.49(17),	14.99(17),					
O(11B)-C(11B) /	0M =	10.06(16),	11.16(16),	0.82(16),	10.06(16),	46.55(16),	47.18(16),	50.03(14),	39.09(15),	16.54(15),	17.04(15),
	1M =	9.68(16),	33.83(15),	18.89(18),	16.04(15),	9.72(15),	20.26(16),	14.09(15),	4.01(15),	6.9(3),	14.77(15),
	2M =	32.37(15),	18.93(17),	5.2(3),	16.54(15),	32.59(15),	20.26(16),	9.68(16),	4.01(15),	47.39(15),	48.67(15),
	3M =	10.10(17),	11.69(17),	16.31(18),	0.53(17),	7.75(17),					
O(12A)-C(11A) /	0M =	6.34(16),	7.84(16),	7.49(16),	6.34(16),	38.48(16),	39.52(16),	42.73(14),	46.82(15),	11.75(15),	12.57(15),
	1M =	5.92(16),	41.75(15),	16.02(18),	12.54(15),	6.20(15),	25.37(16),	20.28(15),	7.91(15),	14.0(3),	21.70(15),
	2M =	40.05(15),	13.95(17),	11.4(3),	11.75(15),	25.19(15),	25.37(16),	5.93(16),	7.91(15),	39.28(15),	40.95(15),
	3M =	18.41(17),	19.99(17),	10.94(18),	7.75(17),	3.46(17),					
O(12B)-C(11B) /	0M =	12.16(16),	10.30(16),	48.98(16),	12.16(16),	63.95(16),	57.43(16),	53.20(13),	13.34(15),	22.48(15),	20.63(14),
	1M =	12.21(15),	18.60(14),	11.83(17),	13.98(15),	10.74(15),	24.62(16),	14.08(15),	32.16(14),	26.0(3),	19.03(15),
	2M =	20.02(14),	25.03(16),	20.2(3),	22.48(15),	80.54(14),	24.62(16),	12.21(15),	32.16(14),	64.70(14),	58.08(14),
	3M =	39.24(17),	36.80(17),	26.38(17),	47.17(17),	14.56(17),					
O(21A)-C(21A) /	0M =	4.24(16),	3.00(16),	7.68(16),	4.24(16),	34.90(16),	34.37(16),	36.60(13),	41.24(15),	2.08(15),	2.61(14),
	1M =	4.62(15),	37.11(14),	4.95(17),	1.83(15),	4.51(15),	15.70(16),	28.07(15),	2.59(14),	20.0(3),	28.03(15),
	2M =	34.57(14),	4.48(16),	19.2(3),	2.08(15),	29.84(14),	15.70(16),	4.62(15),	2.59(14),	35.90(14),	35.96(14),
	3M =	18.12(17),	20.25(17),	1.89(17),	8.67(17),	6.67(17),					
O(21B)-C(21B) /	0M =	35.97(16),	38.71(16),	11.93(16),	35.97(16),	29.54(16),	35.10(16),	40.15(14),	53.66(15),	35.77(15),	37.89(15),
	1M =	35.46(16),	48.43(15),	47.14(18),	41.97(15),	36.59(15),	58.62(16),	2.94(15),	45.82(15),	2.2(3),	2.74(15),
	2M =	50.66(15),	36.51(17),	9.9(3),	35.77(15),	1.54(15),	58.62(16),	35.46(16),	45.82(15),	29.39(15),	35.34(15),
	3M =	20.86(17),	20.17(17),	32.27(18),	9.82(17),	31.27(17),					
O(22A)-C(21A) /	0M =	34.93(16),	37.85(16),	15.90(16),	34.93(16),	24.70(16),	30.34(16),	35.38(14),	56.20(15),	33.70(15),	35.96(15),

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O(22B)-C(21B) /	1M =	34.42(16),	51.35(15),	46.03(18),	40.67(15),	35.70(15),	63.58(16),	1.73(15),	50.19(15),	0.0(3),	4.40(15),
	2M =	53.94(15),	34.18(17),	8.2(3),	33.70(15),	6.50(15),	63.58(16),	34.42(16),	50.19(15),	24.52(15),	30.54(15),
	3M =	24.44(17),	23.54(17),	29.90(18),	13.63(17),	30.02(17),					
	0M =	6.36(16),	5.28(16),	5.93(16),	6.36(16),	35.23(16),	34.19(16),	36.06(13),	37.97(15),	0.40(15),	0.78(14),
O(41A)-C(41A) /	1M =	6.73(15),	34.02(14),	2.49(17),	0.40(15),	6.72(15),	12.01(16),	28.70(15),	6.30(14),	20.0(3),	28.07(14),
	2M =	31.35(14),	2.88(16),	19.9(3),	0.40(15),	32.58(14),	12.01(16),	6.73(15),	6.30(14),	36.29(14),	35.81(14),
	3M =	16.16(17),	18.42(17),	0.50(17),	7.11(17),	8.53(17),					
	0M =	0.59(16),	0.89(16),	10.31(16),	0.59(16),	34.20(16),	34.51(16),	37.30(14),	46.35(15),	4.98(15),	5.73(15),
O(42A)-C(41A) /	1M =	1.01(16),	41.89(15),	9.07(18),	5.60(15),	0.74(15),	21.68(16),	26.59(15),	3.46(15),	19.6(3),	27.49(15),
	2M =	39.61(15),	7.22(17),	17.7(3),	4.98(15),	25.38(15),	21.68(16),	1.01(16),	3.46(15),	35.11(15),	36.02(15),
	3M =	21.03(17),	22.92(17),	4.33(18),	10.95(17),	3.42(17),					
	0M =	0.70(16),	0.97(16),	39.95(16),	0.70(16),	54.48(16),	48.16(16),	44.65(13),	10.55(15),	11.04(15),	9.33(14),
O(51A)-C(51A) /	1M =	0.73(15),	15.11(14),	1.27(17),	2.96(15),	0.67(15),	28.15(16),	2.62(15),	39.37(14),	14.6(3),	8.00(15),
	2M =	17.32(14),	13.66(16),	8.4(3),	11.04(15),	81.95(14),	28.15(16),	0.73(15),	39.37(14),	55.46(14),	49.14(14),
	3M =	31.37(17),	28.61(17),	14.76(17),	37.62(17),	2.86(17),					
	0M =	39.60(16),	41.94(16),	3.37(16),	39.60(16),	38.64(16),	44.22(16),	49.26(13),	46.34(15),	41.21(15),	43.03(14),
O(52A)-C(51A) /	1M =	39.11(15),	40.77(14),	50.54(17),	45.87(15),	39.95(15),	49.92(16),	7.50(15),	38.91(14),	8.3(3),	2.63(15),
	2M =	42.59(14),	42.37(16),	15.1(3),	41.21(15),	6.96(14),	49.92(16),	39.11(15),	38.91(14),	38.47(14),	44.46(14),
	3M =	12.69(17),	12.23(17),	38.28(17),	1.42(17),	35.39(17),					
	0M =	5.37(16),	4.80(16),	2.56(16),	5.37(16),	41.28(16),	39.25(16),	40.28(14),	29.10(15),	2.53(15),	2.50(15),
C(1A)f-C(2A)f /	1M =	5.68(16),	25.02(15),	2.29(18),	0.17(15),	5.96(15),	4.51(16),	23.66(15),	13.08(15),	13.9(3),	21.93(15),
	2M =	22.43(15),	5.17(17),	15.2(3),	2.53(15),	41.65(15),	4.51(16),	5.68(16),	13.08(15),	42.43(15),	40.91(15),
	3M =	7.45(17),	9.82(17),	3.37(18),	1.17(17),	6.77(17),					
	0M =	36.23(18),	34.09(18),	34.20(18),	36.23(18),	0.25(18),	1.12(18),	0.81(16),	42.27(17),	32.14(17),	31.09(17),
-C(6A)f /	1M =	36.70(18),	42.69(17),	25.5(2),	29.90(18),	36.02(18),	10.02(18),	63.91(17),	8.64(17),	55.1(3),	63.07(17),
	2M =	38.58(17),	30.06(19),	55.0(3),	32.14(17),	8.10(17),	10.02(18),	36.70(18),	8.64(17),	1.37(17),	0.50(17),
	3M =	41.71(19),	44.74(19),	33.1(2),	36.56(19),	39.87(19),					
	0M =	41.19(19),	43.31(18),	14.86(18),	41.19(19),	11.54(19),	5.32(19),	2.21(16),	17.10(17),	31.00(17),	32.99(17),
-C(11A) /	1M =	41.07(18),	17.68(17),	41.7(2),	39.77(18),	42.67(18),	48.85(18),	26.67(18),	68.26(17),	15.8(3),	18.89(17),
	2M =	21.71(17),	28.56(19),	25.1(3),	31.00(17),	45.15(17),	48.85(18),	41.07(18),	68.26(17),	12.55(17),	6.41(17),
	3M =	12.94(19),	9.86(19),	26.8(2),	11.35(19),	38.1(2),					
	0M =	1.99(17),	1.32(17),	59.38(17),	1.99(17),	14.89(18),	10.46(18),	5.53(15),	72.61(16),	6.78(16),	4.22(16),
C(1B)f-C(2B)f /	1M =	2.45(17),	77.57(16),	7.63(19),	2.21(16),	0.73(17),	61.05(17),	31.98(16),	45.68(16),	38.7(3),	39.85(16),
	2M =	79.25(16),	7.07(18),	28.9(3),	6.78(16),	35.12(16),	61.05(17),	2.45(17),	45.68(16),	14.67(16),	9.81(16),
	3M =	67.50(18),	65.95(18),	11.27(19),	57.14(18),	7.23(19),					
	0M =	36.09(18),	34.03(18),	32.84(18),	36.09(18),	1.29(18),	0.19(18),	1.66(16),	41.42(17),	31.74(17),	30.76(17),
-C(11B) /	1M =	36.56(18),	41.69(17),	25.5(2),	29.76(18),	35.93(18),	9.13(18),	63.09(17),	9.62(17),	54.0(3),	61.97(17),
	2M =	37.59(17),	29.61(19),	54.3(3),	31.74(17),	9.45(17),	9.13(18),	36.56(18),	9.62(17),	2.42(17),	1.45(17),
	3M =	40.35(19),	43.38(19),	32.6(2),	35.22(19),	39.62(19),					
	0M =	1.87(17),	5.14(17),	53.02(17),	1.87(17),	8.10(17),	3.71(17),	1.22(15),	78.64(16),	2.06(16),	0.43(16),
C(2A)f-C(3A)f /	1M =	1.38(17),	82.13(16),	11.98(19),	6.50(16),	3.04(16),	63.36(17),	29.51(16),	45.92(16),	34.9(3),	37.09(16),
	2M =	85.39(16),	2.12(18),	25.4(3),	2.06(16),	29.26(16),	63.36(17),	1.38(17),	45.92(16),	7.87(16),	3.04(16),
	3M =	61.92(18),	60.86(18),	6.37(19),	51.01(18),	3.37(18),					
	0M =	4.49(19),	7.80(18),	54.22(18),	4.49(19),	11.81(19),	6.92(19),	1.91(16),	71.95(17),	0.53(17),	2.05(17),
-C(21A) /	1M =	4.03(18),	75.15(17),	14.0(2),	8.59(18),	5.77(18),	67.60(18),	25.48(17),	51.74(17),	32.2(3),	33.33(17),
	2M =	78.49(17),	0.92(19),	22.4(3),	0.53(17),	35.44(17),	67.60(18),	4.03(18),	51.74(17),	11.71(17),	6.43(17),
	3M =	61.41(19),	59.65(19),	5.1(2),	51.66(19),	0.7(2),					
	0M =	43.73(17),	45.69(17),	11.32(17),	43.73(17),	9.83(18),	3.73(18),	0.86(15),	14.02(16),	33.46(16),	35.35(16),

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Cu(2)g-0(6W)g /	1M =	9.37(9),	3.95(6),	6.49(12),	5.94(8),	10.52(8),	23.31(9),	11.64(8),	38.70(7),	0.3(2), 6.54(7),
	2M =	6.73(7),	3.61(11),	5.4(2),	0.85(8),	67.68(7),	23.31(9),	9.37(9),	38.70(7),	47.09(7), 41.76(7),
	3M =	17.20(11),	14.34(11),	3.94(12),	22.99(11),	8.04(12),				
	0M =	86.89(10),	86.94(10),	26.19(10),	86.89(10),	36.62(10),	42.13(10),	43.80(5),	4.37(8),	80.61(8), 82.71(7),
	1M =	86.43(9),	0.32(7),	81.59(12),	86.75(8),	86.55(9),	28.18(10),	54.08(8),	36.37(8),	51.2(2), 47.83(8),
	2M =	3.70(8),	78.29(11),	60.3(2),	80.61(8),	4.58(7),	28.18(10),	86.43(9),	36.37(8),	35.47(8), 40.72(7),
	3M =	21.99(12),	24.03(12),	75.97(12),	29.56(12),	82.39(12),				
	-0(12A) /	0M =	2.70(10),	3.62(9),	26.48(9),	2.70(10),	52.41(10),	47.19(10),	45.21(5),	3.30(8), 7.32(8), 6.15(7),
	1M =	2.79(9),	1.03(6),	0.60(12),	0.94(8),	3.86(8),	17.54(9),	7.86(8),	31.99(7),	3.8(2), 3.50(7),
	2M =	3.44(7),	10.11(11),	0.9(2),	7.32(8),	67.62(7),	17.54(9),	2.79(9),	31.99(7),	53.61(7), 48.60(7),
	3M =	17.36(11),	14.70(11),	10.16(12),	24.46(11),	1.74(12),				
	-0(12B) /	0M =	76.28(10),	77.27(10),	18.06(10),	76.28(10),	21.09(10),	26.52(10),	28.21(5),	2.83(8), 65.98(8), 67.47(7),
-0(12A) /	1M =	76.30(9),	0.12(7),	71.01(12),	72.47(8),	77.53(8),	31.85(9),	54.97(8),	44.98(7),	47.3(2), 47.17(8),
	2M =	4.01(7),	63.29(11),	57.4(2),	65.98(8),	9.75(7),	31.85(9),	76.30(9),	44.98(7),	19.93(7), 25.10(7),
	3M =	16.63(12),	19.25(12),	62.25(12),	21.61(12),	73.88(12),				
	0M =	0.78(10),	3.89(10),	45.80(10),	0.78(10),	0.98(10),	4.65(10),	9.35(5),	88.80(8),	1.09(8), 1.18(7),
	1M =	0.28(9),	84.27(7),	11.66(12),	6.21(8),	1.72(8),	56.53(10),	32.19(8),	37.48(8),	34.8(2), 38.88(8),
	2M =	82.71(7),	0.57(11),	26.4(2),	1.09(8),	17.53(7),	56.53(10),	0.28(9),	37.48(8),	1.37(8), 5.53(7),
	3M =	56.21(12),	56.28(12),	4.84(12),	44.61(12),	4.30(12),				
	-0(41A) /	0M =	2.72(10),	0.23(9),	55.02(9),	2.72(10),	48.18(10),	41.79(10),	37.13(4),	28.59(7), 12.55(7), 10.29(6),
	1M =	2.90(8),	33.32(6),	0.24(12),	3.00(8),	1.19(8),	41.86(9),	14.09(7),	47.36(7),	26.0(2), 20.76(7),
	2M =	35.38(7),	14.71(10),	17.9(2),	12.55(7),	79.34(6),	41.86(9),	2.90(8),	47.36(7),	48.69(7), 42.14(6),
	3M =	48.11(11),	45.13(11),	17.09(12),	52.04(11),	6.25(11),				
	-0(42A) /	0M =	3.61(10),	0.39(10),	53.90(10),	3.61(10),	7.25(10),	3.51(10),	1.24(5),	81.51(8), 6.63(8), 4.23(7),
Na(1)g-0(21B) /	1M =	4.10(9),	87.47(7),	6.89(12),	1.39(8),	2.53(8),	56.41(10),	35.76(8),	38.61(7),	40.1(2), 43.08(8),
	2M =	84.93(7),	6.40(11),	31.0(2),	6.63(8),	24.74(7),	56.41(10),	4.10(9),	38.61(7),	6.87(7), 2.65(7),
	3M =	64.07(12),	63.82(12),	10.68(12),	52.53(12),	8.81(12),				
	0M =	28.03(10),	31.34(9),	33.34(9),	28.03(10),	0.02(10),	6.08(10),	10.98(5),	56.52(8),	22.12(8), 24.74(7),
	1M =	27.59(9),	55.64(7),	36.90(12),	31.68(8),	29.37(8),	88.55(9),	1.75(8),	71.49(7),	8.4(2), 9.53(7),
	2M =	59.75(7),	21.33(11),	1.5(2),	22.12(8),	32.47(7),	88.55(9),	27.59(9),	71.49(7),	0.36(7), 6.00(7),
	3M =	38.40(11),	36.26(11),	17.37(12),	30.22(11),	22.84(12),				
	-0(11A) /	0M =	10.17(10),	9.42(9),	29.64(9),	10.17(10),	64.64(10),	60.03(10),	58.42(5),	7.13(8), 19.99(8), 18.98(7),
	1M =	10.04(9),	2.00(6),	13.89(12),	14.06(8),	9.07(8),	8.36(9),	1.11(8),	20.63(7),	12.0(2), 4.18(7),
	2M =	0.39(7),	22.79(11),	8.9(2),	19.99(8),	64.32(7),	8.36(9),	10.04(9),	20.63(7),	65.87(7), 61.52(7),
	3M =	19.30(11),	17.12(11),	22.49(12),	28.42(11),	10.75(12),				
	-0(4W)g /	0M =	43.80(11),	42.07(11),	28.64(11),	43.80(11),	0.63(12),	3.13(12),	2.04(8),	31.91(10), 38.14(10), 37.53(9),
-0(5W)g /	1M =	44.23(10),	32.49(9),	33.63(13),	37.53(10),	43.84(10),	0.30(11),	65.43(10),	18.82(9),	54.2(3), 61.50(9),
	2M =	28.37(9),	35.75(12),	57.4(3),	38.14(10),	13.14(9),	0.30(11),	44.23(10),	18.82(9),	0.56(9), 1.47(9),
	3M =	34.64(13),	37.77(13),	38.23(13),	31.45(13),	46.72(13),				
	0M =	29.83(11),	33.11(11),	32.52(11),	29.83(11),	2.46(11),	3.80(11),	8.60(7),	51.80(9),	23.12(9), 25.75(9),
	1M =	29.41(10),	51.36(9),	37.94(13),	32.94(10),	31.23(10),	83.98(11),	1.37(9),	76.60(9),	6.1(3), 6.54(9),
	2M =	55.49(9),	22.08(12),	3.9(3),	23.12(9),	35.95(9),	83.98(11),	29.41(10),	76.60(9),	2.90(9), 3.59(9),
	3M =	36.51(13),	34.14(13),	18.29(13),	29.24(13),	24.73(13),				
	-0(52A) /	0M =	38.27(10),	35.50(10),	47.49(10),	38.27(10),	11.08(10),	11.59(10),	8.98(5),	47.74(8), 36.94(8), 35.30(7),
	1M =	38.78(9),	49.85(7),	27.10(12),	32.20(8),	37.64(8),	16.90(9),	70.83(8),	0.39(7),	65.9(2), 73.71(7),
	2M =	45.78(7),	35.40(11),	62.6(2),	36.94(8),	5.20(7),	16.90(9),	38.78(9),	0.39(7),	10.03(7), 10.03(7),
	3M =	54.57(11),	57.67(11),	39.14(12),	49.88(11),	42.85(12),				
	-0(41A) /	0M =	32.26(10),	31.22(10),	40.46(10),	32.26(10),	86.80(10),	81.93(10),	78.39(5),	3.14(8), 42.28(8), 41.10(7),

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Na(2)g-O(1W)g /	1M =	32.17(9),	2.75(7),	34.69(12),	35.64(8),	31.08(8),	0.52(9),	21.78(8),	6.94(7),	31.5(2),	23.44(7),
	2M =	2.80(7),	45.06(11),	30.1(2),	42.28(8),	55.40(7),	0.52(9),	32.17(9),	6.94(7),	87.91(7),	83.04(7),
	3M =	29.51(11),	28.32(12),	44.93(12),	40.69(11),	33.13(12),					
	0M =	31.33(10),	28.82(10),	40.87(10),	31.33(10),	2.08(10),	2.45(10),	0.20(5),	50.96(8),	28.88(8),	27.44(7),
	1M =	31.82(9),	51.69(7),	20.25(12),	25.08(8),	30.88(8),	18.86(9),	62.54(8),	0.37(7),	56.7(2),	64.57(7),
	2M =	47.57(7),	27.15(11),	53.9(2),	28.88(8),	1.13(7),	18.86(9),	31.82(9),	0.37(7),	1.05(7),	0.89(7),
	3M =	49.36(12),	52.26(12),	30.71(12),	42.82(11),	35.55(12),					
	-O(3W)g /	0M =	35.70(10),	38.96(9),	26.90(9),	35.70(10),	0.30(10),	6.70(10),	11.33(5),	46.46(8),	28.65(8),
	1M =	35.30(9),	45.61(6),	43.41(12),	38.56(8),	37.13(8),	78.66(9),	7.51(8),	80.16(7),	0.0(2),	0.39(7),
	2M =	49.74(7),	27.47(11),	10.0(2),	28.65(8),	34.27(7),	78.66(9),	35.30(9),	80.16(7),	0.25(7),	6.33(7),
	3M =	30.49(11),	28.08(11),	23.78(12),	23.56(11),	30.65(12),					
	-O(41A) /	0M =	43.88(10),	41.30(10),	43.05(10),	43.88(10),	10.99(10),	12.31(10),	10.26(5),	40.84(8),	41.40(8),
O(11A)-C(11A) /	1M =	44.38(9),	42.79(7),	32.77(12),	37.66(8),	43.39(8),	9.82(9),	74.63(8),	7.44(7),	66.3(2),	74.25(7),
	2M =	38.70(7),	39.58(11),	65.8(2),	41.40(8),	1.06(7),	9.82(9),	44.38(9),	7.44(7),	9.87(7),	10.69(7),
	3M =	48.97(12),	52.12(12),	43.01(12),	45.79(11),	48.16(12),					
	0M =	42.68(16),	44.00(16),	11.55(16),	42.68(16),	54.75(16),	60.29(16),	65.34(13),	32.66(15),	47.84(15),	48.85(14),
	1M =	42.27(15),	26.80(14),	51.84(17),	48.81(15),	42.46(15),	34.13(16),	14.58(15),	25.36(14),	18.3(3),	11.42(14),
	2M =	28.00(14),	49.83(16),	23.1(3),	47.84(15),	22.14(14),	34.13(16),	42.27(15),	25.36(14),	54.56(14),	60.56(14),
	3M =	1.61(17),	1.63(17),	46.41(17),	13.14(17),	39.82(17),					
	O(11B)-C(11B) /	0M =	0.64(16),	0.82(16),	11.16(16),	0.64(16),	49.81(16),	47.30(16),	47.82(14),	22.90(15),	9.21(15),
	1M =	0.38(16),	18.34(15),	7.25(18),	5.78(15),	0.12(15),	1.37(16),	15.22(15),	14.79(15),	5.2(3),	13.18(15),
	2M =	16.13(15),	11.94(17),	6.9(3),	9.21(15),	48.93(15),	1.37(16),	0.38(16),	14.79(15),	50.98(15),	48.96(15),
	3M =	0.95(17),	1.32(17),	10.52(18),	9.89(17),	0.20(17),					
	O(12A)-C(11A) /	0M =	7.65(16),	7.49(16),	7.84(16),	7.65(16),	42.75(16),	39.68(16),	39.85(14),	21.70(15),	1.04(15),
O(12B)-C(11B) /	1M =	7.90(16),	17.78(15),	1.04(18),	2.53(15),	8.41(15),	2.96(16),	22.02(15),	20.28(15),	11.4(3),	19.25(15),
	2M =	15.07(15),	3.78(17),	14.0(3),	1.04(15),	48.26(15),	2.96(16),	7.90(16),	20.28(15),	43.96(15),	41.32(15),
	3M =	1.72(17),	4.26(17),	2.50(18),	6.15(17),	8.38(17),					
	0M =	47.38(16),	48.98(16),	10.30(16),	47.38(16),	50.94(16),	56.94(16),	61.91(13),	33.00(15),	51.49(15),	52.80(14),
	1M =	46.94(15),	27.32(14),	57.10(17),	53.63(15),	47.30(15),	38.25(16),	17.71(15),	30.81(14),	20.2(3),	13.85(15),
	2M =	28.99(14),	53.18(16),	26.0(3),	51.49(15),	17.16(14),	38.25(16),	46.94(15),	30.81(14),	50.59(14),	56.94(14),
	3M =	0.91(17),	1.26(17),	49.44(17),	12.22(17),	44.10(17),					
	O(21A)-C(21A) /	0M =	8.52(16),	7.68(16),	3.00(16),	8.52(16),	36.11(16),	34.42(16),	35.78(13),	33.34(15),	1.16(15),
	1M =	8.86(15),	29.56(14),	0.20(17),	2.74(15),	8.99(15),	7.13(16),	28.63(15),	11.12(14),	19.2(3),	27.23(15),
	2M =	26.77(14),	1.41(16),	20.0(3),	1.16(15),	36.54(14),	7.13(16),	8.86(15),	11.12(14),	37.23(14),	36.06(14),
	3M =	12.94(17),	15.34(17),	0.66(17),	4.41(17),	10.31(17),					
	O(21B)-C(21B) /	0M =	9.90(16),	11.93(16),	38.71(16),	9.90(16),	42.02(16),	35.57(16),	31.81(14),	18.37(15),	0.35(15),
O(22A)-C(21A) /	1M =	9.81(16),	22.10(15),	10.63(18),	8.40(15),	11.36(15),	40.04(16),	2.11(15),	52.44(15),	9.9(3),	4.44(15),
	2M =	24.96(15),	2.82(17),	2.2(3),	0.35(15),	76.52(15),	40.04(16),	9.81(16),	52.44(15),	42.91(15),	36.44(15),
	3M =	32.37(17),	29.31(17),	4.47(18),	35.71(17),	7.09(17),					
	0M =	13.73(16),	15.90(16),	37.85(16),	13.73(16),	37.29(16),	30.81(16),	26.97(14),	21.38(15),	3.57(15),	5.61(15),
	1M =	13.61(16),	24.74(15),	15.01(18),	12.56(15),	15.21(15),	44.53(16),	3.66(15),	57.40(15),	8.2(3),	3.26(15),
	2M =	27.83(15),	1.17(17),	0.0(3),	3.57(15),	72.36(15),	44.53(16),	13.61(16),	57.40(15),	38.15(15),	31.65(15),
	3M =	32.50(17),	29.37(17),	0.69(18),	34.66(17),	10.67(17),					
	O(22B)-C(21B) /	0M =	6.95(16),	5.93(16),	5.28(16),	6.95(16),	35.39(16),	34.20(16),	35.94(13),	36.88(15),	0.04(15),
	1M =	7.31(15),	32.99(14),	1.78(17),	1.03(15),	7.33(15),	10.83(16),	28.77(15),	7.47(14),	19.9(3),	27.96(14),
	2M =	30.27(14),	2.46(16),	20.0(3),	0.04(15),	33.50(14),	10.83(16),	7.31(15),	7.47(14),	36.47(14),	35.83(14),
	3M =	15.44(17),	17.74(17),	0.15(17),	6.53(17),	9.03(17),					
	O(41A)-C(41A) /	0M =	10.83(16),	10.31(16),	0.89(16),	10.83(16),	37.10(16),	34.61(16),	35.34(14),	27.49(15),	2.78(15),

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O(42A)-C(41A) /	1M =	11.13(16),	23.88(15),	3.26(18),	5.33(15),	11.44(15),	1.12(16),	27.91(15),	17.02(15),	17.7(3),	25.61(15),
	2M =	20.98(15),	0.11(17),	19.6(3),	2.78(15),	41.48(15),	1.12(16),	11.13(16),	17.02(15),	38.28(15),	36.27(15),
	3M =	8.65(17),	11.21(17),	1.79(18),	0.79(17),	12.11(17),					
	0M =	37.85(16),	39.95(16),	0.97(16),	37.85(16),	42.40(16),	47.71(16),	52.75(13),	44.80(15),	40.51(15),	42.12(14),
O(51A)-C(51A) /	1M =	37.38(15),	39.04(14),	48.50(17),	44.18(15),	38.05(15),	45.56(16),	6.63(15),	34.17(14),	8.4(3),	2.29(15),
	2M =	40.48(14),	41.95(16),	14.6(3),	40.51(15),	11.45(14),	45.56(16),	37.38(15),	34.17(14),	42.31(14),	48.08(14),
	3M =	10.69(17),	10.48(17),	38.02(17),	0.75(17),	33.97(17),					
	0M =	1.49(16),	3.37(16),	41.94(16),	1.49(16),	51.13(16),	44.68(16),	40.91(13),	14.82(15),	8.82(15),	6.97(14),
O(52A)-C(51A) /	1M =	1.43(15),	19.23(14),	1.69(17),	0.34(15),	2.91(15),	32.88(16),	3.07(15),	43.72(14),	15.1(3),	8.93(15),
	2M =	21.58(14),	11.36(16),	8.3(3),	8.82(15),	83.94(14),	32.88(16),	1.43(15),	43.72(14),	52.02(14),	45.56(14),
	3M =	34.01(17),	31.13(17),	12.77(17),	39.35(17),	1.02(17),					
	0M =	1.35(16),	2.56(16),	4.80(16),	1.35(16),	39.24(16),	39.17(16),	41.66(14),	41.24(15),	7.66(15),	8.20(15),
C(1A)g-C(2A)g /	1M =	0.96(16),	36.60(15),	10.45(18),	7.39(15),	1.06(15),	18.03(16),	22.81(15),	0.38(15),	15.2(3),	23.13(15),
	2M =	34.47(15),	10.04(17),	13.9(3),	7.66(15),	30.70(15),	18.03(16),	0.96(16),	0.38(15),	40.19(15),	40.73(15),
	3M =	15.50(17),	17.41(17),	7.41(18),	5.50(17),	1.08(17),					
	0M =	36.33(18),	34.20(18),	34.09(18),	36.33(18),	0.27(18),	1.12(18),	0.79(16),	42.11(17),	32.22(17),	31.17(17),
-C(6A)g /	1M =	36.80(18),	42.52(17),	25.6(2),	30.00(18),	36.13(18),	9.86(18),	63.93(17),	8.81(17),	55.0(3),	63.04(17),
	2M =	38.41(17),	30.13(19),	55.1(3),	32.22(17),	8.21(17),	9.86(18),	36.80(18),	8.81(17),	1.39(17),	0.50(17),
	3M =	41.58(19),	44.61(19),	33.2(2),	36.46(19),	39.96(19),					
	0M =	11.61(19),	14.86(18),	43.31(18),	11.61(19),	0.02(19),	4.88(19),	9.89(16),	77.23(17),	8.05(17),	10.53(17),
-C(11A) /	1M =	11.12(18),	75.86(17),	21.9(2),	16.44(18),	12.73(18),	70.45(18),	20.43(18),	51.35(17),	25.1(3),	27.75(17),
	2M =	79.72(17),	8.05(19),	15.8(3),	8.05(17),	25.02(17),	70.45(18),	11.12(18),	51.35(17),	0.11(17),	5.40(17),
	3M =	51.79(19),	50.67(19),	3.8(2),	41.09(19),	6.4(2),					
	0M =	57.24(17),	59.38(17),	1.32(17),	57.24(17),	4.01(18),	10.05(18),	12.78(15),	13.64(16),	47.07(16),	49.06(16),
C(1B)g-C(2B)g /	1M =	57.10(17),	12.55(16),	57.29(19),	55.75(16),	58.73(17),	45.61(17),	38.55(16),	62.60(16),	28.9(3),	30.52(16),
	2M =	16.68(16),	44.63(18),	38.7(3),	47.07(16),	29.08(16),	45.61(17),	57.10(17),	62.60(16),	2.94(16),	8.86(16),
	3M =	1.30(18),	1.57(18),	42.81(19),	2.24(18),	53.91(19),					
	0M =	34.99(18),	32.84(18),	34.03(18),	34.99(18),	1.09(18),	0.19(18),	1.80(16),	43.21(17),	30.94(17),	29.87(17),
-C(11B) /	1M =	35.46(18),	43.50(17),	24.3(2),	28.65(18),	34.78(18),	10.93(18),	62.86(17),	7.81(17),	54.3(3),	62.29(17),
	2M =	39.40(17),	28.87(19),	54.0(3),	30.94(17),	8.26(17),	10.93(18),	35.46(18),	7.81(17),	2.20(17),	1.43(17),
	3M =	41.75(19),	44.76(19),	32.0(2),	36.32(19),	38.64(19),					
	0M =	51.09(17),	53.02(17),	5.14(17),	51.09(17),	2.71(17),	3.30(17),	5.99(15),	12.49(16),	40.81(16),	42.69(16),
C(2A)g-C(3A)g /	1M =	51.00(17),	12.12(16),	50.54(19),	49.19(16),	52.54(16),	44.80(17),	35.92(16),	63.36(16),	25.4(3),	27.99(16),
	2M =	16.24(16),	38.30(18),	34.9(3),	40.81(16),	35.34(16),	44.80(17),	51.00(17),	63.36(16),	3.78(16),	2.09(16),
	3M =	3.99(18),	0.99(18),	36.72(19),	1.61(18),	48.15(18),					
	0M =	51.79(19),	54.22(18),	7.80(18),	51.79(19),	0.23(19),	6.49(19),	9.63(16),	18.94(17),	41.87(17),	44.02(17),
-C(21A) /	1M =	51.60(18),	18.24(17),	53.4(2),	51.07(18),	53.32(18),	51.18(18),	32.04(17),	68.91(17),	22.4(3),	24.01(17),
	2M =	22.37(17),	39.58(19),	32.2(3),	41.87(17),	33.88(17),	51.18(18),	51.60(18),	68.91(17),	0.76(17),	5.41(17),
	3M =	7.84(19),	4.96(19),	37.4(2),	4.24(19),	48.1(2),					
	0M =	8.09(17),	11.32(17),	45.69(17),	8.09(17),	1.29(18),	3.31(18),	8.28(15),	80.35(16),	4.73(16),	7.18(16),
C(2B)g-C(6B)g /	1M =	7.59(17),	79.50(16),	18.49(19),	12.99(17),	9.19(17),	67.07(17),	24.06(16),	48.20(16),	28.5(3),	31.34(16),
	2M =	83.34(16),	4.81(18),	19.3(3),	4.73(16),	24.65(16),	67.07(17),	7.59(17),	48.20(16),	1.12(16),	3.92(16),
	3M =	54.62(18),	53.68(18),	0.53(19),	43.65(18),	2.87(19),					
	0M =	46.11(19),	48.31(18),	11.30(18),	46.11(19),	6.41(19),	0.20(19),	2.88(16),	17.29(18),	35.97(17),	38.01(17),
-C(21B) /	1M =	45.97(18),	17.31(17),	46.9(2),	44.85(18),	47.60(18),	49.50(18),	29.74(18),	68.62(17),	19.3(3),	21.82(17),
	2M =	21.41(17),	33.57(19),	28.8(3),	35.97(17),	40.11(17),	49.50(18),	45.97(18),	68.62(17),	7.42(17),	1.30(17),
	3M =	10.15(19),	7.15(19),	31.7(2),	7.76(19),	42.8(2),					
	0M =	5.61(17),	8.89(17),	50.35(17),	5.61(17),	6.48(17),	1.80(17),	3.18(15),	77.40(16),	1.52(16),	4.03(16),

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C(3A)g-C(4A)g /	1M =	5.13(17),	79.28(16),	15.65(19),	10.18(16),	6.80(17),	67.10(17),	25.70(16),	49.33(16),	31.2(3),	33.28(16),
	2M =	83.28(16),	1.39(18),	21.7(3),	1.52(16),	29.55(16),	67.10(17),	5.13(17),	49.33(16),	6.32(16),	1.23(16),
	3M =	58.73(18),	57.48(18),	2.85(19),	48.12(18),	0.37(18),					
	0M =	11.39(19),	14.63(18),	43.36(18),	11.39(19),	0.10(19),	4.93(19),	9.94(17),	77.56(18),	7.88(18),	10.34(17),
C(4A)g-C(5A)g /	1M =	10.90(18),	76.14(17),	21.7(2),	16.24(18),	12.50(18),	70.12(18),	20.69(18),	51.01(17),	25.3(3),	28.00(17),
	2M =	79.98(17),	7.89(19),	16.0(3),	7.88(18),	24.80(17),	70.12(18),	10.90(18),	51.01(17),	0.20(17),	5.46(17),
	3M =	51.9(2),	50.8(2),	3.6(2),	41.2(2),	6.2(2),					
	0M =	36.82(18),	34.66(18),	34.61(18),	36.82(18),	0.39(19),	1.78(19),	0.15(16),	42.06(17),	32.78(17),	31.72(17),
-C(41A) /	1M =	37.29(18),	42.57(17),	26.1(2),	30.48(18),	36.60(18),	9.84(18),	64.57(17),	8.76(17),	55.7(3),	63.70(17),
	2M =	38.45(17),	30.70(19),	55.7(3),	32.78(17),	7.69(17),	9.84(18),	37.29(18),	8.76(17),	0.74(17),	0.15(17),
	3M =	42.02(19),	45.07(19),	33.8(2),	37.00(19),	40.48(19),					
	0M =	54.51(18),	56.74(17),	4.18(17),	54.51(18),	1.74(18),	7.87(18),	10.74(15),	15.41(16),	44.40(16),	46.44(16),
C(5A)g-C(6A)g /	1M =	54.36(17),	14.56(16),	55.06(19),	53.25(17),	56.01(17),	47.56(17),	35.87(16),	65.06(16),	26.1(3),	27.85(16),
	2M =	18.69(16),	42.00(18),	35.9(3),	44.40(16),	31.69(16),	47.56(17),	54.36(17),	65.06(16),	0.70(16),	6.71(16),
	3M =	4.03(18),	1.13(19),	40.08(19),	0.61(18),	51.09(19),					
	0M =	51.34(19),	53.74(18),	8.05(18),	51.34(19),	0.35(19),	5.90(19),	9.02(16),	18.72(18),	41.39(18),	43.53(17),
-C(51A) /	1M =	51.16(18),	18.08(17),	52.8(2),	50.55(18),	52.86(18),	50.98(18),	31.93(18),	68.89(17),	22.2(3),	23.91(17),
	2M =	22.21(17),	39.08(19),	32.0(3),	41.39(18),	34.41(17),	50.98(18),	51.16(18),	68.89(17),	1.35(17),	4.81(17),
	3M =	8.0(2),	5.1(2),	36.9(2),	4.48(19),	47.7(2),					
	0M =	6.06(17),	9.33(17),	49.14(17),	6.06(17),	5.01(18),	0.38(18),	4.59(15),	78.66(16),	2.21(16),	4.70(16),
Cu(1)h-O(7W)h /	1M =	5.58(17),	79.92(16),	16.23(19),	10.74(16),	7.22(17),	66.90(17),	25.54(16),	48.75(16),	30.7(3),	33.04(16),
	2M =	84.04(16),	2.15(18),	21.3(3),	2.21(16),	28.01(16),	66.90(17),	5.58(17),	48.75(16),	4.84(16),	0.21(16),
	3M =	57.76(18),	56.62(18),	2.10(19),	47.00(18),	0.83(19),					
	0M =	83.90(10),	81.52(10),	31.87(10),	83.90(10),	40.62(10),	45.75(10),	46.86(5),	0.17(8),	85.71(8),	86.40(7),
-O(11A) /	1M =	83.95(9),	4.15(7),	77.05(12),	82.47(8),	82.44(9),	22.76(10),	57.29(8),	30.60(8),	55.9(2),	51.76(8),
	2M =	0.93(8),	82.95(11),	64.4(2),	85.71(8),	9.68(7),	22.76(10),	83.95(9),	30.60(8),	39.43(8),	44.25(7),
	3M =	27.36(12),	29.29(12),	81.59(12),	35.21(12),	84.27(12),					
	0M =	75.96(10),	76.24(10),	20.23(10),	75.96(10),	20.86(10),	26.07(10),	27.49(5),	0.19(8),	65.96(8),	67.15(7),
-O(11B) /	1M =	76.09(9),	2.87(7),	69.10(12),	71.27(8),	76.98(8),	28.98(10),	57.84(8),	42.54(7),	49.8(2),	49.99(8),
	2M =	1.04(7),	63.19(11),	59.9(2),	65.96(8),	9.00(7),	28.98(10),	76.09(9),	42.54(7),	19.67(8),	24.61(7),
	3M =	19.18(12),	21.85(12),	62.64(12),	23.79(12),	74.57(12),					
	0M =	9.30(10),	10.40(9),	25.39(9),	9.30(10),	45.92(10),	40.41(10),	38.16(5),	0.12(8),	0.85(8),	0.46(7),
Cu(2)h-O(6W)h /	1M =	9.37(9),	3.95(6),	6.49(12),	5.94(8),	10.52(8),	23.31(9),	11.64(8),	38.70(7),	0.3(2),	6.54(7),
	2M =	6.73(7),	3.61(11),	5.4(2),	0.85(8),	67.68(7),	23.31(9),	9.37(9),	38.70(7),	47.09(7),	41.76(7),
	3M =	17.20(11),	14.34(11),	3.94(12),	22.99(11),	8.04(12),					
	0M =	86.89(10),	86.94(10),	26.19(10),	86.89(10),	36.62(10),	42.13(10),	43.80(5),	4.37(8),	80.61(8),	82.71(7),
-O(12A) /	1M =	86.43(9),	0.32(7),	81.59(12),	86.75(8),	86.55(9),	28.18(10),	54.08(8),	36.37(8),	51.2(2),	47.83(8),
	2M =	3.70(8),	78.29(11),	60.3(2),	80.61(8),	4.58(7),	28.18(10),	86.43(9),	36.37(8),	35.47(8),	40.72(7),
	3M =	21.99(12),	24.03(12),	75.97(12),	29.56(12),	82.39(12),					
	0M =	2.70(10),	3.62(9),	26.48(9),	2.70(10),	52.41(10),	47.19(10),	45.21(5),	3.30(8),	7.32(8),	6.15(7),
-O(12B) /	1M =	2.79(9),	1.03(6),	0.60(12),	0.94(8),	3.86(8),	17.54(9),	7.86(8),	31.99(7),	3.8(2),	3.50(7),
	2M =	3.44(7),	10.11(11),	0.9(2),	7.32(8),	67.62(7),	17.54(9),	2.79(9),	31.99(7),	53.61(7),	48.60(7),
	3M =	17.36(11),	14.70(11),	10.16(12),	24.46(11),	1.74(12),					
	0M =	76.28(10),	77.27(10),	18.06(10),	76.28(10),	21.09(10),	26.52(10),	28.21(5),	2.83(8),	65.98(8),	67.47(7),
Na(1)h-O(4W)h /	1M =	76.30(9),	0.12(7),	71.01(12),	72.47(8),	77.53(8),	31.85(9),	54.97(8),	44.98(7),	47.3(2),	47.17(8),
	2M =	4.01(7),	63.29(11),	57.4(2),	65.98(8),	9.75(7),	31.85(9),	76.30(9),	44.98(7),	19.93(7),	25.10(7),
	3M =	16.63(12),	19.25(12),	62.25(12),	21.61(12),	73.88(12),					
	0M =	43.80(11),	42.07(11),	28.64(11),	43.80(11),	0.63(12),	3.13(12),	2.04(8),	31.91(10),	38.14(10),	37.53(9),

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	1M =	44.23(10),	32.49(9),	33.63(13),	37.53(10),	43.84(10),	0.30(11),	65.43(10),	18.82(9),	54.2(3),	61.50(9),
	2M =	28.37(9),	35.75(12),	57.4(3),	38.14(10),	13.14(9),	0.30(11),	44.23(10),	18.82(9),	0.56(9),	1.47(9),
	3M =	34.64(13),	37.77(13),	38.23(13),	31.45(13),	46.72(13),					
-O(5W)h /	0M =	29.83(11),	33.11(11),	32.52(11),	29.83(11),	2.46(11),	3.80(11),	8.60(7),	51.80(9),	23.12(9),	25.75(9),
	1M =	29.41(10),	51.36(9),	37.94(13),	32.94(10),	31.23(10),	83.98(11),	1.37(9),	76.60(9),	6.1(3),	6.54(9),
	2M =	55.49(9),	22.08(12),	3.9(3),	23.12(9),	35.95(9),	83.98(11),	29.41(10),	76.60(9),	2.90(9),	3.59(9),
	3M =	36.51(13),	34.14(13),	18.29(13),	29.24(13),	24.73(13),					
-O(52A) /	0M =	38.27(10),	35.50(10),	47.49(10),	38.27(10),	11.08(10),	11.59(10),	8.98(5),	47.74(8),	36.94(8),	35.30(7),
	1M =	38.78(9),	49.85(7),	27.10(12),	32.20(8),	37.64(8),	16.90(9),	70.83(8),	0.39(7),	65.9(2),	73.71(7),
	2M =	45.78(7),	35.40(11),	62.6(2),	36.94(8),	5.20(7),	16.90(9),	38.78(9),	0.39(7),	10.03(7),	10.03(7),
	3M =	54.57(11),	57.67(11),	39.14(12),	49.88(11),	42.85(12),					
Na(2)h-O(1W)h /	0M =	31.33(10),	28.82(10),	40.87(10),	31.33(10),	2.08(10),	2.45(10),	0.20(5),	50.96(8),	28.88(8),	27.44(7),
	1M =	31.82(9),	51.69(7),	20.25(12),	25.08(8),	30.88(8),	18.86(9),	62.54(8),	0.37(7),	56.7(2),	64.57(7),
	2M =	47.57(7),	27.15(11),	53.9(2),	28.88(8),	1.13(7),	18.86(9),	31.82(9),	0.37(7),	1.05(7),	0.89(7),
	3M =	49.36(12),	52.26(12),	30.71(12),	42.82(11),	35.55(12),					
-O(3W)h /	0M =	35.70(10),	38.96(9),	26.90(9),	35.70(10),	0.30(10),	6.70(10),	11.33(5),	46.46(8),	28.65(8),	31.27(7),
	1M =	35.30(9),	45.61(6),	43.41(12),	38.56(8),	37.13(8),	78.66(9),	7.51(8),	80.16(7),	0.0(2),	0.39(7),
	2M =	49.74(7),	27.47(11),	10.0(2),	28.65(8),	34.27(7),	78.66(9),	35.30(9),	80.16(7),	0.25(7),	6.33(7),
	3M =	30.49(11),	28.08(11),	23.78(12),	23.56(11),	30.65(12),					
-O(41A) /	0M =	43.88(10),	41.30(10),	43.05(10),	43.88(10),	10.99(10),	12.31(10),	10.26(5),	40.84(8),	41.40(8),	40.02(7),
	1M =	44.38(9),	42.79(7),	32.77(12),	37.66(8),	43.39(8),	9.82(9),	74.63(8),	7.44(7),	66.3(2),	74.25(7),
	2M =	38.70(7),	39.58(11),	65.8(2),	41.40(8),	1.06(7),	9.82(9),	44.38(9),	7.44(7),	9.87(7),	10.69(7),
	3M =	48.97(12),	52.12(12),	43.01(12),	45.79(11),	48.16(12),					
O(11A)-C(11A) /	0M =	42.68(16),	44.00(16),	11.55(16),	42.68(16),	54.75(16),	60.29(16),	65.34(13),	32.66(15),	47.84(15),	48.85(14),
	1M =	42.27(15),	26.80(14),	51.84(17),	48.81(15),	42.46(15),	34.13(16),	14.58(15),	25.36(14),	18.3(3),	11.42(14),
	2M =	28.00(14),	49.83(16),	23.1(3),	47.84(15),	22.14(14),	34.13(16),	42.27(15),	25.36(14),	54.56(14),	60.56(14),
	3M =	1.61(17),	1.63(17),	46.41(17),	13.14(17),	39.82(17),					
O(11B)-C(11B) /	0M =	0.64(16),	0.82(16),	11.16(16),	0.64(16),	49.81(16),	47.30(16),	47.82(14),	22.90(15),	9.21(15),	8.90(15),
	1M =	0.38(16),	18.34(15),	7.25(18),	5.78(15),	0.12(15),	1.37(16),	15.22(15),	14.79(15),	5.2(3),	13.18(15),
	2M =	16.13(15),	11.94(17),	6.9(3),	9.21(15),	48.93(15),	1.37(16),	0.38(16),	14.79(15),	50.98(15),	48.96(15),
	3M =	0.95(17),	1.32(17),	10.52(18),	9.89(17),	0.20(17),					
O(12A)-C(11A) /	0M =	7.65(16),	7.49(16),	7.84(16),	7.65(16),	42.75(16),	39.68(16),	39.85(14),	21.70(15),	1.04(15),	0.67(15),
	1M =	7.90(16),	17.78(15),	1.04(18),	2.53(15),	8.41(15),	2.96(16),	22.02(15),	20.28(15),	11.4(3),	19.25(15),
	2M =	15.07(15),	3.78(17),	14.0(3),	1.04(15),	48.26(15),	2.96(16),	7.90(16),	20.28(15),	43.96(15),	41.32(15),
	3M =	1.72(17),	4.26(17),	2.50(18),	6.15(17),	8.38(17),					
O(12B)-C(11B) /	0M =	47.38(16),	48.98(16),	10.30(16),	47.38(16),	50.94(16),	56.94(16),	61.91(13),	33.00(15),	51.49(15),	52.80(14),
	1M =	46.94(15),	27.32(14),	57.10(17),	53.63(15),	47.30(15),	38.25(16),	17.71(15),	30.81(14),	20.2(3),	13.85(15),
	2M =	28.99(14),	53.18(16),	26.0(3),	51.49(15),	17.16(14),	38.25(16),	46.94(15),	30.81(14),	50.59(14),	56.94(14),
	3M =	0.91(17),	1.26(17),	49.44(17),	12.22(17),	44.10(17),					
O(21A)-C(21A) /	0M =	8.52(16),	7.68(16),	3.00(16),	8.52(16),	36.11(16),	34.42(16),	35.78(13),	33.34(15),	1.16(15),	0.99(14),
	1M =	8.86(15),	29.56(14),	0.20(17),	2.74(15),	8.99(15),	7.13(16),	28.63(15),	11.12(14),	19.2(3),	27.23(15),
	2M =	26.77(14),	1.41(16),	20.0(3),	1.16(15),	36.54(14),	7.13(16),	8.86(15),	11.12(14),	37.23(14),	36.06(14),
	3M =	12.94(17),	15.34(17),	0.66(17),	4.41(17),	10.31(17),					
O(21B)-C(21B) /	0M =	9.90(16),	11.93(16),	38.71(16),	9.90(16),	42.02(16),	35.57(16),	31.81(14),	18.37(15),	0.35(15),	1.60(15),
	1M =	9.81(16),	22.10(15),	10.63(18),	8.40(15),	11.36(15),	40.04(16),	2.11(15),	52.44(15),	9.9(3),	4.44(15),
	2M =	24.96(15),	2.82(17),	2.2(3),	0.35(15),	76.52(15),	40.04(16),	9.81(16),	52.44(15),	42.91(15),	36.44(15),
	3M =	32.37(17),	29.31(17),	4.47(18),	35.71(17),	7.09(17),					
O(22A)-C(21A) /	0M =	13.73(16),	15.90(16),	37.85(16),	13.73(16),	37.29(16),	30.81(16),	26.97(14),	21.38(15),	3.57(15),	5.61(15),

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	1M =	13.61(16),	24.74(15),	15.01(18),	12.56(15),	15.21(15),	44.53(16),	3.66(15),	57.40(15),	8.2(3),	3.26(15),
	2M =	27.83(15),	1.17(17),	0.0(3),	3.57(15),	72.36(15),	44.53(16),	13.61(16),	57.40(15),	38.15(15),	31.65(15),
	3M =	32.50(17),	29.37(17),	0.69(18),	34.66(17),	10.67(17),					
0(22B)-C(21B) /	0M =	6.95(16),	5.93(16),	5.28(16),	6.95(16),	35.39(16),	34.20(16),	35.94(13),	36.88(15),	0.04(15),	0.28(14),
	1M =	7.31(15),	32.99(14),	1.78(17),	1.03(15),	7.33(15),	10.83(16),	28.77(15),	7.47(14),	19.9(3),	27.96(14),
	2M =	30.27(14),	2.46(16),	20.0(3),	0.04(15),	33.50(14),	10.83(16),	7.31(15),	7.47(14),	36.47(14),	35.83(14),
	3M =	15.44(17),	17.74(17),	0.15(17),	6.53(17),	9.03(17),					
0(41A)-C(41A) /	0M =	10.83(16),	10.31(16),	0.89(16),	10.83(16),	37.10(16),	34.61(16),	35.34(14),	27.49(15),	2.78(15),	2.88(15),
	1M =	11.13(16),	23.88(15),	3.26(18),	5.33(15),	11.44(15),	1.12(16),	27.91(15),	17.02(15),	17.7(3),	25.61(15),
	2M =	20.98(15),	0.11(17),	19.6(3),	2.78(15),	41.48(15),	1.12(16),	11.13(16),	17.02(15),	38.28(15),	36.27(15),
	3M =	8.65(17),	11.21(17),	1.79(18),	0.79(17),	12.11(17),					
0(42A)-C(41A) /	0M =	37.85(16),	39.95(16),	0.97(16),	37.85(16),	42.40(16),	47.71(16),	52.75(13),	44.80(15),	40.51(15),	42.12(14),
	1M =	37.38(15),	39.04(14),	48.50(17),	44.18(15),	38.05(15),	45.56(16),	6.63(15),	34.17(14),	8.4(3),	2.29(15),
	2M =	40.48(14),	41.95(16),	14.6(3),	40.51(15),	11.45(14),	45.56(16),	37.38(15),	34.17(14),	42.31(14),	48.08(14),
	3M =	10.69(17),	10.48(17),	38.02(17),	0.75(17),	33.97(17),					
0(51A)-C(51A) /	0M =	1.49(16),	3.37(16),	41.94(16),	1.49(16),	51.13(16),	44.68(16),	40.91(13),	14.82(15),	8.82(15),	6.97(14),
	1M =	1.43(15),	19.23(14),	1.69(17),	0.34(15),	2.91(15),	32.88(16),	3.07(15),	43.72(14),	15.1(3),	8.93(15),
	2M =	21.58(14),	11.36(16),	8.3(3),	8.82(15),	83.94(14),	32.88(16),	1.43(15),	43.72(14),	52.02(14),	45.56(14),
	3M =	34.01(17),	31.13(17),	12.77(17),	39.35(17),	1.02(17),					
0(52A)-C(51A) /	0M =	1.35(16),	2.56(16),	4.80(16),	1.35(16),	39.24(16),	39.17(16),	41.66(14),	41.24(15),	7.66(15),	8.20(15),
	1M =	0.96(16),	36.60(15),	10.45(18),	7.39(15),	1.06(15),	18.03(16),	22.81(15),	0.38(15),	15.2(3),	23.13(15),
	2M =	34.47(15),	10.04(17),	13.9(3),	7.66(15),	30.70(15),	18.03(16),	0.96(16),	0.38(15),	40.19(15),	40.73(15),
	3M =	15.50(17),	17.41(17),	7.41(18),	5.50(17),	1.08(17),					
C(1A)h-C(2A)h /	0M =	36.33(18),	34.20(18),	34.09(18),	36.33(18),	0.27(18),	1.12(18),	0.79(16),	42.11(17),	32.22(17),	31.17(17),
	1M =	36.80(18),	42.52(17),	25.6(2),	30.00(18),	36.13(18),	9.86(18),	63.93(17),	8.81(17),	55.0(3),	63.04(17),
	2M =	38.41(17),	30.13(19),	55.1(3),	32.22(17),	8.21(17),	9.86(18),	36.80(18),	8.81(17),	1.39(17),	0.50(17),
	3M =	41.58(19),	44.61(19),	33.2(2),	36.46(19),	39.96(19),					
-C(6A)h /	0M =	11.61(19),	14.86(18),	43.31(18),	11.61(19),	0.02(19),	4.88(19),	9.89(16),	77.23(17),	8.05(17),	10.53(17),
	1M =	11.12(18),	75.86(17),	21.9(2),	16.44(18),	12.73(18),	70.45(18),	20.43(18),	51.35(17),	25.1(3),	27.75(17),
	2M =	79.72(17),	8.05(19),	15.8(3),	8.05(17),	25.02(17),	70.45(18),	11.12(18),	51.35(17),	0.11(17),	5.40(17),
	3M =	51.79(19),	50.67(19),	3.8(2),	41.09(19),	6.4(2),					
-C(11A) /	0M =	57.24(17),	59.38(17),	1.32(17),	57.24(17),	4.01(18),	10.05(18),	12.78(15),	13.64(16),	47.07(16),	49.06(16),
	1M =	57.10(17),	12.55(16),	57.29(19),	55.75(16),	58.73(17),	45.61(17),	38.55(16),	62.60(16),	28.9(3),	30.52(16),
	2M =	16.68(16),	44.63(18),	38.7(3),	47.07(16),	29.08(16),	45.61(17),	57.10(17),	62.60(16),	2.94(16),	8.86(16),
	3M =	1.30(18),	1.57(18),	42.81(19),	2.24(18),	53.91(19),					
C(1B)h-C(6B) /	0M =	9.87(19),	13.16(18),	47.23(18),	9.87(19),	4.78(19),	0.20(19),	5.22(16),	74.72(17),	5.55(17),	8.09(17),
	1M =	9.40(18),	75.36(17),	19.8(2),	14.35(18),	11.07(18),	71.41(18),	21.32(17),	53.28(17),	26.9(3),	28.92(17),
	2M =	79.49(17),	5.34(19),	17.3(3),	5.55(17),	29.92(17),	71.41(18),	9.40(18),	53.28(17),	4.72(17),	0.67(17),
	3M =	55.03(19),	53.58(19),	1.1(2),	44.80(19),	4.6(2),					
-C(2B)h /	0M =	34.99(18),	32.84(18),	34.03(18),	34.99(18),	1.09(18),	0.19(18),	1.80(16),	43.21(17),	30.94(17),	29.87(17),
	1M =	35.46(18),	43.50(17),	24.3(2),	28.65(18),	34.78(18),	10.93(18),	62.86(17),	7.81(17),	54.3(3),	62.29(17),
	2M =	39.40(17),	28.87(19),	54.0(3),	30.94(17),	8.26(17),	10.93(18),	35.46(18),	7.81(17),	2.20(17),	1.43(17),
	3M =	41.75(19),	44.76(19),	32.0(2),	36.32(19),	38.64(19),					
-C(11B) /	0M =	51.09(17),	53.02(17),	5.14(17),	51.09(17),	2.71(17),	3.30(17),	5.99(15),	12.49(16),	40.81(16),	42.69(16),
	1M =	51.00(17),	12.12(16),	50.54(19),	49.19(16),	52.54(16),	44.80(17),	35.92(16),	63.36(16),	25.4(3),	27.99(16),
	2M =	16.24(16),	38.30(18),	34.9(3),	40.81(16),	35.34(16),	44.80(17),	51.00(17),	63.36(16),	3.78(16),	2.09(16),
	3M =	3.99(18),	0.99(18),	36.72(19),	1.61(18),	48.15(18),					
C(2A)h-C(3A)h /	0M =	51.79(19),	54.22(18),	7.80(18),	51.79(19),	0.23(19),	6.49(19),	9.63(16),	18.94(17),	41.87(17),	44.02(17),

	1M =	51.60(18),	18.24(17),	53.4(2),	51.07(18),	53.32(18),	51.18(18),	32.04(17),	68.91(17),	22.4(3),	24.01(17),
	2M =	22.37(17),	39.58(19),	32.2(3),	41.87(17),	33.88(17),	51.18(18),	51.60(18),	68.91(17),	0.76(17),	5.41(17),
	3M =	7.84(19),	4.96(19),	37.4(2),	4.24(19),	48.1(2),					
-C(21A) /	0M =	8.09(17),	11.32(17),	45.69(17),	8.09(17),	1.29(18),	3.31(18),	8.28(15),	80.35(16),	4.73(16),	7.18(16),
	1M =	7.59(17),	79.50(16),	18.49(19),	12.99(17),	9.19(17),	67.07(17),	24.06(16),	48.20(16),	28.5(3),	31.34(16),
	2M =	83.34(16),	4.81(18),	19.3(3),	4.73(16),	24.65(16),	67.07(17),	7.59(17),	48.20(16),	1.12(16),	3.92(16),
	3M =	54.62(18),	53.68(18),	0.53(19),	43.65(18),	2.87(19),					
C(2B)h-C(6B)h /	0M =	46.11(19),	48.31(18),	11.30(18),	46.11(19),	6.41(19),	0.20(19),	2.88(16),	17.29(18),	35.97(17),	38.01(17),
	1M =	45.97(18),	17.31(17),	46.9(2),	44.85(18),	47.60(18),	49.50(18),	29.74(18),	68.62(17),	19.3(3),	21.82(17),
	2M =	21.41(17),	33.57(19),	28.8(3),	35.97(17),	40.11(17),	49.50(18),	45.97(18),	68.62(17),	7.42(17),	1.30(17),
	3M =	10.15(19),	7.15(19),	31.7(2),	7.76(19),	42.8(2),					
-C(21B) /	0M =	5.61(17),	8.89(17),	50.35(17),	5.61(17),	6.48(17),	1.80(17),	3.18(15),	77.40(16),	1.52(16),	4.03(16),
	1M =	5.13(17),	79.28(16),	15.65(19),	10.18(16),	6.80(17),	67.10(17),	25.70(16),	49.33(16),	31.2(3),	33.28(16),
	2M =	83.28(16),	1.39(18),	21.7(3),	1.52(16),	29.55(16),	67.10(17),	5.13(17),	49.33(16),	6.32(16),	1.23(16),
	3M =	58.73(18),	57.48(18),	2.85(19),	48.12(18),	0.37(18),					
C(3A)h-C(4A)h /	0M =	11.39(19),	14.63(18),	43.36(18),	11.39(19),	0.10(19),	4.93(19),	9.94(17),	77.56(18),	7.88(18),	10.34(17),
	1M =	10.90(18),	76.14(17),	21.7(2),	16.24(18),	12.50(18),	70.12(18),	20.69(18),	51.01(17),	25.3(3),	28.00(17),
	2M =	79.98(17),	7.89(19),	16.0(3),	7.88(18),	24.80(17),	70.12(18),	10.90(18),	51.01(17),	0.20(17),	5.46(17),
	3M =	51.9(2),	50.8(2),	3.6(2),	41.2(2),	6.2(2),					
C(4A)h-C(5A)h /	0M =	36.82(18),	34.66(18),	34.61(18),	36.82(18),	0.39(19),	1.78(19),	0.15(16),	42.06(17),	32.78(17),	31.72(17),
	1M =	37.29(18),	42.57(17),	26.1(2),	30.48(18),	36.60(18),	9.84(18),	64.57(17),	8.76(17),	55.7(3),	63.70(17),
	2M =	38.45(17),	30.70(19),	55.7(3),	32.78(17),	7.69(17),	9.84(18),	37.29(18),	8.76(17),	0.74(17),	0.15(17),
	3M =	42.02(19),	45.07(19),	33.8(2),	37.00(19),	40.48(19),					
-C(41A) /	0M =	54.51(18),	56.74(17),	4.18(17),	54.51(18),	1.74(18),	7.87(18),	10.74(15),	15.41(16),	44.40(16),	46.44(16),
	1M =	54.36(17),	14.56(16),	55.06(19),	53.25(17),	56.01(17),	47.56(17),	35.87(16),	65.06(16),	26.1(3),	27.85(16),
	2M =	18.69(16),	42.00(18),	35.9(3),	44.40(16),	31.69(16),	47.56(17),	54.36(17),	65.06(16),	0.70(16),	6.71(16),
	3M =	4.03(18),	1.13(19),	40.08(19),	0.61(18),	51.09(19),					
C(5A)h-C(6A)h /	0M =	51.34(19),	53.74(18),	8.05(18),	51.34(19),	0.35(19),	5.90(19),	9.02(16),	18.72(18),	41.39(18),	43.53(17),
	1M =	51.16(18),	18.08(17),	52.8(2),	50.55(18),	52.86(18),	50.98(18),	31.93(18),	68.89(17),	22.2(3),	23.91(17),
	2M =	22.21(17),	39.08(19),	32.0(3),	41.39(18),	34.41(17),	50.98(18),	51.16(18),	68.89(17),	1.35(17),	4.81(17),
	3M =	8.0(2),	5.1(2),	36.9(2),	4.48(19),	47.7(2),					
-C(51A) /	0M =	6.06(17),	9.33(17),	49.14(17),	6.06(17),	5.01(18),	0.38(18),	4.59(15),	78.66(16),	2.21(16),	4.70(16),
	1M =	5.58(17),	79.92(16),	16.23(19),	10.74(16),	7.22(17),	66.90(17),	25.54(16),	48.75(16),	30.7(3),	33.04(16),
	2M =	84.04(16),	2.15(18),	21.3(3),	2.21(16),	28.01(16),	66.90(17),	5.58(17),	48.75(16),	4.84(16),	0.21(16),
	3M =	57.76(18),	56.62(18),	2.10(19),	47.00(18),	0.83(19),					
Cu(1)i-O(51A) /	0M =	0.59(10),	2.63(10),	51.85(10),	0.59(10),	5.63(10),	1.66(10),	3.15(5),	82.95(8),	3.68(8),	1.27(7),
	1M =	1.09(9),	87.48(7),	9.89(12),	4.39(8),	0.49(8),	59.18(10),	32.76(8),	41.08(7),	37.1(2),	40.06(8),
	2M =	87.95(7),	3.49(11),	28.0(2),	3.68(8),	24.70(7),	59.18(10),	1.09(9),	41.08(7),	5.30(8),	0.86(7),
	3M =	61.71(12),	61.25(12),	7.77(12),	50.29(12),	5.80(12),					
-O(52A) /	0M =	0.33(10),	2.25(9),	54.83(9),	0.33(10),	44.78(10),	38.41(10),	33.73(4),	31.20(7),	10.01(7),	7.70(6),
	1M =	0.53(8),	35.74(6),	3.05(12),	0.36(8),	1.21(8),	45.30(9),	13.33(7),	50.52(7),	25.1(2),	20.27(7),
	2M =	37.98(7),	12.10(10),	16.7(2),	10.01(7),	76.49(6),	45.30(9),	0.53(8),	50.52(7),	45.28(7),	38.73(6),
	3M =	48.78(11),	45.72(11),	14.63(12),	51.67(11),	4.03(11),					
-O(22B) /	0M =	1.28(10),	4.45(10),	48.13(10),	1.28(10),	1.76(10),	2.16(10),	6.94(5),	86.76(8),	1.25(8),	1.10(7),
	1M =	0.78(9),	86.46(7),	11.97(12),	6.48(8),	2.29(8),	59.07(10),	31.36(8),	40.33(8),	34.9(2),	38.38(8),
	2M =	86.42(7),	0.91(11),	26.1(2),	1.25(8),	21.16(7),	59.07(10),	0.78(9),	40.33(8),	1.42(8),	2.97(7),
	3M =	58.19(12),	57.93(12),	5.19(12),	46.68(12),	3.88(12),					
-O(7W)i /	0M =	83.90(10),	81.52(10),	31.87(10),	83.90(10),	40.62(10),	45.75(10),	46.86(5),	0.17(8),	85.71(8),	86.40(7),

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	1M =	83.95(9),	4.15(7),	77.05(12),	82.47(8),	82.44(9),	22.76(10),	57.29(8),	30.60(8),	55.9(2),	51.76(8),
	2M =	0.93(8),	82.95(11),	64.4(2),	85.71(8),	9.68(7),	22.76(10),	83.95(9),	30.60(8),	39.43(8),	44.25(7),
	3M =	27.36(12),	29.29(12),	81.59(12),	35.21(12),	84.27(12),					
-O(11A) /	0M =	75.96(10),	76.24(10),	20.23(10),	75.96(10),	20.86(10),	26.07(10),	27.49(5),	0.19(8),	65.96(8),	67.15(7),
	1M =	76.09(9),	2.87(7),	69.10(12),	71.27(8),	76.98(8),	28.98(10),	57.84(8),	42.54(7),	49.8(2),	49.99(8),
	2M =	1.04(7),	63.19(11),	59.9(2),	65.96(8),	9.00(7),	28.98(10),	76.09(9),	42.54(7),	19.67(8),	24.61(7),
	3M =	19.18(12),	21.85(12),	62.64(12),	23.79(12),	74.57(12),					
-O(11B) /	0M =	9.30(10),	10.40(9),	25.39(9),	9.30(10),	45.92(10),	40.41(10),	38.16(5),	0.12(8),	0.85(8),	0.46(7),
	1M =	9.37(9),	3.95(6),	6.49(12),	5.94(8),	10.52(8),	23.31(9),	11.64(8),	38.70(7),	0.3(2),	6.54(7),
	2M =	6.73(7),	3.61(11),	5.4(2),	0.85(8),	67.68(7),	23.31(9),	9.37(9),	38.70(7),	47.09(7),	41.76(7),
	3M =	17.20(11),	14.34(11),	3.94(12),	22.99(11),	8.04(12),					
Cu(2)i-O(6W)i /	0M =	86.89(10),	86.94(10),	26.19(10),	86.89(10),	36.62(10),	42.13(10),	43.80(5),	4.37(8),	80.61(8),	82.71(7),
	1M =	86.43(9),	0.32(7),	81.59(12),	86.75(8),	86.55(9),	28.18(10),	54.08(8),	36.37(8),	51.2(2),	47.83(8),
	2M =	3.70(8),	78.29(11),	60.3(2),	80.61(8),	4.58(7),	28.18(10),	86.43(9),	36.37(8),	35.47(8),	40.72(7),
	3M =	21.99(12),	24.03(12),	75.97(12),	29.56(12),	82.39(12),					
-O(12A) /	0M =	2.70(10),	3.62(9),	26.48(9),	2.70(10),	52.41(10),	47.19(10),	45.21(5),	3.30(8),	7.32(8),	6.15(7),
	1M =	2.79(9),	1.03(6),	0.60(12),	0.94(8),	3.86(8),	17.54(9),	7.86(8),	31.99(7),	3.8(2),	3.50(7),
	2M =	3.44(7),	10.11(11),	0.9(2),	7.32(8),	67.62(7),	17.54(9),	2.79(9),	31.99(7),	53.61(7),	48.60(7),
	3M =	17.36(11),	14.70(11),	10.16(12),	24.46(11),	1.74(12),					
-O(12B) /	0M =	76.28(10),	77.27(10),	18.06(10),	76.28(10),	21.09(10),	26.52(10),	28.21(5),	2.83(8),	65.98(8),	67.47(7),
	1M =	76.30(9),	0.12(7),	71.01(12),	72.47(8),	77.53(8),	31.85(9),	54.97(8),	44.98(7),	47.3(2),	47.17(8),
	2M =	4.01(7),	63.29(11),	57.4(2),	65.98(8),	9.75(7),	31.85(9),	76.30(9),	44.98(7),	19.93(7),	25.10(7),
	3M =	16.63(12),	19.25(12),	62.25(12),	21.61(12),	73.88(12),					
Na(1)i-O(11A) /	0M =	10.17(10),	9.42(9),	29.64(9),	10.17(10),	64.64(10),	60.03(10),	58.42(5),	7.13(8),	19.99(8),	18.98(7),
	1M =	10.04(9),	2.00(6),	13.89(12),	14.06(8),	9.07(8),	8.36(9),	1.11(8),	20.63(7),	12.0(2),	4.18(7),
	2M =	0.39(7),	22.79(11),	8.9(2),	19.99(8),	64.32(7),	8.36(9),	10.04(9),	20.63(7),	65.87(7),	61.52(7),
	3M =	19.30(11),	17.12(11),	22.49(12),	28.42(11),	10.75(12),					
-O(21B) /	0M =	28.03(10),	31.34(9),	33.34(9),	28.03(10),	0.02(10),	6.08(10),	10.98(5),	56.52(8),	22.12(8),	24.74(7),
	1M =	27.59(9),	55.64(7),	36.90(12),	31.68(8),	29.37(8),	88.55(9),	1.75(8),	71.49(7),	8.4(2),	9.53(7),
	2M =	59.75(7),	21.33(11),	1.5(2),	22.12(8),	32.47(7),	88.55(9),	27.59(9),	71.49(7),	0.36(7),	6.00(7),
	3M =	38.40(11),	36.26(11),	17.37(12),	30.22(11),	22.84(12),					
-O(4W)i /	0M =	43.80(11),	42.07(11),	28.64(11),	43.80(11),	0.63(12),	3.13(12),	2.04(8),	31.91(10),	38.14(10),	37.53(9),
	1M =	44.23(10),	32.49(9),	33.63(13),	37.53(10),	43.84(10),	0.30(11),	65.43(10),	18.82(9),	54.2(3),	61.50(9),
	2M =	28.37(9),	35.75(12),	57.4(3),	38.14(10),	13.14(9),	0.30(11),	44.23(10),	18.82(9),	0.56(9),	1.47(9),
	3M =	34.64(13),	37.77(13),	38.23(13),	31.45(13),	46.72(13),					
-O(5W)i /	0M =	29.83(11),	33.11(11),	32.52(11),	29.83(11),	2.46(11),	3.80(11),	8.60(7),	51.80(9),	23.12(9),	25.75(9),
	1M =	29.41(10),	51.36(9),	37.94(13),	32.94(10),	31.23(10),	83.98(11),	1.37(9),	76.60(9),	6.1(3),	6.54(9),
	2M =	55.49(9),	22.08(12),	3.9(3),	23.12(9),	35.95(9),	83.98(11),	29.41(10),	76.60(9),	2.90(9),	3.59(9),
	3M =	36.51(13),	34.14(13),	18.29(13),	29.24(13),	24.73(13),					
-O(52A) /	0M =	38.27(10),	35.50(10),	47.49(10),	38.27(10),	11.08(10),	11.59(10),	8.98(5),	47.74(8),	36.94(8),	35.30(7),
	1M =	38.78(9),	49.85(7),	27.10(12),	32.20(8),	37.64(8),	16.90(9),	70.83(8),	0.39(7),	65.9(2),	73.71(7),
	2M =	45.78(7),	35.40(11),	62.6(2),	36.94(8),	5.20(7),	16.90(9),	38.78(9),	0.39(7),	10.03(7),	10.03(7),
	3M =	54.57(11),	57.67(11),	39.14(12),	49.88(11),	42.85(12),					
Na(2)i-O(52A) /	0M =	36.09(10),	35.46(10),	35.13(10),	36.09(10),	81.96(10),	84.41(10),	84.47(5),	9.10(8),	45.65(8),	44.84(7),
	1M =	35.94(9),	3.16(7),	39.82(12),	40.12(8),	35.05(8),	6.67(9),	21.42(8),	0.04(7),	30.0(2),	22.01(7),
	2M =	3.39(7),	48.45(11),	30.1(2),	45.65(8),	48.48(7),	6.67(9),	35.94(9),	0.04(7),	82.00(7),	85.97(7),
	3M =	24.29(11),	23.40(12),	47.61(12),	35.74(11),	36.27(12),					
-O(1W)i /	0M =	31.33(10),	28.82(10),	40.87(10),	31.33(10),	2.08(10),	2.45(10),	0.20(5),	50.96(8),	28.88(8),	27.44(7),

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	1M =	31.82(9),	51.69(7),	20.25(12),	25.08(8),	30.88(8),	18.86(9),	62.54(8),	0.37(7),	56.7(2),	64.57(7),
	2M =	47.57(7),	27.15(11),	53.9(2),	28.88(8),	1.13(7),	18.86(9),	31.82(9),	0.37(7),	1.05(7),	0.89(7),
	3M =	49.36(12),	52.26(12),	30.71(12),	42.82(11),	35.55(12),					
-O(3W)i /	0M =	35.70(10),	38.96(9),	26.90(9),	35.70(10),	0.30(10),	6.70(10),	11.33(5),	46.46(8),	28.65(8),	31.27(7),
	1M =	35.30(9),	45.61(6),	43.41(12),	38.56(8),	37.13(8),	78.66(9),	7.51(8),	80.16(7),	0.0(2),	0.39(7),
	2M =	49.74(7),	27.47(11),	10.0(2),	28.65(8),	34.27(7),	78.66(9),	35.30(9),	80.16(7),	0.25(7),	6.33(7),
	3M =	30.49(11),	28.08(11),	23.78(12),	23.56(11),	30.65(12),					
-O(41A) /	0M =	43.88(10),	41.30(10),	43.05(10),	43.88(10),	10.99(10),	12.31(10),	10.26(5),	40.84(8),	41.40(8),	40.02(7),
	1M =	44.38(9),	42.79(7),	32.77(12),	37.66(8),	43.39(8),	9.82(9),	74.63(8),	7.44(7),	66.3(2),	74.25(7),
	2M =	38.70(7),	39.58(11),	65.8(2),	41.40(8),	1.06(7),	9.82(9),	44.38(9),	7.44(7),	9.87(7),	10.69(7),
	3M =	48.97(12),	52.12(12),	43.01(12),	45.79(11),	48.16(12),					
O(11A)-C(11A) /	0M =	42.68(16),	44.00(16),	11.55(16),	42.68(16),	54.75(16),	60.29(16),	65.34(13),	32.66(15),	47.84(15),	48.85(14),
	1M =	42.27(15),	26.80(14),	51.84(17),	48.81(15),	42.46(15),	34.13(16),	14.58(15),	25.36(14),	18.3(3),	11.42(14),
	2M =	28.00(14),	49.83(16),	23.1(3),	47.84(15),	22.14(14),	34.13(16),	42.27(15),	25.36(14),	54.56(14),	60.56(14),
	3M =	1.61(17),	1.63(17),	46.41(17),	13.14(17),	39.82(17),					
O(11B)-C(11B) /	0M =	0.64(16),	0.82(16),	11.16(16),	0.64(16),	49.81(16),	47.30(16),	47.82(14),	22.90(15),	9.21(15),	8.90(15),
	1M =	0.38(16),	18.34(15),	7.25(18),	5.78(15),	0.12(15),	1.37(16),	15.22(15),	14.79(15),	5.2(3),	13.18(15),
	2M =	16.13(15),	11.94(17),	6.9(3),	9.21(15),	48.93(15),	1.37(16),	0.38(16),	14.79(15),	50.98(15),	48.96(15),
	3M =	0.95(17),	1.32(17),	10.52(18),	9.89(17),	0.20(17),					
O(12A)-C(11A) /	0M =	7.65(16),	7.49(16),	7.84(16),	7.65(16),	42.75(16),	39.68(16),	39.85(14),	21.70(15),	1.04(15),	0.67(15),
	1M =	7.90(16),	17.78(15),	1.04(18),	2.53(15),	8.41(15),	2.96(16),	22.02(15),	20.28(15),	11.4(3),	19.25(15),
	2M =	15.07(15),	3.78(17),	14.0(3),	1.04(15),	48.26(15),	2.96(16),	7.90(16),	20.28(15),	43.96(15),	41.32(15),
	3M =	1.72(17),	4.26(17),	2.50(18),	6.15(17),	8.38(17),					
O(12B)-C(11B) /	0M =	47.38(16),	48.98(16),	10.30(16),	47.38(16),	50.94(16),	56.94(16),	61.91(13),	33.00(15),	51.49(15),	52.80(14),
	1M =	46.94(15),	27.32(14),	57.10(17),	53.63(15),	47.30(15),	38.25(16),	17.71(15),	30.81(14),	20.2(3),	13.85(15),
	2M =	28.99(14),	53.18(16),	26.0(3),	51.49(15),	17.16(14),	38.25(16),	46.94(15),	30.81(14),	50.59(14),	56.94(14),
	3M =	0.91(17),	1.26(17),	49.44(17),	12.22(17),	44.10(17),					
O(21A)-C(21A) /	0M =	8.52(16),	7.68(16),	3.00(16),	8.52(16),	36.11(16),	34.42(16),	35.78(13),	33.34(15),	1.16(15),	0.99(14),
	1M =	8.86(15),	29.56(14),	0.20(17),	2.74(15),	8.99(15),	7.13(16),	28.63(15),	11.12(14),	19.2(3),	27.23(15),
	2M =	26.77(14),	1.41(16),	20.0(3),	1.16(15),	36.54(14),	7.13(16),	8.86(15),	11.12(14),	37.23(14),	36.06(14),
	3M =	12.94(17),	15.34(17),	0.66(17),	4.41(17),	10.31(17),					
O(21B)-C(21B) /	0M =	9.90(16),	11.93(16),	38.71(16),	9.90(16),	42.02(16),	35.57(16),	31.81(14),	18.37(15),	0.35(15),	1.60(15),
	1M =	9.81(16),	22.10(15),	10.63(18),	8.40(15),	11.36(15),	40.04(16),	2.11(15),	52.44(15),	9.9(3),	4.44(15),
	2M =	24.96(15),	2.82(17),	2.2(3),	0.35(15),	76.52(15),	40.04(16),	9.81(16),	52.44(15),	42.91(15),	36.44(15),
	3M =	32.37(17),	29.31(17),	4.47(18),	35.71(17),	7.09(17),					
O(22A)-C(21A) /	0M =	13.73(16),	15.90(16),	37.85(16),	13.73(16),	37.29(16),	30.81(16),	26.97(14),	21.38(15),	3.57(15),	5.61(15),
	1M =	13.61(16),	24.74(15),	15.01(18),	12.56(15),	15.21(15),	44.53(16),	3.66(15),	57.40(15),	8.2(3),	3.26(15),
	2M =	27.83(15),	1.17(17),	0.0(3),	3.57(15),	72.36(15),	44.53(16),	13.61(16),	57.40(15),	38.15(15),	31.65(15),
	3M =	32.50(17),	29.37(17),	0.69(18),	34.66(17),	10.67(17),					
O(22B)-C(21B) /	0M =	6.95(16),	5.93(16),	5.28(16),	6.95(16),	35.39(16),	34.20(16),	35.94(13),	36.88(15),	0.04(15),	0.28(14),
	1M =	7.31(15),	32.99(14),	1.78(17),	1.03(15),	7.33(15),	10.83(16),	28.77(15),	7.47(14),	19.9(3),	27.96(14),
	2M =	30.27(14),	2.46(16),	20.0(3),	0.04(15),	33.50(14),	10.83(16),	7.31(15),	7.47(14),	36.47(14),	35.83(14),
	3M =	15.44(17),	17.74(17),	0.15(17),	6.53(17),	9.03(17),					
O(41A)-C(41A) /	0M =	10.83(16),	10.31(16),	0.89(16),	10.83(16),	37.10(16),	34.61(16),	35.34(14),	27.49(15),	2.78(15),	2.88(15),
	1M =	11.13(16),	23.88(15),	3.26(18),	5.33(15),	11.44(15),	1.12(16),	27.91(15),	17.02(15),	17.7(3),	25.61(15),
	2M =	20.98(15),	0.11(17),	19.6(3),	2.78(15),	41.48(15),	1.12(16),	11.13(16),	17.02(15),	38.28(15),	36.27(15),
	3M =	8.65(17),	11.21(17),	1.79(18),	0.79(17),	12.11(17),					
O(42A)-C(41A) /	0M =	37.85(16),	39.95(16),	0.97(16),	37.85(16),	42.40(16),	47.71(16),	52.75(13),	44.80(15),	40.51(15),	42.12(14),

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	1M =	37.38(15),	39.04(14),	48.50(17),	44.18(15),	38.05(15),	45.56(16),	6.63(15),	34.17(14),	8.4(3),	2.29(15),
	2M =	40.48(14),	41.95(16),	14.6(3),	40.51(15),	11.45(14),	45.56(16),	37.38(15),	34.17(14),	42.31(14),	48.08(14),
	3M =	10.69(17),	10.48(17),	38.02(17),	0.75(17),	33.97(17),					
O(51A)-C(51A) /	0M =	1.49(16),	3.37(16),	41.94(16),	1.49(16),	51.13(16),	44.68(16),	40.91(13),	14.82(15),	8.82(15),	6.97(14),
	1M =	1.43(15),	19.23(14),	1.69(17),	0.34(15),	2.91(15),	32.88(16),	3.07(15),	43.72(14),	15.1(3),	8.93(15),
	2M =	21.58(14),	11.36(16),	8.3(3),	8.82(15),	83.94(14),	32.88(16),	1.43(15),	43.72(14),	52.02(14),	45.56(14),
	3M =	34.01(17),	31.13(17),	12.77(17),	39.35(17),	1.02(17),					
O(52A)-C(51A) /	0M =	1.35(16),	2.56(16),	4.80(16),	1.35(16),	39.24(16),	39.17(16),	41.66(14),	41.24(15),	7.66(15),	8.20(15),
	1M =	0.96(16),	36.60(15),	10.45(18),	7.39(15),	1.06(15),	18.03(16),	22.81(15),	0.38(15),	15.2(3),	23.13(15),
	2M =	34.47(15),	10.04(17),	13.9(3),	7.66(15),	30.70(15),	18.03(16),	0.96(16),	0.38(15),	40.19(15),	40.73(15),
	3M =	15.50(17),	17.41(17),	7.41(18),	5.50(17),	1.08(17),					
C(1A)i-C(2A)i /	0M =	36.33(18),	34.20(18),	34.09(18),	36.33(18),	0.27(18),	1.12(18),	0.80(16),	42.11(17),	32.22(17),	31.17(17),
	1M =	36.80(18),	42.52(17),	25.6(2),	30.00(18),	36.13(18),	9.86(18),	63.93(17),	8.81(17),	55.0(3),	63.04(17),
	2M =	38.41(17),	30.13(19),	55.1(3),	32.22(17),	8.21(17),	9.86(18),	36.80(18),	8.81(17),	1.39(17),	0.50(17),
	3M =	41.58(19),	44.61(19),	33.2(2),	36.46(19),	39.96(19),					
-C(6A)i /	0M =	11.61(19),	14.86(18),	43.31(18),	11.61(19),	0.02(19),	4.88(19),	9.89(16),	77.23(17),	8.05(17),	10.53(17),
	1M =	11.12(18),	75.86(17),	21.9(2),	16.44(18),	12.73(18),	70.45(18),	20.43(18),	51.35(17),	25.1(3),	27.75(17),
	2M =	79.72(17),	8.05(19),	15.8(3),	8.05(17),	25.02(17),	70.45(18),	11.12(18),	51.35(17),	0.11(17),	5.40(17),
	3M =	51.79(19),	50.67(19),	3.8(2),	41.09(19),	6.4(2),					
-C(11A) /	0M =	57.24(17),	59.38(17),	1.32(17),	57.24(17),	4.01(18),	10.05(18),	12.78(15),	13.64(16),	47.07(16),	49.06(16),
	1M =	57.10(17),	12.55(16),	57.29(19),	55.75(16),	58.73(17),	45.61(17),	38.55(16),	62.60(16),	28.9(3),	30.52(16),
	2M =	16.68(16),	44.63(18),	38.7(3),	47.07(16),	29.08(16),	45.61(17),	57.10(17),	62.60(16),	2.94(16),	8.86(16),
	3M =	1.30(18),	1.57(18),	42.81(19),	2.24(18),	53.91(19),					
C(1B)i-C(2B)i /	0M =	34.99(18),	32.84(18),	34.03(18),	34.99(18),	1.09(18),	0.19(18),	1.80(16),	43.21(17),	30.94(17),	29.87(17),
	1M =	35.46(18),	43.50(17),	24.3(2),	28.65(18),	34.78(18),	10.93(18),	62.86(17),	7.81(17),	54.3(3),	62.29(17),
	2M =	39.40(17),	28.87(19),	54.0(3),	30.94(17),	8.26(17),	10.93(18),	35.46(18),	7.81(17),	2.20(17),	1.43(17),
	3M =	41.75(19),	44.76(19),	32.0(2),	36.32(19),	38.64(19),					
-C(11B) /	0M =	51.09(17),	53.02(17),	5.14(17),	51.09(17),	2.71(17),	3.30(17),	5.99(15),	12.49(16),	40.81(16),	42.69(16),
	1M =	51.00(17),	12.12(16),	50.54(19),	49.19(16),	52.54(16),	44.80(17),	35.92(16),	63.36(16),	25.4(3),	27.99(16),
	2M =	16.24(16),	38.30(18),	34.9(3),	40.81(16),	35.34(16),	44.80(17),	51.00(17),	63.36(16),	3.78(16),	2.09(16),
	3M =	3.99(18),	0.99(18),	36.72(19),	1.61(18),	48.15(18),					
C(2A)i-C(3A)i /	0M =	51.79(19),	54.22(18),	7.80(18),	51.79(19),	0.23(19),	6.49(19),	9.63(16),	18.94(17),	41.87(17),	44.02(17),
	1M =	51.60(18),	18.24(17),	53.4(2),	51.07(18),	53.32(18),	51.18(18),	32.04(17),	68.91(17),	22.4(3),	24.01(17),
	2M =	22.37(17),	39.58(19),	32.2(3),	41.87(17),	33.88(17),	51.18(18),	51.60(18),	68.91(17),	0.76(17),	5.41(17),
	3M =	7.84(19),	4.96(19),	37.4(2),	4.24(19),	48.1(2),					
-C(21A) /	0M =	8.09(17),	11.32(17),	45.69(17),	8.09(17),	1.29(18),	3.31(18),	8.28(15),	80.35(16),	4.73(16),	7.18(16),
	1M =	7.59(17),	79.50(16),	18.49(19),	12.99(17),	9.19(17),	67.07(17),	24.06(16),	48.20(16),	28.5(3),	31.34(16),
	2M =	83.34(16),	4.81(18),	19.3(3),	4.73(16),	24.65(16),	67.07(17),	7.59(17),	48.20(16),	1.12(16),	3.92(16),
	3M =	54.62(18),	53.68(18),	0.53(19),	43.65(18),	2.87(19),					
C(2B)i-C(6B)i /	0M =	46.11(19),	48.31(18),	11.30(18),	46.11(19),	6.41(19),	0.20(19),	2.88(16),	17.29(18),	35.97(17),	38.01(17),
	1M =	45.97(18),	17.31(17),	46.9(2),	44.85(18),	47.60(18),	49.50(18),	29.74(18),	68.62(17),	19.3(3),	21.82(17),
	2M =	21.41(17),	33.57(19),	28.8(3),	35.97(17),	40.11(17),	49.50(18),	45.97(18),	68.62(17),	7.42(17),	1.30(17),
	3M =	10.15(19),	7.15(19),	31.7(2),	7.76(19),	42.8(2),					
-C(21B) /	0M =	5.61(17),	8.89(17),	50.35(17),	5.61(17),	6.48(17),	1.80(17),	3.18(15),	77.40(16),	1.52(16),	4.03(16),
	1M =	5.13(17),	79.28(16),	15.65(19),	10.18(16),	6.80(17),	67.10(17),	25.70(16),	49.33(16),	31.2(3),	33.28(16),
	2M =	83.28(16),	1.39(18),	21.7(3),	1.52(16),	29.55(16),	67.10(17),	5.13(17),	49.33(16),	6.32(16),	1.23(16),
	3M =	58.73(18),	57.48(18),	2.85(19),	48.12(18),	0.37(18),					
C(3A)i-C(4A)i /	0M =	11.39(19),	14.63(18),	43.36(18),	11.39(19),	0.10(19),	4.93(19),	9.94(17),	77.56(18),	7.88(18),	10.34(17),

C(4A)i-C(5A)i /	1M =	10.90(18),	76.14(17),	21.7(2),	16.24(18),	12.50(18),	70.12(18),	20.69(18),	51.01(17),	25.3(3),	28.00(17),	
	2M =	79.98(17),	7.89(19),	16.0(3),	7.88(18),	24.80(17),	70.12(18),	10.90(18),	51.01(17),	0.20(17),	5.46(17),	
	3M =	51.9(2),	50.8(2),	3.6(2),	41.2(2),	6.2(2),						
	0M =	36.82(18),	34.66(18),	34.61(18),	36.82(18),	0.39(19),	1.78(19),	0.15(16),	42.06(17),	32.78(17),	31.72(17),	
	1M =	37.29(18),	42.57(17),	26.1(2),	30.48(18),	36.60(18),	9.84(18),	64.57(17),	8.76(17),	55.7(3),	63.70(17),	
	2M =	38.45(17),	30.70(19),	55.7(3),	32.78(17),	7.69(17),	9.84(18),	37.29(18),	8.76(17),	0.74(17),	0.15(17),	
	3M =	42.02(19),	45.07(19),	33.8(2),	37.00(19),	40.48(19),						
	-C(41A) /	0M =	54.51(18),	56.74(17),	4.18(17),	54.51(18),	1.74(18),	7.87(18),	10.74(15),	15.41(16),	44.40(16),	46.44(16),
	1M =	54.36(17),	14.56(16),	55.06(19),	53.25(17),	56.01(17),	47.56(17),	35.87(16),	65.06(16),	26.1(3),	27.85(16),	
	2M =	18.69(16),	42.00(18),	35.9(3),	44.40(16),	31.69(16),	47.56(17),	54.36(17),	65.06(16),	0.70(16),	6.71(16),	
	3M =	4.03(18),	1.13(19),	40.08(19),	0.61(18),	51.09(19),						
	C(5A)i-C(6A)i /	0M =	51.34(19),	53.74(18),	8.05(18),	51.34(19),	0.35(19),	5.90(19),	9.02(16),	18.72(18),	41.39(18),	43.53(17),
1M =	51.16(18),	18.08(17),	52.8(2),	50.55(18),	52.86(18),	50.98(18),	31.93(18),	68.89(17),	22.2(3),	23.91(17),		
2M =	22.21(17),	39.08(19),	32.0(3),	41.39(18),	34.41(17),	50.98(18),	51.16(18),	68.89(17),	1.35(17),	4.81(17),		
3M =	8.0(2),	5.1(2),	36.9(2),	4.48(19),	47.7(2),							
-C(51A) /	0M =	6.06(17),	9.33(17),	49.14(17),	6.06(17),	5.01(18),	0.38(18),	4.59(15),	78.66(16),	2.21(16),	4.70(16),	
1M =	5.58(17),	79.92(16),	16.23(19),	10.74(16),	7.22(17),	66.90(17),	25.54(16),	48.75(16),	30.7(3),	33.04(16),		
2M =	84.04(16),	2.15(18),	21.3(3),	2.21(16),	28.01(16),	66.90(17),	5.58(17),	48.75(16),	4.84(16),	0.21(16),		
3M =	57.76(18),	56.62(18),	2.10(19),	47.00(18),	0.83(19),							
Cu(1)j-O(7W)j /	0M =	35.01(10),	31.87(10),	81.52(10),	35.01(10),	48.47(10),	46.05(10),	41.64(5),	38.16(8),	42.59(8),	39.96(7),	
1M =	35.36(9),	44.05(7),	27.79(12),	32.68(8),	33.50(9),	26.27(10),	52.43(8),	19.12(8),	64.4(2),	58.74(8),		
2M =	42.73(8),	43.64(11),	55.9(2),	42.59(8),	46.20(7),	26.27(10),	35.36(9),	19.12(8),	47.77(8),	44.94(7),		
3M =	72.45(12),	72.07(12),	47.44(12),	83.96(12),	39.72(12),							
-O(11A) /	0M =	23.54(10),	20.23(10),	76.24(10),	23.54(10),	29.25(10),	26.39(10),	21.90(5),	57.74(8),	28.59(8),	26.03(7),	
1M =	23.99(9),	63.53(7),	14.16(12),	19.55(8),	22.23(8),	39.85(10),	51.29(8),	27.30(7),	59.9(2),	59.32(8),		
2M =	61.70(7),	28.84(11),	49.8(2),	28.59(8),	36.50(7),	39.85(10),	23.99(9),	27.30(7),	28.66(8),	25.34(7),		
3M =	87.04(12),	87.75(12),	33.05(12),	76.00(12),	28.75(12),							
-O(11B) /	0M =	23.22(10),	25.39(9),	10.40(9),	23.22(10),	36.11(10),	40.05(10),	44.76(5),	54.94(8),	26.00(8),	27.52(7),	
1M =	22.74(9),	48.98(6),	33.97(12),	29.55(8),	23.46(8),	44.46(9),	7.88(8),	28.71(7),	5.4(2),	11.86(7),		
2M =	49.30(7),	27.55(11),	0.3(2),	26.00(8),	11.15(7),	44.46(9),	22.74(9),	28.71(7),	36.39(7),	40.89(7),		
3M =	20.92(11),	21.29(11),	23.73(12),	9.30(11),	19.31(12),							
Cu(2)j-O(6W)j /	0M =	29.35(10),	26.19(10),	86.94(10),	29.35(10),	45.61(10),	42.48(10),	37.83(5),	42.41(8),	36.82(8),	34.19(7),	
1M =	29.70(9),	48.36(7),	22.02(12),	26.92(8),	27.85(9),	32.02(10),	48.66(8),	24.71(8),	60.3(2),	55.59(8),		
2M =	47.39(8),	37.86(11),	51.2(2),	36.82(8),	48.51(7),	32.02(10),	29.70(9),	24.71(8),	45.04(8),	41.51(7),		
3M =	76.26(12),	74.98(12),	41.67(12),	86.67(12),	34.12(12),							
-O(12A) /	0M =	24.67(10),	26.48(9),	3.62(9),	24.67(10),	43.20(10),	46.85(10),	51.41(5),	47.99(8),	28.77(8),	29.99(7),	
1M =	24.22(9),	42.05(6),	34.86(12),	30.98(8),	24.70(8),	37.91(9),	4.76(8),	23.19(7),	0.9(2),	7.92(7),		
2M =	42.16(7),	30.62(11),	3.8(2),	28.77(8),	18.26(7),	37.91(9),	24.22(9),	23.19(7),	43.53(7),	47.78(7),		
3M =	14.30(11),	14.86(11),	27.09(12),	2.71(11),	21.26(12),							
-O(12B) /	0M =	21.36(10),	18.06(10),	77.27(10),	21.36(10),	30.05(10),	26.86(10),	22.25(5),	57.87(8),	26.80(8),	24.22(7),	
1M =	21.80(9),	63.78(7),	12.23(12),	17.58(8),	20.01(8),	42.03(9),	48.45(8),	30.04(7),	57.4(2),	56.46(8),		
2M =	62.38(7),	27.18(11),	47.3(2),	26.80(8),	39.05(7),	42.03(9),	21.80(9),	30.04(7),	29.52(7),	25.89(7),		
3M =	87.65(12),	85.44(12),	31.36(12),	76.26(12),	26.54(12),							
Na(1)j-O(4W)j /	0M =	31.20(11),	28.64(11),	42.07(11),	31.20(11),	2.95(12),	3.21(12),	0.50(8),	51.77(10),	29.01(10),	27.51(9),	
1M =	31.70(10),	52.65(9),	20.09(13),	24.98(10),	30.72(10),	19.75(11),	62.78(10),	1.35(9),	57.4(3),	65.16(9),		
2M =	48.52(9),	27.33(12),	54.2(3),	29.01(10),	0.10(9),	19.75(11),	31.70(10),	1.35(9),	1.94(9),	1.67(9),		
3M =	50.60(13),	53.50(13),	30.95(13),	44.00(13),	35.50(13),							
-O(5W)j /	0M =	29.44(11),	32.52(11),	33.11(11),	29.44(11),	10.76(11),	4.30(11),	0.22(7),	42.37(9),	21.14(9),	23.69(9),	

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	1M =	29.10(10),	43.11(9),	35.46(13),	31.16(10),	30.95(10),	72.81(11),	5.21(9),	83.58(9),	3.9(3),	2.82(9),
	2M =	47.14(9),	19.57(12),	6.1(3),	21.14(9),	45.61(9),	72.81(11),	29.10(10),	83.58(9),	11.36(9),	4.75(9),
	3M =	34.48(13),	31.69(13),	16.27(13),	29.59(13),	24.75(13),					
-O(52A) /	0M =	49.65(10),	47.49(10),	35.50(10),	49.65(10),	9.15(10),	11.52(10),	10.26(5),	31.96(8),	45.21(8),	44.31(7),
	1M =	50.12(9),	33.57(7),	38.90(12),	43.32(8),	49.44(8),	0.54(9),	73.97(8),	16.90(7),	62.6(2),	69.44(7),
	2M =	29.46(7),	42.99(11),	65.9(2),	45.21(8),	5.59(7),	0.54(9),	50.12(9),	16.90(7),	7.96(7),	9.86(7),
	3M =	40.34(11),	43.49(11),	45.80(12),	38.53(11),	53.22(12),					
Na(2)j-O(12B) /	0M =	8.89(10),	8.08(9),	30.08(9),	8.89(10),	63.61(10),	58.79(10),	57.01(5),	6.00(8),	18.78(7),	17.72(7),
	1M =	8.77(8),	0.94(6),	12.43(12),	12.69(8),	7.77(8),	9.95(9),	0.62(8),	22.31(7),	11.6(2),	3.90(7),
	2M =	0.75(7),	21.57(10),	8.2(2),	18.78(7),	65.67(7),	9.95(9),	8.77(8),	22.31(7),	64.84(7),	60.25(6),
	3M =	19.85(11),	17.61(11),	21.37(12),	28.75(11),	9.58(11),					
-O(22A) /	0M =	26.64(10),	29.95(10),	34.55(10),	26.64(10),	0.48(10),	5.56(10),	10.49(5),	57.94(8),	20.84(8),	23.46(7),
	1M =	26.19(9),	57.13(7),	35.59(12),	30.35(8),	27.96(8),	89.60(9),	3.24(8),	70.27(7),	9.9(2),	11.02(7),
	2M =	61.24(7),	20.09(11),	0.0(2),	20.84(8),	32.52(7),	89.60(9),	26.19(9),	70.27(7),	0.79(7),	5.52(7),
	3M =	39.77(11),	37.66(11),	16.10(12),	31.46(11),	21.43(12),					
-O(1W)j /	0M =	42.62(10),	40.87(10),	28.82(10),	42.62(10),	0.02(10),	2.37(10),	1.20(5),	33.00(8),	37.07(8),	36.42(7),
	1M =	43.05(9),	33.49(7),	32.42(12),	36.34(8),	42.64(8),	0.76(9),	64.91(8),	17.83(7),	53.9(2),	61.30(7),
	2M =	29.38(7),	34.70(11),	56.7(2),	37.07(8),	13.10(7),	0.76(9),	43.05(9),	17.83(7),	1.20(7),	0.71(7),
	3M =	35.05(12),	38.17(12),	37.23(12),	31.57(11),	45.60(12),					
-O(3W)j /	0M =	23.76(10),	26.90(9),	38.96(9),	23.76(10),	13.55(10),	7.20(10),	2.49(5),	47.00(8),	15.79(8),	18.37(7),
	1M =	23.41(9),	48.27(6),	30.32(12),	25.81(8),	25.26(8),	74.73(9),	0.93(8),	77.58(7),	10.0(2),	8.97(7),
	2M =	52.21(7),	14.35(11),	0.0(2),	15.79(8),	47.36(7),	74.73(9),	23.41(9),	77.58(7),	14.04(7),	7.50(7),
	3M =	40.61(11),	37.83(11),	10.91(12),	35.47(11),	18.98(12),					
-O(41A) /	0M =	45.54(10),	43.05(10),	41.30(10),	45.54(10),	10.71(10),	12.30(10),	10.44(5),	38.57(8),	42.61(8),	41.33(7),
	1M =	46.04(9),	40.45(7),	34.48(12),	39.28(8),	45.11(8),	7.46(9),	75.16(8),	9.82(7),	65.8(2),	73.55(7),
	2M =	36.36(7),	40.69(11),	66.3(2),	42.61(8),	0.50(7),	7.46(9),	46.04(9),	9.82(7),	9.57(7),	10.67(7),
	3M =	46.90(12),	50.05(12),	43.99(12),	44.13(11),	49.68(12),					
O(11A)-C(11A) /	0M =	13.10(16),	11.55(16),	44.00(16),	13.10(16),	67.13(16),	60.75(16),	57.02(13),	7.26(15),	23.43(15),	21.81(14),
	1M =	13.10(15),	12.55(14),	13.95(17),	15.57(15),	11.76(15),	19.18(16),	11.50(15),	27.97(14),	23.1(3),	15.80(14),
	2M =	13.94(14),	26.09(16),	18.3(3),	23.43(15),	76.13(14),	19.18(16),	13.10(15),	27.97(14),	68.08(14),	61.66(14),
	3M =	33.91(17),	31.61(17),	26.96(17),	42.49(17),	14.99(17),					
O(11B)-C(11B) /	0M =	10.06(16),	11.16(16),	0.82(16),	10.06(16),	46.55(16),	47.18(16),	50.03(14),	39.09(15),	16.54(15),	17.04(15),
	1M =	9.68(16),	33.83(15),	18.89(18),	16.04(15),	9.72(15),	20.26(16),	14.09(15),	4.01(15),	6.9(3),	14.77(15),
	2M =	32.37(15),	18.93(17),	5.2(3),	16.54(15),	32.59(15),	20.26(16),	9.68(16),	4.01(15),	47.39(15),	48.67(15),
	3M =	10.10(17),	11.69(17),	16.31(18),	0.53(17),	7.75(17),					
O(12A)-C(11A) /	0M =	6.34(16),	7.84(16),	7.49(16),	6.34(16),	38.48(16),	39.52(16),	42.73(14),	46.82(15),	11.75(15),	12.57(15),
	1M =	5.92(16),	41.75(15),	16.02(18),	12.54(15),	6.20(15),	25.37(16),	20.28(15),	7.91(15),	14.0(3),	21.70(15),
	2M =	40.05(15),	13.95(17),	11.4(3),	11.75(15),	25.19(15),	25.37(16),	5.93(16),	7.91(15),	39.28(15),	40.95(15),
	3M =	18.41(17),	19.99(17),	10.94(18),	7.75(17),	3.46(17),					
O(12B)-C(11B) /	0M =	12.16(16),	10.30(16),	48.98(16),	12.16(16),	63.95(16),	57.43(16),	53.20(13),	13.34(15),	22.48(15),	20.63(14),
	1M =	12.21(15),	18.60(14),	11.83(17),	13.98(15),	10.74(15),	24.62(16),	14.08(15),	32.16(14),	26.0(3),	19.03(15),
	2M =	20.02(14),	25.03(16),	20.2(3),	22.48(15),	80.54(14),	24.62(16),	12.21(15),	32.16(14),	64.70(14),	58.08(14),
	3M =	39.24(17),	36.80(17),	26.38(17),	47.17(17),	14.56(17),					
O(21A)-C(21A) /	0M =	4.24(16),	3.00(16),	7.68(16),	4.24(16),	34.90(16),	34.37(16),	36.60(13),	41.24(15),	2.08(15),	2.61(14),
	1M =	4.62(15),	37.11(14),	4.95(17),	1.83(15),	4.51(15),	15.70(16),	28.07(15),	2.59(14),	20.0(3),	28.03(15),
	2M =	34.57(14),	4.48(16),	19.2(3),	2.08(15),	29.84(14),	15.70(16),	4.62(15),	2.59(14),	35.90(14),	35.96(14),
	3M =	18.12(17),	20.25(17),	1.89(17),	8.67(17),	6.67(17),					
O(21B)-C(21B) /	0M =	35.97(16),	38.71(16),	11.93(16),	35.97(16),	29.54(16),	35.10(16),	40.15(14),	53.66(15),	35.77(15),	37.89(15),

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O(22A)-C(21A) /	1M =	35.46(16),	48.43(15),	47.14(18),	41.97(15),	36.59(15),	58.62(16),	2.94(15),	45.82(15),	2.2(3),	2.74(15),
	2M =	50.66(15),	36.51(17),	9.9(3),	35.77(15),	1.54(15),	58.62(16),	35.46(16),	45.82(15),	29.39(15),	35.34(15),
	3M =	20.86(17),	20.17(17),	32.27(18),	9.82(17),	31.27(17),					
	0M =	34.93(16),	37.85(16),	15.90(16),	34.93(16),	24.70(16),	30.34(16),	35.38(14),	56.20(15),	33.70(15),	35.96(15),
O(22B)-C(21B) /	1M =	34.42(16),	51.35(15),	46.03(18),	40.67(15),	35.70(15),	63.58(16),	1.73(15),	50.19(15),	0.0(3),	4.40(15),
	2M =	53.94(15),	34.18(17),	8.2(3),	33.70(15),	6.50(15),	63.58(16),	34.42(16),	50.19(15),	24.52(15),	30.54(15),
	3M =	24.44(17),	23.54(17),	29.90(18),	13.63(17),	30.02(17),					
	0M =	6.36(16),	5.28(16),	5.93(16),	6.36(16),	35.23(16),	34.19(16),	36.06(13),	37.97(15),	0.40(15),	0.78(14),
O(41A)-C(41A) /	1M =	6.73(15),	34.02(14),	2.49(17),	0.40(15),	6.72(15),	12.01(16),	28.70(15),	6.30(14),	20.0(3),	28.07(14),
	2M =	31.35(14),	2.88(16),	19.9(3),	0.40(15),	32.58(14),	12.01(16),	6.73(15),	6.30(14),	36.29(14),	35.81(14),
	3M =	16.16(17),	18.42(17),	0.50(17),	7.11(17),	8.53(17),					
	0M =	0.59(16),	0.89(16),	10.31(16),	0.59(16),	34.20(16),	34.51(16),	37.30(14),	46.35(15),	4.98(15),	5.73(15),
O(42A)-C(41A) /	1M =	1.01(16),	41.89(15),	9.07(18),	5.60(15),	0.74(15),	21.68(16),	26.59(15),	3.46(15),	19.6(3),	27.49(15),
	2M =	39.61(15),	7.22(17),	17.7(3),	4.98(15),	25.38(15),	21.68(16),	1.01(16),	3.46(15),	35.11(15),	36.02(15),
	3M =	21.03(17),	22.92(17),	4.33(18),	10.95(17),	3.42(17),					
	0M =	0.70(16),	0.97(16),	39.95(16),	0.70(16),	54.48(16),	48.16(16),	44.65(13),	10.55(15),	11.04(15),	9.33(14),
O(51A)-C(51A) /	1M =	0.73(15),	15.11(14),	1.27(17),	2.96(15),	0.67(15),	28.15(16),	2.62(15),	39.37(14),	14.6(3),	8.00(15),
	2M =	17.32(14),	13.66(16),	8.4(3),	11.04(15),	81.95(14),	28.15(16),	0.73(15),	39.37(14),	55.46(14),	49.14(14),
	3M =	31.37(17),	28.61(17),	14.76(17),	37.62(17),	2.86(17),					
	0M =	39.60(16),	41.94(16),	3.37(16),	39.60(16),	38.64(16),	44.22(16),	49.26(13),	46.34(15),	41.21(15),	43.03(14),
O(52A)-C(51A) /	1M =	39.11(15),	40.77(14),	50.54(17),	45.87(15),	39.95(15),	49.92(16),	7.50(15),	38.91(14),	8.3(3),	2.63(15),
	2M =	42.59(14),	42.37(16),	15.1(3),	41.21(15),	6.96(14),	49.92(16),	39.11(15),	38.91(14),	38.47(14),	44.46(14),
	3M =	12.69(17),	12.23(17),	38.28(17),	1.42(17),	35.39(17),					
	0M =	5.37(16),	4.80(16),	2.56(16),	5.37(16),	41.28(16),	39.25(16),	40.28(14),	29.10(15),	2.53(15),	2.50(15),
C(1A)j-C(2A)j /	1M =	5.68(16),	25.02(15),	2.29(18),	0.17(15),	5.96(15),	4.51(16),	23.66(15),	13.08(15),	13.9(3),	21.93(15),
	2M =	22.43(15),	5.17(17),	15.2(3),	2.53(15),	41.65(15),	4.51(16),	5.68(16),	13.08(15),	42.43(15),	40.91(15),
	3M =	7.45(17),	9.82(17),	3.37(18),	1.17(17),	6.77(17),					
	0M =	36.23(18),	34.09(18),	34.20(18),	36.23(18),	0.25(18),	1.12(18),	0.81(16),	42.27(17),	32.14(17),	31.09(17),
-C(6A)j /	1M =	36.70(18),	42.69(17),	25.5(2),	29.90(18),	36.02(18),	10.02(18),	63.91(17),	8.64(17),	55.1(3),	63.07(17),
	2M =	38.58(17),	30.06(19),	55.0(3),	32.14(17),	8.10(17),	10.02(18),	36.70(18),	8.64(17),	1.37(17),	0.50(17),
	3M =	41.71(19),	44.74(19),	33.1(2),	36.56(19),	39.87(19),					
	0M =	41.19(19),	43.31(18),	14.86(18),	41.19(19),	11.54(19),	5.32(19),	2.21(16),	17.10(17),	31.00(17),	32.99(17),
-C(11A) /	1M =	41.07(18),	17.68(17),	41.7(2),	39.77(18),	42.67(18),	48.85(18),	26.67(18),	68.26(17),	15.8(3),	18.89(17),
	2M =	21.71(17),	28.56(19),	25.1(3),	31.00(17),	45.15(17),	48.85(18),	41.07(18),	68.26(17),	12.55(17),	6.41(17),
	3M =	12.94(19),	9.86(19),	26.8(2),	11.35(19),	38.1(2),					
	0M =	1.99(17),	1.32(17),	59.38(17),	1.99(17),	14.89(18),	10.46(18),	5.53(15),	72.61(16),	6.78(16),	4.22(16),
C(1B)j-C(2B)j /	1M =	2.45(17),	77.57(16),	7.63(19),	2.21(16),	0.73(17),	61.05(17),	31.98(16),	45.68(16),	38.7(3),	39.85(16),
	2M =	79.25(16),	7.07(18),	28.9(3),	6.78(16),	35.12(16),	61.05(17),	2.45(17),	45.68(16),	14.67(16),	9.81(16),
	3M =	67.50(18),	65.95(18),	11.27(19),	57.14(18),	7.23(19),					
	0M =	36.09(18),	34.03(18),	32.84(18),	36.09(18),	1.29(18),	0.19(18),	1.66(16),	41.42(17),	31.74(17),	30.76(17),
-C(11B) /	1M =	36.56(18),	41.69(17),	25.5(2),	29.76(18),	35.93(18),	9.13(18),	63.09(17),	9.62(17),	54.0(3),	61.97(17),
	2M =	37.59(17),	29.61(19),	54.3(3),	31.74(17),	9.45(17),	9.13(18),	36.56(18),	9.62(17),	2.42(17),	1.45(17),
	3M =	40.35(19),	43.38(19),	32.6(2),	35.22(19),	39.62(19),					
	0M =	1.87(17),	5.14(17),	53.02(17),	1.87(17),	8.10(17),	3.71(17),	1.22(15),	78.64(16),	2.06(16),	0.43(16),
C(2A)j-C(3A)j /	1M =	1.38(17),	82.13(16),	11.98(19),	6.50(16),	3.04(16),	63.36(17),	29.51(16),	45.92(16),	34.9(3),	37.09(16),
	2M =	85.39(16),	2.12(18),	25.4(3),	2.06(16),	29.26(16),	63.36(17),	1.38(17),	45.92(16),	7.87(16),	3.04(16),
	3M =	61.92(18),	60.86(18),	6.37(19),	51.01(18),	3.37(18),					
	0M =	4.49(19),	7.80(18),	54.22(18),	4.49(19),	11.81(19),	6.92(19),	1.91(16),	71.95(17),	0.53(17),	2.05(17),

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	1M =	4.03(18),	75.15(17),	14.0(2),	8.59(18),	5.77(18),	67.60(18),	25.48(17),	51.74(17),	32.2(3),	33.33(17),
	2M =	78.49(17),	0.92(19),	22.4(3),	0.53(17),	35.44(17),	67.60(18),	4.03(18),	51.74(17),	11.71(17),	6.43(17),
	3M =	61.41(19),	59.65(19),	5.1(2),	51.66(19),	0.7(2),					
-C(21A) /	0M =	43.73(17),	45.69(17),	11.32(17),	43.73(17),	9.83(18),	3.73(18),	0.86(15),	14.02(16),	33.46(16),	35.35(16),
	1M =	43.64(17),	14.40(16),	43.49(19),	41.92(17),	45.18(17),	46.00(17),	30.28(16),	65.37(16),	19.3(3),	22.52(16),
	2M =	18.47(16),	30.95(18),	28.5(3),	33.46(16),	42.69(16),	46.00(17),	43.64(17),	65.37(16),	10.88(16),	4.90(16),
	3M =	9.30(18),	6.22(18),	29.36(19),	7.82(18),	40.84(19),					
C(2B)j-C(6B)j /	0M =	8.02(19),	11.30(18),	48.31(18),	8.02(19),	5.06(19),	0.24(19),	4.77(16),	76.52(18),	3.89(17),	6.41(17),
	1M =	7.54(18),	77.47(17),	18.1(2),	12.58(18),	9.20(18),	69.30(18),	23.34(18),	51.19(17),	28.8(3),	30.90(17),
	2M =	81.59(17),	3.74(19),	19.3(3),	3.89(17),	29.20(17),	69.30(18),	7.54(18),	51.19(17),	4.94(17),	0.29(17),
	3M =	56.47(19),	55.15(19),	0.5(2),	46.00(19),	2.8(2),					
-C(21B) /	0M =	48.22(17),	50.35(17),	8.89(17),	48.22(17),	4.76(17),	1.38(17),	4.32(15),	15.62(16),	38.03(16),	40.02(16),
	1M =	48.10(17),	15.46(16),	48.55(19),	46.76(16),	49.70(17),	47.91(17),	32.11(16),	66.79(16),	21.7(3),	24.18(16),
	2M =	19.58(16),	35.60(18),	31.2(3),	38.03(16),	38.12(16),	47.91(17),	48.10(17),	66.79(16),	5.80(16),	0.24(16),
	3M =	7.80(18),	4.80(18),	33.80(19),	5.35(18),	45.03(18),					
C(3A)j-C(4A)j /	0M =	41.25(19),	43.36(18),	14.63(18),	41.25(19),	11.57(19),	5.37(19),	2.28(17),	16.76(18),	31.05(18),	33.03(17),
	1M =	41.14(18),	17.34(17),	41.7(2),	39.79(18),	42.73(18),	48.51(18),	26.92(18),	67.93(17),	16.0(3),	19.15(17),
	2M =	21.37(17),	28.61(19),	25.3(3),	31.05(18),	45.11(17),	48.51(18),	41.14(18),	67.93(17),	12.59(17),	6.47(17),
	3M =	12.7(2),	9.6(2),	26.8(2),	11.1(2),	38.2(2),					
C(4A)j-C(5A)j /	0M =	36.77(18),	34.61(18),	34.66(18),	36.77(18),	0.39(19),	1.78(19),	0.15(16),	42.13(17),	32.75(17),	31.69(17),
	1M =	37.25(18),	42.64(17),	26.0(2),	30.44(18),	36.56(18),	9.91(18),	64.56(17),	8.69(17),	55.7(3),	63.71(17),
	2M =	38.52(17),	30.67(19),	55.7(3),	32.75(17),	7.64(17),	9.91(18),	37.25(18),	8.69(17),	0.73(17),	0.15(17),
	3M =	42.08(19),	45.12(19),	33.8(2),	37.05(19),	40.44(19),					
-C(41A) /	0M =	0.87(18),	4.18(17),	56.74(17),	0.87(18),	12.88(18),	8.29(18),	3.31(15),	73.44(16),	3.89(16),	1.33(16),
	1M =	0.40(17),	77.64(16),	10.51(19),	5.09(17),	2.13(17),	63.80(17),	29.32(16),	47.95(16),	35.9(3),	37.15(16),
	2M =	80.22(16),	4.18(18),	26.1(3),	3.89(16),	34.50(16),	63.80(17),	0.40(17),	47.95(16),	12.70(16),	7.69(16),
	3M =	64.63(18),	63.07(19),	8.38(19),	54.40(18),	4.37(19),					
C(5A)j-C(6A)j /	0M =	4.74(19),	8.05(18),	53.74(18),	4.74(19),	11.21(19),	6.33(19),	1.32(16),	72.48(18),	0.19(18),	2.38(17),
	1M =	4.27(18),	75.54(17),	14.3(2),	8.89(18),	6.01(18),	67.75(18),	25.38(18),	51.64(17),	32.0(3),	33.21(17),
	2M =	78.97(17),	0.56(19),	22.2(3),	0.19(18),	34.85(17),	67.75(18),	4.27(18),	51.64(17),	11.11(17),	5.83(17),
	3M =	61.1(2),	59.3(2),	4.7(2),	51.21(19),	0.5(2),					
-C(51A) /	0M =	47.09(17),	49.14(17),	9.33(17),	47.09(17),	6.16(18),	0.04(18),	2.86(15),	14.87(16),	36.86(16),	38.81(16),
	1M =	46.98(17),	14.86(16),	47.16(19),	45.48(16),	48.56(17),	47.11(17),	31.89(16),	66.18(16),	21.3(3),	24.01(16),
	2M =	18.97(16),	34.39(18),	30.7(3),	36.86(16),	39.31(16),	47.11(17),	46.98(17),	66.18(16),	7.20(16),	1.20(16),
	3M =	7.94(18),	4.92(18),	32.68(19),	5.80(18),	44.01(19),					

Ring Puckering Analysis (Cremer & Pople) - (e.s.d. following Norrestam, Acta Cryst. (1981), A37, 764-765)

Symmetrical Forms

References

6-Membered Rings : C : Chair - Th = 0.0
 H : Half-Chair- Th = 50.8; Phi = k X 60 + 30
 E : Envelope - Th = 54.7; Phi = k X 60
 S : Screw-Boat- Th = 67.5; Phi = k X 60 + 30
 B : Boat - Th = 90.0; Phi = k X 60
 T : Twist-Boat- Th = 90.0; Phi = k X 60 + 30

J.C.A. Boeyens, J.Cryst.Mol.Struct. 8,(1978),317-320

Definitions (All Values Rounded on Esd)

Dev - Deviation of Atom I from Cremer&Pople Plane (Defined Differently from Least-Squares Plane)
 Cs(I),C2(I) - Mirror Plane and 2-Axis Asym. Par. for Atom I (See Duax et al., Topics in Stereochemistry,V-9, (1976) pp.271-383)
 Cs(I-J),C2(I-J)- Asymmetry Parameters for Bond I-J
 Tors(I-J) - Torsion Angle for Bond I-J

Descriptors for Torsion Angles

Descriptors for Ring Substituents (J.Appl.Cryst.,1983,16,431)

Torsion Angle Range	Full Descriptor	Short Descriptor
0 to 30 Deg	+ Syn-Periplanar	+sp
30 to 90	+ Syn-Clinal	+sc
90 to 150	+ Anti-Clinal	+ac
150 to 180	+ Anti-Periplanar	+ap
0 to -30	- Syn-Periplanar	-sp
-30 to -90	- Syn-Clinal	-sc
-90 to -150	- Anti-Clinal	-ac
-150 to -180	- Anti-Periplanar	-ap

Angle Range of Subst.	Full Descriptor	Short Descriptor
0 to 30 Deg.	Axial	ax
30 to 60	Bisectional	bi
60 to 90	Equatorial	eq

*** NOTE *** - For Ring Puckering Comparisons: Make Sure that the Absolute Configuration, Pivot Atom and Cyclic Sense Agree.
 - The "RING AT1 AT2 AT3 ... ATn" Instruction Gives the User Explicit Choice of Pivot Atom (AT1) and Sense (AT2).
 - Use TRNS Instructions to Obtain the Required Absolute Configuration.
 - The Values of Theta and Phi [= Phi(2)] Depend on the Abs. Conf. and the Choice of the First and Second Ring Atom.
 - Alternatively, Appropriate Phase Shifts may be Applied to the Same Effect (see Below)

For Correct Usage of C&P Puckering Parameters see also: D. Cremer, Acta Cryst. (1984). B40, 498-500.

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=====
4-Membered Ring ( 1)  Cu(1)  -->  O(51A)  -->  C(51A)  -->  O(52A)  -->
-----
```

		sp3	sp2	
Dev. (Ang)	0.0143(10)	-0.014(2)	0.014(3)	-0.014(2)
Cs(I)-Asym-Par (Deg)	0.9(3)	1.6(2)	0.9(3)	1.6(2)
C2(I)-Asym-Par (Deg)	5.3(2)	5.1(2)	5.3(2)	5.1(2)
Ring Bond Angle(Deg)	52.16(6)	111.36(15)	123.9(2)	72.45(15)
Tors(I-J) (Deg)	-1.79(15)	3.9(3)	-2.6(2)	1.81(15)
Cs(I-J)-Asym-Par (Deg)	5.7(3)	4.4(3)	5.7(3)	4.4(3)
C2(I-J)-Asym-Par (Deg)	2.1(3)	0.8(3)	2.1(3)	0.8(3)
Ring Bond Distance (Ang)	1.9568(18)	1.284(3)	1.240(3)	2.805(2)

Weighted Average Ring Bond Distance = 2.0306(11,999) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 2.15(9, 37) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Angle between Cu(1) O(51A)O(52A) and O(51A)C(51A)O(52A) = 176.4(3) deg.

Angle between Cu(1) O(51A)C(51A) and Cu(1) C(51A)O(52A) = 176.8(3) deg.

No C & P - Puckering Analysis since <Tau> = 2.1 < 5.0 Deg.

Centroid Cg(1) : x ,y ,z	0.02637(10)	0.17557(6)	0.10392(6)
X0,Y0,Z0	-0.0225(8)	2.9679(9)	1.5993(9)

```
=====
4-Membered Ring ( 2)   Cu(2)  -->   O(41A)  -->   C(41A)  -->   O(42A)  -->
-----
```

			sp2	sp3
Dev. (Ang)	0.0094(10)	-0.009(2)	0.009(3)	-0.009(2)
Cs(I)-Asym-Par (Deg)	0.5(3)	1.0(2)	0.5(3)	1.0(2)
C2(I)-Asym-Par (Deg)	3.3(2)	3.2(2)	3.3(2)	3.2(2)
Ring Bond Angle(Deg)	54.69(6)	75.21(14)	123.0(2)	107.07(15)
Tors(I-J) (Deg)	-1.17(15)	1.7(2)	-2.4(3)	1.15(14)
Cs(I-J)-Asym-Par (Deg)	2.9(2)	3.6(3)	2.9(2)	3.6(3)
C2(I-J)-Asym-Par (Deg)	0.6(2)	1.2(3)	0.6(2)	1.2(3)
Ring Bond Distance (Ang)	2.6738(19)	1.245(3)	1.284(3)	1.9670(18)

Weighted Average Ring Bond Distance = 2.0161(11,999) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 1.37(9, 22) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Angle between Cu(2) O(41A)O(42A) and O(41A)C(41A)O(42A) = 177.7(3) deg.

Angle between Cu(2) O(41A)C(41A) and Cu(2) C(41A)O(42A) = 177.9(3) deg.

No C & P - Puckering Analysis since <Tau> = 1.4 < 5.0 Deg.

Centroid Cg(2) : x ,y ,z	-0.32645(10)	0.32744(5)	-0.25029(6)
X0,Y0,Z0	-2.0687(8)	5.5352(9)	-3.8519(9)

```
=====
4-Membered Ring ( 3)  O(41A) -->  C(41A) -->  O(42A) -->  Cu(2)c -->
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```

		sp2	sp3	
Dev. (Ang)	-0.009(2)	0.009(3)	-0.009(2)	0.0094(10)
Cs(I)-Asym-Par (Deg)	1.0(2)	0.5(3)	1.0(2)	0.5(3)
C2(I)-Asym-Par (Deg)	3.2(2)	3.3(2)	3.2(2)	3.3(2)
Ring Bond Angle(Deg)	75.21(14)	123.0(2)	107.07(15)	54.69(6)
Tors(I-J) (Deg)	1.7(2)	-2.4(3)	1.15(14)	-1.17(15)
Cs(I-J)-Asym-Par (Deg)	3.6(3)	2.9(2)	3.6(3)	2.9(2)
C2(I-J)-Asym-Par (Deg)	1.2(3)	0.6(2)	1.2(3)	0.6(2)
Ring Bond Distance (Ang)	1.245(3)	1.284(3)	1.9670(18)	2.6738(19)

Weighted Average Ring Bond Distance = 2.0161(11,999) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 1.37(9, 22) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Angle between O(41A)C(41A)Cu(2)c and C(41A)O(42A)Cu(2)c = 177.9(3) deg.

Angle between O(41A)C(41A)O(42A) and O(41A)O(42A)Cu(2)c = 177.7(3) deg.

No C & P - Puckering Analysis since <Tau> = 1.4 < 5.0 Deg.

Centroid Cg(3) : x , y , z	0.32645(10)	-0.17256(5)	-0.24971(6)
X0,Y0,Z0	3.2016(8)	-2.9170(9)	-3.8430(9)


```
=====
4-Membered Ring ( 4)  O(51A) -->  C(51A) -->  O(52A) -->  Cu(1)i -->
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	sp3	sp2		
Dev. (Ang)	0.014(2)	-0.014(3)	0.014(2)	-0.0143(10)
Cs(I)-Asym-Par (Deg)	1.6(2)	0.9(3)	1.6(2)	0.9(3)
C2(I)-Asym-Par (Deg)	5.1(2)	5.3(2)	5.1(2)	5.3(2)
Ring Bond Angle(Deg)	111.36(15)	123.9(2)	72.45(15)	52.16(6)
Tors(I-J) (Deg)	-3.9(3)	2.6(2)	-1.81(15)	1.79(15)
Cs(I-J)-Asym-Par (Deg)	4.4(3)	5.7(3)	4.4(3)	5.7(3)
C2(I-J)-Asym-Par (Deg)	0.8(3)	2.1(3)	0.8(3)	2.1(3)
Ring Bond Distance (Ang)	1.284(3)	1.240(3)	2.805(2)	1.9568(18)

Weighted Average Ring Bond Distance = 2.0306(11,999) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 2.15(9, 37) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Angle between O(51A)C(51A)Cu(1)i and C(51A)O(52A)Cu(1)i = 176.8(3) deg.

Angle between O(51A)C(51A)O(52A) and O(51A)O(52A)Cu(1)i = 176.4(3) deg.

No C & P - Puckering Analysis since <Tau> = 2.1 < 5.0 Deg.

Centroid Cg(4) : x , y , z	-0.02637(10)	-0.17557(6)	-0.10392(6)
X0,Y0,Z0	0.0225(8)	-2.9679(9)	-1.5993(9)

6-Membered Ring (5)	C(1A) -->	C(2A) -->	C(3A) -->	C(4A) -->	C(5A) -->	C(6A) -->
	sp2	sp2	sp2	sp2	sp2	sp2
Dev. (Ang)	-0.002(3)	0.004(3)	-0.001(3)	-0.004(3)	0.006(3)	-0.003(3)
Cs(I)-Asym-Par (Deg)	1.0(3)	0.1(3)	1.1(3)	1.0(3)	0.1(3)	1.1(3)
C2(I)-Asym-Par (Deg)	0.8(3)	1.2(3)	0.6(3)	0.8(3)	1.2(3)	0.6(3)
Ring Bond Angle(Deg)	119.4(2)	119.0(2)	121.3(2)	119.7(2)	119.2(2)	121.5(2)
Tors(I-J) (Deg)	0.6(4)	-0.5(4)	-0.3(4)	0.9(4)	-0.9(4)	0.1(4)
Cs(I-J)-Asym-Par (Deg)	0.9(4)	0.7(4)	0.4(4)	0.9(4)	0.7(4)	0.4(4)
C2(I-J)-Asym-Par (Deg)	0.6(4)	0.9(4)	1.5(4)	0.6(4)	0.9(4)	1.5(4)
Ring Bond Distance (Ang)	1.403(4)	1.399(4)	1.388(4)	1.400(4)	1.390(4)	1.396(4)

Weighted Average Ring Bond Distance = 1.3960(16, 24) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.55(16, 13) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 0.6 < 5.0 Deg.

Centroid Cg(5) : x , y , z	0.16880(12)	0.02042(6)	-0.16071(7)
X0,Y0,Z0	1.7270(10)	0.3451(11)	-2.4733(11)

6-Membered Ring (6)	C(1B) -->	C(2B) -->	C(6B) -->	C(1B)h -->	C(2B)h -->	C(6B)h -->
	sp2	sp2	sp2	sp2	sp2	sp2
Dev. (Ang)	-0.002(3)	0.002(3)	-0.002(3)	0.002(3)	-0.002(3)	0.002(3)
Cs(I)-Asym-Par (Deg)	0.00	0.00	0.00	0.00	0.00	0.00
C2(I)-Asym-Par (Deg)	1.4(3)	1.4(3)	1.4(3)	1.4(3)	1.4(3)	1.4(3)
Ring Bond Angle(Deg)	118.9(2)	119.2(2)	121.9(2)	118.9(2)	119.2(2)	121.9(2)
Tors(I-J) (Deg)	0.7(4)	-0.7(4)	0.7(4)	-0.7(4)	0.7(4)	-0.7(4)
Cs(I-J)-Asym-Par (Deg)	1.4(4)	1.4(4)	1.4(4)	1.4(4)	1.4(4)	1.4(4)
C2(I-J)-Asym-Par (Deg)	0.00	0.00	0.00	0.00	0.00	0.00
Ring Bond Distance (Ang)	1.403(4)	1.395(4)	1.399(4)	1.403(4)	1.395(4)	1.399(4)

Weighted Average Ring Bond Distance = 1.3990(16, 15) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.70(16, 0) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 0.7 < 5.0 Deg.

Centroid Cg(6) : x ,y ,z	-0.50000(12)	0.50000(6)	0.00000(7)
X0,Y0,Z0	-4.0371(10)	8.4522(11)	0.0000(11)

=====

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 Deg.

=====

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(1)	[1]	-> Cg(2)	[4555.01]	3.8915(12)	-0.2639-0.5448 0.7960 2.3148	62.82	45.56	47.03	2.653	2.725	
Cg(1)	[1]	-> Cg(3)	[3555.01]	3.8915(12)	0.2639 0.5448-0.7960 -2.3148	62.82	45.56	47.03	2.653	2.725	
Cg(1)	[1]	-> Cg(5)	[1555.01]	5.1503(14)	0.4030-0.1154 0.9079 -1.5893	55.22	3.49	58.52	2.690	5.141	
Cg(2)	[1]	-> Cg(1)	[4554.01]	3.8914(12)	-0.2871-0.4970 0.8189 -8.0361	62.82	47.03	45.56	2.725	2.653	
Cg(2)	[1]	-> Cg(4)	[2554.01]	3.8914(12)	0.2871 0.4970-0.8189 8.0361	62.82	47.03	45.56	2.725	2.653	
Cg(2)	[1]	-> Cg(6)	[1555.01]	5.2173(14)	0.3835-0.0043 0.9235 -1.5848	50.83	7.34	57.67	2.790	5.175	
Cg(2)	[1]	-> Cg(6)	[3465.01]	5.2173(14)	-0.3835 0.0043-0.9235 1.5848	50.83	7.34	57.67	2.790	5.175	
Cg(3)	[1]	-> Cg(1)	[3555.01]	3.8914(12)	0.2871-0.4970-0.8189 2.7912	62.82	47.03	45.56	2.725	2.653	
Cg(3)	[1]	-> Cg(4)	[1555.01]	3.8914(12)	-0.2871 0.4970 0.8189 -2.7912	62.82	47.03	45.56	2.725	2.653	
Cg(3)	[1]	-> Cg(6)	[2544.01]	5.2173(14)	-0.3835-0.0043-0.9235 5.1241	50.83	7.34	57.67	2.790	5.175	
Cg(3)	[1]	-> Cg(6)	[4654.01]	5.2173(14)	0.3835 0.0043 0.9235 -5.1241	50.83	7.34	57.67	2.790	5.175	
Cg(4)	[1]	-> Cg(2)	[2544.01]	3.8915(12)	0.2639 0.5448-0.7960 2.3148	62.82	45.56	47.03	2.653	2.725	
Cg(4)	[1]	-> Cg(3)	[1555.01]	3.8915(12)	-0.2639-0.5448 0.7960 -2.3148	62.82	45.56	47.03	2.653	2.725	
Cg(4)	[1]	-> Cg(5)	[3555.01]	5.1503(14)	-0.4030 0.1154-0.9079 -1.5893	55.22	3.49	58.52	2.690	5.141	
Cg(5)	[1]	-> Cg(1)	[1555.01]	5.1504(14)	-0.2871 0.4970 0.8189 2.7912	55.22	58.52	3.49	5.141	2.690	
Cg(5)	[1]	-> Cg(4)	[3555.01]	5.1504(14)	0.2871-0.4970-0.8189 -2.7912	55.22	58.52	3.49	5.141	2.690	
Cg(6)	[1]	-> Cg(2)	[1555.01]	5.2174(14)	-0.2639 0.5448 0.7960 0.4950	50.83	57.67	7.34	5.175	2.790	
Cg(6)	[1]	-> Cg(2)	[3465.01]	5.2174(14)	0.2639-0.5448-0.7960 -10.8441	50.83	57.67	7.34	5.175	2.790	
Cg(6)	[1]	-> Cg(3)	[2554.01]	5.2174(14)	0.2639-0.5448-0.7960 -0.4950	50.83	57.67	7.34	5.175	2.790	
Cg(6)	[1]	-> Cg(3)	[4455.01]	5.2174(14)	-0.2639 0.5448 0.7960 10.8441	50.83	57.67	7.34	5.175	2.790	
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Min or Max				3.891		50.83	3.49	58.52	2.653	2.653	

- [4555] = X,1/2-Y,1/2+Z
- [3555] = -X,-Y,-Z
- [1555] = X,Y,Z
- [4554] = X,1/2-Y,-1/2+Z
- [2554] = -X,1/2+Y,-1/2-Z
- [3465] = -1-X,1-Y,-Z
- [2544] = -X,-1/2+Y,-1/2-Z
- [4654] = 1+X,1/2-Y,-1/2+Z
- [4455] = -1+X,1/2-Y,1/2+Z

=====
 Geometry around Metals Involving Ring centroids
 =====

Cg(4)	--	Cu(1)	1.7477(10)
Cg(4)	--	Cu(1) -- O(7W)	85.01(6)
Cg(4)	--	Cu(1) -- O(11A)	83.75(6)
Cg(4)	--	Cu(1) -- O(11B)	125.04(6)
Cg(4)	--	Cu(1) -- O(22B)b	147.35(6)
O(7W)	--	Cu(1)	2.0079(19)
O(7W)	--	Cu(1) -- O(11A)	160.24(7)
O(7W)	--	Cu(1) -- O(11B)	86.56(7)
O(7W)	--	Cu(1) -- O(22B)b	90.75(8)
O(11A)	--	Cu(1)	1.9505(18)
O(11A)	--	Cu(1) -- O(11B)	113.19(7)
O(11A)	--	Cu(1) -- O(22B)b	90.00(8)
O(11B)	--	Cu(1)	2.3539(19)
O(11B)	--	Cu(1) -- O(22B)b	86.83(7)
O(22B)b	--	Cu(1)	1.9466(18)
Cg(3)	--	Cu(2)	1.6941(10)
Cg(3)	--	Cu(2) -- O(6W)	87.58(6)
Cg(3)	--	Cu(2) -- O(12A)	123.06(6)
Cg(3)	--	Cu(2) -- O(12B)	84.30(6)
Cg(3)	--	Cu(2) -- O(21A)a	142.57(6)
O(6W)	--	Cu(2)	2.0242(19)
O(6W)	--	Cu(2) -- O(12A)	89.33(7)
O(6W)	--	Cu(2) -- O(12B)	164.37(7)
O(6W)	--	Cu(2) -- O(21A)a	86.72(8)
O(12A)	--	Cu(2)	2.2233(18)
O(12A)	--	Cu(2) -- O(12B)	106.29(7)
O(12A)	--	Cu(2) -- O(21A)a	93.84(7)
O(12B)	--	Cu(2)	1.9792(18)
O(12B)	--	Cu(2) -- O(21A)a	91.65(8)
O(21A)a	--	Cu(2)	1.9459(18)
Cg(1)	--	Na(1)	2.9463(14)
Cg(1)	--	Na(1) -- O(4W)	165.29(8)
Cg(1)	--	Na(1) -- O(5W)	91.88(9)
Cg(1)	--	Na(1) -- O(41A)a	106.51(6)
Cg(1)	--	Na(1) -- O(21B)g	93.13(6)
Cg(1)	--	Na(1) -- O(11A)i	53.61(5)
O(4W)	--	Na(1)	2.275(3)
O(4W)	--	Na(1) -- O(5W)	83.93(11)
O(4W)	--	Na(1) -- O(41A)a	87.45(8)
O(4W)	--	Na(1) -- O(21B)g	91.53(9)
O(4W)	--	Na(1) -- O(11A)i	113.46(8)
O(5W)	--	Na(1)	2.377(3)
O(5W)	--	Na(1) -- O(41A)a	87.51(10)
O(5W)	--	Na(1) -- O(21B)g	174.81(10)
O(5W)	--	Na(1) -- O(11A)i	102.22(10)

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O(41A)a -- Na(1)                2.367(2)
O(41A)a -- Na(1) -- O(21B)g     89.80(7)
O(41A)a -- Na(1) -- O(11A)i    157.54(8)
O(21B)g -- Na(1)                2.413(2)
O(21B)g -- Na(1) -- O(11A)i     81.87(7)
O(11A)i -- Na(1)                2.449(2)
Cg(2)   -- Na(2)                2.9888(14)
Cg(2)   -- Na(2) -- O(1W)       166.78(7)
Cg(2)   -- Na(2) -- O(3W)       102.21(7)
Cg(2)   -- Na(2) -- O(52A)b     105.89(6)
Cg(2)   -- Na(2) -- O(12B)c     52.41(5)
Cg(2)   -- Na(2) -- O(22A)e     89.03(5)
Cg(3)   -- Na(2)                2.9888(14)
Cg(3)   -- Na(2) -- O(1W)       166.78(7)
Cg(3)   -- Na(2) -- O(3W)       102.21(7)
Cg(3)   -- Na(2) -- O(52A)b     105.89(6)
Cg(3)   -- Na(2) -- O(12B)c     52.41(5)
Cg(3)   -- Na(2) -- O(22A)e     89.03(5)
O(1W)   -- Na(2)                2.323(2)
O(1W)   -- Na(2) -- O(3W)       82.46(8)
O(1W)   -- Na(2) -- O(52A)b     86.87(7)
O(1W)   -- Na(2) -- O(12B)c    114.38(8)
O(1W)   -- Na(2) -- O(22A)e     89.02(7)
O(3W)   -- Na(2)                2.473(2)
O(3W)   -- Na(2) -- O(52A)b     82.95(9)
O(3W)   -- Na(2) -- O(12B)c    115.05(8)
O(3W)   -- Na(2) -- O(22A)e    164.33(9)
O(52A)b -- Na(2)                2.371(2)
O(52A)b -- Na(2) -- O(12B)c    152.90(8)
O(52A)b -- Na(2) -- O(22A)e     83.47(8)
O(12B)c -- Na(2)                2.538(2)
O(12B)c -- Na(2) -- O(22A)e     80.45(7)
O(22A)e -- Na(2)                2.391(2)

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Analysis of Y-X...Cg(Pi-Ring) Interactions (X..Cg < 4.0 Ang. - Gamma < 30.0 Deg)

Y--X(I)	Res(I)	Cg(J)	[	ARU(J)]	X..Cg	Transformed J-Plane P, Q, R, S				X-Perp	Gamma	Y-X..Cg	Y..Cg	Y-X, Pi	
Na(2)	-O(3W)	[1] -> Cg(6)	[	2544.01]	3.677(3)	-0.3835	-0.0043	-0.9235	5.1241	3.642	7.81	80.32(7)	4.0713(15)	7.20	
Na(2)	-O(3W)	[1] -> Cg(6)	[	4654.01]	3.677(3)	0.3835	0.0043	0.9235	-5.1241	3.642	7.81	80.32(7)	4.0713(15)	7.20	
Na(1)	-O(5W)	[1] -> Cg(5)	[	3555.01]	3.530(3)	-0.4030	0.1154	-0.9079	-1.5893	3.470	10.57	91.93(9)	4.3217(15)	2.46	

					Min or Max	3.530					3.470	7.81	91.93	4.071	7.20

[2544] = -X, -1/2+Y, -1/2-Z
 [4654] = 1+X, 1/2-Y, -1/2+Z
 [3555] = -X, -Y, -Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.02637(10)	0.17557(6)	0.10392(6)	-0.0225(8)	2.9679(9)	1.5993(9)
Cg(2)	-0.32645(10)	0.32744(5)	-0.25029(6)	-2.0687(8)	5.5352(9)	-3.8519(9)
Cg(3)	0.32645(10)	-0.17256(5)	-0.24971(6)	3.2016(8)	-2.9170(9)	-3.8430(9)
Cg(4)	-0.02637(10)	-0.17557(6)	-0.10392(6)	0.0225(8)	-2.9679(9)	-1.5993(9)
Cg(5)	0.16880(12)	0.02042(6)	-0.16071(7)	1.7270(10)	0.3451(11)	-2.4733(11)
Cg(6)	-0.50000(12)	0.50000(6)	0.00000(7)	-4.0371(10)	8.4522(11)	0.0000(11)

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Analysis of Short Intra- and Inter-molecular Contacts , d(I-J) < R(I) + R(J) + Tolr, With Tolr = 0.2 Ang. (X - I...J) > 100. Deg.

Contact Radii : C H Cu Na O
(Angstrom) 1.70 1.20 2.32 1.77 1.52

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

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***** ARU = 1555.01 *****

=====

At(I)[1555.01]	At(J)	[	ARU(J)	]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J	
Cu(1)		0(2W)	[		]	3.534(2)<<	3.84	-0.31		0.0411	0.2651	0.0493	-0.0156	0.4620	0.1156	0(11A)	144.61(7)
Cu(1)		0(12A)	[		]	3.112(2)<<	3.84	-0.73	Intra	0.0411	0.2651	0.0493	-0.1160	0.1821	-0.1219	0(7W)	149.90(6)
Cu(1)		0(21B)	[	1655.01]		3.1352(17)<<	3.84	-0.70	Intra	0.0411	0.2651	0.0493	0.4283	0.2950	0.0735	0(11B)	132.06(6)
Cu(1)		0(1W)	[	2654.01]		3.765(2) <	3.84	-0.07	Intra	0.0411	0.2651	0.0493	0.0907	0.3865	-0.1482	0(7W)	121.92(6)
Cu(1)		0(52A)	[	3555.01]		2.805(2)<<	3.84	-1.03	Intra	0.0411	0.2651	0.0493	0.1540	0.1346	0.1530	0(11B)	147.27(6)
Cu(1)		0(6W)	[	4555.01]		4.0290(18)	3.84	0.19		0.0411	0.2651	0.0493	-0.3107	0.3177	0.1993	0(11A)	151.73(6)
Cu(1)		0(22A)	[	4555.01]		3.858(2)	3.84	0.02		0.0411	0.2651	0.0493	0.2691	0.2736	0.2850	0(11A)	119.70(6)
																0(11B)	126.79(6)
Cu(2)		0(11B)	[		]	3.347(2)<<	3.84	-0.49	Intra	-0.3392	0.2436	-0.1920	-0.1881	0.3429	-0.0114	0(6W)	152.37(6)
Cu(2)		0(22A)	[	1455.01]		3.1443(17)<<	3.84	-0.70	Intra	-0.3392	0.2436	-0.1920	-0.7309	0.2264	-0.2150	0(12A)	137.95(6)
Cu(2)		0(41A)	[	2554.01]		2.6738(19)<<	3.84	-1.17	Intra	-0.3392	0.2436	-0.1920	-0.4578	0.3619	-0.2973	0(12A)	147.42(6)
Cu(2)		0(4W)	[	3455.01]		3.672(2) <	3.84	-0.17	Intra	-0.3392	0.2436	-0.1920	-0.3966	0.1313	0.0035	0(6W)	118.10(7)
Cu(2)		0(7W)	[	4554.01]		4.0102(17)	3.84	0.17		-0.3392	0.2436	-0.1920	0.0147	0.1847	-0.3365	0(12B)	149.54(6)
Cu(2)		0(21B)	[	4554.01]		3.907(2)	3.84	0.07		-0.3392	0.2436	-0.1920	-0.5717	0.2050	-0.4265	0(12A)	128.69(6)
																0(12B)	124.61(6)
0(1W)		0(3W)	[		]	3.163(3)	3.04	0.12	Intra	0.9093	-0.1135	-0.3518	0.6832	0.0100	-0.2696		
0(1W)		0(42A)	[	1655.01]		2.719(2)<<	3.04	-0.32	Intra	0.9093	-0.1135	-0.3518	1.2039	-0.1708	-0.2681	Na(2)	117.81(9)
0(1W)		0(52A)	[	1655.01]		3.227(3)	3.04	0.19	Intra	0.9093	-0.1135	-0.3518	0.8460	-0.1346	-0.1530		
0(1W)		C(5A)	[	1655.01]		3.419(3)	3.22	0.20	Intra	0.9093	-0.1135	-0.3518	1.0851	-0.0509	-0.1501		
0(1W)		Cu(1)	[	2644.01]		3.765(2) <	3.84	-0.07	Intra	0.9093	-0.1135	-0.3518	0.9589	-0.2349	-0.5493	Na(2)	116.88(7)
0(1W)		0(22B)	[	2544.01]		2.712(3)<<	3.04	-0.33	Intra	0.9093	-0.1135	-0.3518	0.8169	-0.1480	-0.5223	Na(2)	104.53(8)
0(1W)		C(21B)	[	2544.01]		3.360(3)	3.22	0.14	Intra	0.9093	-0.1135	-0.3518	0.6563	-0.1488	-0.5392		
0(1W)		0(2W)	[	4654.02]		2.697(3)<<	3.04	-0.34		0.9093	-0.1135	-0.3518	0.9844	0.0380	-0.3844	Na(2)	116.96(9)
0(3W)		0(1W)	[		]	3.163(3)	3.04	0.12	Intra	0.6832	0.0100	-0.2696	0.9093	-0.1135	-0.3518		
0(3W)		0(6W)	[	1655.01]		2.955(3) <	3.04	-0.09	Intra	0.6832	0.0100	-0.2696	0.6893	0.1823	-0.3007	Na(2)	163.79(12)
0(3W)		0(52A)	[	1655.01]		3.209(3)	3.04	0.17	Intra	0.6832	0.0100	-0.2696	0.8460	-0.1346	-0.1530		
0(3W)		C(3A)	[		]	3.332(4)	3.22	0.11	Intra	0.6832	0.0100	-0.2696	0.3150	0.0199	-0.1973		

0(3W)		C(6A)	[1655.01]	3.291(4)	3.22	0.07	Intra	0.6832	0.0100-0.2696	1.0224	0.0205-0.1244		
0(3W)		H(3A)	[]	2.39<<	2.72	-0.33	Intra	0.6832	0.0100-0.2696	0.4153	0.0195-0.2226		
0(4W)		O(5W)	[]	3.112(4)	3.04	0.07	Intra	-0.6034-0.1313-0.0035		-0.3417-0.0149-0.0611			
0(4W)		O(41A)	[1455.01]	3.209(3)	3.04	0.17	Intra	-0.6034-0.1313-0.0035		-0.5422-0.1381-0.2027			
0(4W)		O(51A)	[1455.01]	2.707(3)<<	3.04	-0.33	Intra	-0.6034-0.1313-0.0035		-0.9088-0.1767-0.0838	Na(1)	120.21(11)	
0(4W)		C(4A)	[1455.01]	3.269(4)	3.22	0.05	Intra	-0.6034-0.1313-0.0035		-0.7674-0.0509-0.1875			
0(4W)		C(41A)	[1455.01]	3.344(3)	3.22	0.12	Intra	-0.6034-0.1313-0.0035		-0.6951-0.1249-0.2201			
0(4W)		Cu(2)	[3455.01]	3.672(2) <	3.84	-0.17	Intra	-0.6034-0.1313-0.0035		-0.6608-0.2436 0.1920	Na(1)	118.63(9)	
0(4W)		O(5W)	[3455.01]	2.729(4)<<	3.04	-0.31	Intra	-0.6034-0.1313-0.0035		-0.6583 0.0149 0.0611	Na(1)	120.41(12)	
0(4W)		O(21A)	[3555.01]	2.721(3)<<	3.04	-0.32	Intra	-0.6034-0.1313-0.0035		-0.5064-0.1607 0.1684	Na(1)	104.84(10)	
0(4W)		C(21A)	[3555.01]	3.393(3)	3.22	0.17	Intra	-0.6034-0.1313-0.0035		-0.3471-0.1663 0.1856			
0(5W)		O(4W)	[]	3.112(4)	3.04	0.07	Intra	-0.3417-0.0149-0.0611		-0.6034-0.1313-0.0035			
0(5W)		O(52A)	[]	3.010(4) <	3.04	-0.03	Intra	-0.3417-0.0149-0.0611		-0.1540-0.1346-0.1530			
0(5W)		C(3A)	[1455.01]	3.288(4)	3.22	0.07	Intra	-0.3417-0.0149-0.0611		-0.6850 0.0199-0.1973			
0(5W)		C(6A)	[]	3.289(4)	3.22	0.07	Intra	-0.3417-0.0149-0.0611		0.0224 0.0205-0.1244	Na(1)	105.05(12)	
0(5W)		H(6A)	[]	2.37<<	2.72	-0.35	Intra	-0.3417-0.0149-0.0611		-0.0785 0.0208-0.0997	Na(1)	109	
0(5W)		O(4W)	[3455.01]	2.729(4)<<	3.04	-0.31	Intra	-0.3417-0.0149-0.0611		-0.3966 0.1313 0.0035	Na(1)	153.38(15)	
0(6W)		O(3W)	[1455.01]	2.955(3) <	3.04	-0.09	Intra	-0.3107 0.1823-0.3007		-0.3168 0.0100-0.2696	Cu(2)	111.16(9)	
0(6W)		O(12A)	[]	2.989(3) <	3.04	-0.05	Intra	-0.3107 0.1823-0.3007		-0.1160 0.1821-0.1219			
0(6W)		O(21A)	[1455.01]	2.726(3)<<	3.04	-0.31	Intra	-0.3107 0.1823-0.3007		-0.4936 0.1607-0.1684			
0(6W)		O(42A)	[2554.01]	2.789(3)<<	3.04	-0.25	Intra	-0.3107 0.1823-0.3007		-0.2039 0.3291-0.2319			
0(6W)		C(41A)	[2554.01]	3.274(3)	3.22	0.05	Intra	-0.3107 0.1823-0.3007		-0.3049 0.3751-0.2799			
0(6W)		Cu(1)	[4554.01]	4.0290(18)	3.84	0.19		-0.3107 0.1823-0.3007		0.0411 0.2349-0.4507	Cu(2)	123.12(7)	
0(6W)		O(7W)	[4554.01]	2.764(2)<<	3.04	-0.28		-0.3107 0.1823-0.3007		0.0147 0.1847-0.3365	Cu(2)	112.84(8)	
0(6W)		O(21B)	[4554.01]	2.687(3)<<	3.04	-0.35		-0.3107 0.1823-0.3007		-0.5717 0.2050-0.4265	Cu(2)	111.29(8)	
0(7W)		O(2W)	[]	2.590(3)<<	3.04	-0.45		0.0147 0.3153 0.1635		-0.0156 0.4620 0.1156			
0(7W)		O(11B)	[]	3.001(3) <	3.04	-0.04	Intra	0.0147 0.3153 0.1635		-0.1881 0.3429-0.0114			
0(7W)		O(22B)	[1655.01]	2.815(3)<<	3.04	-0.22	Intra	0.0147 0.3153 0.1635		0.1831 0.3520 0.0223			
0(7W)		O(51A)	[3555.01]	2.731(3)<<	3.04	-0.31	Intra	0.0147 0.3153 0.1635		-0.0912 0.1767 0.0838			
0(7W)		C(51A)	[3555.01]	3.244(3)	3.22	0.02	Intra	0.0147 0.3153 0.1635		0.0016 0.1260 0.1296			
0(7W)		Cu(2)	[4555.01]	4.0103(18)	3.84	0.17		0.0147 0.3153 0.1635		-0.3392 0.2564 0.3080	Cu(1)	124.53(7)	
0(7W)		O(6W)	[4555.01]	2.764(2)<<	3.04	-0.28		0.0147 0.3153 0.1635		-0.3107 0.3177 0.1993	Cu(1)	114.25(8)	
0(7W)		O(22A)	[4555.01]	2.676(3)<<	3.04	-0.36		0.0147 0.3153 0.1635		0.2691 0.2736 0.2850	Cu(1)	110.12(8)	
0(7W)		C(2A)	[4555.01]	3.373(3)	3.22	0.15		0.0147 0.3153 0.1635		0.2533 0.4082 0.3292	Cu(1)	138.65(8)	
0(7W)		C(21A)	[4555.01]	3.313(3)	3.22	0.09		0.0147 0.3153 0.1635		0.3471 0.3337 0.3144	Cu(1)	119.15(8)	
0(11A)		O(21B)	[1655.01]	3.185(3)	3.04	0.14	Intra	0.1300 0.1988-0.0359		0.4283 0.2950 0.0735	C(11A)	164.51(16)	
0(11A)		O(22A)	[]	3.186(3)	3.04	0.15	Intra	0.1300 0.1988-0.0359		0.2691 0.2264-0.2150	Cu(1)	136.23(9)	
0(11A)		O(22B)	[1655.01]	2.756(3)<<	3.04	-0.28	Intra	0.1300 0.1988-0.0359		0.1831 0.3520 0.0223	C(11A)	135.98(16)	
0(11A)		C(21A)	[]	3.160(3) <	3.22	-0.06	Intra	0.1300 0.1988-0.0359		0.3471 0.1663-0.1856	Cu(1)	154.08(10)	
0(11A)		C(21B)	[1655.01]	3.223(3)	3.22	0.00	Intra	0.1300 0.1988-0.0359		0.3437 0.3512 0.0392	C(11A)	150.54(17)	
0(11A)		Na(1)	[3555.01]	2.449(2)<<	3.29	-0.84	Intra	0.1300 0.1988-0.0359		0.3713 0.1548 0.0668	C(11A)	133.72(16)	
0(11A)		O(51A)	[3555.01]	2.787(2)<<	3.04	-0.25	Intra	0.1300 0.1988-0.0359		-0.0912 0.1767 0.0838			
0(11A)		O(52A)	[3555.01]	3.112(3)	3.04	0.07	Intra	0.1300 0.1988-0.0359		0.1540 0.1346 0.1530	C(11A)	119.09(16)	
0(11A)		C(51A)	[3555.01]	3.162(3) <	3.22	-0.06	Intra	0.1300 0.1988-0.0359		0.0016 0.1260 0.1296	C(11A)	100.64(15)	
0(11B)		Cu(2)	[]	3.347(2)<<	3.84	-0.49	Intra	-0.1881 0.3429-0.0114		-0.3392 0.2436-0.1920	Cu(1)	103.02(7)	
0(11B)		O(2W)	[]	3.016(3) <	3.04	-0.02		-0.1881 0.3429-0.0114		-0.0156 0.4620 0.1156	C(11B)	119.48(17)	
0(11B)		O(7W)	[]	3.001(3) <	3.04	-0.04	Intra	-0.1881 0.3429-0.0114		0.0147 0.3153 0.1635	C(11B)	140.83(17)	
0(11B)		O(22B)	[1655.01]	2.970(2) <	3.04	-0.07	Intra	-0.1881 0.3429-0.0114		0.1831 0.3520 0.0223	C(11B)	160.21(18)	

0(11B)		O(51A)	[3555.01]	3.220(3)	3.04	0.18	Intra	-0.1881	0.3429-0.0114	-0.0912	0.1767	0.0838	C(11B)	119.59(16)	
0(11B)		H(6B)	[3465.01]	2.82	2.72	0.10	Intra	-0.1881	0.3429-0.0114	-0.2492	0.5025-0.0575		Cu(1)	137	
0(12A)		Cu(1)	[]	3.112(2)<<	3.84	-0.73	Intra	-0.1160	0.1821-0.1219	0.0411	0.2651	0.0493	Cu(2)	114.17(7)	
0(12A)		O(6W)	[]	2.989(3) <	3.04	-0.05	Intra	-0.1160	0.1821-0.1219	-0.3107	0.1823-0.3007		C(11A)	130.03(17)	
0(12A)		O(21A)	[1455.01]	3.051(2)	3.04	0.01	Intra	-0.1160	0.1821-0.1219	-0.4936	0.1607-0.1684		C(11A)	158.44(17)	
0(12A)		H(6A)	[]	2.76	2.72	0.04	Intra	-0.1160	0.1821-0.1219	-0.0785	0.0208-0.0997		Cu(2)	126	
0(12A)		O(42A)	[2554.01]	3.043(3)	3.04	0.00	Intra	-0.1160	0.1821-0.1219	-0.2039	0.3291-0.2319		C(11A)	120.72(16)	
0(12A)		O(51A)	[3555.01]	3.177(3)	3.04	0.14	Intra	-0.1160	0.1821-0.1219	-0.0912	0.1767	0.0838	Cu(2)	115.80(7)	
0(12B)		O(21A)	[1455.01]	2.815(3)<<	3.04	-0.22	Intra	-0.4206	0.3151-0.1065	-0.4936	0.1607-0.1684		C(11B)	143.74(17)	
0(12B)		O(21B)	[]	3.231(3)	3.04	0.19	Intra	-0.4206	0.3151-0.1065	-0.5717	0.2950	0.0735	Cu(2)	136.25(9)	
0(12B)		O(22A)	[1455.01]	3.185(3)	3.04	0.14	Intra	-0.4206	0.3151-0.1065	-0.7309	0.2264-0.2150		C(11B)	159.92(16)	
0(12B)		C(21A)	[1455.01]	3.269(3)	3.22	0.05	Intra	-0.4206	0.3151-0.1065	-0.6529	0.1663-0.1856		C(11B)	154.61(17)	
0(12B)		C(21B)	[]	3.223(3)	3.22	0.00	Intra	-0.4206	0.3151-0.1065	-0.6563	0.3512	0.0392	Cu(2)	151.19(9)	
0(12B)		Na(2)	[2554.01]	2.538(2)<<	3.29	-0.75	Intra	-0.4206	0.3151-0.1065	-0.6695	0.3648-0.2111		C(11B)	126.24(16)	
0(12B)		O(41A)	[2554.01]	3.045(3)	3.04	0.01	Intra	-0.4206	0.3151-0.1065	-0.4578	0.3619-0.2973		C(11B)	123.22(16)	
0(12B)		O(42A)	[2554.01]	2.814(2)<<	3.04	-0.23	Intra	-0.4206	0.3151-0.1065	-0.2039	0.3291-0.2319				
0(12B)		C(41A)	[2554.01]	3.148(3) <	3.22	-0.07	Intra	-0.4206	0.3151-0.1065	-0.3049	0.3751-0.2799		C(11B)	105.41(15)	
0(21A)		O(6W)	[1655.01]	2.726(3)<<	3.04	-0.31	Intra	0.5064	0.1607-0.1684	0.6893	0.1823-0.3007		C(21A)	118.13(17)	
0(21A)		O(12A)	[1655.01]	3.051(2)	3.04	0.01	Intra	0.5064	0.1607-0.1684	0.8840	0.1821-0.1219		C(21A)	168.75(17)	
0(21A)		O(12B)	[1655.01]	2.815(3)<<	3.04	-0.22	Intra	0.5064	0.1607-0.1684	0.5794	0.3151-0.1065				
0(21A)		H(3A)	[]	2.60 <	2.72	-0.12	Intra	0.5064	0.1607-0.1684	0.4153	0.0195-0.2226				
0(21A)		O(4W)	[3555.01]	2.721(3)<<	3.04	-0.32	Intra	0.5064	0.1607-0.1684	0.6034	0.1313	0.0035	C(21A)	110.83(17)	
0(21B)		Cu(1)	[1455.01]	3.1352(17)<<	3.84	-0.70	Intra	-0.5717	0.2950	0.0735	-0.9589	0.2651	0.0493		
0(21B)		O(11A)	[1455.01]	3.185(3)	3.04	0.14	Intra	-0.5717	0.2950	0.0735	-0.8700	0.1988-0.0359			
0(21B)		O(12B)	[]	3.231(3)	3.04	0.19	Intra	-0.5717	0.2950	0.0735	-0.4206	0.3151-0.1065			
0(21B)		C(11B)	[]	3.028(3) <	3.22	-0.19	Intra	-0.5717	0.2950	0.0735	-0.3349	0.3551-0.0458			
0(21B)		Cu(2)	[4555.01]	3.907(2)	3.84	0.07		-0.5717	0.2950	0.0735	-0.3392	0.2564	0.3080	C(21B)	133.39(16)
0(21B)		O(6W)	[4555.01]	2.687(3)<<	3.04	-0.35		-0.5717	0.2950	0.0735	-0.3107	0.3177	0.1993	C(21B)	121.79(17)
0(22A)		Cu(2)	[1655.01]	3.1443(17)<<	3.84	-0.70	Intra	0.2691	0.2264-0.2150	0.6608	0.2436-0.1920				
0(22A)		O(11A)	[]	3.186(3)	3.04	0.15	Intra	0.2691	0.2264-0.2150	0.1300	0.1988-0.0359				
0(22A)		O(12B)	[1655.01]	3.185(3)	3.04	0.14	Intra	0.2691	0.2264-0.2150	0.5794	0.3151-0.1065				
0(22A)		C(11A)	[]	3.028(3) <	3.22	-0.19	Intra	0.2691	0.2264-0.2150	0.0315	0.1642-0.0971				
0(22A)		O(52A)	[2554.01]	3.170(3)	3.04	0.13	Intra	0.2691	0.2264-0.2150	0.1540	0.3654-0.3470		C(21A)	157.93(17)	
0(22A)		Cu(1)	[4554.01]	3.858(2)	3.84	0.02		0.2691	0.2264-0.2150	0.0411	0.2349-0.4507		C(21A)	121.68(16)	
0(22A)		O(7W)	[4554.01]	2.676(3)<<	3.04	-0.36		0.2691	0.2264-0.2150	0.0147	0.1847-0.3365		C(21A)	109.86(16)	
0(22B)		O(2W)	[1455.02]	2.970(3) <	3.04	-0.07		-0.8169	0.3520	0.0223	-1.0156	0.4620	0.1156	C(21B)	120.51(16)
0(22B)		O(7W)	[1455.01]	2.815(3)<<	3.04	-0.22	Intra	-0.8169	0.3520	0.0223	-0.9853	0.3153	0.1635	C(21B)	115.23(16)
0(22B)		O(11A)	[1455.01]	2.756(3)<<	3.04	-0.28	Intra	-0.8169	0.3520	0.0223	-0.8700	0.1988-0.0359			
0(22B)		O(11B)	[1455.01]	2.970(2) <	3.04	-0.07	Intra	-0.8169	0.3520	0.0223	-1.1881	0.3429-0.0114		C(21B)	176.14(17)
0(22B)		H(6B)	[]	2.56 <	2.72	-0.16	Intra	-0.8169	0.3520	0.0223	-0.7508	0.4975	0.0575		
0(22B)		O(1W)	[2554.01]	2.712(3)<<	3.04	-0.33	Intra	-0.8169	0.3520	0.0223	-0.9093	0.3865-0.1482		C(21B)	109.11(16)
0(41A)		O(4W)	[1655.01]	3.209(3)	3.04	0.17	Intra	0.4578-0.1381-0.2027		0.3966-0.1313-0.0035			Na(2)	141.87(9)	
0(41A)		O(52A)	[1655.01]	3.118(2)	3.04	0.08	Intra	0.4578-0.1381-0.2027		0.8460-0.1346-0.1530			C(41A)	168.54(17)	
0(41A)		H(3A)	[]	2.70 <	2.72	-0.02	Intra	0.4578-0.1381-0.2027		0.4153	0.0195-0.2226				
0(41A)		Cu(2)	[2544.01]	2.6738(19)<<	3.84	-1.17	Intra	0.4578-0.1381-0.2027		0.3392-0.2564-0.3080					
0(41A)		O(12B)	[2544.01]	3.045(3)	3.04	0.01	Intra	0.4578-0.1381-0.2027		0.4206-0.1849-0.3935					
0(42A)		O(1W)	[1455.01]	2.719(2)<<	3.04	-0.32	Intra	0.2039-0.1708-0.2681		-0.0907-0.1135-0.3518			C(41A)	120.01(16)	
0(42A)		O(51A)	[]	3.134(3)	3.04	0.09	Intra	0.2039-0.1708-0.2681		0.0912-0.1767-0.0838					

0(42A)		C(51A)	[		]	3.002(3)<<	3.22	-0.22	Intra	0.2039-0.1708-0.2681	-0.0016-0.1260-0.1296		
0(42A)		0(6W)	[	2544.01]		2.789(3)<<	3.04	-0.25	Intra	0.2039-0.1708-0.2681	0.3107-0.3177-0.1993	C(41A)	100.40(15)
0(42A)		0(12A)	[	2544.01]		3.043(3)	3.04	0.00	Intra	0.2039-0.1708-0.2681	0.1160-0.3179-0.3781	C(41A)	153.85(16)
0(42A)		0(12B)	[	2544.01]		2.814(2)<<	3.04	-0.23	Intra	0.2039-0.1708-0.2681	0.4206-0.1849-0.3935		
0(42A)		C(11B)	[	2544.01]		3.253(3)	3.22	0.03	Intra	0.2039-0.1708-0.2681	0.3349-0.1449-0.4542	C(41A)	100.05(15)
0(51A)		0(4W)	[	1655.01]		2.707(3)<<	3.04	-0.33	Intra	0.0912-0.1767-0.0838	0.3966-0.1313-0.0035	C(51A)	119.05(16)
0(51A)		0(42A)	[		]	3.134(3)	3.04	0.09	Intra	0.0912-0.1767-0.0838	0.2039-0.1708-0.2681		
0(51A)		C(41A)	[		]	3.051(3) <	3.22	-0.17	Intra	0.0912-0.1767-0.0838	0.3049-0.1249-0.2201		
0(51A)		0(7W)	[	3555.01]		2.731(3)<<	3.04	-0.31	Intra	0.0912-0.1767-0.0838	-0.0147-0.3153-0.1635	C(51A)	101.65(15)
0(51A)		0(11A)	[	3555.01]		2.787(2)<<	3.04	-0.25	Intra	0.0912-0.1767-0.0838	-0.1300-0.1988 0.0359		
0(51A)		0(11B)	[	3555.01]		3.220(3)	3.04	0.18	Intra	0.0912-0.1767-0.0838	0.1881-0.3429 0.0114	C(51A)	157.08(16)
0(51A)		0(12A)	[	3555.01]		3.177(3)	3.04	0.14	Intra	0.0912-0.1767-0.0838	0.1160-0.1821 0.1219	C(51A)	121.66(16)
0(51A)		C(11A)	[	3555.01]		3.123(3) <	3.22	-0.10	Intra	0.0912-0.1767-0.0838	-0.0315-0.1642 0.0971	C(51A)	102.69(15)
0(52A)		0(1W)	[	1455.01]		3.227(3)	3.04	0.19	Intra	-0.1540-0.1346-0.1530	-0.0907-0.1135-0.3518	Na(1)	141.95(8)
0(52A)		0(3W)	[	1455.01]		3.209(3)	3.04	0.17	Intra	-0.1540-0.1346-0.1530	-0.3168 0.0100-0.2696	C(51A)	112.55(17)
0(52A)		0(5W)	[		]	3.010(4) <	3.04	-0.03	Intra	-0.1540-0.1346-0.1530	-0.3417-0.0149-0.0611	C(51A)	109.17(17)
0(52A)		0(41A)	[	1455.01]		3.118(2)	3.04	0.08	Intra	-0.1540-0.1346-0.1530	-0.5422-0.1381-0.2027	C(51A)	173.66(18)
0(52A)		H(6A)	[		]	2.80	2.72	0.08	Intra	-0.1540-0.1346-0.1530	-0.0785 0.0208-0.0997		
0(52A)		0(22A)	[	2544.01]		3.170(3)	3.04	0.13	Intra	-0.1540-0.1346-0.1530	-0.2691-0.2736-0.2850	C(51A)	117.53(16)
0(52A)		Cu(1)	[	3555.01]		2.805(2)<<	3.84	-1.03	Intra	-0.1540-0.1346-0.1530	-0.0411-0.2651-0.0493		
0(52A)		0(11A)	[	3555.01]		3.112(3)	3.04	0.07	Intra	-0.1540-0.1346-0.1530	-0.1300-0.1988 0.0359		
C(2A)		0(7W)	[	4554.01]		3.373(3)	3.22	0.15		0.2533 0.0918-0.1708	0.0147 0.1847-0.3365	C(3A)	111.53(17)
C(3A)		0(3W)	[		]	3.332(4)	3.22	0.11	Intra	0.3150 0.0199-0.1973	0.6832 0.0100-0.2696	C(2A)	121.12(17)
												C(4A)	117.32(17)
C(3A)		0(5W)	[	1655.01]		3.288(4)	3.22	0.07	Intra	0.3150 0.0199-0.1973	0.6583-0.0149-0.0611	C(2A)	105.57(17)
C(4A)		0(4W)	[	1655.01]		3.269(4)	3.22	0.05	Intra	0.2326-0.0509-0.1875	0.3966-0.1313-0.0035	C(3A)	108.34(17)
C(5A)		0(1W)	[	1455.01]		3.419(3)	3.22	0.20	Intra	0.0851-0.0509-0.1501	-0.0907-0.1135-0.3518	C(6A)	114.37(17)
C(6A)		0(3W)	[	1455.01]		3.291(4)	3.22	0.07	Intra	0.0224 0.0205-0.1244	-0.3168 0.0100-0.2696	C(1A)	109.45(17)
C(6A)		0(5W)	[		]	3.289(4)	3.22	0.07	Intra	0.0224 0.0205-0.1244	-0.3417-0.0149-0.0611	C(1A)	130.48(18)
												C(5A)	107.85(17)
C(6B)		0(2W)	[	3465.02]		3.377(3)	3.22	0.16		-0.6483 0.4985 0.0342	-0.9844 0.5380-0.1156	C(2B)	111.41(17)
C(11A)		0(22A)	[		]	3.028(3) <	3.22	-0.19	Intra	0.0315 0.1642-0.0971	0.2691 0.2264-0.2150	0(12A)	113.18(17)
C(11B)		0(21B)	[		]	3.028(3) <	3.22	-0.19	Intra	-0.3349 0.3551-0.0458	-0.5717 0.2950 0.0735	0(11B)	109.16(17)
C(21A)		0(11A)	[		]	3.160(3) <	3.22	-0.06	Intra	0.3471 0.1663-0.1856	0.1300 0.1988-0.0359	0(21A)	120.55(17)
C(21A)		0(4W)	[	3555.01]		3.393(3)	3.22	0.17	Intra	0.3471 0.1663-0.1856	0.6034 0.1313 0.0035	0(22A)	132.24(18)
C(21A)		0(7W)	[	4554.01]		3.313(3)	3.22	0.09		0.3471 0.1663-0.1856	0.0147 0.1847-0.3365	0(21A)	147.29(18)
C(21B)		0(12B)	[		]	3.223(3)	3.22	0.00	Intra	-0.6563 0.3512 0.0392	-0.4206 0.3151-0.1065	0(22B)	122.69(17)
C(21B)		0(1W)	[	2554.01]		3.360(3)	3.22	0.14	Intra	-0.6563 0.3512 0.0392	-0.9093 0.3865-0.1482	0(21B)	137.23(18)
C(41A)		0(51A)	[		]	3.051(3) <	3.22	-0.17	Intra	0.3049-0.1249-0.2201	0.0912-0.1767-0.0838	0(41A)	116.15(17)
C(51A)		0(42A)	[		]	3.002(3)<<	3.22	-0.22	Intra	-0.0016-0.1260-0.1296	0.2039-0.1708-0.2681	0(52A)	112.86(18)
H(3A)		0(3W)	[		]	2.39<<	2.72	-0.33	Intra	0.4153 0.0195-0.2226	0.6832 0.0100-0.2696	C(3A)	173
H(3A)		0(21A)	[		]	2.60 <	2.72	-0.12	Intra	0.4153 0.0195-0.2226	0.5064 0.1607-0.1684		
H(3A)		0(41A)	[		]	2.70 <	2.72	-0.02	Intra	0.4153 0.0195-0.2226	0.4578-0.1381-0.2027		
H(6A)		0(5W)	[		]	2.37<<	2.72	-0.35	Intra	-0.0785 0.0208-0.0997	-0.3417-0.0149-0.0611	C(6A)	163
H(6A)		0(12A)	[		]	2.76	2.72	0.04	Intra	-0.0785 0.0208-0.0997	-0.1160 0.1821-0.1219		
H(6A)		0(52A)	[		]	2.80	2.72	0.08	Intra	-0.0785 0.0208-0.0997	-0.1540-0.1346-0.1530		
H(6B)		0(2W)	[	1455.02]		2.51<<	2.72	-0.21		-0.7508 0.4975 0.0575	-1.0156 0.4620 0.1156	C(6B)	167
H(6B)		0(22B)	[		]	2.56 <	2.72	-0.16	Intra	-0.7508 0.4975 0.0575	-0.8169 0.3520 0.0223		

H(6B) O(11B) [3465.01] 2.82 2.72 0.10 Intra -0.7508 0.4975 0.0575 -0.8119 0.6571 0.0114

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 1 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact Resd.			
1	[1555.02]	3	2.5900	-0.45	0 Cu(1)	- O(7W) ...	O(2W)	-	0	<<	1555.02			
2	[4555.01]	9	2.6760	-0.36	0 Cu(1)	- O(7W) ...	O(22A)	-C(21A)	0	<<	3555.01	3565.01	3665.01	4455.01
3	[4554.01]	9	2.6760	-0.36	0 C(21A)	- O(22A) ...	O(7W)	-Cu(1)	0	<<	3554.01	3564.01	3664.01	4454.01
4	[4654.02]	1	2.6970	-0.34	0 Na(2)	- O(1W) ...	O(2W)	-	0	<<	4654.02			
5	[1455.02]	2	2.5100	-0.21	1 C(6B)	- H(6B) ...	O(2W)	-	0	<<	1455.02			
6	[3465.02]	1	3.3770	0.16	0 C(2B)	- C(6B) ...	O(2W)	-	0		3465.02			
7	[4455.01]	9	2.6760	-0.36	0 Cu(1)	- O(7W) ...	O(22A)	-C(21A)	0	<<	3455.01	3465.01	3565.01	4355.01
8	[4454.01]	9	2.6760	-0.36	0 C(21A)	- O(22A) ...	O(7W)	-Cu(1)	0	<<	3454.01	3464.01	3564.01	4354.01
9	[4554.02]	1	2.6970	-0.34	0 Na(2)	- O(1W) ...	O(2W)	-	0	<<	4554.02			
10	[1355.02]	2	2.5100	-0.21	1 C(6B)	- H(6B) ...	O(2W)	-	0	<<	1355.02			
11	[3365.02]	1	3.3770	0.16	0 C(2B)	- C(6B) ...	O(2W)	-	0		3365.02			
12	[1655.02]	3	2.5900	-0.45	0 Cu(1)	- O(7W) ...	O(2W)	-	0	<<	1655.02			
13	[4655.01]	9	2.6760	-0.36	0 Cu(1)	- O(7W) ...	O(22A)	-C(21A)	0	<<	3655.01	3665.01	3765.01	4555.01
14	[4654.01]	9	2.6760	-0.36	0 C(21A)	- O(22A) ...	O(7W)	-Cu(1)	0	<<	3654.01	3664.01	3764.01	4554.01
15	[4754.02]	1	2.6970	-0.34	0 Na(2)	- O(1W) ...	O(2W)	-	0	<<	4754.02			
16	[3565.02]	1	3.3770	0.16	0 C(2B)	- C(6B) ...	O(2W)	-	0		3565.02			
17	[2544.02]	3	2.5900	-0.45	0 Cu(1)	- O(7W) ...	O(2W)	-	0	<<	2544.02			
18	[3455.02]	1	2.6970	-0.34	0 Na(2)	- O(1W) ...	O(2W)	-	0	<<	3455.02			
19	[2644.02]	2	2.5100	-0.21	1 C(6B)	- H(6B) ...	O(2W)	-	0	<<	2644.02			
20	[2554.02]	3	2.5900	-0.45	0 Cu(1)	- O(7W) ...	O(2W)	-	0	<<	2554.02			
21	[3564.01]	9	2.6760	-0.36	0 Cu(1)	- O(7W) ...	O(22A)	-C(21A)	0	<<	3464.01	3564.01	3664.01	4464.01
22	[3565.01]	9	2.6760	-0.36	0 C(21A)	- O(22A) ...	O(7W)	-Cu(1)	0	<<	3465.01	3565.01	3665.01	4465.01
23	[2654.02]	2	2.5100	-0.21	1 C(6B)	- H(6B) ...	O(2W)	-	0	<<	2654.02			
24	[4664.02]	1	3.3770	0.16	0 C(2B)	- C(6B) ...	O(2W)	-	0		4664.02			
25	[3555.02]	1	2.6970	-0.34	0 Na(2)	- O(1W) ...	O(2W)	-	0	<<	3555.02			
26	[2744.02]	2	2.5100	-0.21	1 C(6B)	- H(6B) ...	O(2W)	-	0	<<	2744.02			
27	[3664.01]	9	2.6760	-0.36	0 Cu(1)	- O(7W) ...	O(22A)	-C(21A)	0	<<	3564.01	3664.01	3764.01	4564.01
28	[3665.01]	9	2.6760	-0.36	0 C(21A)	- O(22A) ...	O(7W)	-Cu(1)	0	<<	3565.01	3665.01	3765.01	4565.01
29	[2754.02]	2	2.5100	-0.21	1 C(6B)	- H(6B) ...	O(2W)	-	0	<<	2754.02			
30	[4764.02]	1	3.3770	0.16	0 C(2B)	- C(6B) ...	O(2W)	-	0		4764.02			
31	[2444.01]	9	2.6760	-0.36	0 Cu(1)	- O(7W) ...	O(22A)	-C(21A)	0	<<	1345.01	1445.01	1455.01	2344.01
32	[2445.01]	9	2.6760	-0.36	0 C(21A)	- O(22A) ...	O(7W)	-Cu(1)	0	<<	1346.01	1446.01	1456.01	2345.01
33	[2345.02]	1	2.6970	-0.34	0 Na(2)	- O(1W) ...	O(2W)	-	0	<<	2345.02			
34	[1545.02]	1	3.3770	0.16	0 C(2B)	- C(6B) ...	O(2W)	-	0		1545.02			
35	[2454.01]	9	2.6760	-0.36	0 Cu(1)	- O(7W) ...	O(22A)	-C(21A)	0	<<	1355.01	1455.01	1465.01	2354.01
36	[2455.01]	9	2.6760	-0.36	0 C(21A)	- O(22A) ...	O(7W)	-Cu(1)	0	<<	1356.01	1456.01	1466.01	2355.01
37	[2355.02]	1	2.6970	-0.34	0 Na(2)	- O(1W) ...	O(2W)	-	0	<<	2355.02			
38	[2544.01]	9	2.6760	-0.36	0 Cu(1)	- O(7W) ...	O(22A)	-C(21A)	0	<<	1445.01	1545.01	1555.01	2444.01
39	[2545.01]	9	2.6760	-0.36	0 C(21A)	- O(22A) ...	O(7W)	-Cu(1)	0	<<	1446.01	1546.01	1556.01	2445.01

40	[	2445.02]	1	2.6970	-0.34	0	Na(2)	-	O(1W)	...	O(2W)	-	0	<<	2445.02
41	[	3655.02]	2	2.5100	-0.21	1	C(6B)	-	H(6B)	...	O(2W)	-	0	<<	3655.02
42	[	1645.02]	1	3.3770	0.16	0	C(2B)	-	C(6B)	...	O(2W)	-	0		1645.02
43	[	4445.02]	3	2.5900	-0.45	0	Cu(1)	-	O(7W)	...	O(2W)	-	0	<<	4445.02
44	[	4345.02]	2	2.5100	-0.21	1	C(6B)	-	H(6B)	...	O(2W)	-	0	<<	4345.02
45	[	2335.02]	1	3.3770	0.16	0	C(2B)	-	C(6B)	...	O(2W)	-	0		2335.02

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
 Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 =====
 ARU = 1555.02
 =====

At(I)[1555.02]	At(J)	[	ARU(J)	]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
O(2W)		Cu(1)	[		]	3.534(2)<<	3.84	-0.31	-0.0156	0.4620	0.1156	0.0411	0.2651	0.0493		
O(2W)		O(7W)	[		]	2.590(3)<<	3.04	-0.45	-0.0156	0.4620	0.1156	0.0147	0.3153	0.1635		
O(2W)		O(11B)	[		]	3.016(3) <	3.04	-0.02	-0.0156	0.4620	0.1156	-0.1881	0.3429	-0.0114		
O(2W)		O(22B)	[	1655.01]		2.970(3) <	3.04	-0.07	-0.0156	0.4620	0.1156	0.1831	0.3520	0.0223		
O(2W)		H(6B)	[	1655.01]		2.51<<	2.72	-0.21	-0.0156	0.4620	0.1156	0.2492	0.4975	0.0575		
O(2W)		C(6B)	[	3465.01]		3.377(3)	3.22	0.16	-0.0156	0.4620	0.1156	-0.3517	0.5015	-0.0342		
O(2W)		O(1W)	[	4455.01]		2.697(3)<<	3.04	-0.34	-0.0156	0.4620	0.1156	-0.0907	0.6135	0.1482		

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 2 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn	X	-	At(I)	At(J)	-	Y	YHn	Note	Partaking ARU's in Close Contact	Resd.
1	[1555.01]	3	2.5900	-0.45	0		-	O(2W)	...	O(7W)	-Cu(1)	0	<<	1455.01 1555.01 1655.01	2544.01
2	[1655.01]	2	2.5100	-0.21	0		-	O(2W)	...	H(6B)	-C(6B)	1	<<	1555.01 1655.01 1755.01	2644.01
3	[3465.01]	1	3.3770	0.16	0		-	O(2W)	...	C(6B)	-C(2B)	0		3365.01 3465.01 3565.01	4365.01
4	[4455.01]	1	2.6970	-0.34	0		-	O(2W)	...	O(1W)	-Na(2)	0	<<	3455.01 3465.01 3565.01	4355.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
 Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

=====

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)	
[1455.01]	= -1+x, y, z	= [	1	-1	0	0	1	-1.495	-0.244	0.002
[1655.01]	= 1+x, y, z	= [	1	1	0	0	1	0.505	-0.244	0.002
[2544.01]	= -x, -1/2+y, -1/2-z	= [	2	0	-1	-1	1	0.495	-0.744	-0.502
[2554.01]	= -x, 1/2+y, -1/2-z	= [	2	0	0	-1	1	0.495	0.256	-0.502
[2644.01]	= 1-x, -1/2+y, -1/2-z	= [	2	1	-1	-1	1	1.495	-0.744	-0.502
[2654.01]	= 1-x, 1/2+y, -1/2-z	= [	2	1	0	-1	1	1.495	0.256	-0.502
[3455.01]	= -1-x, -y, -z	= [	3	-1	0	0	1	-0.505	0.244	-0.002
[3465.01]	= -1-x, 1-y, -z	= [	3	-1	1	0	1	-0.505	1.244	-0.002
[3555.01]	= -x, -y, -z	= [	3	0	0	0	1	0.495	0.244	-0.002
[4445.01]	= -1+x, -1/2-y, 1/2+z	= [	4	-1	-1	0	1	-1.495	-0.256	0.502
[4555.01]	= x, 1/2-y, 1/2+z	= [	4	0	0	0	1	-0.495	0.744	0.502
[4554.01]	= x, 1/2-y, -1/2+z	= [	4	0	0	-1	1	-0.495	0.744	-0.498
[4654.02]	= 1+x, 1/2-y, -1/2+z	= [	4	1	0	-1	2	0.984	0.038	-0.384
[1455.02]	= -1+x, y, z	= [	1	-1	0	0	2	-1.016	0.462	0.116
[3465.02]	= -1-x, 1-y, -z	= [	3	-1	1	0	2	-0.984	0.538	-0.116
[4455.01]	= -1+x, 1/2-y, 1/2+z	= [	4	-1	0	0	1	-1.495	0.744	0.502

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,

SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

Analysis of Short Non-Hydrogen Inter-Molecular Contacts For Inter-Molecular Clusters and/or Networks (Minor Disorder Excluded)

Contact-Nr	Atom I[	ARU	]	Atom J[	ARU	]	d(I-J)	Del
1	Cu(1)	[	1555.01]	...	O(2W)	[	1555.02]	= 3.534 -0.31
2	O(1W)	[	1555.01]	...	O(2W)	[	4654.02]	= 2.697 -0.34
3	O(6W)	[	1555.01]	...	O(7W)	[	4554.01]	= 2.764 -0.28
4	O(6W)	[	1555.01]	...	O(21B)	[	4554.01]	= 2.687 -0.35
5	O(7W)	[	1555.01]	...	O(2W)	[	1555.02]	= 2.590 -0.45
6	O(7W)	[	1555.01]	...	O(6W)	[	4555.01]	= 2.764 -0.28
7	O(7W)	[	1555.01]	...	O(22A)	[	4555.01]	= 2.676 -0.36
8	O(21B)	[	1555.01]	...	O(6W)	[	4555.01]	= 2.687 -0.35
9	O(22A)	[	1555.01]	...	O(7W)	[	4554.01]	= 2.676 -0.36
10	O(2W)	[	1555.02]	...	Cu(1)	[	1555.01]	= 3.534 -0.31
11	O(2W)	[	1555.02]	...	O(7W)	[	1555.01]	= 2.590 -0.45
12	O(2W)	[	1555.02]	...	O(1W)	[	4455.01]	= 2.697 -0.34

Cluster = 1

(N:M)	:	ARU	--	Connected with (N) Interactions to/from (M) ARU(S).								T = Translated Molecule (Infinite chain etc.)			
9 14	1555.01	--		1455.01*	1655.01*	2544.01*	2554.01*	2644.01*	2654.01*	3455.01*	3465.01*	3555.01*	4445.01*	1555.02	
				4654.02	4554.01T	4555.01T									
9 14	2544.01	--		2644.01*	2444.01*	1545.01*	1555.01*	1445.01*	1455.01*	4644.01*	4654.01*	4544.01*	3644.01*	2544.02	
				3455.02	3555.01T	3554.01T									
9 14	3455.01	--		3555.01*	3355.01*	4455.01*	4445.01*	4355.01*	4345.01*	1555.01*	1545.01*	1455.01*	2554.01*	3455.02	
				2345.02T	2445.01T	2444.01T									
9 14	4445.01	--		4345.01*	4545.01*	3455.01*	3445.01*	3555.01*	3545.01*	2345.01*	2335.01*	2445.01*	1356.01*	4445.02T	
				1545.02T	1445.01T	1446.01T									
3 2	1555.02	--		1555.01	4455.01T										
3 2	4654.02	--		4654.01T	1555.01										
3 2	2544.02	--		2544.01	3654.01T										
3 2	3455.02	--		3455.01	2544.01										

:: Starred ARUs belong (chemically) to the previous ARU

:: Analysis of Polymeric Structure(s)

:: Resd # 0 - Infinite Three-Dimensional Framework :: Det = 1, Base Vectors: #1 =[0 1 0], #2 =[0 0 1], #3 =[1 0 0],

=====
 Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg
 =====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
 =====

Nr	Typ	Res	Donor	---	H...Acceptor	[	ARU	]	D - H	H...A	D...A	D - H...A	A...H...A*	A'...H...A"	Sum(XY,YZ)	Sum(XZ)
1	Intra	1	C(3A)	--H(3A)	..O(3W)	[		]	0.95	2.39	3.332(4)	173				
2	Intra	1	C(6A)	--H(6A)	..O(5W)	[		]	0.95	2.37	3.289(4)	163				
3		1	C(6B)	--H(6B)	..O(2W)	[	1455.02	]	0.95	2.51	3.446(3)	167				

:: No Classic Hydrogen Bonds Found

Translation of ARU-code to Equivalent Position Code

=====

[1455.] = -1+x,y,z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

 2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
 4-Centre (trifurcated)

The List May be Limited to the Shortest Distances.

=====													
3.6 Angstrom Coordination Sphere Around Atom I = Cu(1) [ARU = 1555.01]								0.04108	0.26508	0.04931	0.2200	4.4810	0.7589

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0 Y0 Z0

1	1.9466(18)	--	O(22B)b	[1+x,y,z	=	1655.01]	Intra	50.57	-12.32	0.18310	0.35198	0.02233	1.4278 5.9500 0.3437
2	1.9505(18)	--	O(11A)	[	=	]	Intra	-50.87	-42.26	0.13000	0.19884	-0.03592	1.1310 3.3613 -0.5528
3	1.9568(18)	--	O(51A)i	[-x,-y,-z	=	3555.01]	Intra	-127.48	15.72	-0.09120	0.17665	0.08376	-0.9261 2.9862 1.2891
4	2.0079(19)	--	O(7W)	[	=	]	Intra	119.04	61.05	0.01470	0.31534	0.16348	-0.2517 5.3306 2.5159
5	2.3539(19)	--	O(11B)	[	=	]	Intra	142.46	-23.40	-0.18810	0.34295	-0.01144	-1.4928 5.7974 -0.1761
6	2.805(2)	--	O(52A)i	[-x,-y,-z	=	3555.01]	Intra	-72.94	34.67	0.15400	0.13460	0.15299	0.8968 2.2753 2.3545
7	2.703(3)	<<	C(51A)i	[-x,-y,-z	=	3555.01]	Intra	-102.02	27.20	0.00160	0.12596	0.12961	-0.2807 2.1293 1.9947
8	2.837(3)	<<	C(11A)	[	=	]	Intra	-81.51	-52.59	0.03150	0.16424	-0.09713	0.4744 2.7764 -1.4948
9	2.868(2)	<<	C(21B)b	[1+x,y,z	=	1655.01]	Intra	30.55	-3.11	0.34370	0.35120	0.03919	2.6863 5.9368 0.6031
10	3.112(2)	<<	O(12A)	[	=	]	Intra	-122.12	-57.85	-0.11600	0.18213	-0.12188	-0.6605 3.0788 -1.8757
11	3.1352(17)	<<	O(21B)b	[1+x,y,z	=	1655.01]	Intra	9.34	6.82	0.42830	0.29498	0.07349	3.2917 4.9865 1.1310
12	3.2318(12)	<<	Na(1)i	[-x,-y,-z	=	3555.01]	Intra	-35.35	4.78	0.37130	0.15484	0.06681	2.8466 2.6175 1.0282
13	3.523(3)	<<	C(11B)	[	=	]	Intra	151.66	-24.56	-0.33490	0.35506	-0.04584	-2.6002 6.0021 -0.7055
14	3.534(2)	<<	O(2W)	[	=	02]		100.35	16.79	-0.01560	0.46199	0.11565	-0.3880 7.8097 1.7798

Bond Valence Analysis

N.E. Brese & M. O'Keeffe (1991) Acta Cryst. B47, 192-197.

I.D. Brown (2002). The Chemical Bond in Inorganic Chemistry: The Bond Valence Model. Oxford University Press.

Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 1 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu(1) O(22B)b	1.9466	1.6100	0.37	0.403	0.403	0.597	
2	Cu(1) O(11A)	1.9505	1.6100	0.37	0.398	0.801	0.199	
3	Cu(1) O(51A)i	1.9568	1.6100	0.37	0.392	1.193	0.193	
4	Cu(1) O(7W)	2.0079	1.6100	0.37	0.341	1.534	0.534	
5	Cu(1) O(11B)	2.3539	1.6100	0.37	0.134	1.668	0.668	
	Cu(1) O(52A)i	2.8050						(Contribution below Minimum, Skipped)
	Cu(1) C(51A)i	2.7030						(Contribution below Minimum, Skipped)
	Cu(1) C(11A)	2.8370						(Contribution below Minimum, Skipped)
	Cu(1) C(21B)b	2.8680						(Contribution below Minimum, Skipped)
	Cu(1) O(12A)	3.1120						(Contribution below Minimum, Skipped)
	Cu(1) O(21B)b	3.1352						(Contribution below Minimum, Skipped)
	Cu(1) Na(1)i	3.2318						(Contribution not Tabulated, Result Dubious !)
	Cu(1) C(11B)	3.5230						(Contribution below Minimum, Skipped)
	Cu(1) O(2W)	3.5340						(Contribution below Minimum, Skipped)

Bond Valence Analysis

N.E. Brese & M. O'Keeffe (1991) Acta Cryst. B47, 192-197.

I.D. Brown (2002). The Chemical Bond in Inorganic Chemistry: The Bond Valence Model. Oxford University Press.

Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 2 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu(1) O(22B)b	1.9466	1.6790	0.37	0.485	0.485	1.515	
2	Cu(1) O(11A)	1.9505	1.6790	0.37	0.480	0.965	1.035	
3	Cu(1) O(51A)i	1.9568	1.6790	0.37	0.472	1.437	0.563	
4	Cu(1) O(7W)	2.0079	1.6790	0.37	0.411	1.848	0.152	
5	Cu(1) O(11B)	2.3539	1.6790	0.37	0.161	2.010	0.010	
	Cu(1) O(52A)i	2.8050						(Contribution below Minimum, Skipped)
	Cu(1) C(51A)i	2.7030						(Contribution below Minimum, Skipped)
	Cu(1) C(11A)	2.8370						(Contribution below Minimum, Skipped)
	Cu(1) C(21B)b	2.8680						(Contribution below Minimum, Skipped)
	Cu(1) O(12A)	3.1120						(Contribution below Minimum, Skipped)
	Cu(1) O(21B)b	3.1352						(Contribution below Minimum, Skipped)
	Cu(1) Na(1)i	3.2318						(Contribution not Tabulated, Result Dubious !)
	Cu(1) C(11B)	3.5230						(Contribution below Minimum, Skipped)
	Cu(1) O(2W)	3.5340						(Contribution below Minimum, Skipped)

===== Bond Valence Analysis =====

N.E. Brese & M. O'Keeffe (1991) Acta Cryst. B47, 192-197.

I.D. Brown (2002). The Chemical Bond in Inorganic Chemistry: The Bond Valence Model. Oxford University Press.

Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 3 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu(1) O(22B)b	1.9466	1.7350	0.37	0.564	0.564	2.436	
2	Cu(1) O(11A)	1.9505	1.7350	0.37	0.559	1.123	1.877	
3	Cu(1) O(51A)i	1.9568	1.7350	0.37	0.549	1.672	1.328	
4	Cu(1) O(7W)	2.0079	1.7350	0.37	0.478	2.150	0.850	
5	Cu(1) O(11B)	2.3539	1.7350	0.37	0.188	2.338	0.662	
	Cu(1) O(52A)i	2.8050						(Contribution below Minimum, Skipped)
	Cu(1) C(51A)i	2.7030						(Contribution below Minimum, Skipped)
	Cu(1) C(11A)	2.8370						(Contribution below Minimum, Skipped)
	Cu(1) C(21B)b	2.8680						(Contribution below Minimum, Skipped)
	Cu(1) O(12A)	3.1120						(Contribution below Minimum, Skipped)
	Cu(1) O(21B)b	3.1352						(Contribution below Minimum, Skipped)
	Cu(1) Na(1)i	3.2318						(Contribution not Tabulated, Result Dubious !)
	Cu(1) C(11B)	3.5230						(Contribution below Minimum, Skipped)
	Cu(1) O(2W)	3.5340						(Contribution below Minimum, Skipped)

Octahedral Volume 11.520 Ang**3, Quadratic Elongation 1.142, Angle Variance 306.57 Deg**2 [K.Robinson +, Science 1971,172,567-570]

Angles (Degrees) At1...V...At2 with Vertex V = Cu(1)

O(22B)b, O(11A)	90.00(8)	O(22B)b, O(51A)i	176.11(8)	O(22B)b, O(7W)	90.75(8)	O(22B)b, O(11B)	86.83(7)
O(22B)b, O(52A)i	124.40(6)	O(22B)b, C(51A)i	150.33(8)	O(22B)b, C(11A)	103.20(8)	O(22B)b, C(21B)b	21.85(7)
O(22B)b, O(12A)	109.57(7)	O(22B)b, O(21B)b	45.23(6)	O(22B)b, Na(1)i	87.06(6)	O(22B)b, C(11B)	94.72(7)
O(22B)b, O(2W)	57.15(7)	O(11A) , O(51A)i	90.99(8)	O(11A) , O(7W)	160.24(7)	O(11A) , O(11B)	113.19(7)
O(11A) , O(52A)i	79.54(7)	O(11A) , C(51A)i	83.95(8)	O(11A) , C(11A)	22.93(7)	O(11A) , C(21B)b	81.56(7)
O(11A) , O(12A)	45.90(6)	O(11A) , O(21B)b	73.43(6)	O(11A) , Na(1)i	49.11(6)	O(11A) , C(11B)	110.02(7)
O(11A) , O(2W)	144.61(7)	O(51A)i, O(7W)	87.05(8)	O(51A)i, O(11B)	96.24(7)	O(51A)i, O(52A)i	52.16(6)
O(51A)i, C(51A)i	26.25(7)	O(51A)i, C(11A)	78.98(7)	O(51A)i, C(21B)b	154.97(7)	O(51A)i, O(12A)	73.71(6)
O(51A)i, O(21B)b	131.67(6)	O(51A)i, Na(1)i	90.74(6)	O(51A)i, C(11B)	88.49(7)	O(51A)i, O(2W)	122.71(7)
O(7W) , O(11B)	86.56(7)	O(7W) , O(52A)i	83.78(7)	O(7W) , C(51A)i	85.67(8)	O(7W) , C(11A)	166.03(7)
O(7W) , C(21B)b	91.99(7)	O(7W) , O(12A)	149.90(6)	O(7W) , O(21B)b	93.33(6)	O(7W) , Na(1)i	111.22(5)
O(7W) , C(11B)	89.60(7)	O(7W) , O(2W)	46.24(7)	O(11B) , O(52A)i	147.27(6)	O(11B) , C(51A)i	122.23(7)
O(11B) , C(11A)	94.92(7)	O(11B) , C(21B)b	108.68(7)	O(11B) , O(12A)	73.13(6)	O(11B) , O(21B)b	132.06(6)
O(11B) , Na(1)i	161.26(5)	O(11B) , C(11B)	8.49(6)	O(11B) , O(2W)	57.51(6)	O(52A)i, C(51A)i	25.93(6)
O(52A)i, C(11A)	87.58(7)	O(52A)i, C(21B)b	102.86(6)	O(52A)i, O(12A)	101.28(5)	O(52A)i, O(21B)b	79.80(5)
O(52A)i, Na(1)i	45.82(4)	O(52A)i, C(11B)	140.27(5)	O(52A)i, O(2W)	128.15(6)	C(51A)i, C(11A)	81.78(8)
C(51A)i, C(21B)b	128.73(7)	C(51A)i, O(12A)	86.71(7)	C(51A)i, O(21B)b	105.51(6)	C(51A)i, Na(1)i	67.10(6)
C(51A)i, C(11B)	114.67(7)	C(51A)i, O(2W)	130.95(7)	C(11A) , C(21B)b	100.64(7)	C(11A) , O(12A)	23.38(6)
C(11A) , O(21B)b	95.93(6)	C(11A) , Na(1)i	69.32(5)	C(11A) , C(11B)	90.06(7)	C(11A) , O(2W)	144.17(6)
C(21B)b, O(12A)	115.22(6)	C(21B)b, O(21B)b	23.38(6)	C(21B)b, Na(1)i	66.32(5)	C(21B)b, C(11B)	116.53(7)
C(21B)b, O(2W)	71.67(6)	O(12A) , O(21B)b	116.77(5)	O(12A) , Na(1)i	92.33(4)	O(12A) , C(11B)	67.43(5)
O(12A) , O(2W)	128.34(5)	O(21B)b, Na(1)i	44.50(4)	O(21B)b, C(11B)	139.82(5)	O(21B)b, O(2W)	88.99(5)
Na(1)i , C(11B)	159.10(5)	Na(1)i , O(2W)	131.21(5)	C(11B) , O(2W)	64.90(6)		

=====													
3.6 Angstrom Coordination Sphere Around Atom I = Cu(2) [ARU = 1555.01]								-0.33918	0.24358	-0.19199	-2.3036	4.1175	-2.9547

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0 Y0 Z0

1	1.9459(18)	--	O(21A)a	[-1+x,y,z	=	1455.01]	Intra	-132.85	10.73	-0.49360	0.16066	-0.16844	-3.6038 2.7159 -2.5923
2	1.9670(18)	--	O(42A)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	50.73	-18.20	-0.20390	0.32915	-0.23192	-1.1209 5.5641 -3.5692
3	1.9792(18)	--	O(12B)	[	=	]	Intra	125.15	41.67	-0.42060	0.31509	-0.10649	-3.1547 5.3264 -1.6389
4	2.0242(19)	--	O(6W)	[	=	]	Intra	-65.30	-55.74	-0.31070	0.18233	-0.30069	-1.8274 3.0822 -4.6276
5	2.2233(18)	--	O(12A)	[	=	]	Intra	-32.30	29.03	-0.11600	0.18213	-0.12188	-0.6605 3.0788 -1.8757
6	2.6738(19)	--	O(41A)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	109.77	-37.33	-0.45780	0.36194	-0.29734	-3.0227 6.1184 -4.5760
7	2.646(3)	<<	C(41A)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	77.92	-30.76	-0.30490	0.37509	-0.27990	-1.8277 6.3407 -4.3076
8	2.865(2)	<<	C(21A)a	[-1+x,y,z	=	1455.01]	Intra	-152.86	1.97	-0.65290	0.16631	-0.18560	-4.8511 2.8114 -2.8563
9	2.949(3)	<<	C(11B)	[	=	]	Intra	98.94	49.70	-0.33490	0.35506	-0.04584	-2.6002 6.0021 -0.7055
10	3.1443(17)	<<	O(22A)a	[-1+x,y,z	=	1455.01]	Intra	-174.66	-6.47	-0.73090	0.22636	-0.21500	-5.4143 3.8265 -3.3088
11	3.3420(11)	<<	Na(2)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	142.01	-5.06	-0.66950	0.36479	-0.21114	-4.9273 6.1666 -3.2494
12	3.347(2)	<<	O(11B)	[	=	]	Intra	64.24	56.13	-0.18810	0.34295	-0.01144	-1.4928 5.7974 -0.1761
13	3.413(3)	<<	C(11A)	[	=	]	Intra	-25.77	25.33	0.03150	0.16424	-0.09713	0.4744 2.7764 -1.4948

Bond Valence Analysis

N.E. Brese & M. O'Keeffe (1991) Acta Cryst. B47, 192-197.

I.D. Brown (2002). The Chemical Bond in Inorganic Chemistry: The Bond Valence Model. Oxford University Press.

Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 1 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu(2) O(21A)a	1.9459	1.6100	0.37	0.403	0.403	0.597	
2	Cu(2) O(42A)d	1.9670	1.6100	0.37	0.381	0.784	0.216	
3	Cu(2) O(12B)	1.9792	1.6100	0.37	0.369	1.153	0.153	
4	Cu(2) O(6W)	2.0242	1.6100	0.37	0.326	1.480	0.480	
5	Cu(2) O(12A)	2.2233	1.6100	0.37	0.191	1.670	0.670	
6	Cu(2) O(41A)d	2.6738	1.6100	0.37	0.056	1.727	0.727	
	Cu(2) C(41A)d	2.6460						(Contribution below Minimum, Skipped)
	Cu(2) C(21A)a	2.8650						(Contribution below Minimum, Skipped)
	Cu(2) C(11B)	2.9490						(Contribution below Minimum, Skipped)
	Cu(2) O(22A)a	3.1443						(Contribution below Minimum, Skipped)
	Cu(2) Na(2)d	3.3420						(Contribution not Tabulated, Result Dubious !)
	Cu(2) O(11B)	3.3470						(Contribution below Minimum, Skipped)
	Cu(2) C(11A)	3.4130						(Contribution below Minimum, Skipped)

Bond Valence Analysis

N.E. Brese & M. O'Keefe (1991) Acta Cryst. B47, 192-197.

I.D. Brown (2002). The Chemical Bond in Inorganic Chemistry: The Bond Valence Model. Oxford University Press.

Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 2 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu(2) O(21A)a	1.9459	1.6790	0.37	0.486	0.486	1.514	
2	Cu(2) O(42A)d	1.9670	1.6790	0.37	0.459	0.945	1.055	
3	Cu(2) O(12B)	1.9792	1.6790	0.37	0.444	1.390	0.610	
4	Cu(2) O(6W)	2.0242	1.6790	0.37	0.393	1.783	0.217	
5	Cu(2) O(12A)	2.2233	1.6790	0.37	0.230	2.013	0.013	
	Cu(2) O(41A)d	2.6738						(Contribution below Minimum, Skipped)
6	Cu(2) C(41A)d	2.6460	1.7200	0.37	0.082	2.094	0.094	
	Cu(2) C(21A)a	2.8650						(Contribution below Minimum, Skipped)
	Cu(2) C(11B)	2.9490						(Contribution below Minimum, Skipped)
	Cu(2) O(22A)a	3.1443						(Contribution below Minimum, Skipped)
	Cu(2) Na(2)d	3.3420						(Contribution not Tabulated, Result Dubious !)
	Cu(2) O(11B)	3.3470						(Contribution below Minimum, Skipped)
	Cu(2) C(11A)	3.4130						(Contribution below Minimum, Skipped)

Bond Valence Analysis

N.E. Brese & M. O'Keeffe (1991) Acta Cryst. B47, 192-197.

I.D. Brown (2002). The Chemical Bond in Inorganic Chemistry: The Bond Valence Model. Oxford University Press.

Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 3 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu(2) O(21A)a	1.9459	1.7350	0.37	0.566	0.566	2.434	
2	Cu(2) O(42A)d	1.9670	1.7350	0.37	0.534	1.100	1.900	
3	Cu(2) O(12B)	1.9792	1.7350	0.37	0.517	1.617	1.383	
4	Cu(2) O(6W)	2.0242	1.7350	0.37	0.458	2.074	0.926	
5	Cu(2) O(12A)	2.2233	1.7350	0.37	0.267	2.341	0.659	
	Cu(2) O(41A)d	2.6738						(Contribution below Minimum, Skipped)
	Cu(2) C(41A)d	2.6460						(Contribution below Minimum, Skipped)
	Cu(2) C(21A)a	2.8650						(Contribution below Minimum, Skipped)
	Cu(2) C(11B)	2.9490						(Contribution below Minimum, Skipped)
	Cu(2) O(22A)a	3.1443						(Contribution below Minimum, Skipped)
	Cu(2) Na(2)d	3.3420						(Contribution not Tabulated, Result Dubious !)
	Cu(2) O(11B)	3.3470						(Contribution below Minimum, Skipped)
	Cu(2) C(11A)	3.4130						(Contribution below Minimum, Skipped)

Octahedral Volume 11.526 Ang**3, Quadratic Elongation 1.099, Angle Variance 222.91 Deg**2 [K.Robinson +, Science 1971,172,567-570]

Angles (Degrees) At1...V...At2 with Vertex V = Cu(2)

O(21A)a, O(42A)d	171.77(8)	O(21A)a, O(12B)	91.65(8)	O(21A)a, O(6W)	86.72(8)	O(21A)a, O(12A)	93.84(7)
O(21A)a, O(41A)d	118.18(7)	O(21A)a, C(41A)d	145.16(8)	O(21A)a, C(21A)a	21.71(7)	O(21A)a, C(11B)	104.54(8)
O(21A)a, O(22A)a	45.03(6)	O(21A)a, Na(2)d	86.19(6)	O(21A)a, O(11B)	111.64(7)	O(21A)a, C(11A)	100.44(7)
O(42A)d, O(12B)	90.98(7)	O(42A)d, O(6W)	88.65(7)	O(42A)d, O(12A)	92.91(7)	O(42A)d, O(41A)d	54.69(6)
O(42A)d, C(41A)d	27.64(7)	O(42A)d, C(21A)a	151.74(7)	O(42A)d, C(11B)	80.14(7)	O(42A)d, O(22A)a	128.89(6)
O(42A)d, Na(2)d	89.63(5)	O(42A)d, O(11B)	75.20(6)	O(42A)d, C(11A)	86.17(7)	O(12B) , O(6W)	164.37(7)
O(12B) , O(12A)	106.29(7)	O(12B) , O(41A)d	80.24(7)	O(12B) , C(41A)d	84.50(8)	O(12B) , C(21A)a	82.72(7)
O(12B) , C(11B)	19.86(7)	O(12B) , O(22A)a	72.90(6)	O(12B) , Na(2)d	49.20(5)	O(12B) , O(11B)	41.03(6)
O(12B) , C(11A)	107.80(7)	O(6W) , O(12A)	89.33(7)	O(6W) , O(41A)d	86.84(7)	O(6W) , C(41A)d	87.99(8)
O(6W) , C(21A)a	90.25(7)	O(6W) , C(11B)	168.74(7)	O(6W) , O(22A)a	95.30(6)	O(6W) , Na(2)d	115.18(5)
O(6W) , O(11B)	152.37(6)	O(6W) , C(11A)	87.77(7)	O(12A) , O(41A)d	147.42(6)	O(12A) , C(41A)d	120.52(7)
O(12A) , C(21A)a	115.31(7)	O(12A) , C(11B)	90.16(7)	O(12A) , O(22A)a	137.95(6)	O(12A) , Na(2)d	155.43(6)
O(12A) , O(11B)	69.67(6)	O(12A) , C(11A)	6.89(6)	O(41A)d, C(41A)d	27.06(6)	O(41A)d, C(21A)a	97.06(6)
O(41A)d, C(11B)	87.55(6)	O(41A)d, O(22A)a	74.63(5)	O(41A)d, Na(2)d	43.66(4)	O(41A)d, O(11B)	101.13(5)
O(41A)d, C(11A)	140.57(6)	C(41A)d, C(21A)a	124.11(7)	C(41A)d, C(11B)	82.60(8)	C(41A)d, O(22A)a	101.43(6)
C(41A)d, Na(2)d	65.22(6)	C(41A)d, O(11B)	87.66(7)	C(41A)d, C(11A)	113.74(7)	C(21A)a, C(11B)	100.12(7)
C(21A)a, O(22A)a	23.34(6)	C(21A)a, Na(2)d	65.44(5)	C(21A)a, O(11B)	114.57(6)	C(21A)a, C(11A)	122.01(7)
C(11B) , O(22A)a	92.61(6)	C(11B) , Na(2)d	66.21(5)	C(11B) , O(11B)	21.63(6)	C(11B) , C(11A)	90.39(7)
O(22A)a, Na(2)d	43.13(4)	O(22A)a, O(11B)	112.31(5)	O(22A)a, C(11A)	144.80(6)	Na(2)d , O(11B)	87.46(4)
Na(2)d , C(11A)	156.59(5)	O(11B) , C(11A)	69.20(5)				

3.6 Angstrom Coordination Sphere Around Atom I = Na(1) [ARU = 1555.01] -0.37130 -0.15484 -0.06681 -2.8466 -2.6175 -1.0282

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.275(3)	--	O(4W)	[	=		Intra	168.83	25.34	-0.60340	-0.13127	-0.00353	-4.8640	-2.2190	-0.0543
2	2.367(2)	--	O(41A)a	[-1+x,y,z	=	1455.01]	Intra	165.18	-62.06	-0.54220	-0.13806	-0.20266	-3.9187	-2.3338	-3.1189
3	2.377(3)	--	O(5W)	[	=		Intra	84.54	2.12	-0.34170	-0.01494	-0.06110	-2.6205	-0.2526	-0.9403
4	2.383(2)	--	O(52A)	[	=		Intra	9.95	-33.82	-0.15400	-0.13460	-0.15299	-0.8968	-2.2753	-2.3545
5	2.413(2)	--	O(21B)g	[-1-x,-y,-z	=	3455.01]	Intra	-100.64	-2.44	-0.42830	-0.29498	-0.07349	-3.2917	-4.9865	-1.1310
6	2.449(2)	--	O(11A)i	[-x,-y,-z	=	3555.01]	Intra	-23.44	40.22	-0.13000	-0.19884	0.03592	-1.1310	-3.3613	0.5528
7	3.2318(12)	<<	Cu(1)i	[-x,-y,-z	=	3555.01]	Intra	-35.35	4.78	-0.04108	-0.26508	-0.04931	-0.2200	-4.4810	-0.7589
8	3.310(3)	<	C(51A)	[	=		Intra	8.87	-16.98	-0.00160	-0.12596	-0.12961	0.2807	-2.1293	-1.9947
9	3.311(3)	<	C(41A)a	[-1+x,y,z	=	1455.01]	Intra	167.42	-45.44	-0.69510	-0.12491	-0.22010	-5.1137	-2.1115	-3.3873
10	3.350(3)	<	C(21B)g	[-1-x,-y,-z	=	3455.01]	Intra	-87.24	7.29	-0.34370	-0.35120	-0.03919	-2.6863	-5.9368	-0.6031
11	3.467(3)	<	C(11A)i	[-x,-y,-z	=	3555.01]	Intra	-3.83	46.70	-0.03150	-0.16424	0.09713	-0.4744	-2.7764	1.4948
12	3.5329(15)	<	Na(2)a	[-1+x,y,z	=	1455.01]	Intra	21.73	-75.30	-0.33050	-0.13521	-0.28886	-2.0141	-2.2856	-4.4455

Octahedral Volume 16.964 Ang**3, Quadratic Elongation 1.037, Angle Variance 122.92 Deg**2 [K.Robinson +, Science 1971,172,567-570]

Angles (Degrees) At1...V...At2 with Vertex V = Na(1)

O(4W)	,	O(41A)a	87.45(8)	O(4W)	,	O(5W)	83.93(11)	O(4W)	,	O(52A)	159.82(10)	O(4W)	,	O(21B)g	91.53(9)
O(4W)	,	O(11A)i	113.46(8)	O(4W)	,	Cu(1)i	141.81(8)	O(4W)	,	C(51A)	159.56(9)	O(4W)	,	C(41A)a	70.80(8)
O(4W)	,	C(21B)g	99.30(8)	O(4W)	,	C(11A)i	107.65(8)	O(4W)	,	Na(2)a	127.34(7)	O(41A)a,	O(5W)		87.51(10)
O(41A)a,	O(52A)		82.05(7)	O(41A)a,	O(21B)g		89.80(7)	O(41A)a,	O(11A)i		157.54(8)	O(41A)a,	Cu(1)i		120.72(6)
O(41A)a,	C(51A)		98.77(7)	O(41A)a,	C(41A)a		16.66(6)	O(41A)a,	C(21B)g		104.63(7)	O(41A)a,	C(11A)i		163.42(7)
O(41A)a,	Na(2)a		40.62(5)	O(5W)	,	O(52A)	78.46(10)	O(5W)	,	O(21B)g	174.81(10)	O(5W)	,	O(11A)i	102.22(10)
O(5W)	,	Cu(1)i	119.55(9)	O(5W)	,	C(51A)	76.95(9)	O(5W)	,	C(41A)a	86.53(9)	O(5W)	,	C(21B)g	167.52(10)
O(5W)	,	C(11A)i	87.34(9)	O(5W)	,	Na(2)a	85.41(8)	O(52A)	,	O(21B)g	105.56(8)	O(52A)	,	O(11A)i	80.20(7)
O(52A)	,	Cu(1)i	57.60(5)	O(52A)	,	C(51A)	16.87(6)	O(52A)	,	C(41A)a	98.15(7)	O(52A)	,	C(21B)g	100.01(7)
O(52A)	,	C(11A)i	81.48(7)	O(52A)	,	Na(2)a	41.87(5)	O(21B)g,	O(11A)i		81.87(7)	O(21B)g,	Cu(1)i		65.63(5)
O(21B)g,	C(51A)		107.86(7)	O(21B)g,	C(41A)a		89.62(7)	O(21B)g,	C(21B)g		16.54(6)	O(21B)g,	C(11A)i		96.45(7)
O(21B)g,	Na(2)a		95.42(6)	O(11A)i,	Cu(1)i		37.02(5)	O(11A)i,	C(51A)		64.62(7)	O(11A)i,	C(41A)a		170.49(8)
O(11A)i,	C(21B)g		65.39(7)	O(11A)i,	C(11A)i		15.59(6)	O(11A)i,	Na(2)a		119.21(6)	Cu(1)i,	C(51A)		48.81(5)
Cu(1)i,	C(41A)a		134.75(6)	Cu(1)i,	C(21B)g		51.63(5)	Cu(1)i,	C(11A)i		49.97(5)	Cu(1)i,	Na(2)a		86.75(3)
C(51A)	,	C(41A)a	114.61(7)	C(51A)	,	C(21B)g	97.93(7)	C(51A)	,	C(11A)i	64.70(6)	C(51A)	,	Na(2)a	58.73(5)
C(41A)a,	C(21B)g		105.94(7)	C(41A)a,	C(11A)i		173.81(7)	C(41A)a,	Na(2)a		57.16(5)	C(21B)g,	C(11A)i		80.18(7)
C(21B)g,	Na(2)a		101.80(6)	C(11A)i,	Na(2)a		123.16(5)								

3.6 Angstrom Coordination Sphere Around Atom I = Na(2) [ARU = 1555.01] 0.66950 -0.13521 -0.28886 6.0601 -2.2856 -4.4455

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.322(2)	--	O(41A)	[	=		Intra	-178.55	34.85	0.45780	-0.13806	-0.20266	4.1555	-2.3338	-3.1189
2	2.323(2)	--	O(1W)	[	=		Intra	10.02	-24.65	0.90930	-0.11348	-0.35181	8.1390	-1.9183	-5.4143
3	2.371(2)	--	O(52A)b	[1+x,y,z	=	1655.01]	Intra	0.53	61.88	0.84600	-0.13460	-0.15299	7.1774	-2.2753	-2.3545
4	2.391(2)	--	O(22A)e	[1-x,-1/2+y,-1/2-z	=	2644.01]	Intra	-78.24	1.42	0.73090	-0.27364	-0.28500	6.5472	-4.6257	-4.3861
5	2.473(2)	--	O(3W)	[	=		Intra	88.44	6.88	0.68320	0.00998	-0.26961	6.1272	0.1687	-4.1492
6	2.538(2)	--	O(12B)c	[-x,-1/2+y,-1/2-z	=	2544.01]	Intra	-154.64	-39.39	0.42060	-0.18491	-0.39351	4.2876	-3.1258	-6.0560
7	3.280(3)	.<	C(41A)	[	=		Intra	176.78	18.82	0.30490	-0.12491	-0.22010	2.9605	-2.1115	-3.3873
8	3.3420(11)	<<	Cu(2)c	[-x,-1/2+y,-1/2-z	=	2544.01]	Intra	-142.01	-5.06	0.33918	-0.25642	-0.30801	3.4365	-4.3347	-4.7402
9	3.361(3)	.<	C(51A)b	[1+x,y,z	=	1655.01]	Intra	3.90	46.82	0.99840	-0.12596	-0.12961	8.3549	-2.1293	-1.9947
10	3.379(3)	.<	C(21A)e	[1-x,-1/2+y,-1/2-z	=	2644.01]	Intra	-91.30	-6.68	0.65290	-0.33369	-0.31440	5.9840	-5.6408	-4.8386
11	3.452(3)	.<	C(11B)c	[-x,-1/2+y,-1/2-z	=	2544.01]	Intra	-175.96	-47.48	0.33490	-0.14494	-0.45416	3.7330	-2.4501	-6.9894
12	3.517(3)	..	C(1B)c	[-x,-1/2+y,-1/2-z	=	2544.01]	Intra	145.32	-57.48	0.42290	-0.07158	-0.48154	4.5056	-1.2100	-7.4108
13	3.5329(15)	.<	Na(1)b	[1+x,y,z	=	1655.01]	Intra	-158.27	75.30	0.62870	-0.15484	-0.06681	5.2276	-2.6175	-1.0282
14	3.57	..	H(3A)	[	=		Intra	130.10	16.61	0.41530	0.01950	-0.22260	3.8576	0.3296	-3.4258

Octahedral Volume 17.241 Ang**3, Quadratic Elongation 1.049, Angle Variance 157.82 Deg**2 [K.Robinson +, Science 1971,172,567-570]

Angles (Degrees) At1...V...At2 with Vertex V = Na(2)

O(41A) , O(1W)	167.39(8)	O(41A) , O(52A)b	83.27(7)	O(41A) , O(22A)e	97.62(7)	O(41A) , O(3W)	88.53(8)
O(41A) , O(12B)c	77.45(7)	O(41A) , C(41A)	16.55(6)	O(41A) , Cu(2)c	52.67(5)	O(41A) , C(51A)b	98.30(7)
O(41A) , C(21A)e	91.57(7)	O(41A) , C(11B)c	82.36(7)	O(41A) , C(1B)c	97.21(7)	O(41A) , Na(1)b	41.58(5)
O(1W) , O(52A)b	86.87(7)	O(1W) , O(22A)e	89.02(7)	O(1W) , O(3W)	82.46(8)	O(1W) , O(12B)c	114.38(8)
O(1W) , C(41A)	166.40(8)	O(1W) , Cu(2)c	139.71(6)	O(1W) , C(51A)b	71.68(7)	O(1W) , C(21A)e	97.39(7)
O(1W) , C(11B)c	107.67(7)	O(1W) , C(1B)c	89.75(7)	O(1W) , Na(1)b	128.99(6)	O(52A)b , O(22A)e	83.47(8)
O(52A)b , O(3W)	82.95(9)	O(52A)b , O(12B)c	152.90(8)	O(52A)b , C(41A)	99.24(7)	O(52A)b , Cu(2)c	116.77(6)
O(52A)b , C(51A)b	15.19(6)	O(52A)b , C(21A)e	96.75(7)	O(52A)b , C(11B)c	165.46(7)	O(52A)b , C(1B)c	161.94(8)
O(52A)b , Na(1)b	42.13(5)	O(22A)e , O(3W)	164.33(9)	O(22A)e , O(12B)c	80.45(7)	O(22A)e , C(41A)	103.68(7)
O(22A)e , Cu(2)c	64.03(5)	O(22A)e , C(51A)b	83.59(7)	O(22A)e , C(21A)e	15.35(6)	O(22A)e , C(11B)c	96.26(7)
O(22A)e , C(1B)c	114.23(7)	O(22A)e , Na(1)b	86.10(6)	O(3W) , O(12B)c	115.05(8)	O(3W) , C(41A)	86.23(8)
O(3W) , Cu(2)c	129.82(7)	O(3W) , C(51A)b	81.26(8)	O(3W) , C(21A)e	179.67(9)	O(3W) , C(11B)c	98.85(8)
O(3W) , C(1B)c	79.01(8)	O(3W) , Na(1)b	89.07(7)	O(12B)c , C(41A)	64.04(6)	O(12B)c , Cu(2)c	36.18(4)
O(12B)c , C(51A)b	162.73(7)	O(12B)c , C(21A)e	65.28(6)	O(12B)c , C(11B)c	17.39(6)	O(12B)c , C(1B)c	42.05(6)
O(12B)c , Na(1)b	114.72(6)	C(41A) , Cu(2)c	47.09(5)	C(41A) , C(51A)b	114.05(7)	C(41A) , C(21A)e	93.95(7)
C(41A) , C(11B)c	66.62(6)	C(41A) , C(1B)c	80.68(7)	C(41A) , Na(1)b	58.01(5)	Cu(2)c , C(51A)b	128.96(5)
Cu(2)c , C(21A)e	50.45(4)	Cu(2)c , C(11B)c	51.43(5)	Cu(2)c , C(1B)c	76.48(5)	Cu(2)c , Na(1)b	80.95(3)
C(51A)b , C(21A)e	98.42(7)	C(51A)b , C(11B)c	179.33(7)	C(51A)b , C(1B)c	154.48(7)	C(51A)b , Na(1)b	57.31(5)
C(21A)e , C(11B)c	81.48(6)	C(21A)e , C(1B)c	101.28(7)	C(21A)e , Na(1)b	90.80(5)	C(11B)c , C(1B)c	25.19(6)
C(11B)c , Na(1)b	123.34(5)	C(1B)c , Na(1)b	137.75(5)				

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3.6 Angstrom Coordination Sphere Around Atom I = O(1W) [ARU = 1555.01] 0.90930 -0.11348 -0.35181 8.1390 -1.9183 -5.4143

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.323(2) --	Na(2)	[	=	]	Intra	-169.98	24.65	0.66950	-0.13521	-0.28886	6.0601	-2.2856	-4.4455
2	2.697(3) <<	O(2W)k	[1+x, 1/2-y, -1/2+z	=	4654.02]		75.13	-10.70	0.98440	0.03801	-0.38435	8.8191	0.6425	-5.9151
3	2.712(3) <<	O(22B)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra	-121.64	-75.35	0.81690	-0.14802	-0.52233	7.7793	-2.5022	-8.0386
4	2.719(2) <<	O(42A)b	[1+x, y, z	=	1655.01]	Intra	-23.90	28.29	1.20390	-0.17085	-0.26808	10.3279	-2.8881	-4.1257
5	3.163(3) ..	O(3W)	[	=	]	Intra	133.95	23.58	0.68320	0.00998	-0.26961	6.1272	0.1687	-4.1492
6	3.227(3) ..	O(52A)b	[1+x, y, z	=	1655.01]	Intra	-159.63	71.47	0.84600	-0.13460	-0.15299	7.1774	-2.2753	-2.3545
7	3.305(3) ..	O(22A)e	[1-x, -1/2+y, -1/2-z	=	2644.01]	Intra	-120.45	18.13	0.73090	-0.27364	-0.28500	6.5472	-4.6257	-4.3861
8	3.360(3) ..	C(21B)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra	-159.75	-59.12	0.65630	-0.14880	-0.53919	6.5207	-2.5154	-8.2980
9	3.396(3) ..	O(11B)e	[1-x, -1/2+y, -1/2-z	=	2644.01]	Intra	-16.05	-38.30	1.18810	-0.15705	-0.48856	10.6999	-2.6548	-7.5188
10	3.419(3) ..	C(5A)b	[1+x, y, z	=	1655.01]	Intra	47.73	65.26	1.08510	-0.05085	-0.15006	9.1013	-0.8596	-2.3094
11	3.433(3) ..	C(51A)b	[1+x, y, z	=	1655.01]	Intra	-44.33	84.95	0.99840	-0.12596	-0.12961	8.3549	-2.1293	-1.9947
12	3.520(3) ..	C(2B)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra	163.66	-46.15	0.57320	-0.07289	-0.51676	5.7990	-1.2322	-7.9528
13	3.538(3) ..	C(4A)b	[1+x, y, z	=	1655.01]	Intra	25.30	45.60	1.23260	-0.05090	-0.18754	10.3772	-0.8604	-2.8862
14	3.540(3) ..	C(41A)b	[1+x, y, z	=	1655.01]	Intra	-3.82	34.93	1.30490	-0.12491	-0.22010	11.0347	-2.1115	-3.3873

Angles (Degrees) At1...V...At2 with Vertex V = O(1W)

Na(2) , O(2W)k	116.96(9)	Na(2) , O(22B)c	104.53(8)	Na(2) , O(42A)b	117.81(9)	Na(2) , O(3W)	50.82(6)
Na(2) , O(52A)b	47.19(5)	Na(2) , O(22A)e	46.34(5)	Na(2) , C(21B)c	84.19(7)	Na(2) , O(11B)e	154.05(9)
Na(2) , C(5A)b	85.53(8)	Na(2) , C(51A)b	68.35(7)	Na(2) , C(2B)c	74.73(7)	Na(2) , C(4A)b	108.39(8)
Na(2) , C(41A)b	118.99(9)	O(2W)k , O(22B)c	93.34(9)	O(2W)k , O(42A)b	102.93(9)	O(2W)k , O(3W)	66.92(8)
O(2W)k , O(52A)b	110.87(9)	O(2W)k , O(22A)e	163.20(9)	O(2W)k , C(21B)c	97.52(9)	O(2W)k , O(11B)e	84.30(8)
O(2W)k , C(5A)b	78.67(8)	O(2W)k , C(51A)b	103.15(9)	O(2W)k , C(2B)c	81.29(8)	O(2W)k , C(4A)b	71.89(8)
O(2W)k , C(41A)b	87.24(8)	O(22B)c , O(42A)b	119.24(9)	O(22B)c , O(3W)	116.40(9)	O(22B)c , O(52A)b	148.65(8)
O(22B)c , O(22A)e	93.49(8)	O(22B)c , C(21B)c	21.18(6)	O(22B)c , O(11B)e	56.88(6)	O(22B)c , C(5A)b	169.33(9)
O(22B)c , C(51A)b	163.51(9)	O(22B)c , C(2B)c	41.93(6)	O(22B)c , C(4A)b	147.09(8)	O(22B)c , C(41A)b	130.60(8)
O(42A)b , O(3W)	123.91(9)	O(42A)b , O(52A)b	75.59(7)	O(42A)b , O(22A)e	87.03(7)	O(42A)b , C(21B)c	136.98(9)
O(42A)b , O(11B)e	67.00(6)	O(42A)b , C(5A)b	56.87(7)	O(42A)b , C(51A)b	57.00(7)	O(42A)b , C(2B)c	161.18(9)
O(42A)b , C(4A)b	42.16(6)	O(42A)b , C(41A)b	18.30(6)	O(3W) , O(52A)b	60.28(7)	O(3W) , O(22A)e	96.30(7)
O(3W) , C(21B)c	98.87(8)	O(3W) , O(11B)e	150.55(9)	O(3W) , C(5A)b	67.14(7)	O(3W) , C(51A)b	71.47(8)
O(3W) , C(2B)c	74.75(7)	O(3W) , C(4A)b	85.37(8)	O(3W) , C(41A)b	109.11(8)	O(52A)b , O(22A)e	58.05(6)
O(52A)b , C(21B)c	130.58(8)	O(52A)b , O(11B)e	142.03(8)	O(52A)b , C(5A)b	42.01(6)	O(52A)b , C(51A)b	21.17(5)
O(52A)b , C(2B)c	120.48(7)	O(52A)b , C(4A)b	62.88(6)	O(52A)b , C(41A)b	72.23(6)	O(22A)e , C(21B)c	83.65(7)
O(22A)e , O(11B)e	112.24(7)	O(22A)e , C(5A)b	96.13(7)	O(22A)e , C(51A)b	70.73(7)	O(22A)e , C(2B)c	93.66(7)
O(22A)e , C(4A)b	109.11(8)	O(22A)e , C(41A)b	99.86(7)	C(21B)c , O(11B)e	78.04(7)	C(21B)c , C(5A)b	165.94(8)
C(21B)c , C(51A)b	150.96(8)	C(21B)c , C(2B)c	25.26(6)	C(21B)c , C(4A)b	166.15(9)	C(21B)c , C(41A)b	151.12(8)
O(11B)e , C(5A)b	114.69(7)	O(11B)e , C(51A)b	123.82(7)	O(11B)e , C(2B)c	95.55(7)	O(11B)e , C(4A)b	91.75(6)
O(11B)e , C(41A)b	74.10(6)	C(5A)b , C(51A)b	25.40(6)	C(5A)b , C(2B)c	141.42(8)	C(5A)b , C(4A)b	23.14(6)
C(5A)b , C(41A)b	42.83(6)	C(51A)b , C(2B)c	140.55(8)	C(51A)b , C(4A)b	42.85(6)	C(51A)b , C(41A)b	51.30(6)
C(2B)c , C(4A)b	151.34(9)	C(2B)c , C(41A)b	165.32(8)	C(4A)b , C(41A)b	24.46(6)		

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3.6 Angstrom Coordination Sphere Around Atom I = O(2W) [ARU = 1555.02] -0.01560 0.46199 0.11565 -0.3880 7.8097 1.7798

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.590(3)	<<	O(7W)	[	= 01]			-86.85	16.51	0.01470	0.31534	0.16348	-0.2517	5.3306	2.5159
2	2.697(3)	<<	O(1W)k	[-1+x,1/2-y,1/2+z	= 4455.01]			104.87	10.70	-0.09070	0.61348	0.14819	-1.0681	10.3705	2.2806
3	2.970(3)	.<	O(22B)b	[1+x,y,z	= 1655.01]			-45.68	-28.92	0.18310	0.35198	0.02233	1.4278	5.9500	0.3437
4	3.016(3)	.<	O(11B)	[	= 01]			-118.77	-40.43	-0.18810	0.34295	-0.01144	-1.4928	5.7974	-0.1761
5	3.254(4)	..	O(3W)k	[-1+x,1/2-y,1/2+z	= 4455.01]			170.02	32.86	-0.31680	0.49002	0.23039	-3.0799	8.2835	3.5457
6	3.377(3)	..	C(6B)h	[-1-x,1-y,-z	= 3465.01]			164.30	-43.08	-0.35170	0.50147	-0.03422	-2.7622	8.4770	-0.5266
7	3.446(3)	..	C(6B)b	[1+x,y,z	= 1655.01]			11.09	-21.32	0.35170	0.49853	0.03422	2.7622	8.4274	0.5266
8	3.534(2)	<<	Cu(1)	[	= 01]			-79.65	-16.79	0.04108	0.26508	0.04931	0.2200	4.4810	0.7589
9	2.51	<<	H(6B)b	[1+x,y,z	= 1655.01]			14.81	-20.87	0.24920	0.49750	0.05750	1.8818	8.4099	0.8849
10	3.13	..	H(6B)h	[-1-x,1-y,-z	= 3465.01]			155.37	-58.34	-0.24920	0.50250	-0.05750	-1.8818	8.4945	-0.8849

Angles (Degrees) At1...V...At2 with Vertex V = O(2W)

O(7W)	,	O(1W)k	150.41(11)	O(7W)	,	O(22B)b	60.38(7)	O(7W)	,	O(11B)	64.21(7)	O(7W)	,	O(3W)k	91.64(9)
O(7W)	,	C(6B)h	114.86(10)	O(7W)	,	C(6B)b	103.11(9)	O(7W)	,	Cu(1)	34.05(5)	O(1W)k	,	O(22B)b	147.01(10)
O(1W)k	,	O(11B)	131.43(10)	O(1W)k	,	O(3W)k	63.40(7)	O(1W)k	,	C(6B)h	76.22(8)	O(1W)k	,	C(6B)b	97.35(9)
O(1W)k	,	Cu(1)	172.50(10)	O(22B)b	,	O(11B)	59.50(6)	O(22B)b	,	O(3W)k	149.26(10)	O(22B)b	,	C(6B)h	102.91(9)
O(22B)b	,	C(6B)b	51.49(7)	O(22B)b	,	Cu(1)	33.42(4)	O(11B)	,	O(3W)k	98.40(9)	O(11B)	,	C(6B)h	55.34(7)
O(11B)	,	C(6B)b	102.63(9)	O(11B)	,	Cu(1)	41.17(5)	O(3W)k	,	C(6B)h	76.13(8)	O(3W)k	,	C(6B)b	158.04(10)
O(3W)k	,	Cu(1)	115.86(8)	C(6B)h	,	C(6B)b	111.03(9)	C(6B)h	,	Cu(1)	96.30(7)	C(6B)b	,	Cu(1)	84.64(7)

3.6 Angstrom Coordination Sphere Around Atom I = O(3W)	[ARU = 1555.01]	0.68320	0.00998	-0.26961	6.1272	0.1687	-4.1492

Nr	d(I, J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.473(2)	--	Na(2)	[	=	]	Intra	-91.56	-6.88	0.66950	-0.13521	-0.28886	6.0601	-2.2856	-4.4455
2	2.955(3)	.<	O(6W)b	[1+x, y, z	=	1655.01]	Intra	87.65	-9.32	0.68930	0.18233	-0.30069	6.2468	3.0822	-4.6276
3	3.163(3)	..	O(1W)	[	=	]	Intra	-46.05	-23.58	0.90930	-0.11348	-0.35181	8.1390	-1.9183	-5.4143
4	3.209(3)	..	O(52A)b	[1+x, y, z	=	1655.01]	Intra	-66.75	34.01	0.84600	-0.13460	-0.15299	7.1774	-2.2753	-2.3545
5	3.254(4)	..	O(2W)k	[1+x, 1/2-y, -1/2+z	=	4654.02]		9.98	-32.86	0.98440	0.03801	-0.38435	8.8191	0.6425	-5.9151
6	3.291(4)	..	C(6A)b	[1+x, y, z	=	1655.01]	Intra	4.24	42.76	1.02240	0.02055	-0.12442	8.5370	0.3474	-1.9148
7	3.306(4)	..	O(5W)b	[1+x, y, z	=	1655.01]	Intra	-147.97	76.10	0.65830	-0.01494	-0.06110	5.4537	-0.2526	-0.9403
8	3.332(4)	..	C(3A)	[	=	]	Intra	176.94	19.50	0.31500	0.01989	-0.19732	2.9904	0.3362	-3.0367
9	3.348(3)	..	O(41A)	[	=	]	Intra	-128.23	17.92	0.45780	-0.13806	-0.20266	4.1555	-2.3338	-3.1189
10	3.414(3)	..	O(21A)	[	=	]	Intra	123.04	27.13	0.50640	0.16066	-0.16844	4.4704	2.7159	-2.5923
11	2.39	<<	H(3A)	[	=	]	Intra	175.94	17.64	0.41530	0.01950	-0.22260	3.8576	0.3296	-3.4258
12	3.04	..	H(6A)b	[1+x, y, z	=	1655.01]	Intra	6.78	59.34	0.92150	0.02080	-0.09970	7.6663	0.3516	-1.5344

Angles (Degrees) At1...V...At2 with Vertex V = 0(3W)

[illegible]

3.6 Angstrom Coordination Sphere Around Atom I = O(4W) [ARU = 1555.01] -0.60340 -0.13127 -0.00353 -4.8640 -2.2190 -0.0543

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.275(3) --	Na(1)	[	=	]	Intra	-11.17	-25.34	-0.37130	-0.15484	-0.06681	-2.8466	-2.6175	-1.0282
2	2.707(3) <<	O(51A)a	[-1+x,y,z	=	1455.01]	Intra	-161.44	-27.13	-0.90880	-0.17665	-0.08376	-7.1481	-2.9862	-1.2891
3	2.721(3) <<	O(21A)i	[-x,-y,-z	=	3555.01]	Intra	-51.61	76.53	-0.50640	-0.16066	0.16844	-4.4704	-2.7159	2.5923
4	2.729(4) <<	O(5W)g	[-1-x,-y,-z	=	3455.01]	Intra	103.42	21.38	-0.65830	0.01494	0.06110	-5.4537	0.2526	0.9403
5	3.112(4) ..	O(5W)	[	=	]	Intra	41.24	-16.54	-0.34170	-0.01494	-0.06110	-2.6205	-0.2526	-0.9403
6	3.209(3) ..	O(41A)a	[-1+x,y,z	=	1455.01]	Intra	-6.92	-72.74	-0.54220	-0.13806	-0.20266	-3.9187	-2.3338	-3.1189
7	3.269(4) ..	C(4A)a	[-1+x,y,z	=	1455.01]	Intra	123.73	-60.02	-0.76740	-0.05090	-0.18754	-5.7712	-0.8604	-2.8862
8	3.311(3) ..	O(12A)g	[-1-x,-y,-z	=	3455.01]	Intra	-161.37	35.65	-0.88400	-0.18213	0.12188	-7.4137	-3.0788	1.8757
9	3.344(3) ..	C(41A)a	[-1+x,y,z	=	1455.01]	Intra	156.71	-85.34	-0.69510	-0.12491	-0.22010	-5.1137	-2.1115	-3.3873
10	3.360(3) ..	O(21B)g	[-1-x,-y,-z	=	3455.01]	Intra	-60.40	-18.69	-0.42830	-0.29498	-0.07349	-3.2917	-4.9865	-1.1310
11	3.393(3) ..	C(21A)i	[-x,-y,-z	=	3555.01]	Intra	-19.85	59.06	-0.34710	-0.16631	0.18560	-3.2231	-2.8114	2.8563
12	3.420(3) ..	C(5A)a	[-1+x,y,z	=	1455.01]	Intra	148.09	-41.25	-0.91490	-0.05085	-0.15006	-7.0471	-0.8596	-2.3094
13	3.515(3) ..	C(51A)a	[-1+x,y,z	=	1455.01]	Intra	178.24	-33.51	-1.00160	-0.12596	-0.12961	-7.7935	-2.1293	-1.9947
14	3.539(3) ..	O(12B)g	[-1-x,-y,-z	=	3455.01]	Intra	-91.02	28.58	-0.57940	-0.31509	0.10649	-4.9195	-5.3264	1.6389

Angles (Degrees) At1...V...At2 with Vertex V = O(4W)

Na(1) , O(51A)a	120.21(11)	Na(1) , O(21A)i	104.84(10)	Na(1) , O(5W)g	120.41(12)	Na(1) , O(5W)	49.43(8)
Na(1) , O(41A)a	47.45(6)	Na(1) , C(4A)a	87.02(9)	Na(1) , O(12A)g	152.46(11)	Na(1) , C(41A)a	69.22(8)
Na(1) , O(21B)g	45.87(6)	Na(1) , C(21A)i	84.71(9)	Na(1) , C(5A)a	110.69(10)	Na(1) , C(51A)a	120.48(10)
Na(1) , O(12B)g	93.72(9)	O(51A)a, O(21A)i	120.92(10)	O(51A)a, O(5W)g	103.92(11)	O(51A)a, O(5W)	131.10(11)
O(51A)a, O(41A)a	78.63(8)	O(51A)a, C(4A)a	59.24(7)	O(51A)a, O(12A)g	62.78(7)	O(51A)a, C(41A)a	59.44(7)
O(51A)a, O(21B)g	90.88(8)	O(51A)a, C(21A)i	138.56(10)	O(51A)a, C(5A)a	43.41(7)	O(51A)a, C(51A)a	18.62(6)
O(51A)a, O(12B)g	87.49(8)	O(21A)i, O(5W)g	80.92(10)	O(21A)i, O(5W)	106.74(10)	O(21A)i, O(41A)a	151.59(10)
O(21A)i, C(4A)a	163.41(11)	O(21A)i, O(12A)g	59.81(7)	O(21A)i, C(41A)a	170.38(11)	O(21A)i, O(21B)g	95.37(9)
O(21A)i, C(21A)i	20.62(6)	O(21A)i, C(5A)a	143.71(10)	O(21A)i, C(51A)a	131.46(10)	O(21A)i, O(12B)g	51.44(6)
O(5W)g , O(5W)	71.77(10)	O(5W)g , O(41A)a	116.37(11)	O(5W)g , C(4A)a	83.07(10)	O(5W)g , O(12A)g	81.74(10)
O(5W)g , C(41A)a	108.55(11)	O(5W)g , O(21B)g	164.57(12)	O(5W)g , C(21A)i	87.13(10)	O(5W)g , C(5A)a	75.07(10)
O(5W)g , C(51A)a	89.88(10)	O(5W)g , O(12B)g	128.13(10)	O(5W) , O(41A)a	62.51(8)	O(5W) , C(4A)a	71.99(9)
O(5W) , O(12A)g	152.26(11)	O(5W) , C(41A)a	75.51(9)	O(5W) , O(21B)g	95.27(9)	O(5W) , C(21A)i	90.34(9)
O(5W) , C(5A)a	91.22(9)	O(5W) , C(51A)a	115.31(10)	O(5W) , O(12B)g	134.61(10)	O(41A)a, C(4A)a	43.07(6)
O(41A)a, O(12A)g	140.73(9)	O(41A)a, C(41A)a	21.77(5)	O(41A)a, O(21B)g	61.75(6)	O(41A)a, C(21A)i	132.10(9)
O(41A)a, C(5A)a	64.70(7)	O(41A)a, C(51A)a	73.70(7)	O(41A)a, O(12B)g	115.47(8)	C(4A)a , O(12A)g	113.52(9)
C(4A)a , C(41A)a	26.18(6)	C(4A)a , O(21B)g	101.22(8)	C(4A)a , C(21A)i	161.75(10)	C(4A)a , C(5A)a	24.03(6)
C(4A)a , C(51A)a	43.94(7)	C(4A)a , O(12B)g	140.80(9)	O(12A)g, C(41A)a	122.12(9)	O(12A)g, O(21B)g	109.47(8)
O(12A)g, C(21A)i	80.04(7)	O(12A)g, C(5A)a	89.77(8)	O(12A)g, C(51A)a	71.74(7)	O(12A)g, O(12B)g	58.74(6)
C(41A)a, O(21B)g	75.05(7)	C(41A)a, C(21A)i	153.72(10)	C(41A)a, C(5A)a	44.15(7)	C(41A)a, C(51A)a	52.18(7)
C(41A)a, O(12B)g	120.26(9)	O(21B)g, C(21A)i	84.54(8)	O(21B)g, C(5A)a	114.50(9)	O(21B)g, C(51A)a	103.54(8)
O(21B)g, O(12B)g	55.77(6)	C(21A)i, C(5A)a	160.65(10)	C(21A)i, C(51A)a	151.76(10)	C(21A)i, O(12B)g	56.22(6)
C(5A)a , C(51A)a	25.04(6)	C(5A)a , O(12B)g	130.87(9)	C(51A)a, O(12B)g	105.87(8)		

3.6 Angstrom Coordination Sphere Around Atom I = O(5W) [ARU = 1555.01] -0.34170 -0.01494 -0.06110 -2.6205 -0.2526 -0.9403

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.377(3)	--	Na(1)	[	=	] Intra	-95.46	-2.12	-0.37130	-0.15484	-0.06681	-2.8466	-2.6175	-1.0282
2	2.729(4)	<<	O(4W)g	[-1-x, -y, -z	= 3455.01]	Intra	103.42	21.38	-0.39660	0.13127	0.00353	-3.2102	2.2190	0.0543
3	3.010(4)	<	O(52A)	[	=	] Intra	-49.56	-28.02	-0.15400	-0.13460	-0.15299	-0.8968	-2.2753	-2.3545
4	3.112(4)	..	O(4W)	[	=	] Intra	-138.76	16.54	-0.60340	-0.13127	-0.00353	-4.8640	-2.2190	-0.0543
5	3.281(4)	..	O(41A)a	[-1+x, y, z	= 1455.01]	Intra	-121.95	-41.61	-0.54220	-0.13806	-0.20266	-3.9187	-2.3338	-3.1189
6	3.288(4)	..	C(3A)a	[-1+x, y, z	= 1455.01]	Intra	166.56	-39.62	-0.68500	0.01989	-0.19732	-5.0838	0.3362	-3.0367
7	3.289(4)	..	C(6A)	[	=	] Intra	11.01	-17.24	0.02240	0.02055	-0.12442	0.4628	0.3474	-1.9148
8	3.306(4)	..	O(3W)a	[-1+x, y, z	= 1455.01]	Intra	32.03	-76.10	-0.31680	0.00998	-0.26961	-1.9470	0.1687	-4.1492
9	3.438(5)	..	O(5W)g	[-1-x, -y, -z	= 3455.01]	Intra	169.89	33.16	-0.65830	0.01494	0.06110	-5.4537	0.2526	0.9403
10	3.537(3)	..	O(21A)a	[-1+x, y, z	= 1455.01]	Intra	108.33	-27.85	-0.49360	0.16066	-0.16844	-3.6038	2.7159	-2.5923
11	3.580(4)	..	C(6A)i	[-x, -y, -z	= 3555.01]	Intra	-2.52	52.89	-0.02240	-0.02055	0.12442	-0.4628	-0.3474	1.9148
12	3.591(4)	..	C(1A)i	[-x, -y, -z	= 3555.01]	Intra	-41.46	56.80	-0.10440	-0.09196	0.13415	-1.1469	-1.5545	2.0645
13	2.37	<<	H(6A)	[	=	] Intra	15.27	-14.52	-0.07850	0.02080	-0.09970	-0.4079	0.3516	-1.5344
14	3.01	..	H(3A)a	[-1+x, y, z	= 1455.01]	Intra	159.96	-55.64	-0.58470	0.01950	-0.22260	-4.2166	0.3296	-3.4258

Angles (Degrees) At1...V...At2 with Vertex V = O(5W)

Na(1) , O(4W)g	153.38(15)	Na(1) , O(52A)	50.85(7)	Na(1) , O(4W)	46.64(8)	Na(1) , O(41A)a	46.11(7)
Na(1) , C(3A)a	94.78(11)	Na(1) , C(6A)	105.05(12)	Na(1) , O(3W)a	96.33(11)	Na(1) , O(5W)g	95.05(11)
Na(1) , O(21A)a	142.30(13)	Na(1) , C(6A)i	93.47(10)	Na(1) , C(1A)i	73.10(9)	O(4W)g , O(52A)	154.63(14)
O(4W)g , O(4W)	108.23(12)	O(4W)g , O(41A)a	136.98(13)	O(4W)g , C(3A)a	84.74(11)	O(4W)g , C(6A)	98.36(11)
O(4W)g , O(3W)a	106.41(11)	O(4W)g , O(5W)g	59.30(9)	O(4W)g , O(21A)a	49.45(8)	O(4W)g , C(6A)i	82.16(10)
O(4W)g , C(1A)i	96.44(11)	O(52A) , O(4W)	97.00(10)	O(52A) , O(41A)a	59.23(7)	O(52A) , C(3A)a	104.47(11)
O(52A) , C(6A)	56.40(8)	O(52A) , O(3W)a	60.86(8)	O(52A) , O(5W)g	145.85(12)	O(52A) , O(21A)a	120.25(11)
O(52A) , C(6A)i	90.67(10)	O(52A) , C(1A)i	85.10(9)	O(4W) , O(41A)a	60.19(8)	O(4W) , C(3A)a	75.79(10)
O(4W) , C(6A)	151.10(12)	O(4W) , O(3W)a	120.25(11)	O(4W) , O(5W)g	48.93(8)	O(4W) , O(21A)a	117.58(11)
O(4W) , C(6A)i	100.99(10)	O(4W) , C(1A)i	80.13(9)	O(41A)a , C(3A)a	52.68(7)	O(41A)a , C(6A)	106.85(10)
O(41A)a , O(3W)a	61.11(7)	O(41A)a , O(5W)g	97.49(10)	O(41A)a , O(21A)a	96.45(9)	O(41A)a , C(6A)i	138.70(11)
O(41A)a , C(1A)i	119.21(10)	C(3A)a , C(6A)	118.74(11)	C(3A)a , O(3W)a	60.72(8)	C(3A)a , O(5W)g	72.85(9)
C(3A)a , O(21A)a	48.97(7)	C(3A)a , C(6A)i	164.76(12)	C(3A)a , C(1A)i	154.95(12)	C(6A) , O(3W)a	59.88(8)
C(6A) , O(5W)g	155.22(12)	C(6A) , O(21A)a	88.23(9)	C(6A) , C(6A)i	71.10(9)	C(6A) , C(1A)i	85.95(10)
O(3W)a , O(5W)g	132.86(12)	O(3W)a , O(21A)a	59.75(7)	O(3W)a , C(6A)i	130.90(11)	O(3W)a , C(1A)i	140.79(12)
O(5W)g , O(21A)a	84.44(9)	O(5W)g , C(6A)i	93.69(10)	O(5W)g , C(1A)i	86.20(9)	O(21A)a , C(6A)i	124.22(10)
O(21A)a , C(1A)i	144.02(10)	C(6A)i , C(1A)i	22.44(6)				

3.6 Angstrom Coordination Sphere Around Atom I = O(6W) [ARU = 1555.01] -0.31070 0.18233 -0.30069 -1.8274 3.0822 -4.6276

Nr	d(I, J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.0242(19)	--	Cu(2)	[	=	]	Intra	114.70	55.74	-0.33918	0.24358	-0.19199	-2.3036	4.1175	-2.9547
2	2.687(3)	<<	O(21B)	k	[x, 1/2-y, -1/2+z	= 4554.01]		168.11	-46.12	-0.57170	0.20502	-0.42651	-3.6497	3.4657	-6.5639
3	2.726(3)	<<	O(21A)	a	[-1+x, y, z	= 1455.01]	Intra	-168.35	48.29	-0.49360	0.16066	-0.16844	-3.6038	2.7159	-2.5923
4	2.764(2)	<<	O(7W)	k	[x, 1/2-y, -1/2+z	= 4554.01]		0.83	-11.51	0.01470	0.18466	-0.33652	0.8811	3.1216	-5.1790
5	2.789(3)	<<	O(42A)	d	[-x, 1/2+y, -1/2-z	= 2554.01]	Intra	74.11	22.30	-0.20390	0.32915	-0.23192	-1.1209	5.5641	-3.5692
6	2.955(3)	<	O(3W)	a	[-1+x, y, z	= 1455.01]	Intra	-92.35	9.32	-0.31680	0.00998	-0.26961	-1.9470	0.1687	-4.1492
7	2.989(3)	<	O(12A)	[	=	]	Intra	-0.17	67.02	-0.11600	0.18213	-0.12188	-0.6605	3.0788	-1.8757
8	3.263(3)	..	O(41A)	d	[-x, 1/2+y, -1/2-z	= 2554.01]	Intra	111.49	0.91	-0.45780	0.36194	-0.29734	-3.0227	6.1184	-4.5760
9	3.274(3)	..	C(41A)	d	[-x, 1/2+y, -1/2-z	= 2554.01]	Intra	90.00	5.61	-0.30490	0.37509	-0.27990	-1.8277	6.3407	-4.3076
10	3.505(3)	..	C(21B)	k	[x, 1/2-y, -1/2+z	= 4554.01]		-166.86	-44.67	-0.65630	0.14880	-0.46081	-4.2550	2.5154	-7.0918
11	3.515(3)	..	C(21A)	a	[-1+x, y, z	= 1455.01]	Intra	-174.88	30.26	-0.65290	0.16631	-0.18560	-4.8511	2.8114	-2.8563
12	3.586(3)	..	O(11B)	k	[x, 1/2-y, -1/2+z	= 4554.01]		-16.24	-64.77	-0.18810	0.15705	-0.51144	-0.3600	2.6548	-7.8710

Angles (Degrees) At1...V...At2 with Vertex V = 0(6W)

Cu(2) , O(21B)k	111.29(8)	Cu(2) , O(21A)a	45.45(5)	Cu(2) , O(7W)k	112.84(8)	Cu(2) , O(42A)d	44.83(5)
Cu(2) , O(3W)a	111.16(9)	Cu(2) , O(12A)	48.05(5)	Cu(2) , O(41A)d	54.89(5)	Cu(2) , C(41A)d	53.86(6)
Cu(2) , C(21B)k	120.05(8)	Cu(2) , C(21A)a	54.59(6)	Cu(2) , O(11B)k	154.81(9)	O(21B)k, O(21A)a	96.62(7)
O(21B)k, O(7W)k	121.25(9)	O(21B)k, O(42A)d	108.56(8)	O(21B)k, O(3W)a	103.30(9)	O(21B)k, O(12A)	158.21(9)
O(21B)k, O(41A)d	68.29(6)	O(21B)k, C(41A)d	85.89(8)	O(21B)k, C(21B)k	17.56(6)	O(21B)k, C(21A)a	77.92(7)
O(21B)k, O(11B)k	69.06(6)	O(21A)a, O(7W)k	142.12(9)	O(21A)a, O(42A)d	90.08(8)	O(21A)a, O(3W)a	73.76(8)
O(21A)a, O(12A)	64.34(6)	O(21A)a, O(41A)d	82.79(7)	O(21A)a, C(41A)d	93.48(8)	O(21A)a, C(21B)k	92.97(7)
O(21A)a, C(21A)a	18.71(6)	O(21A)a, O(11B)k	157.82(8)	O(7W)k , O(42A)d	79.33(7)	O(7W)k , O(3W)a	94.94(8)
O(7W)k , O(12A)	78.53(7)	O(7W)k , O(41A)d	110.41(7)	O(7W)k , C(41A)d	90.31(8)	O(7W)k , C(21B)k	122.73(8)
O(7W)k , C(21A)a	160.83(9)	O(7W)k , O(11B)k	54.57(6)	O(42A)d, O(3W)a	145.71(9)	O(42A)d, O(12A)	63.43(6)
O(42A)d, O(41A)d	42.17(5)	O(42A)d, C(41A)d	22.68(6)	O(42A)d, C(21B)k	125.88(8)	O(42A)d, C(21A)a	95.47(7)
O(42A)d, O(11B)k	110.22(7)	O(3W)a , O(12A)	82.28(8)	O(3W)a , O(41A)d	154.15(8)	O(3W)a , C(41A)d	164.89(10)
O(3W)a , C(21B)k	85.77(8)	O(3W)a , C(21A)a	78.91(8)	O(3W)a , O(11B)k	92.61(8)	O(12A) , O(41A)d	97.44(7)
O(12A) , C(41A)d	84.91(7)	O(12A) , C(21B)k	156.55(8)	O(12A) , C(21A)a	82.64(7)	O(12A) , O(11B)k	132.29(7)
O(41A)d, C(41A)d	21.95(5)	O(41A)d, C(21B)k	84.71(7)	O(41A)d, C(21A)a	75.44(6)	O(41A)d, O(11B)k	105.97(7)
C(41A)d, C(21B)k	103.27(8)	C(41A)d, C(21A)a	91.57(7)	C(41A)d, O(11B)k	101.95(7)	C(21B)k, C(21A)a	75.29(7)
C(21B)k, O(11B)k	68.18(6)	C(21A)a, O(11B)k	143.01(7)				

3.6 Angstrom Coordination Sphere Around Atom I = O(7W) [ARU = 1555.01] 0.01470 0.31534 0.16348 -0.2517 5.3306 2.5159

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.0079(19)	--	Cu(1)	[	=	] Intra	-60.96	-61.05	0.04108	0.26508	0.04931	0.2200	4.4810	0.7589
2	2.590(3)	<<	O(2W)	[	=	02]	93.15	-16.51	-0.01560	0.46199	0.11565	-0.3880	7.8097	1.7798
3	2.676(3)	<<	O(22A)k	[x,1/2-y,1/2+z	=	4555.01]	-21.62	44.35	0.26910	0.27364	0.28500	1.5270	4.6257	4.3861
4	2.731(3)	<<	O(51A)i	[-x,-y,-z	=	3555.01] Intra	-106.05	-26.70	-0.09120	0.17665	0.08376	-0.9261	2.9862	1.2891
5	2.764(2)	<<	O(6W)k	[x,1/2-y,1/2+z	=	4555.01]	179.17	11.51	-0.31070	0.31767	0.19931	-2.9602	5.3700	3.0673
6	2.815(3)	<<	O(22B)b	[1+x,y,z	=	1655.01] Intra	20.24	-50.51	0.18310	0.35198	0.02233	1.4278	5.9500	0.3437
7	3.001(3)	<	O(11B)	[	=	] Intra	159.39	-63.78	-0.18810	0.34295	-0.01144	-1.4928	5.7974	-0.1761
8	3.244(3)	..	C(51A)i	[-x,-y,-z	=	3555.01] Intra	-90.52	-9.25	0.00160	0.12596	0.12961	-0.2807	2.1293	1.9947
9	3.268(3)	..	O(52A)i	[-x,-y,-z	=	3555.01] Intra	-69.40	-2.83	0.15400	0.13460	0.15299	0.8968	2.2753	2.3545
10	3.313(3)	..	C(21A)k	[x,1/2-y,1/2+z	=	4555.01]	7.55	44.51	0.34710	0.33369	0.31440	2.0902	5.6408	4.8386
11	3.373(3)	..	C(2A)k	[x,1/2-y,1/2+z	=	4555.01]	45.33	49.15	0.25330	0.40816	0.32924	1.2992	6.8997	5.0669
12	3.497(3)	..	C(1A)k	[x,1/2-y,1/2+z	=	4555.01]	80.38	62.96	0.10440	0.40804	0.36585	0.0140	6.8977	5.6304
13	3.545(3)	..	O(42A)i	[-x,-y,-z	=	3555.01] Intra	-129.34	27.01	-0.20390	0.17085	0.26808	-2.2537	2.8881	4.1257
14	3.558(3)	..	C(21B)b	[1+x,y,z	=	1655.01] Intra	11.66	-32.52	0.34370	0.35120	0.03919	2.6863	5.9368	0.6031

Angles (Degrees) At1...V...At2 with Vertex V = O(7W)

Cu(1)	,	O(2W)	99.71(9)	Cu(1)	,	O(22A)k	110.12(8)	Cu(1)	,	O(51A)i	45.70(5)	Cu(1)	,	O(6W)k	114.25(8)
Cu(1)	,	O(22B)b	43.75(5)	Cu(1)	,	O(11B)	51.54(6)	Cu(1)	,	C(51A)i	56.21(6)	Cu(1)	,	O(52A)i	58.57(6)
Cu(1)	,	C(21A)k	119.15(8)	Cu(1)	,	C(2A)k	138.65(8)	Cu(1)	,	C(1A)k	162.03(8)	Cu(1)	,	O(42A)i	103.80(7)
Cu(1)	,	C(21B)b	53.68(6)	O(2W)	,	O(22A)k	119.07(9)	O(2W)	,	O(51A)i	132.94(10)	O(2W)	,	O(6W)k	89.51(8)
O(2W)	,	O(22B)b	66.51(8)	O(2W)	,	O(11B)	64.81(8)	O(2W)	,	C(51A)i	153.98(10)	O(2W)	,	O(52A)i	154.09(9)
O(2W)	,	C(21A)k	98.44(9)	O(2W)	,	C(2A)k	78.10(8)	O(2W)	,	C(1A)k	80.11(8)	O(2W)	,	O(42A)i	139.38(9)
O(2W)	,	C(21B)b	74.19(8)	O(22A)k,	O(51A)i	104.60(8)	O(22A)k,	O(6W)k	121.05(9)	O(22A)k,	O(22B)b	101.58(7)			
O(22A)k,	O(11B)	160.56(9)	O(22A)k,	C(51A)i	81.85(8)	O(22A)k,	O(52A)i	63.55(6)	O(22A)k,	C(21A)k	20.72(6)				
O(22A)k,	C(2A)k	44.61(6)	O(22A)k,	C(1A)k	56.29(7)	O(22A)k,	O(42A)i	82.91(7)	O(22A)k,	C(21B)b	82.63(7)				
O(51A)i,	O(6W)k	81.94(7)	O(51A)i,	O(22B)b	89.40(8)	O(51A)i,	O(11B)	68.18(7)	O(51A)i,	C(51A)i	22.81(6)				
O(51A)i,	O(52A)i	42.43(5)	O(51A)i,	C(21A)k	124.75(8)	O(51A)i,	C(2A)k	148.52(9)	O(51A)i,	C(1A)k	143.49(9)				
O(51A)i,	O(42A)i	58.19(6)	O(51A)i,	C(21B)b	96.24(7)	O(6W)k,	O(22B)b	137.34(9)	O(6W)k,	O(11B)	76.79(7)				
O(6W)k,	C(51A)i	92.14(8)	O(6W)k,	O(52A)i	111.56(8)	O(6W)k,	C(21A)k	123.47(8)	O(6W)k,	C(2A)k	107.04(8)				
O(6W)k,	C(1A)k	83.71(7)	O(6W)k,	O(42A)i	50.64(6)	O(6W)k,	C(21B)b	156.05(9)	O(22B)b,	O(11B)	61.33(6)				
O(22B)b,	C(51A)i	95.65(8)	O(22B)b,	O(52A)i	87.59(7)	O(22B)b,	C(21A)k	95.66(7)	O(22B)b,	C(2A)k	101.95(8)				
O(22B)b,	C(1A)k	122.92(8)	O(22B)b,	O(42A)i	147.04(8)	O(22B)b,	C(21B)b	19.07(6)	O(11B),	C(51A)i	90.32(8)				
O(11B),	O(52A)i	104.27(7)	O(11B),	C(21A)k	155.06(8)	O(11B),	C(2A)k	142.78(9)	O(11B),	C(1A)k	139.53(8)				
O(11B),	O(42A)i	106.32(7)	O(11B),	C(21B)b	80.37(7)	C(51A)i,	O(52A)i	21.95(5)	C(51A)i,	C(21A)k	102.21(8)				
C(51A)i,	C(2A)k	125.79(8)	C(51A)i,	C(1A)k	125.88(8)	C(51A)i,	O(42A)i	52.26(6)	C(51A)i,	C(21B)b	95.12(7)				
O(52A)i,	C(21A)k	82.75(7)	O(52A)i,	C(2A)k	108.10(7)	O(52A)i,	C(1A)k	115.87(8)	O(52A)i,	O(42A)i	64.96(5)				
O(52A)i,	C(21B)b	80.94(6)	C(21A)k,	C(2A)k	25.99(6)	C(21A)k,	C(1A)k	43.93(6)	C(21A)k,	O(42A)i	98.36(7)				
C(21A)k,	C(21B)b	77.13(7)	C(2A)k,	C(1A)k	23.49(6)	C(2A)k,	O(42A)i	103.70(7)	C(2A)k,	C(21B)b	87.00(7)				
C(1A)k,	O(42A)i	86.98(7)	C(1A)k,	C(21B)b	109.86(7)	O(42A)i,	C(21B)b	145.89(8)							

3.6 Angstrom Coordination Sphere Around Atom I = O(11A) [ARU = 1555.01] 0.13000 0.19884 -0.03592 1.1310 3.3613 -0.5528

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.289(3)	--	C(11A)	[	=		Intra	-138.31	-46.97	0.03150	0.16424	-0.09713	0.4744	2.7764	-1.4948
2	1.9505(18)	--	Cu(1)	[	=		Intra	129.13	42.26	0.04108	0.26508	0.04931	0.2200	4.4810	0.7589
3	2.449(2)	--	Na(1)i	[-x, -y, -z	=	3555.01]	Intra	-23.44	40.22	0.37130	0.15484	0.06681	2.8466	2.6175	1.0282
4	2.245(2)	<<	O(12A)	[	=		Intra	-171.04	-36.11	-0.11600	0.18213	-0.12188	-0.6605	3.0788	-1.8757
5	2.356(3)	<<	C(1A)	[	=		Intra	-89.50	-39.92	0.10440	0.09196	-0.13415	1.1469	1.5545	-2.0645
6	2.756(3)	<<	O(22B)b	[1+x, y, z	=	1655.01]	Intra	83.46	18.99	0.18310	0.35198	0.02233	1.4278	5.9500	0.3437
7	2.787(2)	<<	O(51A)i	[-x, -y, -z	=	3555.01]	Intra	-169.67	41.37	-0.09120	0.17665	0.08376	-0.9261	2.9862	1.2891
8	3.045(3)	<	C(2A)	[	=		Intra	-54.27	-42.96	0.25330	0.09184	-0.17076	2.4321	1.5525	-2.6280
9	3.112(3)	..	O(52A)i	[-x, -y, -z	=	3555.01]	Intra	-102.17	69.09	0.15400	0.13460	0.15299	0.8968	2.2753	2.3545
10	3.160(3)	<	C(21A)	[	=		Intra	-14.73	-46.80	0.34710	0.16631	-0.18560	3.2231	2.8114	-2.8563
11	3.162(3)	<	C(51A)i	[-x, -y, -z	=	3555.01]	Intra	-138.89	53.66	0.00160	0.12596	0.12961	-0.2807	2.1293	1.9947
12	3.185(3)	..	O(21B)b	[1+x, y, z	=	1655.01]	Intra	36.95	31.91	0.42830	0.29498	0.07349	3.2917	4.9865	1.1310
13	3.186(3)	..	O(22A)	[	=		Intra	16.92	-59.89	0.26910	0.22636	-0.21500	2.6599	3.8265	-3.3088
14	3.223(3)	..	C(21B)b	[1+x, y, z	=	1655.01]	Intra	58.87	21.02	0.34370	0.35120	0.03919	2.6863	5.9368	0.6031
15	3.374(3)	..	C(6A)	[	=		Intra	-102.50	-23.81	0.02240	0.02055	-0.12442	0.4628	0.3474	-1.9148
16	3.52	..	H(6A)	[	=		Intra	-117.08	-16.19	-0.07850	0.02080	-0.09970	-0.4079	0.3516	-1.5344

Angles (Degrees) At1...V...At2 with Vertex V = O(11A)

C(11A) , Cu(1)	120.94(15)	C(11A) , Na(1)i	133.72(16)	C(11A) , O(12A)	26.55(13)	C(11A) , C(1A)	35.54(14)
C(11A) , O(22B)b	135.98(16)	C(11A) , O(51A)i	92.63(14)	C(11A) , C(2A)	56.63(14)	C(11A) , O(52A)i	119.09(16)
C(11A) , C(21A)	74.07(14)	C(11A) , C(51A)i	100.64(15)	C(11A) , O(21B)b	164.51(16)	C(11A) , O(22A)	71.24(14)
C(11A) , C(21B)b	150.54(17)	C(11A) , C(6A)	36.74(14)	Cu(1) , Na(1)i	93.87(8)	Cu(1) , O(12A)	95.50(8)
Cu(1) , C(1A)	151.04(11)	Cu(1) , O(22B)b	44.95(5)	Cu(1) , O(51A)i	44.60(5)	Cu(1) , C(2A)	177.40(9)
Cu(1) , O(52A)i	62.42(6)	Cu(1) , C(21A)	154.08(10)	Cu(1) , C(51A)i	58.22(7)	Cu(1) , O(21B)b	70.64(6)
Cu(1) , O(22A)	136.23(9)	Cu(1) , C(21B)b	61.67(7)	Cu(1) , C(6A)	133.77(9)	Na(1)i , O(12A)	154.34(10)
Na(1)i , C(1A)	100.17(9)	Na(1)i , O(22B)b	89.99(7)	Na(1)i , O(51A)i	92.84(7)	Na(1)i , C(2A)	87.72(7)
Na(1)i , O(52A)i	48.98(5)	Na(1)i , C(21A)	87.36(7)	Na(1)i , C(51A)i	70.99(7)	Na(1)i , O(21B)b	48.58(5)
Na(1)i , O(22A)	105.47(7)	Na(1)i , C(21B)b	70.92(7)	Na(1)i , C(6A)	97.36(8)	O(12A) , C(1A)	62.01(9)
O(12A) , O(22B)b	113.32(9)	O(12A) , O(51A)i	77.49(8)	O(12A) , C(2A)	82.22(9)	O(12A) , O(52A)i	116.52(9)
O(12A) , C(21A)	94.41(9)	O(12A) , C(51A)i	93.98(9)	O(12A) , O(21B)b	156.51(10)	O(12A) , O(22A)	83.77(8)
O(12A) , C(21B)b	134.19(10)	O(12A) , C(6A)	59.45(8)	C(1A) , O(22B)b	158.21(11)	C(1A) , O(51A)i	109.02(10)
C(1A) , C(2A)	26.39(8)	C(1A) , O(52A)i	109.41(10)	C(1A) , C(21A)	52.72(8)	C(1A) , C(51A)i	102.78(10)
C(1A) , O(21B)b	136.55(9)	C(1A) , O(22A)	63.49(8)	C(1A) , C(21B)b	147.11(10)	C(1A) , C(6A)	19.49(8)
O(22B)b , O(51A)i	89.48(7)	O(22B)b , C(2A)	137.21(9)	O(22B)b , O(52A)i	91.83(7)	O(22B)b , C(21A)	109.23(8)
O(22B)b , C(51A)i	98.74(8)	O(22B)b , O(21B)b	43.58(5)	O(22B)b , O(22A)	95.31(7)	O(22B)b , C(21B)b	23.17(6)
O(22B)b , C(6A)	172.65(9)	O(51A)i , C(2A)	133.31(9)	O(51A)i , O(52A)i	43.95(5)	O(51A)i , C(21A)	161.29(9)
O(51A)i , C(51A)i	23.87(6)	O(51A)i , O(21B)b	102.71(7)	O(51A)i , O(22A)	161.04(8)	O(51A)i , C(21B)b	103.11(8)
O(51A)i , C(6A)	90.02(7)	C(2A) , O(52A)i	117.49(8)	C(2A) , C(21A)	27.98(7)	C(2A) , C(51A)i	120.56(9)
C(2A) , O(21B)b	111.94(8)	C(2A) , O(22A)	44.94(6)	C(2A) , C(21B)b	120.86(8)	C(2A) , C(6A)	43.86(7)
O(52A)i , C(21A)	132.07(8)	O(52A)i , C(51A)i	22.78(6)	O(52A)i , O(21B)b	74.65(6)	O(52A)i , O(22A)	153.53(7)

O(52A)i, C(21B)b	88.86(7)	O(52A)i, C(6A)	92.90(7)	C(21A) , C(51A)i	144.59(9)	C(21A) , O(21B)b	91.44(7)
C(21A) , O(22A)	22.64(6)	C(21A) , C(21B)b	94.65(8)	C(21A) , C(6A)	71.42(7)	C(51A)i, O(21B)b	94.35(8)
C(51A)i, O(22A)	165.47(9)	C(51A)i, C(21B)b	103.76(8)	C(51A)i, C(6A)	83.61(8)	O(21B)b, O(22A)	93.28(6)
O(21B)b, C(21B)b	22.38(6)	O(21B)b, C(6A)	143.47(8)	O(22A) , C(21B)b	87.82(7)	O(22A) , C(6A)	82.89(7)
C(21B)b, C(6A)	162.57(8)						

3.6 Angstrom Coordination Sphere Around Atom I = O(11B) [ARU = 1555.01] -0.18810 0.34295 -0.01144 -1.4928 5.7974 -0.1761

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.244(3)	--	C(11B)	[	=		Intra	169.53	-25.18	-0.33490	0.35506	-0.04584	-2.6002	6.0021	-0.7055
2	2.3539(19)	--	Cu(1)	[	=		Intra	-37.54	23.40	0.04108	0.26508	0.04931	0.2200	4.4810	0.7589
3	2.264(3)	<<	O(12B)	[	=		Intra	-164.18	-40.26	-0.42060	0.31509	-0.10649	-3.1547	5.3264	-1.6389
4	2.374(3)	<<	C(1B)	[	=		Intra	142.46	-2.61	-0.42290	0.42842	-0.01846	-3.3728	7.2422	-0.2841
5	2.970(2)	.<	O(22B)b	[1+x,y,z	=	1655.01]	Intra	2.99	10.08	0.18310	0.35198	0.02233	1.4278	5.9500	0.3437
6	2.986(3)	<<	C(6B)h	[-1-x,1-y,-z	=	3465.01]	Intra	115.35	-6.74	-0.35170	0.50147	-0.03422	-2.7622	8.4770	-0.5266
7	3.001(3)	.<	O(7W)	[	=		Intra	-20.61	63.78	0.01470	0.31534	0.16348	-0.2517	5.3306	2.5159
8	3.016(3)	.<	O(2W)	[	=	02]		61.23	40.43	-0.01560	0.46199	0.11565	-0.3880	7.8097	1.7798
9	3.220(3)	..	O(51A)i	[-x,-y,-z	=	3555.01]	Intra	-78.60	27.06	-0.09120	0.17665	0.08376	-0.9261	2.9862	1.2891
10	3.312(3)	..	O(12A)	[	=		Intra	-72.98	-30.87	-0.11600	0.18213	-0.12188	-0.6605	3.0788	-1.8757
11	3.347(2)	<<	Cu(2)	[	=		Intra	-115.76	-56.13	-0.33918	0.24358	-0.19199	-2.3036	4.1175	-2.9547
12	3.396(3)	..	O(1W)f	[1-x,1/2+y,-1/2-z	=	2654.01]	Intra	16.05	-38.30	0.09070	0.38652	-0.14819	1.0681	6.5339	-2.2806
13	3.421(3)	..	O(42A)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	-32.09	-82.63	-0.20390	0.32915	-0.23192	-1.1209	5.5641	-3.5692
14	3.505(3)	..	C(2B)	[	=		Intra	155.85	7.11	-0.57320	0.42711	0.01676	-4.6661	7.2200	0.2579
15	3.586(3)	..	O(6W)k	[x,1/2-y,1/2+z	=	4555.01]		-163.76	64.77	-0.31070	0.31767	0.19931	-2.9602	5.3700	3.0673
16	2.82	..	H(6B)h	[-1-x,1-y,-z	=	3465.01]	Intra	98.21	-14.58	-0.24920	0.50250	-0.05750	-1.8818	8.4945	-0.8849

Angles (Degrees) At1...V...At2 with Vertex V = O(11B)

C(11B), Cu(1)	155.30(18)	C(11B), O(12B)	26.61(14)	C(11B), C(1B)	34.48(14)	C(11B), O(22B)b	160.21(18)
C(11B), C(6B)h	54.84(15)	C(11B), O(7W)	140.83(17)	C(11B), O(2W)	119.48(17)	C(11B), O(51A)i	119.59(16)
C(11B), O(12A)	98.07(16)	C(11B), Cu(2)	60.91(14)	C(11B), O(1W)f	111.83(16)	C(11B), O(42A)d	71.70(15)
C(11B), C(2B)	34.93(14)	C(11B), O(6W)k	92.31(15)	Cu(1), O(12B)	132.42(10)	Cu(1), C(1B)	159.21(11)
Cu(1), O(22B)b	40.87(5)	Cu(1), C(6B)h	149.08(9)	Cu(1), O(7W)	41.91(5)	Cu(1), O(2W)	81.31(7)
Cu(1), O(51A)i	37.16(4)	Cu(1), O(12A)	64.02(6)	Cu(1), Cu(2)	103.02(7)	Cu(1), O(1W)f	79.55(6)
Cu(1), O(42A)d	106.06(7)	Cu(1), C(2B)	146.79(9)	Cu(1), O(6W)k	82.64(6)	O(12B), C(1B)	61.03(9)
O(12B), O(22B)b	147.74(10)	O(12B), C(6B)h	78.39(9)	O(12B), O(7W)	148.33(10)	O(12B), O(2W)	145.78(10)
O(12B), O(51A)i	103.98(9)	O(12B), O(12A)	71.47(8)	O(12B), Cu(2)	35.03(5)	O(12B), O(1W)f	101.44(9)
O(12B), O(42A)d	54.88(7)	O(12B), C(2B)	59.98(7)	O(12B), O(6W)k	105.03(8)	C(1B), O(22B)b	139.07(11)
C(1B), C(6B)h	27.33(8)	C(1B), O(7W)	117.59(10)	C(1B), O(2W)	85.04(10)	C(1B), O(51A)i	133.75(10)
C(1B), O(12A)	132.48(10)	C(1B), Cu(2)	94.35(8)	C(1B), O(1W)f	115.92(10)	C(1B), O(42A)d	94.73(9)
C(1B), C(2B)	16.53(8)	C(1B), O(6W)k	77.85(8)	O(22B)b, C(6B)h	113.11(9)	O(22B)b, O(7W)	56.25(6)
O(22B)b, O(2W)	59.47(7)	O(22B)b, O(51A)i	78.01(6)	O(22B)b, O(12A)	83.39(6)	O(22B)b, Cu(2)	114.16(7)
O(22B)b, O(1W)f	49.89(5)	O(22B)b, O(42A)d	94.02(7)	O(22B)b, C(2B)	147.97(9)	O(22B)b, O(6W)k	104.49(7)
C(6B)h, O(7W)	114.88(9)	C(6B)h, O(2W)	68.47(8)	C(6B)h, O(51A)i	155.74(9)	C(6B)h, O(12A)	141.55(9)
C(6B)h, Cu(2)	104.48(7)	C(6B)h, O(1W)f	93.05(8)	C(6B)h, O(42A)d	89.48(8)	C(6B)h, C(2B)	42.72(7)
C(6B)h, O(6W)k	92.25(7)	O(7W), O(2W)	50.99(6)	O(7W), O(51A)i	51.93(6)	O(7W), O(12A)	103.22(7)
O(7W), Cu(2)	140.08(8)	O(7W), O(1W)f	106.13(7)	O(7W), O(42A)d	146.52(7)	O(7W), C(2B)	109.06(8)
O(7W), O(6W)k	48.64(5)	O(2W), O(51A)i	102.88(8)	O(2W), O(12A)	142.03(8)	O(2W), Cu(2)	164.18(8)
O(2W), O(1W)f	88.91(7)	O(2W), O(42A)d	130.45(8)	O(2W), C(2B)	88.89(8)	O(2W), O(6W)k	69.07(7)

O(51A)i, O(12A)	58.18(6)	O(51A)i, Cu(2)	88.98(6)	O(51A)i, O(1W)f	109.79(7)	O(51A)i, O(42A)d	111.87(7)
O(51A)i, C(2B)	117.22(7)	O(51A)i, O(6W)k	63.67(6)	O(12A), Cu(2)	39.00(4)	O(12A), O(1W)f	70.76(6)
O(12A), O(42A)d	53.69(6)	O(12A), C(2B)	128.63(8)	O(12A), O(6W)k	117.98(7)	Cu(2), O(1W)f	77.11(5)
Cu(2), O(42A)d	33.77(4)	Cu(2), C(2B)	95.00(6)	Cu(2), O(6W)k	126.31(6)	O(1W)f, O(42A)d	47.01(5)
O(1W)f, C(2B)	132.19(8)	O(1W)f, O(6W)k	153.53(7)	O(42A)d, C(2B)	104.41(7)	O(42A)d, O(6W)k	158.99(7)
C(2B), O(6W)k	64.27(6)						

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3.6 Angstrom Coordination Sphere Around Atom I = O(12A) [ARU = 1555.01] -0.11600 0.18213 -0.12188 -0.6605 3.0788 -1.8757

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	1.235(3)	--	C(11A)	[	=		Intra	-14.92	17.97	0.03150	0.16424	-0.09713	0.4744	2.7764	-1.4948
2	2.2233(18)	--	Cu(2)	[	=		Intra	147.70	-29.03	-0.33918	0.24358	-0.19199	-2.3036	4.1175	-2.9547

3	2.245(2)	<<	O(11A)	[	=		Intra	8.96	36.11	0.13000	0.19884	-0.03592	1.1310	3.3613	-0.5528
4	2.372(3)	<<	C(1A)	[	=		Intra	-40.14	-4.57	0.10440	0.09196	-0.13415	1.1469	1.5545	-2.0645
5	2.954(3)	<<	C(6A)	[	=		Intra	-67.65	-0.76	0.02240	0.02055	-0.12442	0.4628	0.3474	-1.9148
6	2.989(3)	<	O(6W)	[	=		Intra	179.83	-67.02	-0.31070	0.18233	-0.30069	-1.8274	3.0822	-4.6276
7	3.043(3)	..	O(42A)d	[-x, 1/2+y, -1/2-z	=	2554.01]	Intra	100.50	-33.82	-0.20390	0.32915	-0.23192	-1.1209	5.5641	-3.5692
8	3.051(2)	..	O(21A)a	[-1+x, y, z	=	1455.01]	Intra	-172.97	-13.58	-0.49360	0.16066	-0.16844	-3.6038	2.7159	-2.5923
9	3.112(2)	<<	Cu(1)	[	=		Intra	57.88	57.85	0.04108	0.26508	0.04931	0.2200	4.4810	0.7589
10	3.177(3)	..	O(51A)i	[-x, -y, -z	=	3555.01]	Intra	-160.78	84.92	-0.09120	0.17665	0.08376	-0.9261	2.9862	1.2891
11	3.311(3)	..	O(4W)g	[-1-x, -y, -z	=	3455.01]	Intra	-161.37	35.65	-0.39660	0.13127	0.00353	-3.2102	2.2190	0.0543
12	3.312(3)	..	O(11B)	[	=		Intra	107.02	30.87	-0.18810	0.34295	-0.01144	-1.4928	5.7974	-0.1761
13	3.366(2)	..	O(12B)	[	=		Intra	137.98	4.04	-0.42060	0.31509	-0.10649	-3.1547	5.3264	-1.6389
14	3.530(3)	..	C(2A)	[	=		Intra	-26.27	-12.31	0.25330	0.09184	-0.17076	2.4321	1.5525	-2.6280

15	2.76	..	H(6A)	[	=		Intra	-84.71	7.10	-0.07850	0.02080	-0.09970	-0.4079	0.3516	-1.5344

Angles (Degrees) At1...V...At2 with Vertex V = O(12A)

C(11A) , Cu(2)	160.64(18)	C(11A) , O(11A)	27.81(14)	C(11A) , C(1A)	33.57(14)	C(11A) , C(6A)	55.11(15)
C(11A) , O(6W)	130.03(17)	C(11A) , O(42A)d	120.72(16)	C(11A) , O(21A)a	158.44(17)	C(11A) , Cu(1)	65.74(15)
C(11A) , O(51A)i	76.26(15)	C(11A) , O(4W)g	117.67(17)	C(11A) , O(11B)	105.89(16)	C(11A) , O(12B)	145.38(17)
C(11A) , C(2A)	32.28(14)	Cu(2) , O(11A)	144.79(10)	Cu(2) , C(1A)	145.57(11)	Cu(2) , C(6A)	134.97(9)
Cu(2) , O(6W)	42.62(5)	Cu(2) , O(42A)d	40.22(5)	Cu(2) , O(21A)a	39.52(5)	Cu(2) , Cu(1)	114.17(7)
Cu(2) , O(51A)i	115.80(7)	Cu(2) , O(4W)g	80.51(6)	Cu(2) , O(11B)	71.33(6)	Cu(2) , O(12B)	34.36(4)
Cu(2) , C(2A)	138.25(9)	O(11A) , C(1A)	61.29(9)	O(11A) , C(6A)	79.67(9)	O(11A) , O(6W)	148.65(10)
O(11A) , O(42A)d	110.24(9)	O(11A) , O(21A)a	157.41(10)	O(11A) , Cu(1)	38.61(6)	O(11A) , O(51A)i	58.90(7)
O(11A) , O(4W)g	107.68(9)	O(11A) , O(11B)	78.16(8)	O(11A) , O(12B)	117.77(9)	O(11A) , C(2A)	58.72(7)
C(1A) , C(6A)	27.73(8)	C(1A) , O(6W)	103.00(10)	C(1A) , O(42A)d	126.58(10)	C(1A) , O(21A)a	129.79(10)
C(1A) , Cu(1)	98.13(9)	C(1A) , O(51A)i	97.14(9)	C(1A) , O(4W)g	117.79(10)	C(1A) , O(11B)	139.44(10)
C(1A) , O(12B)	178.05(10)	C(1A) , C(2A)	15.75(8)	C(6A) , O(6W)	97.89(8)	C(6A) , O(42A)d	143.67(9)
C(6A) , O(21A)a	104.70(8)	C(6A) , Cu(1)	108.68(8)	C(6A) , O(51A)i	91.03(8)	C(6A) , O(4W)g	93.47(8)
C(6A) , O(11B)	149.47(9)	C(6A) , O(12B)	154.19(8)	C(6A) , C(2A)	42.62(7)	O(6W) , O(42A)d	55.08(6)
O(6W) , O(21A)a	53.65(6)	O(6W) , Cu(1)	152.80(8)	O(6W) , O(51A)i	152.18(7)	O(6W) , O(4W)g	103.67(7)
O(6W) , O(11B)	111.92(7)	O(6W) , O(12B)	76.98(6)	O(6W) , C(2A)	98.41(7)	O(42A)d , O(21A)a	79.66(6)
O(42A)d , Cu(1)	98.40(6)	O(42A)d , O(51A)i	124.44(8)	O(42A)d , O(4W)g	114.83(7)	O(42A)d , O(11B)	64.99(6)
O(42A)d , O(12B)	51.80(5)	O(42A)d , C(2A)	111.54(7)	O(21A)a , Cu(1)	121.70(7)	O(21A)a , O(51A)i	98.62(7)
O(21A)a , O(4W)g	50.44(6)	O(21A)a , O(11B)	88.61(6)	O(21A)a , O(12B)	51.76(5)	O(21A)a , C(2A)	138.05(8)
Cu(1) , O(51A)i	36.24(4)	Cu(1) , O(4W)g	80.87(6)	Cu(1) , O(11B)	42.85(4)	Cu(1) , O(12B)	81.33(5)
Cu(1) , C(2A)	97.32(6)	O(51A)i , O(4W)g	49.27(6)	O(51A)i , O(11B)	59.46(6)	O(51A)i , O(12B)	83.54(6)
O(51A)i , C(2A)	105.84(7)	O(4W)g , O(11B)	73.77(7)	O(4W)g , O(12B)	64.01(6)	O(4W)g , C(2A)	133.36(8)
O(11B) , O(12B)	39.61(5)	O(11B) , C(2A)	133.19(7)	O(12B) , C(2A)	162.36(8)		

3.6 Angstrom Coordination Sphere Around Atom I = O(12B) [ARU = 1555.01] -0.42060 0.31509 -0.10649 -3.1547 5.3264 -1.6389

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.279(3)	--	C(11B)	[	=		Intra	50.62	46.88	-0.33490	0.35506	-0.04584	-2.6002	6.0021	-0.7055
2	1.9792(18)	--	Cu(2)	[	=		Intra	-54.85	-41.67	-0.33918	0.24358	-0.19199	-2.3036	4.1175	-2.9547
3	2.538(2)	--	Na(2)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	154.64	-39.39	-0.66950	0.36479	-0.21114	-4.9273	6.1666	-3.2494
4	2.264(3)	<<	O(11B)	[	=		Intra	15.82	40.26	-0.18810	0.34295	-0.01144	-1.4928	5.7974	-0.1761
5	2.357(3)	<<	C(1B)	[	=		Intra	96.49	35.09	-0.42290	0.42842	-0.01846	-3.3728	7.2422	-0.2841
6	2.814(2)	<<	O(42A)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	6.67	-43.31	-0.20390	0.32915	-0.23192	-1.1209	5.5641	-3.5692
7	2.815(3)	<<	O(21A)a	[-1+x,y,z	=	1455.01]	Intra	-99.76	-19.80	-0.49360	0.16066	-0.16844	-3.6038	2.7159	-2.5923
8	3.045(3)	..	O(41A)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	80.53	-74.71	-0.45780	0.36194	-0.29734	-3.0227	6.1184	-4.5760
9	3.077(3)	<	C(2B)	[	=		Intra	128.59	38.06	-0.57320	0.42711	0.01676	-4.6661	7.2200	0.2579
10	3.148(3)	<	C(41A)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	37.39	-57.96	-0.30490	0.37509	-0.27990	-1.8277	6.3407	-4.3076
11	3.185(3)	..	O(22A)a	[-1+x,y,z	=	1455.01]	Intra	-146.42	-31.62	-0.73090	0.22636	-0.21500	-5.4143	3.8265	-3.3088
12	3.223(3)	..	C(21B)	[	=		Intra	164.71	44.08	-0.65630	0.35120	0.03919	-5.3879	5.9368	0.6031
13	3.231(3)	..	O(21B)	[	=		Intra	-168.20	59.02	-0.57170	0.29498	0.07349	-4.7825	4.9865	1.1310
14	3.269(3)	..	C(21A)a	[-1+x,y,z	=	1455.01]	Intra	-124.00	-21.87	-0.65290	0.16631	-0.18560	-4.8511	2.8114	-2.8563
15	3.364(3)	..	C(6B)h	[-1-x,1-y,-z	=	3465.01]	Intra	82.90	19.31	-0.35170	0.50147	-0.03422	-2.7622	8.4770	-0.5266
16	3.366(2)	..	O(12A)	[	=		Intra	-42.02	-4.04	-0.11600	0.18213	-0.12188	-0.6605	3.0788	-1.8757
17	3.539(3)	..	O(4W)g	[-1-x,-y,-z	=	3455.01]	Intra	-91.02	28.58	-0.39660	0.13127	0.00353	-3.2102	2.2190	0.0543
18	3.50	..	H(6B)h	[-1-x,1-y,-z	=	3465.01]	Intra	68.11	12.45	-0.24920	0.50250	-0.05750	-1.8818	8.4945	-0.8849

Angles (Degrees) At1...V...At2 with Vertex V = O(12B)

C(11B)	,	Cu(2)	128.43(16)	C(11B)	,	Na(2)d	126.24(16)	C(11B)	,	O(11B)	25.84(13)	C(11B)	,	C(1B)	36.00(14)
C(11B)	,	O(42A)d	98.20(15)	C(11B)	,	O(21A)a	143.74(17)	C(11B)	,	O(41A)d	123.22(16)	C(11B)	,	C(2B)	55.80(14)
C(11B)	,	C(41A)d	105.41(15)	C(11B)	,	O(22A)a	159.92(16)	C(11B)	,	C(21B)	72.10(14)	C(11B)	,	O(21B)	69.41(14)
C(11B)	,	C(21A)a	154.61(17)	C(11B)	,	C(6B)h	38.12(14)	C(11B)	,	O(12A)	94.75(14)	C(11B)	,	O(4W)g	96.98(15)
Cu(2)	,	Na(2)d	94.63(7)	Cu(2)	,	O(11B)	103.95(9)	Cu(2)	,	C(1B)	156.72(11)	Cu(2)	,	O(42A)d	44.34(5)
Cu(2)	,	O(21A)a	43.70(5)	Cu(2)	,	O(41A)d	59.93(6)	Cu(2)	,	C(2B)	175.52(9)	Cu(2)	,	C(41A)d	56.77(6)
Cu(2)	,	O(22A)a	70.66(6)	Cu(2)	,	C(21B)	151.19(9)	Cu(2)	,	O(21B)	136.25(9)	Cu(2)	,	C(21A)a	60.37(6)
Cu(2)	,	C(6B)h	137.87(9)	Cu(2)	,	O(12A)	39.35(5)	Cu(2)	,	O(4W)g	77.79(7)	Na(2)d	,	O(11B)	148.65(10)
Na(2)d	,	C(1B)	91.78(9)	Na(2)d	,	O(42A)d	92.38(7)	Na(2)d	,	O(21A)a	88.89(7)	Na(2)d	,	O(41A)d	48.09(5)
Na(2)d	,	C(2B)	81.05(7)	Na(2)d	,	C(41A)d	69.50(7)	Na(2)d	,	O(22A)a	47.76(5)	Na(2)d	,	C(21B)	83.96(7)
Na(2)d	,	O(21B)	103.12(7)	Na(2)d	,	C(21A)a	69.87(6)	Na(2)d	,	C(6B)h	88.93(7)	Na(2)d	,	O(12A)	133.94(8)
Na(2)d	,	O(4W)g	125.68(8)	O(11B)	,	C(1B)	61.79(9)	O(11B)	,	O(42A)d	83.98(8)	O(11B)	,	O(21A)a	121.93(9)
O(11B)	,	O(41A)d	122.51(9)	O(11B)	,	C(2B)	80.46(9)	O(11B)	,	C(41A)d	99.86(9)	O(11B)	,	O(22A)a	163.28(10)
O(11B)	,	C(21B)	91.13(9)	O(11B)	,	O(21B)	80.66(8)	O(11B)	,	C(21A)a	141.43(10)	O(11B)	,	C(6B)h	60.38(8)
O(11B)	,	O(12A)	68.92(7)	O(11B)	,	O(4W)g	83.40(8)	C(1B)	,	O(42A)d	113.11(10)	C(1B)	,	O(21A)a	159.04(11)
C(1B)	,	O(41A)d	110.31(10)	C(1B)	,	C(2B)	25.82(8)	C(1B)	,	C(41A)d	105.33(10)	C(1B)	,	O(22A)a	128.22(9)
C(1B)	,	C(21B)	51.83(8)	C(1B)	,	O(21B)	63.00(8)	C(1B)	,	C(21A)a	142.34(10)	C(1B)	,	C(6B)h	19.84(8)
C(1B)	,	O(12A)	130.68(9)	C(1B)	,	O(4W)g	115.93(10)	O(42A)d	,	O(21A)a	87.78(7)	O(42A)d	,	O(41A)d	44.36(5)
O(42A)d	,	C(2B)	136.54(9)	O(42A)d	,	C(41A)d	24.03(6)	O(42A)d	,	O(22A)a	101.12(7)	O(42A)d	,	C(21B)	164.16(9)

O(42A)d,	O(21B)	163.98(8)	O(42A)d,	C(21A)a	100.64(8)	O(42A)d,	C(6B)h	93.63(8)	O(42A)d,	O(12A)	58.17(6)
O(42A)d,	O(4W)g	114.43(8)	O(21A)a,	O(41A)d	85.49(7)	O(21A)a,	C(2B)	134.51(9)	O(21A)a,	C(41A)d	94.53(8)
O(21A)a,	O(22A)a	43.33(5)	O(21A)a,	C(21B)	107.50(8)	O(21A)a,	O(21B)	96.45(7)	O(21A)a,	C(21A)a	22.73(6)
O(21A)a,	C(6B)h	177.45(8)	O(21A)a,	O(12A)	58.34(6)	O(21A)a,	O(4W)g	49.11(6)	O(41A)d,	C(2B)	117.12(8)
O(41A)d,	C(41A)d	23.11(6)	O(41A)d,	O(22A)a	69.36(6)	O(41A)d,	C(21B)	130.68(8)	O(41A)d,	O(21B)	151.19(7)
O(41A)d,	C(21A)a	82.15(7)	O(41A)d,	C(6B)h	94.03(7)	O(41A)d,	O(12A)	94.23(7)	O(41A)d,	O(4W)g	133.67(8)
C(2B) ,	C(41A)d	122.10(9)	C(2B) ,	O(22A)a	105.34(7)	C(2B) ,	C(21B)	27.65(7)	C(2B) ,	O(21B)	44.66(6)
C(2B) ,	C(21A)a	116.63(8)	C(2B) ,	C(6B)h	43.71(7)	C(2B) ,	O(12A)	144.92(8)	C(2B) ,	O(4W)g	103.75(8)
C(41A)d,	O(22A)a	90.36(7)	C(41A)d,	C(21B)	145.16(9)	C(41A)d,	O(21B)	166.66(9)	C(41A)d,	C(21A)a	98.68(8)
C(41A)d,	C(6B)h	85.95(8)	C(41A)d,	O(12A)	80.97(7)	C(41A)d,	O(4W)g	134.03(8)	O(22A)a,	C(21B)	87.84(7)
O(22A)a,	O(21B)	92.44(6)	O(22A)a,	C(21A)a	22.21(6)	O(22A)a,	C(6B)h	134.20(8)	O(22A)a,	O(12A)	100.04(7)
O(22A)a,	O(4W)g	79.99(7)	C(21B) ,	O(21B)	22.23(6)	C(21B) ,	C(21A)a	92.59(8)	C(21B) ,	C(6B)h	70.94(7)
C(21B) ,	O(12A)	133.55(8)	C(21B) ,	O(4W)g	79.78(7)	O(21B) ,	C(21A)a	88.68(7)	O(21B) ,	C(6B)h	82.76(7)
O(21B) ,	O(12A)	111.31(7)	O(21B) ,	O(4W)g	59.31(6)	C(21A)a,	C(6B)h	154.72(8)	C(21A)a,	O(12A)	81.06(7)
C(21A)a,	O(4W)g	59.64(7)	C(6B)h ,	O(12A)	124.21(7)	C(6B)h ,	O(4W)g	131.75(8)	O(12A) ,	O(4W)g	57.25(6)

3.6 Angstrom Coordination Sphere Around Atom I = O(21A) [ARU = 1555.01] 0.50640 0.16066 -0.16844 4.4704 2.7159 -2.5923

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.279(3)	--	C(21A)	[	=		Intra	175.62	-11.92	0.34710	0.16631	-0.18560	3.2231	2.8114	-2.8563
2	1.9459(18)	--	Cu(2)b	[1+x,y,z	=	1655.01]	Intra	47.15	-10.73	0.66082	0.24358	-0.19199	5.7706	4.1175	-2.9547
3	2.242(2)	<<	O(22A)	[	=		Intra	148.47	-18.64	0.26910	0.22636	-0.21500	2.6599	3.8265	-3.3088
4	2.347(3)	<<	C(2A)	[	=		Intra	-150.28	-0.87	0.25330	0.09184	-0.17076	2.4321	1.5525	-2.6280
5	2.721(3)	<<	O(4W)i	[-x,-y,-z	=	3555.01]	Intra	-51.61	76.53	0.60340	0.13127	0.00353	4.8640	2.2190	0.0543
6	2.726(3)	<<	O(6W)b	[1+x,y,z	=	1655.01]	Intra	11.65	-48.29	0.68930	0.18233	-0.30069	6.2468	3.0822	-4.6276
7	2.815(3)	<<	O(12B)b	[1+x,y,z	=	1655.01]	Intra	80.24	19.80	0.57940	0.31509	-0.10649	4.9195	5.3264	-1.6389
8	2.837(3)	<<	C(3A)	[	=		Intra	-121.88	-9.01	0.31500	0.01989	-0.19732	2.9904	0.3362	-3.0367
9	3.051(2)	..	O(12A)b	[1+x,y,z	=	1655.01]	Intra	7.03	13.58	0.88400	0.18213	-0.12188	7.4137	3.0788	-1.8757
10	3.414(3)	..	O(3W)	[	=		Intra	-56.96	-27.13	0.68320	0.00998	-0.26961	6.1272	0.1687	-4.1492
11	3.537(3)	..	O(5W)b	[1+x,y,z	=	1655.01]	Intra	-71.67	27.85	0.65830	-0.01494	-0.06110	5.4537	-0.2526	-0.9403
12	3.560(3)	..	C(1A)	[	=		Intra	-160.74	8.52	0.10440	0.09196	-0.13415	1.1469	1.5545	-2.0645
13	2.60	.<	H(3A)	[	=		Intra	-104.40	-18.69	0.41530	0.01950	-0.22260	3.8576	0.3296	-3.4258

Angles (Degrees) At1...V...At2 with Vertex V = O(21A)

C(21A) , Cu(2)b	124.03(17)	C(21A) , O(22A)	27.00(13)	C(21A) , C(2A)	35.58(14)	C(21A) , O(4W)i	110.83(17)
C(21A) , O(6W)b	118.13(17)	C(21A) , O(12B)b	98.99(15)	C(21A) , C(3A)	61.41(14)	C(21A) , O(12A)b	168.75(17)
C(21A) , O(3W)	115.78(16)	C(21A) , O(5W)b	115.49(16)	C(21A) , C(1A)	31.15(14)	Cu(2)b , O(22A)	97.08(9)
Cu(2)b , C(2A)	159.13(12)	Cu(2)b , O(4W)i	102.48(9)	Cu(2)b , O(6W)b	47.84(6)	Cu(2)b , O(12B)b	44.65(5)
Cu(2)b , C(3A)	157.44(11)	Cu(2)b , O(12A)b	46.64(5)	Cu(2)b , O(3W)	97.37(7)	Cu(2)b , O(5W)b	120.39(9)
Cu(2)b , C(1A)	152.42(9)	O(22A) , C(2A)	62.57(9)	O(22A) , O(4W)i	121.21(10)	O(22A) , O(6W)b	102.77(9)
O(22A) , O(12B)b	77.15(8)	O(22A) , C(3A)	86.80(9)	O(22A) , O(12A)b	142.69(10)	O(22A) , O(3W)	128.01(10)
O(22A) , O(5W)b	142.16(10)	O(22A) , C(1A)	56.97(7)	C(2A) , O(4W)i	92.86(10)	C(2A) , O(6W)b	128.40(11)
C(2A) , O(12B)b	127.10(10)	C(2A) , C(3A)	29.42(8)	C(2A) , O(12A)b	154.20(11)	C(2A) , O(3W)	92.56(9)
C(2A) , O(5W)b	80.36(10)	C(2A) , C(1A)	14.03(8)	O(4W)i , O(6W)b	131.02(9)	O(4W)i , O(12B)b	79.45(8)
O(4W)i , C(3A)	94.28(9)	O(4W)i , O(12A)b	69.75(8)	O(4W)i , O(3W)	103.72(9)	O(4W)i , O(5W)b	49.63(8)
O(4W)i , C(1A)	86.06(8)	O(6W)b , O(12B)b	91.39(8)	O(6W)b , C(3A)	109.61(9)	O(6W)b , O(12A)b	62.01(6)
O(6W)b , O(3W)	56.19(7)	O(6W)b , O(5W)b	106.28(8)	O(6W)b , C(1A)	139.72(9)	O(12B)b , C(3A)	156.06(9)
O(12B)b , O(12A)b	69.90(6)	O(12B)b , O(3W)	140.25(8)	O(12B)b , O(5W)b	125.16(9)	O(12B)b , C(1A)	113.66(8)
C(3A) , O(12A)b	129.77(9)	C(3A) , O(3W)	63.64(7)	C(3A) , O(5W)b	60.94(8)	C(3A) , C(1A)	42.49(7)
O(12A)b , O(3W)	74.20(7)	O(12A)b , O(5W)b	73.85(7)	O(12A)b , C(1A)	154.78(9)	O(3W) , O(5W)b	56.76(7)
O(3W) , C(1A)	106.10(7)	O(5W)b , C(1A)	85.21(8)				

3.6 Angstrom Coordination Sphere Around Atom I = O(21B) [ARU = 1555.01] -0.57170 0.29498 0.07349 -4.7825 4.9865 1.1310

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.244(3)	--	C(21B)	[	=		Intra	122.50	-25.10	-0.65630	0.35120	0.03919	-5.3879	5.9368	0.6031
2	2.413(2)	--	Na(1)g	[-1-x, -y, -z	=	3455.01]	Intra	-100.64	-2.44	-0.62870	0.15484	0.06681	-5.2276	2.6175	1.0282
3	2.241(2)	<<	O(22B)	[	=		Intra	152.66	-20.57	-0.81690	0.35198	0.02233	-6.6464	5.9500	0.3437
4	2.401(3)	<<	C(2B)	[	=		Intra	87.02	-21.32	-0.57320	0.42711	0.01676	-4.6661	7.2200	0.2579
5	2.687(3)	<<	O(6W)k	[x, 1/2-y, 1/2+z	=	4555.01]		11.89	46.12	-0.31070	0.31767	0.19931	-2.9602	5.3700	3.0673
6	3.013(3)	<<	C(1B)	[	=		Intra	58.00	-28.01	-0.42290	0.42842	-0.01846	-3.3728	7.2422	-0.2841
7	3.028(3)	<	C(11B)	[	=		Intra	24.96	-37.34	-0.33490	0.35506	-0.04584	-2.6002	6.0021	-0.7055
8	3.1352(17)	<<	Cu(1)a	[-1+x, y, z	=	1455.01]	Intra	-170.66	-6.82	-0.95892	0.26508	0.04931	-7.8542	4.4810	0.7589
9	3.185(3)	..	O(11A)a	[-1+x, y, z	=	1455.01]	Intra	-143.05	-31.91	-0.87000	0.19884	-0.03592	-6.9432	3.3613	-0.5528
10	3.231(3)	..	O(12B)	[	=		Intra	11.80	-59.02	-0.42060	0.31509	-0.10649	-3.1547	5.3264	-1.6389
11	3.360(3)	..	O(4W)g	[-1-x, -y, -z	=	3455.01]	Intra	-60.40	-18.69	-0.39660	0.13127	0.00353	-3.2102	2.2190	0.0543
12	3.374(3)	..	O(41A)i	[-x, -y, -z	=	3555.01]	Intra	-76.70	36.10	-0.45780	0.13806	0.20266	-4.1555	2.3338	3.1189
13	3.534(3)	..	C(6B)	[	=		Intra	98.75	-9.85	-0.64830	0.49853	0.03422	-5.3120	8.4274	0.5266

Angles (Degrees) At1...V...At2 with Vertex V = O(21B)

C(21B) , Na(1)g	129.95(16)	C(21B) , O(22B)	28.11(13)	C(21B) , C(2B)	32.73(14)	C(21B) , O(6W)k	121.79(17)
C(21B) , C(1B)	57.08(14)	C(21B) , C(11B)	80.63(15)	C(21B) , Cu(1)a	66.18(13)	C(21B) , O(11A)a	80.53(15)
C(21B) , O(12B)	78.52(15)	C(21B) , O(4W)g	136.12(17)	C(21B) , O(41A)i	160.21(16)	C(21B) , C(6B)	27.22(14)
Na(1)g , O(22B)	104.70(9)	Na(1)g , C(2B)	155.08(11)	Na(1)g , O(6W)k	107.22(8)	Na(1)g , C(1B)	143.27(10)
Na(1)g , C(11B)	115.88(9)	Na(1)g , Cu(1)a	69.87(5)	Na(1)g , O(11A)a	49.56(5)	Na(1)g , O(12B)	99.19(7)
Na(1)g , O(4W)g	42.60(6)	Na(1)g , O(41A)i	44.55(5)	Na(1)g , C(6B)	157.11(8)	O(22B) , C(2B)	60.83(9)
O(22B) , O(6W)k	139.11(10)	O(22B) , C(1B)	84.39(9)	O(22B) , C(11B)	104.01(10)	O(22B) , Cu(1)a	38.07(5)
O(22B) , O(11A)a	57.96(7)	O(22B) , O(12B)	94.16(8)	O(22B) , O(4W)g	129.10(10)	O(22B) , O(41A)i	134.40(9)
O(22B) , C(6B)	52.89(7)	C(2B) , O(6W)k	95.53(9)	C(2B) , C(1B)	27.14(8)	C(2B) , C(11B)	55.42(9)
C(2B) , Cu(1)a	98.88(8)	C(2B) , O(11A)a	108.38(9)	C(2B) , O(12B)	64.27(8)	C(2B) , O(4W)g	128.83(10)
C(2B) , O(41A)i	159.51(10)	C(2B) , C(6B)	16.09(8)	O(6W)k , C(1B)	85.08(8)	O(6W)k , C(11B)	84.28(8)
O(6W)k , Cu(1)a	140.64(8)	O(6W)k , O(11A)a	156.07(9)	O(6W)k , O(12B)	105.14(7)	O(6W)k , O(4W)g	91.78(7)
O(6W)k , O(41A)i	63.99(6)	O(6W)k , C(6B)	94.93(8)	C(1B) , C(11B)	29.16(7)	C(1B) , Cu(1)a	121.56(8)
C(1B) , O(11A)a	116.82(9)	C(1B) , O(12B)	44.18(6)	C(1B) , O(4W)g	104.31(8)	C(1B) , O(41A)i	141.12(8)
C(1B) , C(6B)	42.33(7)	C(11B) , Cu(1)a	133.50(8)	C(11B) , O(11A)a	109.84(8)	C(11B) , O(12B)	23.29(6)
C(11B) , O(4W)g	75.20(7)	C(11B) , O(41A)i	119.16(8)	C(11B) , C(6B)	71.19(7)	Cu(1)a , O(11A)a	35.94(4)
Cu(1)a , O(12B)	114.13(7)	Cu(1)a , O(4W)g	106.72(7)	Cu(1)a , O(41A)i	97.20(6)	Cu(1)a , C(6B)	89.42(6)
O(11A)a , O(12B)	86.69(7)	O(11A)a , O(4W)g	74.20(7)	O(11A)a , O(41A)i	92.09(6)	O(11A)a , C(6B)	107.75(7)
O(12B) , O(4W)g	64.92(6)	O(12B) , O(41A)i	119.62(7)	O(12B) , C(6B)	80.00(7)	O(4W)g , O(41A)i	56.92(6)
O(4W)g , C(6B)	144.82(8)	O(41A)i , C(6B)	153.42(8)				

3.6 Angstrom Coordination Sphere Around Atom I = O(22A) [ARU = 1555.01] 0.26910 0.22636 -0.21500 2.6599 3.8265 -3.3088

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.246(3)	--	C(21A)	[	=		Intra	-60.98	21.29	0.34710	0.16631	-0.18560	3.2231	2.8114	-2.8563
2	2.391(2)	--	Na(2)f	[1-x,1/2+y,-1/2-z	=	2654.01]	Intra	78.24	1.42	0.33050	0.36479	-0.21114	3.1469	6.1666	-3.2494
3	2.242(2)	<<	O(21A)	[	=		Intra	-31.53	18.64	0.50640	0.16066	-0.16844	4.4704	2.7159	-2.5923
4	2.385(3)	<<	C(2A)	[	=		Intra	-95.72	16.59	0.25330	0.09184	-0.17076	2.4321	1.5525	-2.6280
5	2.676(3)	<<	O(7W)k	[x,1/2-y,-1/2+z	=	4554.01]		-158.38	-44.35	0.01470	0.18466	-0.33652	0.8811	3.1216	-5.1790
6	3.000(3)	<<	C(1A)	[	=		Intra	-123.66	24.51	0.10440	0.09196	-0.13415	1.1469	1.5545	-2.0645
7	3.028(3)	<	C(11A)	[	=		Intra	-154.34	36.80	0.03150	0.16424	-0.09713	0.4744	2.7764	-1.4948
8	3.1443(17)	<<	Cu(2)b	[1+x,y,z	=	1655.01]	Intra	5.34	6.47	0.66082	0.24358	-0.19199	5.7706	4.1175	-2.9547
9	3.170(3)	..	O(52A)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	105.01	-39.86	0.15400	0.36540	-0.34701	2.0297	6.1769	-5.3404
10	3.185(3)	..	O(12B)b	[1+x,y,z	=	1655.01]	Intra	33.58	31.62	0.57940	0.31509	-0.10649	4.9195	5.3264	-1.6389
11	3.186(3)	..	O(11A)	[	=		Intra	-163.08	59.89	0.13000	0.19884	-0.03592	1.1310	3.3613	-0.5528
12	3.305(3)	..	O(1W)f	[1-x,1/2+y,-1/2-z	=	2654.01]	Intra	120.45	18.13	0.09070	0.38652	-0.14819	1.0681	6.5339	-2.2806
13	3.516(3)	..	C(3A)	[	=		Intra	-84.59	4.44	0.31500	0.01989	-0.19732	2.9904	0.3362	-3.0367
14	3.547(3)	..	O(41A)f	[1-x,1/2+y,-1/2-z	=	2654.01]	Intra	43.78	-20.93	0.54220	0.36194	-0.29734	5.0515	6.1184	-4.5760

Angles (Degrees) At1...V...At2 with Vertex V = O(22A)

C(21A) , Na(2)f	134.13(16)	C(21A) , O(21A)	27.77(13)	C(21A) , C(2A)	33.13(14)	C(21A) , O(7W)k	109.86(16)
C(21A) , C(1A)	57.34(14)	C(21A) , C(11A)	79.99(15)	C(21A) , Cu(2)b	65.63(13)	C(21A) , O(52A)d	157.93(17)
C(21A) , O(12B)b	82.68(15)	C(21A) , O(11A)	77.51(15)	C(21A) , O(1W)f	140.55(17)	C(21A) , C(3A)	28.45(14)
C(21A) , O(41A)f	110.58(15)	Na(2)f , O(21A)	108.21(9)	Na(2)f , C(2A)	161.03(11)	Na(2)f , O(7W)k	114.25(9)
Na(2)f , C(1A)	146.48(10)	Na(2)f , C(11A)	118.13(9)	Na(2)f , Cu(2)b	72.85(5)	Na(2)f , O(52A)d	47.99(6)
Na(2)f , O(12B)b	51.80(5)	Na(2)f , O(11A)	102.66(8)	Na(2)f , O(1W)f	44.65(5)	Na(2)f , C(3A)	161.87(8)
Na(2)f , O(41A)f	40.45(5)	O(21A) , C(2A)	60.89(9)	O(21A) , O(7W)k	129.04(10)	O(21A) , C(1A)	84.23(9)
O(21A) , C(11A)	102.69(10)	O(21A) , Cu(2)b	37.89(5)	O(21A) , O(52A)d	137.12(9)	O(21A) , O(12B)b	59.52(7)
O(21A) , O(11A)	92.22(9)	O(21A) , O(1W)f	134.07(10)	O(21A) , C(3A)	53.67(7)	O(21A) , O(41A)f	83.67(7)
C(2A) , O(7W)k	83.39(9)	C(2A) , C(1A)	27.28(8)	C(2A) , C(11A)	55.20(9)	C(2A) , Cu(2)b	98.66(8)
C(2A) , O(52A)d	150.58(10)	C(2A) , O(12B)b	111.54(10)	C(2A) , O(11A)	64.40(8)	C(2A) , O(1W)f	130.27(10)
C(2A) , C(3A)	16.34(8)	C(2A) , O(41A)f	141.51(9)	O(7W)k , C(1A)	75.82(8)	O(7W)k , C(11A)	81.23(8)
O(7W)k , Cu(2)b	139.54(8)	O(7W)k , O(52A)d	67.37(7)	O(7W)k , O(12B)b	164.20(9)	O(7W)k , O(11A)	104.31(7)
O(7W)k , O(1W)f	96.49(7)	O(7W)k , C(3A)	81.67(7)	O(7W)k , O(41A)f	111.64(8)	C(1A) , C(11A)	28.94(7)
C(1A) , Cu(2)b	121.49(8)	C(1A) , O(52A)d	136.64(8)	C(1A) , O(12B)b	119.80(9)	C(1A) , O(11A)	44.65(7)
C(1A) , O(1W)f	104.39(8)	C(1A) , C(3A)	42.57(7)	C(1A) , O(41A)f	167.88(8)	C(11A) , Cu(2)b	132.74(8)
C(11A) , O(52A)d	119.84(8)	C(11A) , O(12B)b	111.18(8)	C(11A) , O(11A)	23.76(6)	C(11A) , O(1W)f	75.53(7)
C(11A) , C(3A)	71.17(7)	C(11A) , O(41A)f	157.64(9)	Cu(2)b , O(52A)d	101.55(6)	Cu(2)b , O(12B)b	36.44(4)
Cu(2)b , O(11A)	113.01(7)	Cu(2)b , O(1W)f	111.45(6)	Cu(2)b , C(3A)	89.44(6)	Cu(2)b , O(41A)f	46.63(4)
O(52A)d , O(12B)b	97.35(7)	O(52A)d , O(11A)	124.56(7)	O(52A)d , O(1W)f	59.75(6)	O(52A)d , C(3A)	143.53(9)
O(52A)d , O(41A)f	54.97(5)	O(12B)b , O(11A)	87.46(7)	O(12B)b , O(1W)f	78.04(6)	O(12B)b , C(3A)	111.11(7)
O(12B)b , O(41A)f	53.46(5)	O(11A) , O(1W)f	67.62(6)	O(11A) , C(3A)	80.40(7)	O(11A) , O(41A)f	136.64(7)
O(1W)f , C(3A)	146.55(8)	O(1W)f , O(41A)f	84.64(6)	C(3A) , O(41A)f	127.28(7)		

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3.6 Angstrom Coordination Sphere Around Atom I = O(22B) [ARU = 1555.01] -0.81690 0.35198 0.02233 -6.6464 5.9500 0.3437

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.285(3)	--	C(21B)	[	=		Intra	-0.60	11.65	-0.65630	0.35120	0.03919	-5.3879	5.9368	0.6031
2	1.9466(18)	--	Cu(1)a	[-1+x,y,z	=	1455.01]	Intra	-129.43	12.32	-0.95892	0.26508	0.04931	-7.8542	4.4810	0.7589
3	2.241(2)	<<	O(21B)	[	=		Intra	-27.34	20.57	-0.57170	0.29498	0.07349	-4.7825	4.9865	1.1310
4	2.354(3)	<<	C(2B)	[	=		Intra	32.67	-2.09	-0.57320	0.42711	0.01676	-4.6661	7.2200	0.2579
5	2.712(3)	<<	O(1W)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	121.64	-75.35	-0.90930	0.38652	-0.14819	-7.0061	6.5339	-2.2806
6	2.756(3)	<<	O(11A)a	[-1+x,y,z	=	1455.01]	Intra	-96.54	-18.99	-0.87000	0.19884	-0.03592	-6.9432	3.3613	-0.5528
7	2.815(3)	<<	O(7W)a	[-1+x,y,z	=	1455.01]	Intra	-159.76	50.51	-0.98530	0.31534	0.16348	-8.3259	5.3306	2.5159
8	2.820(3)	<<	C(6B)	[	=		Intra	61.69	3.72	-0.64830	0.49853	0.03422	-5.3120	8.4274	0.5266
9	2.970(3)	.<	O(2W)k	[-1+x,y,z	=	1455.02]		134.32	28.92	-1.01560	0.46199	0.11565	-8.4622	7.8097	1.7798
10	2.970(2)	.<	O(11B)a	[-1+x,y,z	=	1455.01]	Intra	-177.01	-10.08	-1.18810	0.34295	-0.01144	-9.5670	5.7974	-0.1761
11	3.575(3)	..	C(1B)	[	=		Intra	21.54	-10.11	-0.42290	0.42842	-0.01846	-3.3728	7.2422	-0.2841
12	2.56	.<	H(6B)	[	=		Intra	79.54	12.21	-0.75080	0.49750	0.05750	-6.1924	8.4099	0.8849

Angles (Degrees) At1...V...At2 with Vertex V = O(22B)

C(21B) , Cu(1)a	123.84(17)	C(21B) , O(21B)	27.14(13)	C(21B) , C(2B)	35.81(14)	C(21B) , O(1W)d	109.11(16)
C(21B) , O(11A)a	99.30(15)	C(21B) , O(7W)a	115.23(16)	C(21B) , C(6B)	62.13(14)	C(21B) , O(2W)k	120.51(16)
C(21B) , O(11B)a	176.14(17)	C(21B) , C(1B)	30.95(13)	Cu(1)a , O(21B)	96.70(9)	Cu(1)a , C(2B)	159.53(11)
Cu(1)a , O(1W)d	106.65(8)	Cu(1)a , O(11A)a	45.06(5)	Cu(1)a , O(7W)a	45.50(5)	Cu(1)a , C(6B)	160.53(10)
Cu(1)a , O(2W)k	89.43(7)	Cu(1)a , O(11B)a	52.30(6)	Cu(1)a , C(1B)	151.45(9)	O(21B) , C(2B)	62.94(9)
O(21B) , O(1W)d	122.87(9)	O(21B) , O(11A)a	78.46(8)	O(21B) , O(7W)a	97.50(9)	O(21B) , C(6B)	87.79(9)
O(21B) , O(2W)k	127.44(10)	O(21B) , O(11B)a	149.00(10)	O(21B) , C(1B)	57.01(7)	C(2B) , O(1W)d	87.72(9)
C(2B) , O(11A)a	125.84(10)	C(2B) , O(7W)a	130.45(10)	C(2B) , C(6B)	29.58(8)	C(2B) , O(2W)k	101.19(10)
C(2B) , O(11B)a	148.04(11)	C(2B) , C(1B)	13.67(8)	O(1W)d , O(11A)a	82.72(8)	O(1W)d , O(7W)a	135.64(8)
O(1W)d , C(6B)	86.36(9)	O(1W)d , O(2W)k	104.60(8)	O(1W)d , O(11B)a	73.23(7)	O(1W)d , C(1B)	82.75(7)
O(11A)a , O(7W)a	88.86(7)	O(11A)a , C(6B)	153.82(9)	O(11A)a , O(2W)k	132.83(8)	O(11A)a , O(11B)a	77.81(7)
O(11A)a , C(1B)	112.40(8)	O(7W)a , C(6B)	115.19(9)	O(7W)a , O(2W)k	53.11(7)	O(7W)a , O(11B)a	62.42(6)
O(7W)a , C(1B)	139.59(8)	C(6B) , O(2W)k	73.01(8)	C(6B) , O(11B)a	121.45(9)	C(6B) , C(1B)	42.31(7)
O(2W)k , O(11B)a	61.03(7)	O(2W)k , C(1B)	114.74(8)	O(11B)a , C(1B)	152.65(9)		

3.6 Angstrom Coordination Sphere Around Atom I = O(41A) [ARU = 1555.01] 0.45780 -0.13806 -0.20266 4.1555 -2.3338 -3.1189

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.245(3)	--	C(41A)	[	=		Intra	169.46	-12.45	0.30490	-0.12491	-0.22010	2.9605	-2.1115	-3.3873
2	2.322(2)	--	Na(2)	[	=		Intra	1.45	-34.85	0.66950	-0.13521	-0.28886	6.0601	-2.2856	-4.4455
3	2.367(2)	--	Na(1)b	[1+x,y,z	=	1655.01]	Intra	-14.82	62.06	0.62870	-0.15484	-0.06681	5.2276	-2.6175	-1.0282
4	2.6738(19)	--	Cu(2)c	[-x,-1/2+y,-1/2-z	=	2544.01]	Intra	-109.77	-37.33	0.33918	-0.25642	-0.30801	3.4365	-4.3347	-4.7402
5	2.222(2)	<<	O(42A)	[	=		Intra	-163.75	-26.94	0.20390	-0.17085	-0.26808	2.2537	-2.8881	-4.1257
6	2.379(3)	<<	C(4A)	[	=		Intra	141.50	5.61	0.23260	-0.05090	-0.18754	2.3030	-0.8604	-2.8862
7	2.914(3)	<<	C(3A)	[	=		Intra	113.57	1.62	0.31500	0.01989	-0.19732	2.9904	0.3362	-3.0367
8	3.045(3)	..	O(12B)c	[-x,-1/2+y,-1/2-z	=	2544.01]	Intra	-80.53	-74.71	0.42060	-0.18491	-0.39351	4.2876	-3.1258	-6.0560
9	3.118(2)	..	O(52A)b	[1+x,y,z	=	1655.01]	Intra	1.11	14.19	0.84600	-0.13460	-0.15299	7.1774	-2.2753	-2.3545
10	3.209(3)	..	O(4W)b	[1+x,y,z	=	1655.01]	Intra	173.08	72.74	0.39660	-0.13127	-0.00353	3.2102	-2.2190	-0.0543
11	3.263(3)	..	O(6W)c	[-x,-1/2+y,-1/2-z	=	2544.01]	Intra	-111.49	0.91	0.31070	-0.31767	-0.19931	2.9602	-5.3700	-3.0673
12	3.281(4)	..	O(5W)b	[1+x,y,z	=	1655.01]	Intra	58.05	41.61	0.65830	-0.01494	-0.06110	5.4537	-0.2526	-0.9403
13	3.348(3)	..	O(3W)	[	=		Intra	51.77	-17.92	0.68320	0.00998	-0.26961	6.1272	0.1687	-4.1492
14	3.374(3)	..	O(21B)i	[-x,-y,-z	=	3555.01]	Intra	-76.70	36.10	0.57170	-0.29498	-0.07349	4.7825	-4.9865	-1.1310
15	3.547(3)	..	O(22A)e	[1-x,-1/2+y,-1/2-z	=	2644.01]	Intra	-43.78	-20.93	0.73090	-0.27364	-0.28500	6.5472	-4.6257	-4.3861
16	3.552(3)	..	C(5A)	[	=		Intra	154.77	13.17	0.08510	-0.05085	-0.15006	1.0271	-0.8596	-2.3094
17	2.70	.<	H(3A)	[	=		Intra	96.38	-6.53	0.41530	0.01950	-0.22260	3.8576	0.3296	-3.4258

Tetrahedral Volume 3.788 Ang**3, Quadratic Elongation 1.298, Angle Variance 623.37 Deg**2 [K.Robinson +, Science 1971,172,567-570]

Angles (Degrees) At1...V...At2 with Vertex V = O(41A)

C(41A) , Na(2)	131.35(17)	C(41A) , Na(1)b	130.30(17)	C(41A) , Cu(2)c	75.21(14)	C(41A) , O(42A)	28.98(14)
C(41A) , C(4A)	33.15(14)	C(41A) , C(3A)	57.23(15)	C(41A) , O(12B)c	83.11(15)	C(41A) , O(52A)b	168.54(17)
C(41A) , O(4W)b	85.22(15)	C(41A) , O(6W)c	79.51(15)	C(41A) , O(5W)b	114.19(17)	C(41A) , O(3W)	111.44(16)
C(41A) , O(21B)i	116.48(16)	C(41A) , O(22A)e	133.29(16)	C(41A) , C(5A)	29.48(14)	Na(2) , Na(1)b	97.80(7)
Na(2) , Cu(2)c	83.67(6)	Na(2) , O(42A)	116.64(10)	Na(2) , C(4A)	133.00(11)	Na(2) , C(3A)	108.97(9)
Na(2) , O(12B)c	54.45(6)	Na(2) , O(52A)b	49.04(5)	Na(2) , O(4W)b	141.87(9)	Na(2) , O(6W)c	109.20(7)
Na(2) , O(5W)b	92.39(8)	Na(2) , O(3W)	47.59(6)	Na(2) , O(21B)i	101.57(7)	Na(2) , O(22A)e	41.93(5)
Na(2) , C(5A)	147.59(9)	Na(1)b , Cu(2)c	124.60(8)	Na(1)b , O(42A)	139.29(10)	Na(1)b , C(4A)	109.92(10)
Na(1)b , C(3A)	105.43(9)	Na(1)b , O(12B)c	143.26(8)	Na(1)b , O(52A)b	49.20(5)	Na(1)b , O(4W)b	45.10(6)
Na(1)b , O(6W)c	92.32(7)	Na(1)b , O(5W)b	46.38(7)	Na(1)b , O(3W)	95.43(8)	Na(1)b , O(21B)i	45.66(5)
Na(1)b , O(22A)e	86.14(6)	Na(1)b , C(5A)	104.32(8)	Cu(2)c , O(42A)	46.25(6)	Cu(2)c , C(4A)	108.27(9)
Cu(2)c , C(3A)	126.53(8)	Cu(2)c , O(12B)c	39.84(4)	Cu(2)c , O(52A)b	115.05(7)	Cu(2)c , O(4W)b	121.78(8)
Cu(2)c , O(6W)c	38.27(4)	Cu(2)c , O(5W)b	169.68(9)	Cu(2)c , O(3W)	122.08(8)	Cu(2)c , O(21B)i	79.57(6)
Cu(2)c , O(22A)e	58.74(5)	Cu(2)c , C(5A)	102.24(6)	O(42A) , C(4A)	62.11(9)	O(42A) , C(3A)	84.21(9)
O(42A) , O(12B)c	62.30(7)	O(42A) , O(52A)b	160.97(10)	O(42A) , O(4W)b	100.92(9)	O(42A) , O(6W)c	57.43(7)
O(42A) , O(5W)b	142.92(10)	O(42A) , O(3W)	123.43(10)	O(42A) , O(21B)i	103.29(8)	O(42A) , O(22A)e	104.72(8)
O(42A) , C(5A)	56.84(7)	C(4A) , C(3A)	28.15(8)	C(4A) , O(12B)c	106.81(9)	C(4A) , O(52A)b	136.00(10)
C(4A) , O(4W)b	69.82(9)	C(4A) , O(6W)c	106.83(9)	C(4A) , O(5W)b	81.39(10)	C(4A) , O(3W)	91.48(9)

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C(4A) ,	O(21B)i	125.04(9)	C(4A) ,	O(22A)e	163.85(10)	C(4A) ,	C(5A)	15.10(8)	C(3A) ,	O(12B)c	106.43(8)
C(3A) ,	O(52A)b	111.31(8)	C(3A) ,	O(4W)b	79.78(8)	C(3A) ,	O(6W)c	134.87(8)	C(3A) ,	O(5W)b	63.78(8)
C(3A) ,	O(3W)	63.85(7)	C(3A) ,	O(21B)i	141.08(9)	C(3A) ,	O(22A)e	150.66(9)	C(3A) ,	C(5A)	42.37(7)
O(12B)c,	O(52A)b	101.50(7)	O(12B)c,	O(4W)b	160.60(8)	O(12B)c,	O(6W)c	77.83(6)	O(12B)c,	O(5W)b	142.04(9)
O(12B)c,	O(3W)	82.65(7)	O(12B)c,	O(21B)i	110.84(7)	O(12B)c,	O(22A)e	57.18(5)	O(12B)c,	C(5A)	111.47(7)
O(52A)b,	O(4W)b	92.91(7)	O(52A)b,	O(6W)c	111.63(7)	O(52A)b,	O(5W)b	56.06(7)	O(52A)b,	O(3W)	59.38(6)
O(52A)b,	O(21B)i	71.95(6)	O(52A)b,	O(22A)e	56.37(5)	O(52A)b,	C(5A)	142.19(8)	O(4W)b ,	O(6W)c	84.85(7)
O(4W)b ,	O(5W)b	57.30(8)	O(4W)b ,	O(3W)	116.14(8)	O(4W)b ,	O(21B)i	61.33(6)	O(4W)b ,	O(22A)e	124.26(8)
O(4W)b ,	C(5A)	60.53(7)	O(6W)c ,	O(5W)b	136.44(9)	O(6W)c ,	O(3W)	156.33(8)	O(6W)c ,	O(21B)i	47.72(5)
O(6W)c ,	O(22A)e	69.60(5)	O(6W)c ,	C(5A)	93.44(6)	O(5W)b ,	O(3W)	59.82(8)	O(5W)b ,	O(21B)i	91.95(8)
O(5W)b ,	O(22A)e	112.36(8)	O(5W)b ,	C(5A)	86.21(8)	O(3W) ,	O(21B)i	131.27(7)	O(3W) ,	O(22A)e	88.62(6)
O(3W) ,	C(5A)	106.17(8)	O(21B)i,	O(22A)e	64.98(5)	O(21B)i,	C(5A)	110.84(7)	O(22A)e,	C(5A)	160.67(8)

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3.6 Angstrom Coordination Sphere Around Atom I = O(42A) [ARU = 1555.01] 0.20390 -0.17085 -0.26808 2.2537 -2.8881 -4.1257

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.284(3)	--	C(41A)	[	=		Intra	47.69	35.11	0.30490	-0.12491	-0.22010	2.9605	-2.1115	-3.3873
2	1.9670(18)	--	Cu(2)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra	-50.73	-18.20	0.33918	-0.25642	-0.30801	3.4365	-4.3347	-4.7402
3	2.222(2)	<<	O(41A)	[	=		Intra	16.25	26.94	0.45780	-0.13806	-0.20266	4.1555	-2.3338	-3.1189
4	2.377(3)	<<	C(4A)	[	=		Intra	88.61	31.43	0.23260	-0.05090	-0.18754	2.3030	-0.8604	-2.8862
5	2.719(2)	<<	O(1W)a	[-1+x, y, z	=	1455.01]	Intra	156.10	-28.29	-0.09070	-0.11348	-0.35181	0.0648	-1.9183	-5.4143
6	2.789(3)	<<	O(6W)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra	-74.11	22.30	0.31070	-0.31767	-0.19931	2.9602	-5.3700	-3.0673
7	2.814(2)	<<	O(12B)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra	-6.67	-43.31	0.42060	-0.18491	-0.39351	4.2876	-3.1258	-6.0560
8	2.986(3)	<<	C(5A)	[	=		Intra	121.16	37.46	0.08510	-0.05085	-0.15006	1.0271	-0.8596	-2.3094
9	3.002(3)	<<	C(51A)	[	=		Intra	158.96	45.23	-0.00160	-0.12596	-0.12961	0.2807	-2.1293	-1.9947
10	3.043(3)	..	O(12A)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra	-100.50	-33.82	0.11600	-0.31787	-0.37812	1.7933	-5.3734	-5.8192
11	3.134(3)	..	O(51A)	[	=		Intra	-175.78	64.86	0.09120	-0.17665	-0.08376	0.9261	-2.9862	-1.2891
12	3.253(3)	..	C(11B)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra	16.49	-61.69	0.33490	-0.14494	-0.45416	3.7330	-2.4501	-6.9894
13	3.421(3)	..	O(11B)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra	32.09	-82.63	0.18810	-0.15705	-0.48856	2.6257	-2.6548	-7.5188
14	3.482(3)	..	C(3A)	[	=		Intra	77.13	18.22	0.31500	0.01989	-0.19732	2.9904	0.3362	-3.0367
15	3.545(3)	..	O(7W)i	[-x, -y, -z	=	3555.01]	Intra	-129.34	27.01	-0.01470	-0.31534	-0.16348	0.2517	-5.3306	-2.5159

Angles (Degrees) At1...V...At2 with Vertex V = O(42A)

C(41A) , Cu(2)c	107.07(15)	C(41A) , O(41A)	28.02(13)	C(41A) , C(4A)	34.17(14)	C(41A) , O(1W)a	120.01(16)
C(41A) , O(6W)c	100.40(15)	C(41A) , O(12B)c	92.74(14)	C(41A) , C(5A)	57.68(14)	C(41A) , C(51A)	78.50(15)
C(41A) , O(12A)c	153.85(16)	C(41A) , O(51A)	74.42(14)	C(41A) , C(11B)c	100.05(15)	C(41A) , O(11B)c	117.99(15)
C(41A) , C(3A)	31.07(13)	C(41A) , O(7W)i	117.81(16)	Cu(2)c , O(41A)	79.07(8)	Cu(2)c , C(4A)	141.06(10)
Cu(2)c , O(1W)a	126.75(9)	Cu(2)c , O(6W)c	46.51(5)	Cu(2)c , O(12B)c	44.69(5)	Cu(2)c , C(5A)	159.48(10)
Cu(2)c , C(51A)	143.41(10)	Cu(2)c , O(12A)c	46.87(5)	Cu(2)c , O(51A)	120.97(8)	Cu(2)c , C(11B)c	63.29(7)
Cu(2)c , O(11B)c	71.03(6)	Cu(2)c , C(3A)	130.65(8)	Cu(2)c , O(7W)i	88.55(7)	O(41A) , C(4A)	62.18(9)
O(41A) , O(1W)a	144.57(10)	O(41A) , O(6W)c	80.40(8)	O(41A) , O(12B)c	73.34(7)	O(41A) , C(5A)	84.64(9)
O(41A) , C(51A)	100.24(9)	O(41A) , O(12A)c	125.84(9)	O(41A) , O(51A)	87.72(8)	O(41A) , C(11B)c	88.63(8)
O(41A) , O(11B)c	109.83(8)	O(41A) , C(3A)	56.38(7)	O(41A) , O(7W)i	116.71(9)	C(4A) , O(1W)a	87.68(9)
C(4A) , O(6W)c	123.78(10)	C(4A) , O(12B)c	114.50(10)	C(4A) , C(5A)	27.37(8)	C(4A) , C(51A)	55.09(9)
C(4A) , O(12A)c	171.97(10)	C(4A) , O(51A)	64.11(8)	C(4A) , C(11B)c	109.56(10)	C(4A) , O(11B)c	117.18(10)
C(4A) , C(3A)	16.80(8)	C(4A) , O(7W)i	111.27(9)	O(1W)a , O(6W)c	134.52(9)	O(1W)a , O(12B)c	106.67(8)
O(1W)a , C(5A)	73.46(8)	O(1W)a , C(51A)	73.57(8)	O(1W)a , O(12A)c	84.59(7)	O(1W)a , O(51A)	95.69(7)
O(1W)a , C(11B)c	84.31(8)	O(1W)a , O(11B)c	66.00(6)	O(1W)a , C(3A)	89.33(8)	O(1W)a , O(7W)i	90.36(7)
O(6W)c , O(12B)c	90.12(7)	O(6W)c , C(5A)	118.54(9)	O(6W)c , C(51A)	97.01(8)	O(6W)c , O(12A)c	61.49(6)
O(6W)c , O(51A)	74.69(7)	O(6W)c , C(11B)c	109.80(8)	O(6W)c , O(11B)c	114.17(8)	O(6W)c , C(3A)	130.67(8)
O(6W)c , O(7W)i	50.03(5)	O(12B)c , C(5A)	140.48(9)	O(12B)c , C(51A)	169.55(9)	O(12B)c , O(12A)c	70.04(6)
O(12B)c , O(51A)	157.60(8)	O(12B)c , C(11B)c	22.90(6)	O(12B)c , O(11B)c	41.14(5)	O(12B)c , C(3A)	98.04(7)
O(12B)c , O(7W)i	131.41(8)	C(5A) , C(51A)	29.13(7)	C(5A) , O(12A)c	146.23(8)	C(5A) , O(51A)	45.30(7)
C(5A) , C(11B)c	129.11(9)	C(5A) , O(11B)c	126.98(8)	C(5A) , C(3A)	42.92(7)	C(5A) , O(7W)i	87.70(7)
C(51A) , O(12A)c	120.15(8)	C(51A) , O(51A)	24.04(6)	C(51A) , C(11B)c	152.86(9)	C(51A) , O(11B)c	139.32(8)
C(51A) , C(3A)	71.52(7)	C(51A) , O(7W)i	58.71(6)	O(12A)c , O(51A)	114.47(7)	O(12A)c , C(11B)c	71.87(7)
O(12A)c , O(11B)c	61.32(6)	O(12A)c , C(3A)	164.26(9)	O(12A)c , O(7W)i	66.70(6)	O(51A) , C(11B)c	173.65(9)

O(51A) , O(11B)c	161.08(7)	O(51A) , C(3A)	80.53(7)	O(51A) , O(7W)i	47.78(5)	C(11B)c, O(11B)c	21.30(5)
C(11B)c, C(3A)	93.12(8)	C(11B)c, O(7W)i	138.54(8)	O(11B)c, C(3A)	102.95(7)	O(11B)c, O(7W)i	123.97(7)
C(3A) , O(7W)i	127.99(7)						

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3.6 Angstrom Coordination Sphere Around Atom I = O(51A) [ARU = 1555.01] 0.09120 -0.17665 -0.08376 0.9261 -2.9862 -1.2891

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.284(3)	--	C(51A)	[	=		Intra	126.99	-33.34	-0.00160	-0.12596	-0.12961	0.2807	-2.1293	-1.9947
2	1.9568(18)	--	Cu(1)i	[-x, -y, -z	=	3555.01]	Intra	-127.48	15.72	-0.04108	-0.26508	-0.04931	-0.2200	-4.4810	-0.7589
3	2.228(2)	<<	O(52A)	[	=		Intra	158.70	-28.57	-0.15400	-0.13460	-0.15299	-0.8968	-2.2753	-2.3545
4	2.361(3)	<<	C(5A)	[	=		Intra	87.28	-25.61	0.08510	-0.05085	-0.15006	1.0271	-0.8596	-2.3094
5	2.707(3)	<<	O(4W)b	[1+x, y, z	=	1655.01]	Intra	18.56	27.13	0.39660	-0.13127	-0.00353	3.2102	-2.2190	-0.0543
6	2.731(3)	<<	O(7W)i	[-x, -y, -z	=	3555.01]	Intra	-106.05	-26.70	-0.01470	-0.31534	-0.16348	0.2517	-5.3306	-2.5159
7	2.787(2)	<<	O(11A)i	[-x, -y, -z	=	3555.01]	Intra	-169.67	41.37	-0.13000	-0.19884	0.03592	-1.1310	-3.3613	0.5528
8	2.994(3)	<<	C(4A)	[	=		Intra	57.07	-32.24	0.23260	-0.05090	-0.18754	2.3030	-0.8604	-2.8862
9	3.051(3)	<	C(41A)	[	=		Intra	23.26	-43.46	0.30490	-0.12491	-0.22010	2.9605	-2.1115	-3.3873
10	3.123(3)	<	C(11A)i	[-x, -y, -z	=	3555.01]	Intra	171.48	63.04	-0.03150	-0.16424	0.09713	-0.4744	-2.7764	1.4948
11	3.134(3)	..	O(42A)	[	=		Intra	4.22	-64.86	0.20390	-0.17085	-0.26808	2.2537	-2.8881	-4.1257
12	3.177(3)	..	O(12A)i	[-x, -y, -z	=	3555.01]	Intra	-160.78	84.92	0.11600	-0.18213	0.12188	0.6605	-3.0788	1.8757
13	3.220(3)	..	O(11B)i	[-x, -y, -z	=	3555.01]	Intra	-78.60	27.06	0.18810	-0.34295	0.01144	1.4928	-5.7974	0.1761
14	3.423(3)	..	C(6A)	[	=		Intra	97.91	-10.53	0.02240	0.02055	-0.12442	0.4628	0.3474	-1.9148

Angles (Degrees) At1...V...At2 with Vertex V = O(51A)

C(51A) , Cu(1)i	111.36(15)	C(51A) , O(52A)	27.50(13)	C(51A) , C(5A)	35.20(14)	C(51A) , O(4W)b	119.05(16)
C(51A) , O(7W)i	101.65(15)	C(51A) , O(11A)i	94.70(15)	C(51A) , C(4A)	57.60(14)	C(51A) , C(41A)	76.46(15)
C(51A) , C(11A)i	102.69(15)	C(51A) , O(42A)	72.22(14)	C(51A) , O(12A)i	121.66(16)	C(51A) , O(11B)i	157.08(16)
C(51A) , C(6A)	35.08(13)	Cu(1)i , O(52A)	83.92(8)	Cu(1)i , C(5A)	146.12(10)	Cu(1)i , O(4W)b	125.95(10)
Cu(1)i , O(7W)i	47.25(6)	Cu(1)i , O(11A)i	44.41(5)	Cu(1)i , C(4A)	162.98(10)	Cu(1)i , C(41A)	142.75(10)
Cu(1)i , C(11A)i	63.08(7)	Cu(1)i , O(42A)	121.15(8)	Cu(1)i , O(12A)i	70.06(6)	Cu(1)i , O(11B)i	46.60(5)
Cu(1)i , C(6A)	135.57(8)	O(52A) , C(5A)	62.67(9)	O(52A) , O(4W)b	144.88(11)	O(52A) , O(7W)i	81.78(8)
O(52A) , O(11A)i	75.82(8)	O(52A) , C(4A)	83.95(9)	O(52A) , C(41A)	97.20(9)	O(52A) , C(11A)i	92.17(9)
O(52A) , O(42A)	84.48(8)	O(52A) , O(12A)i	114.66(9)	O(52A) , O(11B)i	129.80(9)	O(52A) , C(6A)	59.41(8)
C(5A) , O(4W)b	84.60(10)	C(5A) , O(7W)i	126.14(10)	C(5A) , O(11A)i	116.01(10)	C(5A) , C(4A)	27.16(8)
C(5A) , C(41A)	54.27(9)	C(5A) , C(11A)i	110.11(10)	C(5A) , O(42A)	64.05(8)	C(5A) , O(12A)i	117.41(10)
C(5A) , O(11B)i	167.27(10)	C(5A) , C(6A)	18.13(8)	O(4W)b , O(7W)i	131.04(9)	O(4W)b , O(11A)i	111.07(9)
O(4W)b , C(4A)	69.77(8)	O(4W)b , C(41A)	70.72(8)	O(4W)b , C(11A)i	87.29(8)	O(4W)b , O(42A)	92.67(8)
O(4W)b , O(12A)i	67.95(7)	O(4W)b , O(11B)i	83.77(8)	O(4W)b , C(6A)	85.51(8)	O(7W)i , O(11A)i	89.95(7)
O(7W)i , C(4A)	118.91(9)	O(7W)i , C(41A)	95.85(8)	O(7W)i , C(11A)i	110.33(8)	O(7W)i , O(42A)	74.02(7)
O(7W)i , O(12A)i	113.69(8)	O(7W)i , O(11B)i	59.89(6)	O(7W)i , C(6A)	136.10(9)	O(11A)i , C(4A)	141.96(9)
O(11A)i , C(41A)	170.24(9)	O(11A)i , C(11A)i	24.34(6)	O(11A)i , O(42A)	156.26(8)	O(11A)i , O(12A)i	43.61(5)
O(11A)i , O(11B)i	73.24(6)	O(11A)i , C(6A)	98.74(8)	C(4A) , C(41A)	28.71(7)	C(4A) , C(11A)i	129.34(9)
C(4A) , O(42A)	45.58(7)	C(4A) , O(12A)i	126.19(8)	C(4A) , O(11B)i	141.40(8)	C(4A) , C(6A)	43.40(7)
C(41A) , C(11A)i	153.23(9)	C(41A) , O(42A)	23.91(6)	C(41A) , O(12A)i	138.52(8)	C(41A) , O(11B)i	116.48(8)
C(41A) , C(6A)	71.66(7)	C(11A)i , O(42A)	174.13(9)	C(11A)i , O(12A)i	22.58(6)	C(11A)i , O(11B)i	74.46(7)
C(11A)i , C(6A)	92.11(8)	O(42A) , O(12A)i	159.73(7)	O(42A) , O(11B)i	111.38(7)	O(42A) , C(6A)	82.03(7)
O(12A)i , O(11B)i	62.36(6)	O(12A)i , C(6A)	101.49(7)	O(11B)i , C(6A)	163.15(8)		

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3.6 Angstrom Coordination Sphere Around Atom I = O(52A) [ARU = 1555.01] -0.15400 -0.13460 -0.15299 -0.8968 -2.2753 -2.3545

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	1.240(3)	--	C(51A)	[	=		Intra	7.07	16.87	-0.00160	-0.12596	-0.12961	0.2807	-2.1293	-1.9947
2	2.371(2)	--	Na(2)a	[-1+x,y,z	=	1455.01]	Intra	-179.47	-61.88	-0.33050	-0.13521	-0.28886	-2.0141	-2.2856	-4.4455
3	2.383(2)	--	Na(1)	[	=		Intra	-170.05	33.82	-0.37130	-0.15484	-0.06681	-2.8466	-2.6175	-1.0282
4	2.805(2)	--	Cu(1)i	[-x,-y,-z	=	3555.01]	Intra	-72.94	34.67	-0.04108	-0.26508	-0.04931	-0.2200	-4.4810	-0.7589

5	2.228(2)	<<	O(51A)	[	=		Intra	-21.30	28.57	0.09120	-0.17665	-0.08376	0.9261	-2.9862	-1.2891
6	2.389(3)	<<	C(5A)	[	=		Intra	36.35	1.08	0.08510	-0.05085	-0.15006	1.0271	-0.8596	-2.3094
7	2.987(3)	<<	C(6A)	[	=		Intra	62.60	8.47	0.02240	0.02055	-0.12442	0.4628	0.3474	-1.9148
8	3.010(4)	<	O(5W)	[	=		Intra	130.44	28.02	-0.34170	-0.01494	-0.06110	-2.6205	-0.2526	-0.9403
9	3.112(3)	..	O(11A)i	[-x,-y,-z	=	3555.01]	Intra	-102.17	69.09	-0.13000	-0.19884	0.03592	-1.1310	-3.3613	0.5528
10	3.118(2)	..	O(41A)a	[-1+x,y,z	=	1455.01]	Intra	-178.89	-14.19	-0.54220	-0.13806	-0.20266	-3.9187	-2.3338	-3.1189
11	3.170(3)	..	O(22A)c	[-x,-1/2+y,-1/2-z	=	2544.01]	Intra	-105.01	-39.86	-0.26910	-0.27364	-0.28500	-1.5270	-4.6257	-4.3861
12	3.209(3)	..	O(3W)a	[-1+x,y,z	=	1455.01]	Intra	113.25	-34.01	-0.31680	0.00998	-0.26961	-1.9470	0.1687	-4.1492
13	3.227(3)	..	O(1W)a	[-1+x,y,z	=	1455.01]	Intra	20.37	-71.47	-0.09070	-0.11348	-0.35181	0.0648	-1.9183	-5.4143
14	3.268(3)	..	O(7W)i	[-x,-y,-z	=	3555.01]	Intra	-69.40	-2.83	-0.01470	-0.31534	-0.16348	0.2517	-5.3306	-2.5159
15	3.539(3)	..	C(4A)	[	=		Intra	23.85	-8.64	0.23260	-0.05090	-0.18754	2.3030	-0.8604	-2.8862

16	2.80	..	H(6A)	[	=		Intra	79.46	17.06	-0.07850	0.02080	-0.09970	-0.4079	0.3516	-1.5344

Tetrahedral Volume 3.631 Ang**3, Quadratic Elongation 1.405, Angle Variance 799.20 Deg**2 [K.Robinson +, Science 1971,172,567-570]

Angles (Degrees) At1...V...At2 with Vertex V = O(52A)

C(51A)	,	Na(2)a	134.75(18)	C(51A)	,	Na(1)	129.23(18)	C(51A)	,	Cu(1)i	72.45(15)	C(51A)	,	O(51A)	28.57(14)
C(51A)	,	C(5A)	32.85(14)	C(51A)	,	C(6A)	54.66(15)	C(51A)	,	O(5W)	109.17(17)	C(51A)	,	O(11A)i	80.88(16)
C(51A)	,	O(41A)a	173.66(18)	C(51A)	,	O(22A)c	117.53(16)	C(51A)	,	O(3W)a	112.55(17)	C(51A)	,	O(1W)a	88.81(15)
C(51A)	,	O(7W)i	77.92(15)	C(51A)	,	C(4A)	30.44(14)	Na(2)a	,	Na(1)	96.01(7)	Na(2)a	,	Cu(1)i	127.73(8)
Na(2)a	,	O(51A)	143.71(11)	Na(2)a	,	C(5A)	113.50(10)	Na(2)a	,	C(6A)	110.38(9)	Na(2)a	,	O(5W)	98.48(9)
Na(2)a	,	O(11A)i	141.90(8)	Na(2)a	,	O(41A)a	47.69(5)	Na(2)a	,	O(22A)c	48.54(6)	Na(2)a	,	O(3W)a	49.89(6)
Na(2)a	,	O(1W)a	45.95(5)	Na(2)a	,	O(7W)i	96.78(8)	Na(2)a	,	C(4A)	107.18(8)	Na(1)	,	Cu(1)i	76.58(6)
Na(1)	,	O(51A)	110.95(10)	Na(1)	,	C(5A)	137.18(11)	Na(1)	,	C(6A)	114.62(9)	Na(1)	,	O(5W)	50.69(7)
Na(1)	,	O(11A)i	50.83(5)	Na(1)	,	O(41A)a	48.75(5)	Na(1)	,	O(22A)c	95.02(7)	Na(1)	,	O(3W)a	98.79(8)
Na(1)	,	O(1W)a	141.95(8)	Na(1)	,	O(7W)i	100.42(8)	Na(1)	,	C(4A)	151.75(9)	Cu(1)i	,	O(51A)	43.92(6)
Cu(1)i	,	C(5A)	105.12(9)	Cu(1)i	,	C(6A)	119.79(8)	Cu(1)i	,	O(5W)	113.53(9)	Cu(1)i	,	O(11A)i	38.05(4)
Cu(1)i	,	O(41A)a	111.01(7)	Cu(1)i	,	O(22A)c	80.19(6)	Cu(1)i	,	O(3W)a	174.84(8)	Cu(1)i	,	O(1W)a	123.67(7)
Cu(1)i	,	O(7W)i	37.65(4)	Cu(1)i	,	C(4A)	100.47(6)	O(51A)	,	C(5A)	61.39(9)	O(51A)	,	C(6A)	80.64(9)
O(51A)	,	O(5W)	117.27(11)	O(51A)	,	O(11A)i	60.23(7)	O(51A)	,	O(41A)a	154.74(10)	O(51A)	,	O(22A)c	103.45(9)
O(51A)	,	O(3W)a	141.10(10)	O(51A)	,	O(1W)a	104.18(8)	O(51A)	,	O(7W)i	55.79(7)	O(51A)	,	C(4A)	57.29(7)
C(5A)	,	C(6A)	27.16(8)	C(5A)	,	O(5W)	93.10(11)	C(5A)	,	O(11A)i	104.46(10)	C(5A)	,	O(41A)a	142.78(11)
C(5A)	,	O(22A)c	127.70(10)	C(5A)	,	O(3W)a	79.79(9)	C(5A)	,	O(1W)a	73.29(9)	C(5A)	,	O(7W)i	105.78(9)
C(5A)	,	C(4A)	15.80(8)	C(6A)	,	O(5W)	66.51(9)	C(6A)	,	O(11A)i	101.72(8)	C(6A)	,	O(41A)a	119.59(9)
C(6A)	,	O(22A)c	146.71(9)	C(6A)	,	O(3W)a	64.06(8)	C(6A)	,	O(1W)a	84.65(8)	C(6A)	,	O(7W)i	131.93(8)

C(6A) , C(4A)	42.22(7)	O(5W) , O(11A)i	75.67(8)	O(5W) , O(41A)a	64.71(8)	O(5W) , O(22A)c	133.27(9)
O(5W) , O(3W)a	64.12(8)	O(5W) , O(1W)a	122.80(9)	O(5W) , O(7W)i	148.50(9)	O(5W) , C(4A)	108.64(9)
O(11A)i, O(41A)a	98.60(7)	O(11A)i, O(22A)c	108.97(8)	O(11A)i, O(3W)a	139.78(9)	O(11A)i, O(1W)a	161.21(8)
O(11A)i, O(7W)i	75.31(6)	O(11A)i, C(4A)	110.36(7)	O(41A)a, O(22A)c	68.67(6)	O(41A)a, O(3W)a	63.89(7)
O(41A)a, O(1W)a	93.35(7)	O(41A)a, O(7W)i	108.12(7)	O(41A)a, C(4A)	147.90(9)	O(22A)c, O(3W)a	98.12(8)
O(22A)c, O(1W)a	62.20(6)	O(22A)c, O(7W)i	49.08(5)	O(22A)c, C(4A)	112.33(7)	O(3W)a , O(1W)a	58.87(7)
O(3W)a , O(7W)i	143.08(9)	O(3W)a , C(4A)	84.69(7)	O(1W)a , O(7W)i	87.24(7)	O(1W)a , C(4A)	62.86(6)
O(7W)i , C(4A)	92.79(7)						

>>>>>>>>>>>>>>> : Symmetry operations refer to the coordinates listed in the fractional coordinate table given above

=====													
5.0 Angstrom Coordination Sphere Around Atom I = Cu(1) [ARU = 1555.01]													

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	ZO

1	3.2318(12)	<<	Na(1)i	[-x, -y, -z	=	3555.01]	Intra	-35.35	4.78	0.37130	0.15484	0.06681	1.0282
2	4.5046(5)	.<	Cu(2)	[	=		Intra	-171.80	-55.53	-0.33918	0.24358	-0.19199	-2.9547
3	4.6508(11)	..	Na(2)k	[1-x, -y, -z	=	3655.01]		-50.74	52.44	0.33050	0.13521	0.28886	4.4455

5.0 Angstrom Coordination Sphere Around Atom I = Cu(2) [ARU = 1555.01]										-0.33918	0.24358	-0.19199	-2.3036	4.1175	-2.9547
Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	3.3420(11)	<<	Na(2)d	[-x,1/2+y,-1/2-z	=	2554.01]	Intra	142.01	-5.06	-0.66950	0.36479	-0.21114	-4.9273	6.1666	-3.2494
2	4.4650(11)	..	Na(1)k	[-1-x,1/2+y,-1/2-z	=	2454.01]		136.21	-56.24	-0.62870	0.34516	-0.43319	-4.0948	5.8347	-6.6667
3	4.5046(5)	.<	Cu(1)	[	=	]	Intra	8.20	55.53	0.04108	0.26508	0.04931	0.2200	4.4810	0.7589

=====

5.0 Angstrom Coordination Sphere Around Atom I = Na(1) [ARU = 1555.01] -0.37130 -0.15484 -0.06681 -2.8466 -2.6175 -1.0282

Nr	d(I, J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	3.2318(12)	<<	Cu(1)i	[-x, -y, -z	=	3555.01]	Intra	-35.35	4.78	-0.04108	-0.26508	-0.04931	-0.2200	-4.4810	-0.7589
2	3.5329(15)	.<	Na(2)a	[-1+x, y, z	=	1455.01]	Intra	21.73	-75.30	-0.33050	-0.13521	-0.28886	-2.0141	-2.2856	-4.4455
3	4.4650(11)	..	Cu(2)k	[-1-x, -1/2+y, -1/2-z	=	2444.01]		-136.21	-56.24	-0.66082	-0.25642	-0.30801	-4.6377	-4.3346	-4.7402

=====															
5.0 Angstrom Coordination Sphere Around Atom I = Na(2) [ARU = 1555.01]									0.66950	-0.13521	-0.28886	6.0601	-2.2856	-4.4455	

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	3.3420(11)	<<	Cu(2)c	[-x, -1/2+y, -1/2-z	=	2544.01]	Intra-142.01	-5.06		0.33918	-0.25642	-0.30801	3.4365	-4.3347	-4.7402
2	3.5329(15)	.<	Na(1)b	[1+x, y, z	=	1655.01]	Intra-158.27	75.30		0.62870	-0.15484	-0.06681	5.2276	-2.6175	-1.0282
3	4.6508(11)	..	Cu(1)k	[1-x, -y, -z	=	3655.01]		-50.74	52.44	0.95892	-0.26508	-0.04931	7.8542	-4.4810	-0.7589

=====

Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6

=====

van der Waals (or ion) Radii used in the Analysis

C	H	Cu	Na	O
1.70	1.20	2.32	1.77	1.52

:: Grid: X-Axis Step = 0.0278 = Points 36, Angstrom Step = 0.22

:: Grid: Z-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.22

:: Grid: Y-Axis Step = 0.0119 = Points 84, Angstrom Step = 0.20

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 10 Kmax = 22 Lmax= 20 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 27.831 Deg. (Applied Theta Limit: 27.840 Deg.)

Space Group P21/c No: 14, Laue: 2/m [Hall: -P 2ybc]

Lattice Type mP, Centric, Monoclinic, Order 4(2) [Schoenflies: C2h^5]

Nr ***** Symmetry Operation(s) *****

1	H ,	K ,	L
2	- H ,	1/2 + K ,	1/2 - L
3	- H ,	- K ,	- L
4	H ,	1/2 - K ,	1/2 + L

:: Number of Independent Type H, K, L Reflections = 5001

Table 0 - Crystal Data and Details of the Structure Determination
for: c:xtal u u_kno~1knoR = 0.03

Crystal Data

Formula	C15 H3 Cu2 Na2 O18, O
Formula Weight	660.25
Crystal System	Monoclinic
Space group	P21/c (No. 14)
a, b, c [Angstrom]	8.0742(1) 16.9044(3) 15.5557(3)
alpha, beta, gamma [deg]	90 98.375(1) 90
V [Ang**3]	2100.55(6)
Z	4
D(calc) [g/cm**3]	2.088
Mu(MoKa) [/mm]	2.168
F(000)	1300
Crystal Size [mm]	0.20 x 0.20 x 0.20

Data Collection

Temperature (K)	113
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	3.0, 27.8
Dataset	-10: 10 ; -22: 22 ; -20: 20
Tot., Uniq. Data, R(int)	29251, 4988, 0.068
Observed data [I > 2.0 sigma(I)]	4274

Refinement

Nref, Npar	4988, 343
R, wR2, S	0.0324, 0.0891, 1.00
w = 1/[S2^(F02^)+(0.0323P)2^+7.0886P] WHERE P=(F02^+2FC2^)/3'	
Max. and Av. Shift/Error	0.02, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.70, 0.87

=====

=====

***** N O T I C E *****

=====

- PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13
- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow
- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)
- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.
- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.
- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@chem.uu.nl
- Recent versions of PLATON may be obtained by Anonymous FTP from xraysoft.chem.uu.nl
- More INFO can be found on <http://www.cryst.chem.uu.nl/platon/>

Page - Index

Page 1	---	GENERAL
Page 2	---	ADDSYM
Page 3	---	GEOMETRY
Page 16	---	ADP-Anal
Page 20	---	GEOMETRY
Page 108	---	SelGeom
Page 110	---	INTER
Page 118	---	H-BONDS
Page 119	---	COORDN
Page 157	---	METAL
Page 162	---	VOIDS
Page 163	---	EXPECT
Page 164	---	SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed 'TRUE'

:: >>> Network Analysis may be INCORRECT when FALSE

W: Structure contains 1 isolated O-atom(s).

W: Structure contains 4 Intra/Inter contacts < Sum(vdWrad) -1.00 A (max -1.17)

N: Number of Isotropic Non-H Atoms 2

W: Number of valency check faults for H & C 1

:: Input Xtal Data from File cuclrhom-modified.cif - Data Type CIF

:: NORMAL END of PLATON : 166 Pages on:

:: cuclrhom-modified.lis (ASCII, 132 Characters Wide)

:: cuclrhom-modified.lps (PostScript Version of .lis)

::

:: SPF File on :cuclrhom-modified.eld

PLATON(V-201207)-Run for: c:xtal uP-1tkins3watR = 0.07cuace2na

TIME: Jan 11 10:54:58 2008

(C) 1980-2007 A.L.Spek

Crystal Data

Input Cell (Lattice Type: P)		Temp = 100K	Reduced Cell		(Acta Cryst.(1976),A32,297-298)
a = 7.8427(2) Angstrom	alpha = 92.310(1) Degree		a = 7.843	alpha = 92.31	V = 928.7
b = 10.5462(2)	beta = 105.606(1)		b = 10.546	beta = 105.61	
c = 11.6728(3)	gamma = 91.073(1)		c = 11.673	gamma = 91.07	
V = 928.68(4) Cubic-Angstrom	d(100) = 7.5500 Angstrom		Niggli Values		
Lambda(MoKa) = 0.71073 Angstrom	d(010) = 10.5327		61.508	111.222	136.254
	d(001) = 11.2300		-4.962	-24.628	-1.549

Orthogonalization Matrices

(See e.g. J.D.Dunitz, Xray Analysis and Structure Determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

(X0) (7.84270 -0.19749 -3.14022) (X) , (X) (0.12751 0.00239 0.03577) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 10.54435 -0.52938)*(Y) , (Y) = (0 0.09484 0.00447)*(Y0) are defined as:
 (Z0) (0 0 11.23001) (Z) , (Z) (0 0 0.08905) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group P-1 No: 2, Laue: -1 [Hall: -P 1]

Lattice Type aP, Centric, Triclinic, Order 2(1) [Schoenflies: Ci^1]

Nr ***** Symmetry Operation(s) *****

1	X ,	Y ,	Z
2	- X ,	- Y ,	- Z

ADDSYM - CHECK (cf. MISSYM (C): Le Page, Y., J. Appl. Cryst. (1987), 20, 264-269; J. Appl. Cryst. (1988), 21, 983-984)

- ADDSYM Search on ALL NON-H Chemical Types [Max NonFit 20 Perc]

:: Excluded Disorder Atoms From ADDSYM Analysis:

02W 03W 05W 08W

- Number of Excluded Disordered Input Atoms = 4
 - Number of Input Atoms Included in Search 26 (Unitcell 52)
 - Density based on Input Atom Set = 1.829 g.cm-3 - Vol / Non-H atom = 16.6 Ang+3
 - The Structure Implies the Following Symmetry Elements Subject to the Criteria:
 Criteria: 1.00 Deg (Metric), 0.25 Ang (Rot.), 0.45 Ang (Inv), 0.45 Ang (Transl)

Symm.	Input	Reduced	(Ang)	(Deg)	(%)	(Ang)	Input Cell
Elem	Cell_Row	Cell_Row	d	Typ	Dot	Angle	Fit
-1	=====		100	0	at	0	0 0 0

T.R.A.N.S.F.O.R.M.A.T.I.O.N M.A.T.R.I.X for CELL and HKL DATA

Reduced->Convent	Input->Reduced	T = Input->Convent:	a' = T a
(1 0 0)	(1 0 0)	(1 0 0)	Det(T)
(0 1 0)	(0 1 0)	(0 1 0)	=
(0 0 1)	(0 0 1)	(0 0 1)	1.000

Cell Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input	aP	7.843	10.546	11.673	92.31	105.61	91.07	929	Triclinic -1
Reduced	P	7.843	10.546	11.673	92.31	105.61	91.07	929	
Convent	aP	7.843	10.546	11.673	92.31	105.61	91.07	929	Triclinic -1

:: *** No Obvious Extra Crystallographic Symmetry was Detected ***

:: Note: Rerun in EQUAL Atom Type Mode for more Checks

(1:19-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

 Site = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
 ***** Move = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
 SYMBOLS: Type = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
 ***** El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
 ARU = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
 RESIDUE = collection of ARU's constituting an isolated unit (= molecule, ion).
 FLAGS : d = determined, c = calculated, R = riding G = group

Atom Types : C H Cu Na O
 Cov.Rad(Ang): 0.68 0.35 1.52 0.97 0.68
 Atom Volume : 13.87 5.08 26.90 26.00 11.39
 Atom Number : 6 1 29 11 8
 Atom Weight : 12.010 1.008 63.55 22.99 16.00
 Scat.Fact.f0: 5.999 1.000 28.986 10.992 7.999
 Scat.Fact.f': 0.003 0.000 0.320 0.036 0.011
 Scat.Fact.f": 0.002 0.000 1.265 0.025 0.006
 Mu/Rho(MoKa): 0.58 0.37 49.09 3.04 1.22
 Elem. Type : -- -- TR AK --

Sources - Cov. Radii : Manual Cambridge Crystallographic Data Base
 - Atom Volume: D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493
 - Atomic Wt. : SHELXL97
 - Scat. Fact.: SHELXL97 (International Tables)
 - mu/rho : International Tables C, table 4.2.4.2, p193-199

NOMOVE

 =====
 Residue = 1
 =====

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	Cu(1)	0.37342(11)	0.00315(8)	0.13751(8)	2.4962(9)	-0.0396(8)	1.5442(9)	1	1	1	-	Met
d	Cu(2)	0.00515(11)	0.13533(8)	0.03133(8)	-0.0847(9)	1.4104(8)	0.3518(9)	1	1	1	-	Met
d	Na(1)	1.0070(9)	0.3647(5)	0.2180(5)	7.141(7)	3.730(5)	2.448(6)	1	1	1	-	Met
d	O(1)	0.1675(7)	0.0051(5)	0.0040(5)	1.300(6)	0.052(5)	0.045(6)	1	1	1	-	D/A
d	O(4W)	1.0143(13)	0.5780(10)	0.1715(10)	7.302(11)	6.004(11)	1.926(11)	1	1	1	-	D/A
d	*O(5W)	0.811(5)	0.408(2)	0.334(2)	5.23(4)	4.13(2)	3.75(2)	1	1/2	1/2	-	D/A
d	O(6W)	1.309(3)	0.4146(15)	0.332(2)	9.14(2)	4.196(16)	3.73(2)	1	1	1	-	D/A
d	O(11A)	0.4360(7)	0.1820(5)	0.1031(5)	3.060(6)	1.864(5)	1.158(6)	1	1	1	-	D/A
d	O(11B)	0.0501(8)	0.1385(6)	0.2275(5)	-0.349(6)	1.340(6)	2.555(6)	1	1	1	-	D/A
d	O(12A)	0.1711(7)	0.2722(5)	0.0309(6)	1.191(6)	2.854(5)	0.347(7)	1	1	1	-	D/A
d	O(12B)	0.2122(8)	-0.0370(6)	0.2561(5)	0.867(6)	-0.526(6)	2.876(6)	1	1	1	-	D/A
d	O(21A)	0.5920(7)	0.1841(5)	-0.1062(5)	4.940(6)	1.997(5)	-1.193(6)	1	1	1	-	D/A
d	O(21B)	-0.4254(7)	0.0170(5)	0.2756(5)	-4.205(6)	0.033(5)	3.095(6)	1	1	1	-	D/A
d	O(22A)	0.8324(7)	0.2629(5)	0.0357(5)	6.364(6)	2.753(5)	0.401(6)	1	1	1	-	D/A

d	O(22B)	-0.2305(8)	-0.0749(7)	0.1898(5)	-2.389(6)	-0.890(7)	2.131(6)	1	1	1	-	D/A
d	C(1A)	0.4259(10)	0.3869(7)	0.0259(7)	3.182(8)	4.066(7)	0.291(8)	1	1	1	-	-
d	C(1B)	0.0460(11)	0.0153(9)	0.3924(7)	-0.874(9)	-0.046(9)	4.407(8)	1	1	1	-	-
d	C(2A)	0.5822(10)	0.3842(7)	-0.0094(7)	4.520(8)	4.056(7)	-0.106(8)	1	1	1	-	-
d	C(2B)	-0.1317(11)	-0.0053(8)	0.3915(7)	-2.261(9)	-0.263(8)	4.397(8)	1	1	1	-	-
d	C(3A)	0.6555(10)	0.4980(7)	-0.0342(7)	5.150(8)	5.269(7)	-0.384(8)	1	1	1	-	-
d	C(3B)	-0.1775(11)	-0.0200(9)	0.4977(7)	-2.951(9)	-0.474(9)	5.589(8)	1	1	1	-	-
d	C(11A)	0.3403(10)	0.2686(7)	0.0559(7)	2.440(8)	2.803(7)	0.628(8)	1	1	1	-	-
d	C(11B)	0.1038(10)	0.0406(8)	0.2832(7)	-0.083(8)	0.278(8)	3.180(8)	1	1	1	-	-
d	C(21A)	0.6739(10)	0.2658(7)	-0.0277(7)	5.320(8)	2.817(7)	-0.311(8)	1	1	1	-	-
d	C(21B)	-0.2717(11)	-0.0230(8)	0.2756(7)	-2.992(9)	-0.388(8)	3.095(8)	1	1	1	-	-
cR	H(3A)	0.76280	0.49710	-0.05730	6.0642	5.2719	-0.6435	1	1	1	-	-
cR	H(3B)	-0.29830	-0.03320	0.49620	-3.8911	-0.6128	5.5723	1	1	1	-	-
d	Cu(1)a	-0.62658(11)	0.00315(8)	0.13751(8)	-5.3465(9)	-0.0396(8)	1.5442(9)	1	1	1	1.455	Met
d	Cu(2)a	-0.99485(11)	0.13533(8)	0.03133(8)	-7.9274(9)	1.4104(8)	0.3518(9)	1	1	1	1.455	Met
d	Na(1)a	0.0070(9)	0.3647(5)	0.2180(5)	-0.702(7)	3.730(5)	2.448(6)	1	1	1	1.455	Met
d	O(1)a	-0.8325(7)	0.0051(5)	0.0040(5)	-6.543(6)	0.052(5)	0.045(6)	1	1	1	1.455	D/A
d	O(4W)a	0.0143(13)	0.5780(10)	0.1715(10)	-0.541(11)	6.004(11)	1.926(11)	1	1	1	1.455	D/A
d	*O(5W)a	-0.189(5)	0.408(2)	0.334(2)	-2.61(4)	4.13(2)	3.75(2)	1	1/2	1/2	1.455	D/A
d	O(6W)a	0.309(3)	0.4146(15)	0.332(2)	1.30(2)	4.196(16)	3.73(2)	1	1	1	1.455	D/A
d	O(11A)a	-0.5640(7)	0.1820(5)	0.1031(5)	-4.783(6)	1.864(5)	1.158(6)	1	1	1	1.455	D/A
d	O(11B)a	-0.9499(8)	0.1385(6)	0.2275(5)	-8.192(6)	1.340(6)	2.555(6)	1	1	1	1.455	D/A
d	O(12A)a	-0.8289(7)	0.2722(5)	0.0309(6)	-6.652(6)	2.854(5)	0.347(7)	1	1	1	1.455	D/A
d	O(12B)a	-0.7878(8)	-0.0370(6)	0.2561(5)	-6.975(6)	-0.526(6)	2.876(6)	1	1	1	1.455	D/A
d	O(21A)a	-0.4080(7)	0.1841(5)	-0.1062(5)	-2.903(6)	1.997(5)	-1.193(6)	1	1	1	1.455	D/A
d	O(21B)a	-1.4254(7)	0.0170(5)	0.2756(5)	-12.048(6)	0.033(5)	3.095(6)	1	1	1	1.455	D/A
d	O(22A)a	-0.1676(7)	0.2629(5)	0.0357(5)	-1.478(6)	2.753(5)	0.401(6)	1	1	1	1.455	D/A
d	O(22B)a	-1.2305(8)	-0.0749(7)	0.1898(5)	-10.232(6)	-0.890(7)	2.131(6)	1	1	1	1.455	D/A
d	C(1A)a	-0.5741(10)	0.3869(7)	0.0259(7)	-4.660(8)	4.066(7)	0.291(8)	1	1	1	1.455	-
d	C(1B)a	-0.9540(11)	0.0153(9)	0.3924(7)	-8.717(9)	-0.046(9)	4.407(8)	1	1	1	1.455	-
d	C(2A)a	-0.4178(10)	0.3842(7)	-0.0094(7)	-3.323(8)	4.056(7)	-0.106(8)	1	1	1	1.455	-
d	C(2B)a	-1.1317(11)	-0.0053(8)	0.3915(7)	-10.104(9)	-0.263(8)	4.397(8)	1	1	1	1.455	-
d	C(3A)a	-0.3445(10)	0.4980(7)	-0.0342(7)	-2.693(8)	5.269(7)	-0.384(8)	1	1	1	1.455	-
d	C(3B)a	-1.1775(11)	-0.0200(9)	0.4977(7)	-10.794(9)	-0.474(9)	5.589(8)	1	1	1	1.455	-
d	C(11A)a	-0.6597(10)	0.2686(7)	0.0559(7)	-5.402(8)	2.803(7)	0.628(8)	1	1	1	1.455	-
d	C(11B)a	-0.8962(10)	0.0406(8)	0.2832(7)	-7.926(8)	0.278(8)	3.180(8)	1	1	1	1.455	-
d	C(21A)a	-0.3261(10)	0.2658(7)	-0.0277(7)	-2.523(8)	2.817(7)	-0.311(8)	1	1	1	1.455	-
d	C(21B)a	-1.2717(11)	-0.0230(8)	0.2756(7)	-10.834(9)	-0.388(8)	3.095(8)	1	1	1	1.455	-
cR	H(3A)a	-0.23720	0.49710	-0.05730	-1.7785	5.2719	-0.6435	1	1	1	1.455	-
cR	H(3B)a	-1.29830	-0.03320	0.49620	-11.7338	-0.6128	5.5723	1	1	1	1.455	-
d	Cu(1)b	1.37342(11)	0.00315(8)	0.13751(8)	10.3389(9)	-0.0396(8)	1.5442(9)	1	1	1	1.655	Met
d	Cu(2)b	1.00515(11)	0.13533(8)	0.03133(8)	7.7580(9)	1.4104(8)	0.3518(9)	1	1	1	1.655	Met
d	Na(1)b	2.0070(9)	0.3647(5)	0.2180(5)	14.984(7)	3.730(5)	2.448(6)	1	1	1	1.655	Met
d	O(1)b	1.1675(7)	0.0051(5)	0.0040(5)	9.143(6)	0.052(5)	0.045(6)	1	1	1	1.655	D/A

d	O(4W)b	2.0143(13)	0.5780(10)	0.1715(10)	15.145(11)	6.004(11)	1.926(11)	1	1	1	1.655	D/A
d	*O(5W)b	1.811(5)	0.408(2)	0.334(2)	13.07(4)	4.13(2)	3.75(2)	1	1/2	1/2	1.655	D/A
d	O(6W)b	2.309(3)	0.4146(15)	0.332(2)	16.98(2)	4.196(16)	3.73(2)	1	1	1	1.655	D/A
d	O(11A)b	1.4360(7)	0.1820(5)	0.1031(5)	10.902(6)	1.864(5)	1.158(6)	1	1	1	1.655	D/A
d	O(11B)b	1.0501(8)	0.1385(6)	0.2275(5)	7.494(6)	1.340(6)	2.555(6)	1	1	1	1.655	D/A
d	O(12A)b	1.1711(7)	0.2722(5)	0.0309(6)	9.034(6)	2.854(5)	0.347(7)	1	1	1	1.655	D/A
d	O(12B)b	1.2122(8)	-0.0370(6)	0.2561(5)	8.710(6)	-0.526(6)	2.876(6)	1	1	1	1.655	D/A
d	O(21A)b	1.5920(7)	0.1841(5)	-0.1062(5)	12.783(6)	1.997(5)	-1.193(6)	1	1	1	1.655	D/A
d	O(21B)b	0.5746(7)	0.0170(5)	0.2756(5)	3.638(6)	0.033(5)	3.095(6)	1	1	1	1.655	D/A
d	O(22A)b	1.8324(7)	0.2629(5)	0.0357(5)	14.207(6)	2.753(5)	0.401(6)	1	1	1	1.655	D/A
d	O(22B)b	0.7695(8)	-0.0749(7)	0.1898(5)	5.454(6)	-0.890(7)	2.131(6)	1	1	1	1.655	D/A
d	C(1A)b	1.4259(10)	0.3869(7)	0.0259(7)	11.025(8)	4.066(7)	0.291(8)	1	1	1	1.655	-
d	C(1B)b	1.0460(11)	0.0153(9)	0.3924(7)	6.968(9)	-0.046(9)	4.407(8)	1	1	1	1.655	-
d	C(2A)b	1.5822(10)	0.3842(7)	-0.0094(7)	12.362(8)	4.056(7)	-0.106(8)	1	1	1	1.655	-
d	C(2B)b	0.8683(11)	-0.0053(8)	0.3915(7)	5.581(9)	-0.263(8)	4.397(8)	1	1	1	1.655	-
d	C(3A)b	1.6555(10)	0.4980(7)	-0.0342(7)	12.993(8)	5.269(7)	-0.384(8)	1	1	1	1.655	-
d	C(3B)b	0.8225(11)	-0.0200(9)	0.4977(7)	4.892(9)	-0.474(9)	5.589(8)	1	1	1	1.655	-
d	C(11A)b	1.3403(10)	0.2686(7)	0.0559(7)	10.283(8)	2.803(7)	0.628(8)	1	1	1	1.655	-
d	C(11B)b	1.1038(10)	0.0406(8)	0.2832(7)	7.759(8)	0.278(8)	3.180(8)	1	1	1	1.655	-
d	C(21A)b	1.6739(10)	0.2658(7)	-0.0277(7)	13.162(8)	2.817(7)	-0.311(8)	1	1	1	1.655	-
d	C(21B)b	0.7283(11)	-0.0230(8)	0.2756(7)	4.851(9)	-0.388(8)	3.095(8)	1	1	1	1.655	-
cR	H(3A)b	1.76280	0.49710	-0.05730	13.9069	5.2719	-0.6435	1	1	1	1.655	-
cR	H(3B)b	0.70170	-0.03320	0.49620	3.9516	-0.6128	5.5723	1	1	1	1.655	-
d	Cu(1)c	-0.37342(11)	-0.00315(8)	-0.13751(8)	-2.4962(9)	0.0396(8)	-1.5442(9)	1	1	1	2.555	Met
d	Cu(2)c	-0.00515(11)	-0.13533(8)	-0.03133(8)	0.0847(9)	-1.4104(8)	-0.3518(9)	1	1	1	2.555	Met
d	Na(1)c	-1.0070(9)	-0.3647(5)	-0.2180(5)	-7.141(7)	-3.730(5)	-2.448(6)	1	1	1	2.555	Met
d	O(1)c	-0.1675(7)	-0.0051(5)	-0.0040(5)	-1.300(6)	-0.052(5)	-0.045(6)	1	1	1	2.555	D/A
d	O(4W)c	-1.0143(13)	-0.5780(10)	-0.1715(10)	-7.302(11)	-6.004(11)	-1.926(11)	1	1	1	2.555	D/A
d	*O(5W)c	-0.811(5)	-0.408(2)	-0.334(2)	-5.23(4)	-4.13(2)	-3.75(2)	1	1/2	1/2	2.555	D/A
d	O(6W)c	-1.309(3)	-0.4146(15)	-0.332(2)	-9.14(2)	-4.196(16)	-3.73(2)	1	1	1	2.555	D/A
d	O(11A)c	-0.4360(7)	-0.1820(5)	-0.1031(5)	-3.060(6)	-1.864(5)	-1.158(6)	1	1	1	2.555	D/A
d	O(11B)c	-0.0501(8)	-0.1385(6)	-0.2275(5)	0.349(6)	-1.340(6)	-2.555(6)	1	1	1	2.555	D/A
d	O(12A)c	-0.1711(7)	-0.2722(5)	-0.0309(6)	-1.191(6)	-2.854(5)	-0.347(7)	1	1	1	2.555	D/A
d	O(12B)c	-0.2122(8)	0.0370(6)	-0.2561(5)	-0.867(6)	0.526(6)	-2.876(6)	1	1	1	2.555	D/A
d	O(21A)c	-0.5920(7)	-0.1841(5)	0.1062(5)	-4.940(6)	-1.997(5)	1.193(6)	1	1	1	2.555	D/A
d	O(21B)c	0.4254(7)	-0.0170(5)	-0.2756(5)	4.205(6)	-0.033(5)	-3.095(6)	1	1	1	2.555	D/A
d	O(22A)c	-0.8324(7)	-0.2629(5)	-0.0357(5)	-6.364(6)	-2.753(5)	-0.401(6)	1	1	1	2.555	D/A
d	O(22B)c	0.2305(8)	0.0749(7)	-0.1898(5)	2.389(6)	0.890(7)	-2.131(6)	1	1	1	2.555	D/A
d	C(1A)c	-0.4259(10)	-0.3869(7)	-0.0259(7)	-3.182(8)	-4.066(7)	-0.291(8)	1	1	1	2.555	-
d	C(1B)c	-0.0460(11)	-0.0153(9)	-0.3924(7)	0.874(9)	0.046(9)	-4.407(8)	1	1	1	2.555	-
d	C(2A)c	-0.5822(10)	-0.3842(7)	0.0094(7)	-4.520(8)	-4.056(7)	0.106(8)	1	1	1	2.555	-
d	C(2B)c	0.1317(11)	0.0053(8)	-0.3915(7)	2.261(9)	0.263(8)	-4.397(8)	1	1	1	2.555	-
d	C(3A)c	-0.6555(10)	-0.4980(7)	0.0342(7)	-5.150(8)	-5.269(7)	0.384(8)	1	1	1	2.555	-
d	C(3B)c	0.1775(11)	0.0200(9)	-0.4977(7)	2.951(9)	0.474(9)	-5.589(8)	1	1	1	2.555	-
d	C(11A)c	-0.3403(10)	-0.2686(7)	-0.0559(7)	-2.440(8)	-2.803(7)	-0.628(8)	1	1	1	2.555	-
d	C(11B)c	-0.1038(10)	-0.0406(8)	-0.2832(7)	0.083(8)	-0.278(8)	-3.180(8)	1	1	1	2.555	-

d	C(21A)c	-0.6739(10)	-0.2658(7)	0.0277(7)	-5.320(8)	-2.817(7)	0.311(8)	1	1	1	2.555	-
d	C(21B)c	0.2717(11)	0.0230(8)	-0.2756(7)	2.992(9)	0.388(8)	-3.095(8)	1	1	1	2.555	-
cR	H(3A)c	-0.76280	-0.49710	0.05730	-6.0642	-5.2719	0.6435	1	1	1	2.555	-
cR	H(3B)c	0.29830	0.03320	-0.49620	3.8911	0.6128	-5.5723	1	1	1	2.555	-
d	Cu(1)d	-0.37342(11)	-0.00315(8)	0.86249(8)	-5.6364(9)	-0.4898(8)	9.6858(9)	1	1	1	2.556	Met
d	Cu(2)d	-0.00515(11)	-0.13533(8)	0.96867(8)	-3.0555(9)	-1.9398(8)	10.8782(9)	1	1	1	2.556	Met
d	Na(1)d	-1.0070(9)	-0.3647(5)	0.7820(5)	-10.281(7)	-4.260(5)	8.782(6)	1	1	1	2.556	Met
d	O(1)d	-0.1675(7)	-0.0051(5)	0.9960(5)	-4.440(6)	-0.581(5)	11.185(6)	1	1	1	2.556	D/A
d	O(4W)d	-1.0143(13)	-0.5780(10)	0.8285(10)	-10.442(11)	-6.533(11)	9.304(11)	1	1	1	2.556	D/A
d	*O(5W)d	-0.811(5)	-0.408(2)	0.666(2)	-8.37(4)	-4.65(2)	7.48(2)	1	1/2	1/2	2.556	D/A
d	O(6W)d	-1.309(3)	-0.4146(15)	0.668(2)	-12.28(2)	-4.725(16)	7.50(2)	1	1	1	2.556	D/A
d	O(11A)d	-0.4360(7)	-0.1820(5)	0.8969(5)	-6.200(6)	-2.394(5)	10.072(6)	1	1	1	2.556	D/A
d	O(11B)d	-0.0501(8)	-0.1385(6)	0.7725(5)	-2.791(6)	-1.869(6)	8.675(6)	1	1	1	2.556	D/A
d	O(12A)d	-0.1711(7)	-0.2722(5)	0.9691(6)	-4.331(6)	-3.383(5)	10.883(7)	1	1	1	2.556	D/A
d	O(12B)d	-0.2122(8)	0.0370(6)	0.7439(5)	-4.008(6)	-0.004(6)	8.354(6)	1	1	1	2.556	D/A
d	O(21A)d	-0.5920(7)	-0.1841(5)	1.1062(5)	-8.080(6)	-2.527(5)	12.423(6)	1	1	1	2.556	D/A
d	O(21B)d	0.4254(7)	-0.0170(5)	0.7244(5)	1.065(6)	-0.563(5)	8.135(6)	1	1	1	2.556	D/A
d	O(22A)d	-0.8324(7)	-0.2629(5)	0.9643(5)	-9.504(6)	-3.283(5)	10.829(6)	1	1	1	2.556	D/A
d	O(22B)d	0.2305(8)	0.0749(7)	0.8102(5)	-0.751(6)	0.361(7)	9.099(6)	1	1	1	2.556	D/A
d	C(1A)d	-0.4259(10)	-0.3869(7)	0.9741(7)	-6.323(8)	-4.595(7)	10.939(8)	1	1	1	2.556	-
d	C(1B)d	-0.0460(11)	-0.0153(9)	0.6076(7)	-2.266(9)	-0.483(9)	6.823(8)	1	1	1	2.556	-
d	C(2A)d	-0.5822(10)	-0.3842(7)	1.0094(7)	-7.660(8)	-4.585(7)	11.336(8)	1	1	1	2.556	-
d	C(2B)d	0.1317(11)	0.0053(8)	0.6085(7)	-0.879(9)	-0.266(8)	6.833(8)	1	1	1	2.556	-
d	C(3A)d	-0.6555(10)	-0.4980(7)	1.0342(7)	-8.290(8)	-5.799(7)	11.614(8)	1	1	1	2.556	-
d	C(3B)d	0.1775(11)	0.0200(9)	0.5023(7)	-0.189(9)	-0.055(9)	5.641(8)	1	1	1	2.556	-
d	C(11A)d	-0.3403(10)	-0.2686(7)	0.9441(7)	-5.581(8)	-3.332(7)	10.602(8)	1	1	1	2.556	-
d	C(11B)d	-0.1038(10)	-0.0406(8)	0.7168(7)	-3.057(8)	-0.808(8)	8.050(8)	1	1	1	2.556	-
d	C(21A)d	-0.6739(10)	-0.2658(7)	1.0277(7)	-8.460(8)	-3.347(7)	11.541(8)	1	1	1	2.556	-
d	C(21B)d	0.2717(11)	0.0230(8)	0.7244(7)	-0.148(9)	-0.141(8)	8.135(8)	1	1	1	2.556	-
cR	H(3A)d	-0.76280	-0.49710	1.05730	-9.2044	-5.8013	11.8735	1	1	1	2.556	-
cR	H(3B)d	0.29830	0.03320	0.50380	0.7509	0.0834	5.6577	1	1	1	2.556	-
d	Cu(1)e	0.62658(11)	-0.00315(8)	-0.13751(8)	5.3465(9)	0.0396(8)	-1.5442(9)	1	1	1	2.655	Met
d	Cu(2)e	0.99485(11)	-0.13533(8)	-0.03133(8)	7.9274(9)	-1.4104(8)	-0.3518(9)	1	1	1	2.655	Met
d	Na(1)e	-0.0070(9)	-0.3647(5)	-0.2180(5)	0.702(7)	-3.730(5)	-2.448(6)	1	1	1	2.655	Met
d	O(1)e	0.8325(7)	-0.0051(5)	-0.0040(5)	6.543(6)	-0.052(5)	-0.045(6)	1	1	1	2.655	D/A
d	O(4W)e	-0.0143(13)	-0.5780(10)	-0.1715(10)	0.541(11)	-6.004(11)	-1.926(11)	1	1	1	2.655	D/A
d	*O(5W)e	0.189(5)	-0.408(2)	-0.334(2)	2.61(4)	-4.13(2)	-3.75(2)	1	1/2	1/2	2.655	D/A
d	O(6W)e	-0.309(3)	-0.4146(15)	-0.332(2)	-1.30(2)	-4.196(16)	-3.73(2)	1	1	1	2.655	D/A
d	O(11A)e	0.5640(7)	-0.1820(5)	-0.1031(5)	4.783(6)	-1.864(5)	-1.158(6)	1	1	1	2.655	D/A
d	O(11B)e	0.9499(8)	-0.1385(6)	-0.2275(5)	8.192(6)	-1.340(6)	-2.555(6)	1	1	1	2.655	D/A
d	O(12A)e	0.8289(7)	-0.2722(5)	-0.0309(6)	6.652(6)	-2.854(5)	-0.347(7)	1	1	1	2.655	D/A
d	O(12B)e	0.7878(8)	0.0370(6)	-0.2561(5)	6.975(6)	0.526(6)	-2.876(6)	1	1	1	2.655	D/A
d	O(21A)e	0.4080(7)	-0.1841(5)	0.1062(5)	2.903(6)	-1.997(5)	1.193(6)	1	1	1	2.655	D/A
d	O(21B)e	1.4254(7)	-0.0170(5)	-0.2756(5)	12.048(6)	-0.033(5)	-3.095(6)	1	1	1	2.655	D/A

d	O(22A)e	0.1676(7)	-0.2629(5)	-0.0357(5)	1.478(6)	-2.753(5)	-0.401(6)	1	1	1	2.655	D/A
d	O(22B)e	1.2305(8)	0.0749(7)	-0.1898(5)	10.232(6)	0.890(7)	-2.131(6)	1	1	1	2.655	D/A
d	C(1A)e	0.5741(10)	-0.3869(7)	-0.0259(7)	4.660(8)	-4.066(7)	-0.291(8)	1	1	1	2.655	-
d	C(1B)e	0.9540(11)	-0.0153(9)	-0.3924(7)	8.717(9)	0.046(9)	-4.407(8)	1	1	1	2.655	-
d	C(2A)e	0.4178(10)	-0.3842(7)	0.0094(7)	3.323(8)	-4.056(7)	0.106(8)	1	1	1	2.655	-
d	C(2B)e	1.1317(11)	0.0053(8)	-0.3915(7)	10.104(9)	0.263(8)	-4.397(8)	1	1	1	2.655	-
d	C(3A)e	0.3445(10)	-0.4980(7)	0.0342(7)	2.693(8)	-5.269(7)	0.384(8)	1	1	1	2.655	-
d	C(3B)e	1.1775(11)	0.0200(9)	-0.4977(7)	10.794(9)	0.474(9)	-5.589(8)	1	1	1	2.655	-
d	C(11A)e	0.6597(10)	-0.2686(7)	-0.0559(7)	5.402(8)	-2.803(7)	-0.628(8)	1	1	1	2.655	-
d	C(11B)e	0.8962(10)	-0.0406(8)	-0.2832(7)	7.926(8)	-0.278(8)	-3.180(8)	1	1	1	2.655	-
d	C(21A)e	0.3261(10)	-0.2658(7)	0.0277(7)	2.523(8)	-2.817(7)	0.311(8)	1	1	1	2.655	-
d	C(21B)e	1.2717(11)	0.0230(8)	-0.2756(7)	10.834(9)	0.388(8)	-3.095(8)	1	1	1	2.655	-
cR	H(3A)e	0.23720	-0.49710	0.05730	1.7785	-5.2719	0.6435	1	1	1	2.655	-
cR	H(3B)e	1.29830	0.03320	-0.49620	11.7338	0.6128	-5.5723	1	1	1	2.655	-
d	Cu(1)f	0.62658(11)	0.99685(8)	-0.13751(8)	5.1490(9)	10.5839(8)	-1.5442(9)	1	1	1	2.665	Met
d	Cu(2)f	0.99485(11)	0.86467(8)	-0.03133(8)	7.7299(9)	9.1340(8)	-0.3518(9)	1	1	1	2.665	Met
d	Na(1)f	-0.0070(9)	0.6353(5)	-0.2180(5)	0.504(7)	6.814(5)	-2.448(6)	1	1	1	2.665	Met
d	O(1)f	0.8325(7)	0.9949(5)	-0.0040(5)	6.345(6)	10.493(5)	-0.045(6)	1	1	1	2.665	D/A
d	O(4W)f	-0.0143(13)	0.4220(10)	-0.1715(10)	0.343(11)	4.541(11)	-1.926(11)	1	1	1	2.665	D/A
d	*O(5W)f	0.189(5)	0.592(2)	-0.334(2)	2.41(4)	6.42(2)	-3.75(2)	1	1/2	1/2	2.665	D/A
d	O(6W)f	-0.309(3)	0.5854(15)	-0.332(2)	-1.50(2)	6.348(16)	-3.73(2)	1	1	1	2.665	D/A
d	O(11A)f	0.5640(7)	0.8180(5)	-0.1031(5)	4.585(6)	8.680(5)	-1.158(6)	1	1	1	2.665	D/A
d	O(11B)f	0.9499(8)	0.8615(6)	-0.2275(5)	7.994(6)	9.204(6)	-2.555(6)	1	1	1	2.665	D/A
d	O(12A)f	0.8289(7)	0.7278(5)	-0.0309(6)	6.454(6)	7.691(5)	-0.347(7)	1	1	1	2.665	D/A
d	O(12B)f	0.7878(8)	1.0370(6)	-0.2561(5)	6.778(6)	11.070(6)	-2.876(6)	1	1	1	2.665	D/A
d	O(21A)f	0.4080(7)	0.8159(5)	0.1062(5)	2.705(6)	8.547(5)	1.193(6)	1	1	1	2.665	D/A
d	O(21B)f	1.4254(7)	0.9830(5)	-0.2756(5)	11.850(6)	10.511(5)	-3.095(6)	1	1	1	2.665	D/A
d	O(22A)f	0.1676(7)	0.7371(5)	-0.0357(5)	1.281(6)	7.791(5)	-0.401(6)	1	1	1	2.665	D/A
d	O(22B)f	1.2305(8)	1.0749(7)	-0.1898(5)	10.034(6)	11.435(7)	-2.131(6)	1	1	1	2.665	D/A
d	C(1A)f	0.5741(10)	0.6131(7)	-0.0259(7)	4.463(8)	6.478(7)	-0.291(8)	1	1	1	2.665	-
d	C(1B)f	0.9540(11)	0.9847(9)	-0.3924(7)	8.520(9)	10.591(9)	-4.407(8)	1	1	1	2.665	-
d	C(2A)f	0.4178(10)	0.6158(7)	0.0094(7)	3.126(8)	6.488(7)	0.106(8)	1	1	1	2.665	-
d	C(2B)f	1.1317(11)	1.0053(8)	-0.3915(7)	9.906(9)	10.807(8)	-4.397(8)	1	1	1	2.665	-
d	C(3A)f	0.3445(10)	0.5020(7)	0.0342(7)	2.495(8)	5.275(7)	0.384(8)	1	1	1	2.665	-
d	C(3B)f	1.1775(11)	1.0200(9)	-0.4977(7)	10.596(9)	11.019(9)	-5.589(8)	1	1	1	2.665	-
d	C(11A)f	0.6597(10)	0.7314(7)	-0.0559(7)	5.205(8)	7.742(7)	-0.628(8)	1	1	1	2.665	-
d	C(11B)f	0.8962(10)	0.9594(8)	-0.2832(7)	7.728(8)	10.266(8)	-3.180(8)	1	1	1	2.665	-
d	C(21A)f	0.3261(10)	0.7342(7)	0.0277(7)	2.326(8)	7.727(7)	0.311(8)	1	1	1	2.665	-
d	C(21B)f	1.2717(11)	1.0230(8)	-0.2756(7)	10.637(9)	10.933(8)	-3.095(8)	1	1	1	2.665	-
cR	H(3A)f	0.23720	0.50290	0.05730	1.5810	5.2724	0.6435	1	1	1	2.665	-
cR	H(3B)f	1.29830	1.03320	-0.49620	11.5363	11.1571	-5.5723	1	1	1	2.665	-

```

=====
*****
Residue = 2 *****
=====

```

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	O(1W)	0.5738(19)	0.2534(10)	0.3945(9)	3.211(15)	2.463(11)	4.430(10)	1	1	1	-	D/A

```

=====
*****
Residue = 3 *****
=====

```

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	>O(2W)	0.709(3)	0.2649(12)	0.6409(10)	3.50(2)	2.454(13)	7.197(11)	1	0.700	0.700	-	D/A

```

=====
*****
Residue = 4 *****
=====

```

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	>O(3W)	1.078(5)	0.337(3)	0.571(3)	6.59(4)	3.25(3)	6.41(3)	1	0.600	0.600	-	D/A

```

=====
*****
Residue = 5 *****
=====

```

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	O(7W)	0.626(3)	0.6731(12)	0.2986(13)	3.84(2)	6.939(13)	3.353(15)	1	1	1	-	D/A

```

=====
*****
Residue = 6 *****
=====

```

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type

Disordered Atoms with S.O.F < 0.5

d	<O(8W)	1	1/2	1/2	6.1738	5.0075	5.6150	-1	2	0.150	0.300	-	D/A

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)	
a =[1455.01]	= -1+x, y, z	= [	1	-1	0	0	1	-1	0	0
b =[1655.01]	= 1+x, y, z	= [	1	1	0	0	1	1	0	0
c =[2555.01]	= -x, -y, -z	= [	2	0	0	0	1	0	0	0
d =[2556.01]	= -x, -y, 1-z	= [	2	0	0	1	1	0	0	1
e =[2655.01]	= 1-x, -y, -z	= [	2	1	0	0	1	1	0	0
f =[2665.01]	= 1-x, 1-y, -z	= [	2	1	1	0	1	1	1	0

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

$X(J) = X(sym) + TX$, $Y(J) = Y(sym) + TY$, $Z(J) = Z(sym) + TZ$,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

:: Starred ARUs belong (chemically) to the previous ARU

:: Analysis of Polymeric Structure(s)

:: Resd # 1 - Infinite Three-Dimensional Framework :: Det = 1, Base Vectors: #1 = [1 0 0], #2 = [0 1 0], #3 = [0 0 1],

NOTE: Atoms preceded by > * or < indicate disordered positions (SOF : < 50%, 50%, > 50%)

Disordered Structure

Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)

Resd	Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	H	Cu	Na	O
1	1	-0.003	0.007	0.020	912.41	1	1	20	4	4	2	23
2	1	0.574	0.253	0.394	16.00	1	2	-	-	-	-	1
3	1	0.709	0.265	0.641	11.20	0.700	2	-	-	-	-	1
4	1	1.078	0.337	0.571	9.60	0.600	2	-	-	-	-	1
5	1	0.626	0.673	0.299	16.00	1	2	-	-	-	-	1
6	-1	1	1/2	1/2	4.80	0.300	1	-	-	-	-	1

Unit Cell Weight = 1022.81 20 4 4 2 30

Calculated Analysis (Percent) = 23.5 0.4 24.9 4.5 46.8

Moiety_Formula = C20 H4 Cu4 Na2 O23, 4(0), 1.4(0), 1.2(0), 0.3(0)

Sum_Formula = C20 H4 Cu4 Na2 O29.90

Formula_Weight = 1022.81 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 1

SpaceGroup_Z = 2 ==> Z' = 1 / 2 = 0.500

Calculated Density = 1.8289(1) g cm-3 [= Mg m-3]

F(000) = 501.2 [502.86]

mu(MoKa) = 23.86 cm-1 = 2.386 mm-1

Resonant Scattering = 4.50 Percent - (E. Girard et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 797.9[782.9] Ang**3, 298[100]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)

** WARNING **

Please Check the Derived Crystal Data.
They may be Incorrect for Disordered,
Incomplete or Polymeric Structures.

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f, f' & f''

=====
 (An)isotropic, Equivalent and Main Axes Displacement Parameters - Unusual Values Marked with a # - [Optional Coordinate Split-up]
 =====

 =====
 ***** Residue = 1 *****
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Cu1	0.0033(5)	0.0068(5)	0.0084(5)	0.0010(3)	-0.0004(3)	0.0004(3)	0.0065(3)	0.0030	0.0067	0.0099	3.34
		[0.3732	0.0043	0.1412]	[0.3736	0.0020	0.1338]					
2	Cu2	0.0018(5)	0.0041(5)	0.0116(5)	0.0000(3)	0.0029(3)	0.0006(3)	0.0056(3)	0.0010	0.0042	0.0116	11.19#
		[0.0110	0.1354	0.0377]	[-0.0007	0.1352	0.0250]					
3	Na1	0.092(5)	0.030(3)	0.044(3)	-0.006(2)	0.005(3)	0.003(3)	0.058(2)	0.0269	0.0465	0.1009	3.75
		[1.0260	0.3655	0.2167]	[0.9880	0.3639	0.2193]					
4	O1	0.005(2)	0.007(2)	0.008(2)	0.0006(19)	0.0017(19)	0.0033(19)	0.0066(12)	0.0026	0.0080	0.0093	3.60
		[0.1715	0.0082	0.0037]	[0.1635	0.0020	0.0043]					
5	O4W	0.046(6)	0.047(6)	0.073(7)	0.025(5)	0.006(5)	0.002(4)	0.057(4)	0.0328	0.0464	0.0908	2.77
		[1.0152	0.5842	0.1805]	[1.0134	0.5718	0.1625]					
6	*O5W	0.26(4)	0.046(12)	0.067(15)	-0.045(11)	0.11(2)	-0.092(19)	0.114(15)	0.0091	0.0237	0.3097	33.93#
		[0.8698	0.3976	0.3454]	[0.7522	0.4184	0.3226]					
7	O6W	0.145(17)	0.064(10)	0.21(2)	-0.012(12)	-0.101(17)	0.007(10)	0.169(9)	0.0547	0.0655	0.3867	7.06
		[1.3368	0.4155	0.3091]	[1.2812	0.4137	0.3549]					
8	O11A	0.003(2)	0.008(3)	0.021(3)	0.002(2)	0.001(2)	-0.0019(19)	0.0111(16)	0.0023	0.0085	0.0225	9.94#
		[0.4396	0.1841	0.1121]	[0.4324	0.1799	0.0941]					
9	O11B	0.017(3)	0.022(3)	0.008(3)	-0.003(2)	0.005(2)	-0.004(2)	0.0155(17)	0.0067	0.0145	0.0253	3.77
		[0.0437	0.1440	0.2261]	[0.0565	0.1330	0.2289]					
10	O12A	0.003(2)	0.007(3)	0.030(3)	0.003(2)	0.008(2)	0.0030(19)	0.0126(16)	0.0001	0.0074	0.0301	213.97#
		[0.1841	0.2746	0.0442]	[0.1581	0.2698	0.0176]					
11	O12B	0.016(3)	0.030(3)	0.011(3)	0.005(2)	0.008(2)	0.004(2)	0.0180(17)	0.0067	0.0161	0.0312	4.68
		[0.2173	-0.0287	0.2580]	[0.2071	-0.0453	0.2542]					
12	O21A	0.008(3)	0.007(3)	0.018(3)	-0.003(2)	-0.002(2)	0.000(2)	0.0122(17)	0.0054	0.0077	0.0233	4.29
		[0.5903	0.1828	-0.1000]	[0.5937	0.1854	-0.1124]					
13	O21B	0.011(3)	0.014(3)	0.012(3)	0.002(2)	-0.002(2)	0.000(2)	0.0133(17)	0.0074	0.0136	0.0189	2.57
		[-0.4216	0.0154	0.2728]	[-0.4292	0.0186	0.2784]					
14	O22A	0.002(2)	0.010(3)	0.019(3)	0.000(2)	0.001(2)	0.0012(19)	0.0107(16)	0.0018	0.0101	0.0202	11.08#
		[0.8363	0.2626	0.0445]	[0.8285	0.2632	0.0269]					
15	O22B	0.014(3)	0.039(4)	0.008(3)	-0.001(3)	0.007(2)	-0.012(3)	0.0198(19)	0.0031	0.0114	0.0448	14.55#
		[-0.2405	-0.0621	0.1887]	[-0.2205	-0.0877	0.1909]					
16	C1A	0.0104(15)						0.0104(15)				
17	C1B	0.011(4)	0.028(5)	0.009(4)	0.000(3)	0.005(3)	-0.005(3)	0.016(3)	0.0061	0.0110	0.0299	4.92
		[0.0415	0.0236	0.3920]	[0.0505	0.0070	0.3928]					
18	C2A	0.0110(15)						0.0110(15)				
19	C2B	0.0133(16)						0.0133(16)				
20	C3A	0.0100(14)						0.0100(14)				

21	C3B	0.006(3)	0.037(5)	0.009(4)	0.002(3)	0.002(3)	-0.005(3)	0.017(2)	0.0049	0.0089	0.0383	7.75
		[-0.1805	-0.0084	0.4983]	[-0.1745	-0.0316	0.4971]					
22	C11A	0.0085(14)						0.0085(14)				
23	C11B	0.0119(15)						0.0119(15)				
24	C21A	0.0093(14)						0.0093(14)				
25	C21B	0.009(4)	0.025(4)	0.010(4)	0.005(3)	0.001(3)	-0.007(3)	0.015(2)	0.0058	0.0088	0.0302	5.17
		[-0.2763	-0.0149	0.2775]	[-0.2671	-0.0311	0.2737]					
26	H3A	0.01200						0.01200				
27	H3B	0.02100						0.02100				
U(i,j)-Average		0.0363	0.0240	0.0321	-0.0014	0.0032	-0.0057	0.0321	0.0205	0.0321	0.0437	2.13

 =====
 Residue = 2
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	01W	0.126(11)	0.043(6)	0.041(6)	-0.008(4)	0.019(6)	-0.003(6)	0.071(5)	0.0322	0.0519	0.1291	4.01
		[0.5971	0.2531	0.3956]	[0.5505	0.2537	0.3934]					
U(i,j)-Average		0.1260	0.0430	0.0410	-0.0080	0.0190	-0.0030	0.0710	0.0322	0.0519	0.1291	4.01

 =====
 Residue = 3
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	>02W	0.21(2)	0.025(6)	0.011(5)	0.011(5)	0.005(8)	-0.031(9)	0.087(7)	0.0032	0.0256	0.2321	71.98#
		[0.7626	0.2598	0.6409]	[0.6554	0.2700	0.6409]					
U(i,j)-Average		0.2100	0.0250	0.0110	0.0110	0.0050	-0.0310	0.0870	0.0032	0.0256	0.2321	71.98

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=====
*****Residue = 4*****
=====

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Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	>O3W	0.129(11)						0.129(11)				

```

=====
*****Residue = 5*****
=====

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Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	07W	0.28(3)	0.039(7)	0.068(9)	0.003(6)	-0.012(12)	0.040(11)	0.140(11)	0.0322	0.0648	0.3229	10.03#
		[0.6740	0.6769	0.2955]	[0.5780	0.6693	0.3017]					
U(i,j)-Average		0.2800	0.0390	0.0680	0.0030	-0.0120	0.0400	0.1400	0.0322	0.0648	0.3229	10.03

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=====
*****Residue = 6*****
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Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	<O8W	0.051(11)						0.051(11)				

=====
The Displacement Factor has the Form of $\text{Exp}(-T)$

where

$T = 8 \cdot (\pi^2) \cdot U_{\text{iso}} \cdot \sin^2(\theta/\lambda)$, for Isotropic Atoms,

$T = 2 \cdot (\pi^2) \cdot (U_{11} \cdot (h \cdot a)^2 + U_{22} \cdot (k \cdot b)^2 + U_{33} \cdot (l \cdot c)^2 + 2 \cdot U_{23} \cdot k \cdot l \cdot b \cdot c + 2 \cdot U_{13} \cdot h \cdot l \cdot a \cdot c + 2 \cdot U_{12} \cdot h \cdot k \cdot a \cdot b)$, for Anisotr. Atoms

$U_{\text{eq}} = 1/3 \sum(i,j) (U_{ij} \cdot a(i) \cdot a(j) \cdot a(i) \cdot a(j))$

U1, U2, U3 are the three Main Axes Components of U_{ij}

Reference U_{eq} : R.X. Fischer & E. Tillmanns, Acta Cryst. (1988). C44, 775-776

U_{eq} [or U_{iso}] Averages per Element

	Non-H	C	H	Cu	Na	O
Average	0.0377	0.0122	0.0165	0.0060	0.0580	0.0552
Minimum	0.0056	0.0085	0.0120	0.0056	0.0580	0.0066
Maximum	0.1690	0.0170	0.0210	0.0065	0.0580	0.1690
Ratio	9.9999	2.0000	1.7500	1.1607	1.0000	9.9999
Number	30	10	2	2	1	17

Residue = 1

:: No TLS-Analysis for Polymeric or Disordered Structures

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Rigid-Body Model Libration Corrections for Bond Distances and "Hirshfeld Rigid-Bond" Test (Acta Cryst, (1976), A32, 239-244)

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Bond		Bond Distance		Components of the Correction			Vibration Along the Interatomic Bond				Angle with Lib. Axes		
Atom(I)	Atom(J)	Obsd	Calcd	Del(L)	Del(M)	Del(N)	I to J	J to I	Difference	Sqrt(Diff)	L(1)	L(2)	L(3)

Cu(1)	- O(1)	1.9201	0	0	0	0	0.0041(5)	0.0061(20)	0.0020(21)	0.0450	0.00	0.00	0.00
Cu(1)	- O(11A)	2.0230	0	0	0	0	0.0068(5)	0.0070(27)	0.0002(27)	0.0133	0.00	0.00	0.00
Cu(1)	- O(12B)	2.1594	0	0	0	0	0.0085(5)	0.0079(30)	0.0006(30)	0.0245	0.00	0.00	0.00
Cu(1)	- O(21B)b	1.9269	0	0	0	0	0.0044(5)	0.0075(30)	0.0031(30)	0.0561	0.00	0.00	0.00
Cu(1)	- O(21A)e	2.0303	0	0	0	0	0.0070(5)	0.0066(30)	0.0004(30)	0.0206	0.00	0.00	0.00
Cu(2)	- O(1)	1.9642	0	0	0	0	0.0022(5)	0.0031(20)	0.0008(21)	0.0289	0.00	0.00	0.00
Cu(2)	- O(11B)	2.2199	0	0	0	0	0.0115(5)	0.0076(30)	0.0039(30)	0.0627	0.00	0.00	0.00
Cu(2)	- O(12A)	1.9265	0	0	0	0	0.0034(5)	0.0063(27)	0.0029(27)	0.0543	0.00	0.00	0.00
Cu(2)	- O(22A)a	1.9360	0	0	0	0	0.0020(5)	0.0053(27)	0.0033(27)	0.0571	0.00	0.00	0.00
Cu(2)	- O(1)c	1.9422	0	0	0	0	0.0036(5)	0.0091(20)	0.0056(21)	0.0745	0.00	0.00	0.00
O(21B)	- C(21B)	1.2845	0	0	0	0	0.0143(30)	0.0174(40)	0.0031(50)	0.0555	0.00	0.00	0.00
O(22B)	- C(21B)	1.2424	0	0	0	0	0.0146(33)	0.0202(40)	0.0057(52)	0.0753	0.00	0.00	0.00
C(1B)	- C(3B)d	1.4117	0	0	0	0	0.0115(43)	0.0080(40)	0.0035(59)	0.0596	0.00	0.00	0.00
C(3B)	- C(1B)d	1.4117	0	0	0	0	0.0080(40)	0.0115(43)	0.0035(59)	0.0596	0.00	0.00	0.00

Sqrt(Sum(DelIJ**2)/Nrb) = 0.0031

- Indicates bonds exceeding the 5.0 sigma test level

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Analysis of Bond Distance and Angle Values - Identification of Chiral Center(s) and Their (R/S)-Configuration (Cahn-Ingold-Prelog)

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The Following Tests are done. Faults are Marked Under Note

- V : Valency Check Fault for H, C
- S : Bond Too Short
- A : Unusual Bond Angle Values (PLEASE CHECK)

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*** PLEASE NOTE: R/S ASSIGNMENTS ARE TENTATIVE *** (CIP Special rules NOT Implemented)

*** See Angew.Chem.Intern. Ed. Eng., (1966), 5, 385 & (1982), 21, 567 for Authoritative Details for Special Cases

***** Residue = 1 *****

Flag Label - Connected to (May be Incomplete for Polymeric Structures)										=A.N.G.L.E.S=				=B.O.N.D.S=						
										nra	min	max	Aver	min	max	nrb	tnr	Hyb	RS	Note
d	Cu(1)	- O(1)	O(11A)	O(12B)	O(21B)b	O(21A)e	-----	-----	-----	-----	10	87	175	107.5	1.920	2.159	5	196		
d	Cu(2)	- O(1)	O(11B)	O(12A)	O(22A)a	O(1)c	-----	-----	-----	-----	10	84	172	107.8	1.926	2.220	5	198		
d	Na(1)	- O(4W)	*O(5W)	O(6W)	O(22A)	O(11B)b	-----	-----	-----	-----	6	71	164	109.5	2.338	2.420	5	184		
d	O(1)	- Cu(1)	Cu(2)	Cu(2)c	-----	-----	-----	-----	-----	-----	3	96	121	109.3	1.920	1.964	3	179		
d	O(4W)	- Na(1)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.338	2.338	1	136	sp2	
d	*O(5W)	- Na(1)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.345	2.345	2	136	sp2	
d	O(6W)	- Na(1)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.420	2.420	1	136	sp2	
d	O(11A)	- Cu(1)	C(11A)	-----	-----	-----	-----	-----	-----	-----	1	131	131	130.8	1.243	2.023	2	170	sp3	
d	O(11B)	- Cu(2)	C(11B)	Na(1)a	-----	-----	-----	-----	-----	-----	3	87	152	119.5	1.261	2.418	3	177		
d	O(12A)	- Cu(2)	C(11A)	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.0	1.281	1.926	2	175	sp3	
d	O(12B)	- Cu(1)	C(11B)	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.4	1.282	2.159	2	171	sp3	
d	O(21A)	- C(21A)	Cu(1)e	-----	-----	-----	-----	-----	-----	-----	1	133	133	133.4	1.262	2.030	2	157	sp3	
d	O(21B)	- C(21B)	Cu(1)a	-----	-----	-----	-----	-----	-----	-----	1	123	123	123.2	1.285	1.927	2	150	sp3	
d	O(22A)	- Na(1)	C(21A)	Cu(2)b	-----	-----	-----	-----	-----	-----	3	94	137	119.6	1.266	2.398	3	162		
d	O(22B)	- C(21B)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	123	sp2	
d	C(1A)	- C(2A)	C(11A)	C(3A)f	-----	-----	-----	-----	-----	-----	3	118	122	120.0	1.394	1.503	3	66	sp2	
d	C(1B)	- C(2B)	C(11B)	C(3B)d	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.404	1.495	3	68	sp2	
d	C(2A)	- C(1A)	C(3A)	C(21A)	-----	-----	-----	-----	-----	-----	3	117	124	120.0	1.395	1.489	3	61	sp2	
d	C(2B)	- C(1B)	C(3B)	C(21B)	-----	-----	-----	-----	-----	-----	3	119	120	119.9	1.394	1.498	3	55	sp2	
d	C(3A)	- C(2A)	H(3A)	C(1A)f	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.395	3	33	sp2	
d	C(3B)	- C(2B)	H(3B)	C(1B)d	-----	-----	-----	-----	-----	-----	3	120	121	120.0	0.950	1.412	3	29	sp2	
d	C(11A)	- O(11A)	O(12A)	C(1A)	-----	-----	-----	-----	-----	-----	3	113	128	120.0	1.243	1.503	3	104	sp2	
d	C(11B)	- O(11B)	O(12B)	C(1B)	-----	-----	-----	-----	-----	-----	3	117	125	120.0	1.261	1.495	3	106	sp2	
d	C(21A)	- O(21A)	O(22A)	C(2A)	-----	-----	-----	-----	-----	-----	3	114	127	120.0	1.262	1.489	3	99	sp2	
d	C(21B)	- O(21B)	O(22B)	C(2B)	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.498	3	90	sp2	
cR	H(3A)	- C(3A)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	9		
cR	H(3B)	- C(3B)	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	7		
d	Cu(1)a	- O(21B)	O(1)a	O(11A)a	O(12B)a	O(21A)c	-----	-----	-----	-----	10	87	175	107.5	1.920	2.159	5	190		
d	Cu(2)a	- O(1)a	O(11B)a	O(12A)a	-----	-----	-----	-----	-----	-----	3	93	103	97.2	1.926	2.220	3	189		
d	Na(1)a	- O(11B)	O(4W)a	*O(5W)a	O(6W)a	O(22A)a	-----	-----	-----	-----	6	71	164	109.5	2.338	2.420	5	186		
d	O(1)a	- Cu(1)a	Cu(2)a	-----	-----	-----	-----	-----	-----	-----	1	110	110	110.5	1.920	1.964	2	151		
d	O(4W)a	- Na(1)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.338	2.338	1	138		
d	*O(5W)a	- Na(1)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.345	2.345	2	138		
d	O(6W)a	- Na(1)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.420	2.420	1	138		
d	O(11A)a	- Cu(1)a	C(11A)a	-----	-----	-----	-----	-----	-----	-----	1	131	131	130.8	1.243	2.023	2	149		
d	O(11B)a	- Cu(2)a	C(11B)a	-----	-----	-----	-----	-----	-----	-----	1	120	120	119.6	1.261	2.220	2	145		
d	O(12A)a	- Cu(2)a	C(11A)a	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.0	1.281	1.926	2	146		
d	O(12B)a	- Cu(1)a	C(11B)a	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.4	1.282	2.159	2	148		

d	O(21A)a- C(21A)a Cu(1)c	-----	-----	-----	-----	-----	-----	-----	-----	1	133	133	133.4	1.262	2.030	2	167	
d	O(21B)a- C(21B)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	111	
d	O(22A)a- Cu(2) Na(1)a C(21A)a	-----	-----	-----	-----	-----	-----	-----	-----	3	94	137	119.6	1.266	2.398	3	176	
d	O(22B)a- C(21B)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	111	
d	C(1A)a - C(2A)a C(11A)a	-----	-----	-----	-----	-----	-----	-----	-----	1	122	122	122.1	1.395	1.503	2	54	?
d	C(1B)a - C(2B)a C(11B)a	-----	-----	-----	-----	-----	-----	-----	-----	1	123	123	123.4	1.404	1.495	2	53	?
d	C(2A)a - C(1A)a C(3A)a C(21A)a	-----	-----	-----	-----	-----	-----	-----	-----	3	117	124	120.0	1.395	1.489	3	67	
d	C(2B)a - C(1B)a C(3B)a C(21B)a	-----	-----	-----	-----	-----	-----	-----	-----	3	119	120	119.9	1.394	1.498	3	42	
d	C(3A)a - C(2A)a H(3A)a	-----	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.4	0.950	1.395	2	38	?
d	C(3B)a - C(2B)a H(3B)a	-----	-----	-----	-----	-----	-----	-----	-----	1	120	120	119.8	0.950	1.394	2	20	?
d	C(11A)a- O(11A)a O(12A)a C(1A)a	-----	-----	-----	-----	-----	-----	-----	-----	3	113	128	120.0	1.243	1.503	3	92	
d	C(11B)a- O(11B)a O(12B)a C(1B)a	-----	-----	-----	-----	-----	-----	-----	-----	3	117	125	120.0	1.261	1.495	3	93	
d	C(21A)a- O(21A)a O(22A)a C(2A)a	-----	-----	-----	-----	-----	-----	-----	-----	3	114	127	120.0	1.262	1.489	3	105	
d	C(21B)a- O(21B)a O(22B)a C(2B)a	-----	-----	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.498	3	72	
cR	H(3A)a - C(3A)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	13	
cR	H(3B)a - C(3B)a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	2	
d	Cu(1)b - O(1)b O(11A)b O(12B)b	-----	-----	-----	-----	-----	-----	-----	-----	3	89	123	100.9	1.920	2.159	3	191	
d	Cu(2)b - O(22A) O(1)b O(11B)b O(12A)b O(1)e	-----	-----	-----	-----	-----	-----	-----	-----	10	84	172	107.8	1.926	2.220	5	194	
d	Na(1)b - O(4W)b *O(5W)b O(6W)b O(22A)b	-----	-----	-----	-----	-----	-----	-----	-----	3	83	143	109.6	2.338	2.420	4	181	
d	O(1)b - Cu(1)b Cu(2)b Cu(2)e	-----	-----	-----	-----	-----	-----	-----	-----	3	96	121	109.3	1.920	1.964	3	163	
d	O(4W)b - Na(1)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.338	2.338	1	132	
d	*O(5W)b - Na(1)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.345	2.345	2	132	
d	O(6W)b - Na(1)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.420	2.420	1	132	
d	O(11A)b- Cu(1)b C(11A)b	-----	-----	-----	-----	-----	-----	-----	-----	1	131	131	130.8	1.243	2.023	2	152	
d	O(11B)b- Na(1) Cu(2)b C(11B)b	-----	-----	-----	-----	-----	-----	-----	-----	3	87	152	119.5	1.261	2.418	3	161	
d	O(12A)b- Cu(2)b C(11A)b	-----	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.0	1.281	1.926	2	160	
d	O(12B)b- Cu(1)b C(11B)b	-----	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.4	1.282	2.159	2	153	
d	O(21A)b- C(21A)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.262	1.262	1	119	
d	O(21B)b- Cu(1) C(21B)b	-----	-----	-----	-----	-----	-----	-----	-----	1	123	123	123.2	1.285	1.927	2	168	
d	O(22A)b- Na(1)b C(21A)b	-----	-----	-----	-----	-----	-----	-----	-----	1	137	137	136.6	1.266	2.398	2	133	
d	O(22B)b- C(21B)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	127	
d	C(1A)b - C(2A)b C(11A)b	-----	-----	-----	-----	-----	-----	-----	-----	1	122	122	122.1	1.395	1.503	2	59	?
d	C(1B)b - C(2B)b C(11B)b	-----	-----	-----	-----	-----	-----	-----	-----	1	123	123	123.4	1.404	1.495	2	60	?
d	C(2A)b - C(1A)b C(3A)b C(21A)b	-----	-----	-----	-----	-----	-----	-----	-----	3	117	124	120.0	1.395	1.489	3	46	
d	C(2B)b - C(1B)b C(3B)b C(21B)b	-----	-----	-----	-----	-----	-----	-----	-----	3	119	120	119.9	1.394	1.498	3	62	
d	C(3A)b - C(2A)b H(3A)b	-----	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.4	0.950	1.395	2	24	?
d	C(3B)b - C(2B)b H(3B)b	-----	-----	-----	-----	-----	-----	-----	-----	1	120	120	119.8	0.950	1.394	2	34	?
d	C(11A)b- O(11A)b O(12A)b C(1A)b	-----	-----	-----	-----	-----	-----	-----	-----	3	113	128	120.0	1.243	1.503	3	97	
d	C(11B)b- O(11B)b O(12B)b C(1B)b	-----	-----	-----	-----	-----	-----	-----	-----	3	117	125	120.0	1.261	1.495	3	98	
d	C(21A)b- O(21A)b O(22A)b C(2A)b	-----	-----	-----	-----	-----	-----	-----	-----	3	114	127	120.0	1.262	1.489	3	84	
d	C(21B)b- O(21B)b O(22B)b C(2B)b	-----	-----	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.498	3	100	
cR	H(3A)b - C(3A)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	5	
cR	H(3B)b - C(3B)b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	10	
d	Cu(1)c - O(21A)a O(1)c O(11A)c O(12B)c	-----	-----	-----	-----	-----	-----	-----	-----	6	89	145	105.4	1.920	2.159	4	195	

d	Cu(2)c - O(1)	O(1)c	O(11B)c	O(12A)c	O(22A)e	-----	-----	-----	-----	10	84	172	107.8	1.926	2.220	5	197	
d	Na(1)c - O(4W)c	*O(5W)c	O(6W)c	O(22A)c	-----	-----	-----	-----	-----	3	83	143	109.6	2.338	2.420	4	183	
d	O(1)c - Cu(2)	Cu(1)c	Cu(2)c	-----	-----	-----	-----	-----	-----	3	96	121	109.3	1.920	1.964	3	178	
d	O(4W)c - Na(1)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.338	2.338	1	128	
d	*O(5W)c - Na(1)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.345	2.345	2	128	
d	O(6W)c - Na(1)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.420	2.420	1	128	
d	O(11A)c- Cu(1)c	C(11A)c	-----	-----	-----	-----	-----	-----	-----	1	131	131	130.8	1.243	2.023	2	165	
d	O(11B)c- Cu(2)c	C(11B)c	Na(1)e	-----	-----	-----	-----	-----	-----	3	87	152	119.5	1.261	2.418	3	173	
d	O(12A)c- Cu(2)c	C(11A)c	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.0	1.281	1.926	2	172	
d	O(12B)c- Cu(1)c	C(11B)c	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.4	1.282	2.159	2	166	
d	O(21A)c- Cu(1)a	C(21A)c	-----	-----	-----	-----	-----	-----	-----	1	133	133	133.4	1.262	2.030	2	147	
d	O(21B)c- C(21B)c	Cu(1)e	-----	-----	-----	-----	-----	-----	-----	1	123	123	123.2	1.285	1.927	2	154	
d	O(22A)c- Na(1)c	C(21A)c	-----	-----	-----	-----	-----	-----	-----	1	137	137	136.6	1.266	2.398	2	129	
d	O(22B)c- C(21B)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	125	
d	C(1A)c - C(2A)c	C(11A)c	-----	-----	-----	-----	-----	-----	-----	1	122	122	122.1	1.395	1.503	2	63	?
d	C(1B)c - C(2B)c	C(11B)c	-----	-----	-----	-----	-----	-----	-----	1	123	123	123.4	1.404	1.495	2	64	?
d	C(2A)c - C(1A)c	C(3A)c	C(21A)c	-----	-----	-----	-----	-----	-----	3	117	124	120.0	1.395	1.489	3	52	
d	C(2B)c - C(1B)c	C(3B)c	C(21B)c	-----	-----	-----	-----	-----	-----	3	119	120	119.9	1.394	1.498	3	56	
d	C(3A)c - C(2A)c	H(3A)c	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.4	0.950	1.395	2	30	?
d	C(3B)c - C(2B)c	H(3B)c	-----	-----	-----	-----	-----	-----	-----	1	120	120	119.8	0.950	1.394	2	31	?
d	C(11A)c- O(11A)c	O(12A)c	C(1A)c	-----	-----	-----	-----	-----	-----	3	113	128	120.0	1.243	1.503	3	101	
d	C(11B)c- O(11B)c	O(12B)c	C(1B)c	-----	-----	-----	-----	-----	-----	3	117	125	120.0	1.261	1.495	3	102	
d	C(21A)c- O(21A)c	O(22A)c	C(2A)c	-----	-----	-----	-----	-----	-----	3	114	127	120.0	1.262	1.489	3	91	
d	C(21B)c- O(21B)c	O(22B)c	C(2B)c	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.498	3	94	
cR	H(3A)c - C(3A)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	6	
cR	H(3B)c - C(3B)c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	8	
d	Cu(1)d - O(1)d	O(11A)d	O(12B)d	-----	-----	-----	-----	-----	-----	3	89	123	100.9	1.920	2.159	3	187	
d	Cu(2)d - O(1)d	O(11B)d	O(12A)d	-----	-----	-----	-----	-----	-----	3	93	103	97.2	1.926	2.220	3	187	
d	Na(1)d - O(4W)d	*O(5W)d	O(6W)d	O(22A)d	-----	-----	-----	-----	-----	3	83	143	109.6	2.338	2.420	4	180	
d	O(1)d - Cu(1)d	Cu(2)d	-----	-----	-----	-----	-----	-----	-----	1	110	110	110.5	1.920	1.964	2	141	
d	O(4W)d - Na(1)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.338	2.338	1	130	
d	*O(5W)d - Na(1)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.345	2.345	2	130	
d	O(6W)d - Na(1)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.420	2.420	1	130	
d	O(11A)d- Cu(1)d	C(11A)d	-----	-----	-----	-----	-----	-----	-----	1	131	131	130.8	1.243	2.023	2	139	
d	O(11B)d- Cu(2)d	C(11B)d	-----	-----	-----	-----	-----	-----	-----	1	120	120	119.6	1.261	2.220	2	140	
d	O(12A)d- Cu(2)d	C(11A)d	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.0	1.281	1.926	2	139	
d	O(12B)d- Cu(1)d	C(11B)d	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.4	1.282	2.159	2	140	
d	O(21A)d- C(21A)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.262	1.262	1	117	
d	O(21B)d- C(21B)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	115	
d	O(22A)d- Na(1)d	C(21A)d	-----	-----	-----	-----	-----	-----	-----	1	137	137	136.6	1.266	2.398	2	131	
d	O(22B)d- C(21B)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	115	
d	C(1A)d - C(2A)d	C(11A)d	-----	-----	-----	-----	-----	-----	-----	1	122	122	122.1	1.395	1.503	2	48	?
d	C(1B)d - C(3B)	C(2B)d	C(11B)d	-----	-----	-----	-----	-----	-----	3	117	123	120.0	1.404	1.495	3	49	
d	C(2A)d - C(1A)d	C(3A)d	C(21A)d	-----	-----	-----	-----	-----	-----	3	117	124	120.0	1.395	1.489	3	45	
d	C(2B)d - C(1B)d	C(3B)d	C(21B)d	-----	-----	-----	-----	-----	-----	3	119	120	119.9	1.394	1.498	3	44	
d	C(3A)d - C(2A)d	H(3A)d	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.4	0.950	1.395	2	23	?

d	C(3B)d - C(1B)	C(2B)d	H(3B)d	-----	-----	-----	-----	-----	-----	3	120	121	120.0	0.950	1.412	3	40		
d	C(11A)d- O(11A)d	O(12A)d	C(1A)d	-----	-----	-----	-----	-----	-----	3	113	128	120.0	1.243	1.503	3	86		
d	C(11B)d- O(11B)d	O(12B)d	C(1B)d	-----	-----	-----	-----	-----	-----	3	117	125	120.0	1.261	1.495	3	87		
d	C(21A)d- O(21A)d	O(22A)d	C(2A)d	-----	-----	-----	-----	-----	-----	3	114	127	120.0	1.262	1.489	3	83		
d	C(21B)d- O(21B)d	O(22B)d	C(2B)d	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.498	3	76		
cR	H(3A)d - C(3A)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	4		
cR	H(3B)d - C(3B)d	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	14		
d	Cu(1)e - O(21A)	O(21B)c	O(1)e	O(11A)e	O(12B)e	-----	-----	-----	-----	10	87	175	107.5	1.920	2.159	5	192		
d	Cu(2)e - O(1)b	O(1)e	O(11B)e	O(12A)e	-----	-----	-----	-----	-----	6	84	168	106.5	1.926	2.220	4	193		
d	Na(1)e - O(11B)c	O(4W)e	*O(5W)e	O(6W)e	O(22A)e	-----	-----	-----	-----	6	71	164	109.5	2.338	2.420	5	185		
d	O(1)e - Cu(2)b	Cu(1)e	Cu(2)e	-----	-----	-----	-----	-----	-----	3	96	121	109.3	1.920	1.964	3	164		
d	O(4W)e - Na(1)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.338	2.338	1	137		
d	*O(5W)e - Na(1)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.345	2.345	2	137		
d	O(6W)e - Na(1)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.420	2.420	1	137		
d	O(11A)e- Cu(1)e	C(11A)e	-----	-----	-----	-----	-----	-----	-----	1	131	131	130.8	1.243	2.023	2	156		
d	O(11B)e- Cu(2)e	C(11B)e	-----	-----	-----	-----	-----	-----	-----	1	120	120	119.6	1.261	2.220	2	158		
d	O(12A)e- Cu(2)e	C(11A)e	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.0	1.281	1.926	2	159		
d	O(12B)e- Cu(1)e	C(11B)e	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.4	1.282	2.159	2	155		
d	O(21A)e- Cu(1)	C(21A)e	-----	-----	-----	-----	-----	-----	-----	1	133	133	133.4	1.262	2.030	2	169		
d	O(21B)e- C(21B)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	113		
d	O(22A)e- Cu(2)c	Na(1)e	C(21A)e	-----	-----	-----	-----	-----	-----	3	94	137	119.6	1.266	2.398	3	174		
d	O(22B)e- C(21B)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	113		
d	C(1A)e - C(2A)e	C(11A)e	-----	-----	-----	-----	-----	-----	-----	1	122	122	122.1	1.395	1.503	2	58		?
d	C(1B)e - C(2B)e	C(11B)e	-----	-----	-----	-----	-----	-----	-----	1	123	123	123.4	1.404	1.495	2	57		?
d	C(2A)e - C(1A)e	C(3A)e	C(21A)e	-----	-----	-----	-----	-----	-----	3	117	124	120.0	1.395	1.489	3	65		
d	C(2B)e - C(1B)e	C(3B)e	C(21B)e	-----	-----	-----	-----	-----	-----	3	119	120	119.9	1.394	1.498	3	43		
d	C(3A)e - C(2A)e	H(3A)e	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.4	0.950	1.395	2	35		?
d	C(3B)e - C(2B)e	H(3B)e	-----	-----	-----	-----	-----	-----	-----	1	120	120	119.8	0.950	1.394	2	21		?
d	C(11A)e- O(11A)e	O(12A)e	C(1A)e	-----	-----	-----	-----	-----	-----	3	113	128	120.0	1.243	1.503	3	95		
d	C(11B)e- O(11B)e	O(12B)e	C(1B)e	-----	-----	-----	-----	-----	-----	3	117	125	120.0	1.261	1.495	3	96		
d	C(21A)e- O(21A)e	O(22A)e	C(2A)e	-----	-----	-----	-----	-----	-----	3	114	127	120.0	1.262	1.489	3	103		
d	C(21B)e- O(21B)e	O(22B)e	C(2B)e	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.498	3	74		
cR	H(3A)e - C(3A)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	11		
cR	H(3B)e - C(3B)e	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	3		
d	Cu(1)f - O(1)f	O(11A)f	O(12B)f	-----	-----	-----	-----	-----	-----	3	89	123	100.9	1.920	2.159	3	188		
d	Cu(2)f - O(1)f	O(11B)f	O(12A)f	-----	-----	-----	-----	-----	-----	3	93	103	97.2	1.926	2.220	3	188		
d	Na(1)f - O(4W)f	*O(5W)f	O(6W)f	O(22A)f	-----	-----	-----	-----	-----	3	83	143	109.6	2.338	2.420	4	182		
d	O(1)f - Cu(1)f	Cu(2)f	-----	-----	-----	-----	-----	-----	-----	1	110	110	110.5	1.920	1.964	2	144		
d	O(4W)f - Na(1)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.338	2.338	1	134		
d	*O(5W)f - Na(1)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.345	2.345	2	134		
d	O(6W)f - Na(1)f	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	2.420	2.420	1	134		
d	O(11A)f- Cu(1)f	C(11A)f	-----	-----	-----	-----	-----	-----	-----	1	131	131	130.8	1.243	2.023	2	143		
d	O(11B)f- Cu(2)f	C(11B)f	-----	-----	-----	-----	-----	-----	-----	1	120	120	119.6	1.261	2.220	2	142		
d	O(12A)f- Cu(2)f	C(11A)f	-----	-----	-----	-----	-----	-----	-----	1	128	128	128.0	1.281	1.926	2	143		

d	O(12B)f- Cu(1)f	C(11B)f	-----	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.4	1.282	2.159	2	142						
d	O(21A)f- C(21A)f	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.262	1.262	1	121						
d	O(21B)f- C(21B)f	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.285	1.285	1	109						
d	O(22A)f- Na(1)f	C(21A)f	-----	-----	-----	-----	-----	-----	-----	-----	1	137	137	136.6	1.266	2.398	2	135						
d	O(22B)f- C(21B)f	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	109						
d	C(1A)f - C(3A)	C(2A)f	C(11A)f	-----	-----	-----	-----	-----	-----	-----	3	118	122	120.0	1.394	1.503	3	51						
d	C(1B)f - C(2B)f	C(11B)f	-----	-----	-----	-----	-----	-----	-----	-----	1	123	123	123.4	1.404	1.495	2	50					?	
d	C(2A)f - C(1A)f	C(3A)f	C(21A)f	-----	-----	-----	-----	-----	-----	-----	3	117	124	120.0	1.395	1.489	3	47						
d	C(2B)f - C(1B)f	C(3B)f	C(21B)f	-----	-----	-----	-----	-----	-----	-----	3	119	120	119.9	1.394	1.498	3	41						
d	C(3A)f - C(1A)	C(2A)f	H(3A)f	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.395	3	37						
d	C(3B)f - C(2B)f	H(3B)f	-----	-----	-----	-----	-----	-----	-----	-----	1	120	120	119.8	0.950	1.394	2	19					?	
d	C(11A)f- O(11A)f	O(12A)f	C(1A)f	-----	-----	-----	-----	-----	-----	-----	3	113	128	120.0	1.243	1.503	3	89						
d	C(11B)f- O(11B)f	O(12B)f	C(1B)f	-----	-----	-----	-----	-----	-----	-----	3	117	125	120.0	1.261	1.495	3	88						
d	C(21A)f- O(21A)f	O(22A)f	C(2A)f	-----	-----	-----	-----	-----	-----	-----	3	114	127	120.0	1.262	1.489	3	85						
d	C(21B)f- O(21B)f	O(22B)f	C(2B)f	-----	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.498	3	70						
=====																								
cR	H(3A)f - C(3A)f	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	12						
cR	H(3B)f - C(3B)f	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	1						

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 ***** Residue = 2 *****
 =====

														=A.N.G.L.E.S=			=B.O.N.D.S=					
Flag	Label	-	Connected to	(May be Incomplete for Polymeric Structures)					nra	min	max	Aver	min	max	nrb	tnr	Hyb	RS	Note			

d	O(1W)	-	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.000	0.000	0	107			V			

=====

 =====
 ***** Residue = 3 *****
 =====

		=A.N.G.L.E.S=			=B.O.N.D.S=								
Flag	Label	-	Connected to	(May be Incomplete for Polymeric Structures)	nra	min	max	Aver	min	max	nrb	tnr	Hyb RS Note
d	>O(2W)	-	-----	-----	0	0	0	0.0	0.000	0.000	0	107	

=====

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=====
***** Residue = 4 *****
=====

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		=A.N.G.L.E.S=			=B.O.N.D.S=								
Flag	Label	-	Connected to	(May be Incomplete for Polymeric Structures)	nra	min	max	Aver	min	max	nrb	tnr	Hyb RS Note
d	>O(3W)	-	-----	-----	-----	-----	-----	0	0	0	0.0	0.000	0.000 0 107

```

=====
*****
Residue = 5 *****
=====

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Flag	Label	- Connected to	(May be Incomplete for Polymeric Structures)	=A.N.G.L.E.S=			=B.O.N.D.S=			nr	tnr	Hyb	RS	Note
				nra	min	max	Aver	min	max					
d	O(7W)	-	-----	0	0	0	0.0	0.000	0.000	0	107			V

 =====
 ***** Residue = 6 *****
 =====

Flag Label - Connected to (May be Incomplete for Polymeric Structures) =A.N.G.L.E.S= =B.O.N.D.S=
 ----- nra min max Aver min max nrb tnr Hyb RS Note -----

Disordered Atoms with S.O.F < 0.5

d <0(8W) - ----- 0 0 0 0.0 0.000 0.000 0 107

Asymmetric Residue Unit (= ARU) Code List
 =====

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)	
a =[1455.01]	= -1+x,y,z	= [	1	-1	0	0	1	-1.003	0.007	0.020
b =[1655.01]	= 1+x,y,z	= [	1	1	0	0	1	0.997	0.007	0.020
c =[2555.01]	= -x,-y,-z	= [	2	0	0	0	1	0.003	-0.007	-0.020
d =[2556.01]	= -x,-y,1-z	= [	2	0	0	1	1	0.003	-0.007	0.980
e =[2655.01]	= 1-x,-y,-z	= [	2	1	0	0	1	1.003	-0.007	-0.020
f =[2665.01]	= 1-x,1-y,-z	= [	2	1	1	0	1	1.003	0.993	-0.020

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

=====

Analysis of the IntraMolecular Geometry in Terms of Unique Molecule(s)/Ions, with Bond Criterium: d(i-j) < R(i) + R(j) + Tol

- Tol = 0.40 Ang. for Normal Bonds + 0.70 for (Earth)alkali-NonMetal Contacts and adjusted by -.40 Ang. for Metal-Metal Distances
- Disordered Atoms are Indicated with > or < Attached to the Atom Label, indicating Major and Minor Form Respectively
- The Bond Distance and Angle su's have been Incremented to Include the Effect of the Unit-cell su.
(Rel.Error in Dist. 0.0000 Ang. , Abs. Angle Error 0.001 Deg.)
- Bonds below with '>' or '<' Substituted for '-' have Distances that Deviate from Expected Values(Based on the hybridisations).
-

=====

***** Residue = 1 *****

=====

Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

=====

Cu(1) - O(1)	1.920(6)	Cu(1) - O(11A)	2.023(5)	Cu(1) - O(12B)	2.159(6)	Cu(1) - O(21B)b	1.927(6)
Cu(1) - O(21A)e	2.030(5)	Cu(2) - O(1)	1.964(6)	Cu(2) - O(11B)	2.220(6)	Cu(2) - O(12A)	1.927(6)
Cu(2) - O(22A)a	1.936(6)	Cu(2) - O(1)c	1.942(6)	Na(1) - O(4W)	2.339(12)	Na(1) - *O(5W)	2.35(4)
Na(1) - O(6W)	2.42(2)	Na(1) - O(22A)	2.398(8)	Na(1) - O(11B)b	2.418(8)	O(11A) - C(11A)	1.243(9)
O(11B) - C(11B)	1.261(10)	O(12A) - C(11A)	1.281(10)	O(12B) - C(11B)	1.282(10)	O(21A) - C(21A)	1.262(9)
O(21B) - C(21B)	1.285(11)	O(22A) - C(21A)	1.266(10)	O(22B) - C(21B)	1.242(10)	C(1A) - C(2A)	1.395(11)
C(1A) > C(11A)	1.503(11)	C(1A) - C(3A)f	1.394(11)	C(1B) - C(2B)	1.404(13)	C(1B) > C(11B)	1.495(11)
C(1B) - C(3B)d	1.412(11)	C(2A) - C(3A)	1.395(11)	C(2A) > C(21A)	1.489(11)	C(2B) - C(3B)	1.394(12)
C(2B) > C(21B)	1.498(11)						
C(3A) - H(3A)	0.95	C(3B) - H(3B)	0.95				

Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().

=====

O(1) - Cu(1) - O(11A)	88.8(2)	O(1) - Cu(1) - O(12B)	91.3(2)	O(1) - Cu(1) - O(21B)b	174.6(2)
O(1) - Cu(1) - O(21A)e	92.0(2)	O(11A) - Cu(1) - O(12B)	122.7(2)	O(11A) - Cu(1) - O(21B)b	87.3(2)
O(11A) - Cu(1) - O(21A)e	145.0(2)	O(12B) - Cu(1) - O(21B)b	87.7(2)	O(12B) - Cu(1) - O(21A)e	92.3(2)
O(21B)b - Cu(1) - O(21A)e	93.3(2)	O(1) - Cu(2) - O(11B)	102.5(2)	O(1) - Cu(2) - O(12A)	92.9(2)
O(1) - Cu(2) - O(22A)a	172.5(2)	O(1) - Cu(2) - O(1)c	83.6(2)	O(11B) - Cu(2) - O(12A)	96.0(3)
O(11B) - Cu(2) - O(22A)a	84.9(2)	O(11B) - Cu(2) - O(1)c	96.0(2)	O(12A) - Cu(2) - O(22A)a	87.5(2)
O(12A) - Cu(2) - O(1)c	167.9(3)	O(22A)a - Cu(2) - O(1)c	94.4(2)	O(4W) - Na(1) - *O(5W)	90.9(6)
O(4W) - Na(1) - O(6W)	82.8(5)	O(4W) - Na(1) - O(22A)	103.2(4)	O(4W) - Na(1) - O(11B)b	163.9(4)
*O(5W) - Na(1) - O(6W)	110.3(9)	*O(5W) - Na(1) - O(22A)	106.2(8)	*O(5W) - Na(1) - O(11B)b	105.1(6)
O(6W) - Na(1) - O(22A)	142.9(6)	O(6W) - Na(1) - O(11B)b	92.7(5)	O(22A) - Na(1) - O(11B)b	71.5(2)
Cu(1) - O(1) - Cu(2)	110.5(3)	Cu(1) - O(1) - Cu(2)c	120.9(3)	Cu(2) - O(1) - Cu(2)c	96.4(3)
Cu(1) - O(11A) - C(11A)	130.8(5)	Cu(2) - O(11B) - C(11B)	119.6(5)	Cu(2) - O(11B) - Na(1)a	86.7(2)
C(11B) - O(11B) - Na(1)a	152.3(5)	Cu(2) - O(12A) - C(11A)	128.0(5)	Cu(1) - O(12B) - C(11B)	124.4(5)
C(21A) - O(21A) - Cu(1)e	133.4(5)	C(21B) - O(21B) - Cu(1)a	123.2(5)	Na(1) - O(22A) - C(21A)	136.6(5)
Na(1) - O(22A) - Cu(2)b	94.1(3)	C(21A) - O(22A) - Cu(2)b	128.0(5)	C(2A) - C(1A) - C(11A)	122.1(7)
C(2A) - C(1A) - C(3A)f	119.9(7)	C(11A) - C(1A) - C(3A)f	118.1(7)	C(2B) - C(1B) - C(11B)	123.4(7)
C(2B) - C(1B) - C(3B)d	119.0(7)	C(11B) - C(1B) - C(3B)d	117.5(8)	C(1A) - C(2A) - C(3A)	118.9(7)
C(1A) - C(2A) - C(21A)	124.1(7)	C(3A) - C(2A) - C(21A)	117.0(7)	C(1B) - C(2B) - C(3B)	120.4(8)
C(1B) - C(2B) - C(21B)	120.1(7)	C(3B) - C(2B) - C(21B)	119.3(8)	C(2A) - C(3A) - C(1A)f	121.2(7)

C(2B) - C(3B) - C(1B)d	120.6(8)	0(11A) - C(11A) - 0(12A)	127.6(7)	0(11A) - C(11A) - C(1A)	118.9(7)
0(12A) - C(11A) - C(1A)	113.5(7)	0(11B) - C(11B) - 0(12B)	124.5(7)	0(11B) - C(11B) - C(1B)	118.6(7)
0(12B) - C(11B) - C(1B)	116.8(7)	0(21A) - C(21A) - 0(22A)	127.5(7)	0(21A) - C(21A) - C(2A)	118.4(7)
0(22A) - C(21A) - C(2A)	114.1(7)	0(21B) - C(21B) - 0(22B)	126.2(8)	0(21B) - C(21B) - C(2B)	115.7(7)
0(22B) - C(21B) - C(2B)	118.1(8)				

C(2A) - C(3A) - H(3A)	119	H(3A) - C(3A) - C(1A)f	119	C(2B) - C(3B) - H(3B)	120
H(3B) - C(3B) - C(1B)d	120				

Torsion/Dihedral Angles (Deg.) - Klyne & Prelog Convention (Dunitz, p241) - (Excl. Minor Disorder & Embedded Bond Angl. > 160. Deg.)

0(11A) Cu(1) 0(1) Cu(2)	-63.5(3)	0(11A) Cu(1) 0(1) Cu(2)c	-174.8(3)	0(12B) Cu(1) 0(1) Cu(2)	59.2(3)
0(12B) Cu(1) 0(1) Cu(2)c	-52.1(3)	0(21A)eCu(1) 0(1) Cu(2)	151.5(3)	0(21A)eCu(1) 0(1) Cu(2)c	40.3(3)
0(1) Cu(1) 0(11A) C(11A)	28.4(7)	0(12B) Cu(1) 0(11A) C(11A)	-62.4(7)	0(21B)bCu(1) 0(11A) C(11A)	-147.9(7)
0(21A)eCu(1) 0(11A) C(11A)	120.3(7)	0(1) Cu(1) 0(12B) C(11B)	-67.3(6)	0(11A) Cu(1) 0(12B) C(11B)	22.2(7)
0(21B)bCu(1) 0(12B) C(11B)	107.5(6)	0(21A)eCu(1) 0(12B) C(11B)	-159.3(6)	0(11A) Cu(1) 0(21B)bC(21B)b	-94.9(6)
0(12B) Cu(1) 0(21B)bC(21B)b	142.2(6)	0(1) Cu(1) 0(21A)eC(21A)e	1.0(7)	0(11A) Cu(1) 0(21A)eC(21A)e	-89.9(8)
0(12B) Cu(1) 0(21A)eC(21A)e	92.3(7)	0(11B) Cu(2) 0(1) Cu(1)	-31.7(3)	0(11B) Cu(2) 0(1) Cu(2)c	94.7(3)
0(12A) Cu(2) 0(1) Cu(1)	65.2(3)	0(12A) Cu(2) 0(1) Cu(2)c	-168.4(3)	0(1)c Cu(2) 0(1) Cu(1)	-126.4(3)
0(1)c Cu(2) 0(1) Cu(2)c	0.0(2)	0(1) Cu(2) 0(11B) C(11B)	-26.3(7)	0(1) Cu(2) 0(11B) Na(1)a	144.4(3)
0(12A) Cu(2) 0(11B) C(11B)	-120.7(6)	0(12A) Cu(2) 0(11B) Na(1)a	50.0(3)	0(22A)aCu(2) 0(11B) C(11B)	152.4(6)
0(22A)aCu(2) 0(11B) Na(1)a	-37.0(3)	0(1)c Cu(2) 0(11B) C(11B)	58.5(6)	0(1)c Cu(2) 0(11B) Na(1)a	-130.9(3)
0(1) Cu(2) 0(12A) C(11A)	-25.3(7)	0(11B) Cu(2) 0(12A) C(11A)	77.7(7)	0(22A)aCu(2) 0(12A) C(11A)	162.3(7)
0(11B) Cu(2) 0(22A)aNa(1)a	37.4(3)	0(11B) Cu(2) 0(22A)aC(21A)a	-131.1(7)	0(12A) Cu(2) 0(22A)aNa(1)a	-58.9(3)
0(12A) Cu(2) 0(22A)aC(21A)a	132.6(7)	0(1) Cu(2) 0(1)c Cu(1)c	-118.5(3)	0(1) Cu(2) 0(1)c Cu(2)c	0.0(2)
0(11B) Cu(2) 0(1)c Cu(1)c	139.5(3)	0(11B) Cu(2) 0(1)c Cu(2)c	-102.0(2)	0(4W) Na(1) 0(22A) C(21A)	-64.9(8)
0(4W) Na(1) 0(22A) Cu(2)b	128.4(4)	0(5W) Na(1) 0(22A) C(21A)	30.0(10)	0(5W) Na(1) 0(22A) Cu(2)b	-136.7(6)
0(6W) Na(1) 0(22A) C(21A)	-160.4(10)	0(6W) Na(1) 0(22A) Cu(2)b	32.9(9)	0(11B)bNa(1) 0(22A) C(21A)	130.9(8)
0(11B)bNa(1) 0(22A) Cu(2)b	-35.8(2)	0(5W) Na(1) 0(11B)bCu(2)b	133.0(8)	0(5W) Na(1) 0(11B)bC(11B)b	-64.6(15)
0(6W) Na(1) 0(11B)bCu(2)b	-115.1(6)	0(6W) Na(1) 0(11B)bC(11B)b	47.3(14)	0(22A) Na(1) 0(11B)bCu(2)b	30.7(2)
0(22A) Na(1) 0(11B)bC(11B)b	-167.0(13)	Cu(1) 0(11A) C(11A) 0(12A)	10.6(13)	Cu(1) 0(11A) C(11A) C(1A)	-171.4(5)
Cu(2) 0(11B) C(11B) 0(12B)	35.4(11)	Cu(2) 0(11B) C(11B) C(1B)	-148.0(6)	Na(1)a 0(11B) C(11B) 0(12B)	-124.3(11)
Na(1)a 0(11B) C(11B) C(1B)	52.3(16)	Cu(2) 0(12A) C(11A) 0(11A)	-12.0(13)	Cu(2) 0(12A) C(11A) C(1A)	169.9(5)
Cu(1) 0(12B) C(11B) 0(11B)	15.0(11)	Cu(1) 0(12B) C(11B) C(1B)	-161.7(5)	Cu(1)e 0(21A) C(21A) 0(22A)	22.1(13)
Cu(1)e 0(21A) C(21A) C(2A)	-161.8(5)	Cu(1)a 0(21B) C(21B) 0(22B)	0.0(12)	Cu(1)a 0(21B) C(21B) C(2B)	-179.4(5)
Na(1) 0(22A) C(21A) 0(21A)	-161.3(6)	Na(1) 0(22A) C(21A) C(2A)	22.5(11)	Cu(2)b 0(22A) C(21A) 0(21A)	1.8(12)
Cu(2)b 0(22A) C(21A) C(2A)	-174.4(5)	C(11A) C(1A) C(2A) C(3A)	-179.1(7)	C(11A) C(1A) C(2A) C(21A)	3.6(12)
C(3A)f C(1A) C(2A) C(3A)	0.9(12)	C(3A)f C(1A) C(2A) C(21A)	-176.4(7)	C(2A) C(1A) C(11A) 0(11A)	33.4(11)
C(2A) C(1A) C(11A) 0(12A)	-148.3(8)	C(3A)f C(1A) C(11A) 0(11A)	-146.6(8)	C(3A)f C(1A) C(11A) 0(12A)	31.8(10)
C(2A) C(1A) C(3A)f C(2A)f	-0.9(12)	C(11A) C(1A) C(3A)f C(2A)f	179.1(7)	C(11B) C(1B) C(2B) C(3B)	-175.7(8)
C(11B) C(1B) C(2B) C(21B)	9.6(13)	C(3B)d C(1B) C(2B) C(3B)	0.4(13)	C(3B)d C(1B) C(2B) C(21B)	-174.2(8)
C(2B) C(1B) C(11B) 0(11B)	61.9(12)	C(2B) C(1B) C(11B) 0(12B)	-121.2(9)	C(3B)d C(1B) C(11B) 0(11B)	-114.3(9)
C(3B)d C(1B) C(11B) 0(12B)	62.6(11)	C(2B) C(1B) C(3B)d C(2B)d	-0.4(14)	C(11B) C(1B) C(3B)d C(2B)d	176.0(8)
C(1A) C(2A) C(3A) C(1A)f	-0.9(12)	C(21A) C(2A) C(3A) C(1A)f	176.6(7)	C(1A) C(2A) C(21A) 0(21A)	61.2(11)
C(1A) C(2A) C(21A) 0(22A)	-122.2(9)	C(3A) C(2A) C(21A) 0(21A)	-116.2(8)	C(3A) C(2A) C(21A) 0(22A)	60.5(10)
C(1B) C(2B) C(3B) C(1B)d	-0.5(14)	C(21B) C(2B) C(3B) C(1B)d	174.2(8)	C(1B) C(2B) C(21B) 0(21B)	-148.6(8)
C(1B) C(2B) C(21B) 0(22B)	32.0(12)	C(3B) C(2B) C(21B) 0(21B)	36.8(11)	C(3B) C(2B) C(21B) 0(22B)	-142.7(9)

C(2A)	C(1A)	C(3A)f	H(3A)f	179	C(11A)	C(1A)	C(3A)f	H(3A)f	-1	C(2B)	C(1B)	C(3B)d	H(3B)d	179
C(11B)	C(1B)	C(3B)d	H(3B)d	-4	C(1A)	C(2A)	C(3A)	H(3A)	179	C(21A)	C(2A)	C(3A)	H(3A)	-3
C(1B)	C(2B)	C(3B)	H(3B)	179	C(21B)	C(2B)	C(3B)	H(3B)	-6					

[illegible]

Selected Bond Lengths (Angstrom) - see M.F.C. Ladd & R.A. Palmer, Structure Determination by X-Ray Crystallography (1985)

Formal single bonds

C4-C4	1.54	C4-C3	1.52	C4-C2	1.46	C4-N3	1.47	C4-N2	1.47	C4-O2	1.43	C3-C3	1.46	C3-C2	1.45	C3-N3	1.40	C3-N2	1.40
C3-O2	1.36	C2-C2	1.38	C2-N3	1.33	C2-N2	1.33	C2-O2	1.36	N3-N3	1.45	N3-N2	1.45	N3-O2	1.36	N2-N2	1.45	N2-O2	1.41

Formal double bonds

C3-C3 1.34 C3-C2 1.31 C3-N2 1.32 C3-O1 1.22 C2-C2 1.28 C2-N2 1.32 C2-O1 1.16 N3-O1 1.24 N2-N2 1.25 N2-O1 1.21

Formal triple bonds

Aromatic bonds

C2-C2 1.20 C2-N1 1.16 C3-C3 1.40 C2-N2 1.34 N2-N2 1.35

The notation in the table indicates the connectivity of the atoms

For more detailed standard bond distance tabulations see: J. Chem. Soc. Perkin II, (1987), S1-S19; J. Chem. Soc. Dalton Trans. (1989), S1 - S83 or International Tables C, (1992), 707-791.

Automatic Search for Rings (3 to 6-Membered) and Planes Determined by 4 or More Connected Atoms (with Deviation < 0.10 Ang.)

Least-Squares Planes - $P*X+Q*Y+R*Z=S$:: First Line Orthogonal(X0,Y0,Z0), Second Line Fractional(X,Y,Z)
 Ring/Plan/Resd/Lspl N Indicates that the Ring/Plane/Residue Involves N Atoms
 Sigref - R.M.S-Error of the Contributing Atoms
 Sigpln - $\text{Sqrt}(\text{Sum}(j=1:N)(D(j)**2)/(N-3))$
 Chisq - Chi-Squared = $\text{Sum}(j=1:N)(D(j)**2)/\text{Sigref}**2$
 Pl.Hyp. - Result of the Chi.Sq. Test for Planarity (See Stout & Jensen, p424)

Calculated via Substitution in

$D = P*X + Q*Y + R*Z - S$ (2nd Line)

**** - Atoms Deviating by More Than 1.5 Angstrom and Hydrogen Atoms are NOT Listed
 Note - Weights : UNIT
 **** - Maximum Metal Containing Ring Size: 6
 - Maximum Number of Bonds to Ring Metal: 6
 - Deviations from planes are in Angstrom Units
 - The Plane determining Atoms have been Marked #

Nr	1	P	Q	R	S	Sigref	0.004	Sigpln	0.000	Chisq	0.0	Pl.Hyp.
Ring		-0.024(3)	-0.2433(4)	0.9697(2)	0.000(2)	#Cu(2)	0.000(1)	#O(1)	0.000(6)	#Cu(2)c	0.000(1)	#O(1)c 0.000(6)
A 4		-0.19(2)	-2.561(5)	11.093(10)	0.000(2)	Cu(1)	1.448(1)	Na(1)	1.296(6)	O(4W)	0.233(11)	O(11A) 0.596(6)
						O(12A)	-0.386(7)	O(22A)	-0.433(6)	C(1A)	-0.783(8)	C(2A) -1.197(8)
						C(11A)	-0.131(8)	C(21A)	-1.114(8)	Cu(2)a	0.187(1)	Na(1)a 1.483(6)
						O(1)a	0.187(6)	O(4W)a	0.420(11)	O(11A)	0.783(6)	O(12A) -0.199(7)
						O(22A)	-0.246(6)	C(1A)a	-0.596(8)	C(2A)a	-1.010(8)	C(11A) 0.056(8)
						C(21A)	-0.927(8)	Cu(1)b	1.261(1)	Cu(2)b	-0.187(1)	Na(1)b 1.109(6)
						O(1)b	-0.187(6)	O(4W)b	0.046(11)	O(11A)	0.409(6)	O(12A) -0.573(7)
						O(22A)	-0.620(6)	C(1A)b	-0.970(8)	C(2A)b	-1.384(8)	C(11A) -0.318(8)
						C(21A)	-1.301(8)	Cu(1)c	-1.448(1)	Na(1)c	-1.296(6)	O(4W)c -0.233(11)
						O(11A)	-0.596(6)	O(12A)	0.386(7)	O(22A)	0.433(6)	C(1A)c 0.783(8)
						C(2A)c	1.197(8)	C(11A)	0.131(8)	C(21A)	1.114(8)	Cu(2)e -0.187(1)
						Na(1)e	-1.483(6)	O(1)e	-0.187(6)	O(4W)e	-0.420(11)	O(11A) -0.783(6)
						O(12A)	0.199(7)	O(22A)	0.246(6)	C(1A)e	0.596(8)	C(2A)e 1.010(8)
						C(11A)	-0.056(8)	C(21A)	0.927(8)	O(21A)	-0.988(6)	C(3A)f -0.971(8)

Nr	2	P	Q	R	S	Sigref	0.005	Sigpln	0.511	Chisq	26949.8	Pl.Hyp.	P<5
Ring		0.5426(15)	0.7998(10)	0.257(2)	1.162(3)	#Cu(1)	0.557(1)	#Cu(2)	0.011(1)	#O(1)	-0.404(5)	#O(11B)	0.377(6)
A 6		4.255(12)	8.326(10)	0.76(2)	1.162(3)	#O(12B)	-0.373(6)	#C(11B)	-0.168(8)	C(1B)	-0.542(9)	C(2B)	-1.470(9)
						O(21A)	-1.445(5)	O(22A)	0.341(5)	C(1A)a	-0.364(8)	C(2A)a	0.252(8)
						C(3A)a	1.493(8)	C(21A)	-0.357(8)	O(21B)	0.299(5)	O(22B)	0.299(7)
						C(2B)c	-0.853(9)	C(3B)c	-0.616(9)	C(21B)	-0.022(9)	O(1)d	-1.164(5)
						O(12B)	-1.194(6)	O(21B)	1.055(5)	O(22B)	1.055(7)	C(1B)d	-1.026(9)
						C(2B)d	-0.097(9)	C(3B)d	0.140(9)	C(11B)	-1.400(8)	C(21B)	0.734(9)
						Cu(1)e	1.374(1)	O(11A)	-0.355(5)	O(12A)	0.076(6)	O(21A)	-0.878(5)
						C(11A)	-0.633(8)						

Nr	3	P	Q	R	S	Sigref	0.005	Sigpln	0.454	Chisq	23314.3	Pl.Hyp.	P<5
Ring		-0.3610(16)	0.103(2)	0.9268(6)	0.157(5)	#Cu(1)	0.369(1)	#Cu(2)	0.345(1)	#O(1)	-0.580(6)	#O(11A)	0.004(6)
A	6	-2.831(12)	1.16(2)	11.487(8)	0.157(5)	#O(12A)	0.029(7)	#C(11A)	-0.167(8)	Na(1)	-0.081(6)	O(4W)	-0.389(11)
						O(6W)	0.43(2)	C(1A)	-0.617(8)	C(2A)	-1.468(8)	O(21A)	-0.008(6)
						O(22A)	1.032(6)	C(2A)a	1.363(8)	C(3A)a	1.003(8)	C(21A)	0.756(8)
						O(5W)b	-0.98(3)	O(11B)	-0.356(6)	O(12B)	-0.690(6)	O(21B)	1.402(6)
						O(22B)	-0.243(6)	C(1B)b	1.407(8)	C(11B)	0.018(8)	C(21B)	0.920(8)
						Cu(1)c	-0.683(1)	Cu(2)c	-0.660(1)	Na(1)c	-0.233(6)	O(1)c	0.265(6)
						O(4W)c	0.074(11)	O(6W)c	-0.75(2)	O(11A)	-0.318(6)	O(12A)	-0.344(7)
						O(22A)	1.485(6)	C(1A)c	0.302(8)	C(2A)c	1.153(8)	C(11A)	-0.148(8)
						O(21A)	-0.306(6)	O(22A)	-1.347(6)	C(3A)e	-1.318(8)	C(21A)	-1.071(8)
						O(1)f	-1.406(6)	O(21A)	0.854(6)	O(22A)	-0.187(6)	C(1A)f	-1.369(8)
						C(2A)f	-0.518(8)	C(3A)f	-0.157(8)	C(21A)	0.089(8)		
Nr	4	P	Q	R	S	Sigref	0.005	Sigpln	0.341	Chisq	13570.3	Pl.Hyp.	P<5
Ring		-0.5585(13)	-0.2541(19)	0.7897(8)	-0.316(4)	#Cu(1)	0.152(1)	#O(1)	-0.388(6)	#Cu(2)c	0.349(1)	#O(21A)	0.144(6)
A	6	-4.380(10)	-2.57(2)	10.756(10)	-0.316(4)	#O(22A)	-0.127(6)	#C(21A)	-0.131(8)	Cu(2)	0.283(1)	O(5W)	-0.69(3)
						O(11A)	-0.952(6)	O(12A)	-0.800(6)	C(11A)	-1.263(8)	O(4W)a	0.614(11)
						O(6W)a	1.47(2)	O(21A)	0.488(6)	O(22A)	0.759(6)	C(2A)a	1.058(8)
						C(3A)a	0.178(8)	C(21A)	0.764(8)	O(21B)	0.720(6)	O(22B)	-0.820(6)
						C(1B)b	-0.084(8)	C(2B)b	0.738(8)	C(21B)	0.150(8)	Cu(1)c	0.481(1)
						O(1)c	1.020(6)	O(5W)c	1.32(3)	O(12A)	1.433(6)	Na(1)e	-1.061(6)
						O(4W)e	0.019(11)	O(6W)e	-0.84(2)	C(1A)e	-1.483(8)	C(2A)e	-0.426(8)
						C(3A)e	0.454(8)						
Nr	5	P	Q	R	S	Sigref	0.005	Sigpln	0.341	Chisq	13570.3	Pl.Hyp.	P<5
Ring		-0.5585(13)	-0.2541(19)	0.7897(8)	0.316(4)	#Cu(2)	-0.349(1)	#O(21A)	-0.144(6)	#O(22A)	0.127(6)	#C(21A)	0.131(8)
A	6	-4.380(10)	-2.57(2)	10.756(10)	0.316(4)	#Cu(1)c	-0.152(1)	#O(1)c	0.388(6)	Cu(1)	-0.481(1)	O(1)	-1.020(6)
						O(5W)	-1.32(3)	O(12A)	-1.433(6)	Na(1)a	1.061(6)	O(4W)a	-0.019(11)
						O(6W)a	0.84(2)	C(1A)a	1.483(8)	C(2A)a	0.426(8)	C(3A)a	-0.454(8)
						O(21B)	0.088(6)	O(22B)	-1.453(6)	C(1B)b	-0.716(8)	C(2B)b	0.105(8)
						C(3B)b	1.486(8)	C(21B)	-0.483(8)	Cu(2)c	-0.283(1)	O(5W)c	0.69(3)
						O(11A)	0.952(6)	O(12A)	0.800(6)	C(11A)	1.263(8)	O(4W)e	-0.614(11)
						O(6W)e	-1.47(2)	O(21A)	-0.488(6)	O(22A)	-0.759(6)	C(2A)e	-1.058(8)
						C(3A)e	-0.178(8)	C(21A)	-0.764(8)				
Nr	6	P	Q	R	S	Sigref	0.005	Sigpln	0.341	Chisq	13570.3	Pl.Hyp.	P<5
Ring		-0.5585(13)	-0.2541(19)	0.7897(8)	-4.064(7)	#O(21A)	-0.144(6)	#O(22A)	0.127(6)	#C(21A)	0.131(8)	#Cu(2)b	-0.349(1)
A	6	-4.380(10)	-2.57(2)	10.756(10)	-4.064(7)	#Cu(1)e	-0.152(1)	#O(1)e	0.388(6)	Na(1)	1.061(6)	O(4W)	-0.019(11)
						O(6W)	0.84(2)	C(1A)	1.483(8)	C(2A)	0.426(8)	C(3A)	-0.454(8)
						Cu(1)b	-0.481(1)	O(1)b	-1.020(6)	O(5W)b	-1.32(3)	O(12A)	-1.433(6)
						O(21B)	-0.720(6)	O(22B)	0.820(6)	C(1B)c	0.084(8)	C(2B)c	-0.738(8)
						C(21B)	-0.150(8)	Cu(2)e	-0.283(1)	O(5W)e	0.69(3)	O(11A)	0.952(6)

=====												
						O(12A)	0.800(6)	C(11A)	1.263(8)	Na(1)f	0.118(6)	O(4W)f 1.198(11)
						O(6W)f	0.34(2)	O(21A)	1.323(6)	O(22A)	1.052(6)	C(1A)f -0.304(8)
						C(2A)f	0.753(8)	C(11A)	-1.306(8)	C(21A)	1.047(8)	

Nr	7	P	Q	R	S	Sigref	0.008	Sigpln	0.005	Chisq	1.5	Pl.Hyp.

Ring		0.280(3)	0.080(3)	0.9568(10)	1.49(2)	#C(1A)	0.003(8)	#C(2A)	-0.003(8)	#C(3A)	0.003(8)	#C(1A)f -0.003(8)
A 6		2.19(2)	0.79(3)	9.826(15)	1.49(2)	#C(2A)f	0.003(8)	#C(3A)f	-0.003(8)	Cu(1)	0.683(1)	Cu(2) -1.063(1)
						O(1)	-1.078(6)	O(11A)	0.623(6)	O(11B)	0.965(6)	O(12A) -0.596(7)
						O(12B)	1.464(6)	O(21A)	-1.090(6)	O(21B)	0.300(6)	O(22A) 0.893(6)
						O(22B)	-0.188(6)	C(11A)	0.017(8)	C(21A)	-0.075(8)	C(21B) 0.606(8)
						Na(1)a	0.955(6)	O(4W)a	0.682(11)	O(11B)	-1.227(6)	O(12B) -0.728(6)
						O(22A)	-1.299(6)	C(1B)a	0.288(8)	C(2B)a	-0.127(8)	C(3B)a 0.805(8)
						C(11B)	-0.639(8)	Cu(2)b	1.129(1)	O(1)b	1.114(6)	O(21A) 1.102(6)
						Cu(1)e	-1.469(1)	Cu(2)e	0.278(1)	O(1)e	0.293(6)	O(11A) -1.409(6)
						O(12A)	-0.190(7)	O(21A)	0.304(6)	O(21B)	-1.086(6)	O(22B) -0.598(6)
						C(1A)e	-0.789(8)	C(2A)e	-0.783(8)	C(3A)e	-0.789(8)	C(11A) -0.803(8)
						C(21A)	-0.711(8)	C(21B)	-1.391(8)	Cu(1)f	-0.683(1)	Cu(2)f 1.063(1)
						O(1)f	1.078(6)	O(11A)	-0.623(6)	O(11B)	-0.965(6)	O(12A) 0.596(7)
						O(12B)	-1.464(6)	O(21A)	1.090(6)	O(21B)	-0.300(6)	O(22A) -0.893(6)
						O(22B)	0.188(6)	C(11A)	-0.017(8)	C(21A)	0.075(8)	C(21B) -0.606(8)

Nr	8	P	Q	R	S	Sigref	0.009	Sigpln	0.004	Chisq	0.6	Pl.Hyp.

Ring		-0.152(4)	0.9843(7)	0.089(4)	0.48(2)	#C(1B)	0.002(9)	#C(2B)	-0.002(8)	#C(3B)	0.002(9)	#C(1B)d -0.002(9)
A 6		-1.19(3)	10.409(7)	0.96(4)	0.48(2)	#C(2B)d	0.002(8)	#C(3B)d	-0.002(9)	Cu(1)	-0.759(1)	Cu(2) 0.955(1)
						O(1)	-0.621(5)	O(11A)	0.995(5)	O(11B)	1.122(6)	O(12B) -0.872(6)
						O(21A)	0.630(5)	O(21B)	0.471(5)	O(22A)	1.299(5)	O(22B) -0.801(7)
						C(11B)	0.092(8)	C(21A)	1.458(7)	C(21B)	-0.129(8)	Cu(1)a 0.435(1)
						O(1)a	0.573(5)	O(12B)	0.323(6)	O(22B)	0.393(7)	C(1B)a 1.196(9)
						C(2B)a	1.193(8)	C(3B)a	1.196(9)	C(11B)	1.286(8)	C(21B) 1.065(8)
						Cu(2)b	-0.239(1)	Na(1)b	1.130(5)	O(6W)b	1.398(16)	O(11A) -0.199(5)
						O(11B)	-0.073(6)	O(12A)	0.987(5)	O(21A)	-0.564(5)	O(21B) -0.724(5)
						O(22A)	0.105(5)	C(1B)b	-1.193(9)	C(2B)b	-1.196(8)	C(3B)b -1.193(9)
						C(11A)	0.771(7)	C(11B)	-1.103(8)	C(21A)	0.264(7)	C(21B) -1.323(8)
						Cu(1)c	-0.196(1)	O(1)c	-0.335(5)	O(12B)	-0.084(6)	O(21B) -1.426(5)
						O(22B)	-0.155(7)	C(1B)c	-0.957(9)	C(2B)c	-0.954(8)	C(3B)c -0.957(9)
						C(11B)	-1.047(8)	C(21B)	-0.826(8)	Cu(1)d	0.759(1)	Cu(2)d -0.955(1)
						O(1)d	0.621(5)	O(11A)	-0.995(5)	O(11B)	-1.122(6)	O(12B) 0.872(6)
						O(21A)	-0.630(5)	O(21B)	-0.471(5)	O(22A)	-1.299(5)	O(22B) 0.801(7)
						C(11B)	-0.092(8)	C(21A)	-1.458(7)	C(21B)	0.129(8)	Cu(1)e -1.390(1)
						O(12B)	-1.278(6)	O(22B)	-1.349(7)			

Nr	9	P	Q	R	S	Sigref	0.010	Sigpln	3.278	Chisq	999999.9	Pl.Hyp.

Resd		-0.1635	0.8500	0.5008	1.4211	#Cu(1)	-1.090(1)	#Cu(2)	-0.032(1)	#Na(1)	1.808(5)	#O(1) -1.567(5)
A175		-1.2825	8.9948	5.6873	1.4211	#O(4W)	3.452(11)	#O(5W)	3.11(2)	#O(6W)	2.518(18)	#O(11A) 0.243(5)
						#O(11B)	1.054(6)	#O(12A)	0.984(6)	#O(12B)	-0.570(6)	#O(21A) -1.128(5)

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#O(21B) 0.845(5) #O(22A) 0.079(5) #O(22B) -0.720(7) #C(1A) 1.660(8)
#C(1B) 0.889(9) #C(2A) 1.235(8) #C(2B) 0.927(8) #C(3A) 2.023(8)
#C(3B) 1.457(9) #C(11A) 0.876(8) #C(11B) 0.422(8) #C(21A) -0.052(8)
#C(21B) 0.288(8) #Cu(1)a 0.193(1) #Cu(2)a 1.250(1) #Na(1)a 3.090(5)
#O(1)a -0.285(5) #O(4W)a 4.735(11) #O(5W)a 4.39(2) #O(6W)a 3.800(18)
#O(11A) 1.526(5) #O(11B) 2.337(6) #O(12A) 2.266(6) #O(12B) 0.713(6)
#O(21A) 0.154(5) #O(21B) 2.127(5) #O(22A) 1.362(5) #O(22B) 0.563(7)
#C(1A)a 2.943(8) #C(1B)a 2.172(9) #C(2A)a 2.517(8) #C(2B)a 2.209(8)
#C(3A)a 3.306(8) #C(3B)a 2.740(9) #C(11A) 2.159(8) #C(11B) 1.704(8)
#C(21A) 1.230(8) #C(21B) 1.570(8) #Cu(1)b -2.372(1) #Cu(2)b -1.315(1)
#Na(1)b 0.525(5) #O(1)b -2.850(5) #O(4W)b 2.170(11) #O(5W)b 1.83(2)
#O(6W)b 1.235(18) #O(11A) -1.039(5) #O(11B) -0.228(6) #O(12A) -0.299(6)
#O(12B) -1.852(6) #O(21A) -2.411(5) #O(21B) -0.438(5) #O(22A) -1.203(5)
#O(22B) -2.002(7) #C(1A)b 0.378(8) #C(1B)b -0.393(9) #C(2A)b -0.048(8)
#C(2B)b -0.356(8) #C(3A)b 0.741(8) #C(3B)b 0.175(9) #C(11A) -0.406(8)
#C(11B) -0.861(8) #C(21A) -1.335(8) #C(21B) -0.995(8) #Cu(1)c -1.753(1)
#Cu(2)c -2.810(1) #Na(1)c -4.650(5) #O(1)c -1.275(5) #O(4W)c -6.295(11)
#O(5W)c -5.95(2) #O(6W)c -5.360(18) #O(11A) -3.085(5) #O(11B) -3.897(6)
#O(12A) -3.826(6) #O(12B) -2.273(6) #O(21A) -1.714(5) #O(21B) -3.687(5)
#O(22A) -2.921(5) #O(22B) -2.123(7) #C(1A)c -4.502(8) #C(1B)c -3.731(9)
#C(2A)c -4.077(8) #C(2B)c -3.769(8) #C(3A)c -4.865(8) #C(3B)c -4.299(9)
#C(11A) -3.719(8) #C(11B) -3.264(8) #C(21A) -2.790(8) #C(21B) -3.130(8)
#Cu(1)d 3.935(1) #Cu(2)d 2.877(1) #Na(1)d 1.038(5) #O(1)d 4.412(5)
#O(4W)d -0.607(11) #O(5W)d -0.26(2) #O(6W)d 0.328(18) #O(11A) 2.602(5)
#O(11B) 1.791(6) #O(12A) 1.862(6) #O(12B) 3.415(6) #O(21A) 3.974(5)
#O(21B) 2.000(5) #O(22A) 2.766(5) #O(22B) 3.565(7) #C(1A)d 1.185(8)
#C(1B)d 1.956(9) #C(2A)d 1.611(8) #C(2B)d 1.918(8) #C(3A)d 0.822(8)
#C(3B)d 1.388(9) #C(11A) 1.969(8) #C(11B) 2.424(8) #C(21A) 2.897(8)
#C(21B) 2.557(8) #Cu(1)e -3.035(1) #Cu(2)e -4.093(1) #Na(1)e -5.932(5)
#O(1)e -2.557(5) #O(4W)e -7.577(11) #O(5W)e -7.23(2) #O(6W)e -6.642(18)
#O(11A) -4.368(5) #O(11B) -5.179(6) #O(12A) -5.108(6) #O(12B) -3.555(6)
#O(21A) -2.996(5) #O(21B) -4.970(5) #O(22A) -4.204(5) #O(22B) -3.405(7)
#C(1A)e -5.785(8) #C(1B)e -5.014(9) #C(2A)e -5.359(8) #C(2B)e -5.051(8)
#C(3A)e -6.148(8) #C(3B)e -5.582(9) #C(11A) -5.001(8) #C(11B) -4.546(8)
#C(21A) -4.073(8) #C(21B) -4.413(8) #Cu(1)f 5.960(1) #Cu(2)f 4.902(1)
#Na(1)f 3.063(5) #O(1)f 6.437(5) #O(4W)f 1.418(11) #O(5W)f 1.76(2)
#O(6W)f 2.353(18) #O(11A) 4.627(5) #O(11B) 3.816(6) #O(12A) 3.887(6)
#O(12B) 5.440(6) #O(21A) 5.999(5) #O(21B) 4.025(5) #O(22A) 4.791(5)
#O(22B) 5.590(7) #C(1A)f 3.210(8) #C(1B)f 3.981(9) #C(2A)f 3.636(8)
#C(2B)f 3.943(8) #C(3A)f 2.847(8) #C(3B)f 3.413(9) #C(11A) 3.994(8)
#C(11B) 4.449(8) #C(21A) 4.922(8) #C(21B) 4.582(8)

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Nr	10	P	Q	R	S	Sigref	0.006	Sigpln	0.008	Chisq	4.4	Pl.Hyp.	
Plan		0.7652(14)	0.270(2)	-0.5846(16)	0.987(7)	#Cu(1)	0.010(1)	#O(1)	-0.005(6)	#O(21B)	-0.004(6)	#O(21A)	-0.002(6)
A	5	6.001(11)	2.69(2)	-9.110(19)	0.987(7)	#C(21A)	0.001(8)	Cu(2)	-0.877(1)	O(1W)	-0.455(13)	O(11A)	1.180(6)
						O(12A)	0.492(6)	C(11A)	1.270(8)	O(4W)a	-0.906(11)	O(6W)a	-1.04(2)
						C(3A)a	-1.401(8)	C(2B)b	0.643(9)	C(3B)b	-0.640(9)	C(21B)	0.811(9)

=====												
						Cu(2)c	-1.097(1)	O(11B)	0.412(6)	O(12B)	0.172(6)	C(11B) 0.861(8)
						Na(1)e	-0.026(7)	O(4W)e	-1.068(11)	O(6W)e	-0.93(2)	O(22A) -0.364(6)
						C(2A)e	0.399(8)	C(3A)e	-0.573(8)			

Nr 11	P	Q	R	S	Sigref	0.005	Sigpln	0.016	Chisq	10.7	Pl.Hyp.	P<5

Plan	0.630(2)	-0.018(2)	0.7765(17)	2.786(3)	#Cu(1)	-0.014(1)	#O(11A)	0.006(6)	#O(12B)	0.003(6)	#O(21A)	0.005(6)
A 4	4.940(16)	-0.32(2)	6.75(2)	2.786(3)	O(11B)	-1.047(6)	O(21A)	-0.638(6)	O(22A)	1.483(6)	C(1A)	-0.630(8)
					C(1B)	0.086(8)	C(2A)	-0.096(8)	C(2B)	-0.791(8)	C(3A)	0.063(8)
					C(3B)	-0.296(8)	C(11A)	-0.813(8)	C(11B)	-0.374(8)	C(21A)	0.271(8)
					Na(1)a	-1.395(6)	O(6W)a	0.85(2)	Cu(1)d	1.194(1)	O(11A)	1.174(6)
					O(12B)	1.177(6)	O(22A)	-0.303(6)	C(1B)d	1.094(8)	C(2A)d	1.276(8)
					C(3A)d	1.118(8)	C(3B)d	1.476(8)	C(21A)	0.909(8)	Cu(1)e	-0.619(1)
					O(1)e	1.301(6)	O(11A)	-0.638(6)	O(11B)	0.414(6)	O(12A)	1.186(6)
					O(12B)	-0.636(6)	C(1A)e	-0.002(8)	C(1B)e	-0.718(8)	C(2A)e	-0.537(8)
					C(2B)e	0.159(8)	C(3A)e	-0.695(8)	C(3B)e	-0.337(8)	C(11A)	0.181(8)
					C(11B)	-0.259(8)	C(21A)	-0.904(8)	Cu(1)f	-0.937(1)	O(1)f	0.983(6)
					O(11A)	-0.956(6)	O(11B)	0.096(6)	O(12A)	0.868(6)	O(12B)	-0.954(6)
					O(21A)	-0.313(6)	C(1A)f	-0.320(8)	C(1B)f	-1.037(8)	C(2A)f	-0.855(8)
					C(2B)f	-0.159(8)	C(3A)f	-1.013(8)	C(3B)f	-0.655(8)	C(11A)	-0.138(8)
					C(11B)	-0.577(8)	C(21A)	-1.222(8)	C(21B)	1.309(8)		

Nr 12	P	Q	R	S	Sigref	0.005	Sigpln	0.018	Chisq	12.5	Pl.Hyp.	P<5

Plan	0.7002(14)	0.7070(15)	0.100(3)	0.958(3)	#Cu(2)	0.015(1)	#O(1)	-0.007(5)	#O(11B)	-0.001(6)	#O(22A)	-0.007(5)
A 4	5.491(11)	7.317(16)	-1.46(3)	0.958(3)	Cu(1)	0.915(1)	O(12B)	-0.436(6)	C(1B)	-1.165(9)	C(11B)	-0.503(8)
					Na(1)a	1.431(6)	O(5W)a	0.50(3)	C(1A)a	-1.318(8)	C(2A)a	-0.428(8)
					C(3A)a	0.844(8)	C(21A)	-0.764(8)	O(12B)	-1.480(6)	O(22B)	1.132(7)
					C(1B)c	-0.752(9)	C(2B)c	0.374(9)	C(3B)c	0.887(9)	C(11B)	-1.413(8)
					C(21B)	1.103(9)	O(21B)	0.199(6)	O(22B)	-0.324(7)	C(2B)d	-1.082(9)
					C(3B)d	-0.568(9)	C(21B)	-0.352(9)	O(11A)	0.957(6)	O(21A)	-0.219(5)
					C(1A)e	-0.599(8)	C(2A)e	-1.489(8)	C(11A)	0.780(8)	C(21A)	-1.153(8)

Nr 13	P	Q	R	S	Sigref	0.005	Sigpln	0.011	Chisq	5.0	Pl.Hyp.	P<5

Plan	0.7521(14)	-0.6549(15)	0.074(3)	-0.952(4)	#Cu(2)	-0.010(1)	#O(11B)	0.001(6)	#O(12A)	0.004(6)	#O(1)c	0.004(6)
A 4	5.899(11)	-7.054(16)	-1.19(3)	-0.952(4)	O(22B)	-0.105(7)	C(1A)	0.704(8)	C(1B)	0.650(9)	C(2B)	-0.252(9)
					C(3A)	1.346(8)	C(3B)	-0.544(9)	C(11A)	0.998(8)	C(11B)	0.942(8)
					C(21B)	-0.815(9)	O(6W)a	-0.54(2)	Cu(1)c	-1.066(1)	O(4W)c	-0.751(11)
					O(5W)c	-0.56(3)	O(11A)	-0.214(6)	O(12B)	-0.258(6)	O(21A)	-1.368(6)
					C(1A)c	1.199(8)	C(1B)c	1.253(9)	C(2A)c	0.216(8)	C(3A)c	0.557(8)
					C(11A)	0.905(8)	C(11B)	0.961(8)	C(21A)	-1.182(8)	Cu(2)d	0.728(1)
					O(1)d	-1.180(6)	O(11A)	-1.399(6)	O(11B)	0.718(6)	O(12A)	0.714(6)
					O(12B)	-1.442(6)	O(22B)	0.823(7)	C(1A)d	0.014(8)	C(1B)d	0.069(9)
					C(2A)d	-0.968(8)	C(2B)d	0.970(9)	C(3A)d	-0.628(8)	C(3B)d	1.263(9)
					C(11A)	-0.280(8)	C(11B)	-0.223(8)	Cu(2)f	0.758(1)	O(1)f	-1.150(6)
					O(11A)	-1.369(6)	O(11B)	0.748(6)	O(12A)	0.744(6)	O(12B)	-1.412(6)
					O(22B)	0.853(7)	C(1A)f	0.044(8)	C(1B)f	0.098(9)	C(2A)f	-0.939(8)

					C(2B)f	1.000(9)	C(3A)f	-0.598(8)	C(3B)f	1.293(9)	C(11A)	-0.250(8)
					C(11B)	-0.194(8)						
Nr 14	P	Q	R	S	Sigref	0.016	Sigpln	0.021	Chisq	1.7	Pl.Hyp.	
Plan	0.584(9)	0.132(3)	0.801(7)	6.61(5)	#Na(1)	0.017(6)	#O(4W)	-0.007(11)	#O(5W)	0.00(3)	#O(11B)	-0.007(6)
A 4	4.58(7)	1.28(3)	7.10(8)	6.61(5)	O(1W)	-0.856(12)	Cu(1)b	0.661(1)	O(1)b	-1.226(6)	O(11A)	0.932(6)
					O(12A)	-0.678(6)	O(12B)	0.714(6)	O(21A)	0.164(6)	C(1A)b	0.600(8)
					C(1B)b	0.987(8)	C(2A)b	1.061(8)	C(2B)b	0.140(8)	C(3A)b	1.366(8)
					C(3B)b	0.666(8)	C(11A)	0.270(8)	C(11B)	0.509(8)	C(21A)	1.200(8)
					C(21B)	-1.345(8)	Cu(2)d	0.071(1)	O(1)d	-0.312(6)	O(12A)	-0.860(6)
					O(21B)	0.460(6)	O(22B)	0.294(6)	C(21B)	-0.193(8)	Cu(2)f	-1.169(1)
					O(21B)	-0.781(6)	O(22B)	-0.947(6)	C(21B)	-1.433(8)		
Nr 15	P	Q	R	S	Sigref	0.004	Sigpln	0.031	Chisq	103.7	Pl.Hyp.	P<5
Plan	0.5915(8)	0.6664(18)	-0.454(2)	0.762(4)	#Cu(1)	-0.013(1)	#Cu(2)	-0.032(1)	#O(1)	0.021(6)	#O(22A)	0.016(5)
A 5	4.639(6)	6.910(19)	-7.31(3)	0.762(4)	#O(21B)	0.007(5)	O(1W)	0.768(12)	O(2W)	-0.326(17)	O(11B)	-1.235(6)
					Na(1)a	0.197(6)	O(5W)a	-1.26(3)	O(6W)a	1.11(2)	O(21A)	-0.607(6)
					C(1A)a	-0.941(8)	C(2A)a	0.023(8)	C(3A)a	1.331(8)	C(21A)	-0.236(8)
					O(22B)	0.904(7)	C(1B)b	1.329(9)	C(2B)b	0.369(9)	C(3B)b	-0.721(9)
					C(21B)	0.444(8)	Cu(2)c	-1.492(1)	O(11B)	-0.289(6)	O(12B)	0.381(6)
					C(11B)	0.546(8)	O(5W)e	-0.26(3)	O(11A)	1.351(6)	O(12A)	1.429(6)
					O(21A)	-0.917(5)	C(1A)e	-0.583(8)	C(11A)	0.851(8)	C(21A)	-1.288(8)
Nr 16	P	Q	R	S	Sigref	0.006	Sigpln	0.008	Chisq	4.4	Pl.Hyp.	
Plan	0.7652(14)	0.270(2)	-0.5846(16)	5.014(5)	#O(21A)	0.002(6)	#C(21A)	-0.001(8)	#O(21B)	0.004(6)	#Cu(1)e	-0.010(1)
A 5	6.001(11)	2.69(2)	-9.110(19)	5.014(5)	#O(1)e	0.005(6)	Na(1)	0.026(7)	O(4W)	1.068(11)	O(6W)	0.93(2)
					O(22A)	0.364(6)	C(2A)	-0.399(8)	C(3A)	0.573(8)	Cu(2)b	1.097(1)
					O(11B)	-0.412(6)	O(12B)	-0.172(6)	C(11B)	-0.861(8)	C(2B)c	-0.643(9)
					C(3B)c	0.640(9)	C(21B)	-0.811(9)	Cu(2)e	0.877(1)	O(11A)	-1.180(6)
					O(12A)	-0.492(6)	C(11A)	-1.270(8)	Na(1)f	-1.358(7)	O(5W)f	0.76(3)
					O(21A)	-1.335(6)	C(1A)f	0.319(8)	C(2A)f	-0.933(8)	C(11A)	1.425(8)
					C(21A)	-1.331(8)						
Nr 17	P	Q	R	S	Sigref	0.007	Sigpln	0.006	Chisq	1.7	Pl.Hyp.	
Plan	0.316(2)	0.9091(17)	-0.271(4)	-2.143(17)	#O(21B)	0.004(5)	#O(22B)	0.000(7)	#C(2B)	-0.004(8)	#C(21B)	0.004(8)
A 5	2.481(19)	9.523(18)	-4.52(4)	-2.143(17)	#Cu(1)a	-0.003(1)	O(12B)	1.159(6)	C(1B)	0.629(9)	C(3B)	-0.738(9)
					Cu(2)a	0.822(1)	O(1)a	0.108(5)	O(11B)	0.077(6)	O(12B)	-1.322(6)
					C(11B)	-0.974(8)	Cu(2)c	0.983(1)	O(11A)	-0.206(5)	O(12A)	-0.734(5)
					C(11A)	-1.007(8)	O(12B)	-1.394(6)	O(21B)	-0.238(5)	O(22B)	-0.234(7)
					C(1B)d	-0.863(9)	C(2B)d	-0.231(8)	C(3B)d	0.503(9)	C(21B)	-0.239(8)
					Na(1)e	-0.363(6)	O(5W)e	0.24(2)	O(6W)e	-1.072(17)	O(21A)	0.922(5)
					O(22A)	0.216(5)	C(1A)e	-0.001(8)	C(2A)e	-0.522(8)	C(11A)	1.474(8)
					C(21A)	0.295(8)						

Nr 18	P	Q	R	S	Sigref	0.006	Sigpln	0.010	Chisq	3.4	Pl.Hyp.	
Plan	-0.4913(14)	-0.529(4)	0.692(3)	-4.312(12)	#O(21A)	0.003(6)	#O(22A)	0.006(6)	#C(21A)	-0.007(8)	#Cu(2)b	-0.002(1)
A 4	-3.853(11)	-5.48(4)	9.59(3)	-4.312(12)	Na(1)	0.524(6)	O(4W)	-1.120(11)	O(6W)	0.18(2)	C(1A)	0.799(8)
					C(2A)	-0.127(8)	C(3A)	-1.272(8)	Cu(1)b	0.322(1)	O(1)b	-0.176(6)
					O(11A)	-1.230(6)	O(12A)	-1.396(6)	O(21B)	0.123(6)	O(22B)	1.193(6)
					C(1B)c	0.809(9)	C(2B)c	0.020(8)	C(3B)c	-1.255(9)	C(21B)	0.496(8)
					Cu(1)e	0.596(1)	Cu(2)e	0.920(1)	O(1)e	1.094(6)	O(11B)	-0.771(6)
					O(12B)	-1.383(6)	Na(1)f	-1.235(6)	O(4W)f	0.409(11)	O(6W)f	-0.89(2)
					O(21A)	-0.714(6)	O(22A)	-0.717(6)	C(2A)f	-0.583(8)	C(3A)f	0.561(8)
					C(21A)	-0.703(8)						
Nr 19	P	Q	R	S	Sigref	0.008	Sigpln	0.024	Chisq	66.1	Pl.Hyp.	P<5
Plan	0.2977(19)	0.0705(14)	0.9521(6)	1.509(11)	#C(1A)	0.001(8)	#C(2A)	0.021(8)	#C(3A)	0.029(8)	#C(11A)	0.012(8)
A 10	2.334(15)	0.684(15)	9.720(9)	1.509(11)	#C(21A)	-0.024(8)	#C(1A)f	-0.001(8)	#C(2A)f	-0.021(8)	#C(3A)f	-0.029(8)
					#C(11A)	-0.012(8)	#C(21A)	0.024(8)	Cu(1)	0.701(1)	Cu(2)	-1.100(1)
					O(1)	-1.076(6)	O(11A)	0.635(6)	O(11B)	0.914(6)	O(12A)	-0.623(7)
					O(12B)	1.450(6)	O(21A)	-1.034(6)	O(21B)	0.188(6)	O(22A)	0.961(6)
					O(22B)	-0.254(6)	C(21B)	0.519(8)	Na(1)a	0.876(6)	O(4W)a	0.587(11)
					O(11B)	-1.421(6)	O(12B)	-0.884(6)	O(22A)	-1.374(6)	C(1B)a	0.088(8)
					C(2B)a	-0.350(8)	C(3B)a	0.566(8)	C(11B)	-0.821(8)	Cu(2)b	1.234(1)
					O(1)b	1.258(6)	O(21A)	1.301(6)	Cu(1)e	-1.385(1)	Cu(2)e	0.416(1)
					O(1)e	0.392(6)	O(11A)	-1.319(6)	O(12A)	-0.061(7)	O(21A)	0.349(6)
					O(21B)	-0.872(6)	O(22B)	-0.431(6)	C(1A)e	-0.686(8)	C(2A)e	-0.706(8)
					C(3A)e	-0.714(8)	C(11A)	-0.697(8)	C(21A)	-0.661(8)	C(21B)	-1.204(8)
					Cu(1)f	-0.701(1)	Cu(2)f	1.100(1)	O(1)f	1.076(6)	O(11A)	-0.635(6)
					O(11B)	-0.914(6)	O(12A)	0.623(7)	O(12B)	-1.450(6)	O(21A)	1.034(6)
					O(21B)	-0.188(6)	O(22A)	-0.961(6)	O(22B)	0.254(6)	C(21B)	-0.519(8)
Nr 20	P	Q	R	S	Sigref	0.009	Sigpln	0.030	Chisq	60.5	Pl.Hyp.	P<5
Plan	-0.164(3)	0.9804(5)	0.109(2)	0.608(12)	#C(1B)	-0.031(9)	#C(2B)	-0.017(8)	#C(3B)	0.019(9)	#C(11B)	0.024(8)
A 8	-1.29(3)	10.370(5)	1.22(3)	0.608(12)	#C(1B)d	0.031(9)	#C(2B)d	0.017(8)	#C(3B)d	-0.019(9)	#C(11B)	-0.024(8)
					Cu(1)	-0.889(1)	Cu(2)	0.827(1)	O(1)	-0.766(5)	O(11A)	0.843(5)
					O(11B)	1.041(6)	O(12B)	-0.954(6)	O(21A)	0.410(5)	O(21B)	0.452(5)
					O(22A)	1.089(5)	O(22B)	-0.857(7)	C(21A)	1.247(7)	C(21B)	-0.161(8)
					Cu(1)a	0.400(1)	O(1)a	0.523(5)	O(12B)	0.336(6)	O(22B)	0.433(7)
					C(1B)a	1.258(9)	C(2B)a	1.272(8)	C(3B)a	1.308(9)	C(11B)	1.313(8)
					C(21B)	1.128(8)	Cu(2)b	-0.462(1)	Na(1)b	0.852(5)	O(6W)b	1.119(16)
					O(11A)	-0.446(5)	O(11B)	-0.249(6)	O(12A)	0.743(5)	O(21A)	-0.880(5)
					O(21B)	-0.837(5)	O(22A)	-0.200(5)	C(1B)b	-1.320(9)	C(2A)b	1.326(7)
					C(2B)b	-1.306(8)	C(3B)b	-1.271(9)	C(11A)	0.518(7)	C(11B)	-1.265(8)
					C(21A)	-0.043(7)	C(21B)	-1.450(8)	Cu(1)c	-0.326(1)	O(1)c	-0.449(5)
					O(12B)	-0.262(6)	O(22B)	-0.359(7)	C(1B)c	-1.184(9)	C(2B)c	-1.198(8)
					C(3B)c	-1.234(9)	C(11B)	-1.239(8)	C(21B)	-1.054(8)	Cu(1)d	0.889(1)
					Cu(2)d	-0.827(1)	O(1)d	0.766(5)	O(11A)	-0.843(5)	O(11B)	-1.041(6)

=====												
					O(12B)	0.954(6)	O(21A)	-0.410(5)	O(21B)	-0.452(5)	O(22A)	-1.089(5)
					O(22B)	0.857(7)	C(21A)	-1.247(7)	C(21B)	0.161(8)		

Nr 21	P	Q	R	S	Sigref	0.007	Sigpln	0.011	Chisq	2.5	Pl.Hyp.	

Plan	-0.199(4)	0.368(4)	0.9082(16)	1.126(16)	#O(11A)	0.004(6)	#O(12A)	0.003(7)	#C(1A)	0.003(8)	#C(11A)	-0.009(8)
A 4	-1.56(3)	3.92(4)	10.63(2)	1.126(16)	Cu(1)	-0.235(1)	Cu(2)	-0.270(1)	Na(1)	1.051(6)	O(1)	-1.325(6)
					O(4W)	1.382(11)	O(12B)	1.120(6)	O(22A)	-1.014(6)	O(22B)	0.957(6)
					C(2A)	-0.627(8)	C(3A)	-0.559(8)	C(21A)	-1.429(8)	Cu(1)a	1.325(1)
					Cu(2)a	1.290(1)	O(1)a	0.235(6)	O(21A)	-0.896(6)	O(22A)	0.546(6)
					C(2A)a	0.933(8)	C(3A)a	1.002(8)	C(21A)	0.131(8)	Na(1)b	-0.510(6)
					O(4W)b	-0.179(11)	O(5W)b	1.20(2)	O(6W)b	0.43(2)	O(11B)	0.197(6)
					O(12B)	-0.440(6)	O(21B)	0.973(6)	O(22B)	-0.603(6)	C(1B)b	1.473(8)
					C(11B)	0.321(8)	C(21B)	0.577(8)	O(1)c	-0.927(6)	O(21A)	0.204(6)
					O(22A)	-1.238(6)	C(21A)	-0.823(8)	O(21A)	-1.356(6)	Cu(1)f	0.345(1)
					Cu(2)f	0.381(1)	Na(1)f	-0.940(6)	O(1)f	1.435(6)	O(4W)f	-1.271(11)
					O(11A)	0.107(6)	O(12A)	0.107(7)	O(12B)	-1.009(6)	O(22A)	1.125(6)
					O(22B)	-0.847(6)	C(1A)f	0.108(8)	C(2A)f	0.738(8)	C(3A)f	0.669(8)
					C(11A)	0.120(8)						

Nr 22	P	Q	R	S	Sigref	0.007	Sigpln	0.019	Chisq	6.7	Pl.Hyp.	P<5

Plan	0.642(3)	0.516(3)	0.568(4)	1.912(12)	#O(11B)	0.006(6)	#O(12B)	0.006(6)	#C(1B)	0.005(9)	#C(11B)	-0.016(8)
A 4	5.03(3)	5.31(4)	4.09(4)	1.912(12)	Cu(1)	0.546(1)	Cu(2)	-1.039(1)	O(1)	-1.026(6)	O(12A)	0.522(6)
					C(2B)	-1.003(8)	C(3B)	-0.877(9)	C(11A)	1.456(8)	Na(1)a	0.952(6)
					O(5W)a	0.67(3)	O(22A)	-1.212(6)	C(3A)a	-1.139(8)	O(21B)	-0.989(6)
					O(22B)	-1.130(6)	Cu(1)d	-0.282(1)	Cu(2)d	1.302(1)	O(1)d	1.289(6)
					O(11A)	-1.407(6)	O(11B)	0.257(6)	O(12A)	-0.258(6)	O(12B)	0.258(6)
					O(21A)	-1.347(6)	C(1B)d	0.259(9)	C(2B)d	1.266(8)	C(3B)d	1.140(9)
					C(11A)	-1.193(8)	C(11B)	0.280(8)	Cu(1)e	0.662(1)	O(11A)	-0.463(6)
					O(11B)	1.201(6)	O(12A)	0.686(6)	O(12B)	1.201(6)	O(21A)	-0.404(6)
					C(1A)e	-1.186(8)	C(1B)e	1.203(9)	C(11A)	-0.249(8)	C(11B)	1.224(8)
					Na(1)f	0.538(6)	O(4W)f	-0.442(11)	O(5W)f	0.82(3)		

Nr 23	P	Q	R	S	Sigref	0.007	Sigpln	0.022	Chisq	10.2	Pl.Hyp.	P<5

Plan	0.530(3)	0.477(4)	-0.701(2)	4.402(15)	#O(21A)	0.007(6)	#O(22A)	0.007(6)	#C(2A)	0.005(8)	#C(21A)	-0.018(8)
A 4	4.16(3)	4.93(4)	-9.79(3)	4.402(15)	Na(1)	-0.550(6)	O(4W)	0.987(11)	O(6W)	-0.16(2)	C(1A)	-0.977(8)
					C(3A)	1.113(8)	Cu(1)b	-0.020(1)	Cu(2)b	0.139(1)	O(1)b	0.440(6)
					O(11A)	1.459(6)	O(21B)	-0.020(6)	O(22B)	-1.217(6)	C(1B)c	-0.829(9)
					C(2B)c	0.003(8)	C(3B)c	1.305(9)	C(21B)	-0.462(8)	Cu(1)e	-0.466(1)
					Cu(2)e	-0.625(1)	O(1)e	-0.926(6)	O(11B)	1.092(6)	Na(1)f	0.833(6)
					O(4W)f	-0.704(11)	O(6W)f	0.45(2)	O(21A)	0.277(6)	O(22A)	0.277(6)
					C(1A)f	1.261(8)	C(2A)f	0.279(8)	C(3A)f	-0.830(8)	C(21A)	0.302(8)

(Acute) Angles (Degrees) Between Planes (Numbers I,J from List Above)

1, 2= 87.6(2) 1, 3= 28.1(2) 1, 4= 32.8(2) 1, 5= 32.8(2) 1, 6= 32.8(2) 1, 7= 25.6(3) 1, 8= 81.4(4)

1, 9=	73.58(18)	1, 10=	49.4(3)	1, 11=	42.1(3)	1, 12=	84.7(3)	1, 13=	77.7(3)	1, 14=	43.0(7)	1, 15=	52.0(3)
1, 16=	49.4(3)	1, 17=	60.6(3)	1, 18=	35.8(3)	1, 19=	26.0(2)	1, 20=	82.6(3)	1, 21=	37.3(4)	1, 22=	65.8(4)
1, 23=	36.1(4)	2, 3=	82.8(2)	2, 4=	72.3(2)	2, 5=	72.3(2)	2, 6=	72.3(2)	2, 7=	62.5(3)	2, 8=	43.3(3)
2, 9=	43.97(15)	2, 10=	61.3(2)	2, 11=	58.2(2)	2, 12=	13.9(3)	2, 13=	84.5(3)	2, 14=	51.1(7)	2, 15=	42.5(2)
2, 16=	61.3(2)	2, 17=	34.0(3)	2, 18=	59.2(3)	2, 19=	62.5(2)	2, 20=	43.7(3)	2, 21=	65.2(4)	2, 22=	25.0(4)
2, 23=	60.7(4)	3, 4=	24.9(2)	3, 5=	24.9(2)	3, 6=	24.9(2)	3, 7=	37.4(3)	3, 8=	76.2(3)	3, 9=	52.34(16)
3, 10=	37.8(2)	3, 11=	60.6(2)	3, 12=	85.0(3)	3, 13=	74.3(3)	3, 14=	56.9(7)	3, 15=	55.6(2)	3, 16=	37.8(2)
3, 17=	74.2(3)	3, 18=	40.2(3)	3, 19=	38.5(2)	3, 20=	74.9(3)	3, 21=	17.9(4)	3, 22=	69.7(4)	3, 23=	37.7(4)
4, 5=	0.0(2)	4, 6=	0.0(2)	4, 7=	54.6(3)	4, 8=	84.6(3)	4, 9=	74.29(14)	4, 10=	16.8(2)	4, 11=	74.6(2)
4, 12=	60.5(3)	4, 13=	78.7(3)	4, 14=	74.2(7)	4, 15=	30.9(2)	4, 16=	16.8(2)	4, 17=	51.6(3)	4, 18=	17.2(3)
4, 19=	55.4(2)	4, 20=	85.9(3)	4, 21=	42.7(4)	4, 22=	87.6(4)	4, 23=	13.9(3)	5, 6=	0.0(2)	5, 7=	54.6(3)
5, 8=	84.6(3)	5, 9=	74.29(14)	5, 10=	16.8(2)	5, 11=	74.6(2)	5, 12=	60.5(3)	5, 13=	78.7(3)	5, 14=	74.2(7)
5, 15=	30.9(2)	5, 16=	16.8(2)	5, 17=	51.6(3)	5, 18=	17.2(3)	5, 19=	55.4(2)	5, 20=	85.9(3)	5, 21=	42.7(4)
5, 22=	87.6(4)	5, 23=	13.9(3)	6, 7=	54.6(3)	6, 8=	84.6(3)	6, 9=	74.29(14)	6, 10=	16.8(2)	6, 11=	74.6(2)
6, 12=	60.5(3)	6, 13=	78.7(3)	6, 14=	74.2(7)	6, 15=	30.9(2)	6, 16=	16.8(2)	6, 17=	51.6(3)	6, 18=	17.2(3)
6, 19=	55.4(2)	6, 20=	85.9(3)	6, 21=	42.7(4)	6, 22=	87.6(4)	6, 23=	13.9(3)	7, 8=	83.1(4)	7, 9=	59.9(3)
7, 10=	71.1(3)	7, 11=	23.4(3)	7, 12=	69.7(3)	7, 13=	76.8(3)	7, 14=	19.9(7)	7, 15=	77.5(3)	7, 16=	71.1(3)
7, 17=	84.3(4)	7, 18=	61.2(4)	7, 19=	1.2(3)	7, 20=	82.2(4)	7, 21=	32.6(4)	7, 22=	40.2(4)	7, 23=	61.1(4)
8, 9=	25.0(3)	8, 10=	84.4(4)	8, 11=	87.4(4)	8, 12=	53.3(4)	8, 13=	41.2(4)	8, 14=	83.6(8)	8, 15=	58.3(4)
8, 16=	84.4(4)	8, 17=	34.7(4)	8, 18=	67.4(4)	8, 19=	83.8(3)	8, 20=	1.3(4)	8, 21=	61.7(5)	8, 22=	62.6(5)
8, 23=	70.9(4)	9, 10=	79.14(18)	9, 11=	74.32(19)	9, 12=	57.6(2)	9, 13=	50.0(2)	9, 14=	65.3(7)	9, 15=	75.97(18)
9, 16=	79.14(18)	9, 17=	54.2(3)	9, 18=	88.7(3)	9, 19=	60.79(14)	9, 20=	23.9(2)	9, 21=	36.8(3)	9, 22=	51.8(3)
9, 23=	88.2(3)	10, 11=	88.7(3)	10, 12=	48.1(3)	10, 13=	69.2(3)	10, 14=	89.2(7)	10, 15=	26.1(3)	10, 16=	0.0(3)
10, 17=	49.8(3)	10, 18=	22.6(3)	10, 19=	72.0(2)	10, 20=	85.7(3)	10, 21=	54.3(4)	10, 22=	72.7(4)	10, 23=	19.2(4)
11, 12=	59.7(3)	11, 13=	57.1(3)	11, 14=	9.1(7)	11, 15=	89.6(3)	11, 16=	88.7(3)	11, 17=	88.4(3)	11, 18=	76.3(3)
11, 19=	22.3(2)	11, 20=	87.9(3)	11, 21=	55.0(4)	11, 22=	33.4(4)	11, 23=	77.4(4)	12, 13=	85.9(3)	12, 14=	54.4(7)
12, 15=	32.9(3)	12, 16=	48.1(3)	12, 17=	33.2(3)	12, 18=	49.5(3)	12, 19=	69.3(3)	12, 20=	53.9(3)	12, 21=	77.8(4)
12, 22=	29.5(4)	12, 23=	50.3(4)	13, 14=	65.7(7)	13, 15=	88.6(3)	13, 16=	69.2(3)	13, 17=	67.8(3)	13, 18=	88.4(3)
13, 19=	75.6(3)	13, 20=	40.7(3)	13, 21=	71.1(4)	13, 22=	79.3(4)	13, 23=	88.0(4)	14, 15=	86.0(7)	14, 16=	89.2(7)
14, 17=	85.0(7)	14, 18=	78.6(7)	14, 19=	19.0(7)	14, 20=	83.1(7)	14, 21=	48.7(8)	14, 22=	26.2(8)	14, 23=	79.1(8)
15, 16=	26.1(3)	15, 17=	23.7(3)	15, 18=	16.8(3)	15, 19=	77.9(2)	15, 20=	59.6(3)	15, 21=	73.5(4)	15, 22=	62.3(4)
15, 23=	18.2(4)	16, 17=	49.8(3)	16, 18=	22.6(3)	16, 19=	72.0(2)	16, 20=	85.7(3)	16, 21=	54.3(4)	16, 22=	72.7(4)
16, 23=	19.2(4)	17, 18=	34.5(4)	17, 19=	84.3(3)	17, 20=	35.9(4)	17, 21=	88.5(4)	17, 22=	58.8(4)	17, 23=	37.7(4)
18, 19=	61.6(3)	18, 20=	68.7(4)	18, 21=	57.9(4)	18, 22=	78.7(4)	18, 23=	3.8(4)	19, 20=	82.9(3)	19, 21=	33.8(4)
19, 22=	39.9(4)	19, 23=	61.6(3)	20, 21=	60.5(4)	20, 22=	62.5(4)	20, 23=	72.3(4)	21, 22=	54.7(5)	21, 23=	55.5(5)
22, 23=	79.1(5)												

(Acute) Angles (Degrees) Between Axes, Lines, Bonds and L.S.-Plane

Bond	/	Plane	NM --> M	1	2	3	4	5	6	7	8	9	10
Axes 0	---	a	/ OM =	1.37(18),	32.86(15),	21.16(16),	33.95(14),	33.95(14),	33.95(14),	16.2(3),	8.8(3),	9.41,	49.92(18),
			1M =	39.04(19),	44.4(2),	48.8(2),	35.7(7),	36.27(18),	49.92(18),	18.4(3),	29.4(3),	17.32(14),	9.5(2),
			2M =	11.5(3),	39.9(3),	32.0(3),							
		b	/ OM =	14.05(18),	52.14(15),	6.32(16),	14.10(14),	14.10(14),	14.10(14),	4.3(3),	80.8(3),	58.53,	14.80(18),
			1M =	1.73(19),	43.9(2),	42.0(2),	7.0(7),	40.93(18),	14.80(18),	64.6(3),	31.3(3),	3.72(14),	79.5(2),

=====											
	2M =	21.8(3),	30.3(3),	27.9(3),							
c / 0M =	71.86(18),	3.71(15),	79.77(16),	67.14(14),	67.14(14),	67.14(14),	57.3(3),	4.7(3),	29.16,	51.30(18),	
1M =	35.34(19),	7.2(2),	5.8(2),	37.4(7),	38.76(18),	51.30(18),	22.8(3),	55.3(3),	56.38(14),	6.0(2),	
	2M =	65.6(3),	20.5(3),	57.0(3),							
a* / 0M =	13.56(18),	37.31(15),	5.47(16),	19.21(14),	19.21(14),	19.21(14),	31.9(3),	6.0(3),	0.39,	35.70(18),	
1M =	54.66(19),	45.5(2),	47.1(2),	51.3(7),	27.32(18),	35.70(18),	14.3(3),	17.2(3),	33.02(14),	6.4(2),	
	2M =	3.5(3),	51.3(3),	19.3(3),							
b* / 0M =	11.39(18),	54.20(15),	8.44(16),	12.51(14),	12.51(14),	12.51(14),	7.2(3),	80.9(3),	60.76,	14.01(18),	
1M =	1.04(19),	45.3(2),	40.6(2),	9.8(7),	40.11(18),	14.01(18),	63.6(3),	29.7(3),	6.62(14),	79.9(2),	
	2M =	24.3(3),	32.8(3),	26.4(3),							
c* / 0M =	75.85(18),	14.88(15),	67.95(16),	52.15(14),	52.15(14),	52.15(14),	73.1(3),	5.1(3),	30.05,	35.77(18),	
1M =	50.94(19),	5.7(2),	4.2(2),	53.2(7),	27.00(18),	35.77(18),	15.7(3),	43.8(3),	72.19(14),	6.2(2),	
	2M =	65.3(3),	34.6(3),	44.5(3),							
Cu(1) -0(1) / 0M =	48.9(3),	30.0(2),	29.6(2),	16.3(2),	16.3(2),	16.3(2),	66.6(3),	4.1(4),	14.41(18),	0.4(3),	
1M =	88.3(3),	28.7(3),	33.9(3),	79.4(7),	1.0(3),	0.4(3),	3.3(3),	15.0(3),	67.7(2),	3.7(3),	
	2M =	34.6(4),	54.9(4),	13.9(4),							
-0(11A) / 0M =	24.9(2),	58.8(2),	10.4(2),	33.1(2),	33.1(2),	33.1(2),	1.7(3),	60.1(3),	41.21(14),	35.4(2),	
1M =	0.6(2),	57.3(3),	24.9(3),	7.7(7),	61.5(2),	35.4(2),	84.6(3),	50.1(3),	1.9(2),	58.9(3),	
	2M =	6.8(4),	33.8(4),	47.0(3),							
-0(12B) / 0M =	42.1(2),	25.5(2),	55.2(2),	74.9(2),	74.9(2),	74.9(2),	21.2(3),	3.0(3),	13.94(16),	86.8(2),	
1M =	0.5(3),	38.8(3),	22.0(3),	1.4(7),	61.2(2),	86.8(2),	37.6(3),	66.4(3),	20.3(2),	1.7(3),	
	2M =	38.9(4),	14.5(4),	70.0(4),							
-0(21B) / 0M =	49.2(3),	33.9(2),	32.4(2),	17.2(2),	17.2(2),	17.2(2),	69.8(3),	1.1(4),	19.78(18),	0.4(3),	
1M =	85.8(3),	31.4(3),	28.7(3),	84.6(7),	0.6(3),	0.4(3),	0.2(3),	14.2(3),	70.9(2),	1.6(3),	
	2M =	38.8(4),	58.9(4),	13.4(4),							
-0(21A) / 0M =	3.6(2),	45.0(2),	19.4(2),	0.2(2),	0.2(2),	0.2(2),	10.8(3),	84.3(3),	69.91(14),	0.3(2),	
1M =	0.5(2),	34.0(3),	50.3(3),	8.6(7),	26.5(2),	0.3(2),	50.0(3),	17.0(3),	10.0(2),	85.7(3),	
	2M =	33.5(4),	27.9(4),	13.5(3),							
Cu(2) -0(1) / 0M =	0.0(2),	12.2(2),	28.1(2),	20.0(2),	20.0(2),	20.0(2),	0.4(3),	53.3(4),	51.40(18),	26.4(3),	
1M =	19.6(3),	0.6(3),	76.3(3),	11.2(7),	1.6(3),	26.4(3),	21.3(3),	5.1(3),	0.7(2),	54.2(3),	
	2M =	32.5(4),	0.4(4),	8.8(4),							
-0(11B) / 0M =	76.6(2),	9.5(2),	73.6(2),	59.1(2),	59.1(2),	59.1(2),	66.0(3),	4.3(3),	29.31(15),	42.8(2),	
1M =	44.1(2),	0.4(3),	0.3(3),	46.2(7),	32.8(2),	42.8(2),	19.6(3),	49.6(3),	65.1(2),	5.5(3),	
	2M =	66.0(4),	28.1(4),	50.7(4),							
-0(12A) / 0M =	11.6(3),	73.3(2),	9.4(2),	34.2(2),	34.2(2),	34.2(2),	14.0(3),	39.5(4),	31.82(18),	45.3(3),	
1M =	23.7(3),	83.3(3),	0.4(3),	28.9(7),	63.2(3),	45.3(3),	63.0(3),	46.4(3),	14.3(2),	38.7(3),	
	2M =	8.2(4),	54.1(4),	45.3(4),							
-0(22A) / 0M =	7.3(2),	9.8(2),	20.8(2),	14.2(2),	14.2(2),	14.2(2),	7.0(3),	52.6(4),	46.05(18),	22.2(3),	
1M =	26.5(3),	0.6(3),	83.6(3),	18.0(7),	1.4(3),	22.2(3),	23.3(3),	0.2(3),	8.1(2),	53.2(3),	
	2M =	24.9(4),	5.1(4),	3.9(4),							
-0(1)c / 0M =	0.0(2),	83.8(2),	2.4(2),	22.3(2),	22.3(2),	22.3(2),	25.5(3),	41.6(4),	39.78(18),	34.2(3),	
1M =	32.6(3),	82.2(3),	0.4(3),	38.9(7),	51.2(3),	34.2(3),	55.8(3),	34.4(3),	25.7(2),	41.1(3),	
	2M =	19.8(4),	64.9(4),	33.2(4),							
Na(1) -0(4W) / 0M =	27.1(3),	49.3(3),	7.6(3),	27.5(3),	27.5(3),	27.5(3),	6.7(4),	67.9(4),	44.7(3),	26.5(3),	
1M =	8.5(4),	45.5(4),	37.0(4),	0.6(7),	52.2(3),	26.5(3),	75.1(4),	44.7(4),	7.1(3),	66.6(4),	
	2M =	8.1(4),	24.8(5),	41.1(4),							
-0(5W) / 0M =	31.1(10),	9.5(10),	55.7(10),	58.3(10),	58.3(10),	58.3(10),	18.5(10),	19.8(10),	33.7(10),	64.5(10),	
1M =	4.9(10),	23.3(10),	43.0(10),	0.5(12),	38.4(10),	64.5(10),	14.8(10),	44.0(10),	17.4(10),	21.1(10),	

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	2M =	46.8(10),	6.9(10),	47.8(10),							
-O(6W) /	0M =	26.5(5),	47.6(5),	12.2(5),	5.3(5),	5.3(5),	5.3(5),	48.8(5),	6.4(6),	17.1(5),	22.0(5),
	1M =	68.1(5),	50.1(5),	32.3(5),	68.7(8),	22.2(5),	22.0(5),	17.0(5),	8.2(5),	49.7(5),	6.3(5),
	2M =	22.8(6),	68.4(6),	9.2(6),							
-O(22A) /	0M =	46.1(3),	46.1(2),	45.8(2),	22.9(2),	22.9(2),	22.9(2),	70.1(3),	25.3(4),	46.13(19),	8.1(3),
	1M =	59.3(3),	36.9(3),	2.3(3),	68.0(7),	4.3(3),	8.1(3),	14.0(3),	12.5(3),	69.7(2),	26.0(3),
	2M =	59.4(4),	64.5(4),	13.4(4),							
-O(11B) /	0M =	16.3(3),	44.4(2),	6.5(2),	11.8(2),	11.8(2),	11.8(2),	0.2(3),	82.4(4),	57.33(19),	10.4(3),
	1M =	8.3(3),	36.3(3),	49.5(3),	0.6(7),	36.3(3),	10.4(3),	59.8(3),	28.8(3),	0.9(2),	81.2(3),
	2M =	20.7(4),	23.0(4),	25.2(4),							
O(11A)-C(11A) /	0M =	35.8(5),	12.9(4),	7.9(4),	14.5(4),	14.5(4),	14.5(4),	29.2(5),	51.4(5),	30.6(4),	4.1(5),
	1M =	41.2(5),	8.2(5),	64.3(5),	32.2(8),	23.7(5),	4.1(5),	40.1(5),	26.7(5),	30.1(4),	50.9(5),
	2M =	0.6(5),	9.9(5),	23.3(5),							
O(11B)-C(11B) /	0M =	42.9(5),	25.6(5),	17.3(5),	29.2(5),	29.2(5),	29.2(5),	27.8(5),	54.8(5),	30.1(5),	20.9(5),
	1M =	32.2(5),	23.5(5),	48.3(5),	24.2(8),	41.4(5),	20.9(5),	56.5(5),	43.3(5),	28.4(5),	53.8(5),
	2M =	5.7(6),	1.0(6),	39.6(6),							
O(12A)-C(11A) /	0M =	11.5(5),	33.6(5),	8.8(5),	21.2(5),	21.2(5),	21.2(5),	28.6(5),	9.7(5),	4.8(4),	37.4(5),
	1M =	51.7(5),	42.5(5),	50.9(5),	47.7(8),	26.8(5),	37.4(5),	12.3(5),	17.8(5),	29.7(5),	10.1(5),
	2M =	0.6(6),	46.8(6),	20.2(5),							
O(12B)-C(11B) /	0M =	5.5(5),	9.2(5),	33.6(5),	26.3(5),	26.3(5),	26.3(5),	4.0(5),	48.7(5),	50.7(4),	32.5(5),
	1M =	17.1(5),	3.0(5),	72.0(5),	9.2(8),	7.4(5),	32.5(5),	15.7(5),	11.4(5),	2.8(5),	49.7(5),
	2M =	36.5(6),	1.0(6),	15.1(5),							
O(21A)-C(21A) /	0M =	30.8(4),	59.5(4),	37.3(4),	12.6(4),	12.6(4),	12.6(4),	53.5(5),	41.0(5),	58.5(4),	0.2(4),
	1M =	46.0(5),	47.7(5),	8.5(5),	55.2(8),	17.1(4),	0.2(4),	29.8(5),	0.5(5),	53.2(4),	41.5(5),
	2M =	54.5(5),	67.6(5),	1.1(5),							
O(21B)-C(21B) /	0M =	3.3(5),	14.5(5),	22.0(5),	26.4(5),	26.4(5),	26.4(5),	13.8(6),	27.8(6),	25.7(5),	39.4(5),
	1M =	36.9(5),	25.4(5),	67.7(5),	30.5(8),	19.9(5),	39.4(5),	0.0(6),	16.9(6),	15.0(5),	28.5(5),
	2M =	18.0(6),	25.9(6),	20.1(6),							
O(22A)-C(21A) /	0M =	32.6(5),	33.5(5),	12.6(5),	0.2(5),	0.2(5),	0.2(5),	49.9(5),	7.2(5),	6.0(5),	16.8(5),
	1M =	73.2(5),	36.7(5),	44.1(5),	67.8(8),	11.5(5),	16.8(5),	3.6(5),	0.6(5),	51.0(5),	7.1(5),
	2M =	19.2(6),	55.3(6),	1.1(6),							
O(22B)-C(21B) /	0M =	41.7(5),	15.0(5),	69.3(5),	51.3(5),	51.3(5),	51.3(5),	39.7(5),	32.7(6),	54.2(5),	45.7(5),
	1M =	16.8(5),	1.3(5),	34.9(5),	23.1(8),	21.7(5),	45.7(5),	0.2(5),	34.1(5),	38.5(5),	34.1(5),
	2M =	71.7(6),	19.7(6),	37.4(6),							
C(1A) -C(2A) /	0M =	17.3(5),	26.2(5),	37.6(5),	49.3(5),	49.3(5),	49.3(5),	0.3(5),	10.3(5),	17.8(5),	63.9(5),
	1M =	22.5(5),	39.6(5),	44.8(5),	19.3(8),	43.8(5),	63.9(5),	22.0(5),	41.6(5),	0.8(5),	11.3(5),
	2M =	26.8(6),	26.8(6),	44.8(6),							
-C(11A) /	0M =	25.7(5),	61.9(4),	17.4(4),	41.8(4),	41.8(4),	41.8(4),	0.5(5),	47.1(5),	31.4(4),	47.4(5),
	1M =	7.0(5),	66.6(5),	11.3(5),	12.7(8),	72.5(5),	47.4(5),	78.8(5),	57.4(5),	0.4(4),	45.9(5),
	2M =	0.4(5),	38.5(5),	55.1(5),							
-C(3A)f /	0M =	7.7(5),	26.3(5),	19.2(5),	6.2(5),	6.2(5),	6.2(5),	0.3(5),	69.2(5),	58.4(5),	10.5(5),
	1M =	15.9(5),	16.0(5),	69.1(5),	6.9(8),	14.8(5),	10.5(5),	37.9(5),	9.8(5),	1.3(5),	69.9(5),
	2M =	28.6(6),	9.8(6),	6.1(6),							
C(1B) -C(2B) /	0M =	3.1(6),	41.4(6),	19.5(6),	35.8(5),	35.8(5),	35.8(5),	17.2(6),	0.1(6),	1.5(5),	52.5(6),
	1M =	38.7(6),	53.3(6),	40.0(6),	37.1(9),	43.2(6),	52.5(6),	26.8(6),	34.2(6),	18.2(5),	0.6(6),
	2M =	7.7(6),	45.9(6),	36.4(6),							
-C(11B) /	0M =	59.4(5),	14.5(4),	68.3(4),	86.8(4),	86.8(4),	86.8(4),	38.3(5),	3.5(5),	18.2(4),	70.6(5),
	1M =	17.9(5),	26.3(5),	11.3(5),	18.6(8),	56.1(5),	70.6(5),	36.0(5),	70.5(5),	37.5(4),	2.1(5),

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	2M =	50.4(5),	0.8(5),	73.5(5),							
-C(3B)d /	0M =	56.9(5),	28.9(5),	39.4(5),	24.9(5),	24.9(5),	24.9(5),	76.3(5),	0.1(5),	20.7(4),	8.1(5),
	1M =	80.0(5),	25.0(5),	25.7(5),	79.4(8),	6.5(5),	8.1(5),	5.1(5),	21.7(5),	77.5(5),	0.5(5),
	2M =	44.0(6),	53.6(6),	21.0(5),							
C(2A) -C(3A) /	0M =	24.6(5),	62.8(5),	15.0(5),	39.1(5),	39.1(5),	39.1(5),	0.3(5),	50.3(5),	34.4(5),	44.2(5),
	1M =	6.5(5),	65.7(5),	14.1(5),	12.6(8),	69.6(5),	44.2(5),	80.9(5),	55.1(5),	0.3(5),	49.2(5),
	2M =	2.8(6),	38.7(6),	52.6(6),							
-C(21A) /	0M =	3.2(5),	24.2(5),	24.1(5),	11.4(4),	11.4(4),	11.4(4),	2.8(5),	65.9(5),	59.8(4),	15.5(5),
	1M =	14.3(5),	13.1(5),	69.9(5),	5.4(8),	10.0(5),	15.5(5),	33.3(5),	4.6(5),	1.7(4),	66.8(5),
	2M =	32.6(5),	9.4(5),	0.9(5),							
C(2B) -C(3B) /	0M =	61.4(5),	9.8(5),	73.0(5),	82.1(5),	82.1(5),	82.1(5),	41.9(6),	0.1(6),	22.4(5),	66.9(5),
	1M =	20.8(5),	21.6(5),	12.1(5),	22.1(8),	51.5(5),	66.9(5),	31.8(6),	66.3(6),	41.1(5),	1.5(5),
	2M =	55.1(6),	5.2(6),	69.1(6),							
-C(21B) /	0M =	54.2(5),	33.7(4),	39.6(4),	23.1(4),	23.1(4),	23.1(4),	77.0(5),	4.9(5),	25.3(4),	6.4(5),
	1M =	78.7(5),	29.2(5),	22.1(5),	82.7(8),	2.9(5),	6.4(5),	0.3(5),	18.5(5),	78.1(4),	5.5(5),
	2M =	46.3(5),	58.1(5),	18.1(5),							
Cu(1)a-0(21B) /	0M =	49.2(3),	33.9(2),	32.4(2),	17.2(2),	17.2(2),	17.2(2),	69.8(3),	1.1(4),	19.78(18),	0.4(3),
	1M =	85.8(3),	31.4(3),	28.7(3),	84.6(7),	0.6(3),	0.4(3),	0.2(3),	14.2(3),	70.9(2),	1.6(3),
	2M =	38.8(4),	58.9(4),	13.4(4),							
-0(1)a /	0M =	48.9(3),	30.0(2),	29.6(2),	16.3(2),	16.3(2),	16.3(2),	66.6(3),	4.1(4),	14.41(18),	0.4(3),
	1M =	88.3(3),	28.7(3),	33.9(3),	79.4(7),	1.0(3),	0.4(3),	3.3(3),	15.0(3),	67.7(2),	3.7(3),
	2M =	34.6(4),	54.9(4),	13.9(4),							
-0(11A) /	0M =	24.9(2),	58.8(2),	10.4(2),	33.1(2),	33.1(2),	33.1(2),	1.7(3),	60.1(3),	41.21(14),	35.4(2),
	1M =	0.6(2),	57.3(3),	24.9(3),	7.7(7),	61.5(2),	35.4(2),	84.6(3),	50.1(3),	1.9(2),	58.9(3),
	2M =	6.8(4),	33.8(4),	47.0(3),							
-0(12B) /	0M =	42.1(2),	25.5(2),	55.2(2),	74.9(2),	74.9(2),	74.9(2),	21.2(3),	3.0(3),	13.94(16),	86.8(2),
	1M =	0.5(3),	38.8(3),	22.0(3),	1.4(7),	61.2(2),	86.8(2),	37.6(3),	66.4(3),	20.3(2),	1.7(3),
	2M =	38.9(4),	14.5(4),	70.0(4),							
-0(21A) /	0M =	3.6(2),	45.0(2),	19.4(2),	0.2(2),	0.2(2),	0.2(2),	10.8(3),	84.3(3),	69.91(14),	0.3(2),
	1M =	0.5(2),	34.0(3),	50.3(3),	8.6(7),	26.5(2),	0.3(2),	50.0(3),	17.0(3),	10.0(2),	85.7(3),
	2M =	33.5(4),	27.9(4),	13.5(3),							
Cu(2)a-0(1)a /	0M =	0.0(2),	12.2(2),	28.1(2),	20.0(2),	20.0(2),	20.0(2),	0.4(3),	53.3(4),	51.40(18),	26.4(3),
	1M =	19.6(3),	0.6(3),	76.3(3),	11.2(7),	1.6(3),	26.4(3),	21.3(3),	5.1(3),	0.7(2),	54.2(3),
	2M =	32.5(4),	0.4(4),	8.8(4),							
-0(11B) /	0M =	76.6(2),	9.5(2),	73.6(2),	59.1(2),	59.1(2),	59.1(2),	66.0(3),	4.3(3),	29.31(15),	42.8(2),
	1M =	44.1(2),	0.4(3),	0.3(3),	46.2(7),	32.8(2),	42.8(2),	19.6(3),	49.6(3),	65.1(2),	5.5(3),
	2M =	66.0(4),	28.1(4),	50.7(4),							
-0(12A) /	0M =	11.6(3),	73.3(2),	9.4(2),	34.2(2),	34.2(2),	34.2(2),	14.0(3),	39.5(4),	31.82(18),	45.3(3),
	1M =	23.7(3),	83.3(3),	0.4(3),	28.9(7),	63.2(3),	45.3(3),	63.0(3),	46.4(3),	14.3(2),	38.7(3),
	2M =	8.2(4),	54.1(4),	45.3(4),							
Na(1)a-0(11B) /	0M =	16.3(3),	44.4(2),	6.5(2),	11.8(2),	11.8(2),	11.8(2),	0.2(3),	82.4(4),	57.33(19),	10.4(3),
	1M =	8.3(3),	36.3(3),	49.5(3),	0.6(7),	36.3(3),	10.4(3),	59.8(3),	28.8(3),	0.9(2),	81.2(3),
	2M =	20.7(4),	23.0(4),	25.2(4),							
-0(4W)a /	0M =	27.1(3),	49.3(3),	7.6(3),	27.5(3),	27.5(3),	27.5(3),	6.7(4),	67.9(4),	44.7(3),	26.5(3),
	1M =	8.5(4),	45.5(4),	37.0(4),	0.6(7),	52.2(3),	26.5(3),	75.1(4),	44.7(4),	7.1(3),	66.6(4),
	2M =	8.1(4),	24.8(5),	41.1(4),							
-0(5W)a /	0M =	31.1(10),	9.5(10),	55.7(10),	58.3(10),	58.3(10),	58.3(10),	18.5(10),	19.8(10),	33.7(10),	64.5(10),
	1M =	4.9(10),	23.3(10),	43.0(10),	0.5(12),	38.4(10),	64.5(10),	14.8(10),	44.0(10),	17.4(10),	21.1(10),

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	2M =	46.8(10),	6.9(10),	47.8(10),							
-O(6W)a /	0M =	26.5(5),	47.6(5),	12.2(5),	5.3(5),	5.3(5),	5.3(5),	48.8(5),	6.4(6),	17.1(5),	22.0(5),
	1M =	68.1(5),	50.1(5),	32.3(5),	68.7(8),	22.2(5),	22.0(5),	17.0(5),	8.2(5),	49.7(5),	6.3(5),
	2M =	22.8(6),	68.4(6),	9.2(6),							
-O(22A) /	0M =	46.1(3),	46.1(2),	45.8(2),	22.9(2),	22.9(2),	22.9(2),	70.1(3),	25.3(4),	46.13(19),	8.1(3),
	1M =	59.3(3),	36.9(3),	2.3(3),	68.0(7),	4.3(3),	8.1(3),	14.0(3),	12.5(3),	69.7(2),	26.0(3),
	2M =	59.4(4),	64.5(4),	13.4(4),							
O(11A)-C(11A) /	0M =	35.8(5),	12.9(4),	7.9(4),	14.5(4),	14.5(4),	14.5(4),	29.2(5),	51.4(5),	30.6(4),	4.1(5),
	1M =	41.2(5),	8.2(5),	64.3(5),	32.2(8),	23.7(5),	4.1(5),	40.1(5),	26.7(5),	30.1(4),	50.9(5),
	2M =	0.6(5),	9.9(5),	23.3(5),							
O(11B)-C(11B) /	0M =	42.9(5),	25.6(5),	17.3(5),	29.2(5),	29.2(5),	29.2(5),	27.8(5),	54.8(5),	30.1(5),	20.9(5),
	1M =	32.2(5),	23.5(5),	48.3(5),	24.2(8),	41.4(5),	20.9(5),	56.5(5),	43.3(5),	28.4(5),	53.8(5),
	2M =	5.7(6),	1.0(6),	39.6(6),							
O(12A)-C(11A) /	0M =	11.5(5),	33.6(5),	8.8(5),	21.2(5),	21.2(5),	21.2(5),	28.6(5),	9.7(5),	4.8(4),	37.4(5),
	1M =	51.7(5),	42.5(5),	50.9(5),	47.7(8),	26.8(5),	37.4(5),	12.3(5),	17.8(5),	29.7(5),	10.1(5),
	2M =	0.6(6),	46.8(6),	20.2(5),							
O(12B)-C(11B) /	0M =	5.5(5),	9.2(5),	33.6(5),	26.3(5),	26.3(5),	26.3(5),	4.0(5),	48.7(5),	50.7(4),	32.5(5),
	1M =	17.1(5),	3.0(5),	72.0(5),	9.2(8),	7.4(5),	32.5(5),	15.7(5),	11.4(5),	2.8(5),	49.7(5),
	2M =	36.5(6),	1.0(6),	15.1(5),							
O(21A)-C(21A) /	0M =	30.8(4),	59.5(4),	37.3(4),	12.6(4),	12.6(4),	12.6(4),	53.5(5),	41.0(5),	58.5(4),	0.2(4),
	1M =	46.0(5),	47.7(5),	8.5(5),	55.2(8),	17.1(4),	0.2(4),	29.8(5),	0.5(5),	53.2(4),	41.5(5),
	2M =	54.5(5),	67.6(5),	1.1(5),							
O(21B)-C(21B) /	0M =	3.3(5),	14.5(5),	22.0(5),	26.4(5),	26.4(5),	26.4(5),	13.8(6),	27.8(6),	25.7(5),	39.4(5),
	1M =	36.9(5),	25.4(5),	67.7(5),	30.5(8),	19.9(5),	39.4(5),	0.0(6),	16.9(6),	15.0(5),	28.5(5),
	2M =	18.0(6),	25.9(6),	20.1(6),							
O(22A)-C(21A) /	0M =	32.6(5),	33.5(5),	12.6(5),	0.2(5),	0.2(5),	0.2(5),	49.9(5),	7.2(5),	6.0(5),	16.8(5),
	1M =	73.2(5),	36.7(5),	44.1(5),	67.8(8),	11.5(5),	16.8(5),	3.6(5),	0.6(5),	51.0(5),	7.1(5),
	2M =	19.2(6),	55.3(6),	1.1(6),							
O(22B)-C(21B) /	0M =	41.7(5),	15.0(5),	69.3(5),	51.3(5),	51.3(5),	51.3(5),	39.7(5),	32.7(6),	54.2(5),	45.7(5),
	1M =	16.8(5),	1.3(5),	34.9(5),	23.1(8),	21.7(5),	45.7(5),	0.2(5),	34.1(5),	38.5(5),	34.1(5),
	2M =	71.7(6),	19.7(6),	37.4(6),							
C(1A)a-C(2A)a /	0M =	17.3(5),	26.2(5),	37.6(5),	49.3(5),	49.3(5),	49.3(5),	0.3(5),	10.3(5),	17.8(5),	63.9(5),
	1M =	22.5(5),	39.6(5),	44.8(5),	19.3(8),	43.8(5),	63.9(5),	22.0(5),	41.6(5),	0.8(5),	11.3(5),
	2M =	26.8(6),	26.8(6),	44.8(6),							
-C(11A) /	0M =	25.7(5),	61.9(4),	17.4(4),	41.8(4),	41.8(4),	41.8(4),	0.5(5),	47.1(5),	31.4(4),	47.4(5),
	1M =	7.0(5),	66.6(5),	11.3(5),	12.7(8),	72.5(5),	47.4(5),	78.8(5),	57.4(5),	0.4(4),	45.9(5),
	2M =	0.4(5),	38.5(5),	55.1(5),							
C(1B)a-C(2B)a /	0M =	3.1(6),	41.4(6),	19.5(6),	35.8(5),	35.8(5),	35.8(5),	17.2(6),	0.1(6),	1.5(5),	52.5(6),
	1M =	38.7(6),	53.3(6),	40.0(6),	37.1(9),	43.2(6),	52.5(6),	26.8(6),	34.2(6),	18.2(5),	0.6(6),
	2M =	7.7(6),	45.9(6),	36.4(6),							
-C(11B) /	0M =	59.4(5),	14.5(4),	68.3(4),	86.8(4),	86.8(4),	86.8(4),	38.3(5),	3.5(5),	18.2(4),	70.6(5),
	1M =	17.9(5),	26.3(5),	11.3(5),	18.6(8),	56.1(5),	70.6(5),	36.0(5),	70.5(5),	37.5(4),	2.1(5),
	2M =	50.4(5),	0.8(5),	73.5(5),							
C(2A)a-C(3A)a /	0M =	24.6(5),	62.8(5),	15.0(5),	39.1(5),	39.1(5),	39.1(5),	0.3(5),	50.3(5),	34.4(5),	44.2(5),
	1M =	6.5(5),	65.7(5),	14.1(5),	12.6(8),	69.6(5),	44.2(5),	80.9(5),	55.1(5),	0.3(5),	49.2(5),
	2M =	2.8(6),	38.7(6),	52.6(6),							
-C(21A) /	0M =	3.2(5),	24.2(5),	24.1(5),	11.4(4),	11.4(4),	11.4(4),	2.8(5),	65.9(5),	59.8(4),	15.5(5),
	1M =	14.3(5),	13.1(5),	69.9(5),	5.4(8),	10.0(5),	15.5(5),	33.3(5),	4.6(5),	1.7(4),	66.8(5),

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C(2B)a-C(3B)a /	2M =	32.6(5),	9.4(5),	0.9(5),							
	0M =	61.4(5),	9.8(5),	73.0(5),	82.1(5),	82.1(5),	82.1(5),	41.9(6),	0.1(6),	22.4(5),	66.9(5),
	1M =	20.8(5),	21.6(5),	12.1(5),	22.1(8),	51.5(5),	66.9(5),	31.8(6),	66.3(6),	41.1(5),	1.5(5),
-C(21B) /	2M =	55.1(6),	5.2(6),	69.1(6),							
	0M =	54.2(5),	33.7(4),	39.6(4),	23.1(4),	23.1(4),	23.1(4),	77.0(5),	4.9(5),	25.3(4),	6.4(5),
	1M =	78.7(5),	29.2(5),	22.1(5),	82.7(8),	2.9(5),	6.4(5),	0.3(5),	18.5(5),	78.1(4),	5.5(5),
Cu(1)b-O(1)b /	2M =	46.3(5),	58.1(5),	18.1(5),							
	0M =	48.9(3),	30.0(2),	29.6(2),	16.3(2),	16.3(2),	16.3(2),	66.6(3),	4.1(4),	14.41(18),	0.4(3),
	1M =	88.3(3),	28.7(3),	33.9(3),	79.4(7),	1.0(3),	0.4(3),	3.3(3),	15.0(3),	67.7(2),	3.7(3),
-O(11A) /	2M =	34.6(4),	54.9(4),	13.9(4),							
	0M =	24.9(2),	58.8(2),	10.4(2),	33.1(2),	33.1(2),	33.1(2),	1.7(3),	60.1(3),	41.21(14),	35.4(2),
	1M =	0.6(2),	57.3(3),	24.9(3),	7.7(7),	61.5(2),	35.4(2),	84.6(3),	50.1(3),	1.9(2),	58.9(3),
-O(12B) /	2M =	6.8(4),	33.8(4),	47.0(3),							
	0M =	42.1(2),	25.5(2),	55.2(2),	74.9(2),	74.9(2),	74.9(2),	21.2(3),	3.0(3),	13.94(16),	86.8(2),
	1M =	0.5(3),	38.8(3),	22.0(3),	1.4(7),	61.2(2),	86.8(2),	37.6(3),	66.4(3),	20.3(2),	1.7(3),
Cu(2)b-O(22A) /	2M =	38.9(4),	14.5(4),	70.0(4),							
	0M =	7.3(2),	9.8(2),	20.8(2),	14.2(2),	14.2(2),	14.2(2),	7.0(3),	52.6(4),	46.05(18),	22.2(3),
	1M =	26.5(3),	0.6(3),	83.6(3),	18.0(7),	1.4(3),	22.2(3),	23.3(3),	0.2(3),	8.1(2),	53.2(3),
-O(1)b /	2M =	24.9(4),	5.1(4),	3.9(4),							
	0M =	0.0(2),	12.2(2),	28.1(2),	20.0(2),	20.0(2),	20.0(2),	0.4(3),	53.3(4),	51.40(18),	26.4(3),
	1M =	19.6(3),	0.6(3),	76.3(3),	11.2(7),	1.6(3),	26.4(3),	21.3(3),	5.1(3),	0.7(2),	54.2(3),
-O(11B) /	2M =	32.5(4),	0.4(4),	8.8(4),							
	0M =	76.6(2),	9.5(2),	73.6(2),	59.1(2),	59.1(2),	59.1(2),	66.0(3),	4.3(3),	29.31(15),	42.8(2),
	1M =	44.1(2),	0.4(3),	0.3(3),	46.2(7),	32.8(2),	42.8(2),	19.6(3),	49.6(3),	65.1(2),	5.5(3),
-O(12A) /	2M =	66.0(4),	28.1(4),	50.7(4),							
	0M =	11.6(3),	73.3(2),	9.4(2),	34.2(2),	34.2(2),	34.2(2),	14.0(3),	39.5(4),	31.82(18),	45.3(3),
	1M =	23.7(3),	83.3(3),	0.4(3),	28.9(7),	63.2(3),	45.3(3),	63.0(3),	46.4(3),	14.3(2),	38.7(3),
-O(1)e /	2M =	8.2(4),	54.1(4),	45.3(4),							
	0M =	0.0(2),	83.8(2),	2.4(2),	22.3(2),	22.3(2),	22.3(2),	25.5(3),	41.6(4),	39.78(18),	34.2(3),
	1M =	32.6(3),	82.2(3),	0.4(3),	38.9(7),	51.2(3),	34.2(3),	55.8(3),	34.4(3),	25.7(2),	41.1(3),
Na(1)b-O(4W)b /	2M =	19.8(4),	64.9(4),	33.2(4),							
	0M =	27.1(3),	49.3(3),	7.6(3),	27.5(3),	27.5(3),	27.5(3),	6.7(4),	67.9(4),	44.7(3),	26.5(3),
	1M =	8.5(4),	45.5(4),	37.0(4),	0.6(7),	52.2(3),	26.5(3),	75.1(4),	44.7(4),	7.1(3),	66.6(4),
-O(5W)b /	2M =	8.1(4),	24.8(5),	41.1(4),							
	0M =	31.1(10),	9.5(10),	55.7(10),	58.3(10),	58.3(10),	58.3(10),	18.5(10),	19.8(10),	33.7(10),	64.5(10),
	1M =	4.9(10),	23.3(10),	43.0(10),	0.5(12),	38.4(10),	64.5(10),	14.8(10),	44.0(10),	17.4(10),	21.1(10),
-O(6W)b /	2M =	46.8(10),	6.9(10),	47.8(10),							
	0M =	26.5(5),	47.6(5),	12.2(5),	5.3(5),	5.3(5),	5.3(5),	48.8(5),	6.4(6),	17.1(5),	22.0(5),
	1M =	68.1(5),	50.1(5),	32.3(5),	68.7(8),	22.2(5),	22.0(5),	17.0(5),	8.2(5),	49.7(5),	6.3(5),
-O(22A) /	2M =	22.8(6),	68.4(6),	9.2(6),							
	0M =	46.1(3),	46.1(2),	45.8(2),	22.9(2),	22.9(2),	22.9(2),	70.1(3),	25.3(4),	46.13(19),	8.1(3),
	1M =	59.3(3),	36.9(3),	2.3(3),	68.0(7),	4.3(3),	8.1(3),	14.0(3),	12.5(3),	69.7(2),	26.0(3),
O(11A)-C(11A) /	2M =	59.4(4),	64.5(4),	13.4(4),							
	0M =	35.8(5),	12.9(4),	7.9(4),	14.5(4),	14.5(4),	14.5(4),	29.2(5),	51.4(5),	30.6(4),	4.1(5),
	1M =	41.2(5),	8.2(5),	64.3(5),	32.2(8),	23.7(5),	4.1(5),	40.1(5),	26.7(5),	30.1(4),	50.9(5),
O(11B)-C(11B) /	2M =	0.6(5),	9.9(5),	23.3(5),							
	0M =	42.9(5),	25.6(5),	17.3(5),	29.2(5),	29.2(5),	29.2(5),	27.8(5),	54.8(5),	30.1(5),	20.9(5),
	1M =	32.2(5),	23.5(5),	48.3(5),	24.2(8),	41.4(5),	20.9(5),	56.5(5),	43.3(5),	28.4(5),	53.8(5),

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	2M =	5.7(6),	1.0(6),	39.6(6),							
0(12A)-C(11A) /	0M =	11.5(5),	33.6(5),	8.8(5),	21.2(5),	21.2(5),	21.2(5),	28.6(5),	9.7(5),	4.8(4),	37.4(5),
	1M =	51.7(5),	42.5(5),	50.9(5),	47.7(8),	26.8(5),	37.4(5),	12.3(5),	17.8(5),	29.7(5),	10.1(5),
	2M =	0.6(6),	46.8(6),	20.2(5),							
0(12B)-C(11B) /	0M =	5.5(5),	9.2(5),	33.6(5),	26.3(5),	26.3(5),	26.3(5),	4.0(5),	48.7(5),	50.7(4),	32.5(5),
	1M =	17.1(5),	3.0(5),	72.0(5),	9.2(8),	7.4(5),	32.5(5),	15.7(5),	11.4(5),	2.8(5),	49.7(5),
	2M =	36.5(6),	1.0(6),	15.1(5),							
0(21A)-C(21A) /	0M =	30.8(4),	59.5(4),	37.3(4),	12.6(4),	12.6(4),	12.6(4),	53.5(5),	41.0(5),	58.5(4),	0.2(4),
	1M =	46.0(5),	47.7(5),	8.5(5),	55.2(8),	17.1(4),	0.2(4),	29.8(5),	0.5(5),	53.2(4),	41.5(5),
	2M =	54.5(5),	67.6(5),	1.1(5),							
0(21B)-C(21B) /	0M =	3.3(5),	14.5(5),	22.0(5),	26.4(5),	26.4(5),	26.4(5),	13.8(6),	27.8(6),	25.7(5),	39.4(5),
	1M =	36.9(5),	25.4(5),	67.7(5),	30.5(8),	19.9(5),	39.4(5),	0.0(6),	16.9(6),	15.0(5),	28.5(5),
	2M =	18.0(6),	25.9(6),	20.1(6),							
0(22A)-C(21A) /	0M =	32.6(5),	33.5(5),	12.6(5),	0.2(5),	0.2(5),	0.2(5),	49.9(5),	7.2(5),	6.0(5),	16.8(5),
	1M =	73.2(5),	36.7(5),	44.1(5),	67.8(8),	11.5(5),	16.8(5),	3.6(5),	0.6(5),	51.0(5),	7.1(5),
	2M =	19.2(6),	55.3(6),	1.1(6),							
0(22B)-C(21B) /	0M =	41.7(5),	15.0(5),	69.3(5),	51.3(5),	51.3(5),	51.3(5),	39.7(5),	32.7(6),	54.2(5),	45.7(5),
	1M =	16.8(5),	1.3(5),	34.9(5),	23.1(8),	21.7(5),	45.7(5),	0.2(5),	34.1(5),	38.5(5),	34.1(5),
	2M =	71.7(6),	19.7(6),	37.4(6),							
C(1A)b-C(2A)b /	0M =	17.3(5),	26.2(5),	37.6(5),	49.3(5),	49.3(5),	49.3(5),	0.3(5),	10.3(5),	17.8(5),	63.9(5),
	1M =	22.5(5),	39.6(5),	44.8(5),	19.3(8),	43.8(5),	63.9(5),	22.0(5),	41.6(5),	0.8(5),	11.3(5),
	2M =	26.8(6),	26.8(6),	44.8(6),							
-C(11A) /	0M =	25.7(5),	61.9(4),	17.4(4),	41.8(4),	41.8(4),	41.8(4),	0.5(5),	47.1(5),	31.4(4),	47.4(5),
	1M =	7.0(5),	66.6(5),	11.3(5),	12.7(8),	72.5(5),	47.4(5),	78.8(5),	57.4(5),	0.4(4),	45.9(5),
	2M =	0.4(5),	38.5(5),	55.1(5),							
C(1B)b-C(2B)b /	0M =	3.1(6),	41.4(6),	19.5(6),	35.8(5),	35.8(5),	35.8(5),	17.2(6),	0.1(6),	1.5(5),	52.5(6),
	1M =	38.7(6),	53.3(6),	40.0(6),	37.1(9),	43.2(6),	52.5(6),	26.8(6),	34.2(6),	18.2(5),	0.6(6),
	2M =	7.7(6),	45.9(6),	36.4(6),							
-C(11B) /	0M =	59.4(5),	14.5(4),	68.3(4),	86.8(4),	86.8(4),	86.8(4),	38.3(5),	3.5(5),	18.2(4),	70.6(5),
	1M =	17.9(5),	26.3(5),	11.3(5),	18.6(8),	56.1(5),	70.6(5),	36.0(5),	70.5(5),	37.5(4),	2.1(5),
	2M =	50.4(5),	0.8(5),	73.5(5),							
C(2A)b-C(3A)b /	0M =	24.6(5),	62.8(5),	15.0(5),	39.1(5),	39.1(5),	39.1(5),	0.3(5),	50.3(5),	34.4(5),	44.2(5),
	1M =	6.5(5),	65.7(5),	14.1(5),	12.6(8),	69.6(5),	44.2(5),	80.9(5),	55.1(5),	0.3(5),	49.2(5),
	2M =	2.8(6),	38.7(6),	52.6(6),							
-C(21A) /	0M =	3.2(5),	24.2(5),	24.1(5),	11.4(4),	11.4(4),	11.4(4),	2.8(5),	65.9(5),	59.8(4),	15.5(5),
	1M =	14.3(5),	13.1(5),	69.9(5),	5.4(8),	10.0(5),	15.5(5),	33.3(5),	4.6(5),	1.7(4),	66.8(5),
	2M =	32.6(5),	9.4(5),	0.9(5),							
C(2B)b-C(3B)b /	0M =	61.4(5),	9.8(5),	73.0(5),	82.1(5),	82.1(5),	82.1(5),	41.9(6),	0.1(6),	22.4(5),	66.9(5),
	1M =	20.8(5),	21.6(5),	12.1(5),	22.1(8),	51.5(5),	66.9(5),	31.8(6),	66.3(6),	41.1(5),	1.5(5),
	2M =	55.1(6),	5.2(6),	69.1(6),							
-C(21B) /	0M =	54.2(5),	33.7(4),	39.6(4),	23.1(4),	23.1(4),	23.1(4),	77.0(5),	4.9(5),	25.3(4),	6.4(5),
	1M =	78.7(5),	29.2(5),	22.1(5),	82.7(8),	2.9(5),	6.4(5),	0.3(5),	18.5(5),	78.1(4),	5.5(5),
	2M =	46.3(5),	58.1(5),	18.1(5),							
Cu(1)c-0(21A) /	0M =	3.6(2),	45.0(2),	19.4(2),	0.2(2),	0.2(2),	0.2(2),	10.8(3),	84.3(3),	69.91(14),	0.3(2),
	1M =	0.5(2),	34.0(3),	50.3(3),	8.6(7),	26.5(2),	0.3(2),	50.0(3),	17.0(3),	10.0(2),	85.7(3),
	2M =	33.5(4),	27.9(4),	13.5(3),							
-0(1)c /	0M =	48.9(3),	30.0(2),	29.6(2),	16.3(2),	16.3(2),	16.3(2),	66.6(3),	4.1(4),	14.41(18),	0.4(3),
	1M =	88.3(3),	28.7(3),	33.9(3),	79.4(7),	1.0(3),	0.4(3),	3.3(3),	15.0(3),	67.7(2),	3.7(3),

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	2M =	34.6(4),	54.9(4),	13.9(4),							
-O(11A) /	0M =	24.9(2),	58.8(2),	10.4(2),	33.1(2),	33.1(2),	33.1(2),	1.7(3),	60.1(3),	41.21(14),	35.4(2),
	1M =	0.6(2),	57.3(3),	24.9(3),	7.7(7),	61.5(2),	35.4(2),	84.6(3),	50.1(3),	1.9(2),	58.9(3),
	2M =	6.8(4),	33.8(4),	47.0(3),							
-O(12B) /	0M =	42.1(2),	25.5(2),	55.2(2),	74.9(2),	74.9(2),	74.9(2),	21.2(3),	3.0(3),	13.94(16),	86.8(2),
	1M =	0.5(3),	38.8(3),	22.0(3),	1.4(7),	61.2(2),	86.8(2),	37.6(3),	66.4(3),	20.3(2),	1.7(3),
	2M =	38.9(4),	14.5(4),	70.0(4),							
Cu(2)c-O(1) /	0M =	0.0(2),	83.8(2),	2.4(2),	22.3(2),	22.3(2),	22.3(2),	25.5(3),	41.6(4),	39.78(18),	34.2(3),
	1M =	32.6(3),	82.2(3),	0.4(3),	38.9(7),	51.2(3),	34.2(3),	55.8(3),	34.4(3),	25.7(2),	41.1(3),
	2M =	19.8(4),	64.9(4),	33.2(4),							
-O(1)c /	0M =	0.0(2),	12.2(2),	28.1(2),	20.0(2),	20.0(2),	20.0(2),	0.4(3),	53.3(4),	51.40(18),	26.4(3),
	1M =	19.6(3),	0.6(3),	76.3(3),	11.2(7),	1.6(3),	26.4(3),	21.3(3),	5.1(3),	0.7(2),	54.2(3),
	2M =	32.5(4),	0.4(4),	8.8(4),							
-O(11B) /	0M =	76.6(2),	9.5(2),	73.6(2),	59.1(2),	59.1(2),	59.1(2),	66.0(3),	4.3(3),	29.31(15),	42.8(2),
	1M =	44.1(2),	0.4(3),	0.3(3),	46.2(7),	32.8(2),	42.8(2),	19.6(3),	49.6(3),	65.1(2),	5.5(3),
	2M =	66.0(4),	28.1(4),	50.7(4),							
-O(12A) /	0M =	11.6(3),	73.3(2),	9.4(2),	34.2(2),	34.2(2),	34.2(2),	14.0(3),	39.5(4),	31.82(18),	45.3(3),
	1M =	23.7(3),	83.3(3),	0.4(3),	28.9(7),	63.2(3),	45.3(3),	63.0(3),	46.4(3),	14.3(2),	38.7(3),
	2M =	8.2(4),	54.1(4),	45.3(4),							
-O(22A) /	0M =	7.3(2),	9.8(2),	20.8(2),	14.2(2),	14.2(2),	14.2(2),	7.0(3),	52.6(4),	46.05(18),	22.2(3),
	1M =	26.5(3),	0.6(3),	83.6(3),	18.0(7),	1.4(3),	22.2(3),	23.3(3),	0.2(3),	8.1(2),	53.2(3),
	2M =	24.9(4),	5.1(4),	3.9(4),							
Na(1)c-O(4W)c /	0M =	27.1(3),	49.3(3),	7.6(3),	27.5(3),	27.5(3),	27.5(3),	6.7(4),	67.9(4),	44.7(3),	26.5(3),
	1M =	8.5(4),	45.5(4),	37.0(4),	0.6(7),	52.2(3),	26.5(3),	75.1(4),	44.7(4),	7.1(3),	66.6(4),
	2M =	8.1(4),	24.8(5),	41.1(4),							
-O(5W)c /	0M =	31.1(10),	9.5(10),	55.7(10),	58.3(10),	58.3(10),	58.3(10),	18.5(10),	19.8(10),	33.7(10),	64.5(10),
	1M =	4.9(10),	23.3(10),	43.0(10),	0.5(12),	38.4(10),	64.5(10),	14.8(10),	44.0(10),	17.4(10),	21.1(10),
	2M =	46.8(10),	6.9(10),	47.8(10),							
-O(6W)c /	0M =	26.5(5),	47.6(5),	12.2(5),	5.3(5),	5.3(5),	5.3(5),	48.8(5),	6.4(6),	17.1(5),	22.0(5),
	1M =	68.1(5),	50.1(5),	32.3(5),	68.7(8),	22.2(5),	22.0(5),	17.0(5),	8.2(5),	49.7(5),	6.3(5),
	2M =	22.8(6),	68.4(6),	9.2(6),							
-O(22A) /	0M =	46.1(3),	46.1(2),	45.8(2),	22.9(2),	22.9(2),	22.9(2),	70.1(3),	25.3(4),	46.13(19),	8.1(3),
	1M =	59.3(3),	36.9(3),	2.3(3),	68.0(7),	4.3(3),	8.1(3),	14.0(3),	12.5(3),	69.7(2),	26.0(3),
	2M =	59.4(4),	64.5(4),	13.4(4),							
O(11A)-C(11A) /	0M =	35.8(5),	12.9(4),	7.9(4),	14.5(4),	14.5(4),	14.5(4),	29.2(5),	51.4(5),	30.6(4),	4.1(5),
	1M =	41.2(5),	8.2(5),	64.3(5),	32.2(8),	23.7(5),	4.1(5),	40.1(5),	26.7(5),	30.1(4),	50.9(5),
	2M =	0.6(5),	9.9(5),	23.3(5),							
O(11B)-C(11B) /	0M =	42.9(5),	25.6(5),	17.3(5),	29.2(5),	29.2(5),	29.2(5),	27.8(5),	54.8(5),	30.1(5),	20.9(5),
	1M =	32.2(5),	23.5(5),	48.3(5),	24.2(8),	41.4(5),	20.9(5),	56.5(5),	43.3(5),	28.4(5),	53.8(5),
	2M =	5.7(6),	1.0(6),	39.6(6),							
O(12A)-C(11A) /	0M =	11.5(5),	33.6(5),	8.8(5),	21.2(5),	21.2(5),	21.2(5),	28.6(5),	9.7(5),	4.8(4),	37.4(5),
	1M =	51.7(5),	42.5(5),	50.9(5),	47.7(8),	26.8(5),	37.4(5),	12.3(5),	17.8(5),	29.7(5),	10.1(5),
	2M =	0.6(6),	46.8(6),	20.2(5),							
O(12B)-C(11B) /	0M =	5.5(5),	9.2(5),	33.6(5),	26.3(5),	26.3(5),	26.3(5),	4.0(5),	48.7(5),	50.7(4),	32.5(5),
	1M =	17.1(5),	3.0(5),	72.0(5),	9.2(8),	7.4(5),	32.5(5),	15.7(5),	11.4(5),	2.8(5),	49.7(5),
	2M =	36.5(6),	1.0(6),	15.1(5),							
O(21A)-C(21A) /	0M =	30.8(4),	59.5(4),	37.3(4),	12.6(4),	12.6(4),	12.6(4),	53.5(5),	41.0(5),	58.5(4),	0.2(4),
	1M =	46.0(5),	47.7(5),	8.5(5),	55.2(8),	17.1(4),	0.2(4),	29.8(5),	0.5(5),	53.2(4),	41.5(5),

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	2M =	54.5(5),	67.6(5),	1.1(5),							
0(21B)-C(21B) /	0M =	3.3(5),	14.5(5),	22.0(5),	26.4(5),	26.4(5),	26.4(5),	13.8(6),	27.8(6),	25.7(5),	39.4(5),
	1M =	36.9(5),	25.4(5),	67.7(5),	30.5(8),	19.9(5),	39.4(5),	0.0(6),	16.9(6),	15.0(5),	28.5(5),
	2M =	18.0(6),	25.9(6),	20.1(6),							
0(22A)-C(21A) /	0M =	32.6(5),	33.5(5),	12.6(5),	0.2(5),	0.2(5),	0.2(5),	49.9(5),	7.2(5),	6.0(5),	16.8(5),
	1M =	73.2(5),	36.7(5),	44.1(5),	67.8(8),	11.5(5),	16.8(5),	3.6(5),	0.6(5),	51.0(5),	7.1(5),
	2M =	19.2(6),	55.3(6),	1.1(6),							
0(22B)-C(21B) /	0M =	41.7(5),	15.0(5),	69.3(5),	51.3(5),	51.3(5),	51.3(5),	39.7(5),	32.7(6),	54.2(5),	45.7(5),
	1M =	16.8(5),	1.3(5),	34.9(5),	23.1(8),	21.7(5),	45.7(5),	0.2(5),	34.1(5),	38.5(5),	34.1(5),
	2M =	71.7(6),	19.7(6),	37.4(6),							
C(1A)c-C(2A)c /	0M =	17.3(5),	26.2(5),	37.6(5),	49.3(5),	49.3(5),	49.3(5),	0.3(5),	10.3(5),	17.8(5),	63.9(5),
	1M =	22.5(5),	39.6(5),	44.8(5),	19.3(8),	43.8(5),	63.9(5),	22.0(5),	41.6(5),	0.8(5),	11.3(5),
	2M =	26.8(6),	26.8(6),	44.8(6),							
-C(11A) /	0M =	25.7(5),	61.9(4),	17.4(4),	41.8(4),	41.8(4),	41.8(4),	0.5(5),	47.1(5),	31.4(4),	47.4(5),
	1M =	7.0(5),	66.6(5),	11.3(5),	12.7(8),	72.5(5),	47.4(5),	78.8(5),	57.4(5),	0.4(4),	45.9(5),
	2M =	0.4(5),	38.5(5),	55.1(5),							
C(1B)c-C(2B)c /	0M =	3.1(6),	41.4(6),	19.5(6),	35.8(5),	35.8(5),	35.8(5),	17.2(6),	0.1(6),	1.5(5),	52.5(6),
	1M =	38.7(6),	53.3(6),	40.0(6),	37.1(9),	43.2(6),	52.5(6),	26.8(6),	34.2(6),	18.2(5),	0.6(6),
	2M =	7.7(6),	45.9(6),	36.4(6),							
-C(11B) /	0M =	59.4(5),	14.5(4),	68.3(4),	86.8(4),	86.8(4),	86.8(4),	38.3(5),	3.5(5),	18.2(4),	70.6(5),
	1M =	17.9(5),	26.3(5),	11.3(5),	18.6(8),	56.1(5),	70.6(5),	36.0(5),	70.5(5),	37.5(4),	2.1(5),
	2M =	50.4(5),	0.8(5),	73.5(5),							
C(2A)c-C(3A)c /	0M =	24.6(5),	62.8(5),	15.0(5),	39.1(5),	39.1(5),	39.1(5),	0.3(5),	50.3(5),	34.4(5),	44.2(5),
	1M =	6.5(5),	65.7(5),	14.1(5),	12.6(8),	69.6(5),	44.2(5),	80.9(5),	55.1(5),	0.3(5),	49.2(5),
	2M =	2.8(6),	38.7(6),	52.6(6),							
-C(21A) /	0M =	3.2(5),	24.2(5),	24.1(5),	11.4(4),	11.4(4),	11.4(4),	2.8(5),	65.9(5),	59.8(4),	15.5(5),
	1M =	14.3(5),	13.1(5),	69.9(5),	5.4(8),	10.0(5),	15.5(5),	33.3(5),	4.6(5),	1.7(4),	66.8(5),
	2M =	32.6(5),	9.4(5),	0.9(5),							
C(2B)c-C(3B)c /	0M =	61.4(5),	9.8(5),	73.0(5),	82.1(5),	82.1(5),	82.1(5),	41.9(6),	0.1(6),	22.4(5),	66.9(5),
	1M =	20.8(5),	21.6(5),	12.1(5),	22.1(8),	51.5(5),	66.9(5),	31.8(6),	66.3(6),	41.1(5),	1.5(5),
	2M =	55.1(6),	5.2(6),	69.1(6),							
-C(21B) /	0M =	54.2(5),	33.7(4),	39.6(4),	23.1(4),	23.1(4),	23.1(4),	77.0(5),	4.9(5),	25.3(4),	6.4(5),
	1M =	78.7(5),	29.2(5),	22.1(5),	82.7(8),	2.9(5),	6.4(5),	0.3(5),	18.5(5),	78.1(4),	5.5(5),
	2M =	46.3(5),	58.1(5),	18.1(5),							
Cu(1)d-0(1)d /	0M =	48.9(3),	30.0(2),	29.6(2),	16.3(2),	16.3(2),	16.3(2),	66.6(3),	4.1(4),	14.41(18),	0.4(3),
	1M =	88.3(3),	28.7(3),	33.9(3),	79.4(7),	1.0(3),	0.4(3),	3.3(3),	15.0(3),	67.7(2),	3.7(3),
	2M =	34.6(4),	54.9(4),	13.9(4),							
-0(11A) /	0M =	24.9(2),	58.8(2),	10.4(2),	33.1(2),	33.1(2),	33.1(2),	1.7(3),	60.1(3),	41.21(14),	35.4(2),
	1M =	0.6(2),	57.3(3),	24.9(3),	7.7(7),	61.5(2),	35.4(2),	84.6(3),	50.1(3),	1.9(2),	58.9(3),
	2M =	6.8(4),	33.8(4),	47.0(3),							
-0(12B) /	0M =	42.1(2),	25.5(2),	55.2(2),	74.9(2),	74.9(2),	74.9(2),	21.2(3),	3.0(3),	13.94(16),	86.8(2),
	1M =	0.5(3),	38.8(3),	22.0(3),	1.4(7),	61.2(2),	86.8(2),	37.6(3),	66.4(3),	20.3(2),	1.7(3),
	2M =	38.9(4),	14.5(4),	70.0(4),							
Cu(2)d-0(1)d /	0M =	0.0(2),	12.2(2),	28.1(2),	20.0(2),	20.0(2),	20.0(2),	0.4(3),	53.3(4),	51.40(18),	26.4(3),
	1M =	19.6(3),	0.6(3),	76.3(3),	11.2(7),	1.6(3),	26.4(3),	21.3(3),	5.1(3),	0.7(2),	54.2(3),
	2M =	32.5(4),	0.4(4),	8.8(4),							
-0(11B) /	0M =	76.6(2),	9.5(2),	73.6(2),	59.1(2),	59.1(2),	59.1(2),	66.0(3),	4.3(3),	29.31(15),	42.8(2),
	1M =	44.1(2),	0.4(3),	0.3(3),	46.2(7),	32.8(2),	42.8(2),	19.6(3),	49.6(3),	65.1(2),	5.5(3),

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	2M =	66.0(4),	28.1(4),	50.7(4),							
-O(12A) /	0M =	11.6(3),	73.3(2),	9.4(2),	34.2(2),	34.2(2),	34.2(2),	14.0(3),	39.5(4),	31.82(18),	45.3(3),
	1M =	23.7(3),	83.3(3),	0.4(3),	28.9(7),	63.2(3),	45.3(3),	63.0(3),	46.4(3),	14.3(2),	38.7(3),
	2M =	8.2(4),	54.1(4),	45.3(4),							
Na(1)d-O(4W)d /	0M =	27.1(3),	49.3(3),	7.6(3),	27.5(3),	27.5(3),	27.5(3),	6.7(4),	67.9(4),	44.7(3),	26.5(3),
	1M =	8.5(4),	45.5(4),	37.0(4),	0.6(7),	52.2(3),	26.5(3),	75.1(4),	44.7(4),	7.1(3),	66.6(4),
	2M =	8.1(4),	24.8(5),	41.1(4),							
-O(5W)d /	0M =	31.1(10),	9.5(10),	55.7(10),	58.3(10),	58.3(10),	58.3(10),	18.5(10),	19.8(10),	33.7(10),	64.5(10),
	1M =	4.9(10),	23.3(10),	43.0(10),	0.5(12),	38.4(10),	64.5(10),	14.8(10),	44.0(10),	17.4(10),	21.1(10),
	2M =	46.8(10),	6.9(10),	47.8(10),							
-O(6W)d /	0M =	26.5(5),	47.6(5),	12.2(5),	5.3(5),	5.3(5),	5.3(5),	48.8(5),	6.4(6),	17.1(5),	22.0(5),
	1M =	68.1(5),	50.1(5),	32.3(5),	68.7(8),	22.2(5),	22.0(5),	17.0(5),	8.2(5),	49.7(5),	6.3(5),
	2M =	22.8(6),	68.4(6),	9.2(6),							
-O(22A) /	0M =	46.1(3),	46.1(2),	45.8(2),	22.9(2),	22.9(2),	22.9(2),	70.1(3),	25.3(4),	46.13(19),	8.1(3),
	1M =	59.3(3),	36.9(3),	2.3(3),	68.0(7),	4.3(3),	8.1(3),	14.0(3),	12.5(3),	69.7(2),	26.0(3),
	2M =	59.4(4),	64.5(4),	13.4(4),							
O(11A)-C(11A) /	0M =	35.8(5),	12.9(4),	7.9(4),	14.5(4),	14.5(4),	14.5(4),	29.2(5),	51.4(5),	30.6(4),	4.1(5),
	1M =	41.2(5),	8.2(5),	64.3(5),	32.2(8),	23.7(5),	4.1(5),	40.1(5),	26.7(5),	30.1(4),	50.9(5),
	2M =	0.6(5),	9.9(5),	23.3(5),							
O(11B)-C(11B) /	0M =	42.9(5),	25.6(5),	17.3(5),	29.2(5),	29.2(5),	29.2(5),	27.8(5),	54.8(5),	30.1(5),	20.9(5),
	1M =	32.2(5),	23.5(5),	48.3(5),	24.2(8),	41.4(5),	20.9(5),	56.5(5),	43.3(5),	28.4(5),	53.8(5),
	2M =	5.7(6),	1.0(6),	39.6(6),							
O(12A)-C(11A) /	0M =	11.5(5),	33.6(5),	8.8(5),	21.2(5),	21.2(5),	21.2(5),	28.6(5),	9.7(5),	4.8(4),	37.4(5),
	1M =	51.7(5),	42.5(5),	50.9(5),	47.7(8),	26.8(5),	37.4(5),	12.3(5),	17.8(5),	29.7(5),	10.1(5),
	2M =	0.6(6),	46.8(6),	20.2(5),							
O(12B)-C(11B) /	0M =	5.5(5),	9.2(5),	33.6(5),	26.3(5),	26.3(5),	26.3(5),	4.0(5),	48.7(5),	50.7(4),	32.5(5),
	1M =	17.1(5),	3.0(5),	72.0(5),	9.2(8),	7.4(5),	32.5(5),	15.7(5),	11.4(5),	2.8(5),	49.7(5),
	2M =	36.5(6),	1.0(6),	15.1(5),							
O(21A)-C(21A) /	0M =	30.8(4),	59.5(4),	37.3(4),	12.6(4),	12.6(4),	12.6(4),	53.5(5),	41.0(5),	58.5(4),	0.2(4),
	1M =	46.0(5),	47.7(5),	8.5(5),	55.2(8),	17.1(4),	0.2(4),	29.8(5),	0.5(5),	53.2(4),	41.5(5),
	2M =	54.5(5),	67.6(5),	1.1(5),							
O(21B)-C(21B) /	0M =	3.3(5),	14.5(5),	22.0(5),	26.4(5),	26.4(5),	26.4(5),	13.8(6),	27.8(6),	25.7(5),	39.4(5),
	1M =	36.9(5),	25.4(5),	67.7(5),	30.5(8),	19.9(5),	39.4(5),	0.0(6),	16.9(6),	15.0(5),	28.5(5),
	2M =	18.0(6),	25.9(6),	20.1(6),							
O(22A)-C(21A) /	0M =	32.6(5),	33.5(5),	12.6(5),	0.2(5),	0.2(5),	0.2(5),	49.9(5),	7.2(5),	6.0(5),	16.8(5),
	1M =	73.2(5),	36.7(5),	44.1(5),	67.8(8),	11.5(5),	16.8(5),	3.6(5),	0.6(5),	51.0(5),	7.1(5),
	2M =	19.2(6),	55.3(6),	1.1(6),							
O(22B)-C(21B) /	0M =	41.7(5),	15.0(5),	69.3(5),	51.3(5),	51.3(5),	51.3(5),	39.7(5),	32.7(6),	54.2(5),	45.7(5),
	1M =	16.8(5),	1.3(5),	34.9(5),	23.1(8),	21.7(5),	45.7(5),	0.2(5),	34.1(5),	38.5(5),	34.1(5),
	2M =	71.7(6),	19.7(6),	37.4(6),							
C(1A)d-C(2A)d /	0M =	17.3(5),	26.2(5),	37.6(5),	49.3(5),	49.3(5),	49.3(5),	0.3(5),	10.3(5),	17.8(5),	63.9(5),
	1M =	22.5(5),	39.6(5),	44.8(5),	19.3(8),	43.8(5),	63.9(5),	22.0(5),	41.6(5),	0.8(5),	11.3(5),
	2M =	26.8(6),	26.8(6),	44.8(6),							
-C(11A) /	0M =	25.7(5),	61.9(4),	17.4(4),	41.8(4),	41.8(4),	41.8(4),	0.5(5),	47.1(5),	31.4(4),	47.4(5),
	1M =	7.0(5),	66.6(5),	11.3(5),	12.7(8),	72.5(5),	47.4(5),	78.8(5),	57.4(5),	0.4(4),	45.9(5),
	2M =	0.4(5),	38.5(5),	55.1(5),							
C(1B)d-C(3B) /	0M =	56.9(5),	28.9(5),	39.4(5),	24.9(5),	24.9(5),	24.9(5),	76.3(5),	0.1(5),	20.7(4),	8.1(5),
	1M =	80.0(5),	25.0(5),	25.7(5),	79.4(8),	6.5(5),	8.1(5),	5.1(5),	21.7(5),	77.5(5),	0.5(5),

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	2M =	44.0(6),	53.6(6),	21.0(5),							
-C(2B)d /	0M =	3.1(6),	41.4(6),	19.5(6),	35.8(5),	35.8(5),	35.8(5),	17.2(6),	0.1(6),	1.5(5),	52.5(6),
	1M =	38.7(6),	53.3(6),	40.0(6),	37.1(9),	43.2(6),	52.5(6),	26.8(6),	34.2(6),	18.2(5),	0.6(6),
	2M =	7.7(6),	45.9(6),	36.4(6),							
-C(11B) /	0M =	59.4(5),	14.5(4),	68.3(4),	86.8(4),	86.8(4),	86.8(4),	38.3(5),	3.5(5),	18.2(4),	70.6(5),
	1M =	17.9(5),	26.3(5),	11.3(5),	18.6(8),	56.1(5),	70.6(5),	36.0(5),	70.5(5),	37.5(4),	2.1(5),
	2M =	50.4(5),	0.8(5),	73.5(5),							
C(2A)d-C(3A)d /	0M =	24.6(5),	62.8(5),	15.0(5),	39.1(5),	39.1(5),	39.1(5),	0.3(5),	50.3(5),	34.4(5),	44.2(5),
	1M =	6.5(5),	65.7(5),	14.1(5),	12.6(8),	69.6(5),	44.2(5),	80.9(5),	55.1(5),	0.3(5),	49.2(5),
	2M =	2.8(6),	38.7(6),	52.6(6),							
-C(21A) /	0M =	3.2(5),	24.2(5),	24.1(5),	11.4(4),	11.4(4),	11.4(4),	2.8(5),	65.9(5),	59.8(4),	15.5(5),
	1M =	14.3(5),	13.1(5),	69.9(5),	5.4(8),	10.0(5),	15.5(5),	33.3(5),	4.6(5),	1.7(4),	66.8(5),
	2M =	32.6(5),	9.4(5),	0.9(5),							
C(2B)d-C(3B)d /	0M =	61.4(5),	9.8(5),	73.0(5),	82.1(5),	82.1(5),	82.1(5),	41.9(6),	0.1(6),	22.4(5),	66.9(5),
	1M =	20.8(5),	21.6(5),	12.1(5),	22.1(8),	51.5(5),	66.9(5),	31.8(6),	66.3(6),	41.1(5),	1.5(5),
	2M =	55.1(6),	5.2(6),	69.1(6),							
-C(21B) /	0M =	54.2(5),	33.7(4),	39.6(4),	23.1(4),	23.1(4),	23.1(4),	77.0(5),	4.9(5),	25.3(4),	6.4(5),
	1M =	78.7(5),	29.2(5),	22.1(5),	82.7(8),	2.9(5),	6.4(5),	0.3(5),	18.5(5),	78.1(4),	5.5(5),
	2M =	46.3(5),	58.1(5),	18.1(5),							
Cu(1)e-0(21A) /	0M =	3.6(2),	45.0(2),	19.4(2),	0.2(2),	0.2(2),	0.2(2),	10.8(3),	84.3(3),	69.91(14),	0.3(2),
	1M =	0.5(2),	34.0(3),	50.3(3),	8.6(7),	26.5(2),	0.3(2),	50.0(3),	17.0(3),	10.0(2),	85.7(3),
	2M =	33.5(4),	27.9(4),	13.5(3),							
-0(21B) /	0M =	49.2(3),	33.9(2),	32.4(2),	17.2(2),	17.2(2),	17.2(2),	69.8(3),	1.1(4),	19.78(18),	0.4(3),
	1M =	85.8(3),	31.4(3),	28.7(3),	84.6(7),	0.6(3),	0.4(3),	0.2(3),	14.2(3),	70.9(2),	1.6(3),
	2M =	38.8(4),	58.9(4),	13.4(4),							
-0(1)e /	0M =	48.9(3),	30.0(2),	29.6(2),	16.3(2),	16.3(2),	16.3(2),	66.6(3),	4.1(4),	14.41(18),	0.4(3),
	1M =	88.3(3),	28.7(3),	33.9(3),	79.4(7),	1.0(3),	0.4(3),	3.3(3),	15.0(3),	67.7(2),	3.7(3),
	2M =	34.6(4),	54.9(4),	13.9(4),							
-0(11A) /	0M =	24.9(2),	58.8(2),	10.4(2),	33.1(2),	33.1(2),	33.1(2),	1.7(3),	60.1(3),	41.21(14),	35.4(2),
	1M =	0.6(2),	57.3(3),	24.9(3),	7.7(7),	61.5(2),	35.4(2),	84.6(3),	50.1(3),	1.9(2),	58.9(3),
	2M =	6.8(4),	33.8(4),	47.0(3),							
-0(12B) /	0M =	42.1(2),	25.5(2),	55.2(2),	74.9(2),	74.9(2),	74.9(2),	21.2(3),	3.0(3),	13.94(16),	86.8(2),
	1M =	0.5(3),	38.8(3),	22.0(3),	1.4(7),	61.2(2),	86.8(2),	37.6(3),	66.4(3),	20.3(2),	1.7(3),
	2M =	38.9(4),	14.5(4),	70.0(4),							
Cu(2)e-0(1)b /	0M =	0.0(2),	83.8(2),	2.4(2),	22.3(2),	22.3(2),	22.3(2),	25.5(3),	41.6(4),	39.78(18),	34.2(3),
	1M =	32.6(3),	82.2(3),	0.4(3),	38.9(7),	51.2(3),	34.2(3),	55.8(3),	34.4(3),	25.7(2),	41.1(3),
	2M =	19.8(4),	64.9(4),	33.2(4),							
-0(1)e /	0M =	0.0(2),	12.2(2),	28.1(2),	20.0(2),	20.0(2),	20.0(2),	0.4(3),	53.3(4),	51.40(18),	26.4(3),
	1M =	19.6(3),	0.6(3),	76.3(3),	11.2(7),	1.6(3),	26.4(3),	21.3(3),	5.1(3),	0.7(2),	54.2(3),
	2M =	32.5(4),	0.4(4),	8.8(4),							
-0(11B) /	0M =	76.6(2),	9.5(2),	73.6(2),	59.1(2),	59.1(2),	59.1(2),	66.0(3),	4.3(3),	29.31(15),	42.8(2),
	1M =	44.1(2),	0.4(3),	0.3(3),	46.2(7),	32.8(2),	42.8(2),	19.6(3),	49.6(3),	65.1(2),	5.5(3),
	2M =	66.0(4),	28.1(4),	50.7(4),							
-0(12A) /	0M =	11.6(3),	73.3(2),	9.4(2),	34.2(2),	34.2(2),	34.2(2),	14.0(3),	39.5(4),	31.82(18),	45.3(3),
	1M =	23.7(3),	83.3(3),	0.4(3),	28.9(7),	63.2(3),	45.3(3),	63.0(3),	46.4(3),	14.3(2),	38.7(3),
	2M =	8.2(4),	54.1(4),	45.3(4),							
Na(1)e-0(11B) /	0M =	16.3(3),	44.4(2),	6.5(2),	11.8(2),	11.8(2),	11.8(2),	0.2(3),	82.4(4),	57.33(19),	10.4(3),
	1M =	8.3(3),	36.3(3),	49.5(3),	0.6(7),	36.3(3),	10.4(3),	59.8(3),	28.8(3),	0.9(2),	81.2(3),

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	2M =	20.7(4),	23.0(4),	25.2(4),							
-O(4W)e /	0M =	27.1(3),	49.3(3),	7.6(3),	27.5(3),	27.5(3),	27.5(3),	6.7(4),	67.9(4),	44.7(3),	26.5(3),
	1M =	8.5(4),	45.5(4),	37.0(4),	0.6(7),	52.2(3),	26.5(3),	75.1(4),	44.7(4),	7.1(3),	66.6(4),
	2M =	8.1(4),	24.8(5),	41.1(4),							
-O(5W)e /	0M =	31.1(10),	9.5(10),	55.7(10),	58.3(10),	58.3(10),	58.3(10),	18.5(10),	19.8(10),	33.7(10),	64.5(10),
	1M =	4.9(10),	23.3(10),	43.0(10),	0.5(12),	38.4(10),	64.5(10),	14.8(10),	44.0(10),	17.4(10),	21.1(10),
	2M =	46.8(10),	6.9(10),	47.8(10),							
-O(6W)e /	0M =	26.5(5),	47.6(5),	12.2(5),	5.3(5),	5.3(5),	5.3(5),	48.8(5),	6.4(6),	17.1(5),	22.0(5),
	1M =	68.1(5),	50.1(5),	32.3(5),	68.7(8),	22.2(5),	22.0(5),	17.0(5),	8.2(5),	49.7(5),	6.3(5),
	2M =	22.8(6),	68.4(6),	9.2(6),							
-O(22A) /	0M =	46.1(3),	46.1(2),	45.8(2),	22.9(2),	22.9(2),	22.9(2),	70.1(3),	25.3(4),	46.13(19),	8.1(3),
	1M =	59.3(3),	36.9(3),	2.3(3),	68.0(7),	4.3(3),	8.1(3),	14.0(3),	12.5(3),	69.7(2),	26.0(3),
	2M =	59.4(4),	64.5(4),	13.4(4),							
O(11A)-C(11A) /	0M =	35.8(5),	12.9(4),	7.9(4),	14.5(4),	14.5(4),	14.5(4),	29.2(5),	51.4(5),	30.6(4),	4.1(5),
	1M =	41.2(5),	8.2(5),	64.3(5),	32.2(8),	23.7(5),	4.1(5),	40.1(5),	26.7(5),	30.1(4),	50.9(5),
	2M =	0.6(5),	9.9(5),	23.3(5),							
O(11B)-C(11B) /	0M =	42.9(5),	25.6(5),	17.3(5),	29.2(5),	29.2(5),	29.2(5),	27.8(5),	54.8(5),	30.1(5),	20.9(5),
	1M =	32.2(5),	23.5(5),	48.3(5),	24.2(8),	41.4(5),	20.9(5),	56.5(5),	43.3(5),	28.4(5),	53.8(5),
	2M =	5.7(6),	1.0(6),	39.6(6),							
O(12A)-C(11A) /	0M =	11.5(5),	33.6(5),	8.8(5),	21.2(5),	21.2(5),	21.2(5),	28.6(5),	9.7(5),	4.8(4),	37.4(5),
	1M =	51.7(5),	42.5(5),	50.9(5),	47.7(8),	26.8(5),	37.4(5),	12.3(5),	17.8(5),	29.7(5),	10.1(5),
	2M =	0.6(6),	46.8(6),	20.2(5),							
O(12B)-C(11B) /	0M =	5.5(5),	9.2(5),	33.6(5),	26.3(5),	26.3(5),	26.3(5),	4.0(5),	48.7(5),	50.7(4),	32.5(5),
	1M =	17.1(5),	3.0(5),	72.0(5),	9.2(8),	7.4(5),	32.5(5),	15.7(5),	11.4(5),	2.8(5),	49.7(5),
	2M =	36.5(6),	1.0(6),	15.1(5),							
O(21A)-C(21A) /	0M =	30.8(4),	59.5(4),	37.3(4),	12.6(4),	12.6(4),	12.6(4),	53.5(5),	41.0(5),	58.5(4),	0.2(4),
	1M =	46.0(5),	47.7(5),	8.5(5),	55.2(8),	17.1(4),	0.2(4),	29.8(5),	0.5(5),	53.2(4),	41.5(5),
	2M =	54.5(5),	67.6(5),	1.1(5),							
O(21B)-C(21B) /	0M =	3.3(5),	14.5(5),	22.0(5),	26.4(5),	26.4(5),	26.4(5),	13.8(6),	27.8(6),	25.7(5),	39.4(5),
	1M =	36.9(5),	25.4(5),	67.7(5),	30.5(8),	19.9(5),	39.4(5),	0.0(6),	16.9(6),	15.0(5),	28.5(5),
	2M =	18.0(6),	25.9(6),	20.1(6),							
O(22A)-C(21A) /	0M =	32.6(5),	33.5(5),	12.6(5),	0.2(5),	0.2(5),	0.2(5),	49.9(5),	7.2(5),	6.0(5),	16.8(5),
	1M =	73.2(5),	36.7(5),	44.1(5),	67.8(8),	11.5(5),	16.8(5),	3.6(5),	0.6(5),	51.0(5),	7.1(5),
	2M =	19.2(6),	55.3(6),	1.1(6),							
O(22B)-C(21B) /	0M =	41.7(5),	15.0(5),	69.3(5),	51.3(5),	51.3(5),	51.3(5),	39.7(5),	32.7(6),	54.2(5),	45.7(5),
	1M =	16.8(5),	1.3(5),	34.9(5),	23.1(8),	21.7(5),	45.7(5),	0.2(5),	34.1(5),	38.5(5),	34.1(5),
	2M =	71.7(6),	19.7(6),	37.4(6),							
C(1A)e-C(2A)e /	0M =	17.3(5),	26.2(5),	37.6(5),	49.3(5),	49.3(5),	49.3(5),	0.3(5),	10.3(5),	17.8(5),	63.9(5),
	1M =	22.5(5),	39.6(5),	44.8(5),	19.3(8),	43.8(5),	63.9(5),	22.0(5),	41.6(5),	0.8(5),	11.3(5),
	2M =	26.8(6),	26.8(6),	44.8(6),							
-C(11A) /	0M =	25.7(5),	61.9(4),	17.4(4),	41.8(4),	41.8(4),	41.8(4),	0.5(5),	47.1(5),	31.4(4),	47.4(5),
	1M =	7.0(5),	66.6(5),	11.3(5),	12.7(8),	72.5(5),	47.4(5),	78.8(5),	57.4(5),	0.4(4),	45.9(5),
	2M =	0.4(5),	38.5(5),	55.1(5),							
C(1B)e-C(2B)e /	0M =	3.1(6),	41.4(6),	19.5(6),	35.8(5),	35.8(5),	35.8(5),	17.2(6),	0.1(6),	1.5(5),	52.5(6),
	1M =	38.7(6),	53.3(6),	40.0(6),	37.1(9),	43.2(6),	52.5(6),	26.8(6),	34.2(6),	18.2(5),	0.6(6),
	2M =	7.7(6),	45.9(6),	36.4(6),							
-C(11B) /	0M =	59.4(5),	14.5(4),	68.3(4),	86.8(4),	86.8(4),	86.8(4),	38.3(5),	3.5(5),	18.2(4),	70.6(5),
	1M =	17.9(5),	26.3(5),	11.3(5),	18.6(8),	56.1(5),	70.6(5),	36.0(5),	70.5(5),	37.5(4),	2.1(5),

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	2M =	50.4(5),	0.8(5),	73.5(5),							
C(2A)e-C(3A)e /	0M =	24.6(5),	62.8(5),	15.0(5),	39.1(5),	39.1(5),	39.1(5),	0.3(5),	50.3(5),	34.4(5),	44.2(5),
	1M =	6.5(5),	65.7(5),	14.1(5),	12.6(8),	69.6(5),	44.2(5),	80.9(5),	55.1(5),	0.3(5),	49.2(5),
	2M =	2.8(6),	38.7(6),	52.6(6),							
-C(21A) /	0M =	3.2(5),	24.2(5),	24.1(5),	11.4(4),	11.4(4),	11.4(4),	2.8(5),	65.9(5),	59.8(4),	15.5(5),
	1M =	14.3(5),	13.1(5),	69.9(5),	5.4(8),	10.0(5),	15.5(5),	33.3(5),	4.6(5),	1.7(4),	66.8(5),
	2M =	32.6(5),	9.4(5),	0.9(5),							
C(2B)e-C(3B)e /	0M =	61.4(5),	9.8(5),	73.0(5),	82.1(5),	82.1(5),	82.1(5),	41.9(6),	0.1(6),	22.4(5),	66.9(5),
	1M =	20.8(5),	21.6(5),	12.1(5),	22.1(8),	51.5(5),	66.9(5),	31.8(6),	66.3(6),	41.1(5),	1.5(5),
	2M =	55.1(6),	5.2(6),	69.1(6),							
-C(21B) /	0M =	54.2(5),	33.7(4),	39.6(4),	23.1(4),	23.1(4),	23.1(4),	77.0(5),	4.9(5),	25.3(4),	6.4(5),
	1M =	78.7(5),	29.2(5),	22.1(5),	82.7(8),	2.9(5),	6.4(5),	0.3(5),	18.5(5),	78.1(4),	5.5(5),
	2M =	46.3(5),	58.1(5),	18.1(5),							
Cu(1)f-O(1)f /	0M =	48.9(3),	30.0(2),	29.6(2),	16.3(2),	16.3(2),	16.3(2),	66.6(3),	4.1(4),	14.41(18),	0.4(3),
	1M =	88.3(3),	28.7(3),	33.9(3),	79.4(7),	1.0(3),	0.4(3),	3.3(3),	15.0(3),	67.7(2),	3.7(3),
	2M =	34.6(4),	54.9(4),	13.9(4),							
-O(11A) /	0M =	24.9(2),	58.8(2),	10.4(2),	33.1(2),	33.1(2),	33.1(2),	1.7(3),	60.1(3),	41.21(14),	35.4(2),
	1M =	0.6(2),	57.3(3),	24.9(3),	7.7(7),	61.5(2),	35.4(2),	84.6(3),	50.1(3),	1.9(2),	58.9(3),
	2M =	6.8(4),	33.8(4),	47.0(3),							
-O(12B) /	0M =	42.1(2),	25.5(2),	55.2(2),	74.9(2),	74.9(2),	74.9(2),	21.2(3),	3.0(3),	13.94(16),	86.8(2),
	1M =	0.5(3),	38.8(3),	22.0(3),	1.4(7),	61.2(2),	86.8(2),	37.6(3),	66.4(3),	20.3(2),	1.7(3),
	2M =	38.9(4),	14.5(4),	70.0(4),							
Cu(2)f-O(1)f /	0M =	0.0(2),	12.2(2),	28.1(2),	20.0(2),	20.0(2),	20.0(2),	0.4(3),	53.3(4),	51.40(18),	26.4(3),
	1M =	19.6(3),	0.6(3),	76.3(3),	11.2(7),	1.6(3),	26.4(3),	21.3(3),	5.1(3),	0.7(2),	54.2(3),
	2M =	32.5(4),	0.4(4),	8.8(4),							
-O(11B) /	0M =	76.6(2),	9.5(2),	73.6(2),	59.1(2),	59.1(2),	59.1(2),	66.0(3),	4.3(3),	29.31(15),	42.8(2),
	1M =	44.1(2),	0.4(3),	0.3(3),	46.2(7),	32.8(2),	42.8(2),	19.6(3),	49.6(3),	65.1(2),	5.5(3),
	2M =	66.0(4),	28.1(4),	50.7(4),							
-O(12A) /	0M =	11.6(3),	73.3(2),	9.4(2),	34.2(2),	34.2(2),	34.2(2),	14.0(3),	39.5(4),	31.82(18),	45.3(3),
	1M =	23.7(3),	83.3(3),	0.4(3),	28.9(7),	63.2(3),	45.3(3),	63.0(3),	46.4(3),	14.3(2),	38.7(3),
	2M =	8.2(4),	54.1(4),	45.3(4),							
Na(1)f-O(4W)f /	0M =	27.1(3),	49.3(3),	7.6(3),	27.5(3),	27.5(3),	27.5(3),	6.7(4),	67.9(4),	44.7(3),	26.5(3),
	1M =	8.5(4),	45.5(4),	37.0(4),	0.6(7),	52.2(3),	26.5(3),	75.1(4),	44.7(4),	7.1(3),	66.6(4),
	2M =	8.1(4),	24.8(5),	41.1(4),							
-O(5W)f /	0M =	31.1(10),	9.5(10),	55.7(10),	58.3(10),	58.3(10),	58.3(10),	18.5(10),	19.8(10),	33.7(10),	64.5(10),
	1M =	4.9(10),	23.3(10),	43.0(10),	0.5(12),	38.4(10),	64.5(10),	14.8(10),	44.0(10),	17.4(10),	21.1(10),
	2M =	46.8(10),	6.9(10),	47.8(10),							
-O(6W)f /	0M =	26.5(5),	47.6(5),	12.2(5),	5.3(5),	5.3(5),	5.3(5),	48.8(5),	6.4(6),	17.1(5),	22.0(5),
	1M =	68.1(5),	50.1(5),	32.3(5),	68.7(8),	22.2(5),	22.0(5),	17.0(5),	8.2(5),	49.7(5),	6.3(5),
	2M =	22.8(6),	68.4(6),	9.2(6),							
-O(22A) /	0M =	46.1(3),	46.1(2),	45.8(2),	22.9(2),	22.9(2),	22.9(2),	70.1(3),	25.3(4),	46.13(19),	8.1(3),
	1M =	59.3(3),	36.9(3),	2.3(3),	68.0(7),	4.3(3),	8.1(3),	14.0(3),	12.5(3),	69.7(2),	26.0(3),
	2M =	59.4(4),	64.5(4),	13.4(4),							
O(11A)-C(11A) /	0M =	35.8(5),	12.9(4),	7.9(4),	14.5(4),	14.5(4),	14.5(4),	29.2(5),	51.4(5),	30.6(4),	4.1(5),
	1M =	41.2(5),	8.2(5),	64.3(5),	32.2(8),	23.7(5),	4.1(5),	40.1(5),	26.7(5),	30.1(4),	50.9(5),
	2M =	0.6(5),	9.9(5),	23.3(5),							
O(11B)-C(11B) /	0M =	42.9(5),	25.6(5),	17.3(5),	29.2(5),	29.2(5),	29.2(5),	27.8(5),	54.8(5),	30.1(5),	20.9(5),
	1M =	32.2(5),	23.5(5),	48.3(5),	24.2(8),	41.4(5),	20.9(5),	56.5(5),	43.3(5),	28.4(5),	53.8(5),

=====											
O(12A)-C(11A) /	2M =	5.7(6),	1.0(6),	39.6(6),							
	0M =	11.5(5),	33.6(5),	8.8(5),	21.2(5),	21.2(5),	21.2(5),	28.6(5),	9.7(5),	4.8(4),	37.4(5),
	1M =	51.7(5),	42.5(5),	50.9(5),	47.7(8),	26.8(5),	37.4(5),	12.3(5),	17.8(5),	29.7(5),	10.1(5),
O(12B)-C(11B) /	2M =	0.6(6),	46.8(6),	20.2(5),							
	0M =	5.5(5),	9.2(5),	33.6(5),	26.3(5),	26.3(5),	26.3(5),	4.0(5),	48.7(5),	50.7(4),	32.5(5),
	1M =	17.1(5),	3.0(5),	72.0(5),	9.2(8),	7.4(5),	32.5(5),	15.7(5),	11.4(5),	2.8(5),	49.7(5),
O(21A)-C(21A) /	2M =	36.5(6),	1.0(6),	15.1(5),							
	0M =	30.8(4),	59.5(4),	37.3(4),	12.6(4),	12.6(4),	12.6(4),	53.5(5),	41.0(5),	58.5(4),	0.2(4),
	1M =	46.0(5),	47.7(5),	8.5(5),	55.2(8),	17.1(4),	0.2(4),	29.8(5),	0.5(5),	53.2(4),	41.5(5),
O(21B)-C(21B) /	2M =	54.5(5),	67.6(5),	1.1(5),							
	0M =	3.3(5),	14.5(5),	22.0(5),	26.4(5),	26.4(5),	26.4(5),	13.8(6),	27.8(6),	25.7(5),	39.4(5),
	1M =	36.9(5),	25.4(5),	67.7(5),	30.5(8),	19.9(5),	39.4(5),	0.0(6),	16.9(6),	15.0(5),	28.5(5),
O(22A)-C(21A) /	2M =	18.0(6),	25.9(6),	20.1(6),							
	0M =	32.6(5),	33.5(5),	12.6(5),	0.2(5),	0.2(5),	0.2(5),	49.9(5),	7.2(5),	6.0(5),	16.8(5),
	1M =	73.2(5),	36.7(5),	44.1(5),	67.8(8),	11.5(5),	16.8(5),	3.6(5),	0.6(5),	51.0(5),	7.1(5),
O(22B)-C(21B) /	2M =	19.2(6),	55.3(6),	1.1(6),							
	0M =	41.7(5),	15.0(5),	69.3(5),	51.3(5),	51.3(5),	51.3(5),	39.7(5),	32.7(6),	54.2(5),	45.7(5),
	1M =	16.8(5),	1.3(5),	34.9(5),	23.1(8),	21.7(5),	45.7(5),	0.2(5),	34.1(5),	38.5(5),	34.1(5),
C(1A)f-C(3A) /	2M =	71.7(6),	19.7(6),	37.4(6),							
	0M =	7.7(5),	26.3(5),	19.2(5),	6.2(5),	6.2(5),	6.2(5),	0.3(5),	69.2(5),	58.4(5),	10.5(5),
	1M =	15.9(5),	16.0(5),	69.1(5),	6.9(8),	14.8(5),	10.5(5),	37.9(5),	9.8(5),	1.3(5),	69.9(5),
-C(2A)f /	2M =	28.6(6),	9.8(6),	6.1(6),							
	0M =	17.3(5),	26.2(5),	37.6(5),	49.3(5),	49.3(5),	49.3(5),	0.3(5),	10.3(5),	17.8(5),	63.9(5),
	1M =	22.5(5),	39.6(5),	44.8(5),	19.3(8),	43.8(5),	63.9(5),	22.0(5),	41.6(5),	0.8(5),	11.3(5),
-C(11A) /	2M =	26.8(6),	26.8(6),	44.8(6),							
	0M =	25.7(5),	61.9(4),	17.4(4),	41.8(4),	41.8(4),	41.8(4),	0.5(5),	47.1(5),	31.4(4),	47.4(5),
	1M =	7.0(5),	66.6(5),	11.3(5),	12.7(8),	72.5(5),	47.4(5),	78.8(5),	57.4(5),	0.4(4),	45.9(5),
C(1B)f-C(2B)f /	2M =	0.4(5),	38.5(5),	55.1(5),							
	0M =	3.1(6),	41.4(6),	19.5(6),	35.8(5),	35.8(5),	35.8(5),	17.2(6),	0.1(6),	1.5(5),	52.5(6),
	1M =	38.7(6),	53.3(6),	40.0(6),	37.1(9),	43.2(6),	52.5(6),	26.8(6),	34.2(6),	18.2(5),	0.6(6),
-C(11B) /	2M =	7.7(6),	45.9(6),	36.4(6),							
	0M =	59.4(5),	14.5(4),	68.3(4),	86.8(4),	86.8(4),	86.8(4),	38.3(5),	3.5(5),	18.2(4),	70.6(5),
	1M =	17.9(5),	26.3(5),	11.3(5),	18.6(8),	56.1(5),	70.6(5),	36.0(5),	70.5(5),	37.5(4),	2.1(5),
C(2A)f-C(3A)f /	2M =	50.4(5),	0.8(5),	73.5(5),							
	0M =	24.6(5),	62.8(5),	15.0(5),	39.1(5),	39.1(5),	39.1(5),	0.3(5),	50.3(5),	34.4(5),	44.2(5),
	1M =	6.5(5),	65.7(5),	14.1(5),	12.6(8),	69.6(5),	44.2(5),	80.9(5),	55.1(5),	0.3(5),	49.2(5),
-C(21A) /	2M =	2.8(6),	38.7(6),	52.6(6),							
	0M =	3.2(5),	24.2(5),	24.1(5),	11.4(4),	11.4(4),	11.4(4),	2.8(5),	65.9(5),	59.8(4),	15.5(5),
	1M =	14.3(5),	13.1(5),	69.9(5),	5.4(8),	10.0(5),	15.5(5),	33.3(5),	4.6(5),	1.7(4),	66.8(5),
C(2B)f-C(3B)f /	2M =	32.6(5),	9.4(5),	0.9(5),							
	0M =	61.4(5),	9.8(5),	73.0(5),	82.1(5),	82.1(5),	82.1(5),	41.9(6),	0.1(6),	22.4(5),	66.9(5),
	1M =	20.8(5),	21.6(5),	12.1(5),	22.1(8),	51.5(5),	66.9(5),	31.8(6),	66.3(6),	41.1(5),	1.5(5),
-C(21B) /	2M =	55.1(6),	5.2(6),	69.1(6),							
	0M =	54.2(5),	33.7(4),	39.6(4),	23.1(4),	23.1(4),	23.1(4),	77.0(5),	4.9(5),	25.3(4),	6.4(5),
	1M =	78.7(5),	29.2(5),	22.1(5),	82.7(8),	2.9(5),	6.4(5),	0.3(5),	18.5(5),	78.1(4),	5.5(5),
	2M =	46.3(5),	58.1(5),	18.1(5),							

Ring Puckering Analysis (Cremer & Pople) - (e.s.d. following Norrestam, Acta Cryst. (1981), A37, 764-765)

Symmetrical Forms

References

6-Membered Rings : C : Chair - Th = 0.0
 H : Half-Chair- Th = 50.8; Phi = k X 60 + 30
 E : Envelope - Th = 54.7; Phi = k X 60
 S : Screw-Boat- Th = 67.5; Phi = k X 60 + 30
 B : Boat - Th = 90.0; Phi = k X 60
 T : Twist-Boat- Th = 90.0; Phi = k X 60 + 30

J.C.A. Boeyens, J.Cryst.Mol.Struct. 8,(1978),317-320

Definitions (All Values Rounded on Esd)

Dev - Deviation of Atom I from Cremer&Pople Plane (Defined Differently from Least-Squares Plane)
 Cs(I),C2(I) - Mirror Plane and 2-Axis Asym. Par. for Atom I (See Duax et al., Topics in Stereochemistry,V-9, (1976) pp.271-383)
 Cs(I-J),C2(I-J)- Asymmetry Parameters for Bond I-J
 Tors(I-J) - Torsion Angle for Bond I-J

Descriptors for Torsion Angles

Descriptors for Ring Substituents (J.Appl.Cryst.,1983,16,431)

Torsion Angle Range	Full Descriptor	Short Descriptor
0 to 30 Deg	+ Syn-Periplanar	+sp
30 to 90	+ Syn-Clinal	+sc
90 to 150	+ Anti-Clinal	+ac
150 to 180	+ Anti-Periplanar	+ap
0 to -30	- Syn-Periplanar	-sp
-30 to -90	- Syn-Clinal	-sc
-90 to -150	- Anti-Clinal	-ac
-150 to -180	- Anti-Periplanar	-ap

Angle Range of Subst.	Full Descriptor	Short Descriptor
0 to 30 Deg.	Axial	ax
30 to 60	Bisectional	bi
60 to 90	Equatorial	eq

*** NOTE *** - For Ring Puckering Comparisons: Make Sure that the Absolute Configuration, Pivot Atom and Cyclic Sense Agree.
 - The "RING AT1 AT2 AT3 ... ATn" Instruction Gives the User Explicit Choice of Pivot Atom (AT1) and Sense (AT2).
 - Use TRNS Instructions to Obtain the Required Absolute Configuration.
 - The Values of Theta and Phi [= Phi(2)] Depend on the Abs. Conf. and the Choice of the First and Second Ring Atom.
 - Alternatively, Appropriate Phase Shifts may be Applied to the Same Effect (see Below)

For Correct Usage of C&P Puckering Parameters see also: D. Cremer, Acta Cryst. (1984). B40, 498-500.

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4-Membered Ring ( 1)  Cu(2)  -->  O(1)  -->  Cu(2)c -->  O(1)c  -->
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Dev. (Ang)	0.000(2)	0.000(6)	0.000(2)	0.000(6)
Cs(I)-Asym-Par (Deg)	0.00	0.00	0.00	0.00
C2(I)-Asym-Par (Deg)	0.00	0.00	0.00	0.00
Ring Bond Angle(Deg)	83.6(2)	96.4(3)	83.6(2)	96.4(3)
Tors(I-J) (Deg)	0.0(2)	0.0(2)	0.0(2)	0.0(2)
Cs(I-J)-Asym-Par (Deg)	0.00	0.00	0.00	0.00
C2(I-J)-Asym-Par (Deg)	0.00	0.00	0.00	0.00
Ring Bond Distance (Ang)	1.964(6)	1.942(6)	1.964(6)	1.942(6)

Weighted Average Ring Bond Distance = 1.9530(30, 64) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.00(10, 0) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Angle between Cu(2) O(1) O(1)c and O(1) Cu(2)cO(1)c = 180.0(3) deg.

Angle between Cu(2) O(1) Cu(2)c and Cu(2) Cu(2)cO(1)c = 180.0(4) deg.

No C & P - Puckering Analysis since <Tau> = 0.0 < 5.0 Deg.

Centroid Cg(1) : x ,y ,z	0.0000(3)	0.00000(18)	0.00000(18)
X0,Y0,Z0	0.000(2)	0.0000(19)	0.000(2)

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6-Membered Ring (2)	Cu(1) -->	O(1) -->	Cu(2) -->	O(11B) -->	C(11B) -->	O(12B) -->

					sp2	sp3
Dev. (Ang)	-0.608(2)	0.416(6)	0.061(2)	-0.346(7)	0.154(8)	0.323(7)
Cs(I)-Asym-Par (Deg)	11.9(6)	63.4(6)	70.8(6)	11.9(6)	63.4(6)	70.8(6)
C2(I)-Asym-Par (Deg)	85.6(5)	58.8(4)	49.6(7)	85.6(5)	58.8(4)	49.6(7)
Ring Bond Angle(Deg)	91.3(2)	110.5(3)	102.5(2)	119.6(5)	124.5(7)	124.4(5)
Tors(I-J) (Deg)	59.2(3)	-31.7(3)	-26.3(7)	35.4(11)	15.0(11)	-67.3(6)
Cs(I-J)-Asym-Par (Deg)	70.5(5)	32.4(7)	52.5(8)	70.5(5)	32.4(7)	52.5(8)
C2(I-J)-Asym-Par (Deg)	38.6(8)	94.5(8)	56.8(8)	38.6(8)	94.5(8)	56.8(8)
Ring Bond Distance (Ang)	1.920(6)	1.964(6)	2.220(6)	1.261(10)	1.282(10)	2.159(6)

Weighted Average Ring Bond Distance = 1.9446(28,999) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 45.04(19,705) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Cremer & Pople Puckering Parameters [D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97, (1975), 1354-1358]

Q(2) =	0.831(5) Ang.,	Phi(2) =	186.4(4) Deg
Q(3) =	-0.321(6) Ang.		

:: C & P - Puckering Analysis may be DUBIOUS since %(Bond Distance Range/Average) = 49.3 > 25.0 %

Puckering Amplitude (Q) = 0.891(5) Ang, Theta = 111.1(4) Deg, Phi = 186.4(4) Deg

*** NOTE *** - A Change of the Absolute Configuration Transforms Theta into 180 - Theta and Phi into 180 + Phi.
 - A Cyclic Forward Shift of the Pivot Atom from At1 to At2 Transforms Theta into 180 - Theta and Phi into Phi + 120.
 - A Change of the Sense Transforms Theta into 180 - Theta and Phi into 180 - Phi, and Vice Versa.

Conformational Analysis (G.G. Evans & J.A. Boeyens, Acta Cryst. (1989), B45, 581-590)

Coefficients of Primitive and Normalised Forms			
M	Primitive	Coefficient	Angular Value

CosForm	2	0.666	0.568
SinForm		0.185	0.158
	3		0.274
			-1.0
Analysis of Ring Substituents			
=====			
Bond	Distance	Angle with C&P Plane Normal	

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Cu(1)  - O(11A)      2.023(5)      33.4(2)  Bi
Cu(1)  - O(21B)b     1.927(6)      54.0(2)  Bi
Cu(1)  - O(21A)e     2.030(5)      47.0(2)  Bi
O(1)   - Cu(2)c      1.942(6)       5.6(2)  Ax
Cu(2)  - O(12A)      1.927(6)      17.1(2)  Ax
Cu(2)  - O(22A)a     1.936(6)      82.1(2)  Eq
Cu(2)  - O(1)c       1.942(6)       5.6(2)  Ax
O(11B) - Na(1)a      2.418(8)      47.8(2)  Bi
C(11B) - C(1B)       1.495(11)     76.1(4)  Eq
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=====
6-Membered Ring ( 3)  Cu(1)  -->  O(1)  -->  Cu(2)  -->  O(12A)  -->  C(11A)  -->  O(11A)  -->
-----
```

				sp3	sp2	sp3
Dev. (Ang)	0.383(2)	-0.557(6)	0.358(2)	0.015(6)	-0.189(8)	-0.010(6)
Cs(I)-Asym-Par (Deg)	52.8(7)	2.2(6)	54.2(7)	52.8(7)	2.2(6)	54.2(7)
C2(I)-Asym-Par (Deg)	62.2(6)	81.6(4)	61.0(6)	62.2(6)	81.6(4)	61.0(6)
Ring Bond Angle(Deg)	88.8(2)	110.5(3)	92.9(2)	128.0(5)	127.6(7)	130.8(5)
Tors(I-J) (Deg)	-63.5(3)	65.2(3)	-25.3(7)	-12.0(13)	10.6(13)	28.4(7)
Cs(I-J)-Asym-Par (Deg)	67.0(6)	63.9(6)	53.1(9)	67.0(6)	63.9(6)	53.1(9)
C2(I-J)-Asym-Par (Deg)	36.4(8)	39.3(8)	75.7(9)	36.4(8)	39.3(8)	75.7(9)
Ring Bond Distance (Ang)	1.920(6)	1.964(6)	1.927(6)	1.281(10)	1.243(9)	2.023(5)

Weighted Average Ring Bond Distance = 1.8568(26,999) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 56.50(19,734) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Cremer & Pople Puckering Parameters [D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97, (1975), 1354-1358]

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-----
Q(2)  =      0.647(6) Ang.,  Phi(2) =      57.8(5) Deg
Q(3)  =      0.451(6) Ang.
```

:: C & P - Puckering Analysis may be DUBIOUS since %(Bond Distance Range/Average) = 42.0 > 25.0 %

Puckering Amplitude (Q) = 0.788(5) Ang, Theta = 55.1(4) Deg, Phi = 57.8(5) Deg

*** NOTE *** - A Change of the Absolute Configuration Transforms Theta into 180 - Theta and Phi into 180 + Phi.
 - A Cyclic Forward Shift of the Pivot Atom from At1 to At2 Transforms Theta into 180 - Theta and Phi into Phi + 120.
 - A Change of the Sense Transforms Theta into 180 - Theta and Phi into 180 - Phi, and Vice Versa.

Conformational Analysis (G.G. Evans & J.A. Boeyens, Acta Cryst. (1989), B45, 581-590)

	Coefficients of Primitive and Normalised Forms		
M	Primitive	Coefficient	Angular Value

CosForm	2	0.603	0.547
SinForm		0.050	0.045
	3		0.408
			1.0

:: Note: This is a E-Form

Analysis of Ring Substituents

=====

Bond		Distance	Angle with C&P Plane Normal	

Cu(1)	- O(12B)	2.159(6)	34.1(2)	Bi
Cu(1)	- O(21B)b	1.927(6)	57.9(2)	Bi
Cu(1)	- O(21A)e	2.030(5)	71.3(2)	Eq
O(1)	- Cu(2)c	1.942(6)	88.5(2)	Eq
Cu(2)	- O(11B)	2.220(6)	16.4(2)	Ax
Cu(2)	- O(22A)a	1.936(6)	69.5(2)	Eq
Cu(2)	- O(1)c	1.942(6)	88.5(2)	Eq
C(11A)	- C(1A)	1.503(11)	71.8(4)	Eq

=====

6-Membered Ring (4)	Cu(1) -->	O(1) -->	Cu(2)c -->	O(22A) -->	C(21A) -->	O(21A) -->

					sp2	sp3
Dev. (Ang)	-0.132(2)	0.382(6)	-0.373(2)	0.114(6)	0.136(8)	-0.127(6)
Cs(I)-Asym-Par (Deg)	53.7(7)	26.4(7)	27.6(7)	53.7(7)	26.4(7)	27.6(7)
C2(I)-Asym-Par (Deg)	36.4(7)	59.3(4)	58.7(5)	36.4(7)	59.3(4)	58.7(5)
Ring Bond Angle(Deg)	92.0(2)	120.9(3)	94.4(2)	128.0(5)	127.5(7)	133.4(5)
Tors(I-J) (Deg)	40.3(3)	-54.2(3)	35.5(7)	-1.8(12)	-22.1(13)	1.0(7)
Cs(I-J)-Asym-Par (Deg)	38.8(6)	53.6(5)	41.6(9)	38.8(6)	53.6(5)	41.6(9)
C2(I-J)-Asym-Par (Deg)	56.4(8)	3.9(7)	57.6(9)	56.4(8)	3.9(7)	57.6(9)
Ring Bond Distance (Ang)	1.920(6)	1.942(6)	1.936(6)	1.266(10)	1.262(9)	2.030(5)

Weighted Average Ring Bond Distance = 1.8568(26,999) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 41.28(19,689) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Cremer & Pople Puckering Parameters [D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97, (1975), 1354-1358]

Q(2) =	0.509(6) Ang.,	Phi(2) =	268.3(6) Deg
Q(3) =	-0.301(5) Ang.		

:: C & P - Puckering Analysis may be DUBIOUS since %(Bond Distance Range/Average) = 41.4 > 25.0 %

Puckering Amplitude (Q) = 0.592(5) Ang, Theta = 120.6(5) Deg, Phi = 268.3(6) Deg

*** NOTE *** - A Change of the Absolute Configuration Transforms Theta into 180 - Theta and Phi into 180 + Phi.
 - A Cyclic Forward Shift of the Pivot Atom from At1 to At2 Transforms Theta into 180 - Theta and Phi into Phi + 120.
 - A Change of the Sense Transforms Theta into 180 - Theta and Phi into 180 - Phi, and Vice Versa.

Conformational Analysis (G.G. Evans & J.A. Boeyens, Acta Cryst. (1989), B45, 581-590)

Coefficients of Primitive and Normalised Forms			
M	Primitive	Coefficient	Angular Value

CosForm	2	0.030	0.037
SinForm		0.483	0.593
	3		0.370
			-1.0

:: Note: This is Very Similar to a H-Form

Analysis of Ring Substituents

=====

Bond	Distance	Angle with C&P Plane Normal

=====				
Cu(1)	- O(11A)	2.023(5)	56.7(2)	Bi
Cu(1)	- O(12B)	2.159(6)	14.4(2)	Ax
Cu(1)	- O(21B)b	1.927(6)	73.6(2)	Eq
O(1)	- Cu(2)	1.964(6)	69.7(2)	Eq
Cu(2)c	- O(1)c	1.964(6)	69.7(2)	Eq
Cu(2)c	- O(11B)c	2.220(6)	31.6(2)	Bi
Cu(2)c	- O(12A)c	1.927(6)	55.2(2)	Bi
O(22A)e	- Na(1)e	2.398(8)	67.8(2)	Eq
C(21A)e	- C(2A)e	1.489(11)	78.4(4)	Eq

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=====
6-Membered Ring ( 5)  Cu(2)  -->  O(22A)  -->  C(21A)  -->  O(21A)  -->  Cu(1)c  -->  O(1)c  -->
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```

		sp2		sp3			
Dev. (Ang)	0.373(2)	-0.114(6)	-0.136(8)	0.127(6)	0.132(2)	-0.382(6)	
Cs(I)-Asym-Par (Deg)	27.6(7)	53.7(7)	26.4(7)	27.6(7)	53.7(7)	26.4(7)	
C2(I)-Asym-Par (Deg)	58.7(5)	36.4(7)	59.3(4)	58.7(5)	36.4(7)	59.3(4)	
Ring Bond Angle(Deg)	94.4(2)	128.0(5)	127.5(7)	133.4(5)	92.0(2)	120.9(3)	
Tors(I-J) (Deg)	-35.5(7)	1.8(12)	22.1(13)	-1.0(7)	-40.3(3)	54.2(3)	
Cs(I-J)-Asym-Par (Deg)	41.6(9)	38.8(6)	53.6(5)	41.6(9)	38.8(6)	53.6(5)	
C2(I-J)-Asym-Par (Deg)	57.6(9)	56.4(8)	3.9(7)	57.6(9)	56.4(8)	3.9(7)	
Ring Bond Distance (Ang)	1.936(6)	1.266(10)	1.262(9)	2.030(5)	1.920(6)	1.942(6)	

Weighted Average Ring Bond Distance = 1.8568(26,999) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 41.28(19,689) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Cremer & Pople Puckering Parameters [D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97, (1975), 1354-1358]

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-----
Q(2) = 0.509(5) Ang., Phi(2) = 328.3(6) Deg
Q(3) = 0.301(5) Ang.
```

:: C & P - Puckering Analysis may be DUBIOUS since %(Bond Distance Range/Average) = 41.4 > 25.0 %

Puckering Amplitude (Q) = 0.592(5) Ang, Theta = 59.4(5) Deg, Phi = 328.3(6) Deg

*** NOTE *** - A Change of the Absolute Configuration Transforms Theta into 180 - Theta and Phi into 180 + Phi.
 - A Cyclic Forward Shift of the Pivot Atom from At1 to At2 Transforms Theta into 180 - Theta and Phi into Phi + 120.
 - A Change of the Sense Transforms Theta into 180 - Theta and Phi into 180 - Phi, and Vice Versa.

Conformational Analysis (G.G. Evans & J.A. Boeyens, Acta Cryst. (1989), B45, 581-590)

Coefficients of Primitive and Normalised Forms			
M	Primitive	Coefficient	Angular Value

CosForm	2	0.030	0.037 20.0
SinForm		0.483	0.593 22.0
	3		0.370 1.0

:: Note: This is Very Similar to a H-Form

Analysis of Ring Substituents

=====

Bond	Distance	Angle with C&P Plane Normal

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=====
Cu(2)   - O(1)           1.964(6)           69.7(2)   Eq
Cu(2)   - O(11B)         2.220(6)           31.6(2)   Bi
Cu(2)   - O(12A)         1.927(6)           55.2(2)   Bi
O(22A)a - Na(1)a         2.398(8)           67.8(2)   Eq
C(21A)a - C(2A)a        1.489(11)           78.4(4)   Eq
Cu(1)c   - O(11A)c       2.023(5)           56.7(2)   Bi
Cu(1)c   - O(12B)c       2.159(6)           14.4(2)   Ax
O(1)c    - Cu(2)c        1.964(6)           69.7(2)   Eq
=====

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=====
6-Membered Ring ( 6)  O(21A) -->  C(21A) -->  O(22A) -->  Cu(2)b -->  O(1)e  -->  Cu(1)e -->
-----
```

	sp3	sp2				
Dev. (Ang)	-0.127(6)	0.136(8)	0.114(6)	-0.373(2)	0.382(6)	-0.132(2)
Cs(I)-Asym-Par (Deg)	27.6(7)	26.4(7)	53.7(7)	27.6(7)	26.4(7)	53.7(7)
C2(I)-Asym-Par (Deg)	58.7(5)	59.3(4)	36.4(7)	58.7(5)	59.3(4)	36.4(7)
Ring Bond Angle(Deg)	133.4(5)	127.5(7)	128.0(5)	94.4(2)	120.9(3)	92.0(2)
Tors(I-J) (Deg)	22.1(13)	1.8(12)	-35.5(7)	54.2(3)	-40.3(3)	-1.0(7)
Cs(I-J)-Asym-Par (Deg)	53.6(5)	38.8(6)	41.6(9)	53.6(5)	38.8(6)	41.6(9)
C2(I-J)-Asym-Par (Deg)	3.9(7)	56.4(8)	57.6(9)	3.9(7)	56.4(8)	57.6(9)
Ring Bond Distance (Ang)	1.262(9)	1.266(10)	1.936(6)	1.942(6)	1.920(6)	2.030(5)

Weighted Average Ring Bond Distance = 1.8568(26,999) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 41.28(19,689) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Cremer & Pople Puckering Parameters [D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97, (1975), 1354-1358]

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-----
Q(2) = 0.509(5) Ang., Phi(2) = 211.8(6) Deg
Q(3) = 0.301(5) Ang.
```

:: C & P - Puckering Analysis may be DUBIOUS since %(Bond Distance Range/Average) = 41.4 > 25.0 %

Puckering Amplitude (Q) = 0.592(5) Ang, Theta = 59.4(5) Deg, Phi = 211.8(6) Deg

*** NOTE *** - A Change of the Absolute Configuration Transforms Theta into 180 - Theta and Phi into 180 + Phi.
 - A Cyclic Forward Shift of the Pivot Atom from At1 to At2 Transforms Theta into 180 - Theta and Phi into Phi + 120.
 - A Change of the Sense Transforms Theta into 180 - Theta and Phi into 180 - Phi, and Vice Versa.

Conformational Analysis (G.G. Evans & J.A. Boeyens, Acta Cryst. (1989), B45, 581-590)

Coefficients of Primitive and Normalised Forms			
M	Primitive	Coefficient	Angular Value

CosForm	2	0.032	0.039
SinForm		0.481	0.591
	3		0.370
			1.0

:: Note: This is Very Similar to a H-Form

Analysis of Ring Substituents

=====

Bond	Distance	Angle with C&P Plane Normal

C(21A)	- C(2A)	1.489(11)	78.4(4)	Eq
O(22A)	- Na(1)	2.398(8)	67.8(2)	Eq
Cu(2)b	- O(1)b	1.964(6)	69.7(2)	Eq
Cu(2)b	- O(11B)b	2.220(6)	31.6(2)	Bi
Cu(2)b	- O(12A)b	1.927(6)	55.2(2)	Bi
O(1)e	- Cu(2)e	1.964(6)	69.7(2)	Eq
Cu(1)e	- O(21B)c	1.927(6)	73.6(2)	Eq
Cu(1)e	- O(11A)e	2.023(5)	56.7(2)	Bi
Cu(1)e	- O(12B)e	2.159(6)	14.4(2)	Ax

6-Membered Ring (7)	C(1A) -->	C(2A) -->	C(3A) -->	C(1A)f -->	C(2A)f -->	C(3A)f -->
	sp2	sp2	sp2	sp2	sp2	sp2
Dev. (Ang)	-0.003(8)	0.003(8)	-0.003(8)	0.003(8)	-0.003(8)	0.003(8)
Cs(I)-Asym-Par (Deg)	0.00	0.00	0.00	0.00	0.00	0.00
C2(I)-Asym-Par (Deg)	1.8(10)	1.8(10)	1.8(10)	1.8(10)	1.8(10)	1.8(10)
Ring Bond Angle(Deg)	119.9(7)	118.9(7)	121.2(7)	119.9(7)	118.9(7)	121.2(7)
Tors(I-J) (Deg)	0.9(12)	-0.9(12)	0.9(12)	-0.9(12)	0.9(12)	-0.9(12)
Cs(I-J)-Asym-Par (Deg)	1.8(12)	1.8(12)	1.8(12)	1.8(12)	1.8(12)	1.8(12)
C2(I-J)-Asym-Par (Deg)	0.00	0.00	0.00	0.00	0.00	0.00
Ring Bond Distance (Ang)	1.395(11)	1.395(11)	1.394(11)	1.395(11)	1.395(11)	1.394(11)

Weighted Average Ring Bond Distance = 1.3947(45, 1) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.90(49, 0) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 0.9 < 5.0 Deg.

Centroid Cg(7) : x ,y ,z	0.5000(4)	0.5000(3)	0.0000(3)
X0,Y0,Z0	3.823(3)	5.272(3)	0.000(3)

6-Membered Ring (8)	C(1B) -->	C(2B) -->	C(3B) -->	C(1B)d -->	C(2B)d -->	C(3B)d -->
	sp2	sp2	sp2	sp2	sp2	sp2
Dev. (Ang)	-0.002(9)	0.002(9)	-0.002(9)	0.002(9)	-0.002(9)	0.002(9)
Cs(I)-Asym-Par (Deg)	0.00	0.1(11)	0.1(11)	0.00	0.1(11)	0.1(11)
C2(I)-Asym-Par (Deg)	0.9(11)	0.9(11)	0.9(11)	0.9(11)	0.9(11)	0.9(11)
Ring Bond Angle(Deg)	119.0(7)	120.4(8)	120.6(8)	119.0(7)	120.4(8)	120.6(8)
Tors(I-J) (Deg)	0.4(13)	-0.5(14)	0.4(14)	-0.4(13)	0.5(14)	-0.4(14)
Cs(I-J)-Asym-Par (Deg)	0.9(14)	0.8(14)	0.9(14)	0.9(14)	0.8(14)	0.9(14)
C2(I-J)-Asym-Par (Deg)	0.1(14)	0.00	0.1(14)	0.1(14)	0.00	0.1(14)
Ring Bond Distance (Ang)	1.404(13)	1.394(12)	1.412(11)	1.404(13)	1.394(12)	1.412(11)

Weighted Average Ring Bond Distance = 1.4038(49, 34) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.43(56, 2) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 0.4 < 5.0 Deg.

Centroid Cg(8) : x ,y ,z	0.0000(4)	0.0000(4)	0.5000(3)
X0,Y0,Z0	-1.570(4)	-0.265(4)	5.615(3)

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(1)	[1]	-> Cg(8)	[1554.01]	5.836(4)	-0.1522 0.9843 0.0889 -0.4777	81.39	18.14	85.31	0.478	5.546	
Cg(1)	[1]	-> Cg(8)	[1555.01]	5.836(4)	-0.1522 0.9843 0.0889 0.4777	81.39	18.14	85.31	0.478	5.546	
Cg(1)	[1]	-> Cg(8)	[2555.01]	5.836(4)	0.1522-0.9843-0.0889 0.4777	81.39	18.14	85.31	0.478	5.546	
Cg(1)	[1]	-> Cg(8)	[2556.01]	5.836(4)	0.1522-0.9843-0.0889 -0.4777	81.39	18.14	85.31	0.478	5.546	

				Min or Max	5.836	81.39	18.14	85.31	0.478	5.546	

- [1554] = X,Y,-1+Z
- [1555] = X,Y,Z
- [2555] = -X,-Y,-Z
- [2556] = -X,-Y,1-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.0000(3)	0.00000(18)	0.00000(18)	0.000(2)	0.0000(19)	0.000(2)
Cg(7)	0.5000(4)	0.5000(3)	0.0000(3)	3.823(3)	5.272(3)	0.000(3)
Cg(8)	0.0000(4)	0.0000(4)	0.5000(3)	-1.570(4)	-0.265(4)	5.615(3)

=====

Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + \text{Tolr}$, With Tolr = 0.2 Ang. ($X - I...J$) > 100. Deg.

Contact Radii : C H Cu Na O
(Angstrom) 1.70 1.20 2.32 1.77 1.52

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

=====

***** ARU = 1555.01 *****

=====

At(I)[1555.01]	At(J)	[	ARU(J)	]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J	
Cu(1)		0(1W)	[		]	3.886(11)	3.84	0.05		0.3734	0.0032	0.1375	0.5738	0.2534	0.3945	0(1)	131.6(2)
Cu(1)		0(11B)	[		]	3.319(6)<<	3.84	-0.52	Intra	0.3734	0.0032	0.1375	0.0501	0.1385	0.2275		
Cu(1)		0(12A)	[		]	3.392(6)<<	3.84	-0.45	Intra	0.3734	0.0032	0.1375	0.1711	0.2722	0.0309		
Cu(1)		0(22B)	[	1655.01]	]	3.133(7)<<	3.84	-0.71	Intra	0.3734	0.0032	0.1375	0.7695	-0.0749	0.1898	0(1)	138.4(2)
																0(12B)	122.4(2)
Cu(1)		0(11A)	[	2655.01]	]	3.983(6)	3.84	0.14	Intra	0.3734	0.0032	0.1375	0.5640	-0.1820	-0.1031	0(12B)	138.45(19)
Cu(1)		0(22A)	[	2655.01]	]	3.490(5)<<	3.84	-0.35	Intra	0.3734	0.0032	0.1375	0.1676	-0.2629	-0.0357	0(11A)	134.95(19)
Cu(1)		0(22B)	[	2555.01]	]	3.793(6) <	3.84	-0.05	Intra	0.3734	0.0032	0.1375	0.2305	0.0749	-0.1898	0(12B)	129.16(19)
Cu(2)		0(11A)	[		]	3.278(6)<<	3.84	-0.56	Intra	0.0052	0.1353	0.0313	0.4360	0.1820	0.1031		
Cu(2)		0(12B)	[		]	3.321(6)<<	3.84	-0.52	Intra	0.0052	0.1353	0.0313	0.2122	-0.0370	0.2561	0(12A)	104.4(2)
Cu(2)		0(21A)	[	1455.01]	]	3.267(6)<<	3.84	-0.57	Intra	0.0052	0.1353	0.0313	-0.4080	0.1841	-0.1062	0(1)	131.20(19)
																0(11B)	111.9(2)
																0(12A)	115.8(2)
Cu(2)		0(22B)	[		]	3.711(7) <	3.84	-0.13	Intra	0.0052	0.1353	0.0313	-0.2305	-0.0749	0.1898	0(12A)	151.3(2)
Cu(2)		0(4W)	[	2665.01]	]	3.895(11)	3.84	0.06	Intra	0.0052	0.1353	0.0313	-0.0143	0.4220	-0.1715	0(1)	112.8(2)
																0(11B)	128.2(2)
Cu(2)		0(11B)	[	2555.01]	]	4.025(6)	3.84	0.19	Intra	0.0052	0.1353	0.0313	-0.0501	-0.1385	-0.2275	0(11B)	135.06(19)
																0(12A)	116.0(2)
Cu(2)		0(12B)	[	2555.01]	]	3.437(6)<<	3.84	-0.40	Intra	0.0052	0.1353	0.0313	-0.2122	0.0370	-0.2561	0(11B)	153.7(2)
																0(12A)	110.0(2)
Cu(2)		0(22B)	[	2555.01]	]	3.544(6)<<	3.84	-0.30	Intra	0.0052	0.1353	0.0313	0.2305	0.0749	-0.1898	0(11B)	140.7(2)
Cu(2)		C(11B)	[	2555.01]	]	3.919(8) <	4.02	-0.10	Intra	0.0052	0.1353	0.0313	-0.1038	-0.0406	-0.2832	0(11B)	152.4(2)
																0(12A)	107.0(2)
O(1)		0(11A)	[		]	2.761(8)<<	3.04	-0.28	Intra	0.1675	0.0051	0.0040	0.4360	0.1820	0.1031		
O(1)		0(12A)	[		]	2.821(7)<<	3.04	-0.22	Intra	0.1675	0.0051	0.0040	0.1711	0.2722	0.0309		
O(1)		0(12B)	[		]	2.922(8) <	3.04	-0.12	Intra	0.1675	0.0051	0.0040	0.2122	-0.0370	0.2561		
O(1)		C(11A)	[		]	3.034(9) <	3.22	-0.19	Intra	0.1675	0.0051	0.0040	0.3403	0.2686	0.0559		

O(1)		O(1)	[2555.01]	2.604(8)<<	3.04	-0.44	Intra	0.1675	0.0051	0.0040	-0.1675-0.0051-0.0040	Cu(1)	130.3(3)
O(1)		O(11B)	[2555.01]	3.098(8)	3.04	0.06	Intra	0.1675	0.0051	0.0040	-0.0501-0.1385-0.2275	Cu(1)	145.6(3)
												Cu(2)	103.0(2)
O(1)		O(21A)	[2655.01]	2.843(8) <	3.04	-0.20	Intra	0.1675	0.0051	0.0040	0.4080-0.1841 0.1062	Cu(2)	146.4(3)
O(1)		O(22A)	[2655.01]	2.846(7) <	3.04	-0.19	Intra	0.1675	0.0051	0.0040	0.1676-0.2629-0.0357	Cu(2)	138.6(3)
O(1)		O(22B)	[2555.01]	2.574(8)<<	3.04	-0.47	Intra	0.1675	0.0051	0.0040	0.2305 0.0749-0.1898	Cu(1)	114.3(3)
												Cu(2)	101.8(3)
O(1)		C(21A)	[2655.01]	3.130(9) <	3.22	-0.09	Intra	0.1675	0.0051	0.0040	0.3261-0.2658 0.0277	Cu(2)	153.7(3)
O(4W)		O(6W)	[]	3.15(2)	3.04	0.11	Intra	1.0143	0.5780	0.1715	1.3090 0.4146 0.3320		
O(4W)		C(3A)	[]	3.242(14)	3.22	0.02	Intra	1.0143	0.5780	0.1715	0.6555 0.4980-0.0342		
O(4W)		Cu(2)	[2665.01]	3.895(11)	3.84	0.06	Intra	1.0143	0.5780	0.1715	0.9948 0.8647-0.0313	Na(1)	156.9(4)
O(4W)		>O(2W)	[2766.03]	3.044(19)	3.04	0.00		1.0143	0.5780	0.1715	1.2910 0.7351 0.3591	Na(1)	112.2(5)
O(4W)		O(12A)	[2665.01]	2.955(13) <	3.04	-0.09	Intra	1.0143	0.5780	0.1715	0.8289 0.7278-0.0309	Na(1)	135.0(5)
O(4W)		H(3A)	[2765.01]	2.58 <	2.72	-0.14		1.0143	0.5780	0.1715	1.2372 0.5029 0.0573		
*O(5W)		O(1W)	[]	2.70(4)<<	3.04	-0.34		0.8110	0.4080	0.3340	0.5738 0.2534 0.3945	Na(1)	130.1(9)
*O(5W)		O(7W)	[]	3.17(3)	3.04	0.13		0.8110	0.4080	0.3340	0.6260 0.6731 0.2986	Na(1)	116.0(9)
*O(5W)		<O(8W)	[]	2.27(3)<<	3.04	-0.77		0.8110	0.4080	0.3340	1 0.5000 0.5000	Na(1)	100.6(15)
O(6W)		O(1W)	[1655.02]	2.67(2)<<	3.04	-0.37		1.3090	0.4146	0.3320	1.5738 0.2534 0.3945	Na(1)	127.2(7)
O(6W)		O(4W)	[]	3.15(2)	3.04	0.11	Intra	1.3090	0.4146	0.3320	1.0143 0.5780 0.1715		
O(11A)		Cu(2)	[]	3.278(6)<<	3.84	-0.56	Intra	0.4360	0.1820	0.1031	0.0052 0.1353 0.0313		
O(11A)		O(1)	[]	2.761(8)<<	3.04	-0.28	Intra	0.4360	0.1820	0.1031	0.1675 0.0051 0.0040		
O(11A)		O(21A)	[]	3.013(8) <	3.04	-0.03	Intra	0.4360	0.1820	0.1031	0.5920 0.1841-0.1062	Cu(1)	111.4(2)
O(11A)		O(21B)	[1655.01]	2.728(8)<<	3.04	-0.31	Intra	0.4360	0.1820	0.1031	0.5746 0.0170 0.2756	C(11A)	156.2(5)
O(11A)		C(21A)	[]	2.859(10)<<	3.22	-0.36	Intra	0.4360	0.1820	0.1031	0.6739 0.2658-0.0277	Cu(1)	129.2(3)
O(11A)		Cu(1)	[2655.01]	3.983(6)	3.84	0.14	Intra	0.4360	0.1820	0.1031	0.6266-0.0032-0.1375	C(11A)	110.0(5)
O(11B)		Cu(1)	[]	3.319(6)<<	3.84	-0.52	Intra	0.0501	0.1385	0.2275	0.3734 0.0032 0.1375		
O(11B)		Na(1)	[1455.01]	2.418(8)<<	3.29	-0.87	Intra	0.0501	0.1385	0.2275	0.0070 0.3647 0.2180	C(11B)	152.3(5)
O(11B)		O(12A)	[]	3.088(9)	3.04	0.05	Intra	0.0501	0.1385	0.2275	0.1711 0.2722 0.0309	C(11B)	131.5(5)
O(11B)		O(22A)	[1455.01]	2.813(8)<<	3.04	-0.23	Intra	0.0501	0.1385	0.2275	-0.1676 0.2629 0.0357	C(11B)	152.6(5)
O(11B)		O(22B)	[]	3.052(9)	3.04	0.01	Intra	0.0501	0.1385	0.2275	-0.2305-0.0749 0.1898		
O(11B)		C(21B)	[]	3.204(11) <	3.22	-0.02	Intra	0.0501	0.1385	0.2275	-0.2717-0.0230 0.2756	Cu(2)	106.4(3)
O(11B)		Cu(2)	[2555.01]	4.025(6)	3.84	0.19	Intra	0.0501	0.1385	0.2275	-0.0052-0.1353-0.0313		
O(11B)		O(1)	[2555.01]	3.098(8)	3.04	0.06	Intra	0.0501	0.1385	0.2275	-0.1675-0.0051-0.0040		
O(12A)		Cu(1)	[]	3.392(6)<<	3.84	-0.45	Intra	0.1711	0.2722	0.0309	0.3734 0.0032 0.1375		
O(12A)		Na(1)	[1455.01]	2.961(9)<<	3.29	-0.33	Intra	0.1711	0.2722	0.0309	0.0070 0.3647 0.2180	C(11A)	118.7(5)
O(12A)		O(1)	[]	2.821(7)<<	3.04	-0.22	Intra	0.1711	0.2722	0.0309	0.1675 0.0051 0.0040		
O(12A)		O(11B)	[]	3.088(9)	3.04	0.05	Intra	0.1711	0.2722	0.0309	0.0501 0.1385 0.2275	C(11A)	108.1(5)
O(12A)		O(22A)	[1455.01]	2.672(8)<<	3.04	-0.37	Intra	0.1711	0.2722	0.0309	-0.1676 0.2629 0.0357	C(11A)	165.5(6)
O(12A)		O(4W)	[2665.01]	2.955(13) <	3.04	-0.09	Intra	0.1711	0.2722	0.0309	-0.0143 0.4220-0.1715	Cu(2)	103.9(3)
												C(11A)	118.1(5)
O(12A)		H(3A)	[2665.01]	2.47<<	2.72	-0.25	Intra	0.1711	0.2722	0.0309	0.2372 0.5029 0.0573	Cu(2)	147
O(12B)		Cu(2)	[]	3.321(6)<<	3.84	-0.52	Intra	0.2122-0.0370	0.2561		0.0052 0.1353 0.0313		
O(12B)		O(1)	[]	2.922(8) <	3.04	-0.12	Intra	0.2122-0.0370	0.2561		0.1675 0.0051 0.0040	C(11B)	102.5(5)
O(12B)		O(21B)	[1655.01]	2.835(9)<<	3.04	-0.20	Intra	0.2122-0.0370	0.2561		0.5746 0.0170 0.2756	C(11B)	125.7(5)
O(12B)		Cu(2)	[2555.01]	3.437(6)<<	3.84	-0.40	Intra	0.2122-0.0370	0.2561		-0.0052-0.1353-0.0313	C(11B)	102.5(5)
O(12B)		>O(2W)	[2656.03]	2.737(14)<<	3.04	-0.30		0.2122-0.0370	0.2561		0.2910-0.2649 0.3591	Cu(1)	111.7(5)
												C(11B)	123.7(7)
O(12B)		O(21A)	[2655.01]	3.024(8) <	3.04	-0.02	Intra	0.2122-0.0370	0.2561		0.4080-0.1841 0.1062	C(11B)	159.5(5)

O(12B)		H(3B)	[2556.01]	2.85	2.72	0.13	Intra	0.2122-0.0370 0.2561	0.2983 0.0332 0.5038	Cu(1)	126
O(21A)		Cu(2)	[1655.01]	3.267(6)<<	3.84	-0.57	Intra	0.5920 0.1841-0.1062	1.0051 0.1353 0.0313		
O(21A)		O(11A)	[]	3.013(8) <	3.04	-0.03	Intra	0.5920 0.1841-0.1062	0.4360 0.1820 0.1031		
O(21A)		C(11A)	[]	3.195(10) <	3.22	-0.03	Intra	0.5920 0.1841-0.1062	0.3403 0.2686 0.0559		
O(21A)		O(1)	[2655.01]	2.843(8) <	3.04	-0.20	Intra	0.5920 0.1841-0.1062	0.8325-0.0051-0.0040		
O(21A)		O(7W)	[2665.05]	2.922(17) <	3.04	-0.12		0.5920 0.1841-0.1062	0.3740 0.3269-0.2986	C(21A)	106.0(5)
O(21A)		O(12B)	[2655.01]	3.024(8) <	3.04	-0.02	Intra	0.5920 0.1841-0.1062	0.7878 0.0370-0.2561	C(21A)	120.2(5)
O(21A)		O(21B)	[2555.01]	2.878(8) <	3.04	-0.16	Intra	0.5920 0.1841-0.1062	0.4254-0.0170-0.2756	C(21A)	175.3(5)
O(21A)		O(22B)	[2555.01]	2.935(9) <	3.04	-0.11	Intra	0.5920 0.1841-0.1062	0.2305 0.0749-0.1898	C(21A)	136.9(5)
O(21A)		C(21B)	[2555.01]	3.163(10) <	3.22	-0.06	Intra	0.5920 0.1841-0.1062	0.2717 0.0230-0.2756	C(21A)	159.3(5)
O(21B)		O(1W)	[1455.02]	2.805(12)<<	3.04	-0.23		-0.4254 0.0170 0.2756	-0.4262 0.2534 0.3945	C(21B)	115.3(6)
O(21B)		O(11A)	[1455.01]	2.728(8)<<	3.04	-0.31	Intra	-0.4254 0.0170 0.2756	-0.5640 0.1820 0.1031	C(21B)	114.9(5)
O(21B)		O(12B)	[1455.01]	2.835(9)<<	3.04	-0.20	Intra	-0.4254 0.0170 0.2756	-0.7878-0.0370 0.2561	C(21B)	149.1(5)
O(21B)		H(3B)	[]	2.58 <	2.72	-0.14	Intra	-0.4254 0.0170 0.2756	-0.2983-0.0332 0.4962		
O(21B)		O(21A)	[2555.01]	2.878(8) <	3.04	-0.16	Intra	-0.4254 0.0170 0.2756	-0.5920-0.1841 0.1062		
O(22A)		O(11B)	[1655.01]	2.813(8)<<	3.04	-0.23	Intra	0.8324 0.2629 0.0357	1.0501 0.1385 0.2275	C(21A)	142.0(5)
O(22A)		O(12A)	[1655.01]	2.672(8)<<	3.04	-0.37	Intra	0.8324 0.2629 0.0357	1.1711 0.2722 0.0309	C(21A)	144.2(5)
O(22A)		H(3A)	[]	2.74	2.72	0.02	Intra	0.8324 0.2629 0.0357	0.7628 0.4971-0.0573		
O(22A)		Cu(1)	[2655.01]	3.490(5)<<	3.84	-0.35	Intra	0.8324 0.2629 0.0357	0.6266-0.0032-0.1375	Na(1)	152.5(2)
O(22A)		O(1)	[2655.01]	2.846(7) <	3.04	-0.19	Intra	0.8324 0.2629 0.0357	0.8325-0.0051-0.0040	Na(1)	121.0(3)
O(22B)		Cu(1)	[1455.01]	3.133(7)<<	3.84	-0.71	Intra	-0.2305-0.0749 0.1898	-0.6266 0.0032 0.1375		
O(22B)		Cu(2)	[]	3.711(7) <	3.84	-0.13	Intra	-0.2305-0.0749 0.1898	0.0052 0.1353 0.0313	C(21B)	115.0(6)
O(22B)		O(11B)	[]	3.052(9)	3.04	0.01	Intra	-0.2305-0.0749 0.1898	0.0501 0.1385 0.2275		
O(22B)		C(11B)	[]	2.790(10)<<	3.22	-0.43	Intra	-0.2305-0.0749 0.1898	0.1038 0.0406 0.2832		
O(22B)		Cu(1)	[2555.01]	3.793(6) <	3.84	-0.05	Intra	-0.2305-0.0749 0.1898	-0.3734-0.0032-0.1375	C(21B)	129.7(5)
O(22B)		Cu(2)	[2555.01]	3.544(6)<<	3.84	-0.30	Intra	-0.2305-0.0749 0.1898	-0.0052-0.1353-0.0313	C(21B)	160.3(6)
O(22B)		O(1)	[2555.01]	2.574(8)<<	3.04	-0.47	Intra	-0.2305-0.0749 0.1898	-0.1675-0.0051-0.0040	C(21B)	136.8(6)
O(22B)		O(21A)	[2555.01]	2.935(9) <	3.04	-0.11	Intra	-0.2305-0.0749 0.1898	-0.5920-0.1841 0.1062		
O(22B)		C(11A)	[2555.01]	3.358(10)	3.22	0.14	Intra	-0.2305-0.0749 0.1898	-0.3403-0.2686-0.0559	C(21B)	149.3(6)
C(2A)		O(7W)	[2665.05]	3.356(17)	3.22	0.14		0.5822 0.3842-0.0094	0.3740 0.3269-0.2986		
C(3A)		O(4W)	[]	3.242(14)	3.22	0.02	Intra	0.6555 0.4980-0.0342	1.0143 0.5780 0.1715	C(2A)	110.8(5)
C(11A)		O(21A)	[]	3.195(10) <	3.22	-0.03	Intra	0.3403 0.2686 0.0559	0.5920 0.1841-0.1062	O(12A)	130.4(6)
C(11A)		O(22B)	[2555.01]	3.358(10)	3.22	0.14	Intra	0.3403 0.2686 0.0559	0.2305 0.0749-0.1898	C(1A)	107.6(5)
C(11B)		O(22B)	[]	2.790(10)<<	3.22	-0.43	Intra	0.1038 0.0406 0.2832	-0.2305-0.0749 0.1898	O(12B)	105.1(5)
C(11B)		Cu(2)	[2555.01]	3.919(8) <	4.02	-0.10	Intra	0.1038 0.0406 0.2832	-0.0052-0.1353-0.0313	C(1B)	132.0(5)
C(21A)		O(11A)	[]	2.859(10)<<	3.22	-0.36	Intra	0.6739 0.2658-0.0277	0.4360 0.1820 0.1031	O(22A)	110.3(5)
C(21B)		O(7W)	[1445.05]	3.328(16)	3.22	0.11		-0.2717-0.0230 0.2756	-0.3740-0.3269 0.2986		
C(21B)		O(11B)	[]	3.204(11) <	3.22	-0.02	Intra	-0.2717-0.0230 0.2756	0.0501 0.1385 0.2275	O(21B)	127.0(6)
H(3A)		O(22A)	[]	2.74	2.72	0.02	Intra	0.7628 0.4971-0.0573	0.8324 0.2629 0.0357		
H(3A)		O(4W)	[2765.01]	2.58 <	2.72	-0.14		0.7628 0.4971-0.0573	0.9857 0.4220-0.1715	C(3A)	158
H(3A)		O(12A)	[2665.01]	2.47<<	2.72	-0.25	Intra	0.7628 0.4971-0.0573	0.8289 0.7278-0.0309		
H(3B)		O(21B)	[]	2.58 <	2.72	-0.14	Intra	-0.2983-0.0332 0.4962	-0.4254 0.0170 0.2756		
H(3B)		O(12B)	[2556.01]	2.85	2.72	0.13	Intra	-0.2983-0.0332 0.4962	-0.2122 0.0370 0.7439		

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 1 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact Resd.			
1	[1555.02]	2	2.7000	-0.34	0 Na(1)	-*O(5W) ...	O(1W)	-	0	<<	1555.02			
2	[2766.03]	1	3.0440	0.00	0 Na(1)	- O(4W) ...	*O(2W)	-	0		2766.03			
3	[2765.01]	2	2.5800	-0.14	1 C(3A)	- H(3A) ...	O(4W)	-Na(1)	0	<	1665.01	1764.01	1765.01	2665.01
4	[1555.05]	1	3.1700	0.13	0 Na(1)	-*O(5W) ...	O(7W)	-	0		1555.05			
5	[1555.06]	1	2.2700	-0.77	0 Na(1)	-*O(5W) ...	*O(8W)	-	0	<<	1555.06			
6	[1655.02]	1	2.6700	-0.37	0 Na(1)	- O(6W) ...	O(1W)	-	0	<<	1655.02			
7	[2656.03]	1	2.7370	-0.30	0 Cu(1)	- O(12B) ...	*O(2W)	-	0	<<	2656.03			
8	[2665.05]	2	2.9220	-0.12	0 C(21A)	- O(21A) ...	O(7W)	-	0	<	2665.05			
9	[1455.02]	1	2.8050	-0.24	0 C(21B)	- O(21B) ...	O(1W)	-	0	<<	1455.02			
10	[1445.05]	1	3.3280	0.11	0 O(21B)	- C(21B) ...	O(7W)	-	0		1445.05			
11	[2666.03]	1	3.0440	0.00	0 Na(1)	- O(4W) ...	*O(2W)	-	0		2666.03			
12	[2665.01]	2	2.5800	-0.14	1 C(3A)	- H(3A) ...	O(4W)	-Na(1)	0	<	1565.01	1664.01	1665.01	2565.01
13	[1455.05]	1	3.1700	0.13	0 Na(1)	-*O(5W) ...	O(7W)	-	0		1455.05			
14	[1455.06]	1	2.2700	-0.77	0 Na(1)	-*O(5W) ...	*O(8W)	-	0	<<	1455.06			
15	[2556.03]	1	2.7370	-0.30	0 Cu(1)	- O(12B) ...	*O(2W)	-	0	<<	2556.03			
16	[2565.05]	2	2.9220	-0.12	0 C(21A)	- O(21A) ...	O(7W)	-	0	<	2565.05			
17	[1355.02]	1	2.8050	-0.24	0 C(21B)	- O(21B) ...	O(1W)	-	0	<<	1355.02			
18	[1345.05]	1	3.3280	0.11	0 O(21B)	- C(21B) ...	O(7W)	-	0		1345.05			
19	[2866.03]	1	3.0440	0.00	0 Na(1)	- O(4W) ...	*O(2W)	-	0		2866.03			
20	[2865.01]	2	2.5800	-0.14	1 C(3A)	- H(3A) ...	O(4W)	-Na(1)	0	<	1765.01	1864.01	1865.01	2765.01
21	[1655.05]	1	3.1700	0.13	0 Na(1)	-*O(5W) ...	O(7W)	-	0		1655.05			
22	[1655.06]	1	2.2700	-0.77	0 Na(1)	-*O(5W) ...	*O(8W)	-	0	<<	1655.06			
23	[1755.02]	1	2.6700	-0.37	0 Na(1)	- O(6W) ...	O(1W)	-	0	<<	1755.02			
24	[2756.03]	1	2.7370	-0.30	0 Cu(1)	- O(12B) ...	*O(2W)	-	0	<<	2756.03			
25	[2765.05]	2	2.9220	-0.12	0 C(21A)	- O(21A) ...	O(7W)	-	0	<	2765.05			
26	[1545.05]	1	3.3280	0.11	0 O(21B)	- C(21B) ...	O(7W)	-	0		1545.05			
27	[2555.02]	2	2.7000	-0.34	0 Na(1)	-*O(5W) ...	O(1W)	-	0	<<	2555.02			
28	[1344.03]	1	3.0440	0.00	0 Na(1)	- O(4W) ...	*O(2W)	-	0		1344.03			
29	[1345.01]	2	2.5800	-0.14	1 C(3A)	- H(3A) ...	O(4W)	-Na(1)	0	<	1245.01	1345.01	1445.01	2345.01
30	[2555.05]	1	3.1700	0.13	0 Na(1)	-*O(5W) ...	O(7W)	-	0		2555.05			
31	[2555.06]	1	2.2700	-0.77	0 Na(1)	-*O(5W) ...	*O(8W)	-	0	<<	2555.06			
32	[2455.02]	1	2.6700	-0.37	0 Na(1)	- O(6W) ...	O(1W)	-	0	<<	2455.02			
33	[1454.03]	1	2.7370	-0.30	0 Cu(1)	- O(12B) ...	*O(2W)	-	0	<<	1454.03			
34	[2655.02]	1	2.8050	-0.24	0 C(21B)	- O(21B) ...	O(1W)	-	0	<<	2655.02			
35	[2556.02]	2	2.7000	-0.34	0 Na(1)	-*O(5W) ...	O(1W)	-	0	<<	2556.02			
36	[1345.03]	1	3.0440	0.00	0 Na(1)	- O(4W) ...	*O(2W)	-	0		1345.03			
37	[1346.01]	2	2.5800	-0.14	1 C(3A)	- H(3A) ...	O(4W)	-Na(1)	0	<	1246.01	1346.01	1446.01	2346.01
38	[2556.05]	1	3.1700	0.13	0 Na(1)	-*O(5W) ...	O(7W)	-	0		2556.05			
39	[2556.06]	1	2.2700	-0.77	0 Na(1)	-*O(5W) ...	*O(8W)	-	0	<<	2556.06			
40	[2456.02]	1	2.6700	-0.37	0 Na(1)	- O(6W) ...	O(1W)	-	0	<<	2456.02			

41	[	1455.03]	1	2.7370	-0.30	0	Cu(1)	-	O(12B)	...	*O(2W)	-	0	<<	1455.03			
42	[	1446.05]	2	2.9220	-0.12	0	C(21A)	-	O(21A)	...	O(7W)	-	0	<	1446.05			
43	[	2656.02]	1	2.8050	-0.24	0	C(21B)	-	O(21B)	...	O(1W)	-	0	<<	2656.02			
44	[	2666.05]	1	3.3280	0.11	0	O(21B)	-	C(21B)	...	O(7W)	-	0		2666.05			
45	[	1444.03]	1	3.0440	0.00	0	Na(1)	-	O(4W)	...	*O(2W)	-	0		1444.03			
46	[	1445.01]	2	2.5800	-0.14	1	C(3A)	-	H(3A)	...	O(4W)	-Na(1)	0	<	1345.01	1445.01	1545.01	2445.01
47	[	2655.05]	1	3.1700	0.13	0	Na(1)	-	*O(5W)	...	O(7W)	-	0		2655.05			
48	[	2655.06]	1	2.2700	-0.77	0	Na(1)	-	*O(5W)	...	*O(8W)	-	0	<<	2655.06			
49	[	1554.03]	1	2.7370	-0.30	0	Cu(1)	-	O(12B)	...	*O(2W)	-	0	<<	1554.03			
50	[	2755.02]	1	2.8050	-0.24	0	C(21B)	-	O(21B)	...	O(1W)	-	0	<<	2755.02			
50	[	2665.02]	2	2.7000	-0.34	0	Na(1)	-	*O(5W)	...	O(1W)	-	0	<<	2665.02			
50	[	1455.01]	2	2.5800	-0.14	1	C(3A)	-	H(3A)	...	O(4W)	-Na(1)	0	<	1355.01	1455.01	1555.01	2455.01
50	[	2665.06]	1	2.2700	-0.77	0	Na(1)	-	*O(5W)	...	*O(8W)	-	0	<<	2665.06			
50	[	2565.02]	1	2.6700	-0.37	0	Na(1)	-	O(6W)	...	O(1W)	-	0	<<	2565.02			
50	[	1564.03]	1	2.7370	-0.30	0	Cu(1)	-	O(12B)	...	*O(2W)	-	0	<<	1564.03			
50	[	2765.02]	1	2.8050	-0.24	0	C(21B)	-	O(21B)	...	O(1W)	-	0	<<	2765.02			
50	[	2775.05]	1	3.3280	0.11	0	O(21B)	-	C(21B)	...	O(7W)	-	0		2775.05			

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
 Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 =====
 ARU = 1555.02
 =====

At(I)[1555.02]	At(J)	[	ARU(J)	]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
O(1W)		Cu(1)	[		]	3.886(11)	3.84	0.05	0.5738	0.2534	0.3945	0.3734	0.0032	0.1375		
O(1W)		>O(2W)	[		]	2.782(15)<<	3.04	-0.26	0.5738	0.2534	0.3945	0.7090	0.2649	0.6409		
O(1W)		*O(5W)	[		]	2.70(4)<<	3.04	-0.34	0.5738	0.2534	0.3945	0.8110	0.4080	0.3340		
O(1W)		O(6W)	[	1455.01]		2.67(2)<<	3.04	-0.37	0.5738	0.2534	0.3945	0.3090	0.4146	0.3320		
O(1W)		O(21B)	[	1655.01]		2.805(12)<<	3.04	-0.23	0.5738	0.2534	0.3945	0.5746	0.0170	0.2756		

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 2 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact	Resd.
1	[1555.01]	2	2.7000	-0.34	0	- O(1W)	... *O(5W)	-Na(1)	0	<<	1455.01	1555.01
2	[1555.03]	1	2.7820	-0.26	0	- O(1W)	... *O(2W)	-	0	<<	1555.03	
3	[1455.01]	1	2.6700	-0.37	0	- O(1W)	... O(6W)	-Na(1)	0	<<	1355.01	1455.01
4	[1655.01]	1	2.8050	-0.24	0	- O(1W)	... O(21B)	-C(21B)	0	<<	1555.01	1655.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
 Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 ARU = 1555.03

At(I)[1555.03]	At(J)	[ARU(J)]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
>O(2W)		O(1W)	[	2.782(15)<<	3.04	-0.26	0.7090	0.2649	0.6409	0.5738	0.2534	0.3945		
>O(2W)		O(4W)	[2766.01]	3.044(19)	3.04	0.00	0.7090	0.2649	0.6409	0.9857	0.4220	0.8285		
>O(2W)		O(7W)	[2666.05]	2.98(3)	<	3.04	-0.06	0.7090	0.2649	0.6409	0.3740	0.3269	0.7014	
>O(2W)		O(12B)	[2656.01]	2.737(14)<<	3.04	-0.30	0.7090	0.2649	0.6409	0.7878	0.0370	0.7439		

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 3 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn	X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact	Resd.
1	[1555.02]	1	2.7820	-0.26	0		-*O(2W) ...	O(1W)	-	0	<<	1555.02	
2	[2766.01]	1	3.0440	0.00	0		-*O(2W) ...	O(4W)	-Na(1)	0		1666.01	1765.01 1766.01 2666.01
3	[2666.05]	1	2.9800	-0.06	0		-*O(2W) ...	O(7W)	-	0	<	2666.05	
4	[2656.01]	1	2.7370	-0.30	0		-*O(2W) ...	O(12B)	-Cu(1)	0	<<	1556.01	1655.01 1656.01 2556.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
 Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 ARU = 1555.04

At(I)[1555.04]	At(J)	[ARU(J)]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
>O(3W)		<O(8W)	[	1.97(3)<<	3.04	-1.07	1.0780	0.3370	0.5710		1	0.5000	0.5000	
>O(3W)		O(7W)	[2766.05]	2.42(4)<<	3.04	-0.62	1.0780	0.3370	0.5710	1.3740	0.3269	0.7014		
>O(3W)		<O(8W)	[2766.06]	1.97(3)<<	3.04	-1.07	1.0780	0.3370	0.5710		1	0.5000	0.5000	

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 4 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact	Resd.
1 [	1555.06]	1	1.9700	-1.07	0	-*O(3W) ...	*O(8W)	-	0	<<	1555.06	
2 [	2766.05]	1	2.4200	-0.62	0	-*O(3W) ...	O(7W)	-	0	<<	2766.05	
3 [	2766.06]	1	1.9700	-1.07	0	-*O(3W) ...	*O(8W)	-	0	<<	2766.06	

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
 Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 ARU = 1555.05

At(I)[1555.05]	At(J)	[ARU(J)]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
O(7W)		*O(5W) [	3.17(3)	3.04	0.13		0.6260	0.6731	0.2986	0.8110	0.4080	0.3340		
O(7W)		C(21B) [1665.01]	3.328(16)	3.22	0.11		0.6260	0.6731	0.2986	0.7283	0.9770	0.2756		
O(7W)		>O(2W) [2666.03]	2.98(3)	< 3.04	-0.06		0.6260	0.6731	0.2986	0.2910	0.7351	0.3591		
O(7W)		>O(3W) [2766.04]	2.42(4)	<< 3.04	-0.62		0.6260	0.6731	0.2986	0.9220	0.6630	0.4290		
O(7W)		O(21A) [2665.01]	2.922(17)	< 3.04	-0.12		0.6260	0.6731	0.2986	0.4080	0.8159	0.1062		
O(7W)		C(2A) [2665.01]	3.356(17)	3.22	0.14		0.6260	0.6731	0.2986	0.4178	0.6158	0.0094		

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 5 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact	Resd.
1 [	1555.01]	1	3.1700	0.13	0	- O(7W) ...	*O(5W)	-Na(1)	0		1455.01	1555.01
2 [	1665.01]	1	3.3280	0.11	0	- O(7W) ...	C(21B)	-O(21B)	0		1565.01	1665.01
3 [	2666.03]	1	2.9800	-0.06	0	- O(7W) ...	*O(2W)	-	0	<	2666.03	
4 [	2766.04]	1	2.4200	-0.62	0	- O(7W) ...	*O(3W)	-	0	<<	2766.04	

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
 Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 ARU = 1555.06

At(I)[1555.06]	At(J)	[ARU(J)]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
<O(8W)		>O(3W)	[	1.97(3)<< 3.04	-1.07		1	0.5000	0.5000	1.0780	0.3370	0.5710		
<O(8W)		*O(5W)	[	2.27(3)<< 3.04	-0.77		1	0.5000	0.5000	0.8110	0.4080	0.3340		
<O(8W)		>O(3W)	[2766.04]	1.97(3)<< 3.04	-1.07		1	0.5000	0.5000	0.9220	0.6630	0.4290		
<O(8W)		*O(5W)	[2766.01]	2.27(3)<< 3.04	-0.77		1	0.5000	0.5000	1.1890	0.5920	0.6660		

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 6 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact	Resd.
1	[1555.04]	1	1.9700	-1.07	0	-*O(8W) ...	*O(3W)	-	0	<<	1555.04	
2	[1555.01]	1	2.2700	-0.77	0	-*O(8W) ...	*O(5W)	-Na(1)	0	<<	1455.01 1555.01	1655.01 2555.01
3	[2766.04]	1	1.9700	-1.07	0	-*O(8W) ...	*O(3W)	-	0	<<	2766.04	
4	[2766.01]	1	2.2700	-0.77	0	-*O(8W) ...	*O(5W)	-Na(1)	0	<<	1666.01 1765.01	1766.01 2666.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
 Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)
[1455.01]	= -1+x, y, z	= [	1	-1	0	0 1]	-1.003	0.007	0.020
[1655.01]	= 1+x, y, z	= [	1	1	0	0 1]	0.997	0.007	0.020
[2555.01]	= -x, -y, -z	= [	2	0	0	0 1]	0.003	-0.007	-0.020
[2556.01]	= -x, -y, 1-z	= [	2	0	0	1 1]	0.003	-0.007	0.980
[2655.01]	= 1-x, -y, -z	= [	2	1	0	0 1]	1.003	-0.007	-0.020
[2665.01]	= 1-x, 1-y, -z	= [	2	1	1	0 1]	1.003	0.993	-0.020
[2766.03]	= 2-x, 1-y, 1-z	= [	2	2	1	1 3]	1.291	0.735	0.359
[2765.01]	= 2-x, 1-y, -z	= [	2	2	1	0 1]	2.003	0.993	-0.020
[1655.02]	= 1+x, y, z	= [	1	1	0	0 2]	1.574	0.253	0.394
[2656.03]	= 1-x, -y, 1-z	= [	2	1	0	1 3]	0.291	-0.265	0.359
[2665.05]	= 1-x, 1-y, -z	= [	2	1	1	0 5]	0.374	0.327	-0.299
[1455.02]	= -1+x, y, z	= [	1	-1	0	0 2]	-0.426	0.253	0.394

[1445.05]	= -1+x, -1+y, z	= [1 -1 -1 0 5]	-0.374	-0.327	0.299
[2766.01]	= 2-x, 1-y, 1-z	= [2 2 1 1 1]	2.003	0.993	0.980
[2666.05]	= 1-x, 1-y, 1-z	= [2 1 1 1 5]	0.374	0.327	0.701
[2656.01]	= 1-x, -y, 1-z	= [2 1 0 1 1]	1.003	-0.007	0.980
[2766.05]	= 2-x, 1-y, 1-z	= [2 2 1 1 5]	1.374	0.327	0.701
[2766.06]	= 2-x, 1-y, 1-z	= [2 2 1 1 6]	1	1/2	1/2
[1665.01]	= 1+x, 1+y, z	= [1 1 1 0 1]	0.997	1.007	0.020
[2666.03]	= 1-x, 1-y, 1-z	= [2 1 1 1 3]	0.291	0.735	0.359
[2766.04]	= 2-x, 1-y, 1-z	= [2 2 1 1 4]	0.922	0.663	0.429

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

$X(J) = X(sym) + TX$, $Y(J) = Y(sym) + TY$, $Z(J) = Z(sym) + TZ$,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

Analysis of Short Non-Hydrogen Inter-Molecular Contacts For Inter-Molecular Clusters and/or Networks (Minor Disorder Excluded)

Contact-Nr	Atom I[	ARU	]	Atom J[	ARU	]	d(I-J)	Del
1	*O(5W)	[1555.01]	...	O(1W)	[1555.02]	=	2.700	-0.34
2	O(6W)	[1555.01]	...	O(1W)	[1655.02]	=	2.670	-0.37
3	O(12B)	[1555.01]	...	*O(2W)	[2656.03]	=	2.737	-0.30
4	O(21B)	[1555.01]	...	O(1W)	[1455.02]	=	2.805	-0.23
5	O(1W)	[1555.02]	...	*O(2W)	[1555.03]	=	2.782	-0.26
6	O(1W)	[1555.02]	...	*O(5W)	[1555.01]	=	2.700	-0.34
7	O(1W)	[1555.02]	...	O(6W)	[1455.01]	=	2.670	-0.37
8	O(1W)	[1555.02]	...	O(21B)	[1655.01]	=	2.805	-0.23
9	*O(2W)	[1555.03]	...	O(1W)	[1555.02]	=	2.782	-0.26
10	*O(2W)	[1555.03]	...	O(12B)	[2656.01]	=	2.737	-0.30
11	*O(3W)	[1555.04]	...	O(7W)	[2766.05]	=	2.420	-0.62
12	O(7W)	[1555.05]	...	*O(3W)	[2766.04]	=	2.420	-0.62

***** Cluster = 1 *****

(N:M) : ARU -- Connected with (N) Interactions to/from (M) ARU(S). T = Translated Molecule (Infinite chain etc.)

4	10	1555.01	--	1455.01*	1655.01*	2555.01*	2556.01*	2655.01*	2665.01*	1555.02	1655.02T	2656.03	1455.02T
4	10	2555.01	--	2655.01*	2455.01*	1555.01*	1554.01*	1455.01*	1445.01*	2555.02	2455.02T	1454.03	2655.02T
4	4	1555.02	--	1555.03T	1555.01	1455.01T	1655.01T						
2	2	2656.03	--	2656.02T	1555.01								
4	4	2555.02	--	2555.03T	2555.01	2655.01T	2455.01T						
2	2	1454.03	--	1454.02T	2555.01								

:: Starred ARUs belong (chemically) to the previous ARU

:: Analysis of Polymeric Structure(s)

:: Resd # 0 - Infinite Two-Dimensional Network :: Base Vectors: #1 = [1 0 0], #2 = [0 0 1], - Plane: (0 1 0)

***** Cluster = 2 *****

(N:M) : ARU -- Connected with (N) Interactions to/from (M) ARU(S). T = Translated Molecule (Infinite chain etc.)

1	1	1555.05	--	2766.04	
1	1	2766.04	--	1555.05	

=====

 Cluster = 3

(N:M) : ARU -- Connected with (N) Interactions to/from (M) ARU(S). T = Translated Molecule (Infinite chain etc.)

 1 1 1555.04 -- 2766.05
 1 1 2766.05 -- 1555.04

=====

Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg

=====

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)

=====

Nr	Typ	Res	Donor	---	H...Acceptor	[	ARU	]	D - H	H...A	D...A	D - H...A	A..H..A*	A'..H..A"	Sum(XY,YZ)	Sum(XZ)
1		1	C(3A)	--	H(3A)	..	O(4W)	[	2765.01]	0.95	2.58	3.482(13)			158	

:: No Classic Hydrogen Bonds Found

Translation of ARU-code to Equivalent Position Code

=====

[2765.] = 2-x,1-y,-z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

2-Centre (linear)	D-H...X most prob. angle 160 deg	- also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
3-Centre (bifurcated)	SUM of 3 angl. about H = 360 deg	Springer-Verlag, Berlin, 1991, pp 20.
4-Centre (trifurcated)		

>>>>>>>>>>>> : Symmetry operations refer to the coordinates listed in the fractional coordinate table given above

=====

3.6 Angstrom Coordination Sphere Around Atom I = Cu(1) [ARU = 1555.01] 0.37342 0.00315 0.13751 2.4962 -0.0396 1.5442

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	1.920(6)	--	O(1)	[	=		Intra	175.64	-51.34	0.16750	0.00510	0.00400	1.3001	0.0517	0.0449
2	1.927(6)	--	O(21B)b	[1+x,y,z	=	1655.01]	Intra	3.66	53.59	0.57460	0.01700	0.27560	3.6376	0.0334	3.0950
3	2.023(5)	--	O(11A)	[	=		Intra	73.51	-11.01	0.43600	0.18200	0.10310	3.0597	1.8645	1.1578
4	2.030(5)	--	O(21A)e	[1-x,-y,-z	=	2655.01]	Intra	-78.27	-9.97	0.40800	-0.18410	0.10620	2.9027	-1.9974	1.1926
5	2.159(6)	--	O(12B)	[	=		Intra	-163.38	38.08	0.21220	-0.03700	0.25610	0.8673	-0.5257	2.8760

6	2.841(9)	<<	C(21B)b	[1+x,y,z	=	1655.01]	Intra	-8.43	33.08	0.72830	-0.02300	0.27560	4.8509	-0.3884	3.0950
7	2.987(7)	<<	C(11A)	[	=		Intra	91.13	-17.87	0.34030	0.26860	0.05590	2.4403	2.8026	0.6278
8	3.039(8)	<<	C(21A)e	[1-x,-y,-z	=	2655.01]	Intra	-89.45	-23.94	0.32610	-0.26580	0.02770	2.5230	-2.8174	0.3111
9	3.071(8)	<<	C(11B)	[	=		Intra	172.98	32.19	0.10380	0.04060	0.28320	-0.0833	0.2782	3.1803
10	3.133(7)	<<	O(22B)b	[1+x,y,z	=	1655.01]	Intra	-16.05	10.80	0.76950	-0.07490	0.18980	5.4537	-0.8902	2.1315
11	3.1914(13)	<<	Cu(2)	[	=		Intra	150.67	-21.94	0.00515	0.13533	0.03133	-0.0847	1.4104	0.3518
12	3.319(6)	<<	O(11B)	[	=		Intra	154.13	17.72	0.05010	0.13850	0.22750	-0.3488	1.3400	2.5548
13	3.3600(13)	<<	Cu(2)c	[-x,-y,-z	=	2555.01]	Intra	-150.38	-34.35	-0.00515	-0.13533	-0.03133	0.0847	-1.4104	-0.3518
14	3.392(6)	<<	O(12A)	[	=		Intra	114.28	-20.67	0.17110	0.27220	0.03090	1.1911	2.8538	0.3470
15	3.490(5)	<<	O(22A)e	[1-x,-y,-z	=	2655.01]	Intra	-110.56	-33.87	0.16760	-0.26290	-0.03570	1.4785	-2.7532	-0.4009

Polyhedral Volume 6.667 Ang**3

Angles (Degrees) At1...V...At2 with Vertex V = Cu(1)

O(1)	,	C(21B)b	161.5(2)	O(1)	,	C(11A)	72.8(2)	O(1)	,	C(21A)e	74.5(2)	O(1)	,	C(11B)	83.6(2)
O(1)	,	O(22B)b	138.4(2)	O(1)	,	Cu(2)	35.21(16)	O(1)	,	O(11B)	71.6(2)	O(1)	,	Cu(2)c	29.74(16)
O(1)	,	O(12A)	56.24(19)	O(1)	,	O(22A)e	54.56(18)	O(21B)b,		C(21B)b	22.2(2)	O(21B)b,		C(11A)	102.8(2)
O(21B)b,		C(21A)e	110.9(2)	O(21B)b,		C(11B)	93.7(2)	O(21B)b,		O(22B)b	45.6(2)	O(21B)b,		Cu(2)	139.69(17)
O(21B)b,		O(11B)	104.3(2)	O(21B)b,		Cu(2)c	153.47(17)	O(21B)b,		O(12A)	118.66(19)	O(21B)b,		O(22A)e	130.59(18)
O(11A)	,	C(21B)b	89.4(2)	O(11A)	,	C(11A)	18.4(2)	O(11A)	,	C(21A)e	141.3(2)	O(11A)	,	C(11B)	103.8(2)
O(11A)	,	O(22B)b	91.6(2)	O(11A)	,	Cu(2)	74.11(16)	O(11A)	,	O(11B)	84.6(2)	O(11A)	,	Cu(2)c	118.43(16)
O(11A)	,	O(12A)	40.27(19)	O(11A)	,	O(22A)e	134.95(19)	O(21A)e,		C(21B)b	79.1(2)	O(21A)e,		C(11A)	150.3(2)
O(21A)e,		C(21A)e	17.6(2)	O(21A)e,		C(11B)	111.1(2)	O(21A)e,		O(22B)b	65.3(2)	O(21A)e,		Cu(2)	122.37(16)
O(21A)e,		O(11B)	128.7(2)	O(21A)e,		Cu(2)c	69.67(16)	O(21A)e,		O(12A)	147.0(2)	O(21A)e,		O(22A)e	38.02(18)
O(12B)	,	C(21B)b	105.1(2)	O(12B)	,	C(11A)	112.9(2)	O(12B)	,	C(21A)e	92.9(2)	O(12B)	,	C(11B)	20.2(2)
O(12B)	,	O(22B)b	122.4(2)	O(12B)	,	Cu(2)	73.90(17)	O(12B)	,	O(11B)	42.2(2)	O(12B)	,	Cu(2)c	73.43(16)
O(12B)	,	O(12A)	96.9(2)	O(12B)	,	O(22A)e	87.06(19)	C(21B)b,		C(11A)	107.5(2)	C(21B)b,		C(21A)e	95.9(2)
C(21B)b,		C(11B)	114.7(2)	C(21B)b,		O(22B)b	23.4(2)	C(21B)b,		Cu(2)	158.44(17)	C(21B)b,		O(11B)	126.5(2)
C(21B)b,		Cu(2)c	148.52(17)	C(21B)b,		O(12A)	128.0(2)	C(21B)b,		O(22A)e	116.77(19)	C(11A)	,	C(21A)e	138.2(2)
C(11A)	,	C(11B)	92.8(2)	C(11A)	,	O(22B)b	109.5(2)	C(11A)	,	Cu(2)	55.80(16)	C(11A)	,	O(11B)	71.45(19)
C(11A)	,	Cu(2)c	101.63(16)	C(11A)	,	O(12A)	22.01(18)	C(11A)	,	O(22A)e	124.29(18)	C(21A)e,		C(11B)	108.6(2)
C(21A)e,		O(22B)b	79.6(2)	C(21A)e,		Cu(2)	105.71(15)	C(21A)e,		O(11B)	120.73(19)	C(21A)e,		Cu(2)c	53.45(15)
C(21A)e,		O(12A)	129.77(19)	C(21A)e,		O(22A)e	20.92(18)	C(11B)	,	O(22B)b	136.15(18)	C(11B)	,	Cu(2)	58.18(15)
C(11B)	,	O(11B)	22.32(19)	C(11B)	,	Cu(2)c	74.93(15)	C(11B)	,	O(12A)	77.09(19)	C(11B)	,	O(22A)e	97.61(18)
O(22B)b,		Cu(2)	163.10(12)	O(22B)b,		O(11B)	149.87(15)	O(22B)b,		Cu(2)c	132.26(13)	O(22B)b,		O(12A)	131.37(17)
O(22B)b,		O(22A)e	99.71(16)	Cu(2)	,	O(11B)	39.81(10)	Cu(2)	,	Cu(2)c	52.71(3)	Cu(2)	,	O(12A)	33.85(10)

Cu(2) , O(22A)e	84.79(10)	O(11B) , Cu(2)c	74.11(11)	O(11B) , O(12A)	54.78(15)	O(11B) , O(22A)e	104.06(14)
Cu(2)c , O(12A)	82.69(10)	Cu(2)c , O(22A)e	32.76(9)	O(12A) , O(22A)e	110.75(14)		

Dist. Cu(1) - Polyh_C.G.: 0.207(3) Ang, C.G.: 0.3597(3) -0.0034(2) 0.1490(2) 2.354(3) -0.115(2) 1.673(3)

Real Angles I - Cu(1) - J	Real Edge I - J	Unit Polyhedron	Dihedral Angles	Norm. IJK:IJL	K	L
O(1) , O(21B)	174.6(2)	3.843(8)	-143.00	127.00	90.00	-37.00 O(11A) O(21A)e
O(1) , O(11A)	88.8(2)	2.761(8)	-61.00	-26.00	-35.00	119.00 O(21A)e O(12B)
O(1) , O(21A)	92.0(2)	2.843(8)	78.00	25.00	53.00	102.00 O(11A) O(12B)
O(1) , O(12B)	91.3(2)	2.922(8)	91.00	57.00	34.00	89.00 O(21A)e O(11A)
O(21B) , O(11A)	87.3(2)	2.728(8)	62.00	26.00	35.00	119.00 O(21A)e O(12B)
O(21B) , O(21A)	93.3(2)	2.878(8)	-80.00	-25.00	-55.00	100.00 O(11A) O(12B)
O(21B) , O(12B)	87.7(2)	2.835(9)	90.00	35.00	55.00	90.00 O(11A) O(21A)e
O(11A) , O(21A)	145.0(2)	3.865(7)	-144.00	-74.00	-71.00	35.00 O(1) O(21B)b
O(11A) , O(12B)	122.7(2)	3.670(8)	133.00	65.00	68.00	47.00 O(1) O(21B)b
O(21A) , O(12B)	92.3(2)	3.024(8)	-108.00	-54.00	-54.00	72.00 O(1) O(21B)b

Tau-Descriptor for 5-Coordination (A.W.Addison,T.N.Rao,J.Reedijk,J.van Rijn,G.C.Verschoor, J.Chem.Soc.Dalton Trans.(1984),1349-1356)

Tau = (Beta - Alpha) / 60 = (174.60-145.00) / 60 = 0.49 : (Extreme forms: Tau = 0.00 for SP and 1.00 for TP)

Analysis of Five-Coordination (See R.R. Holmes in Progress in Inorg. Chem. Vol. 32 (1984),119-235 and References Therein)

Idealized Dihedral Angles for Trans Basal Angle : 150.0
 Del(13) & Del(23) Trigonal Bipyramid (TP): 101.5 53.1
 Del(12) & Del(13) Square Pyramid (SP): 118.5 76.9
 Distance Between TP and SP Along Berry Coordinate: 217.7

Pivot(3)	Sum(/Del:C - Del:TP/)	Sum(/Del:C - Del:SP/)	217.7 - Sum(/Del:C - Del:SP/)	Del(24)	Th(24)	Th(15)
O(11A)	104.1 Deg.	320.9 Deg.	-103.2 Deg.	71.53	92.33	174.62
O(21A)e	104.1 Deg.	201.0 Deg.	16.7 Deg.	47.02	122.67	174.62
O(12B)	104.1 Deg.	131.0 Deg.	86.7 Deg.	35.74	144.96	174.62

Trigonal Bipyramid (TP) to Square Pyramid (SP) ::: Perc. Along Berry Pseudorotation Coordinate: 43.8 ::: D3h ---> C2v ---> C4v

NOTE: This Analysis Depends on the Value of the Trans Basal Angle that is used (Default Value = 150 Deg.).

The Pivot Atom that Best Describes a Berry Pseudo Rotation is: O(12B)

The Percentage has been Calculated for the Average value, 95.4 Deg., of the Second and Fourth Table Entry.

The Difference, 17.4 Deg., Between the Second and Fourth Table Entry (for pivot) should be Zero for a True Berry Rotation.

3.6 Angstrom Coordination Sphere Around Atom I = Cu(2) [ARU = 1555.01] 0.00515 0.13533 0.03133 -0.0847 1.4104 0.3518

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.927(6)	--	O(12A)	[	=		Intra	48.53	-0.14	0.17110	0.27220	0.03090	1.1911	2.8538	0.3470
2	1.936(6)	--	O(22A)a	[-1+x,y,z	=	1455.01]	Intra	136.07	1.45	-0.16760	0.26290	0.03570	-1.4785	2.7532	0.4009
3	1.942(6)	--	O(1)c	[-x,-y,-z	=	2555.01]	Intra	-129.74	-11.79	-0.16750	-0.00510	-0.00400	-1.3001	-0.0517	-0.0449
4	1.964(6)	--	O(1)	[	=		Intra	-44.46	-8.99	0.16750	0.00510	0.00400	1.3001	0.0517	0.0449
5	2.220(6)	--	O(11B)	[	=		Intra	-165.07	82.93	0.05010	0.13850	0.22750	-0.3488	1.3400	2.5548
6	2.892(8)	<<	C(21A)a	[-1+x,y,z	=	1455.01]	Intra	150.01	-13.25	-0.32610	0.26580	-0.02770	-2.5230	2.8174	-0.3111
7	2.897(8)	<<	C(11A)	[	=		Intra	28.87	5.47	0.34030	0.26860	0.05590	2.4403	2.8026	0.6278
8	2.9121(12)	<<	Cu(2)c	[-x,-y,-z	=	2555.01]	Intra	-86.56	-13.98	-0.00515	-0.13533	-0.03133	0.0847	-1.4104	-0.3518
9	3.047(8)	<<	C(11B)	[	=		Intra	-89.93	68.18	0.10380	0.04060	0.28320	-0.0833	0.2782	3.1803
10	3.187(6)	<<	Na(1)a	[-1+x,y,z	=	1455.01]	Intra	104.89	41.13	0.00700	0.36470	0.21800	-0.7017	3.7301	2.4481
11	3.1914(13)	<<	Cu(1)	[	=		Intra	-29.33	21.94	0.37342	0.00315	0.13751	2.4962	-0.0396	1.5442
12	3.267(6)	<<	O(21A)a	[-1+x,y,z	=	1455.01]	Intra	168.23	-28.22	-0.40800	0.18410	-0.10620	-2.9027	1.9974	-1.1926
13	3.278(6)	<<	O(11A)	[	=		Intra	8.22	14.23	0.43600	0.18200	0.10310	3.0597	1.8645	1.1578
14	3.321(6)	<<	O(12B)	[	=		Intra	-63.82	49.48	0.21220	-0.03700	0.25610	0.8673	-0.5257	2.8760
15	3.3600(13)	<<	Cu(1)c	[-x,-y,-z	=	2555.01]	Intra	-150.38	-34.35	-0.37342	-0.00315	-0.13751	-2.4962	0.0396	-1.5442
16	3.437(6)	<<	O(12B)c	[-x,-y,-z	=	2555.01]	Intra	-131.50	-69.90	-0.21220	0.03700	-0.25610	-0.8673	0.5257	-2.8760
17	3.544(6)	<<	O(22B)c	[-x,-y,-z	=	2555.01]	Intra	-11.87	-44.49	0.23050	0.07490	-0.18980	2.3890	0.8902	-2.1315

Polyhedral Volume 5.952 Ang**3

Angles (Degrees) At1...V...At2 with Vertex V = Cu(2)

O(12A) , C(21A)a	101.1(2)	O(12A) , C(11A)	20.4(2)	O(12A) , Cu(2)c	133.36(18)	O(12A) , C(11B)	106.3(3)
O(12A) , Na(1)a	65.5(2)	O(12A) , Cu(1)	78.80(17)	O(12A) , O(21A)a	115.8(2)	O(12A) , O(11A)	42.4(2)
O(12A) , O(12B)	104.4(2)	O(12A) , Cu(1)c	141.2(2)	O(12A) , O(12B)c	110.0(2)	O(12A) , O(22B)c	69.3(2)
O(22A)a, C(21A)a	20.2(2)	O(22A)a, C(11A)	107.0(2)	O(22A)a, Cu(2)c	136.04(17)	O(22A)a, C(11B)	103.6(2)
O(22A)a, Na(1)a	48.6(2)	O(22A)a, Cu(1)	152.60(17)	O(22A)a, O(21A)a	42.80(19)	O(22A)a, O(11A)	126.04(19)
O(22A)a, O(12B)	126.3(2)	O(22A)a, Cu(1)c	77.33(17)	O(22A)a, O(12B)c	92.2(2)	O(22A)a, O(22B)c	128.5(2)
O(1)c , C(21A)a	78.0(2)	O(1)c , C(11A)	157.9(2)	O(1)c , Cu(2)c	42.09(17)	O(1)c , C(11B)	84.9(2)
O(1)c , Na(1)a	124.1(2)	O(1)c , Cu(1)	103.91(17)	O(1)c , O(21A)a	59.93(19)	O(1)c , O(11A)	139.01(19)
O(1)c , O(12B)	84.0(2)	O(1)c , Cu(1)c	29.36(17)	O(1)c , O(12B)c	58.1(2)	O(1)c , O(22B)c	100.6(2)
O(1) , C(21A)a	153.5(2)	O(1) , C(11A)	74.5(2)	O(1) , Cu(2)c	41.51(16)	O(1) , C(11B)	83.6(2)
O(1) , Na(1)a	138.0(2)	O(1) , Cu(1)	34.30(17)	O(1) , O(21A)a	131.20(19)	O(1) , O(11A)	57.17(19)
O(1) , O(12B)	60.9(2)	O(1) , Cu(1)c	97.79(17)	O(1) , O(12B)c	80.6(2)	O(1) , O(22B)c	45.3(2)
O(11B) , C(21A)a	98.2(2)	O(11B) , C(11A)	91.4(2)	O(11B) , Cu(2)c	102.47(17)	O(11B) , C(11B)	21.1(2)
O(11B) , Na(1)a	49.25(19)	O(11B) , Cu(1)	73.20(17)	O(11B) , O(21A)a	111.9(2)	O(11B) , O(11A)	82.8(2)
O(11B) , O(12B)	42.4(2)	O(11B) , Cu(1)c	117.50(17)	O(11B) , O(12B)c	153.7(2)	O(11B) , O(22B)c	140.7(2)
C(21A)a, C(11A)	121.5(2)	C(21A)a, Cu(2)c	117.70(15)	C(21A)a, C(11B)	113.2(2)	C(21A)a, Na(1)a	68.5(2)
C(21A)a, Cu(1)	171.29(16)	C(21A)a, O(21A)a	22.62(18)	C(21A)a, O(11A)	142.92(18)	C(21A)a, O(12B)	134.40(19)
C(21A)a, Cu(1)c	57.59(15)	C(21A)a, O(12B)c	73.62(19)	C(21A)a, O(22B)c	119.96(19)	C(11A) , Cu(2)c	115.97(15)
C(11A) , C(11B)	95.2(2)	C(11A) , Na(1)a	75.9(2)	C(11A) , Cu(1)	58.52(15)	C(11A) , O(21A)a	135.29(18)
C(11A) , O(11A)	22.14(18)	C(11A) , O(12B)	87.59(19)	C(11A) , Cu(1)c	151.10(16)	C(11A) , O(12B)c	114.31(19)

C(11A) ,	O(22B)c	61.89(19)	Cu(2)c ,	C(11B)	82.20(16)	Cu(2)c ,	Na(1)a	151.08(11)	Cu(2)c ,	Cu(1)	66.62(3)
Cu(2)c ,	O(21A)a	96.32(10)	Cu(2)c ,	O(11A)	97.92(10)	Cu(2)c ,	O(12B)	66.56(11)	Cu(2)c ,	Cu(1)c	60.67(3)
Cu(2)c ,	O(12B)c	62.42(11)	Cu(2)c ,	O(22B)c	69.38(12)	C(11B) ,	Na(1)a	70.12(19)	C(11B) ,	Cu(1)	58.93(16)
C(11B) ,	O(21A)a	120.41(18)	C(11B) ,	O(11A)	79.79(18)	C(11B) ,	O(12B)	22.70(19)	C(11B) ,	Cu(1)c	111.88(16)
C(11B) ,	O(12B)c	140.92(19)	C(11B) ,	O(22B)c	126.57(19)	Na(1)a ,	Cu(1)	103.98(12)	Na(1)a ,	O(21A)a	90.76(16)
Na(1)a ,	O(11A)	85.59(16)	Na(1)a ,	O(12B)	88.85(15)	Na(1)a ,	Cu(1)c	121.95(13)	Na(1)a ,	O(12B)c	139.55(16)
Na(1)a ,	O(22B)c	134.67(17)	Cu(1) ,	O(21A)a	162.93(10)	Cu(1) ,	O(11A)	36.41(9)	Cu(1) ,	O(12B)	38.67(11)
Cu(1) ,	Cu(1)c	127.29(3)	Cu(1) ,	O(12B)c	114.71(11)	Cu(1) ,	O(22B)c	68.32(10)	O(21A)a ,	O(11A)	156.77(14)
O(21A)a ,	O(12B)	135.36(15)	O(21A)a ,	Cu(1)c	35.65(9)	O(21A)a ,	O(12B)c	53.55(15)	O(21A)a ,	O(22B)c	107.29(14)
O(11A) ,	O(12B)	67.59(15)	O(11A) ,	Cu(1)c	152.11(10)	O(11A) ,	O(12B)c	119.01(15)	O(11A) ,	O(22B)c	61.51(14)
O(12B) ,	Cu(1)c	113.38(11)	O(12B) ,	O(12B)c	128.98(15)	O(12B) ,	O(22B)c	104.30(15)	Cu(1)c ,	O(12B)c	37.03(11)
Cu(1)c ,	O(22B)c	92.62(11)	O(12B)c ,	O(22B)c	57.52(15)						

Dist. Cu(2) - Polyh_C.G.: 0.312(3) Ang, C.G.: 0.0107(3) 0.1347(2) 0.0588(2) -0.127(3) 1.389(2) 0.661(3)

Real Angles I - Cu(2) - J	Real Edge I - J	Unit Polyhedron	Dihedral Angles	Norm. IJK:IJL	K	L
O(12A) , O(22A)	87.5(2)	2.672(8)	62.00	3.00	59.00	118.00 O(1)c O(11B)
O(12A) , O(1)c	167.9(3)	3.847(8)	-176.00	-79.00	-97.00	4.00 O(22A)a O(1)
O(12A) , O(1)	92.9(2)	2.821(7)	55.00	52.00	3.00	125.00 O(11B) O(1)c
O(12A) , O(11B)	96.0(3)	3.088(9)	108.00	61.00	48.00	71.00 O(22A)a O(1)
O(22A) , O(1)c	94.4(2)	2.846(7)	64.00	3.00	61.00	116.00 O(12A) O(11B)
O(22A) , O(1)	172.5(2)	3.892(8)	-176.00	92.00	92.00	-4.00 O(12A) O(1)c
O(22A) , O(11B)	84.9(2)	2.813(8)	-101.00	-53.00	-48.00	79.00 O(12A) O(1)c
O(1)c , O(1)	83.6(2)	2.604(8)	53.00	3.00	50.00	127.00 O(12A) O(11B)
O(1)c , O(11B)	96.0(2)	3.098(8)	-109.00	-57.00	-52.00	71.00 O(22A)a O(1)
O(1) , O(11B)	102.5(2)	3.268(8)	111.00	54.00	57.00	69.00 O(12A) O(1)c

Tau-Descriptor for 5-Coordination (A.W.Addison,T.N.Rao,J.Reedijk,J.van Rijn,G.C.Verschoor, J.Chem.Soc.Dalton Trans.(1984),1349-1356)

Tau = (Beta - Alpha) / 60 = (172.50-167.90) / 60 = 0.08 : (Extreme forms: Tau = 0.00 for SP and 1.00 for TP)

Analysis of Five-Coordination (See R.R. Holmes in Progress in Inorg. Chem. Vol. 32 (1984),119-235 and References Therein)

Idealized Dihedral Angles for Trans Basal Angle : 150.0
 Del(13) & Del(23) Trigonal Bipyramid (TP): 101.5 53.1
 Del(12) & Del(13) Square Pyramid (SP): 118.5 76.9
 Distance Between TP and SP Along Berry Coordinate: 217.7

Pivot(3)	Sum(/Del:C - Del:TP/)	Sum(/Del:C - Del:SP/)	217.7 - Sum(/Del:C - Del:SP/)	Del(24)	Th(24)	Th(15)
O(1)c	219.8 Deg.	335.0 Deg.	-117.2 Deg.	71.60	96.03	172.45
O(12A)	219.8 Deg.	339.0 Deg.	-121.2 Deg.	71.18	95.99	172.45
O(11B)	219.8 Deg.	43.7 Deg.	174.0 Deg.	4.30	167.94	172.45

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Trigonal Bipyramid (TP) to Square Pyramid (SP) ::: Perc. Along Berry Pseudorotation Coordinate: 90.4 ::: D3h ---> C2v ---> C4v

NOTE: This Analysis Depends on the Value of the Trans Basal Angle that is used (Default Value = 150 Deg.).

The Pivot Atom that Best Describes a Berry Pseudo Rotation is: O(11B)

The Percentage has been Calculated for the Average value, 196.9 Deg., of the Second and Fourth Table Entry.

The Difference, 45.8 Deg., Between the Second and Fourth Table Entry (for pivot) should be Zero for a True Berry Rotation.

>> Distance to SP square base plane defined by: O(1) O(12A) O(22A)a O(1)c

O(1) -0.0360(60), O(12A) 0.0350(70), O(22A)a -0.0350(60), O(1)c 0.0360(60), Cu(2) -0.1623(9), O(11B) -2.3560(60)

3.6 Angstrom Coordination Sphere Around Atom I = Na(1) [ARU = 1555.01] 1.00700 0.36470 0.21800 7.1410 3.7301 2.4481

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.339(12)	--	O(4W)	[	=	] Intra	85.95	-12.90	1.01430	0.57800	0.17150	7.3022	6.0038	1.9259
2	2.35(4)	--	*O(5W)	[	=	] Intra	168.31	33.74	0.81100	0.40800	0.33400	5.2310	4.1253	3.7508
3	2.398(8)	--	O(22A)	[	=	] Intra	-128.49	-58.63	0.83240	0.26290	0.03570	6.3642	2.7532	0.4009
4	2.418(8)	--	O(11B)b	[1+x,y,z	= 1655.01]	Intra	-81.60	2.53	1.05010	0.13850	0.22750	7.4939	1.3400	2.5548
5	2.42(2)	--	O(6W)	[	=	] Intra	13.11	31.93	1.30900	0.41460	0.33200	9.1417	4.1959	3.7284
6	2.961(9)	<<	O(12A)b	[1+x,y,z	= 1655.01]	Intra	-24.84	-45.21	1.17110	0.27220	0.03090	9.0338	2.8538	0.3470
7	3.187(6)	<<	Cu(2)b	[1+x,y,z	= 1655.01]	Intra	-75.11	-41.13	1.00515	0.13533	0.03133	7.7580	1.4104	0.3518
8	3.430(10)	<	C(21A)	[	=	] Intra	-153.38	-53.56	0.67390	0.26580	-0.02770	5.3197	2.8174	-0.3111
9	3.549(6)	..	<O(8W)	[	= 06]		127.13	63.16	1	1/2	1/2	6.1738	5.0075	5.6150
10	3.583(10)	..	C(11B)b	[1+x,y,z	= 1655.01]	Intra	-79.84	11.79	1.10380	0.04060	0.28320	7.7594	0.2782	3.1803
11	3.29	..	H(3A)g	[2-x,1-y,-z	= 2765.01]		34.04	-33.23	1.23720	0.50290	0.05730	9.4237	5.2724	0.6435

Polyhedral Volume 10.743 Ang**3

Angles (Degrees) At1...V...At2 with Vertex V = Na(1)

O(4W) , O(12A)b	94.9(4)	O(4W) , Cu(2)b	123.2(3)	O(4W) , C(21A)	96.6(4)	O(4W) , <O(8W)	82.4(3)
O(4W) , C(11B)b	166.1(4)	*O(5W) , O(12A)b	164.7(8)	*O(5W) , Cu(2)b	130.2(7)	*O(5W) , C(21A)	93.4(8)
*O(5W) , <O(8W)	38.9(7)	*O(5W) , C(11B)b	100.9(6)	O(22A) , O(12A)b	58.7(2)	O(22A) , Cu(2)b	37.30(16)
O(22A) , C(21A)	14.7(2)	O(22A) , <O(8W)	145.1(3)	O(22A) , C(11B)b	80.7(2)	O(11B)b , O(12A)b	69.2(2)
O(11B)b , Cu(2)b	44.06(16)	O(11B)b , C(21A)	81.4(2)	O(11B)b , <O(8W)	110.9(2)	O(11B)b , C(11B)b	9.43(19)
O(6W) , O(12A)b	84.5(6)	O(6W) , Cu(2)b	109.2(5)	O(6W) , C(21A)	156.3(6)	O(6W) , <O(8W)	71.6(5)
O(6W) , C(11B)b	86.3(4)	O(12A)b , Cu(2)b	36.29(13)	O(12A)b , C(21A)	71.9(2)	O(12A)b , <O(8W)	156.1(3)
O(12A)b , C(11B)b	75.5(2)	Cu(2)b , C(21A)	51.68(16)	Cu(2)b , <O(8W)	154.38(18)	Cu(2)b , C(11B)b	53.11(15)
C(21A) , <O(8W)	132.0(3)	C(21A) , C(11B)b	90.0(2)	<O(8W) , C(11B)b	102.21(19)		

Dist. Na(1) - Polyh_C.G.: 0.06 Ang, C.G.: 1.0034(12) 0.3604(6) 0.2201(6) 7.107(10) 3.684(6) 2.472(7)

Real Angles I - Na(1) - J	Real Edge I - J	Unit Polyhedron	Dihedral Angles	Norm. IJK:IJL	K	L
O(4W) , *O(5W)	90.9(6)	3.34(3)	89.00	40.00	48.00	92.00
O(4W) , O(22A)	103.2(4)	3.711(12)	-75.00	-61.00	-15.00	104.00
O(4W) , O(11B)	163.9(4)	4.710(12)	160.00	-97.00	-103.00	-20.00
O(4W) , O(6W)	82.8(5)	3.15(2)	66.00	54.00	12.00	114.00
*O(5W) , O(22A)	106.2(8)	3.79(2)	110.00	54.00	55.30(50)	70.70(25)
*O(5W) , O(11B)	105.1(6)	3.78(3)	103.00(50)	57.00	46.00	77.00
*O(5W) , O(6W)	110.3(9)	3.91(5)	-113.00	-69.00	-44.50(40)	66.50(20)
O(22A) , O(11B)	71.5(2)	2.813(8)	-62.40(40)	-49.00	-13.00	118.00
O(22A) , O(6W)	142.9(6)	4.57(2)	161.00	71.00	89.50(60)	19.50(30)
O(11B) , O(6W)	92.7(5)	3.50(2)	-65.60(50)	-50.00	-16.00	114.00
						O(22A) O(6W)
						O(5W) O(6W)
						O(22A) O(6W)
						O(5W) O(22A)
						O(4W) O(11B)b
						O(5W) O(6W)
						O(4W) O(11B)b
						O(5W) O(22A)

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Tau-Descriptor for 5-Coordination (A.W.Addison,T.N.Rao,J.Reedijk,J.van Rijn,G.C.Verschoor, J.Chem.Soc.Dalton Trans.(1984),1349-1356)

Tau = (Beta - Alpha) / 60 = (163.90-142.90) / 60 = 0.35 : (Extreme forms: Tau = 0.00 for SP and 1.00 for TP)

Analysis of Five-Coordination (See R.R. Holmes in Progress in Inorg. Chem. Vol. 32 (1984),119-235 and References Therein)

Idealized Dihedral Angles for Trans Basal Angle : 150.0

Del(13) & Del(23) Trigonal Bipyramid (TP): 101.5 53.1

Del(12) & Del(13) Square Pyramid (SP): 118.5 76.9

Distance Between TP and SP Along Berry Coordinate: 217.7

Pivot(3)	Sum(/Del:C - Del:TP/)	Sum(/Del:C - Del:SP/)	217.7 - Sum(/Del:C - Del:SP/)	Del(24)	Th(24)	Th(15)
O(5W)	142.5 Deg.	75.2 Deg.	142.5 Deg.	19.23	142.92	163.89
O(22A)	142.5 Deg.	275.2 Deg.	-57.5 Deg.	66.98	110.30	163.89
O(6W)	142.5 Deg.	295.6 Deg.	-77.9 Deg.	70.35	106.20	163.89

Trigonal Bipyramid (TP) to Square Pyramid (SP) ::: Perc. Along Berry Pseudorotation Coordinate: 65.4 ::: D3h ---> C2v ---> C4v

NOTE: This Analysis Depends on the Value of the Trans Basal Angle that is used (Default Value = 150 Deg.).

The Pivot Atom that Best Describes a Berry Pseudo Rotation is: O(5W)

The Percentage has been Calculated for the Average value, 142.5 Deg., of the Second and Fourth Table Entry.

The Difference, 0.0 Deg., Between the Second and Fourth Table Entry (for pivot) should be Zero for a True Berry Rotation.

>> Distance to SP square base plane defined by: O(4W) O(6W) O(22A) O(11B)b

O(4W) 0.1810(110), O(6W) -0.1900(200), O(22A) -0.2030(60), O(11B)b 0.2140(60), Na(1) 0.5300(70), O(5W) 2.8500(300)

3.6 Angstrom Coordination Sphere Around Atom I = O(1) [ARU = 1555.01] 0.16750 0.00510 0.00400 1.3001 0.0517 0.0449

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.920(6)	--	Cu(1)	[	=		Intra	-4.36	51.34	0.37342	0.00315	0.13751	2.4962	-0.0396	1.5442
2	1.942(6)	--	Cu(2)c	[-x, -y, -z	=	2555.01]	Intra	-129.74	-11.79	-0.00515	-0.13533	-0.03133	0.0847	-1.4104	-0.3518
3	1.964(6)	--	Cu(2)	[	=		Intra	135.54	8.99	0.00515	0.13533	0.03133	-0.0847	1.4104	0.3518
4	2.574(8)	<<	O(22B)c	[-x, -y, -z	=	2555.01]	Intra	37.60	-57.73	0.23050	0.07490	-0.18980	2.3890	0.8902	-2.1315
5	2.604(8)	<<	O(1)c	[-x, -y, -z	=	2555.01]	Intra	-177.72	-1.98	-0.16750	-0.00510	-0.00400	-1.3001	-0.0517	-0.0449
6	2.761(8)	<<	O(11A)	[	=		Intra	45.85	23.77	0.43600	0.18200	0.10310	3.0597	1.8645	1.1578
7	2.821(7)	<<	O(12A)	[	=		Intra	92.23	6.15	0.17110	0.27220	0.03090	1.1911	2.8538	0.3470
8	2.843(8)	<	O(21A)e	[1-x, -y, -z	=	2655.01]	Intra	-51.97	23.81	0.40800	-0.18410	0.10620	2.9027	-1.9974	1.1926
9	2.846(7)	<	O(22A)e	[1-x, -y, -z	=	2655.01]	Intra	-86.36	-9.01	0.16760	-0.26290	-0.03570	1.4785	-2.7532	-0.4009
10	2.922(8)	<	O(12B)	[	=		Intra	-126.85	75.70	0.21220	-0.03700	0.25610	0.8673	-0.5257	2.8760
11	3.034(9)	<	C(11A)	[	=		Intra	67.49	11.07	0.34030	0.26860	0.05590	2.4403	2.8026	0.6278
12	3.098(8)	..	O(11B)c	[-x, -y, -z	=	2555.01]	Intra	-124.35	-57.04	-0.05010	-0.13850	-0.22750	0.3488	-1.3400	-2.5548
13	3.130(9)	<	C(21A)e	[1-x, -y, -z	=	2655.01]	Intra	-66.91	4.88	0.32610	-0.26580	0.02770	2.5230	-2.8174	0.3111
14	3.268(8)	..	O(11B)	[	=		Intra	142.00	50.18	0.05010	0.13850	0.22750	-0.3488	1.3400	2.5548
15	3.435(10)	..	C(11B)	[	=		Intra	170.70	65.91	0.10380	0.04060	0.28320	-0.0833	0.2782	3.1803
16	3.463(10)	..	C(11B)c	[-x, -y, -z	=	2555.01]	Intra	-164.83	-68.65	-0.10380	-0.04060	-0.28320	0.0833	-0.2782	-3.1803
17	3.583(10)	..	C(21B)c	[-x, -y, -z	=	2555.01]	Intra	11.26	-61.22	0.27170	0.02300	-0.27560	2.9918	0.3884	-3.0950

Angles (Degrees) At1...V...At2 with Vertex V = O(1)

Cu(1)	,	Cu(2)c	120.9(3)	Cu(1)	,	Cu(2)	110.5(3)	Cu(1)	,	O(22B)c	114.3(3)	Cu(1)	,	O(1)c	130.3(3)
Cu(1)	,	O(11A)	47.11(17)	Cu(1)	,	O(12A)	89.3(2)	Cu(1)	,	O(21A)e	45.53(16)	Cu(1)	,	O(22A)e	92.1(2)
Cu(1)	,	O(12B)	47.64(18)	Cu(1)	,	C(11A)	70.1(2)	Cu(1)	,	O(11B)c	145.6(3)	Cu(1)	,	C(21A)e	69.3(2)
Cu(1)	,	O(11B)	74.5(2)	Cu(1)	,	C(11B)	62.7(2)	Cu(1)	,	C(11B)c	160.3(3)	Cu(1)	,	C(21B)c	113.3(3)
Cu(2)c	,	Cu(2)	96.4(3)	Cu(2)c	,	O(22B)c	109.7(3)	Cu(2)c	,	O(1)c	48.56(17)	Cu(2)c	,	O(11A)	167.3(3)
Cu(2)c	,	O(12A)	138.2(3)	Cu(2)c	,	O(21A)e	83.8(2)	Cu(2)c	,	O(22A)e	42.71(16)	Cu(2)c	,	O(12B)	87.5(2)
Cu(2)c	,	C(11A)	163.1(3)	Cu(2)c	,	O(11B)c	45.44(17)	Cu(2)c	,	C(21A)e	64.7(2)	Cu(2)c	,	O(11B)	97.9(2)
Cu(2)c	,	C(11B)	89.1(2)	Cu(2)c	,	C(11B)c	61.2(2)	Cu(2)c	,	C(21B)c	100.8(2)	Cu(2)	,	O(22B)c	101.8(3)
Cu(2)	,	O(1)c	47.84(17)	Cu(2)	,	O(11A)	86.1(2)	Cu(2)	,	O(12A)	43.01(16)	Cu(2)	,	O(21A)e	146.4(3)
Cu(2)	,	O(22A)e	138.6(3)	Cu(2)	,	O(12B)	83.2(2)	Cu(2)	,	C(11A)	66.9(2)	Cu(2)	,	O(11B)c	103.0(2)
Cu(2)	,	C(21A)e	153.7(3)	Cu(2)	,	O(11B)	41.54(16)	Cu(2)	,	C(11B)	61.8(2)	Cu(2)	,	C(11B)c	87.9(2)
Cu(2)	,	C(21B)c	113.9(3)	O(22B)c	,	O(1)c	114.0(3)	O(22B)c	,	O(11A)	81.8(2)	O(22B)c	,	O(12A)	77.5(3)
O(22B)c	,	O(21A)e	109.7(3)	O(22B)c	,	O(22A)e	99.3(3)	O(22B)c	,	O(12B)	161.2(3)	O(22B)c	,	C(11A)	73.0(3)
O(22B)c	,	O(11B)c	64.3(2)	O(22B)c	,	C(21A)e	101.8(3)	O(22B)c	,	O(11B)	137.3(3)	O(22B)c	,	C(11B)	157.0(3)
O(22B)c	,	C(11B)c	52.6(2)	O(22B)c	,	C(21B)c	13.7(2)	O(1)c	,	O(11A)	132.6(3)	O(1)c	,	O(12A)	90.3(2)
O(1)c	,	O(21A)e	123.2(3)	O(1)c	,	O(22A)e	91.0(2)	O(1)c	,	O(12B)	83.0(2)	O(1)c	,	C(11A)	114.7(3)
O(1)c	,	O(11B)c	69.3(2)	O(1)c	,	C(21A)e	110.9(3)	O(1)c	,	O(11B)	62.5(2)	O(1)c	,	C(11B)	68.4(2)
O(1)c	,	C(11B)c	67.2(2)	O(1)c	,	C(21B)c	116.4(3)	O(11A)	,	O(12A)	47.86(19)	O(11A)	,	O(21A)e	87.2(2)
O(11A)	,	O(22A)e	132.1(3)	O(11A)	,	O(12B)	80.4(2)	O(11A)	,	C(11A)	24.18(19)	O(11A)	,	O(11B)c	146.0(3)
O(11A)	,	C(21A)e	108.6(3)	O(11A)	,	O(11B)	75.7(2)	O(11A)	,	C(11B)	81.1(2)	O(11A)	,	C(11B)c	131.5(3)
O(11A)	,	C(21B)c	89.5(2)	O(12A)	,	O(21A)e	134.0(3)	O(12A)	,	O(22A)e	176.8(3)	O(12A)	,	O(12B)	95.0(2)
O(12A)	,	C(11A)	24.9(2)	O(12A)	,	O(11B)c	121.6(3)	O(12A)	,	C(21A)e	156.4(3)	O(12A)	,	O(11B)	60.4(2)

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O(12A) , C(11B)	79.7(2)	O(12A) , C(11B)c	100.4(2)	O(12A) , C(21B)c	91.1(2)	O(21A)e, O(22A)e	46.97(18)				
O(21A)e, O(12B)	63.3(2)	O(21A)e, C(11A)	111.4(3)	O(21A)e, O(11B)c	100.8(2)	O(21A)e, C(21A)e	23.78(19)				
O(21A)e, O(11B)	105.0(2)	O(21A)e, C(11B)	84.6(2)	O(21A)e, C(11B)c	120.4(2)	O(21A)e, C(21B)c	98.9(2)				
O(22A)e, O(12B)	88.1(2)	O(22A)e, C(11A)	154.2(3)	O(22A)e, O(11B)c	56.30(19)	O(22A)e, C(21A)e	23.85(19)				
O(22A)e, O(11B)	122.7(2)	O(22A)e, C(11B)	103.5(2)	O(22A)e, C(11B)c	77.4(2)	O(22A)e, C(21B)c	85.7(2)				
O(12B) , C(11A)	92.8(2)	O(12B) , O(11B)c	132.8(3)	O(12B) , C(21A)e	78.1(2)	O(12B) , O(11B)	42.17(18)				
O(12B) , C(11B)	21.37(19)	O(12B) , C(11B)c	146.3(3)	O(12B) , C(21B)c	159.7(3)	C(11A) , O(11B)c	133.1(3)				
C(11A) , C(21A)e	131.9(3)	C(11A) , O(11B)	71.6(2)	C(11A) , C(11B)	85.2(2)	C(11A) , C(11B)c	113.4(3)				
C(11A) , C(21B)c	84.6(2)	O(11B)c, C(21A)e	77.3(2)	O(11B)c, O(11B)	131.8(2)	O(11B)c, C(11B)	132.2(3)				
O(11B)c, C(11B)c	21.23(18)	O(11B)c, C(21B)c	56.8(2)	C(21A)e, O(11B)	119.6(2)	C(21A)e, C(11B)	98.1(2)				
C(21A)e, C(11B)c	97.4(2)	C(21A)e, C(21B)c	88.6(2)	O(11B) , C(11B)	21.50(18)	O(11B) , C(11B)c	125.1(2)				
O(11B) , C(21B)c	151.0(2)	C(11B) , C(11B)c	135.6(3)	C(11B) , C(21B)c	169.8(3)	C(11B)c, C(21B)c	50.1(2)				

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3.6 Angstrom Coordination Sphere Around Atom I = O(1W) [ARU = 1555.02] 0.57380 0.25340 0.39450 3.2113 2.4631 4.4302

Nr	d(I,J) To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.67(2) <<	O(6W)a	[-1+x,y,z	= 1455.01]		137.82	-15.22	0.30900	0.41460	0.33200	1.2990	4.1959	3.7284
2	2.70(4) <<	*O(5W)	[	= 01]		39.45	-14.56	0.81100	0.40800	0.33400	5.2310	4.1253	3.7508
3	2.782(15) <<	>O(2W)	[	= 03]		-1.85	84.13	0.70900	0.26490	0.64090	3.4956	2.4539	7.1973
4	2.805(12) <<	O(21B)b	[1+x,y,z	= 1655.01]		-80.05	-28.43	0.57460	0.01700	0.27560	3.6376	0.0334	3.0950
5	3.330(12) ..	O(11A)	[	= 01]		-104.21	-79.31	0.43600	0.18200	0.10310	3.0597	1.8645	1.1578
6	3.550(14) ..	C(21B)b	[1+x,y,z	= 1655.01]		-60.10	-22.09	0.72830	-0.02300	0.27560	4.8509	-0.3884	3.0950
7	3.577(15) ..	C(3B)b	[1+x,y,z	= 1655.01]		-60.23	18.90	0.82250	-0.02000	0.49770	4.8917	-0.4744	5.5892
8	3.36 ..	H(3B)b	[1+x,y,z	= 1655.01]		-76.47	19.85	0.70170	-0.03320	0.49620	3.9516	-0.6128	5.5723

Angles (Degrees) At1...V...At2 with Vertex V = O(1W)

O(6W)a , *O(5W)	94.0(9)	O(6W)a , >O(2W)	109.7(7)	O(6W)a , O(21B)b	123.0(6)	O(6W)a , O(11A)	80.0(6)
O(6W)a , C(21B)b	138.8(6)	O(6W)a , C(3B)b	162.4(7)	*O(5W) , >O(2W)	100.1(8)	*O(5W) , O(21B)b	107.4(7)
*O(5W) , O(11A)	84.1(6)	*O(5W) , C(21B)b	93.1(7)	*O(5W) , C(3B)b	103.6(8)	>O(2W) , O(21B)b	117.1(5)
>O(2W) , O(11A)	169.0(5)	>O(2W) , C(21B)b	108.9(5)	>O(2W) , C(3B)b	68.1(4)	O(21B)b, O(11A)	51.9(2)
O(21B)b, C(21B)b	19.1(2)	O(21B)b, C(3B)b	51.1(3)	O(11A) , C(21B)b	60.5(2)	O(11A) , C(3B)b	101.1(3)
C(21B)b, C(3B)b	41.0(2)						

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3.6 Angstrom Coordination Sphere Around Atom I = O(2W) [ARU = 1555.03] 0.70900 0.26490 0.64090 3.4956 2.4539 7.1973

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.737(14)	<<	O(12B)j	[1-x, -y, 1-z	=	2656.01]		-82.13	25.00	0.78780	0.03700	0.74390	3.8352	-0.0037	8.3540
2	2.782(15)	<<	O(1W)	[	=	02]		178.15	-84.13	0.57380	0.25340	0.39450	3.2113	2.4631	4.4302
3	2.98(3)	.<	O(7W)i	[1-x, 1-y, 1-z	=	2666.05]		167.61	13.20	0.37400	0.32690	0.70140	0.6661	3.0756	7.8767
4	3.044(19)	..	O(4W)h	[2-x, 1-y, 1-z	=	2766.01]		45.13	43.80	0.98570	0.42200	0.82850	5.0455	4.0111	9.3041
5	3.39(2)	..	O(6W)h	[2-x, 1-y, 1-z	=	2766.01]		94.92	5.15	0.69100	0.58540	0.66800	3.2060	5.8190	7.5016
6	3.452(16)	..	O(21A)g	[x, y, 1+z	=	1556.01]		-149.83	55.37	0.59200	0.18410	0.89380	1.7998	1.4681	10.0374
7	3.50	..	H(3B)b	[1+x, y, z	=	1655.01]		-81.54	-27.66	0.70170	-0.03320	0.49620	3.9516	-0.6128	5.5723

Angles (Degrees) At1...V...At2 with Vertex V = >O(2W)

O(12B)j,	O(1W)	115.9(5)	O(12B)j,	O(7W)i	102.1(6)	O(12B)j,	O(4W)h	96.0(5)	O(12B)j,	O(6W)h	149.7(6)
O(12B)j,	O(21A)g	57.1(3)	O(1W)	, O(7W)i	97.4(7)	O(1W)	, O(4W)h	137.6(7)	O(1W)	, O(6W)h	94.4(6)
O(1W)	, O(21A)g	140.3(8)	O(7W)i	, O(4W)h	102.7(5)	O(7W)i	, O(6W)h	72.0(6)	O(7W)i	, O(21A)g	53.5(4)
O(4W)h	, O(6W)h	58.3(5)	O(4W)h	, O(21A)g	80.0(3)	O(6W)h	, O(21A)g	99.7(6)			

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3.6 Angstrom Coordination Sphere Around Atom I = O(3W) [ARU = 1555.04] 1.07800 0.33700 0.57100 6.5948 3.2512 6.4123

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.97(3) <<	<O(8W)	[	=	06]		103.48	-23.82	1	1/2	1/2	6.1738	5.0075	5.6150
2	2.42(4) <<	O(7W)h	[2-x,1-y,1-z	=	2766.05]		-5.24	37.30	1.37400	0.32690	0.70140	8.5088	3.0756	7.8767
3	3.37(4) ..	O(4W)g	[2-x,1-y,1-z	=	2766.01]		153.87	59.17	0.98570	0.42200	0.82850	5.0455	4.0111	9.3041
4	3.56(3) ..	C(3B)i	[1-x,-y,1-z	=	2656.01]		-72.24	-12.53	1.17750	0.02000	0.50230	7.6535	-0.0550	5.6408
5	3.56(3) ..	C(2B)i	[1-x,-y,1-z	=	2656.01]		-84.01	6.79	1.13170	0.00530	0.60850	6.9637	-0.2662	6.8335

Angles (Degrees) At1...V...At2 with Vertex V = >O(3W)

<O(8W) , O(7W)h	118.6(16)	<O(8W) , O(4W)g	92.8(12)	<O(8W) , C(3B)i	143.4(14)	<O(8W) , C(2B)i	161.5(16)
O(7W)h , O(4W)g	82.0(10)	O(7W)h , C(3B)i	80.1(10)	O(7W)h , C(2B)i	77.0(9)	O(4W)g , C(3B)i	122.2(10)
O(4W)g , C(2B)i	99.7(9)	C(3B)i , C(2B)i	22.6(3)				

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3.6 Angstrom Coordination Sphere Around Atom I = O(4W) [ARU = 1555.01] 1.01430 0.57800 0.17150 7.3022 6.0038 1.9259

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.339(12)	--	Na(1)	[	=	]	Intra	-94.05	12.90	1.00700	0.36470	0.21800	7.1410	3.7301	2.4481
2	2.955(13)	.<	O(12A)f	[1-x,1-y,-z	=	2665.01]	Intra	116.69	-50.29	0.82890	0.72780	-0.03090	6.4541	7.6905	-0.3470
3	3.044(19)	..	>O(2W)g	[2-x,1-y,1-z	=	2766.03]		45.13	43.80	1.29100	0.73510	0.35910	8.8521	7.5611	4.0327
4	3.15(2)	..	O(6W)	[	=	]	Intra	-44.50	34.95	1.30900	0.41460	0.33200	9.1417	4.1959	3.7284
5	3.242(14)	..	C(3A)	[	=	]	Intra	-161.15	-45.45	0.65550	0.49800	-0.03420	5.1499	5.2692	-0.3841
6	3.34(3)	..	*O(5W)	[	=	]	Intra	-137.79	33.13	0.81100	0.40800	0.33400	5.2310	4.1253	3.7508
7	3.37(4)	..	>O(3W)h	[2-x,1-y,1-z	=	2766.04]		153.87	59.17	0.92200	0.66300	0.42900	5.7529	6.7638	4.8177
8	3.454(12)	..	O(22A)i	[2-x,1-y,-z	=	2765.01]		44.46	-42.36	1.16760	0.73710	-0.03570	9.1237	7.7911	-0.4009
9	3.482(13)	..	C(3A)i	[2-x,1-y,-z	=	2765.01]		-13.50	-26.28	1.34450	0.50200	0.03420	10.3380	5.2752	0.3841
10	2.58	.<	H(3A)i	[2-x,1-y,-z	=	2765.01]		-19.02	-29.75	1.23720	0.50290	0.05730	9.4237	5.2724	0.6435
11	2.94	..	H(3A)	[	=	]	Intra	-149.41	-60.76	0.76280	0.49710	-0.05730	6.0642	5.2719	-0.6435

Angles (Degrees) At1...V...At2 with Vertex V = O(4W)

Na(1)	,	O(12A)f	135.0(5)	Na(1)	,	>O(2W)g	112.2(5)	Na(1)	,	O(6W)	49.7(4)	Na(1)	,	C(3A)	83.9(4)
Na(1)	,	*O(5W)	44.6(5)	Na(1)	,	>O(3W)h	89.8(6)	Na(1)	,	O(22A)i	133.6(4)	Na(1)	,	C(3A)i	87.5(4)
O(12A)f,	>O(2W)g	112.7(4)	O(12A)f,	O(6W)	159.5(6)	O(12A)f,	C(3A)	52.5(2)	O(12A)f,	*O(5W)	124.3(7)				
O(12A)f,	>O(3W)h	113.6(7)	O(12A)f,	O(22A)i	48.5(2)	O(12A)f,	C(3A)i	91.7(3)	>O(2W)g,	O(6W)	66.4(5)				
>O(2W)g,	C(3A)	161.3(5)	>O(2W)g,	*O(5W)	103.0(6)	>O(2W)g,	>O(3W)h	61.6(8)	>O(2W)g,	O(22A)i	86.2(4)				
>O(2W)g,	C(3A)i	88.3(5)	O(6W),	C(3A)	131.8(5)	O(6W),	*O(5W)	74.1(8)	O(6W),	>O(3W)h	84.7(8)				
O(6W),	O(22A)i	112.0(5)	O(6W),	C(3A)i	67.9(5)	C(3A),	*O(5W)	81.4(6)	C(3A),	>O(3W)h	111.0(7)				
C(3A),	O(22A)i	89.3(3)	C(3A),	C(3A)i	102.5(4)	*O(5W),	>O(3W)h	51.1(7)	*O(5W),	O(22A)i	170.6(6)				
*O(5W),	C(3A)i	131.7(6)	>O(3W)h,	O(22A)i	134.8(6)	>O(3W)h,	C(3A)i	146.0(8)	O(22A)i,	C(3A)i	49.5(2)				

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3.6 Angstrom Coordination Sphere Around Atom I = O(5W) [ARU = 1555.01] 0.81100 0.40800 0.33400 5.2310 4.1253 3.7508

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.35(4) --	Na(1)	[	=	]	Intra	-11.69	-33.74	1.00700	0.36470	0.21800	7.1410	3.7301	2.4481
2	2.27(3) <<	O(8W)	[	=	06]		43.10	55.29	1	1/2	1/2	6.1738	5.0075	5.6150
3	2.70(4) <<	O(1W)	[	=	02]		-140.55	14.56	0.57380	0.25340	0.39450	3.2113	2.4631	4.4302
4	3.17(3) ..	O(7W)	[	=	05]		116.32	-7.22	0.62600	0.67310	0.29860	3.8389	6.9393	3.3533
5	3.34(3) ..	O(4W)	[	=	]	Intra	42.21	-33.13	1.01430	0.57800	0.17150	7.3022	6.0038	1.9259

Angles (Degrees) At1...V...At2 with Vertex V = *O(5W)

Na(1)	,	O(8W)	100.6(15)	Na(1)	,	O(1W)	130.1(9)	Na(1)	,	O(7W)	116.0(9)	Na(1)	,	O(4W)	44.5(6)
O(8W)	,	O(1W)	110.1(10)	O(8W)	,	O(7W)	86.6(7)	O(8W)	,	O(4W)	88.4(10)	O(1W)	,	O(7W)	104.5(13)
O(1W)	,	O(4W)	161.3(10)	O(7W)	,	O(4W)	72.8(6)								

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3.6 Angstrom Coordination Sphere Around Atom I = O(6W) [ARU = 1555.01] 1.30900 0.41460 0.33200 9.1417 4.1959 3.7284

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.42(2) --	Na(1)	[	=	]	Intra	-166.89	-31.93	1.00700	0.36470	0.21800	7.1410	3.7301	2.4481
2	2.67(2) <<	O(1W)g	[1+x,y,z	=	1655.02]		-42.18	15.22	1.57380	0.25340	0.39450	11.0540	2.4631	4.4302
3	3.15(2) ..	O(4W)	[	=	]	Intra	135.50	-34.95	1.01430	0.57800	0.17150	7.3022	6.0038	1.9259
4	3.39(2) ..	>O(2W)h	[2-x,1-y,1-z	=	2766.03]		94.92	5.15	1.29100	0.73510	0.35910	8.8521	7.5611	4.0327
5	3.50(2) ..	O(11B)b	[1+x,y,z	=	1655.01]	Intra	-119.98	-19.59	1.05010	0.13850	0.22750	7.4939	1.3400	2.5548
6	3.59(2) ..	C(11A)b	[1+x,y,z	=	1655.01]	Intra	-50.68	-59.85	1.34030	0.26860	0.05590	10.2830	2.8026	0.6278
7	3.28 ..	H(3A)i	[2-x,1-y,-z	=	2765.01]		75.32	-70.16	1.23720	0.50290	0.05730	9.4237	5.2724	0.6435

Angles (Degrees) At1...V...At2 with Vertex V = O(6W)

Na(1) , O(1W)g	127.2(7)	Na(1) , O(4W)	47.5(5)	Na(1) , >O(2W)h	99.7(7)	Na(1) , O(11B)b	43.7(3)
Na(1) , C(11A)b	74.4(6)	O(1W)g , O(4W)	160.2(9)	O(1W)g , >O(2W)h	132.9(9)	O(1W)g , O(11B)b	84.0(5)
O(1W)g , C(11A)b	75.4(6)	O(4W) , >O(2W)h	55.3(5)	O(4W) , O(11B)b	90.1(6)	O(4W) , C(11A)b	85.1(6)
>O(2W)h , O(11B)b	143.1(8)	>O(2W)h , C(11A)b	119.4(6)	O(11B)b , C(11A)b	62.8(4)		

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3.6 Angstrom Coordination Sphere Around Atom I = O(7W) [ARU = 1555.05] 0.62600 0.67310 0.29860 3.8389 6.9393 3.3533

Nr	d(I,J) To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	2.42(4) <<	>O(3W)i	[2-x,1-y,1-z	= 2766.04]		-5.24	37.30	0.92200	0.66300	0.42900	5.7529	6.7638	4.8177
2	2.922(17) .<	O(21A)f	[1-x,1-y,-z	= 2665.01]		125.19	-47.68	0.40800	0.81590	0.10620	2.7052	8.5469	1.1926
3	2.98(3) .<	>O(2W)h	[1-x,1-y,1-z	= 2666.03]		167.61	13.20	0.29100	0.73510	0.35910	1.0094	7.5611	4.0327
4	3.17(3) ..	*O(5W)	[	= 01]		-63.68	7.22	0.81100	0.40800	0.33400	5.2310	4.1253	3.7508
5	3.297(17) ..	O(22B)g	[1+x,1+y,z	= 1665.01]		62.43	-21.75	0.76950	0.92510	0.18980	5.2562	9.6541	2.1315
6	3.328(16) ..	C(21B)g	[1+x,1+y,z	= 1665.01]		75.79	-4.45	0.72830	0.97700	0.27560	4.6534	10.1559	3.0950
7	3.356(17) ..	C(2A)f	[1-x,1-y,-z	= 2665.01]		-147.69	-75.43	0.41780	0.61580	0.00940	3.1255	6.4882	0.1056
8	3.488(18) ..	C(21A)f	[1-x,1-y,-z	= 2665.01]		152.50	-60.72	0.32610	0.73420	0.02770	2.3255	7.7270	0.3111

Angles (Degrees) At1...V...At2 with Vertex V = O(7W)

>O(3W)i , O(21A)f	142.7(11)	>O(3W)i , >O(2W)h	129.1(11)	>O(3W)i , *O(5W)	60.7(10)	>O(3W)i , O(22B)g	86.8(10)
>O(3W)i , C(21B)g	85.6(9)	>O(3W)i , C(2A)f	138.2(12)	>O(3W)i , C(21A)f	152.7(12)	O(21A)f, >O(2W)h	71.6(5)
O(21A)f, *O(5W)	138.8(7)	O(21A)f, O(22B)g	55.9(3)	O(21A)f, C(21B)g	60.4(3)	O(21A)f, C(2A)f	43.6(3)
O(21A)f, C(21A)f	20.4(2)	>O(2W)h , *O(5W)	125.1(9)	>O(2W)h , O(22B)g	108.7(5)	>O(2W)h , C(21B)g	92.8(5)
>O(2W)h , C(2A)f	92.7(6)	>O(2W)h , C(21A)f	74.9(5)	*O(5W) , O(22B)g	126.1(10)	*O(5W) , C(21B)g	139.6(10)
*O(5W) , C(2A)f	95.5(6)	*O(5W) , C(21A)f	120.1(6)	O(22B)g, C(21B)g	21.6(2)	O(22B)g, C(2A)f	81.0(4)
O(22B)g, C(21A)f	71.2(3)	C(21B)g, C(2A)f	96.1(4)	C(21B)g, C(21A)f	79.6(4)	C(2A)f , C(21A)f	25.0(2)

3.6 Angstrom Coordination Sphere Around Atom I = O(11A) [ARU = 1555.01] 0.43600 0.18200 0.10310 3.0597 1.8645 1.1578

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.243(9) --	C(11A) [	=	]		Intra	123.44	-25.24	0.34030	0.26860	0.05590	2.4403	2.8026	0.6278
2	2.023(5) --	Cu(1) [	=	]		Intra	-106.49	11.01	0.37342	0.00315	0.13751	2.4962	-0.0396	1.5442
3	2.265(8) <<	O(12A) [	=	]		Intra	152.10	-20.98	0.17110	0.27220	0.03090	1.1911	2.8538	0.3470
4	2.369(9) <<	C(1A) [	=	]		Intra	86.81	-21.47	0.42590	0.38690	0.02590	3.1825	4.0659	0.2909
5	2.728(8) <<	O(21B)b[1+x,y,z	=	1655.01]		Intra	-72.48	45.25	0.57460	0.01700	0.27560	3.6376	0.0334	3.0950
6	2.761(8) <<	O(1) [	=	]		Intra	-134.15	-23.77	0.16750	0.00510	0.00400	1.3001	0.0517	0.0449
7	2.859(10) <<	C(21A) [	=	]		Intra	22.86	-30.92	0.67390	0.26580	-0.02770	5.3197	2.8174	-0.3111
8	2.921(9) <<	C(2A) [	=	]		Intra	56.33	-25.63	0.58220	0.38420	-0.00940	4.5197	4.0561	-0.1056
9	3.013(8) .<	O(21A) [	=	]		Intra	4.04	-51.27	0.59200	0.18410	-0.10620	4.9400	1.9974	-1.1926
10	3.278(6) <<	Cu(2) [	=	]		Intra	-171.78	-14.23	0.00515	0.13533	0.03133	-0.0847	1.4104	0.3518
11	3.330(12) ..	O(1W) [	=	02]			75.79	79.31	0.57380	0.25340	0.39450	3.2113	2.4631	4.4302
12	3.469(10) ..	C(21B)b[1+x,y,z	=	1655.01]		Intra	-51.51	33.94	0.72830	-0.02300	0.27560	4.8509	-0.3884	3.0950
13	3.496(8) ..	O(22B)c[-x,-y,-z	=	2555.01]		Intra	-124.55	-70.22	0.23050	0.07490	-0.18980	2.3890	0.8902	-2.1315
14	3.505(8) ..	O(22A) [	=	]		Intra	15.05	-12.47	0.83240	0.26290	0.03570	6.3642	2.7532	0.4009
15	3.543(9) ..	C(3A)f [1-x,1-y,-z	=	2665.01]		Intra	99.40	-12.62	0.34450	0.50200	0.03420	2.4953	5.2752	0.3841

Angles (Degrees) At1...V...At2 with Vertex V = O(11A)

C(11A) , Cu(1)	130.8(5)	C(11A) , O(12A)	26.7(4)	C(11A) , C(1A)	33.7(4)	C(11A) , O(21B)b	156.2(5)
C(11A) , O(1)	90.4(5)	C(11A) , C(21A)	85.6(5)	C(11A) , C(2A)	59.9(5)	C(11A) , O(21A)	86.9(5)
C(11A) , Cu(2)	61.4(4)	C(11A) , O(1W)	107.8(5)	C(11A) , C(21B)b	170.3(5)	C(11A) , O(22B)c	73.4(5)
C(11A) , O(22A)	100.7(5)	C(11A) , C(3A)f	25.9(4)	Cu(1) , O(12A)	104.5(3)	Cu(1) , C(1A)	163.5(4)
Cu(1) , O(21B)b	44.88(16)	Cu(1) , O(1)	44.06(16)	Cu(1) , C(21A)	129.2(3)	Cu(1) , C(2A)	158.2(3)
Cu(1) , O(21A)	111.4(2)	Cu(1) , Cu(2)	69.47(16)	Cu(1) , O(1W)	89.7(3)	Cu(1) , C(21B)b	54.97(19)
Cu(1) , O(22B)c	82.2(2)	Cu(1) , O(22A)	122.9(2)	Cu(1) , C(3A)f	154.6(3)	O(12A) , C(1A)	60.4(3)
O(12A) , O(21B)b	136.3(3)	O(12A) , O(1)	67.5(2)	O(12A) , C(21A)	108.8(3)	O(12A) , C(2A)	86.0(3)
O(12A) , O(21A)	102.5(3)	O(12A) , Cu(2)	35.00(16)	O(12A) , O(1W)	108.1(4)	O(12A) , C(21B)b	155.5(3)
O(12A) , O(22B)c	68.1(2)	O(12A) , O(22A)	126.2(3)	O(12A) , C(3A)f	50.9(2)	C(1A) , O(21B)b	150.8(3)
C(1A) , O(1)	119.7(3)	C(1A) , C(21A)	57.4(3)	C(1A) , C(2A)	28.2(3)	C(1A) , O(21A)	69.0(3)
C(1A) , Cu(2)	95.1(3)	C(1A) , O(1W)	101.0(3)	C(1A) , C(21B)b	141.4(3)	C(1A) , O(22B)c	85.7(3)
C(1A) , O(22A)	68.7(3)	C(1A) , C(3A)f	14.9(2)	O(21B)b , O(1)	88.9(2)	O(21B)b , C(21A)	114.9(3)
O(21B)b , C(2A)	134.8(3)	O(21B)b , O(21A)	116.8(2)	O(21B)b , Cu(2)	106.6(2)	O(21B)b , O(1W)	54.1(2)
O(21B)b , C(21B)b	19.63(19)	O(21B)b , O(22B)c	121.5(2)	O(21B)b , O(22A)	97.1(2)	O(21B)b , C(3A)f	146.6(3)
O(1) , C(21A)	121.0(3)	O(1) , C(2A)	129.6(3)	O(1) , O(21A)	96.5(2)	O(1) , Cu(2)	36.72(14)
O(1) , O(1W)	122.9(3)	O(1) , C(21B)b	97.3(2)	O(1) , O(22B)c	46.79(18)	O(1) , O(22A)	132.9(2)
O(1) , C(3A)f	116.3(2)	C(21A) , C(2A)	29.8(2)	C(21A) , O(21A)	24.65(19)	C(21A) , Cu(2)	132.7(3)
C(21A) , O(1W)	114.1(3)	C(21A) , C(21B)b	95.5(3)	C(21A) , O(22B)c	76.2(2)	C(21A) , O(22A)	19.80(19)
C(21A) , C(3A)f	72.1(2)	C(2A) , O(21A)	47.0(2)	C(2A) , Cu(2)	118.5(2)	C(2A) , O(1W)	105.5(3)
C(2A) , C(21B)b	118.1(3)	C(2A) , O(22B)c	84.2(2)	C(2A) , O(22A)	40.97(19)	C(2A) , C(3A)f	42.5(2)
O(21A) , Cu(2)	114.4(2)	O(21A) , O(1W)	136.9(3)	O(21A) , C(21B)b	98.2(2)	O(21A) , O(22B)c	52.98(18)
O(21A) , O(22A)	39.82(16)	O(21A) , C(3A)f	83.5(2)	Cu(2) , O(1W)	108.1(3)	Cu(2) , C(21B)b	122.9(2)
Cu(2) , O(22B)c	62.99(15)	Cu(2) , O(22A)	152.5(2)	Cu(2) , C(3A)f	85.80(18)	O(1W) , C(21B)b	62.9(3)

3.6 Angstrom Coordination Sphere Around Atom I = O(11B) [ARU = 1555.01] 0.05010 0.13850 0.22750 -0.3488 1.3400 2.5548

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.261(10)	--	C(11B)	[	=		Intra	-75.96	29.75	0.10380	0.04060	0.28320	-0.0833	0.2782	3.1803
2	2.220(6)	--	Cu(2)	[	=		Intra	14.93	-82.93	0.00515	0.13533	0.03133	-0.0847	1.4104	0.3518
3	2.418(8)	--	Na(1)a	[-1+x,y,z	=	1455.01]	Intra	98.40	-2.53	0.00700	0.36470	0.21800	-0.7017	3.7301	2.4481
4	2.250(9)	<<	O(12B)	[	=		Intra	-56.90	8.21	0.21220	-0.03700	0.25610	0.8673	-0.5257	2.8760
5	2.372(10)	<<	C(1B)	[	=		Intra	-110.76	51.32	0.04600	0.01530	0.39240	-0.8745	-0.0464	4.4067
6	2.813(8)	<<	O(22A)a	[-1+x,y,z	=	1455.01]	Intra	128.64	-49.97	-0.16760	0.26290	0.03570	-1.4785	2.7532	0.4009
7	3.052(9)	..	O(22B)	[	=		Intra	-132.45	-7.97	-0.23050	-0.07490	0.18980	-2.3890	-0.8902	2.1315
8	3.088(9)	..	O(12A)	[	=		Intra	44.51	-45.63	0.17110	0.27220	0.03090	1.1911	2.8538	0.3470
9	3.098(8)	..	O(1)c	[-x,-y,-z	=	2555.01]	Intra	-124.35	-57.04	-0.16750	-0.00510	-0.00400	-1.3001	-0.0517	-0.0449
10	3.102(10)	.<	C(2B)	[	=		Intra	-140.03	36.43	-0.13170	-0.00530	0.39150	-2.2612	-0.2631	4.3965
11	3.204(11)	.<	C(21B)	[	=		Intra	-146.82	9.71	-0.27170	-0.02300	0.27560	-2.9918	-0.3884	3.0950
12	3.268(8)	..	O(1)	[	=		Intra	-38.00	-50.18	0.16750	0.00510	0.00400	1.3001	0.0517	0.0449
13	3.319(6)	<<	Cu(1)	[	=		Intra	-25.87	-17.72	0.37342	0.00315	0.13751	2.4962	-0.0396	1.5442
14	3.390(10)	..	C(3B)d	[-x,-y,1-z	=	2556.01]	Intra	-83.47	65.54	0.17750	0.02000	0.50230	-0.1892	-0.0550	5.6408
15	3.50(2)	..	O(6W)a	[-1+x,y,z	=	1455.01]	Intra	60.02	19.59	0.30900	0.41460	0.33200	1.2990	4.1959	3.7284
16	3.52	..	H(3B)d	[-x,-y,1-z	=	2556.01]	Intra	-48.81	61.71	0.29830	0.03320	0.50380	0.7509	0.0834	5.6577

Angles (Degrees) At1...V...At2 with Vertex V = O(11B)

C(11B) , Cu(2)	119.6(5)	C(11B) , Na(1)a	152.3(5)	C(11B) , O(12B)	28.0(4)	C(11B) , C(1B)	33.6(5)
C(11B) , O(22A)a	152.6(5)	C(11B) , O(22B)	66.1(5)	C(11B) , O(12A)	131.5(5)	C(11B) , O(1)c	95.9(5)
C(11B) , C(2B)	53.1(5)	C(11B) , C(21B)	68.6(5)	C(11B) , O(1)	86.7(5)	C(11B) , Cu(1)	67.7(5)
C(11B) , C(3B)d	36.1(4)	C(11B) , O(6W)a	114.9(6)	Cu(2) , Na(1)a	86.7(2)	Cu(2) , O(12B)	96.0(3)
Cu(2) , C(1B)	145.0(4)	Cu(2) , O(22A)a	43.28(16)	Cu(2) , O(22B)	88.0(2)	Cu(2) , O(12A)	38.34(15)
Cu(2) , O(1)c	38.57(14)	Cu(2) , C(2B)	132.8(3)	Cu(2) , C(21B)	106.4(3)	Cu(2) , O(1)	35.93(14)
Cu(2) , Cu(1)	66.99(16)	Cu(2) , C(3B)d	155.6(3)	Cu(2) , O(6W)a	104.5(4)	Na(1)a , O(12B)	154.8(4)
Na(1)a , C(1B)	125.4(4)	Na(1)a , O(22A)a	53.9(2)	Na(1)a , O(22B)	128.2(3)	Na(1)a , O(12A)	63.7(2)
Na(1)a , O(1)c	111.2(3)	Na(1)a , C(2B)	116.6(3)	Na(1)a , C(21B)	114.9(3)	Na(1)a , O(1)	115.4(3)
Na(1)a , Cu(1)	121.5(3)	Na(1)a , C(3B)d	117.0(3)	Na(1)a , O(6W)a	43.7(4)	O(12B) , C(1B)	61.6(3)
O(12B) , O(22A)a	138.0(3)	O(12B) , O(22B)	77.0(3)	O(12B) , O(12A)	103.8(3)	O(12B) , O(1)c	85.0(3)
O(12B) , C(2B)	79.6(3)	O(12B) , C(21B)	88.5(3)	O(12B) , O(1)	60.7(2)	O(12B) , Cu(1)	40.15(19)
O(12B) , C(3B)d	60.2(2)	O(12B) , O(6W)a	112.0(4)	C(1B) , O(22A)a	143.4(4)	C(1B) , O(22B)	62.2(3)
C(1B) , O(12A)	162.8(4)	C(1B) , O(1)c	108.9(3)	C(1B) , C(2B)	25.5(3)	C(1B) , C(21B)	51.0(3)
C(1B) , O(1)	118.8(3)	C(1B) , Cu(1)	100.6(3)	C(1B) , C(3B)d	19.9(3)	C(1B) , O(6W)a	108.6(5)
O(22A)a , O(22B)	89.6(2)	O(22A)a , O(12A)	53.60(19)	O(22A)a , O(1)c	57.31(18)	O(22A)a , C(2B)	117.8(3)
O(22A)a , C(21B)	94.0(3)	O(22A)a , O(1)	79.2(2)	O(22A)a , Cu(1)	108.7(2)	O(22A)a , C(3B)d	157.3(3)
O(22A)a , O(6W)a	92.1(4)	O(22B) , O(12A)	126.3(2)	O(22B) , O(1)c	49.47(18)	O(22B) , C(2B)	45.0(2)
O(22B) , C(21B)	22.74(19)	O(22B) , O(1)	86.7(2)	O(22B) , Cu(1)	103.1(2)	O(22B) , C(3B)d	81.8(2)
O(22B) , O(6W)a	163.2(5)	O(12A) , O(1)c	76.9(2)	O(12A) , C(2B)	170.2(3)	O(12A) , C(21B)	142.8(3)
O(12A) , O(1)	52.59(17)	O(12A) , Cu(1)	63.81(16)	O(12A) , C(3B)d	146.0(3)	O(12A) , O(6W)a	66.7(4)
O(1)c , C(2B)	94.4(3)	O(1)c , C(21B)	69.3(2)	O(1)c , O(1)	48.19(17)	O(1)c , Cu(1)	79.69(17)

O(1)c , C(3B)d	126.4(3)	O(1)c , O(6W)a	142.4(4)	C(2B) , C(21B)	27.4(2)	C(2B) , O(1)	124.3(3)
C(2B) , Cu(1)	119.6(3)	C(2B) , C(3B)d	43.6(2)	C(2B) , O(6W)a	120.9(4)	C(21B) , O(1)	109.5(2)
C(21B) , Cu(1)	122.3(2)	C(21B) , C(3B)d	70.3(2)	C(21B) , O(6W)a	140.5(5)	O(1) , Cu(1)	33.88(12)
O(1) , C(3B)d	120.9(3)	O(1) , O(6W)a	110.0(4)	Cu(1) , C(3B)d	93.8(2)	Cu(1) , O(6W)a	92.2(4)
C(3B)d , O(6W)a	90.5(4)						

3.6 Angstrom Coordination Sphere Around Atom I = O(12A) [ARU = 1555.01] 0.17110 0.27220 0.03090 1.1911 2.8538 0.3470

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.281(10)	--	C(11A)	[	=	]	Intra	-2.35	12.66	0.34030	0.26860	0.05590	2.4403	2.8026	0.6278
2	1.927(6)	--	Cu(2)	[	=	]	Intra	-131.47	0.14	0.00515	0.13533	0.03133	-0.0847	1.4104	0.3518
3	2.265(8)	<<	O(11A)	[	=	]	Intra	-27.90	20.98	0.43600	0.18200	0.10310	3.0597	1.8645	1.1578
4	2.332(10)	<<	C(1A)	[	=	]	Intra	31.33	-1.38	0.42590	0.38690	0.02590	3.1825	4.0659	0.2909
5	2.672(8)	<<	O(22A)a	[-1+x,y,z	=	1455.01]	Intra	-177.84	1.16	-0.16760	0.26290	0.03570	-1.4785	2.7532	0.4009
6	2.751(9)	<<	C(3A)f	[1-x,1-y,-z	=	2665.01]	Intra	61.69	0.77	0.34450	0.50200	0.03420	2.4953	5.2752	0.3841
7	2.821(7)	<<	O(1)	[	=	]	Intra	-87.77	-6.15	0.16750	0.00510	0.00400	1.3001	0.0517	0.0449
8	2.955(13)	<	O(4W)f	[1-x,1-y,-z	=	2665.01]	Intra	116.69	-50.29	-0.01430	0.42200	-0.17150	0.3431	4.5405	-1.9259
9	2.961(9)	<<	Na(1)a	[-1+x,y,z	=	1455.01]	Intra	155.16	45.21	0.00700	0.36470	0.21800	-0.7017	3.7301	2.4481
10	3.088(9)	..	O(11B)	[	=	]	Intra	-135.49	45.63	0.05010	0.13850	0.22750	-0.3488	1.3400	2.5548
11	3.381(9)	..	O(22B)c	[-x,-y,-z	=	2555.01]	Intra	-58.61	-47.14	0.23050	0.07490	-0.18980	2.3890	0.8902	-2.1315
12	3.392(6)	<<	Cu(1)	[	=	]	Intra	-65.72	20.67	0.37342	0.00315	0.13751	2.4962	-0.0396	1.5442
13	3.568(10)	..	C(2A)	[	=	]	Intra	19.86	-7.29	0.58220	0.38420	-0.00940	4.5197	4.0561	-0.1056
14	2.47	<<	H(3A)f	[1-x,1-y,-z	=	2665.01]	Intra	80.84	6.90	0.23720	0.50290	0.05730	1.5810	5.2724	0.6435

Angles (Degrees) At1...V...At2 with Vertex V = O(12A)

C(11A) , Cu(2)	128.0(5)	C(11A) , O(11A)	25.8(4)	C(11A) , C(1A)	36.3(4)	C(11A) , O(22A)a	165.5(6)
C(11A) , C(3A)f	64.5(4)	C(11A) , O(1)	86.9(4)	C(11A) , O(4W)f	118.1(5)	C(11A) , Na(1)a	118.7(5)
C(11A) , O(11B)	108.1(5)	C(11A) , O(22B)c	78.0(5)	C(11A) , Cu(1)	60.9(4)	C(11A) , C(2A)	29.8(4)
Cu(2) , O(11A)	102.6(3)	Cu(2) , C(1A)	162.8(4)	Cu(2) , O(22A)a	46.38(17)	Cu(2) , C(3A)f	166.8(3)
Cu(2) , O(1)	44.07(16)	Cu(2) , O(4W)f	103.9(3)	Cu(2) , Na(1)a	78.3(2)	Cu(2) , O(11B)	45.63(18)
Cu(2) , O(22B)c	78.5(2)	Cu(2) , Cu(1)	67.35(16)	Cu(2) , C(2A)	150.5(3)	O(11A) , C(1A)	62.0(3)
O(11A) , O(22A)a	143.2(3)	O(11A) , C(3A)f	89.3(3)	O(11A) , O(1)	64.7(2)	O(11A) , O(4W)f	139.6(4)
O(11A) , Na(1)a	113.8(3)	O(11A) , O(11B)	86.6(3)	O(11A) , O(22B)c	73.5(2)	O(11A) , Cu(1)	35.27(16)
O(11A) , C(2A)	54.8(2)	C(1A) , O(22A)a	150.8(3)	C(1A) , C(3A)f	30.4(3)	C(1A) , O(1)	118.7(3)
C(1A) , O(4W)f	86.0(3)	C(1A) , Na(1)a	114.2(3)	C(1A) , O(11B)	134.3(3)	C(1A) , O(22B)c	89.0(3)
C(1A) , Cu(1)	97.1(3)	C(1A) , C(2A)	12.9(2)	O(22A)a , C(3A)f	120.4(3)	O(22A)a , O(1)	90.2(2)
O(22A)a , O(4W)f	75.5(3)	O(22A)a , Na(1)a	50.1(2)	O(22A)a , O(11B)	57.9(2)	O(22A)a , O(22B)c	110.3(3)
O(22A)a , Cu(1)	110.2(2)	O(22A)a , C(2A)	161.3(3)	C(3A)f , O(1)	149.1(3)	C(3A)f , O(4W)f	69.1(3)
C(3A)f , Na(1)a	91.9(3)	C(3A)f , O(11B)	131.2(3)	C(3A)f , O(22B)c	110.7(3)	C(3A)f , Cu(1)	124.3(3)
C(3A)f , C(2A)	42.5(2)	O(1) , O(4W)f	119.7(3)	O(1) , Na(1)a	113.3(3)	O(1) , O(11B)	67.0(2)
O(1) , O(22B)c	48.00(19)	O(1) , Cu(1)	34.47(13)	O(1) , C(2A)	106.6(2)	O(4W)f , Na(1)a	101.2(3)
O(4W)f , O(11B)	133.4(3)	O(4W)f , O(22B)c	82.5(3)	O(4W)f , Cu(1)	150.3(3)	O(4W)f , C(2A)	88.7(3)
Na(1)a , O(11B)	47.07(18)	Na(1)a , O(22B)c	156.7(3)	Na(1)a , Cu(1)	104.4(2)	Na(1)a , C(2A)	125.9(3)
O(11B) , O(22B)c	114.6(2)	O(11B) , Cu(1)	61.41(16)	O(11B) , C(2A)	136.1(3)	O(22B)c , Cu(1)	68.11(15)
O(22B)c , C(2A)	76.8(2)	Cu(1) , C(2A)	88.47(18)				

3.6 Angstrom Coordination Sphere Around Atom I = O(12B) [ARU = 1555.01] 0.21220 -0.03700 0.25610 0.8673 -0.5257 2.8760

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.282(10)	--	C(11B)	[	=		Intra	139.78	13.74	0.10380	0.04060	0.28320	-0.0833	0.2782	3.1803
2	2.159(6)	--	Cu(1)	[	=		Intra	16.62	-38.08	0.37342	0.00315	0.13751	2.4962	-0.0396	1.5442
3	2.250(9)	<<	O(11B)	[	=		Intra	123.10	-8.21	0.05010	0.13850	0.22750	-0.3488	1.3400	2.5548
4	2.368(10)	<<	C(1B)	[	=		Intra	164.61	40.27	0.04600	0.01530	0.39240	-0.8745	-0.0464	4.4067
5	2.737(14)	<<	>O(2W)g	[1-x,-y,1-z	=	2656.03]		-82.13	25.00	0.29100	-0.26490	0.35910	1.2069	-2.9833	4.0327
6	2.835(9)	<<	O(21B)b	[1+x,y,z	=	1655.01]	Intra	11.41	4.43	0.57460	0.01700	0.27560	3.6376	0.0334	3.0950
7	2.922(8)	.<	O(1)	[	=		Intra	53.15	-75.70	0.16750	0.00510	0.00400	1.3001	0.0517	0.0449
8	2.997(10)	<<	C(3B)d	[-x,-y,1-z	=	2556.01]	Intra	155.99	67.30	0.17750	0.02000	0.50230	-0.1892	-0.0550	5.6408
9	3.024(8)	.<	O(21A)e	[1-x,-y,-z	=	2655.01]	Intra	-35.87	-33.83	0.40800	-0.18410	0.10620	2.9027	-1.9974	1.1926
10	3.321(6)	<<	Cu(2)	[	=		Intra	116.18	-49.48	0.00515	0.13533	0.03133	-0.0847	1.4104	0.3518
11	3.360(9)	..	O(22B)	[	=		Intra	-173.61	-12.80	-0.23050	-0.07490	0.18980	-2.3890	-0.8902	2.1315
12	3.437(6)	<<	Cu(2)c	[-x,-y,-z	=	2555.01]	Intra	-131.50	-69.90	-0.00515	-0.13533	-0.03133	0.0847	-1.4104	-0.3518
13	3.488(11)	..	C(2B)	[	=		Intra	175.20	25.84	-0.13170	-0.00530	0.39150	-2.2612	-0.2631	4.3965
14	2.85	..	H(3B)d	[-x,-y,1-z	=	2556.01]	Intra	100.82	77.43	0.29830	0.03320	0.50380	0.7509	0.0834	5.6577

Angles (Degrees) At1...V...At2 with Vertex V = O(12B)

C(11B) , Cu(1)	124.4(5)	C(11B) , O(11B)	27.5(4)	C(11B) , C(1B)	34.3(5)	C(11B) , >O(2W)g	123.7(7)
C(11B) , O(21B)b	125.7(5)	C(11B) , O(1)	102.5(5)	C(11B) , C(3B)d	54.6(4)	C(11B) , O(21A)e	159.5(5)
C(11B) , Cu(2)	66.6(4)	C(11B) , O(22B)	53.3(5)	C(11B) , Cu(2)c	102.5(5)	C(11B) , C(2B)	35.3(4)
Cu(1) , O(11B)	97.6(3)	Cu(1) , C(1B)	155.2(4)	Cu(1) , >O(2W)g	111.7(5)	Cu(1) , O(21B)b	42.78(16)
Cu(1) , O(1)	41.08(15)	Cu(1) , C(3B)d	143.1(3)	Cu(1) , O(21A)e	42.14(15)	Cu(1) , Cu(2)	67.43(15)
Cu(1) , O(22B)	128.2(2)	Cu(1) , Cu(2)c	69.55(15)	Cu(1) , C(2B)	158.2(3)	O(11B) , C(1B)	61.8(3)
O(11B) , >O(2W)g	150.7(6)	O(11B) , O(21B)b	112.1(3)	O(11B) , O(1)	77.2(2)	O(11B) , C(3B)d	79.1(3)
O(11B) , O(21A)e	133.5(3)	O(11B) , Cu(2)	41.68(18)	O(11B) , O(22B)	62.3(3)	O(11B) , Cu(2)c	87.5(2)
O(11B) , C(2B)	61.0(3)	C(1B) , >O(2W)g	90.0(5)	C(1B) , O(21B)b	129.0(3)	C(1B) , O(1)	134.1(3)
C(1B) , C(3B)d	27.4(3)	C(1B) , O(21A)e	162.5(4)	C(1B) , Cu(2)	99.4(3)	C(1B) , O(22B)	56.8(3)
C(1B) , Cu(2)c	119.5(3)	C(1B) , C(2B)	16.9(3)	>O(2W)g , O(21B)b	91.3(5)	>O(2W)g , O(1)	124.7(4)
>O(2W)g , C(3B)d	78.2(4)	>O(2W)g , O(21A)e	73.4(4)	>O(2W)g , Cu(2)	151.7(4)	>O(2W)g , O(22B)	96.7(5)
>O(2W)g , Cu(2)c	101.2(3)	>O(2W)g , C(2B)	89.7(5)	O(21B)b , O(1)	83.8(2)	O(21B)b , C(3B)d	104.0(3)
O(21B)b , O(21A)e	58.7(2)	O(21B)b , Cu(2)	102.9(2)	O(21B)b , O(22B)	170.3(3)	O(21B)b , Cu(2)c	110.2(2)
O(21B)b , C(2B)	145.9(3)	O(1) , C(3B)d	156.2(3)	O(1) , O(21A)e	57.11(18)	O(1) , Cu(2)	35.97(13)
O(1) , O(22B)	87.2(2)	O(1) , Cu(2)c	34.37(13)	O(1) , C(2B)	122.7(3)	C(3B)d , O(21A)e	145.8(3)
C(3B)d , Cu(2)	120.6(3)	C(3B)d , O(22B)	83.1(2)	C(3B)d , Cu(2)c	145.7(3)	C(3B)d , C(2B)	43.1(2)
O(21A)e , Cu(2)	93.07(18)	O(21A)e , O(22B)	118.4(2)	O(21A)e , Cu(2)c	60.34(15)	O(21A)e , C(2B)	152.0(3)
Cu(2) , O(22B)	67.48(16)	Cu(2) , Cu(2)c	51.02(9)	Cu(2) , C(2B)	91.7(2)	O(22B) , Cu(2)c	62.83(15)
O(22B) , C(2B)	40.15(18)	Cu(2)c , C(2B)	103.0(2)				

3.6 Angstrom Coordination Sphere Around Atom I = O(21A) [ARU = 1555.01] 0.59200 0.18410 -0.10620 4.9400 1.9974 -1.1926

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.262(9) --	C(21A) [		=		Intra	65.15	44.29	0.67390	0.26580	-0.02770	5.3197	2.8174	-0.3111
2	2.030(5) --	Cu(1)e [1-x, -y, -z		=	2655.01]	Intra	-78.27	-9.97	0.62658	-0.00315	-0.13751	5.3465	0.0396	-1.5442
3	2.267(8) <<	O(22A) [		=		Intra	27.95	44.66	0.83240	0.26290	0.03570	6.3642	2.7532	0.4009
4	2.366(9) <<	C(2A) [		=		Intra	101.54	27.36	0.58220	0.38420	-0.00940	4.5197	4.0561	-0.1056
5	2.843(8) .<	O(1)e [1-x, -y, -z		=	2655.01]	Intra	-51.97	23.81	0.83250	-0.00510	-0.00400	6.5426	-0.0517	-0.0449
6	2.878(8) .<	O(21B)c[-x, -y, -z		=	2555.01]	Intra	-109.89	-41.38	0.42540	-0.01700	-0.27560	4.2051	-0.0334	-3.0950
7	2.922(17) .<	O(7W)h [1-x, 1-y, -z		=	2665.05]		125.19	-47.68	0.37400	0.32690	-0.29860	3.8063	3.6050	-3.3533
8	2.935(9) .<	O(22B)c[-x, -y, -z		=	2555.01]	Intra	-156.54	-18.65	0.23050	0.07490	-0.18980	2.3890	0.8902	-2.1315
9	3.013(8) .<	O(11A) [		=		Intra	-175.96	51.27	0.43600	0.18200	0.10310	3.0597	1.8645	1.1578
10	3.024(8) .<	O(12B)e[1-x, -y, -z		=	2655.01]	Intra	-35.87	-33.83	0.78780	0.03700	-0.25610	6.9754	0.5257	-2.8760
11	3.093(10) .<	C(1A) [		=		Intra	130.35	28.66	0.42590	0.38690	0.02590	3.1825	4.0659	0.2909
12	3.163(10) .<	C(21B)c[-x, -y, -z		=	2555.01]	Intra	-140.45	-36.98	0.27170	0.02300	-0.27560	2.9918	0.3884	-3.0950
13	3.195(10) .<	C(11A) [		=		Intra	162.15	34.73	0.34030	0.26860	0.05590	2.4403	2.8026	0.6278
14	3.267(6) <<	Cu(2)b [1+x, y, z		=	1655.01]	Intra	-11.77	28.22	1.00515	0.13533	0.03133	7.7580	1.4104	0.3518
15	3.377(9) ..	C(3A) [		=		Intra	86.33	13.85	0.65550	0.49800	-0.03420	5.1499	5.2692	-0.3841
16	3.452(16) ..	>O(2W)g [x, y, -1+z		=	1554.03]		30.17	-55.37	0.70900	0.26490	-0.35910	6.6358	2.9833	-4.0327
17	3.51 ..	H(3A) [		=		Intra	71.05	9.01	0.76280	0.49710	-0.05730	6.0642	5.2719	-0.6435

Angles (Degrees) At1...V...At2 with Vertex V = O(21A)

C(21A) , Cu(1)e	133.4(5)	C(21A) , O(22A)	26.3(4)	C(21A) , C(2A)	33.6(4)	C(21A) , O(1)e	91.0(5)
C(21A) , O(21B)c	175.3(5)	C(21A) , O(7W)h	106.0(5)	C(21A) , O(22B)c	136.9(5)	C(21A) , O(11A)	70.8(4)
C(21A) , O(12B)e	120.2(5)	C(21A) , C(1A)	53.3(4)	C(21A) , C(21B)c	159.3(5)	C(21A) , C(11A)	71.0(5)
C(21A) , Cu(2)b	61.8(4)	C(21A) , C(3A)	35.4(4)	C(21A) , >O(2W)g	104.0(5)	Cu(1)e , O(22A)	108.5(3)
Cu(1)e , C(2A)	162.6(3)	Cu(1)e , O(1)e	42.45(15)	Cu(1)e , O(21B)c	41.95(15)	Cu(1)e , O(7W)h	118.7(4)
Cu(1)e , O(22B)c	75.8(2)	Cu(1)e , O(11A)	102.6(2)	Cu(1)e , O(12B)e	45.53(17)	Cu(1)e , C(1A)	147.3(3)
Cu(1)e , C(21B)c	61.9(2)	Cu(1)e , C(11A)	119.9(3)	Cu(1)e , Cu(2)b	74.68(17)	Cu(1)e , C(3A)	164.4(3)
Cu(1)e , >O(2W)g	92.0(3)	O(22A) , C(2A)	59.9(3)	O(22A) , O(1)e	66.6(2)	O(22A) , O(21B)c	149.4(3)
O(22A) , O(7W)h	125.5(4)	O(22A) , O(22B)c	153.7(3)	O(22A) , O(11A)	81.9(2)	O(22A) , O(12B)e	97.5(3)
O(22A) , C(1A)	78.3(3)	O(22A) , C(21B)c	168.4(3)	O(22A) , C(11A)	90.4(3)	O(22A) , Cu(2)b	35.47(16)
O(22A) , C(3A)	58.0(2)	O(22A) , >O(2W)g	100.1(4)	C(2A) , O(1)e	122.8(3)	C(2A) , O(21B)c	150.7(3)
C(2A) , O(7W)h	78.0(4)	C(2A) , O(22B)c	108.7(3)	C(2A) , O(11A)	64.5(3)	C(2A) , O(12B)e	143.0(3)
C(2A) , C(1A)	25.4(3)	C(2A) , C(21B)c	127.6(3)	C(2A) , C(11A)	51.7(3)	C(2A) , Cu(2)b	95.3(3)
C(2A) , C(3A)	19.6(2)	C(2A) , >O(2W)g	102.5(3)	O(1)e , O(21B)c	84.4(2)	O(1)e , O(7W)h	156.0(4)
O(1)e , O(22B)c	110.3(2)	O(1)e , O(11A)	90.3(2)	O(1)e , O(12B)e	59.64(19)	O(1)e , C(1A)	127.5(3)
O(1)e , C(21B)c	102.9(2)	O(1)e , C(11A)	113.1(3)	O(1)e , Cu(2)b	36.24(13)	O(1)e , C(3A)	124.5(3)
O(1)e , >O(2W)g	105.1(4)	O(21B)c , O(7W)h	78.5(3)	O(21B)c , O(22B)c	45.61(19)	O(21B)c , O(11A)	109.0(2)
O(21B)c , O(12B)e	57.35(19)	O(21B)c , C(1A)	130.1(3)	O(21B)c , C(21B)c	24.0(2)	O(21B)c , C(11A)	110.8(3)
O(21B)c , Cu(2)b	114.0(2)	O(21B)c , C(3A)	149.1(3)	O(21B)c , >O(2W)g	77.5(3)	O(7W)h , O(22B)c	68.5(4)
O(7W)h , O(11A)	111.0(5)	O(7W)h , O(12B)e	96.7(4)	O(7W)h , C(1A)	76.5(4)	O(7W)h , C(21B)c	66.2(4)
O(7W)h , C(11A)	88.8(5)	O(7W)h , Cu(2)b	141.6(5)	O(7W)h , C(3A)	70.6(3)	O(7W)h , >O(2W)g	54.9(6)
O(22B)c , O(11A)	72.0(2)	O(22B)c , O(12B)e	102.9(2)	O(22B)c , C(1A)	84.9(2)	O(22B)c , C(21B)c	23.1(2)

O(22B)c, C(11A)	66.3(2)	O(22B)c, Cu(2)b	146.4(2)	O(22B)c, C(3A)	119.7(3)	O(22B)c, >O(2W)g	105.8(4)
O(11A) , O(12B)e	146.4(2)	O(11A) , C(1A)	45.64(19)	O(11A) , C(21B)c	93.6(2)	O(11A) , C(11A)	22.85(18)
O(11A) , Cu(2)b	99.30(19)	O(11A) , C(3A)	84.0(2)	O(11A) , >O(2W)g	164.0(4)	O(12B)e, C(1A)	167.2(3)
O(12B)e, C(21B)c	80.3(2)	O(12B)e, C(11A)	165.1(3)	O(12B)e, Cu(2)b	66.11(16)	O(12B)e, C(3A)	124.3(3)
O(12B)e, >O(2W)g	49.5(3)	C(1A) , C(21B)c	106.2(3)	C(1A) , C(11A)	27.6(2)	C(1A) , Cu(2)b	112.6(2)
C(1A) , C(3A)	43.3(2)	C(1A) , >O(2W)g	118.9(3)	C(21B)c, C(11A)	89.4(3)	C(21B)c, Cu(2)b	136.4(2)
C(21B)c, C(3A)	132.5(3)	C(21B)c, >O(2W)g	87.3(4)	C(11A) , Cu(2)b	116.8(2)	C(11A) , C(3A)	70.6(2)
C(11A) , >O(2W)g	141.4(4)	Cu(2)b , C(3A)	90.42(19)	Cu(2)b , >O(2W)g	91.0(4)	C(3A) , >O(2W)g	83.7(3)

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3.6 Angstrom Coordination Sphere Around Atom I = O(21B) [ARU = 1555.01] -0.42540 0.01700 0.27560 -4.2051 0.0334 3.0950

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.285(11)	--	C(21B)	[	=		Intra	-19.17	0.00	-0.27170	-0.02300	0.27560	-2.9918	-0.3884	3.0950
2	1.927(6)	--	Cu(1)a	[-1+x,y,z	=	1455.01]	Intra	-176.34	-53.59	-0.62658	0.00315	0.13751	-5.3465	-0.0396	1.5442
3	2.254(9)	<<	O(22B)	[	=		Intra	-26.96	-25.31	-0.23050	-0.07490	0.18980	-2.3890	-0.8902	2.1315
4	2.358(10)	<<	C(2B)	[	=		Intra	-8.67	33.50	-0.13170	-0.00530	0.39150	-2.2612	-0.2631	4.3965
5	2.728(8)	<<	O(11A)a	[-1+x,y,z	=	1455.01]	Intra	107.52	-45.25	-0.56400	0.18200	0.10310	-4.7830	1.8645	1.1578
6	2.805(12)	<<	O(1W)g	[-1+x,y,z	=	1455.02]		99.95	28.43	-0.42620	0.25340	0.39450	-4.6314	2.4631	4.4302
7	2.835(9)	<<	O(12B)a	[-1+x,y,z	=	1455.01]	Intra	-168.59	-4.43	-0.78780	-0.03700	0.25610	-6.9754	-0.5257	2.8760
8	2.838(10)	<<	C(3B)	[	=		Intra	-22.04	61.52	-0.17750	-0.02000	0.49770	-2.9510	-0.4744	5.5892
9	2.878(8)	.<	O(21A)c	[-x,-y,-z	=	2555.01]	Intra	-109.89	-41.38	-0.59200	-0.18410	0.10620	-4.9400	-1.9974	1.1926
10	3.581(10)	..	C(1B)	[	=		Intra	-1.37	21.49	0.04600	0.01530	0.39240	-0.8745	-0.0464	4.4067
11	2.58	.<	H(3B)	[	=		Intra	-64.08	73.83	-0.29830	-0.03320	0.49620	-3.8911	-0.6128	5.5723

Angles (Degrees) At1...V...At2 with Vertex V = O(21B)

C(21B) , Cu(1)a	123.2(5)	C(21B) , O(22B)	26.4(4)	C(21B) , C(2B)	34.9(4)	C(21B) , O(11A)a	114.9(5)
C(21B) , O(1W)g	115.3(6)	C(21B) , O(12B)a	149.1(5)	C(21B) , C(3B)	61.6(5)	C(21B) , O(21A)c	90.6(5)
C(21B) , C(1B)	27.6(4)	Cu(1)a , O(22B)	96.8(3)	Cu(1)a , C(2B)	158.1(4)	Cu(1)a , O(11A)a	47.80(17)
Cu(1)a , O(1W)g	109.0(3)	Cu(1)a , O(12B)a	49.57(17)	Cu(1)a , C(3B)	164.3(3)	Cu(1)a , O(21A)c	44.77(16)
Cu(1)a , C(1B)	147.7(3)	O(22B) , C(2B)	61.3(3)	O(22B) , O(11A)a	98.2(3)	O(22B) , O(1W)g	132.9(4)
O(22B) , O(12B)a	132.4(3)	O(22B) , C(3B)	86.9(3)	O(22B) , O(21A)c	68.5(2)	O(22B) , C(1B)	53.0(2)
C(2B) , O(11A)a	130.6(3)	C(2B) , O(1W)g	88.4(4)	C(2B) , O(12B)a	145.4(3)	C(2B) , C(3B)	29.3(3)
C(2B) , O(21A)c	119.1(3)	C(2B) , C(1B)	13.6(2)	O(11A)a , O(1W)g	74.0(3)	O(11A)a , O(12B)a	82.6(2)
O(11A)a , C(3B)	146.9(3)	O(11A)a , O(21A)c	87.1(2)	O(11A)a , C(1B)	118.2(3)	O(1W)g , O(12B)a	93.4(4)
O(1W)g , C(3B)	78.7(3)	O(1W)g , O(21A)c	152.5(4)	O(1W)g , C(1B)	89.2(4)	O(12B)a , C(3B)	117.7(3)
O(12B)a , O(21A)c	63.9(2)	O(12B)a , C(1B)	158.9(3)	C(3B) , O(21A)c	124.6(3)	C(3B) , C(1B)	42.5(2)
O(21A)c , C(1B)	117.6(2)						

3.6 Angstrom Coordination Sphere Around Atom I = O(22A) [ARU = 1555.01] 0.83240 0.26290 0.03570 6.3642 2.7532 0.4009

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.266(10)	--	C(21A)	[	=		Intra	176.49	-34.23	0.67390	0.26580	-0.02770	5.3197	2.8174	-0.3111
2	1.936(6)	--	Cu(2)b	[1+x,y,z	=	1655.01]	Intra	-43.93	-1.45	1.00515	0.13533	0.03133	7.7580	1.4104	0.3518
3	2.398(8)	--	Na(1)	[	=		Intra	51.51	58.63	1.00700	0.36470	0.21800	7.1410	3.7301	2.4481
4	2.267(8)	<<	O(21A)	[	=		Intra	-152.05	-44.66	0.59200	0.18410	-0.10620	4.9400	1.9974	-1.1926
5	2.314(10)	<<	C(2A)	[	=		Intra	144.76	-12.64	0.58220	0.38420	-0.00940	4.5197	4.0561	-0.1056
6	2.672(8)	<<	O(12A)b	[1+x,y,z	=	1655.01]	Intra	2.16	-1.16	1.17110	0.27220	0.03090	9.0338	2.8538	0.3470
7	2.813(8)	<<	O(11B)b	[1+x,y,z	=	1655.01]	Intra	-51.36	49.97	1.05010	0.13850	0.22750	7.4939	1.3400	2.5548
8	2.846(7)	<	O(1)e	[1-x,-y,-z	=	2655.01]	Intra	-86.36	-9.01	0.83250	-0.00510	-0.00400	6.5426	-0.0517	-0.0449
9	2.902(9)	<<	C(3A)	[	=		Intra	115.76	-15.69	0.65550	0.49800	-0.03420	5.1499	5.2692	-0.3841
10	3.444(10)	..	C(1A)	[	=		Intra	157.58	-1.83	0.42590	0.38690	0.02590	3.1825	4.0659	0.2909
11	3.454(12)	..	O(4W)g	[2-x,1-y,-z	=	2765.01]		44.46	-42.36	0.98570	0.42200	-0.17150	8.1858	4.5405	-1.9259
12	3.490(5)	<<	Cu(1)e	[1-x,-y,-z	=	2655.01]	Intra	-110.56	-33.87	0.62658	-0.00315	-0.13751	5.3465	0.0396	-1.5442
13	3.505(8)	..	O(11A)	[	=		Intra	-164.95	12.47	0.43600	0.18200	0.10310	3.0597	1.8645	1.1578
14	2.74	..	H(3A)	[	=		Intra	96.79	-22.38	0.76280	0.49710	-0.05730	6.0642	5.2719	-0.6435

Angles (Degrees) At1...V...At2 with Vertex V = O(22A)

C(21A) , Cu(2)b	128.0(5)	C(21A) , Na(1)	136.6(5)	C(21A) , O(21A)	26.2(4)	C(21A) , C(2A)	36.0(4)
C(21A) , O(12A)b	144.2(5)	C(21A) , O(11B)b	142.0(5)	C(21A) , O(1)e	90.8(4)	C(21A) , C(3A)	57.2(4)
C(21A) , C(1A)	36.9(4)	C(21A) , O(4W)g	91.7(5)	C(21A) , Cu(1)e	59.0(4)	C(21A) , O(11A)	49.9(4)
Cu(2)b , Na(1)	94.1(3)	Cu(2)b , O(21A)	101.7(3)	Cu(2)b , C(2A)	163.5(4)	Cu(2)b , O(12A)b	46.08(17)
Cu(2)b , O(11B)b	51.82(18)	Cu(2)b , O(1)e	42.88(16)	Cu(2)b , C(3A)	153.6(3)	Cu(2)b , C(1A)	158.2(3)
Cu(2)b , O(4W)g	87.8(3)	Cu(2)b , Cu(1)e	69.91(16)	Cu(2)b , O(11A)	120.6(2)	Na(1) , O(21A)	160.0(4)
Na(1) , C(2A)	102.5(3)	Na(1) , O(12A)b	71.2(3)	Na(1) , O(11B)b	54.6(2)	Na(1) , O(1)e	121.0(3)
Na(1) , C(3A)	90.8(3)	Na(1) , C(1A)	99.9(3)	Na(1) , O(4W)g	101.2(3)	Na(1) , Cu(1)e	152.5(2)
Na(1) , O(11A)	103.0(3)	O(21A) , C(2A)	62.2(3)	O(21A) , O(12A)b	128.8(3)	O(21A) , O(11B)b	128.5(3)
O(21A) , O(1)e	66.5(2)	O(21A) , C(3A)	80.6(3)	O(21A) , C(1A)	61.6(2)	O(21A) , O(4W)g	91.7(3)
O(21A) , Cu(1)e	33.48(16)	O(21A) , O(11A)	58.3(2)	C(2A) , O(12A)b	140.4(3)	C(2A) , O(11B)b	140.4(3)
C(2A) , O(1)e	124.8(3)	C(2A) , C(3A)	28.3(3)	C(2A) , C(1A)	16.7(2)	C(2A) , O(4W)g	88.9(3)
C(2A) , Cu(1)e	94.8(3)	C(2A) , O(11A)	55.8(2)	O(12A)b , O(11B)b	68.5(2)	O(12A)b , O(1)e	88.4(2)
O(12A)b , C(3A)	112.3(3)	O(12A)b , C(1A)	155.2(3)	O(12A)b , O(4W)g	55.9(2)	O(12A)b , Cu(1)e	108.0(2)
O(12A)b , O(11A)	162.9(3)	O(11B)b , O(1)e	66.4(2)	O(11B)b , C(3A)	144.2(3)	O(11B)b , C(1A)	126.0(3)
O(11B)b , O(4W)g	124.3(3)	O(11B)b , Cu(1)e	98.8(2)	O(11B)b , O(11A)	94.9(2)	O(1)e , C(3A)	147.0(3)
O(1)e , C(1A)	115.4(2)	O(1)e , O(4W)g	111.8(3)	O(1)e , Cu(1)e	33.35(13)	O(1)e , O(11A)	80.97(19)
C(3A) , C(1A)	43.5(2)	C(3A) , O(4W)g	65.8(3)	C(3A) , Cu(1)e	113.7(2)	C(3A) , O(11A)	83.3(2)
C(1A) , O(4W)g	105.6(3)	C(1A) , Cu(1)e	90.52(18)	C(1A) , O(11A)	39.86(17)	O(4W)g , Cu(1)e	100.4(2)
O(4W)g , O(11A)	140.7(3)	Cu(1)e , O(11A)	69.41(14)				

3.6 Angstrom Coordination Sphere Around Atom I = O(22B) [ARU = 1555.01] -0.23050 -0.07490 0.18980 -2.3890 -0.8902 2.1315

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.242(10)	--	C(21B)	[	=	] Intra	140.22	50.85	-0.27170	-0.02300	0.27560	-2.9918	-0.3884	3.0950
2	2.254(9)	<<	O(21B)	[	=	] Intra	153.04	25.31	-0.42540	0.01700	0.27560	-4.2051	0.0334	3.0950
3	2.354(10)	<<	C(2B)	[	=	] Intra	78.49	74.22	-0.13170	-0.00530	0.39150	-2.2612	-0.2631	4.3965
4	2.574(8)	<<	O(1)c	[-x, -y, -z	= 2555.01]	Intra	37.60	-57.73	-0.16750	-0.00510	-0.00400	-1.3001	-0.0517	-0.0449
5	2.790(10)	<<	C(11B)	[	=	] Intra	26.87	22.09	0.10380	0.04060	0.28320	-0.0833	0.2782	3.1803
6	2.861(10)	<<	C(1B)	[	=	] Intra	29.13	52.69	0.04600	0.01530	0.39240	-0.8745	-0.0464	4.4067
7	2.935(9)	<	O(21A)c	[-x, -y, -z	= 2555.01]	Intra	-156.54	-18.65	-0.59200	-0.18410	0.10620	-4.9400	-1.9974	1.1926
8	3.052(9)	..	O(11B)	[	=	] Intra	47.55	7.97	0.05010	0.13850	0.22750	-0.3488	1.3400	2.5548
9	3.133(7)	<<	Cu(1)a	[-1+x, y, z	= 1455.01]	Intra	163.95	-10.80	-0.62658	0.00315	0.13751	-5.3465	-0.0396	1.5442
10	3.297(17)	..	O(7W)g	[-1+x, -1+y, z	= 1445.05]		-117.57	21.75	-0.37400	-0.32690	0.29860	-3.8063	-3.6050	3.3533
11	3.358(10)	..	C(11A)c	[-x, -y, -z	= 2555.01]	Intra	-91.54	-55.27	-0.34030	-0.26860	-0.05590	-2.4403	-2.8026	-0.6278
12	3.360(9)	..	O(12B)	[	=	] Intra	6.39	12.80	0.21220	-0.03700	0.25610	0.8673	-0.5257	2.8760
13	3.381(9)	..	O(12A)c	[-x, -y, -z	= 2555.01]	Intra	-58.61	-47.14	-0.17110	-0.27220	-0.03090	-1.1911	-2.8538	-0.3470
14	3.496(8)	..	O(11A)c	[-x, -y, -z	= 2555.01]	Intra	-124.55	-70.22	-0.43600	-0.18200	-0.10310	-3.0597	-1.8645	-1.1578
15	3.528(10)	..	C(3B)	[	=	] Intra	143.50	78.57	-0.17750	-0.02000	0.49770	-2.9510	-0.4744	5.5892
16	3.544(6)	<<	Cu(2)c	[-x, -y, -z	= 2555.01]	Intra	-11.87	-44.49	-0.00515	-0.13533	-0.03133	0.0847	-1.4104	-0.3518

Angles (Degrees) At1...V...At2 with Vertex V = O(22B)

C(21B) , O(21B)	27.4(5)	C(21B) , C(2B)	34.2(5)	C(21B) , O(1)c	136.8(6)	C(21B) , C(11B)	86.6(5)
C(21B) , C(1B)	61.4(5)	C(21B) , O(21A)c	88.8(5)	C(21B) , O(11B)	85.5(5)	C(21B) , Cu(1)a	65.0(5)
C(21B) , O(7W)g	80.6(6)	C(21B) , C(11A)c	149.3(6)	C(21B) , O(12B)	104.8(5)	C(21B) , O(12A)c	167.1(6)
C(21B) , O(11A)c	138.5(6)	C(21B) , C(3B)	27.7(5)	C(21B) , Cu(2)c	160.3(6)	O(21B) , C(2B)	61.5(3)
O(21B) , O(1)c	124.7(3)	O(21B) , C(11B)	109.5(3)	O(21B) , C(1B)	88.0(3)	O(21B) , O(21A)c	65.9(2)
O(21B) , O(11B)	100.4(3)	O(21B) , Cu(1)a	37.65(18)	O(21B) , O(7W)g	80.4(4)	O(21B) , C(11A)c	124.9(3)
O(21B) , O(12B)	129.9(3)	O(21B) , O(12A)c	146.8(3)	O(21B) , O(11A)c	111.2(3)	O(21B) , C(3B)	53.4(2)
O(21B) , Cu(2)c	157.3(3)	C(2B) , O(1)c	134.7(4)	C(2B) , C(11B)	58.8(3)	C(2B) , C(1B)	29.2(3)
C(2B) , O(21A)c	117.1(3)	C(2B) , O(11B)	68.6(3)	C(2B) , Cu(1)a	99.2(3)	C(2B) , O(7W)g	83.5(4)
C(2B) , C(11A)c	160.6(4)	C(2B) , O(12B)	72.9(3)	C(2B) , O(12A)c	147.2(4)	C(2B) , O(11A)c	172.0(4)
C(2B) , C(3B)	15.0(3)	C(2B) , Cu(2)c	132.5(3)	O(1)c , C(11B)	80.3(3)	O(1)c , C(1B)	110.6(3)
O(1)c , O(21A)c	102.7(3)	O(1)c , O(11B)	66.2(2)	O(1)c , Cu(1)a	98.8(2)	O(1)c , O(7W)g	139.8(4)
O(1)c , C(11A)c	59.8(2)	O(1)c , O(12B)	75.1(2)	O(1)c , O(12A)c	54.52(19)	O(1)c , O(11A)c	51.42(18)
O(1)c , C(3B)	149.1(3)	O(1)c , Cu(2)c	32.86(14)	C(11B) , C(1B)	30.7(2)	C(11B) , O(21A)c	175.3(3)
C(11B) , O(11B)	24.4(2)	C(11B) , Cu(1)a	137.5(3)	C(11B) , O(7W)g	124.1(4)	C(11B) , C(11A)c	124.1(3)
C(11B) , O(12B)	21.6(2)	C(11B) , O(12A)c	103.1(3)	C(11B) , O(11A)c	129.0(3)	C(11B) , C(3B)	73.4(3)
C(11B) , Cu(2)c	75.4(2)	C(1B) , O(21A)c	145.7(3)	C(1B) , O(11B)	47.2(2)	C(1B) , Cu(1)a	124.7(3)
C(1B) , O(7W)g	100.1(4)	C(1B) , C(11A)c	146.1(3)	C(1B) , O(12B)	43.8(2)	C(1B) , O(12A)c	124.5(3)
C(1B) , O(11A)c	158.8(3)	C(1B) , C(3B)	43.1(2)	C(1B) , Cu(2)c	103.4(3)	O(21A)c , O(11B)	154.3(3)
O(21A)c , Cu(1)a	38.92(13)	O(21A)c , O(7W)g	55.6(4)	O(21A)c , C(11A)c	60.6(2)	O(21A)c , O(12B)	162.6(3)
O(21A)c , O(12A)c	81.6(2)	O(21A)c , O(11A)c	55.05(18)	O(21A)c , C(3B)	102.7(3)	O(21A)c , Cu(2)c	109.1(2)
O(11B) , Cu(1)a	117.3(3)	O(11B) , O(7W)g	146.9(4)	O(11B) , C(11A)c	122.7(3)	O(11B) , O(12B)	40.73(18)
O(11B) , O(12A)c	106.8(2)	O(11B) , O(11A)c	117.6(2)	O(11B) , C(3B)	83.4(2)	O(11B) , Cu(2)c	74.80(18)

Cu(1)a , O(7W)g	83.5(4)	Cu(1)a , C(11A)c	89.2(2)	Cu(1)a , O(12B)	158.0(3)	Cu(1)a , O(12A)c	110.8(2)
Cu(1)a , O(11A)c	73.63(16)	Cu(1)a , C(3B)	90.1(2)	Cu(1)a , Cu(2)c	124.58(18)	O(7W)g , C(11A)c	80.2(3)
O(7W)g , O(12B)	115.1(4)	O(7W)g , O(12A)c	86.9(3)	O(7W)g , O(11A)c	92.1(3)	O(7W)g , C(3B)	70.5(3)
O(7W)g , Cu(2)c	116.0(4)	C(11A)c, O(12B)	105.0(2)	C(11A)c, O(12A)c	21.92(18)	C(11A)c, O(11A)c	20.77(16)
C(11A)c, C(3B)	150.5(3)	C(11A)c, Cu(2)c	49.55(16)	O(12B) , O(12A)c	83.2(2)	O(12B) , O(11A)c	115.1(2)
O(12B) , C(3B)	85.7(2)	O(12B) , Cu(2)c	59.65(14)	O(12A)c, O(11A)c	38.41(15)	O(12A)c, C(3B)	147.5(3)
O(12A)c, Cu(2)c	32.20(11)	O(11A)c, C(3B)	157.6(3)	O(11A)c, Cu(2)c	55.50(13)	C(3B) , Cu(2)c	144.6(2)

=====

3.6 Angstrom Coordination Sphere Around Atom I = O(8W) [ARU = 1555.06] 1 1/2 1/2 6.1738 5.0075 5.6150

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.97(3) <<	>O(3W)	[	=	04]		-76.52	23.82	1.07800	0.33700	0.57100	6.5948	3.2512	6.4123
2	1.97(3) <<	>O(3W)h	[2-x,1-y,1-z	=	2766.04]		103.48	-23.82	0.92200	0.66300	0.42900	5.7529	6.7638	4.8177
3	2.27(3) <<	*O(5W)g	[2-x,1-y,1-z	=	2766.01]		43.10	55.29	1.18900	0.59200	0.66600	7.1167	5.8897	7.4792
4	2.27(3) <<	*O(5W)	[	=	01]		-136.90	-55.29	0.81100	0.40800	0.33400	5.2310	4.1253	3.7508
5	3.549(6) ..	Na(1)	[	=	01]		-52.87	-63.16	1.00700	0.36470	0.21800	7.1410	3.7301	2.4481
6	3.549(6) ..	Na(1)g	[2-x,1-y,1-z	=	2766.01]		127.13	63.16	0.99300	0.63530	0.78200	5.2067	6.2848	8.7819

Angles (Degrees) At1...V...At2 with Vertex V = <O(8W)

>O(3W)	,	>O(3W)h	180.00	>O(3W)	,	*O(5W)g	85.7(11)	>O(3W)	,	*O(5W)	94.3(11)	>O(3W)	,	Na(1)	89.0(10)
>O(3W)	,	Na(1)g	91.0(10)	>O(3W)h	,	*O(5W)g	94.3(11)	>O(3W)h	,	*O(5W)	85.7(11)	>O(3W)h	,	Na(1)	91.0(10)
>O(3W)h	,	Na(1)g	89.0(10)	*O(5W)g	,	*O(5W)	180.00	*O(5W)g	,	Na(1)	139.5(9)	*O(5W)g	,	Na(1)g	40.5(9)
*O(5W)	,	Na(1)	40.5(10)	*O(5W)	,	Na(1)g	139.5(10)	Na(1)	,	Na(1)g	180.00				

.....

>>>>>>>>>>>>>>> : Symmetry operations refer to the coordinates listed in the fractional coordinate table given above

=====															
5.0 Angstrom Coordination Sphere Around Atom I = Cu(1) [ARU = 1555.01]										0.37342	0.00315	0.13751	2.4962	-0.0396	1.5442

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	3.1914(13)	<<	Cu(2)	[	=		Intra	150.67	-21.94	0.00515	0.13533	0.03133	-0.0847	1.4104	0.3518
2	3.3600(13)	<<	Cu(2)c	[-x, -y, -z	=	2555.01]	Intra-	150.38	-34.35	-0.00515	-0.13533	-0.03133	0.0847	-1.4104	-0.3518
3	4.2035(13)	<<	Cu(1)e	[1-x, -y, -z	=	2655.01]	Intra	1.59	-47.29	0.62658	-0.00315	-0.13751	5.3465	0.0396	-1.5442

=====															
5.0 Angstrom Coordination Sphere Around Atom I = Cu(2) [ARU = 1555.01]										0.00515	0.13533	0.03133	-0.0847	1.4104	0.3518

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	2.9121(12)	<<	Cu(2)c	[-x, -y, -z	=	2555.01]	Intra	-86.56	-13.98	-0.00515	-0.13533	-0.03133	0.0847	-1.4104	-0.3518
2	3.187(6)	<<	Na(1)a	[-1+x, y, z	=	1455.01]	Intra	104.89	41.13	0.00700	0.36470	0.21800	-0.7017	3.7301	2.4481
3	3.1914(13)	<<	Cu(1)	[	=		Intra	-29.33	21.94	0.37342	0.00315	0.13751	2.4962	-0.0396	1.5442
4	3.3600(13)	<<	Cu(1)c	[-x, -y, -z	=	2555.01]	Intra	-150.38	-34.35	-0.37342	-0.00315	-0.13751	-2.4962	0.0396	-1.5442

=====												
5.0 Angstrom Coordination Sphere Around Atom I = Na(1) [ARU = 1555.01]												

Nr	d(I,J) To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0 Y0 Z0

1	3.187(6) <<	Cu(2)b	[1+x,y,z	=	1655.01]	Intra	-75.11	-41.13	1.00515	0.13533	0.03133	7.7580 1.4104 0.3518

=====

Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6

=====

van der Waals (or ion) Radii used in the Analysis

=====

C	H	Cu	Na	O
1.70	1.20	2.32	1.77	1.52

:: Grid: X-Axis Step = 0.0278 = Points 36, Angstrom Step = 0.22

:: Grid: Y-Axis Step = 0.0208 = Points 48, Angstrom Step = 0.22

:: Grid: Z-Axis Step = 0.0167 = Points 60, Angstrom Step = 0.19

:: Unit cell Contains NO Residual Solvent Accessible Void.

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 9 Kmax = 13 Lmax= 14 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 26.386 Deg. (Applied Theta Limit: 26.390 Deg.)

Space Group P-1 No: 2, Laue: -1 [Hall: -P 1]

Lattice Type aP, Centric, Triclinic, Order 2(1) [Schoenflies: Ci¹]

Nr ***** Symmetry Operation(s) *****

1	H ,	K ,	L
2	- H ,	- K ,	- L

:: Number of Independent Type H, K, L Reflections = 3815

Table 0 - Crystal Data and Details of the Structure Determination
for: c:xtal uP-1tkins3watR = 0.07cuace2na

Crystal Data

Formula	[CU2 (C10 H2 O8) H2O] 5(H2 O) NA
Formula Weight	526.30
Crystal System	Triclinic
Space group	P-1 (No. 2)
a, b, c [Angstrom]	7.8427(2) 10.5462(2) 11.6728(3)
alpha, beta, gamma [deg]	92.310(1) 105.606(1) 91.073(1)
V [Ang**3]	928.68(4)
Z	2
D(calc) [g/cm**3]	1.829
Mu(MoKa) [/mm]	2.388
F(000)	501
Crystal Size [mm]	0.05 x 0.10 x 0.10

Data Collection

Temperature (K)	100
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	2.6, 26.4
Dataset	-9: 9 ; -13: 13 ; -14: 14
Tot., Uniq. Data, R(int)	17649, 3800, 0.043
Observed data [I > 2.0 sigma(I)]	3389

Refinement

Nref, Npar	3800, 225
R, wR2, S	0.0680, 0.2598, 1.19
w = 1/[s^2^(Fo^2^)+(0.1435P)^2^+13.5181P] where P=(Fo^2^+2Fc^2^)/	
Max. and Av. Shift/Error	0.05, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-1.74, 1.46

=====

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***** N O T I C E *****

=====

- PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13
- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow
- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)
- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.
- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.
- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@chem.uu.nl
- Recent versions of PLATON may be obtained by Anonymous FTP from xraysoft.chem.uu.nl
- More INFO can be found on <http://www.cryst.chem.uu.nl/platon/>

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Page - Index

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Page 1 --- GENERAL
 Page 2 --- ADDSYM
 Page 3 --- GEOMETRY
 Page 12 --- ADP-Anal
 Page 17 --- GEOMETRY
 Page 69 --- INTER
 Page 80 --- H-BONDS
 Page 81 --- COORDN
 Page 111 --- METAL
 Page 115 --- VOIDS
 Page 116 --- EXPECT
 Page 117 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR

=====

W: NOMOVE option used.
 :: >>> WARNING: 'CONNECTED INPUT SET' is assumed 'TRUE'
 :: >>> Network Analysis may be INCORRECT when FALSE
 N: DISORDERED structure - ATOMS with Pop. .LT. 1.0 are not moved or as a group.

W: Structure contains 5 isolated 0-atom(s).
 W: Structure contains 3 Intra/Inter contacts < Sum(vdWrad) -1.00 A (max -1.07)
 N: Number of Isotropic Non-H Atoms 8
 W: Number of valency check faults for H & C 2
 W: Number of unusual anisotropic displacement parameters 8

=====

:: Input Xtal Data from File CUACE2NA.cif - Data Type CIF

:: NORMAL END of PLATON : 119 Pages on:
 :: CUACE2NA.lis (ASCII, 132 Characters Wide)
 :: CUACE2NA.lps (PostScript Version of .lis)
 ::
 :: SPF File on :CUACE2NA.eld

PLATON(V-201207)-Run for: C:xtalRUP-1no3pyrcunR = 0.03F

TIME: Jan 11 10:51:56 2008

(C) 1980-2007 A.L.Spek

Crystal Data

Input Cell (Lattice Type: P)		Temp = 113K	Reduced Cell		(Acta Cryst.(1976),A32,297-298)
a = 8.9167(18) Angstrom	alpha = 82.36(3) Degree		a = 8.917	alpha = 82.36	V = 1689.5
b = 11.137(2)	beta = 81.31(3)		b = 11.137	beta = 81.31	
c = 17.481(4)	gamma = 82.37(3)		c = 17.481	gamma = 82.37	
V = 1689.5(6) Cubic-Angstrom	d(100) = 8.7558 Angstrom		Niggli Values		
	d(010) = 10.9649		79.508	124.033	305.585
Lambda(MoKa) = 0.71073 Angstrom	d(001) = 17.1652		25.883	23.551	13.186

Orthogonalization Matrices

(See e.g. J.D.Dunitz, Xray Analysis and Structure Determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

(X0) (8.91670 1.47872 2.64118) (X) , (X) (0.11215 -0.01502 -0.01551) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 11.03839 1.99102)*(Y) , (Y) = (0 0.09059 -0.01051)*(Y0) are defined as:
 (Z0) (0 0 17.16524) (Z) , (Z) (0 0 0.05826) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group P-1 No: 2, Laue: -1 [Hall: -P 1]

Lattice Type aP, Centric, Triclinic, Order 2(1) [Schoenflies: Ci^1]

Nr ***** Symmetry Operation(s) *****

1	X ,	Y ,	Z
2	- X ,	- Y ,	- Z

=====

ADDSYM - CHECK (cf. MISSYM (C): Le Page, Y., J. Appl. Cryst. (1987), 20, 264-269; J. Appl. Cryst. (1988), 21, 983-984)

- ADDSYM Search on ALL NON-H Chemical Types [Max NonFit 20 Perc]
 - Number of Input Atoms Included in Search 50 (Unitcell 100)
 - Density based on Input Atom Set = 1.576 g.cm-3 - Vol / Non-H atom = 16.9 Ang+3
 - The Structure Implies the Following Symmetry Elements Subject to the Criteria:
 Criteria: 1.00 Deg (Metric), 0.25 Ang (Rot.), 0.45 Ang (Inv), 0.45 Ang (Transl)

Symm.	Input	Reduced	(Ang)	(Deg)	(%)	(Ang)	Input	Cell
Elem	Cell_Row	Cell_Row	d	Typ	Dot	Angle	Fit	MaxDev.
-1	=====				100		0	at

T.R.A.N.S.F.O.R.M.A.T.I.O.N M.A.T.R.I.X for CELL and HKL DATA

=====

Reduced->Convent	Input->Reduced	T = Input->Convent:	a' = T a
(1 0 0)	(1 0 0)	(1 0 0)	Det(T)
(0 1 0)	X (0 1 0)	= (0 1 0)	=
(0 0 1)	(0 0 1)	(0 0 1)	1.000

Cell Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input aP	8.917	11.137	17.481	82.36	81.31	82.37	1690	Triclinic	-1
Reduced P	8.917	11.137	17.481	82.36	81.31	82.37	1690		
Convent aP	8.917	11.137	17.481	82.36	81.31	82.37	1690	Triclinic	-1

:: *** No Obvious Extra Crystallographic Symmetry was Detected ***

:: Note: Rerun in EQUAL Atom Type Mode for more Checks

(1:19-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

 Site = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
 ***** Move = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
 SYMBOLS: Type = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
 ***** El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
 ARU = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
 RESIDUE = collection of ARU's constituting an isolated unit (= molecule, ion).
 FLAGS : d = determined, c = calculated, R = riding G = group

Atom Types : C H Cu N O
 Cov.Rad(Ang): 0.68 0.35 1.52 0.68 0.68
 Atom Volume : 13.87 5.08 26.90 11.80 11.39
 Atom Number : 6 1 29 7 8
 Atom Weight : 12.010 1.008 63.55 14.01 16.00
 Scat.Fact.f0: 5.999 1.000 28.986 6.995 7.999
 Scat.Fact.f': 0.003 0.000 0.320 0.006 0.011
 Scat.Fact.f": 0.002 0.000 1.265 0.003 0.006
 Mu/Rho(MoKa): 0.58 0.37 49.09 0.84 1.22
 Elem. Type : -- -- TR -- --

Sources - Cov. Radii : Manual Cambridge Crystallographic Data Base
 - Atom Volume: D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493
 - Atomic Wt. : SHELXL97
 - Scat. Fact.: SHELXL97 (International Tables)
 - mu/rho : International Tables C, table 4.2.4.2, p193-199

NOMOVE

 =====
 ***** Residue = 1 *****
 =====

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	Cu1	0.75664(2)	0.19504(2)	0.23260(1)	7.6495(2)	2.6160(2)	3.9926(2)	1	1	1	-	Met
d	Cu2	1.21202(3)	-0.21291(2)	0.22984(1)	11.0994(3)	-1.8926(2)	3.9452(2)	1	1	1	-	Met
d	O1	0.77323(18)	0.02137(14)	0.17500(8)	7.3885(16)	0.5843(16)	3.0039(14)	1	1	1	-	D/A
d	O2	0.97015(16)	-0.20694(14)	0.19846(8)	8.8687(15)	-1.8891(16)	3.4066(14)	1	1	1	-	D/A
d	O11A	0.89514(14)	0.11740(12)	0.30677(7)	8.9655(13)	1.9067(13)	5.2658(12)	1	1	1	-	D/A
d	O11B	0.62084(15)	0.27894(12)	0.15833(7)	6.3665(14)	3.3943(13)	2.7178(12)	1	1	1	-	D/A
d	O12A	0.87081(17)	0.27409(13)	0.37727(8)	9.1665(15)	3.7767(14)	6.4759(14)	1	1	1	-	D/A
d	O12B	0.53857(17)	0.45479(12)	0.20906(7)	6.0269(15)	5.4364(13)	3.5886(12)	1	1	1	-	D/A
d	O21A	1.14415(15)	-0.09975(12)	0.30950(7)	10.8720(14)	-0.4849(13)	5.3126(12)	1	1	1	-	D/A
d	O21B	0.29071(15)	0.66712(12)	0.15616(7)	3.9911(14)	7.6749(13)	2.6805(12)	1	1	1	-	D/A
d	O22A	0.91494(15)	-0.16648(12)	0.34786(7)	8.8308(14)	-1.1451(13)	5.9711(12)	1	1	1	-	D/A
d	O22B	0.53170(15)	0.71481(12)	0.13573(8)	6.1565(14)	8.1606(13)	2.3298(14)	1	1	1	-	D/A
d	N1C	0.58089(18)	0.14471(14)	0.31169(9)	6.2168(16)	2.2179(16)	5.3502(15)	1	1	1	-	D/A
d	N1D	0.92935(18)	0.26889(15)	0.16218(9)	9.1127(16)	3.2910(17)	2.7839(15)	1	1	1	-	D/A

d	N1E	1.24906(18)	-0.07339(14)	0.14835(9)	11.4208(16)	-0.5147(16)	2.5465(15)	1	1	1	-	D/A
d	N1F	1.21623(18)	-0.34810(15)	0.31782(9)	11.1694(16)	-3.2097(17)	5.4555(15)	1	1	1	-	D/A
d	C1A	0.9580(2)	0.07718(16)	0.43463(10)	9.8043(18)	1.7173(18)	7.4605(17)	1	1	1	-	-
d	C1B	0.5290(2)	0.44835(16)	0.07506(10)	5.5782(18)	5.0985(18)	1.2884(17)	1	1	1	-	-
d	C2A	1.0057(2)	-0.04657(17)	0.42855(10)	10.0305(18)	0.3392(19)	7.3562(17)	1	1	1	-	-
d	C2B	0.4662(2)	0.57029(16)	0.06254(10)	5.1654(18)	6.4196(18)	1.0735(17)	1	1	1	-	-
d	C2C	0.5971(2)	0.03385(17)	0.35267(10)	6.3057(18)	1.0758(19)	6.0537(17)	1	1	1	-	-
d	C2D	1.0283(2)	0.32903(19)	0.18901(12)	10.1548(18)	4.008(2)	3.244(2)	1	1	1	-	-
d	C2E	1.3169(2)	0.02049(18)	0.16215(12)	12.2010(18)	0.549(2)	2.783(2)	1	1	1	-	-
d	C2F	1.3080(2)	-0.3483(2)	0.37193(12)	12.1303(18)	-3.104(2)	6.384(2)	1	1	1	-	-
d	C3C	0.4824(2)	-0.00963(18)	0.40743(11)	5.3633(18)	0.705(2)	6.9936(19)	1	1	1	-	-
d	C3D	1.1328(2)	0.3948(2)	0.14065(13)	11.0561(18)	4.638(2)	2.414(2)	1	1	1	-	-
d	C3E	1.3613(2)	0.1103(2)	0.10417(13)	12.5765(18)	1.425(2)	1.788(2)	1	1	1	-	-
d	C3F	1.3073(3)	-0.4337(2)	0.43696(13)	12.170(3)	-3.917(2)	7.501(2)	1	1	1	-	-
d	C4C	0.3463(2)	0.06381(19)	0.42192(12)	4.2966(18)	1.544(2)	7.242(2)	1	1	1	-	-
d	C4D	1.1374(2)	0.3985(2)	0.06091(13)	10.8920(18)	4.520(2)	1.046(2)	1	1	1	-	-
d	C4E	1.3336(2)	0.1049(2)	0.02873(12)	12.1223(18)	1.215(2)	0.493(2)	1	1	1	-	-
d	C4F	1.2087(3)	-0.5214(2)	0.44700(13)	11.187(3)	-4.865(2)	7.673(2)	1	1	1	-	-
d	C5C	0.3282(2)	0.1771(2)	0.37917(13)	4.1898(18)	2.710(2)	6.509(2)	1	1	1	-	-
d	C5D	1.0391(2)	0.3347(2)	0.03257(12)	9.8463(18)	3.759(2)	0.559(2)	1	1	1	-	-
d	C5E	1.2607(3)	0.0096(2)	0.01464(12)	11.294(3)	0.135(2)	0.251(2)	1	1	1	-	-
d	C5F	1.1137(3)	-0.5214(2)	0.39164(13)	10.194(3)	-4.976(2)	6.723(2)	1	1	1	-	-
d	C6A	0.9532(2)	0.12141(17)	0.50587(10)	10.0150(18)	2.3474(19)	8.6834(17)	1	1	1	-	-
d	C6B	0.5623(2)	0.38027(17)	0.01192(10)	5.6077(18)	4.2213(19)	0.2046(17)	1	1	1	-	-
d	C6C	0.4463(2)	0.21527(19)	0.32484(12)	5.1558(18)	3.023(2)	5.576(2)	1	1	1	-	-
d	C6D	0.9372(2)	0.2714(2)	0.08477(11)	8.9819(18)	3.165(2)	1.4551(19)	1	1	1	-	-
d	C6E	1.2206(2)	-0.07740(19)	0.07516(11)	10.9678(18)	-0.705(2)	1.2901(19)	1	1	1	-	-
d	C6F	1.1217(2)	-0.43442(18)	0.32780(12)	10.2253(18)	-4.143(2)	5.627(2)	1	1	1	-	-
d	C11A	0.9043(2)	0.16478(17)	0.36767(10)	9.2781(18)	2.5509(19)	6.3111(17)	1	1	1	-	-
d	C11B	0.5651(2)	0.39096(17)	0.15462(10)	6.0253(18)	4.6234(19)	2.6541(17)	1	1	1	-	-
d	C21A	1.0200(2)	-0.10669(16)	0.35476(10)	9.8743(18)	-0.4714(18)	6.0895(17)	1	1	1	-	-
d	C21B	0.4292(2)	0.65532(16)	0.12492(10)	5.1260(18)	7.4824(18)	2.1443(17)	1	1	1	-	-
d	H1	0.849(3)	-0.024(2)	0.1756(14)	8.00(3)	0.08(2)	3.01(2)	1	1	1	-	D-H
d	H2	0.706(3)	-0.021(2)	0.1949(14)	6.78(3)	0.16(2)	3.35(2)	1	1	1	-	D-H
cR	H2C	0.69110	-0.01660	0.34360	7.0453	0.5009	5.8980	1	1	1	-	-
cR	H2D	1.02590	0.32600	0.24370	10.2734	4.0837	4.1832	1	1	1	-	-
cR	H2E	1.33500	0.02530	0.21380	12.5059	0.7050	3.6699	1	1	1	-	-
cR	H2F	1.37590	-0.28770	0.36530	12.8079	-2.4484	6.2705	1	1	1	-	-
d	H3	0.934(3)	-0.263(2)	0.1833(14)	8.42(3)	-2.54(2)	3.15(2)	1	1	1	-	D-H
cR	H3C	0.49710	-0.08900	0.43470	5.4490	-0.1169	7.4617	1	1	1	-	-
cR	H3D	1.20030	0.43670	0.16160	11.7753	5.1422	2.7739	1	1	1	-	-
cR	H3E	1.41040	0.17520	0.11570	13.1408	2.1643	1.9860	1	1	1	-	-
cR	H3F	1.37400	-0.43200	0.47420	12.8652	-3.8244	8.1398	1	1	1	-	-
d	H4	0.935(3)	-0.202(2)	0.2434(14)	8.68(3)	-1.75(2)	4.18(2)	1	1	1	-	D-H
cR	H4C	0.26690	0.03710	0.46040	3.6507	1.3262	7.9029	1	1	1	-	-
cR	H4D	1.20710	0.44430	0.02620	11.4895	4.9565	0.4497	1	1	1	-	-
cR	H4E	1.36400	0.16530	-0.01230	12.3743	1.8002	-0.2111	1	1	1	-	-

cR	H4F	1.20600	-0.58090	0.49130	11.1922	-5.4340	8.4333	1	1	1	-	-
cR	H5C	0.23460	0.22850	0.38720	3.4524	3.2932	6.6464	1	1	1	-	-
cR	H5D	1.04170	0.33430	-0.02190	9.7250	3.6465	-0.3759	1	1	1	-	-
cR	H5E	1.23850	0.00430	-0.03620	10.9541	-0.0246	-0.6214	1	1	1	-	-
cR	H5F	1.04400	-0.58060	0.39740	9.5001	-5.6177	6.8215	1	1	1	-	-
cR	H6A	0.92080	0.20540	0.50980	9.8607	3.2823	8.7508	1	1	1	-	-
cR	H6B	0.60570	0.29770	0.02000	5.8939	3.3260	0.3433	1	1	1	-	-
cR	H6C	0.43260	0.29340	0.29580	5.0725	3.8276	5.0775	1	1	1	-	-
cR	H6D	0.86970	0.22770	0.06500	8.2632	2.6429	1.1157	1	1	1	-	-
cR	H6E	1.17100	-0.14290	0.06500	10.4018	-1.4480	1.1157	1	1	1	-	-
cR	H6F	1.05750	-0.43570	0.28930	9.5492	-4.2334	4.9659	1	1	1	-	-
d	Cu1_a	-0.24336(2)	1.19504(2)	0.23260(1)	0.2115(2)	13.6544(2)	3.9926(2)	1	1	1	1.465	Met
d	Cu2_a	0.21202(3)	0.78709(2)	0.22984(1)	3.6614(3)	9.1458(2)	3.9452(2)	1	1	1	1.465	Met
d	O1_a	-0.22677(18)	1.02137(14)	0.17500(8)	-0.0495(16)	11.6227(16)	3.0039(14)	1	1	1	1.465	D/A
d	O2_a	-0.02985(16)	0.79306(14)	0.19846(8)	1.4307(15)	9.1492(16)	3.4066(14)	1	1	1	1.465	D/A
d	O11A_a	-0.10486(14)	1.11740(12)	0.30677(7)	1.5275(13)	12.9451(13)	5.2658(12)	1	1	1	1.465	D/A
d	O11B_a	-0.37916(15)	1.27894(12)	0.15833(7)	-1.0715(14)	14.4327(13)	2.7178(12)	1	1	1	1.465	D/A
d	O12A_a	-0.12919(17)	1.27409(13)	0.37727(8)	1.7285(15)	14.8151(14)	6.4759(14)	1	1	1	1.465	D/A
d	O12B_a	-0.46143(17)	1.45479(12)	0.20906(7)	-1.4110(15)	16.4748(13)	3.5886(12)	1	1	1	1.465	D/A
d	O21A_a	0.14415(15)	0.90025(12)	0.30950(7)	3.4340(14)	10.5535(13)	5.3126(12)	1	1	1	1.465	D/A
d	O21B_a	-0.70929(15)	1.66712(12)	0.15616(7)	-3.4469(14)	18.7132(13)	2.6805(12)	1	1	1	1.465	D/A
d	O22A_a	-0.08506(15)	0.83352(12)	0.34786(7)	1.3928(14)	9.8933(13)	5.9711(12)	1	1	1	1.465	D/A
d	O22B_a	-0.46830(15)	1.71481(12)	0.13573(8)	-1.2815(14)	19.1990(13)	2.3298(14)	1	1	1	1.465	D/A
d	N1C_a	-0.41911(18)	1.14471(14)	0.31169(9)	-1.2211(16)	13.2563(16)	5.3502(15)	1	1	1	1.465	D/A
d	N1D_a	-0.07065(18)	1.26889(15)	0.16218(9)	1.6747(16)	14.3294(17)	2.7839(15)	1	1	1	1.465	D/A
d	N1E_a	0.24906(18)	0.92661(14)	0.14835(9)	3.9828(16)	10.5237(16)	2.5465(15)	1	1	1	1.465	D/A
d	N1F_a	0.21623(18)	0.65190(15)	0.31782(9)	3.7315(16)	7.8287(17)	5.4555(15)	1	1	1	1.465	D/A
d	C1A_a	-0.0420(2)	1.07718(16)	0.43463(10)	2.3663(18)	12.7557(18)	7.4605(17)	1	1	1	1.465	-
d	C1B_a	-0.4710(2)	1.44835(16)	0.07506(10)	-1.8598(18)	16.1369(18)	1.2884(17)	1	1	1	1.465	-
d	C2A_a	0.0057(2)	0.95343(17)	0.42855(10)	2.5926(18)	11.3776(19)	7.3562(17)	1	1	1	1.465	-
d	C2B_a	-0.5338(2)	1.57029(16)	0.06254(10)	-2.2725(18)	17.4580(18)	1.0735(17)	1	1	1	1.465	-
d	C2C_a	-0.4029(2)	1.03385(17)	0.35267(10)	-1.1323(18)	12.1142(19)	6.0537(17)	1	1	1	1.465	-
d	C2D_a	0.0283(2)	1.32903(19)	0.18901(12)	2.7168(18)	15.047(2)	3.244(2)	1	1	1	1.465	-
d	C2E_a	0.3169(2)	1.02049(18)	0.16215(12)	4.7630(18)	11.587(2)	2.783(2)	1	1	1	1.465	-
d	C2F_a	0.3080(2)	0.6517(2)	0.37193(12)	4.6924(18)	7.934(2)	6.384(2)	1	1	1	1.465	-
d	C3C_a	-0.5176(2)	0.99037(18)	0.40743(11)	-2.0747(18)	11.743(2)	6.9936(19)	1	1	1	1.465	-
d	C3D_a	0.1328(2)	1.3948(2)	0.14065(13)	3.6181(18)	15.676(2)	2.414(2)	1	1	1	1.465	-
d	C3E_a	0.3613(2)	1.1103(2)	0.10417(13)	5.1386(18)	12.463(2)	1.788(2)	1	1	1	1.465	-
d	C3F_a	0.3073(3)	0.5663(2)	0.43696(13)	4.732(3)	7.121(2)	7.501(2)	1	1	1	1.465	-
d	C4C_a	-0.6537(2)	1.06381(19)	0.42192(12)	-3.1414(18)	12.583(2)	7.242(2)	1	1	1	1.465	-
d	C4D_a	0.1374(2)	1.3985(2)	0.06091(13)	3.4540(18)	15.558(2)	1.046(2)	1	1	1	1.465	-
d	C4E_a	0.3336(2)	1.1049(2)	0.02873(12)	4.6843(18)	12.254(2)	0.493(2)	1	1	1	1.465	-
d	C4F_a	0.2087(3)	0.4786(2)	0.44700(13)	3.749(3)	6.173(2)	7.673(2)	1	1	1	1.465	-
d	C5C_a	-0.6718(2)	1.1771(2)	0.37917(13)	-3.2482(18)	13.748(2)	6.509(2)	1	1	1	1.465	-
d	C5D_a	0.0391(2)	1.3347(2)	0.03257(12)	2.4083(18)	14.798(2)	0.559(2)	1	1	1	1.465	-
d	C5E_a	0.2607(3)	1.0096(2)	0.01464(12)	3.856(3)	11.174(2)	0.251(2)	1	1	1	1.465	-
d	C5F_a	0.1137(3)	0.4786(2)	0.39164(13)	2.756(3)	6.063(2)	6.723(2)	1	1	1	1.465	-

d	C6A_a	-0.0468(2)	1.12141(17)	0.50587(10)	2.5770(18)	13.3858(19)	8.6834(17)	1	1	1	1.465	-
d	C6B_a	-0.4377(2)	1.38027(17)	0.01192(10)	-1.8303(18)	15.2597(19)	0.2046(17)	1	1	1	1.465	-
d	C6C_a	-0.5537(2)	1.21527(19)	0.32484(12)	-2.2822(18)	14.061(2)	5.576(2)	1	1	1	1.465	-
d	C6D_a	-0.0628(2)	1.2714(2)	0.08477(11)	1.5440(18)	14.203(2)	1.4551(19)	1	1	1	1.465	-
d	C6E_a	0.2206(2)	0.92260(19)	0.07516(11)	3.5298(18)	10.334(2)	1.2901(19)	1	1	1	1.465	-
d	C6F_a	0.1217(2)	0.56558(18)	0.32780(12)	2.7873(18)	6.896(2)	5.627(2)	1	1	1	1.465	-
d	C11A_a	-0.0957(2)	1.16478(17)	0.36767(10)	1.8401(18)	13.5893(19)	6.3111(17)	1	1	1	1.465	-
d	C11B_a	-0.4349(2)	1.39096(17)	0.15462(10)	-1.4127(18)	15.6618(19)	2.6541(17)	1	1	1	1.465	-
d	C21A_a	0.0200(2)	0.89331(16)	0.35476(10)	2.4363(18)	10.5670(18)	6.0895(17)	1	1	1	1.465	-
d	C21B_a	-0.5708(2)	1.65532(16)	0.12492(10)	-2.3120(18)	18.5208(18)	2.1443(17)	1	1	1	1.465	-
d	H1_a	-0.151(3)	0.976(2)	0.1756(14)	0.56(3)	11.12(2)	3.01(2)	1	1	1	1.465	D-H
d	H2_a	-0.294(3)	0.979(2)	0.1949(14)	-0.66(3)	11.19(2)	3.35(2)	1	1	1	1.465	D-H
cR	H2C_a	-0.30890	0.98340	0.34360	-0.3927	11.5393	5.8980	1	1	1	1.465	-
cR	H2D_a	0.02590	1.32600	0.24370	2.8354	15.1221	4.1832	1	1	1	1.465	-
cR	H2E_a	0.33500	1.02530	0.21380	5.0679	11.7433	3.6699	1	1	1	1.465	-
cR	H2F_a	0.37590	0.71230	0.36530	5.3699	8.5900	6.2705	1	1	1	1.465	-
d	H3_a	-0.066(3)	0.737(2)	0.1833(14)	0.99(3)	8.50(2)	3.15(2)	1	1	1	1.465	D-H
cR	H3C_a	-0.50290	0.91100	0.43470	-1.9890	10.9215	7.4617	1	1	1	1.465	-
cR	H3D_a	0.20030	1.43670	0.16160	4.3373	16.1806	2.7739	1	1	1	1.465	-
cR	H3E_a	0.41040	1.17520	0.11570	5.7028	13.2027	1.9860	1	1	1	1.465	-
cR	H3F_a	0.37400	0.56800	0.47420	5.4272	7.2139	8.1398	1	1	1	1.465	-
d	H4_a	-0.065(3)	0.798(2)	0.2434(14)	1.24(3)	9.29(2)	4.18(2)	1	1	1	1.465	D-H
cR	H4C_a	-0.73310	1.03710	0.46040	-3.7873	12.3646	7.9029	1	1	1	1.465	-
cR	H4D_a	0.20710	1.44430	0.02620	4.0516	15.9949	0.4497	1	1	1	1.465	-
cR	H4E_a	0.36400	1.16530	-0.01230	4.9363	12.8386	-0.2111	1	1	1	1.465	-
cR	H4F_a	0.20600	0.41910	0.49130	3.7542	5.6044	8.4333	1	1	1	1.465	-
cR	H5C_a	-0.76540	1.22850	0.38720	-3.9856	14.3316	6.6464	1	1	1	1.465	-
cR	H5D_a	0.04170	1.33430	-0.02190	2.2870	14.6849	-0.3759	1	1	1	1.465	-
cR	H5E_a	0.23850	1.00430	-0.03620	3.5161	11.0138	-0.6214	1	1	1	1.465	-
cR	H5F_a	0.04400	0.41940	0.39740	2.0621	5.4207	6.8215	1	1	1	1.465	-
cR	H6A_a	-0.07920	1.20540	0.50980	2.4227	14.3207	8.7508	1	1	1	1.465	-
cR	H6B_a	-0.39430	1.29770	0.02000	-1.5441	14.3643	0.3433	1	1	1	1.465	-
cR	H6C_a	-0.56740	1.29340	0.29580	-2.3655	14.8660	5.0775	1	1	1	1.465	-
cR	H6D_a	-0.13030	1.22770	0.06500	0.8253	13.6813	1.1157	1	1	1	1.465	-
cR	H6E_a	0.17100	0.85710	0.06500	2.9638	9.5904	1.1157	1	1	1	1.465	-
cR	H6F_a	0.05750	0.56430	0.28930	2.1112	6.8050	4.9659	1	1	1	1.465	-
d	Cu1_b	1.75664(2)	-0.80496(2)	0.23260(1)	15.0874(2)	-8.4224(2)	3.9926(2)	1	1	1	1.645	Met
d	Cu2_b	2.21202(3)	-1.21291(2)	0.22984(1)	18.5374(3)	-12.9310(2)	3.9452(2)	1	1	1	1.645	Met
d	O1_b	1.77323(18)	-0.97863(14)	0.17500(8)	14.8264(16)	-10.4541(16)	3.0039(14)	1	1	1	1.645	D/A
d	O2_b	1.97015(16)	-1.20694(14)	0.19846(8)	16.3067(15)	-12.9275(16)	3.4066(14)	1	1	1	1.645	D/A
d	O11A_b	1.89514(14)	-0.88260(12)	0.30677(7)	16.4035(13)	-9.1317(13)	5.2658(12)	1	1	1	1.645	D/A
d	O11B_b	1.62084(15)	-0.72106(12)	0.15833(7)	13.8045(14)	-7.6441(13)	2.7178(12)	1	1	1	1.645	D/A
d	O12A_b	1.87081(17)	-0.72591(13)	0.37727(8)	16.6045(15)	-7.2617(14)	6.4759(14)	1	1	1	1.645	D/A
d	O12B_b	1.53857(17)	-0.54521(12)	0.20906(7)	13.4649(15)	-5.6020(13)	3.5886(12)	1	1	1	1.645	D/A
d	O21A_b	2.14415(15)	-1.09975(12)	0.30950(7)	18.3100(14)	-11.5233(13)	5.3126(12)	1	1	1	1.645	D/A
d	O21B_b	1.29071(15)	-0.33288(12)	0.15616(7)	11.4291(14)	-3.3635(13)	2.6805(12)	1	1	1	1.645	D/A

d	O22A_b	1.91494(15)	-1.16648(12)	0.34786(7)	16.2688(14)	-12.1835(13)	5.9711(12)	1	1	1	1.645	D/A
d	O22B_b	1.53170(15)	-0.28519(12)	0.13573(8)	13.5945(14)	-2.8778(13)	2.3298(14)	1	1	1	1.645	D/A
d	N1C_b	1.58089(18)	-0.85529(14)	0.31169(9)	13.6548(16)	-8.8204(16)	5.3502(15)	1	1	1	1.645	D/A
d	N1D_b	1.92935(18)	-0.73111(15)	0.16218(9)	16.5507(16)	-7.7474(17)	2.7839(15)	1	1	1	1.645	D/A
d	N1E_b	2.24906(18)	-1.07339(14)	0.14835(9)	18.8588(16)	-11.5531(16)	2.5465(15)	1	1	1	1.645	D/A
d	N1F_b	2.21623(18)	-1.34810(15)	0.31782(9)	18.6074(16)	-14.2481(17)	5.4555(15)	1	1	1	1.645	D/A
d	C1A_b	1.9580(2)	-0.92282(16)	0.43463(10)	17.2422(18)	-9.3211(18)	7.4605(17)	1	1	1	1.645	-
d	C1B_b	1.5290(2)	-0.55165(16)	0.07506(10)	13.0161(18)	-5.9399(18)	1.2884(17)	1	1	1	1.645	-
d	C2A_b	2.0057(2)	-1.04657(17)	0.42855(10)	17.4685(18)	-10.6992(19)	7.3562(17)	1	1	1	1.645	-
d	C2B_b	1.4662(2)	-0.42971(16)	0.06254(10)	12.6034(18)	-4.6188(18)	1.0735(17)	1	1	1	1.645	-
d	C2C_b	1.5971(2)	-0.96615(17)	0.35267(10)	13.7437(18)	-9.9626(19)	6.0537(17)	1	1	1	1.645	-
d	C2D_b	2.0283(2)	-0.67097(19)	0.18901(12)	17.5928(18)	-7.030(2)	3.244(2)	1	1	1	1.645	-
d	C2E_b	2.3169(2)	-0.97951(18)	0.16215(12)	19.6390(18)	-10.489(2)	2.783(2)	1	1	1	1.645	-
d	C2F_b	2.3080(2)	-1.3483(2)	0.37193(12)	19.5683(18)	-14.143(2)	6.384(2)	1	1	1	1.645	-
d	C3C_b	1.4824(2)	-1.00963(18)	0.40743(11)	12.8013(18)	-10.333(2)	6.9936(19)	1	1	1	1.645	-
d	C3D_b	2.1328(2)	-0.6052(2)	0.14065(13)	18.4941(18)	-6.400(2)	2.414(2)	1	1	1	1.645	-
d	C3E_b	2.3613(2)	-0.8897(2)	0.10417(13)	20.0145(18)	-9.613(2)	1.788(2)	1	1	1	1.645	-
d	C3F_b	2.3073(3)	-1.4337(2)	0.43696(13)	19.608(3)	-14.956(2)	7.501(2)	1	1	1	1.645	-
d	C4C_b	1.3463(2)	-0.93619(19)	0.42192(12)	11.7346(18)	-9.494(2)	7.242(2)	1	1	1	1.645	-
d	C4D_b	2.1374(2)	-0.6015(2)	0.06091(13)	18.3300(18)	-6.518(2)	1.046(2)	1	1	1	1.645	-
d	C4E_b	2.3336(2)	-0.8951(2)	0.02873(12)	19.5603(18)	-9.823(2)	0.493(2)	1	1	1	1.645	-
d	C4F_b	2.2087(3)	-1.5214(2)	0.44700(13)	18.625(3)	-15.904(2)	7.673(2)	1	1	1	1.645	-
d	C5C_b	1.3282(2)	-0.8229(2)	0.37917(13)	11.6278(18)	-8.329(2)	6.509(2)	1	1	1	1.645	-
d	C5D_b	2.0391(2)	-0.6653(2)	0.03257(12)	17.2843(18)	-7.279(2)	0.559(2)	1	1	1	1.645	-
d	C5E_b	2.2607(3)	-0.9904(2)	0.01464(12)	18.732(3)	-10.903(2)	0.251(2)	1	1	1	1.645	-
d	C5F_b	2.1137(3)	-1.5214(2)	0.39164(13)	17.632(3)	-16.014(2)	6.723(2)	1	1	1	1.645	-
d	C6A_b	1.9532(2)	-0.87859(17)	0.50587(10)	17.4530(18)	-8.6910(19)	8.6834(17)	1	1	1	1.645	-
d	C6B_b	1.5623(2)	-0.61973(17)	0.01192(10)	13.0456(18)	-6.8171(19)	0.2046(17)	1	1	1	1.645	-
d	C6C_b	1.4463(2)	-0.78473(19)	0.32484(12)	12.5938(18)	-8.015(2)	5.576(2)	1	1	1	1.645	-
d	C6D_b	1.9372(2)	-0.7286(2)	0.08477(11)	16.4199(18)	-7.874(2)	1.4551(19)	1	1	1	1.645	-
d	C6E_b	2.2206(2)	-1.07740(19)	0.07516(11)	18.4058(18)	-11.743(2)	1.2901(19)	1	1	1	1.645	-
d	C6F_b	2.1217(2)	-1.43442(18)	0.32780(12)	17.6632(18)	-15.181(2)	5.627(2)	1	1	1	1.645	-
d	C11A_b	1.9043(2)	-0.83522(17)	0.36767(10)	16.7161(18)	-8.4875(19)	6.3111(17)	1	1	1	1.645	-
d	C11B_b	1.5651(2)	-0.60904(17)	0.15462(10)	13.4633(18)	-6.4150(19)	2.6541(17)	1	1	1	1.645	-
d	C21A_b	2.0200(2)	-1.10669(16)	0.35476(10)	17.3122(18)	-11.5097(18)	6.0895(17)	1	1	1	1.645	-
d	C21B_b	1.4292(2)	-0.34468(16)	0.12492(10)	12.5640(18)	-3.5560(18)	2.1443(17)	1	1	1	1.645	-
d	H1_b	1.849(3)	-1.024(2)	0.1756(14)	15.44(3)	-10.95(2)	3.01(2)	1	1	1	1.645	D-H
d	H2_b	1.706(3)	-1.021(2)	0.1949(14)	14.22(3)	-10.88(2)	3.35(2)	1	1	1	1.645	D-H
cR	H2C_b	1.69110	-1.01660	0.34360	14.4833	-10.5375	5.8980	1	1	1	1.645	-
cR	H2D_b	2.02590	-0.67400	0.24370	17.7113	-6.9547	4.1832	1	1	1	1.645	-
cR	H2E_b	2.33500	-0.97470	0.21380	19.9439	-10.3334	3.6699	1	1	1	1.645	-
cR	H2F_b	2.37590	-1.28770	0.36530	20.2459	-13.4868	6.2705	1	1	1	1.645	-
d	H3_b	1.934(3)	-1.263(2)	0.1833(14)	15.86(3)	-13.58(2)	3.15(2)	1	1	1	1.645	D-H
cR	H3C_b	1.49710	-1.08900	0.43470	12.8870	-11.1553	7.4617	1	1	1	1.645	-
cR	H3D_b	2.20030	-0.56330	0.16160	19.2133	-5.8962	2.7739	1	1	1	1.645	-
cR	H3E_b	2.41040	-0.82480	0.11570	20.5788	-8.8741	1.9860	1	1	1	1.645	-
cR	H3F_b	2.37400	-1.43200	0.47420	20.3032	-14.8628	8.1398	1	1	1	1.645	-

d	H4_b	1.935(3)	-1.202(2)	0.2434(14)	16.12(3)	-12.78(2)	4.18(2)	1	1	1	1.645	D-H
cR	H4C_b	1.26690	-0.96290	0.46040	11.0887	-9.7122	7.9029	1	1	1	1.645	-
cR	H4D_b	2.20710	-0.55570	0.02620	18.9275	-6.0819	0.4497	1	1	1	1.645	-
cR	H4E_b	2.36400	-0.83470	-0.01230	19.8123	-9.2382	-0.2111	1	1	1	1.645	-
cR	H4F_b	2.20600	-1.58090	0.49130	18.6301	-16.4724	8.4333	1	1	1	1.645	-
cR	H5C_b	1.23460	-0.77150	0.38720	10.8904	-7.7452	6.6464	1	1	1	1.645	-
cR	H5D_b	2.04170	-0.66570	-0.02190	17.1630	-7.3919	-0.3759	1	1	1	1.645	-
cR	H5E_b	2.23850	-0.99570	-0.03620	18.3921	-11.0630	-0.6214	1	1	1	1.645	-
cR	H5F_b	2.04400	-1.58060	0.39740	16.9381	-16.6561	6.8215	1	1	1	1.645	-
cR	H6A_b	1.92080	-0.79460	0.50980	17.2987	-7.7561	8.7508	1	1	1	1.645	-
cR	H6B_b	1.60570	-0.70230	0.02000	13.3319	-7.7124	0.3433	1	1	1	1.645	-
cR	H6C_b	1.43260	-0.70660	0.29580	12.5105	-7.2108	5.0775	1	1	1	1.645	-
cR	H6D_b	1.86970	-0.77230	0.06500	15.7012	-8.3955	1.1157	1	1	1	1.645	-
cR	H6E_b	2.17100	-1.14290	0.06500	17.8398	-12.4864	1.1157	1	1	1	1.645	-
cR	H6F_b	2.05750	-1.43570	0.28930	16.9872	-15.2718	4.9659	1	1	1	1.645	-
d	Cu1_c	0.24336(2)	0.80496(2)	-0.23260(1)	2.7460(2)	8.4224(2)	-3.9926(2)	1	1	1	2.665	Met
d	Cu2_c	-0.21202(3)	1.21291(2)	-0.22984(1)	-0.7040(3)	12.9310(2)	-3.9452(2)	1	1	1	2.665	Met
d	O1_c	0.22677(18)	0.97863(14)	-0.17500(8)	3.0070(16)	10.4541(16)	-3.0039(14)	1	1	1	2.665	D/A
d	O2_c	0.02985(16)	1.20694(14)	-0.19846(8)	1.5267(15)	12.9275(16)	-3.4066(14)	1	1	1	2.665	D/A
d	O11A_c	0.10486(14)	0.88260(12)	-0.30677(7)	1.4299(13)	9.1317(13)	-5.2658(12)	1	1	1	2.665	D/A
d	O11B_c	0.37916(15)	0.72106(12)	-0.15833(7)	4.0289(14)	7.6441(13)	-2.7178(12)	1	1	1	2.665	D/A
d	O12A_c	0.12919(17)	0.72591(13)	-0.37727(8)	1.2289(15)	7.2617(14)	-6.4759(14)	1	1	1	2.665	D/A
d	O12B_c	0.46143(17)	0.54521(12)	-0.20906(7)	4.3685(15)	5.6020(13)	-3.5886(12)	1	1	1	2.665	D/A
d	O21A_c	-0.14415(15)	1.09975(12)	-0.30950(7)	-0.4766(14)	11.5233(13)	-5.3126(12)	1	1	1	2.665	D/A
d	O21B_c	0.70929(15)	0.33288(12)	-0.15616(7)	6.4043(14)	3.3635(13)	-2.6805(12)	1	1	1	2.665	D/A
d	O22A_c	0.08506(15)	1.16648(12)	-0.34786(7)	1.5646(14)	12.1835(13)	-5.9711(12)	1	1	1	2.665	D/A
d	O22B_c	0.46830(15)	0.28519(12)	-0.13573(8)	4.2389(14)	2.8778(13)	-2.3298(14)	1	1	1	2.665	D/A
d	N1C_c	0.41911(18)	0.85529(14)	-0.31169(9)	4.1786(16)	8.8204(16)	-5.3502(15)	1	1	1	2.665	D/A
d	N1D_c	0.07065(18)	0.73111(15)	-0.16218(9)	1.2827(16)	7.7474(17)	-2.7839(15)	1	1	1	2.665	D/A
d	N1E_c	-0.24906(18)	1.07339(14)	-0.14835(9)	-1.0254(16)	11.5531(16)	-2.5465(15)	1	1	1	2.665	D/A
d	N1F_c	-0.21623(18)	1.34810(15)	-0.31782(9)	-0.7740(16)	14.2481(17)	-5.4555(15)	1	1	1	2.665	D/A
d	C1A_c	0.0420(2)	0.92282(16)	-0.43463(10)	0.5912(18)	9.3211(18)	-7.4605(17)	1	1	1	2.665	-
d	C1B_c	0.4710(2)	0.55165(16)	-0.07506(10)	4.8173(18)	5.9399(18)	-1.2884(17)	1	1	1	2.665	-
d	C2A_c	-0.0057(2)	1.04657(17)	-0.42855(10)	0.3649(18)	10.6992(19)	-7.3562(17)	1	1	1	2.665	-
d	C2B_c	0.5338(2)	0.42971(16)	-0.06254(10)	5.2300(18)	4.6188(18)	-1.0735(17)	1	1	1	2.665	-
d	C2C_c	0.4029(2)	0.96615(17)	-0.35267(10)	4.0897(18)	9.9626(19)	-6.0537(17)	1	1	1	2.665	-
d	C2D_c	-0.0283(2)	0.67097(19)	-0.18901(12)	0.2406(18)	7.030(2)	-3.244(2)	1	1	1	2.665	-
d	C2E_c	-0.3169(2)	0.97951(18)	-0.16215(12)	-1.8055(18)	10.489(2)	-2.783(2)	1	1	1	2.665	-
d	C2F_c	-0.3080(2)	1.3483(2)	-0.37193(12)	-1.7349(18)	14.143(2)	-6.384(2)	1	1	1	2.665	-
d	C3C_c	0.5176(2)	1.00963(18)	-0.40743(11)	5.0321(18)	10.333(2)	-6.9936(19)	1	1	1	2.665	-
d	C3D_c	-0.1328(2)	0.6052(2)	-0.14065(13)	-0.6607(18)	6.400(2)	-2.414(2)	1	1	1	2.665	-
d	C3E_c	-0.3613(2)	0.8897(2)	-0.10417(13)	-2.1811(18)	9.613(2)	-1.788(2)	1	1	1	2.665	-
d	C3F_c	-0.3073(3)	1.4337(2)	-0.43696(13)	-1.774(3)	14.956(2)	-7.501(2)	1	1	1	2.665	-
d	C4C_c	0.6537(2)	0.93619(19)	-0.42192(12)	6.0988(18)	9.494(2)	-7.242(2)	1	1	1	2.665	-
d	C4D_c	-0.1374(2)	0.6015(2)	-0.06091(13)	-0.4966(18)	6.518(2)	-1.046(2)	1	1	1	2.665	-
d	C4E_c	-0.3336(2)	0.8951(2)	-0.02873(12)	-1.7269(18)	9.823(2)	-0.493(2)	1	1	1	2.665	-
d	C4F_c	-0.2087(3)	1.5214(2)	-0.44700(13)	-0.792(3)	15.904(2)	-7.673(2)	1	1	1	2.665	-

d	C5C_c	0.6718(2)	0.8229(2)	-0.37917(13)	6.2056(18)	8.329(2)	-6.509(2)	1	1	1	2.665	-
d	C5D_c	-0.0391(2)	0.6653(2)	-0.03257(12)	0.5491(18)	7.279(2)	-0.559(2)	1	1	1	2.665	-
d	C5E_c	-0.2607(3)	0.9904(2)	-0.01464(12)	-0.899(3)	10.903(2)	-0.251(2)	1	1	1	2.665	-
d	C5F_c	-0.1137(3)	1.5214(2)	-0.39164(13)	0.202(3)	16.014(2)	-6.723(2)	1	1	1	2.665	-
d	C6A_c	0.0468(2)	0.87859(17)	-0.50587(10)	0.3804(18)	8.6910(19)	-8.6834(17)	1	1	1	2.665	-
d	C6B_c	0.4377(2)	0.61973(17)	-0.01192(10)	4.7878(18)	6.8171(19)	-0.2046(17)	1	1	1	2.665	-
d	C6C_c	0.5537(2)	0.78473(19)	-0.32484(12)	5.2396(18)	8.015(2)	-5.576(2)	1	1	1	2.665	-
d	C6D_c	0.0628(2)	0.7286(2)	-0.08477(11)	1.4135(18)	7.874(2)	-1.4551(19)	1	1	1	2.665	-
d	C6E_c	-0.2206(2)	1.07740(19)	-0.07516(11)	-0.5724(18)	11.743(2)	-1.2901(19)	1	1	1	2.665	-
d	C6F_c	-0.1217(2)	1.43442(18)	-0.32780(12)	0.1702(18)	15.181(2)	-5.627(2)	1	1	1	2.665	-
d	C11A_c	0.0957(2)	0.83522(17)	-0.36767(10)	1.1173(18)	8.4875(19)	-6.3111(17)	1	1	1	2.665	-
d	C11B_c	0.4349(2)	0.60904(17)	-0.15462(10)	4.3701(18)	6.4150(19)	-2.6541(17)	1	1	1	2.665	-
d	C21A_c	-0.0200(2)	1.10669(16)	-0.35476(10)	0.5212(18)	11.5097(18)	-6.0895(17)	1	1	1	2.665	-
d	C21B_c	0.5708(2)	0.34468(16)	-0.12492(10)	5.2694(18)	3.5560(18)	-2.1443(17)	1	1	1	2.665	-
d	H1_c	0.151(3)	1.024(2)	-0.1756(14)	2.40(3)	10.95(2)	-3.01(2)	1	1	1	2.665	D-H
d	H2_c	0.294(3)	1.021(2)	-0.1949(14)	3.62(3)	10.88(2)	-3.35(2)	1	1	1	2.665	D-H
cR	H2C_c	0.30890	1.01660	-0.34360	3.3501	10.5375	-5.8980	1	1	1	2.665	-
cR	H2D_c	-0.02590	0.67400	-0.24370	0.1221	6.9547	-4.1832	1	1	1	2.665	-
cR	H2E_c	-0.33500	0.97470	-0.21380	-2.1105	10.3334	-3.6699	1	1	1	2.665	-
cR	H2F_c	-0.37590	1.28770	-0.36530	-2.4125	13.4868	-6.2705	1	1	1	2.665	-
d	H3_c	0.066(3)	1.263(2)	-0.1833(14)	1.97(3)	13.58(2)	-3.15(2)	1	1	1	2.665	D-H
cR	H3C_c	0.50290	1.08900	-0.43470	4.9464	11.1553	-7.4617	1	1	1	2.665	-
cR	H3D_c	-0.20030	0.56330	-0.16160	-1.3799	5.8962	-2.7739	1	1	1	2.665	-
cR	H3E_c	-0.41040	0.82480	-0.11570	-2.7454	8.8741	-1.9860	1	1	1	2.665	-
cR	H3F_c	-0.37400	1.43200	-0.47420	-2.4698	14.8628	-8.1398	1	1	1	2.665	-
d	H4_c	0.065(3)	1.202(2)	-0.2434(14)	1.71(3)	12.78(2)	-4.18(2)	1	1	1	2.665	D-H
cR	H4C_c	0.73310	0.96290	-0.46040	6.7447	9.7122	-7.9029	1	1	1	2.665	-
cR	H4D_c	-0.20710	0.55570	-0.02620	-1.0941	6.0819	-0.4497	1	1	1	2.665	-
cR	H4E_c	-0.36400	0.83470	0.01230	-1.9789	9.2382	0.2111	1	1	1	2.665	-
cR	H4F_c	-0.20600	1.58090	-0.49130	-0.7967	16.4724	-8.4333	1	1	1	2.665	-
cR	H5C_c	0.76540	0.77150	-0.38720	6.9430	7.7452	-6.6464	1	1	1	2.665	-
cR	H5D_c	-0.04170	0.66570	0.02190	0.6704	7.3919	0.3759	1	1	1	2.665	-
cR	H5E_c	-0.23850	0.99570	0.03620	-0.5587	11.0630	0.6214	1	1	1	2.665	-
cR	H5F_c	-0.04400	1.58060	-0.39740	0.8953	16.6561	-6.8215	1	1	1	2.665	-
cR	H6A_c	0.07920	0.79460	-0.50980	0.5347	7.7561	-8.7508	1	1	1	2.665	-
cR	H6B_c	0.39430	0.70230	-0.02000	4.5015	7.7124	-0.3433	1	1	1	2.665	-
cR	H6C_c	0.56740	0.70660	-0.29580	5.3229	7.2108	-5.0775	1	1	1	2.665	-
cR	H6D_c	0.13030	0.77230	-0.06500	2.1322	8.3955	-1.1157	1	1	1	2.665	-
cR	H6E_c	-0.17100	1.14290	-0.06500	-0.0064	12.4864	-1.1157	1	1	1	2.665	-
cR	H6F_c	-0.05750	1.43570	-0.28930	0.8462	15.2718	-4.9659	1	1	1	2.665	-
d	Cu1_d	1.24336(2)	-0.19504(2)	0.76740(1)	12.8251(2)	-0.6250(2)	13.1727(2)	1	1	1	2.756	Met
d	Cu2_d	0.78798(3)	0.21291(2)	0.77017(1)	9.3752(3)	3.8836(2)	13.2201(2)	1	1	1	2.756	Met
d	O1_d	1.22677(18)	-0.02137(14)	0.82500(8)	13.0861(16)	1.4067(16)	14.1613(14)	1	1	1	2.756	D/A
d	O2_d	1.02985(16)	0.20694(14)	0.80154(8)	11.6059(15)	3.8802(16)	13.7586(14)	1	1	1	2.756	D/A
d	O11A_d	1.10486(14)	-0.11740(12)	0.69323(7)	11.5090(13)	0.0843(13)	11.8995(12)	1	1	1	2.756	D/A
d	O11B_d	1.37916(15)	-0.27894(12)	0.84167(7)	14.1081(14)	-1.4033(13)	14.4475(12)	1	1	1	2.756	D/A

d	O12A_d	1.12919(17)	-0.27409(13)	0.62273(8)	11.3081(15)	-1.7856(14)	10.6893(14)	1	1	1	2.756	D/A
d	O12B_d	1.46143(17)	-0.45479(12)	0.79094(7)	14.4476(15)	-3.4454(13)	13.5767(12)	1	1	1	2.756	D/A
d	O21A_d	0.85585(15)	0.09975(12)	0.69050(7)	9.6026(14)	2.4759(13)	11.8526(12)	1	1	1	2.756	D/A
d	O21B_d	1.70929(15)	-0.66712(12)	0.84384(7)	16.4835(14)	-5.6838(13)	14.4847(12)	1	1	1	2.756	D/A
d	O22A_d	1.08506(15)	0.16648(12)	0.65214(7)	11.6437(14)	3.1361(13)	11.1941(12)	1	1	1	2.756	D/A
d	O22B_d	1.46830(15)	-0.71481(12)	0.86427(8)	14.3181(14)	-6.1696(13)	14.8354(14)	1	1	1	2.756	D/A
d	N1C_d	1.41911(18)	-0.14471(14)	0.68831(9)	14.2577(16)	-0.2269(16)	11.8150(15)	1	1	1	2.756	D/A
d	N1D_d	1.07065(18)	-0.26889(15)	0.83782(9)	11.3619(16)	-1.3000(17)	14.3814(15)	1	1	1	2.756	D/A
d	N1E_d	0.75094(18)	0.07339(14)	0.85165(9)	9.0538(16)	2.5058(16)	14.6188(15)	1	1	1	2.756	D/A
d	N1F_d	0.78377(18)	0.34810(15)	0.68218(9)	9.3051(16)	5.2007(17)	11.7098(15)	1	1	1	2.756	D/A
d	C1A_d	1.0420(2)	-0.07718(16)	0.56537(10)	10.6703(18)	0.2737(18)	9.7047(17)	1	1	1	2.756	-
d	C1B_d	1.4710(2)	-0.44835(16)	0.92494(10)	14.8964(18)	-3.1075(18)	15.8768(17)	1	1	1	2.756	-
d	C2A_d	0.9943(2)	0.04657(17)	0.57145(10)	10.4440(18)	1.6518(19)	9.8091(17)	1	1	1	2.756	-
d	C2B_d	1.5338(2)	-0.57029(16)	0.93746(10)	15.3091(18)	-4.4286(18)	16.0917(17)	1	1	1	2.756	-
d	C2C_d	1.4029(2)	-0.03385(17)	0.64733(10)	14.1689(18)	0.9152(19)	11.1116(17)	1	1	1	2.756	-
d	C2D_d	0.9717(2)	-0.32903(19)	0.81099(12)	10.3198(18)	-2.017(2)	13.921(2)	1	1	1	2.756	-
d	C2E_d	0.6831(2)	-0.02049(18)	0.83785(12)	8.2736(18)	1.442(2)	14.382(2)	1	1	1	2.756	-
d	C2F_d	0.6920(2)	0.3483(2)	0.62807(12)	8.3442(18)	5.095(2)	10.781(2)	1	1	1	2.756	-
d	C3C_d	1.5176(2)	0.00963(18)	0.59257(11)	15.1113(18)	1.286(2)	10.1716(19)	1	1	1	2.756	-
d	C3D_d	0.8672(2)	-0.3948(2)	0.85935(13)	9.4185(18)	-2.647(2)	14.751(2)	1	1	1	2.756	-
d	C3E_d	0.6387(2)	-0.1103(2)	0.89583(13)	7.8980(18)	0.566(2)	15.377(2)	1	1	1	2.756	-
d	C3F_d	0.6927(3)	0.4337(2)	0.56304(13)	8.305(3)	5.908(2)	9.665(2)	1	1	1	2.756	-
d	C4C_d	1.6537(2)	-0.06381(19)	0.57808(12)	16.1780(18)	0.447(2)	9.923(2)	1	1	1	2.756	-
d	C4D_d	0.8626(2)	-0.3985(2)	0.93909(13)	9.5826(18)	-2.529(2)	16.120(2)	1	1	1	2.756	-
d	C4E_d	0.6664(2)	-0.1049(2)	0.97127(12)	8.3523(18)	0.776(2)	16.672(2)	1	1	1	2.756	-
d	C4F_d	0.7913(3)	0.5214(2)	0.55300(13)	9.287(3)	6.856(2)	9.492(2)	1	1	1	2.756	-
d	C5C_d	1.6718(2)	-0.1771(2)	0.62083(13)	16.2848(18)	-0.719(2)	10.657(2)	1	1	1	2.756	-
d	C5D_d	0.9609(2)	-0.3347(2)	0.96743(12)	10.6283(18)	-1.768(2)	16.606(2)	1	1	1	2.756	-
d	C5E_d	0.7393(3)	-0.0096(2)	0.98536(12)	9.180(3)	1.856(2)	16.914(2)	1	1	1	2.756	-
d	C5F_d	0.8863(3)	0.5214(2)	0.60836(13)	10.281(3)	6.967(2)	10.443(2)	1	1	1	2.756	-
d	C6A_d	1.0468(2)	-0.12141(17)	0.49413(10)	10.4596(18)	-0.3564(19)	8.4819(17)	1	1	1	2.756	-
d	C6B_d	1.4377(2)	-0.38027(17)	0.98808(10)	14.8669(18)	-2.2303(19)	16.9606(17)	1	1	1	2.756	-
d	C6C_d	1.5537(2)	-0.21527(19)	0.67516(12)	15.3188(18)	-1.032(2)	11.589(2)	1	1	1	2.756	-
d	C6D_d	1.0628(2)	-0.2714(2)	0.91523(11)	11.4926(18)	-1.174(2)	15.7101(19)	1	1	1	2.756	-
d	C6E_d	0.7794(2)	0.07740(19)	0.92484(11)	9.5068(18)	2.696(2)	15.8751(19)	1	1	1	2.756	-
d	C6F_d	0.8783(2)	0.43442(18)	0.67220(12)	10.2493(18)	6.134(2)	11.538(2)	1	1	1	2.756	-
d	C11A_d	1.0957(2)	-0.16478(17)	0.63233(10)	11.1965(18)	-0.5599(19)	10.8541(17)	1	1	1	2.756	-
d	C11B_d	1.4349(2)	-0.39096(17)	0.84538(10)	14.4493(18)	-2.6324(19)	14.5112(17)	1	1	1	2.756	-
d	C21A_d	0.9800(2)	0.10669(16)	0.64524(10)	10.6003(18)	2.4624(18)	11.0757(17)	1	1	1	2.756	-
d	C21B_d	1.5708(2)	-0.65532(16)	0.87508(10)	15.3486(18)	-5.4914(18)	15.0210(17)	1	1	1	2.756	-
d	H1_d	1.151(3)	0.024(2)	0.8244(14)	12.48(3)	1.91(2)	14.15(2)	1	1	1	2.756	D-H
d	H2_d	1.294(3)	0.021(2)	0.8051(14)	13.70(3)	1.83(2)	13.82(2)	1	1	1	2.756	D-H
cR	H2C_d	1.30890	0.01660	0.65640	13.4293	1.4901	11.2673	1	1	1	2.756	-
cR	H2D_d	0.97410	-0.32600	0.75630	10.2012	-2.0927	12.9821	1	1	1	2.756	-
cR	H2E_d	0.66500	-0.02530	0.78620	7.9687	1.2861	13.4953	1	1	1	2.756	-
cR	H2F_d	0.62410	0.28770	0.63470	7.6667	4.4394	10.8948	1	1	1	2.756	-
d	H3_d	1.066(3)	0.263(2)	0.8167(14)	12.05(3)	4.53(2)	14.02(2)	1	1	1	2.756	D-H

cR	H3C_d	1.50290	0.08900	0.56530	15.0256	2.1079	9.7035	1	1	1	2.756	-
cR	H3D_d	0.79970	-0.43670	0.83840	8.6993	-3.1512	14.3913	1	1	1	2.756	-
cR	H3E_d	0.58960	-0.17520	0.88430	7.3338	-0.1733	15.1792	1	1	1	2.756	-
cR	H3F_d	0.62600	0.43200	0.52580	7.6094	5.8155	9.0255	1	1	1	2.756	-
d	H4_d	1.065(3)	0.202(2)	0.7566(14)	11.79(3)	3.74(2)	12.99(2)	1	1	1	2.756	D-H
cR	H4C_d	1.73310	-0.03710	0.53960	16.8239	0.6648	9.2624	1	1	1	2.756	-
cR	H4D_d	0.79290	-0.44430	0.97380	8.9850	-2.9655	16.7155	1	1	1	2.756	-
cR	H4E_d	0.63600	-0.16530	1.01230	8.1003	0.1909	17.3764	1	1	1	2.756	-
cR	H4F_d	0.79400	0.58090	0.50870	9.2824	7.4250	8.7320	1	1	1	2.756	-
cR	H5C_d	1.76540	-0.22850	0.61280	17.0222	-1.3022	10.5189	1	1	1	2.756	-
cR	H5D_d	0.95830	-0.33430	1.02190	10.7496	-1.6555	17.5412	1	1	1	2.756	-
cR	H5E_d	0.76150	-0.00430	1.03620	9.5205	2.0156	17.7866	1	1	1	2.756	-
cR	H5F_d	0.95600	0.58060	0.60260	10.9745	7.6087	10.3438	1	1	1	2.756	-
cR	H6A_d	1.07920	-0.20540	0.49020	10.6139	-1.2913	8.4144	1	1	1	2.756	-
cR	H6B_d	1.39430	-0.29770	0.98000	14.5807	-1.3349	16.8219	1	1	1	2.756	-
cR	H6C_d	1.56740	-0.29340	0.70420	15.4021	-1.8366	12.0878	1	1	1	2.756	-
cR	H6D_d	1.13030	-0.22770	0.93500	12.2113	-0.6518	16.0495	1	1	1	2.756	-
cR	H6E_d	0.82900	0.14290	0.93500	10.0728	3.4390	16.0495	1	1	1	2.756	-
cR	H6F_d	0.94250	0.43570	0.71070	10.9254	6.2244	12.1993	1	1	1	2.756	-

 =====
 Residue = 2
 =====

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	O1W	0.7331(2)	0.48711(14)	0.30894(9)	8.0731(18)	5.9920(16)	5.3030(15)	1	1	1	-	D/A
d	H1W1	0.767(3)	0.427(2)	0.3321(15)	8.35(3)	5.37(2)	5.70(3)	1	1	1	-	D-H
d	H2W1	0.658(3)	0.468(2)	0.2885(15)	7.32(3)	5.74(2)	4.95(3)	1	1	1	-	D-H

 =====
 Residue = 3
 =====

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	O2W	0.66163(18)	-0.29715(15)	0.37871(10)	6.4604(16)	-2.5260(17)	6.5006(17)	1	1	1	-	D/A
d	H1W2	0.735(3)	-0.269(3)	0.3777(16)	7.15(3)	-2.22(3)	6.48(3)	1	1	1	-	D-H
d	H2W2	0.687(3)	-0.362(2)	0.3617(16)	6.55(3)	-3.28(2)	6.21(3)	1	1	1	-	D-H

 =====
 Residue = 4
 =====

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	O3W	0.82808(18)	0.61448(15)	0.15546(9)	8.7030(16)	7.0924(17)	2.6685(15)	1	1	1	-	D/A
d	H1W3	0.817(3)	0.572(2)	0.1931(15)	8.64(3)	6.70(2)	3.31(3)	1	1	1	-	D-H
d	H2W3	0.744(3)	0.640(2)	0.1463(15)	7.97(3)	7.36(2)	2.51(3)	1	1	1	-	D-H

 =====
 Residue = 5
 =====

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
d	O4W	0.56313(19)	0.85779(15)	0.24452(9)	6.9355(17)	9.9555(17)	4.1972(15)	1	1	1	-	D/A
d	H1W4	0.591(3)	0.813(2)	0.2797(15)	7.21(3)	9.53(2)	4.80(3)	1	1	1	-	D-H
d	H2W4	0.553(3)	0.809(2)	0.2132(15)	6.69(3)	9.35(2)	3.66(3)	1	1	1	-	D-H

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)	
a = [1465.01]	= -1+x, 1+y, z	= [	1	-1	1	0	1	-1	1	0
b = [1645.01]	= 1+x, -1+y, z	= [	1	1	-1	0	1	1	-1	0
c = [2665.01]	= 1-x, 1-y, -z	= [	2	1	1	0	1	1	1	0
d = [2756.01]	= 2-x, -y, 1-z	= [	2	2	0	1	1	2	0	1

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

$X(J) = X(sym) + TX$, $Y(J) = Y(sym) + TY$, $Z(J) = Z(sym) + TZ$,
 SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

:: Starred ARUs belong (chemically) to the previous ARU

:: Analysis of Polymeric Structure(s)

:: Resd # 1 - Infinite Two-Dimensional Network :: Base Vectors: #1 = [1 -1 0], #2 = [0 0 1], - Plane: (1 1 0)

NOTE: A # in the Atom Label Indicates a Label that was Modified to Conform with the Label Convention (A4)

Ordered Structure							Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)					
Resd	Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	H	Cu	N	O
1	1	0.641	0.370	0.073	729.65	1	2	30	26	2	4	10
2	1	0.731	0.483	0.309	18.02	1	2	-	2	-	-	1
3	1	2/3	-0.299	0.378	18.02	1	2	-	2	-	-	1
4	1	0.823	0.614	0.157	18.02	1	2	-	2	-	-	1
5	1	0.564	0.853	0.245	18.02	1	2	-	2	-	-	1

Unit Cell Weight = 1603.42 60 68 4 8 28

Calculated Analysis (Percent) = 44.9 4.3 15.9 7.0 27.9

Moiety_Formula = C30 H26 Cu2 N4 O10, 4(H2 O)

Sum_Formula = C30 H34 Cu2 N4 O14

Formula_Weight = 801.71 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 2

SpaceGroup_Z = 2 ==> Z' = 2 / 2 = 1.000

Calculated Density = 1.5760(6) g cm-3 [= Mg m-3]

F(000) = 824.0 [825.67]

mu(MoKa) = 13.33 cm-1 = 1.333 mm-1

Resonant Scattering = 4.04 Percent - (E. Girard et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 1698.6[1668.7] Ang**3, 298[113]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)

** WARNING **

Please Check the Derived Crystal Data.
They may be Incorrect for Disordered,
Incomplete or Polymeric Structures.

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f, f' & f''

=====
 (An)isotropic, Equivalent and Main Axes Displacement Parameters - Unusual Values Marked with a # - [Optional Coordinate Split-up]
 =====

 Residue = 1 *****
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Cu1	0.00923(12) [0.7582	0.00984(12) 0.1982	0.00586(11) 0.2327]	0.00093(9) [0.7551	-0.00279(9) 0.1918	0.00017(9) 0.2325]	0.00841(7)	0.0043	0.0096	0.0113	2.61
2	Cu2	0.01322(12) [1.2173	0.00929(12) -0.2115	0.00676(11) 0.2299]	-0.00248(9) [1.2068	0.00027(9) -0.2143	0.00149(9) 0.2298]	0.01004(7)	0.0053	0.0094	0.0154	2.90
3	O1	0.0188(8) [0.7774	0.0140(8) 0.0229	0.0145(7) 0.1745]	-0.0019(6) [0.7691	-0.0049(6) 0.0198	0.0024(6) 0.1755]	0.0159(4)	0.0114	0.0141	0.0221	1.94
4	O2	0.0162(7) [0.9708	0.0188(8) -0.2029	0.0123(7) 0.1976]	-0.0058(6) [0.9695	-0.0031(6) -0.2110	-0.0015(6) 0.1994]	0.0153(4)	0.0093	0.0162	0.0205	2.19
5	O11A	0.0114(6) [0.8977	0.0129(7) 0.1216	0.0053(6) 0.3066]	0.0000(5) [0.8926	-0.0035(5) 0.1132	0.0000(5) 0.3070]	0.0098(4)	0.0041	0.0115	0.0140	3.43
6	O11B	0.0142(7) [0.6279	0.0102(7) 0.2805	0.0084(6) 0.1574]	0.0015(5) [0.6138	-0.0060(5) 0.2774	0.0016(5) 0.1592]	0.0110(4)	0.0039	0.0124	0.0167	4.25
7	O12A	0.0318(9) [0.8815	0.0111(7) 0.2755	0.0152(7) 0.3761]	-0.0003(6) [0.8601	-0.0109(6) 0.2726	0.0034(6) 0.3784]	0.0192(4)	0.0082	0.0141	0.0353	4.29
8	O12B	0.0295(8) [0.5494	0.0123(7) 0.4555	0.0072(6) 0.2085]	-0.0022(5) [0.5278	-0.0055(6) 0.4541	0.0001(6) 0.2097]	0.0162(4)	0.0060	0.0122	0.0303	5.07
9	O21A	0.0118(7) [1.1469	0.0127(7) -0.0965	0.0074(6) 0.3090]	-0.0040(5) [1.1414	0.0000(5) -0.1030	0.0005(5) 0.3100]	0.0107(4)	0.0055	0.0120	0.0145	2.62
10	O21B	0.0156(7) [0.2959	0.0119(7) 0.6667	0.0117(7) 0.1568]	-0.0051(5) [0.2855	0.0010(5) 0.6676	0.0001(5) 0.1556]	0.0132(4)	0.0070	0.0149	0.0176	2.50
11	O22A	0.0135(7) [0.9135	0.0155(7) -0.1634	0.0125(7) 0.3471]	-0.0050(5) [0.9164	-0.0021(5) -0.1696	-0.0028(6) 0.3486]	0.0134(4)	0.0091	0.0136	0.0175	1.92
12	O22B	0.0157(7) [0.5360	0.0116(7) 0.7152	0.0132(7) 0.1349]	-0.0035(5) [0.5274	-0.0046(6) 0.7144	-0.0021(5) 0.1365]	0.0130(4)	0.0084	0.0134	0.0171	2.03
13	N1C	0.0123(8) [0.5846	0.0114(8) 0.1441	0.0075(7) 0.3113]	-0.0002(6) [0.5772	-0.0033(6) 0.1453	-0.0014(6) 0.3121]	0.0103(4)	0.0065	0.0115	0.0128	1.98
14	N1D	0.0113(8) [0.9300	0.0138(8) 0.2716	0.0107(8) 0.1626]	0.0009(6) [0.9287	-0.0022(6) 0.2662	0.0003(6) 0.1618]	0.0122(5)	0.0089	0.0117	0.0162	1.82
15	N1E	0.0141(8) [1.2522	0.0109(8) -0.0722	0.0091(7) 0.1483]	-0.0010(6) [1.2459	-0.0013(6) -0.0746	0.0015(6) 0.1484]	0.0117(4)	0.0091	0.0095	0.0165	1.81
16	N1F	0.0137(8) [1.2204	0.0111(8) -0.3463	0.0102(8) 0.3180]	-0.0016(6) [1.2120	0.0002(6) -0.3499	0.0027(6) 0.3176]	0.0122(5)	0.0078	0.0107	0.0181	2.31
17	C1A	0.0074(8) [0.9583	0.0087(9) 0.0788	0.0078(8) 0.4352]	0.0008(7) [0.9577	-0.0004(7) 0.0755	-0.0006(7) 0.4340]	0.0082(5)	0.0065	0.0074	0.0107	1.65
18	C1B	0.0059(8) [0.5276	0.0086(9) 0.4495	0.0094(9) 0.0761]	-0.0003(7) [0.5304	-0.0015(7) 0.4472	-0.0011(7) 0.0741]	0.0080(5)	0.0057	0.0082	0.0099	1.74

19	C2A	0.0057(8)	0.0118(9)	0.0077(8)	-0.0028(7)	-0.0006(7)	-0.0010(7)	0.0083(5)	0.0057	0.0069	0.0122	2.15
		[1.0050	-0.0434	0.4280]	[1.0064	-0.0497	0.4291]					
20	C2B	0.0057(8)	0.0093(9)	0.0080(8)	-0.0023(7)	-0.0008(7)	-0.0012(7)	0.0075(5)	0.0056	0.0070	0.0100	1.80
		[0.4656	0.5725	0.0620]	[0.4668	0.5681	0.0631]					
21	C2C	0.0129(9)	0.0121(10)	0.0097(9)	-0.0023(7)	-0.0043(7)	0.0001(7)	0.0113(5)	0.0075	0.0112	0.0152	2.02
		[0.6005	0.0354	0.3520]	[0.5937	0.0323	0.3533]					
22	C2D	0.0161(10)	0.0156(10)	0.0170(10)	-0.0013(8)	-0.0014(8)	-0.0012(8)	0.0164(6)	0.0152	0.0158	0.0182	1.20
		[1.0291	0.3294	0.1894]	[1.0275	0.3287	0.1886]					
23	C2E	0.0171(10)	0.0151(10)	0.0146(10)	-0.0041(8)	-0.0027(8)	0.0008(8)	0.0156(6)	0.0120	0.0151	0.0196	1.63
		[1.3196	0.0220	0.1617]	[1.3142	0.0190	0.1626]					
24	C2F	0.0188(11)	0.0192(11)	0.0211(11)	0.0001(9)	-0.0069(9)	-0.0011(9)	0.0196(6)	0.0144	0.0202	0.0242	1.68
		[1.3044	-0.3476	0.3731]	[1.3116	-0.3490	0.3708]					
25	C3C	0.0160(10)	0.0125(10)	0.0131(9)	0.0016(8)	-0.0039(8)	-0.0043(8)	0.0137(6)	0.0099	0.0124	0.0188	1.89
		[0.4863	-0.0111	0.4068]	[0.4785	-0.0082	0.4081]					
26	C3D	0.0140(10)	0.0192(11)	0.0291(12)	-0.0028(9)	0.0017(9)	-0.0029(8)	0.0212(6)	0.0130	0.0192	0.0312	2.40
		[1.1347	0.3936	0.1440]	[1.1309	0.3960	0.1373]					
27	C3E	0.0211(11)	0.0150(11)	0.0264(12)	-0.0010(9)	-0.0046(9)	-0.0042(8)	0.0206(7)	0.0140	0.0208	0.0270	1.92
		[1.3577	0.1104	0.1063]	[1.3649	0.1102	0.1020]					
28	C3F	0.0370(14)	0.0292(14)	0.0223(12)	0.0012(10)	-0.0156(11)	0.0022(11)	0.0292(8)	0.0129	0.0317	0.0431	3.34
		[1.3173	-0.4317	0.4355]	[1.2973	-0.4357	0.4384]					
29	C4C	0.0139(10)	0.0218(11)	0.0159(10)	-0.0011(8)	0.0011(8)	-0.0059(8)	0.0173(6)	0.0107	0.0182	0.0230	2.16
		[0.3430	0.0676	0.4218]	[0.3496	0.0600	0.4220]					
30	C4D	0.0155(10)	0.0209(12)	0.0253(11)	0.0090(9)	0.0063(9)	0.0006(9)	0.0228(6)	0.0096	0.0155	0.0433	4.50
		[1.1416	0.4042	0.0646]	[1.1332	0.3928	0.0572]					
31	C4E	0.0218(11)	0.0191(11)	0.0202(11)	0.0074(9)	0.0008(9)	-0.0022(9)	0.0217(6)	0.0106	0.0213	0.0331	3.13
		[1.3362	0.1095	0.0312]	[1.3310	0.1003	0.0262]					
32	C4F	0.0419(15)	0.0229(13)	0.0203(12)	0.0081(10)	-0.0052(11)	0.0036(11)	0.0299(8)	0.0110	0.0315	0.0473	4.30
		[1.2199	-0.5181	0.4474]	[1.1975	-0.5247	0.4466]					
33	C5C	0.0117(10)	0.0198(11)	0.0264(11)	-0.0008(9)	0.0009(9)	0.0023(8)	0.0202(6)	0.0102	0.0206	0.0299	2.94
		[0.3302	0.1796	0.3824]	[0.3262	0.1746	0.3759]					
34	C5D	0.0192(11)	0.0303(13)	0.0135(10)	0.0046(9)	0.0005(8)	0.0035(9)	0.0225(7)	0.0116	0.0170	0.0390	3.37
		[1.0422	0.3416	0.0335]	[1.0360	0.3278	0.0316]					
35	C5E	0.0272(12)	0.0242(12)	0.0114(10)	0.0002(9)	-0.0029(9)	0.0022(9)	0.0216(7)	0.0110	0.0213	0.0324	2.94
		[1.2672	0.0132	0.0146]	[1.2542	0.0060	0.0147]					
36	C5F	0.0294(13)	0.0152(11)	0.0296(12)	0.0010(9)	-0.0007(10)	-0.0048(9)	0.0252(7)	0.0140	0.0277	0.0339	2.42
		[1.1193	-0.5217	0.3938]	[1.1081	-0.5211	0.3895]					
37	C6A	0.0092(9)	0.0079(9)	0.0107(9)	-0.0010(7)	-0.0020(7)	-0.0004(7)	0.0093(5)	0.0077	0.0092	0.0109	1.41
		[0.9518	0.1211	0.5066]	[0.9546	0.1217	0.5051]					
38	C6B	0.0082(8)	0.0075(9)	0.0100(9)	-0.0011(7)	-0.0023(7)	0.0004(7)	0.0086(5)	0.0065	0.0087	0.0105	1.60
		[0.5604	0.3796	0.0127]	[0.5642	0.3810	0.0112]					
39	C6C	0.0146(10)	0.0143(10)	0.0181(10)	0.0017(8)	-0.0019(8)	0.0015(8)	0.0163(6)	0.0108	0.0158	0.0223	2.06
		[0.4478	0.2178	0.3263]	[0.4448	0.2127	0.3234]					
40	C6D	0.0152(10)	0.0242(12)	0.0110(9)	0.0010(8)	-0.0028(8)	0.0012(8)	0.0173(6)	0.0100	0.0149	0.0270	2.70
		[0.9384	0.2769	0.0850]	[0.9360	0.2659	0.0845]					
41	C6E	0.0207(11)	0.0144(10)	0.0122(9)	-0.0031(8)	-0.0030(8)	-0.0007(8)	0.0157(6)	0.0111	0.0148	0.0212	1.91
		[1.2251	-0.0769	0.0749]	[1.2161	-0.0779	0.0754]					
42	C6F	0.0217(11)	0.0133(10)	0.0191(10)	-0.0030(8)	-0.0058(9)	0.0009(8)	0.0179(6)	0.0126	0.0168	0.0242	1.92
		[1.1263	-0.4335	0.3270]	[1.1171	-0.4354	0.3286]					

43	C11A	0.0083(9)	0.0110(9)	0.0094(9)	0.0010(7)	-0.0021(7)	-0.0004(7)	0.0097(5)	0.0071	0.0092	0.0129	1.83
		[0.9036	0.1672	0.3683]	[0.9050	0.1624	0.3670]					
44	C11B	0.0092(9)	0.0099(9)	0.0098(9)	0.0003(7)	-0.0027(7)	-0.0027(7)	0.0095(5)	0.0074	0.0086	0.0124	1.67
		[0.5627	0.3922	0.1551]	[0.5675	0.3897	0.1541]					
45	C21A	0.0137(9)	0.0070(9)	0.0070(8)	0.0006(7)	-0.0028(7)	0.0032(7)	0.0096(5)	0.0041	0.0083	0.0165	4.06
		[1.0265	-0.1046	0.3545]	[1.0135	-0.1088	0.3550]					
46	C21B	0.0138(9)	0.0074(9)	0.0063(8)	0.0006(7)	-0.0035(7)	0.0016(7)	0.0093(5)	0.0043	0.0085	0.0153	3.57
		[0.4354	0.6567	0.1245]	[0.4230	0.6540	0.1253]					
47	H1	0.02400						0.02400				
48	H2	0.02300						0.02300				
49	H2C	0.01400						0.01400				
50	H2D	0.02000						0.02000				
51	H2E	0.01900						0.01900				
52	H2F	0.02300						0.02300				
53	H3	0.02300						0.02300				
54	H3C	0.01600						0.01600				
55	H3D	0.02500						0.02500				
56	H3E	0.02500						0.02500				
57	H3F	0.03500						0.03500				
58	H4	0.02300						0.02300				
59	H4C	0.02100						0.02100				
60	H4D	0.02700						0.02700				
61	H4E	0.02600						0.02600				
62	H4F	0.03600						0.03600				
63	H5C	0.02400						0.02400				
64	H5D	0.02700						0.02700				
65	H5E	0.02600						0.02600				
66	H5F	0.03000						0.03000				
67	H6A	0.01100						0.01100				
68	H6B	0.01000						0.01000				
69	H6C	0.02000						0.02000				
70	H6D	0.02100						0.02100				
71	H6E	0.01900						0.01900				
72	H6F	0.02100						0.02100				
U(i,j)-Average		0.0162	0.0145	0.0135	-0.0004	-0.0026	-0.0001	0.0149	0.0123	0.0149	0.0176	1.44

 =====
 Residue = 2
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	O1W	0.0310(9)	0.0138(8)	0.0280(9)	0.0008(7)	-0.0167(7)	0.0011(7)	0.0236(5)	0.0109	0.0190	0.0408	3.74

=====											
		[	0.7437	0.4877	0.3066]	[	0.7225	0.4865	0.3113]		
2	H1W1		0.03400							0.03400	
3	H2W1		0.03400							0.03400	
U(i,j)-Average											
			0.0310	0.0138	0.0280		0.0008	-0.0167	0.0011	0.0236	0.0109 0.0190 0.0408 3.74

 =====
 Residue = 3
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq (sUeq)	U1	U2	U3	U3/U1
1	O2W	0.0179(8)	0.0192(9)	0.0301(9)	-0.0045(7)	-0.0045(7)	-0.0051(7)	0.0219(5)	0.0141	0.0212	0.0302	2.14
		[0.6595	-0.2991	0.3817]	[0.6638	-0.2952	0.3758]					
2	H1W2	0.03400						0.03400				
3	H2W2	0.03400						0.03400				
U(i, j)-Average		0.0179	0.0192	0.0301	-0.0045	-0.0045	-0.0051	0.0218	0.0141	0.0212	0.0302	2.14

 =====
 Residue = 4
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq (sUeq)	U1	U2	U3	U3/U1
1	O3W	0.0162(8)	0.0217(9)	0.0226(8)	-0.0008(6)	-0.0039(7)	-0.0019(6)	0.0202(5)	0.0157	0.0207	0.0242	1.54
		[0.8265	0.6163	0.1565]	[0.8297	0.6127	0.1544]					
2	H1W3	0.03400						0.03400				
3	H2W3	0.03400						0.03400				
U(i, j)-Average		0.0162	0.0217	0.0226	-0.0008	-0.0039	-0.0019	0.0202	0.0157	0.0207	0.0242	1.54

 =====
 ***** Residue = 5 *****
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	O4W	0.0324(9)	0.0185(9)	0.0199(8)	-0.0082(7)	-0.0115(7)	0.0016(7)	0.0226(5)	0.0109	0.0194	0.0376	3.46
		[0.5725	0.8601	0.2430]	[0.5538	0.8555	0.2460]					
2	H1W4	0.03400						0.03400				
3	H2W4	0.03400						0.03400				
U(i,j)-Average		0.0324	0.0185	0.0199	-0.0082	-0.0115	0.0016	0.0226	0.0109	0.0194	0.0376	3.46

=====
 The Displacement Factor has the Form of Exp(-T)

where

$T = 8 * (\pi^2) * U_{iso} * \sin(\theta / \lambda)^2$, for Isotropic Atoms,

$T = 2 * (\pi^2) * (U_{11} * (h^2) + U_{22} * (k^2) + U_{33} * (l^2) + 2 * U_{23} * k * l + 2 * U_{13} * h * l + 2 * U_{12} * h * k)$, for Anisotr. Atoms

$U_{eq} = 1/3 \sum (U_{ij} * a_i * a_j)$

U1, U2, U3 are the three Main Axes Components of Uij

Reference U(eq): R.X. Fischer & E. Tillmanns, Acta Cryst. (1988). C44, 775-776

Ueq [or U(iso)] Averages per Element

	Non-H	C	H	Cu	N	O
Average	0.0155	0.0161	0.0253	0.0092	0.0116	0.0161
Minimum	0.0075	0.0075	0.0100	0.0084	0.0103	0.0098
Maximum	0.0299	0.0299	0.0360	0.0100	0.0122	0.0236
Ratio	3.9867	3.9867	3.6000	1.1938	1.1845	2.4082
Number	50	30	34	2	4	14

 =====
 ***** Residue = 1 *****
 =====

=====
:: No TLS-Analysis for Polymeric or Disordered Structures

Rigid-Body Model Libration Corrections for Bond Distances and "Hirshfeld Rigid-Bond" Test (Acta Cryst, (1976), A32, 239-244)

Bond		Bond Distance		Components of the Correction			Vibration Along the Interatomic Bond				Angle with Lib. Axes		
Atom(I)	Atom(J)	Obsd	Calcd	Del(L)	Del(M)	Del(N)	I to J	J to I	Difference	Sqrt(Diff)	L(1)	L(2)	L(3)
Cu1	- O1	2.2745	0	0	0	0	0.0108(1)	0.0144(8)	0.0036(8)	0.0601	0.00	0.00	0.00
Cu1	- O11A	1.9637	0	0	0	0	0.0049(1)	0.0056(6)	0.0007(6)	0.0263	0.00	0.00	0.00
Cu1	- O11B	1.9690	0	0	0	0	0.0048(1)	0.0045(7)	0.0004(7)	0.0188	0.00	0.00	0.00
Cu1	- N1C	2.0135	0	0	0	0	0.0094(1)	0.0117(8)	0.0023(8)	0.0482	0.00	0.00	0.00
Cu1	- N1D	2.0144	0	0	0	0	0.0097(1)	0.0123(8)	0.0026(8)	0.0506	0.00	0.00	0.00
Cu2	- O2	2.2948	0	0	0	0	0.0144(1)	0.0147(7)	0.0002(7)	0.0154	0.00	0.00	0.00
Cu2	- O21A	1.9757	0	0	0	0	0.0057(1)	0.0063(7)	0.0006(7)	0.0249	0.00	0.00	0.00
Cu2	- N1E	1.9895	0	0	0	0	0.0100(1)	0.0107(8)	0.0007(8)	0.0270	0.00	0.00	0.00
Cu2	- N1F	2.0051	0	0	0	0	0.0093(1)	0.0109(8)	0.0015(8)	0.0392	0.00	0.00	0.00
Cu2	- O21B_b	1.9677	0	0	0	0	0.0057(1)	0.0071(7)	0.0014(7)	0.0372	0.00	0.00	0.00
O11A	- C11A	1.2671	0	0	0	0	0.0074(6)	0.0117(9)	0.0043(11)	0.0653	0.00	0.00	0.00
O11B	- C11B	1.2772	0	0	0	0	0.0092(7)	0.0107(9)	0.0015(11)	0.0383	0.00	0.00	0.00
O12A	- C11A	1.2418	0	0	0	0	0.0115(8)	0.0118(9)	0.0003(12)	0.0171	0.00	0.00	0.00
O12B	- C11B	1.2386	0	0	0	0	0.0079(7)	0.0114(9)	0.0035(11)	0.0591	0.00	0.00	0.00
O21A	- C21A	1.2646	0	0	0	0	0.0100(7)	0.0133(9)	0.0033(11)	0.0573	0.00	0.00	0.00
O21B	- C21B	1.2699	0	0	0	0	0.0133(7)	0.0139(9)	0.0005(11)	0.0226	0.00	0.00	0.00
O22A	- C21A	1.2477	0	0	0	0	0.0115(7)	0.0160(9)	0.0045(11)	0.0671	0.00	0.00	0.00
O22B	- C21B	1.2475	0	0	0	0	0.0111(7)	0.0137(9)	0.0026(11)	0.0510	0.00	0.00	0.00
N1C	- C2C	1.3443	0	0	0	0	0.0098(8)	0.0120(9)	0.0022(12)	0.0473	0.00	0.00	0.00
N1C	- C6C	1.3509	0	0	0	0	0.0124(8)	0.0124(10)	0.0000(13)	0.0037	0.00	0.00	0.00
N1D	- C2D	1.3463	0	0	0	0	0.0147(8)	0.0178(10)	0.0031(13)	0.0558	0.00	0.00	0.00
N1D	- C6D	1.3411	0	0	0	0	0.0111(8)	0.0115(10)	0.0004(13)	0.0198	0.00	0.00	0.00
N1E	- C2E	1.3403	0	0	0	0	0.0149(8)	0.0166(10)	0.0017(13)	0.0415	0.00	0.00	0.00
N1E	- C6E	1.3489	0	0	0	0	0.0100(8)	0.0118(10)	0.0018(13)	0.0420	0.00	0.00	0.00
N1F	- C2F	1.3406	0	0	0	0	0.0148(8)	0.0161(11)	0.0013(14)	0.0354	0.00	0.00	0.00
N1F	- C6F	1.3384	0	0	0	0	0.0171(8)	0.0199(10)	0.0028(13)	0.0532	0.00	0.00	0.00
C1A	- C2A	1.4005	0	0	0	0	0.0090(8)	0.0109(8)	0.0019(12)	0.0431	0.00	0.00	0.00
C1A	- C6A	1.3917	0	0	0	0	0.0098(8)	0.0102(9)	0.0004(12)	0.0206	0.00	0.00	0.00
C1A	- C11A	1.5142	0	0	0	0	0.0069(8)	0.0074(9)	0.0005(12)	0.0218	0.00	0.00	0.00
C1B	- C2B	1.4006	0	0	0	0	0.0083(9)	0.0093(8)	0.0010(12)	0.0311	0.00	0.00	0.00
C1B	- C6B	1.3946	0	0	0	0	0.0099(9)	0.0091(9)	0.0009(12)	0.0295	0.00	0.00	0.00
C1B	- C11B	1.5135	0	0	0	0	0.0085(9)	0.0085(9)	0.0000(12)	0.0060	0.00	0.00	0.00
C2A	- C21A	1.5119	0	0	0	0	0.0071(8)	0.0086(9)	0.0015(12)	0.0393	0.00	0.00	0.00
C2A	- C6A_d	1.3911	0	0	0	0	0.0100(8)	0.0093(9)	0.0008(12)	0.0279	0.00	0.00	0.00
C2B	- C21B	1.5092	0	0	0	0	0.0071(8)	0.0083(9)	0.0012(12)	0.0351	0.00	0.00	0.00
C2B	- C6B_c	1.3908	0	0	0	0	0.0087(8)	0.0090(9)	0.0002(12)	0.0157	0.00	0.00	0.00
C2C	- C3C	1.3818	0	0	0	0	0.0149(9)	0.0134(10)	0.0015(13)	0.0387	0.00	0.00	0.00
C2D	- C3D	1.3777	0	0	0	0	0.0159(10)	0.0161(11)	0.0002(15)	0.0152	0.00	0.00	0.00
C2E	- C3E	1.3780	0	0	0	0	0.0182(10)	0.0190(11)	0.0008(15)	0.0287	0.00	0.00	0.00
C2F	- C3F	1.3816	0	0	0	0	0.0180(11)	0.0207(13)	0.0027(17)	0.0519	0.00	0.00	0.00
C3C	- C4C	1.3800	0	0	0	0	0.0178(10)	0.0189(10)	0.0010(14)	0.0321	0.00	0.00	0.00

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C3D	- C4D	1.3836	0	0	0	0	0.0303(11)	0.0301(11)	0.0002(16)	0.0153	0.00	0.00	0.00
C3E	- C4E	1.3882	0	0	0	0	0.0253(11)	0.0265(11)	0.0012(16)	0.0345	0.00	0.00	0.00
C3F	- C4F	1.3761	0	0	0	0	0.0391(13)	0.0410(13)	0.0019(19)	0.0440	0.00	0.00	0.00
C4C	- C5C	1.3813	0	0	0	0	0.0203(10)	0.0196(11)	0.0007(15)	0.0257	0.00	0.00	0.00
C4D	- C5D	1.3816	0	0	0	0	0.0375(11)	0.0355(11)	0.0020(16)	0.0447	0.00	0.00	0.00
C4E	- C5E	1.3823	0	0	0	0	0.0277(11)	0.0310(11)	0.0033(16)	0.0574	0.00	0.00	0.00
C4F	- C5F	1.3791	0	0	0	0	0.0337(13)	0.0339(12)	0.0002(18)	0.0153	0.00	0.00	0.00
C5C	- C6C	1.3788	0	0	0	0	0.0164(11)	0.0158(10)	0.0006(15)	0.0248	0.00	0.00	0.00
C5D	- C6D	1.3798	0	0	0	0	0.0190(11)	0.0175(10)	0.0014(15)	0.0378	0.00	0.00	0.00
C5E	- C6E	1.3752	0	0	0	0	0.0179(11)	0.0157(10)	0.0023(15)	0.0475	0.00	0.00	0.00
C5F	- C6F	1.3769	0	0	0	0	0.0202(12)	0.0178(10)	0.0023(16)	0.0482	0.00	0.00	0.00
C6A	- C2A_d	1.3911	0	0	0	0	0.0093(9)	0.0100(8)	0.0008(12)	0.0279	0.00	0.00	0.00
C6B	- C2B_c	1.3908	0	0	0	0	0.0090(9)	0.0087(8)	0.0002(12)	0.0157	0.00	0.00	0.00

Sqrt(Sum(DelIJ**2)/Nrb) = 0.0019

- Indicates bonds exceeding the 5.0 sigma test level

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Analysis of Bond Distance and Angle Values - Identification of Chiral Center(s) and Their (R/S)-Configuration (Cahn-Ingold-Prelog)

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The Following Tests are done. Faults are Marked Under Note

- V : Valency Check Fault for H, C
- S : Bond Too Short
- A : Unusual Bond Angle Values (PLEASE CHECK)

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*** PLEASE NOTE: R/S ASSIGNMENTS ARE TENTATIVE *** (CIP Special rules NOT Implemented)

*** See Angew.Chem.Intern. Ed. Eng., (1966), 5, 385 & (1982), 21, 567 for Authoritative Details for Special Cases

***** Residue = 1 *****

										=A.N.G.L.E.S=				=B.O.N.D.S=						
Flag	Label	-	Connected to	(May be Incomplete for Polymeric Structures)						nra	min	max	Aver	min	max	nrb	tnr	Hyb	RS	Note
d	Cu1	-	O1	O11A	O11B	N1C	N1D	-----	-----	-----	-----	10	87	178	107.9	1.964	2.275	5	281	
d	Cu2	-	O2	O21A	N1E	N1F	O21B_b	-----	-----	-----	-----	10	87	175	107.8	1.968	2.295	5	280	
d	O1	-	Cu1	H1	H2	-----	-----	-----	-----	-----	-----	3	104	118	111.2	0.789	2.275	3	269	
d	O2	-	Cu2	H3	H4	-----	-----	-----	-----	-----	-----	3	90	126	108.3	0.807	2.295	3	260	
d	O11A	-	Cu1	C11A	-----	-----	-----	-----	-----	-----	-----	1	121	121	121.1	1.267	1.964	2	271	sp3
d	O11B	-	Cu1	C11B	-----	-----	-----	-----	-----	-----	-----	1	126	126	125.9	1.277	1.969	2	270	sp3
d	O12A	-	C11A	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	244	sp2
d	O12B	-	C11B	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.239	1.239	1	242	sp2
d	O21A	-	Cu2	C21A	-----	-----	-----	-----	-----	-----	-----	1	122	122	121.6	1.265	1.976	2	262	sp3
d	O21B	-	C21B	Cu2_a	-----	-----	-----	-----	-----	-----	-----	1	122	122	122.3	1.270	1.968	2	259	sp3
d	O22A	-	C21A	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.248	1.248	1	232	sp2
d	O22B	-	C21B	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.248	1.248	1	228	sp2
d	N1C	-	Cu1	C2C	C6C	-----	-----	-----	-----	-----	-----	3	118	124	120.0	1.344	2.013	3	203	
d	N1D	-	Cu1	C2D	C6D	-----	-----	-----	-----	-----	-----	3	118	122	119.8	1.341	2.014	3	203	
d	N1E	-	Cu2	C2E	C6E	-----	-----	-----	-----	-----	-----	3	118	121	119.9	1.340	1.989	3	200	
d	N1F	-	Cu2	C2F	C6F	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.338	2.005	3	200	
d	C1A	-	C2A	C6A	C11A	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.392	1.514	3	143	sp2
d	C1B	-	C2B	C6B	C11B	-----	-----	-----	-----	-----	-----	3	119	121	120.0	1.395	1.514	3	142	sp2
d	C2A	-	C1A	C21A	C6A_d	-----	-----	-----	-----	-----	-----	3	116	125	120.0	1.391	1.512	3	137	sp2
d	C2B	-	C1B	C21B	C6B_c	-----	-----	-----	-----	-----	-----	3	116	124	120.0	1.391	1.509	3	135	sp2
d	C2C	-	N1C	C3C	H2C	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.382	3	153	sp2
d	C2D	-	N1D	C3D	H2D	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.949	1.378	3	153	sp2
d	C2E	-	N1E	C3E	H2E	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.378	3	152	sp2
d	C2F	-	N1F	C3F	H2F	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.382	3	152	sp2
d	C3C	-	C2C	C4C	H3C	-----	-----	-----	-----	-----	-----	3	119	120	120.0	0.950	1.382	3	123	sp2
d	C3D	-	C2D	C4D	H3D	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.949	1.384	3	123	sp2
d	C3E	-	C2E	C4E	H3E	-----	-----	-----	-----	-----	-----	3	119	120	120.0	0.951	1.388	3	117	sp2
d	C3F	-	C2F	C4F	H3F	-----	-----	-----	-----	-----	-----	3	119	120	120.0	0.949	1.382	3	117	sp2
d	C4C	-	C3C	C5C	H4C	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.949	1.381	3	85	sp2
d	C4D	-	C3D	C5D	H4D	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.384	3	85	sp2
d	C4E	-	C3E	C5E	H4E	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.388	3	83	sp2
d	C4F	-	C3F	C5F	H4F	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.949	1.379	3	83	sp2
d	C5C	-	C4C	C6C	H5C	-----	-----	-----	-----	-----	-----	3	120	120	120.0	0.950	1.381	3	123	sp2
d	C5D	-	C4D	C6D	H5D	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.382	3	123	sp2
d	C5E	-	C4E	C6E	H5E	-----	-----	-----	-----	-----	-----	3	119	120	120.0	0.950	1.382	3	117	sp2
d	C5F	-	C4F	C6F	H5F	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.379	3	117	sp2
d	C6A	-	C1A	H6A	C2A_d	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.392	3	103	sp2
d	C6B	-	C1B	H6B	C2B_c	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.395	3	101	sp2
d	C6C	-	N1C	C5C	H6C	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.379	3	153	sp2
d	C6D	-	N1D	C5D	H6D	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.951	1.380	3	153	sp2

d	C6E	- N1E	C5E	H6E	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.375	3	152	sp2
d	C6F	- N1F	C5F	H6F	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.377	3	152	sp2
d	C11A	- 011A	012A	C1A	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.514	3	193	sp2
d	C11B	- 011B	012B	C1B	-----	-----	-----	-----	-----	-----	3	115	126	120.0	1.239	1.514	3	192	sp2
d	C21A	- 021A	022A	C2A	-----	-----	-----	-----	-----	-----	3	116	127	119.9	1.248	1.512	3	191	sp2
d	C21B	- 021B	022B	C2B	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.248	1.509	3	189	sp2
d	H1	- 01	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.789	0.789	1	51	
d	H2	- 01	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.819	0.819	1	51	
cR	H2C	- C2C	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	40	
cR	H2D	- C2D	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	40	
cR	H2E	- C2E	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	37	
cR	H2F	- C2F	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	37	
d	H3	- 02	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.829	0.829	1	50	
cR	H3C	- C3C	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	30	
cR	H3D	- C3D	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	30	
cR	H3E	- C3E	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	29	
cR	H3F	- C3F	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	29	
d	H4	- 02	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.807	0.807	1	50	
cR	H4C	- C4C	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	10	
cR	H4D	- C4D	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	10	
cR	H4E	- C4E	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	7	
cR	H4F	- C4F	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	7	
cR	H5C	- C5C	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	30	
cR	H5D	- C5D	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	30	
cR	H5E	- C5E	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	29	
cR	H5F	- C5F	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	29	
cR	H6A	- C6A	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	20	
cR	H6B	- C6B	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	19	
cR	H6C	- C6C	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	40	
cR	H6D	- C6D	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	40	
cR	H6E	- C6E	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	37	
cR	H6F	- C6F	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	37	
d	Cu1_a	- 01_a	011A_a	011B_a	N1C_a	N1D_a	-----	-----	-----	-----	10	87	178	107.9	1.964	2.275	5	275	
d	Cu2_a	- 021B	02_a	021A_a	N1E_a	N1F_a	-----	-----	-----	-----	10	87	175	107.8	1.968	2.295	5	279	
d	01_a	- Cu1_a	H1_a	H2_a	-----	-----	-----	-----	-----	-----	3	104	118	111.2	0.789	2.275	3	251	
d	02_a	- Cu2_a	H3_a	H4_a	-----	-----	-----	-----	-----	-----	3	90	126	108.3	0.807	2.295	3	257	
d	011A_a	- Cu1_a	C11A_a	-----	-----	-----	-----	-----	-----	-----	1	121	121	121.1	1.267	1.964	2	253	
d	011B_a	- Cu1_a	C11B_a	-----	-----	-----	-----	-----	-----	-----	1	126	126	125.9	1.277	1.969	2	252	
d	012A_a	- C11A_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	220	
d	012B_a	- C11B_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.239	1.239	1	218	
d	021A_a	- Cu2_a	C21A_a	-----	-----	-----	-----	-----	-----	-----	1	122	122	121.6	1.265	1.976	2	258	
d	021B_a	- C21B_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.270	1.270	1	206	
d	022A_a	- C21A_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.248	1.248	1	226	
d	022B_a	- C21B_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.248	1.248	1	206	
d	N1C_a	- Cu1_a	C2C_a	C6C_a	-----	-----	-----	-----	-----	-----	3	118	124	120.0	1.344	2.013	3	197	
d	N1D_a	- Cu1_a	C2D_a	C6D_a	-----	-----	-----	-----	-----	-----	3	118	122	119.8	1.341	2.014	3	197	

d	N1E_a	- Cu2_a	C2E_a	C6E_a	-----	-----	-----	-----	-----	-----	3	118	121	119.9	1.340	1.989	3	199	
d	N1F_a	- Cu2_a	C2F_a	C6F_a	-----	-----	-----	-----	-----	-----	3	118	122	119.9	1.338	2.005	3	199	
d	C1A_a	- C2A_a	C6A_a	C11A_a	-----	-----	-----	-----	-----	-----	3	118	123	120.0	1.392	1.514	3	131	
d	C1B_a	- C2B_a	C6B_a	C11B_a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	1.395	1.514	3	130	
d	C2A_a	- C1A_a	C21A_a	-----	-----	-----	-----	-----	-----	-----	1	125	125	125.0	1.400	1.512	2	134	?
d	C2B_a	- C1B_a	C21B_a	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.3	1.401	1.509	2	124	?
d	C2C_a	- N1C_a	C3C_a	H2C_a	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.382	3	147	
d	C2D_a	- N1D_a	C3D_a	H2D_a	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.949	1.378	3	147	
d	C2E_a	- N1E_a	C3E_a	H2E_a	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.378	3	151	
d	C2F_a	- N1F_a	C3F_a	H2F_a	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.382	3	151	
d	C3C_a	- C2C_a	C4C_a	H3C_a	-----	-----	-----	-----	-----	-----	3	119	120	120.0	0.950	1.382	3	111	
d	C3D_a	- C2D_a	C4D_a	H3D_a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.949	1.384	3	111	
d	C3E_a	- C2E_a	C4E_a	H3E_a	-----	-----	-----	-----	-----	-----	3	119	120	120.0	0.951	1.388	3	115	
d	C3F_a	- C2F_a	C4F_a	H3F_a	-----	-----	-----	-----	-----	-----	3	119	120	120.0	0.949	1.382	3	115	
d	C4C_a	- C3C_a	C5C_a	H4C_a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.949	1.381	3	73	
d	C4D_a	- C3D_a	C5D_a	H4D_a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.384	3	73	
d	C4E_a	- C3E_a	C5E_a	H4E_a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.388	3	81	
d	C4F_a	- C3F_a	C5F_a	H4F_a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.949	1.379	3	81	
d	C5C_a	- C4C_a	C6C_a	H5C_a	-----	-----	-----	-----	-----	-----	3	120	120	120.0	0.950	1.381	3	111	
d	C5D_a	- C4D_a	C6D_a	H5D_a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.382	3	111	
d	C5E_a	- C4E_a	C6E_a	H5E_a	-----	-----	-----	-----	-----	-----	3	119	120	120.0	0.950	1.382	3	115	
d	C5F_a	- C4F_a	C6F_a	H5F_a	-----	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.379	3	115	
d	C6A_a	- C1A_a	H6A_a	-----	-----	-----	-----	-----	-----	-----	1	119	119	118.9	0.950	1.392	2	89	?
d	C6B_a	- C1B_a	H6B_a	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.1	0.950	1.395	2	88	?
d	C6C_a	- N1C_a	C5C_a	H6C_a	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.379	3	147	
d	C6D_a	- N1D_a	C5D_a	H6D_a	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.951	1.380	3	147	
d	C6E_a	- N1E_a	C5E_a	H6E_a	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.375	3	151	
d	C6F_a	- N1F_a	C5F_a	H6F_a	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.377	3	151	
d	C11A_a	- 011A_a	012A_a	C1A_a	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.514	3	181	
d	C11B_a	- 011B_a	012B_a	C1B_a	-----	-----	-----	-----	-----	-----	3	115	126	120.0	1.239	1.514	3	180	
d	C21A_a	- 021A_a	022A_a	C2A_a	-----	-----	-----	-----	-----	-----	3	116	127	119.9	1.248	1.512	3	188	
d	C21B_a	- 021B_a	022B_a	C2B_a	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.248	1.509	3	155	
d	H1_a	- 01_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.789	0.789	1	45	
d	H2_a	- 01_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.819	0.819	1	45	
cR	H2C_a	- C2C_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	34	
cR	H2D_a	- C2D_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	34	
cR	H2E_a	- C2E_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	36	
cR	H2F_a	- C2F_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	36	
d	H3_a	- 02_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.829	0.829	1	49	
cR	H3C_a	- C3C_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	24	
cR	H3D_a	- C3D_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	24	
cR	H3E_a	- C3E_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	28	
cR	H3F_a	- C3F_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	28	
d	H4_a	- 02_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.807	0.807	1	49	
cR	H4C_a	- C4C_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	4	
cR	H4D_a	- C4D_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	4	
cR	H4E_a	- C4E_a	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	6	

cR	H4F_a	-	C4F_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1 6
cR	H5C_a	-	C5C_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1 24
cR	H5D_a	-	C5D_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1 24
cR	H5E_a	-	C5E_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1 28
cR	H5F_a	-	C5F_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1 28
cR	H6A_a	-	C6A_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1 12
cR	H6B_a	-	C6B_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1 11
cR	H6C_a	-	C6C_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1 34
cR	H6D_a	-	C6D_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1 34
cR	H6E_a	-	C6E_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1 36
cR	H6F_a	-	C6F_a	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1 36
d	Cu1_b	-	O1_b	O11A_b	O11B_b	N1C_b	N1D_b	-----	-----	-----	-----	-----	10	87	178	107.9 1.964 2.275 5 276
d	Cu2_b	-	O2_b	O21A_b	N1E_b	N1F_b	-----	-----	-----	-----	-----	-----	6	87	168	105.1 1.976 2.295 4 272
d	O1_b	-	Cu1_b	H1_b	H2_b	-----	-----	-----	-----	-----	-----	-----	3	104	118	111.2 0.789 2.275 3 254
d	O2_b	-	Cu2_b	H3_b	H4_b	-----	-----	-----	-----	-----	-----	-----	3	90	126	108.3 0.807 2.295 3 245
d	O11A_b	-	Cu1_b	C11A_b	-----	-----	-----	-----	-----	-----	-----	-----	1	121	121	121.1 1.267 1.964 2 255
d	O11B_b	-	Cu1_b	C11B_b	-----	-----	-----	-----	-----	-----	-----	-----	1	126	126	125.9 1.277 1.969 2 256
d	O12A_b	-	C11A_b	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0 1.242 1.242 1 222
d	O12B_b	-	C11B_b	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0 1.239 1.239 1 224
d	O21A_b	-	Cu2_b	C21A_b	-----	-----	-----	-----	-----	-----	-----	-----	1	122	122	121.6 1.265 1.976 2 246
d	O21B_b	-	Cu2	C21B_b	-----	-----	-----	-----	-----	-----	-----	-----	1	122	122	122.3 1.270 1.968 2 261
d	O22A_b	-	C21A_b	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0 1.248 1.248 1 212
d	O22B_b	-	C21B_b	-----	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0 1.248 1.248 1 230
d	N1C_b	-	Cu1_b	C2C_b	C6C_b	-----	-----	-----	-----	-----	-----	-----	3	118	124	120.0 1.344 2.013 3 198
d	N1D_b	-	Cu1_b	C2D_b	C6D_b	-----	-----	-----	-----	-----	-----	-----	3	118	122	119.8 1.341 2.014 3 198
d	N1E_b	-	Cu2_b	C2E_b	C6E_b	-----	-----	-----	-----	-----	-----	-----	3	118	121	119.9 1.340 1.989 3 194
d	N1F_b	-	Cu2_b	C2F_b	C6F_b	-----	-----	-----	-----	-----	-----	-----	3	118	122	119.9 1.338 2.005 3 194
d	C1A_b	-	C2A_b	C6A_b	C11A_b	-----	-----	-----	-----	-----	-----	-----	3	118	123	120.0 1.392 1.514 3 132
d	C1B_b	-	C2B_b	C6B_b	C11B_b	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0 1.395 1.514 3 133
d	C2A_b	-	C1A_b	C21A_b	-----	-----	-----	-----	-----	-----	-----	-----	1	125	125	125.0 1.400 1.512 2 127
d	C2B_b	-	C1B_b	C21B_b	-----	-----	-----	-----	-----	-----	-----	-----	1	124	124	124.3 1.401 1.509 2 136
d	C2C_b	-	N1C_b	C3C_b	H2C_b	-----	-----	-----	-----	-----	-----	-----	3	119	123	120.0 0.950 1.382 3 148
d	C2D_b	-	N1D_b	C3D_b	H2D_b	-----	-----	-----	-----	-----	-----	-----	3	119	123	120.0 0.949 1.378 3 148
d	C2E_b	-	N1E_b	C3E_b	H2E_b	-----	-----	-----	-----	-----	-----	-----	3	119	122	120.0 0.950 1.378 3 144
d	C2F_b	-	N1F_b	C3F_b	H2F_b	-----	-----	-----	-----	-----	-----	-----	3	119	122	120.0 0.950 1.382 3 144
d	C3C_b	-	C2C_b	C4C_b	H3C_b	-----	-----	-----	-----	-----	-----	-----	3	119	120	120.0 0.950 1.382 3 113
d	C3D_b	-	C2D_b	C4D_b	H3D_b	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0 0.949 1.384 3 113
d	C3E_b	-	C2E_b	C4E_b	H3E_b	-----	-----	-----	-----	-----	-----	-----	3	119	120	120.0 0.951 1.388 3 105
d	C3F_b	-	C2F_b	C4F_b	H3F_b	-----	-----	-----	-----	-----	-----	-----	3	119	120	120.0 0.949 1.382 3 105
d	C4C_b	-	C3C_b	C5C_b	H4C_b	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0 0.949 1.381 3 75
d	C4D_b	-	C3D_b	C5D_b	H4D_b	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0 0.950 1.384 3 75
d	C4E_b	-	C3E_b	C5E_b	H4E_b	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0 0.950 1.388 3 67
d	C4F_b	-	C3F_b	C5F_b	H4F_b	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0 0.949 1.379 3 67
d	C5C_b	-	C4C_b	C6C_b	H5C_b	-----	-----	-----	-----	-----	-----	-----	3	120	120	120.0 0.950 1.381 3 113
d	C5D_b	-	C4D_b	C6D_b	H5D_b	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0 0.950 1.382 3 113
d	C5E_b	-	C4E_b	C6E_b	H5E_b	-----	-----	-----	-----	-----	-----	-----	3	119	120	120.0 0.950 1.382 3 105
d	C5F_b	-	C4F_b	C6F_b	H5F_b	-----	-----	-----	-----	-----	-----	-----	3	119	121	120.0 0.950 1.379 3 105

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d	C6A_b	- C1A_b	H6A_b	-----	-----	-----	-----	-----	-----	-----	1	119	119	118.9	0.950	1.392	2	90	?
d	C6B_b	- C1B_b	H6B_b	-----	-----	-----	-----	-----	-----	-----	1	119	119	119.1	0.950	1.395	2	91	?
d	C6C_b	- N1C_b	C5C_b	H6C_b	-----	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.379	3	148	
d	C6D_b	- N1D_b	C5D_b	H6D_b	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.951	1.380	3	148	
d	C6E_b	- N1E_b	C5E_b	H6E_b	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.375	3	144	
d	C6F_b	- N1F_b	C5F_b	H6F_b	-----	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.377	3	144	
d	C11A_b	- O11A_b	O12A_b	C1A_b	-----	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.514	3	182	
d	C11B_b	- O11B_b	O12B_b	C1B_b	-----	-----	-----	-----	-----	-----	3	115	126	120.0	1.239	1.514	3	183	
d	C21A_b	- O21A_b	O22A_b	C2A_b	-----	-----	-----	-----	-----	-----	3	116	127	119.9	1.248	1.512	3	177	
d	C21B_b	- O21B_b	O22B_b	C2B_b	-----	-----	-----	-----	-----	-----	3	115	126	119.9	1.248	1.509	3	190	
d	H1_b	- O1_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.789	0.789	1	46	
d	H2_b	- O1_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.819	0.819	1	46	
cR	H2C_b	- C2C_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	35	
cR	H2D_b	- C2D_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	35	
cR	H2E_b	- C2E_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	31	
cR	H2F_b	- C2F_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	31	
d	H3_b	- O2_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.829	0.829	1	42	
cR	H3C_b	- C3C_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	25	
cR	H3D_b	- C3D_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	25	
cR	H3E_b	- C3E_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	21	
cR	H3F_b	- C3F_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	21	
d	H4_b	- O2_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.807	0.807	1	42	
cR	H4C_b	- C4C_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	5	
cR	H4D_b	- C4D_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	5	
cR	H4E_b	- C4E_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	1	
cR	H4F_b	- C4F_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	1	
cR	H5C_b	- C5C_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	25	
cR	H5D_b	- C5D_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	25	
cR	H5E_b	- C5E_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	21	
cR	H5F_b	- C5F_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	21	
cR	H6A_b	- C6A_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	13	
cR	H6B_b	- C6B_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	14	
cR	H6C_b	- C6C_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	35	
cR	H6D_b	- C6D_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	35	
cR	H6E_b	- C6E_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	31	
cR	H6F_b	- C6F_b	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	31	
d	Cu1_c	- O1_c	O11A_c	O11B_c	N1C_c	N1D_c	-----	-----	-----	-----	10	87	178	107.9	1.964	2.275	5	277	
d	Cu2_c	- O2_c	O21A_c	N1E_c	N1F_c	-----	-----	-----	-----	-----	6	87	168	105.1	1.976	2.295	4	273	
d	O1_c	- Cu1_c	H1_c	H2_c	-----	-----	-----	-----	-----	-----	3	104	118	111.2	0.789	2.275	3	263	
d	O2_c	- Cu2_c	H3_c	H4_c	-----	-----	-----	-----	-----	-----	3	90	126	108.3	0.807	2.295	3	247	
d	O11A_c	- Cu1_c	C11A_c	-----	-----	-----	-----	-----	-----	-----	1	121	121	121.1	1.267	1.964	2	264	
d	O11B_c	- Cu1_c	C11B_c	-----	-----	-----	-----	-----	-----	-----	1	126	126	125.9	1.277	1.969	2	265	
d	O12A_c	- C11A_c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.242	1.242	1	234	
d	O12B_c	- C11B_c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.239	1.239	1	236	
d	O21A_c	- Cu2_c	C21A_c	-----	-----	-----	-----	-----	-----	-----	1	122	122	121.6	1.265	1.976	2	248	
d	O21B_c	- C21B_c	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.270	1.270	1	210	

d	022A_c	- C21A_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.248	1.248	1	214	
d	022B_c	- C21B_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	1.248	1.248	1	210	
d	N1C_c	- Cu1_c	C2C_c	C6C_c	-----	-----	-----	-----	-----	3	118	124	120.0	1.344	2.013	3	201	
d	N1D_c	- Cu1_c	C2D_c	C6D_c	-----	-----	-----	-----	-----	3	118	122	119.8	1.341	2.014	3	201	
d	N1E_c	- Cu2_c	C2E_c	C6E_c	-----	-----	-----	-----	-----	3	118	121	119.9	1.340	1.989	3	195	
d	N1F_c	- Cu2_c	C2F_c	C6F_c	-----	-----	-----	-----	-----	3	118	122	119.9	1.338	2.005	3	195	
d	C1A_c	- C2A_c	C6A_c	C11A_c	-----	-----	-----	-----	-----	3	118	123	120.0	1.392	1.514	3	138	
d	C1B_c	- C2B_c	C6B_c	C11B_c	-----	-----	-----	-----	-----	3	119	121	120.0	1.395	1.514	3	139	
d	C2A_c	- C1A_c	C21A_c	-----	-----	-----	-----	-----	-----	1	125	125	125.0	1.400	1.512	2	128	?
d	C2B_c	- C6B	C1B_c	C21B_c	-----	-----	-----	-----	-----	3	116	124	120.0	1.391	1.509	3	126	
d	C2C_c	- N1C_c	C3C_c	H2C_c	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.382	3	149	
d	C2D_c	- N1D_c	C3D_c	H2D_c	-----	-----	-----	-----	-----	3	119	123	120.0	0.949	1.378	3	149	
d	C2E_c	- N1E_c	C3E_c	H2E_c	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.378	3	145	
d	C2F_c	- N1F_c	C3F_c	H2F_c	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.382	3	145	
d	C3C_c	- C2C_c	C4C_c	H3C_c	-----	-----	-----	-----	-----	3	119	120	120.0	0.950	1.382	3	119	
d	C3D_c	- C2D_c	C4D_c	H3D_c	-----	-----	-----	-----	-----	3	119	121	120.0	0.949	1.384	3	119	
d	C3E_c	- C2E_c	C4E_c	H3E_c	-----	-----	-----	-----	-----	3	119	120	120.0	0.951	1.388	3	107	
d	C3F_c	- C2F_c	C4F_c	H3F_c	-----	-----	-----	-----	-----	3	119	120	120.0	0.949	1.382	3	107	
d	C4C_c	- C3C_c	C5C_c	H4C_c	-----	-----	-----	-----	-----	3	119	121	120.0	0.949	1.381	3	77	
d	C4D_c	- C3D_c	C5D_c	H4D_c	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.384	3	77	
d	C4E_c	- C3E_c	C5E_c	H4E_c	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.388	3	69	
d	C4F_c	- C3F_c	C5F_c	H4F_c	-----	-----	-----	-----	-----	3	119	121	120.0	0.949	1.379	3	69	
d	C5C_c	- C4C_c	C6C_c	H5C_c	-----	-----	-----	-----	-----	3	120	120	120.0	0.950	1.381	3	119	
d	C5D_c	- C4D_c	C6D_c	H5D_c	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.382	3	119	
d	C5E_c	- C4E_c	C6E_c	H5E_c	-----	-----	-----	-----	-----	3	119	120	120.0	0.950	1.382	3	107	
d	C5F_c	- C4F_c	C6F_c	H5F_c	-----	-----	-----	-----	-----	3	119	121	120.0	0.950	1.379	3	107	
d	C6A_c	- C1A_c	H6A_c	-----	-----	-----	-----	-----	-----	1	119	119	118.9	0.950	1.392	2	92	?
d	C6B_c	- C2B	C1B_c	H6B_c	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.395	3	97	
d	C6C_c	- N1C_c	C5C_c	H6C_c	-----	-----	-----	-----	-----	3	119	122	120.0	0.950	1.379	3	149	
d	C6D_c	- N1D_c	C5D_c	H6D_c	-----	-----	-----	-----	-----	3	119	123	120.0	0.951	1.380	3	149	
d	C6E_c	- N1E_c	C5E_c	H6E_c	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.375	3	145	
d	C6F_c	- N1F_c	C5F_c	H6F_c	-----	-----	-----	-----	-----	3	119	123	120.0	0.950	1.377	3	145	
d	C11A_c	- 011A_c	012A_c	C1A_c	-----	-----	-----	-----	-----	3	116	126	120.0	1.242	1.514	3	184	
d	C11B_c	- 011B_c	012B_c	C1B_c	-----	-----	-----	-----	-----	3	115	126	120.0	1.239	1.514	3	185	
d	C21A_c	- 021A_c	022A_c	C2A_c	-----	-----	-----	-----	-----	3	116	127	119.9	1.248	1.512	3	178	
d	C21B_c	- 021B_c	022B_c	C2B_c	-----	-----	-----	-----	-----	3	115	126	119.9	1.248	1.509	3	159	
d	H1_c	- 01_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.789	0.789	1	47	
d	H2_c	- 01_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.819	0.819	1	47	
cR	H2C_c	- C2C_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	38	
cR	H2D_c	- C2D_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	38	
cR	H2E_c	- C2E_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	32	
cR	H2F_c	- C2F_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	32	
d	H3_c	- 02_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.829	0.829	1	43	
cR	H3C_c	- C3C_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	26	
cR	H3D_c	- C3D_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	26	
cR	H3E_c	- C3E_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	22	
cR	H3F_c	- C3F_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	22	

d	H4_c	-	O2_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.807	0.807	1	43
cR	H4C_c	-	C4C_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	8
cR	H4D_c	-	C4D_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	8
cR	H4E_c	-	C4E_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	2
cR	H4F_c	-	C4F_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.949	0.949	1	2
cR	H5C_c	-	C5C_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	26
cR	H5D_c	-	C5D_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	26
cR	H5E_c	-	C5E_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	22
cR	H5F_c	-	C5F_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	22
cR	H6A_c	-	C6A_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	15
cR	H6B_c	-	C6B_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	16
cR	H6C_c	-	C6C_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	38
cR	H6D_c	-	C6D_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.951	0.951	1	38
cR	H6E_c	-	C6E_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	32
cR	H6F_c	-	C6F_c	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.950	0.950	1	32
d	Cu1_d	-	O1_d	O11A_d	O11B_d	N1C_d	N1D_d	-----	-----	-----	-10	87	178	107.9	1.964	2.275	5	278
d	Cu2_d	-	O2_d	O21A_d	N1E_d	N1F_d	-----	-----	-----	-----	-6	87	168	105.1	1.976	2.295	4	274
d	O1_d	-	Cu1_d	H1_d	H2_d	-----	-----	-----	-----	-----	-3	104	118	111.2	0.789	2.275	3	266
d	O2_d	-	Cu2_d	H3_d	H4_d	-----	-----	-----	-----	-----	-3	90	126	108.3	0.807	2.295	3	249
d	O11A_d	-	Cu1_d	C11A_d	-----	-----	-----	-----	-----	-----	-1	121	121	121.1	1.267	1.964	2	268
d	O11B_d	-	Cu1_d	C11B_d	-----	-----	-----	-----	-----	-----	-1	126	126	125.9	1.277	1.969	2	267
d	O12A_d	-	C11A_d	-----	-----	-----	-----	-----	-----	-----	-0	0	0	0.0	1.242	1.242	1	240
d	O12B_d	-	C11B_d	-----	-----	-----	-----	-----	-----	-----	-0	0	0	0.0	1.239	1.239	1	238
d	O21A_d	-	Cu2_d	C21A_d	-----	-----	-----	-----	-----	-----	-1	122	122	121.6	1.265	1.976	2	250
d	O21B_d	-	C21B_d	-----	-----	-----	-----	-----	-----	-----	-0	0	0	0.0	1.270	1.270	1	208
d	O22A_d	-	C21A_d	-----	-----	-----	-----	-----	-----	-----	-0	0	0	0.0	1.248	1.248	1	216
d	O22B_d	-	C21B_d	-----	-----	-----	-----	-----	-----	-----	-0	0	0	0.0	1.248	1.248	1	208
d	N1C_d	-	Cu1_d	C2C_d	C6C_d	-----	-----	-----	-----	-----	-3	118	124	120.0	1.344	2.013	3	202
d	N1D_d	-	Cu1_d	C2D_d	C6D_d	-----	-----	-----	-----	-----	-3	118	122	119.8	1.341	2.014	3	202
d	N1E_d	-	Cu2_d	C2E_d	C6E_d	-----	-----	-----	-----	-----	-3	118	121	119.9	1.340	1.989	3	196
d	N1F_d	-	Cu2_d	C2F_d	C6F_d	-----	-----	-----	-----	-----	-3	118	122	119.9	1.338	2.005	3	196
d	C1A_d	-	C2A_d	C6A_d	C11A_d	-----	-----	-----	-----	-----	-3	118	123	120.0	1.392	1.514	3	141
d	C1B_d	-	C2B_d	C6B_d	C11B_d	-----	-----	-----	-----	-----	-3	119	121	120.0	1.395	1.514	3	140
d	C2A_d	-	C6A	C1A_d	C21A_d	-----	-----	-----	-----	-----	-3	116	125	120.0	1.391	1.512	3	129
d	C2B_d	-	C1B_d	C21B_d	-----	-----	-----	-----	-----	-----	-1	124	124	124.3	1.401	1.509	2	125
d	C2C_d	-	N1C_d	C3C_d	H2C_d	-----	-----	-----	-----	-----	-3	119	123	120.0	0.950	1.382	3	150
d	C2D_d	-	N1D_d	C3D_d	H2D_d	-----	-----	-----	-----	-----	-3	119	123	120.0	0.949	1.378	3	150
d	C2E_d	-	N1E_d	C3E_d	H2E_d	-----	-----	-----	-----	-----	-3	119	122	120.0	0.950	1.378	3	146
d	C2F_d	-	N1F_d	C3F_d	H2F_d	-----	-----	-----	-----	-----	-3	119	122	120.0	0.950	1.382	3	146
d	C3C_d	-	C2C_d	C4C_d	H3C_d	-----	-----	-----	-----	-----	-3	119	120	120.0	0.950	1.382	3	121
d	C3D_d	-	C2D_d	C4D_d	H3D_d	-----	-----	-----	-----	-----	-3	119	121	120.0	0.949	1.384	3	121
d	C3E_d	-	C2E_d	C4E_d	H3E_d	-----	-----	-----	-----	-----	-3	119	120	120.0	0.951	1.388	3	109
d	C3F_d	-	C2F_d	C4F_d	H3F_d	-----	-----	-----	-----	-----	-3	119	120	120.0	0.949	1.382	3	109
d	C4C_d	-	C3C_d	C5C_d	H4C_d	-----	-----	-----	-----	-----	-3	119	121	120.0	0.949	1.381	3	79
d	C4D_d	-	C3D_d	C5D_d	H4D_d	-----	-----	-----	-----	-----	-3	119	121	120.0	0.950	1.384	3	79
d	C4E_d	-	C3E_d	C5E_d	H4E_d	-----	-----	-----	-----	-----	-3	119	121	120.0	0.950	1.388	3	71
d	C4F_d	-	C3F_d	C5F_d	H4F_d	-----	-----	-----	-----	-----	-3	119	121	120.0	0.949	1.379	3	71

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d	C5C_d	- C4C_d	C6C_d	H5C_d	-----	-----	-----	-----	-----	-----	3	120	120	120.0	0.950	1.381	3	121																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										

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*****
Residue = 2 *****
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Flag Label - Connected to (May be Incomplete for Polymeric Structures)										=A.N.G.L.E.S=				=B.O.N.D.S=				Hyb RS Note		
										nra	min	max	Aver	min	max	nrb	tnr			
d	O1W	- H1W1	H2W1	-----	-----	-----	-----	-----	-----	1	106	106	106.3	0.784	0.867	2	204	sp3		
d	H1W1	- O1W	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.784	0.784	1	41			
d	H2W1	- O1W	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.867	0.867	1	41			

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*****
Residue = 3 *****
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Flag Label - Connected to (May be Incomplete for Polymeric Structures)											=A.N.G.L.E.S=				=B.O.N.D.S=				Hyb RS Note		
											nra	min	max	Aver	min	max	nrb	tnr			
d	O2W	- H1W2	H2W2	-----	-----	-----	-----	-----	-----	-----	1	106	106	105.8	0.759	0.809	2	204	sp3		
d	H1W2	- O2W	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.759	0.759	1	41			
d	H2W2	- O2W	-----	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.809	0.809	1	41			


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Residue = 4 *****
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Flag Label - Connected to (May be Incomplete for Polymeric Structures)										=A.N.G.L.E.S=				=B.O.N.D.S=				Hyb RS Note		
										nra	min	max	Aver	min	max	nrb	tnr			
d	03W	- H1W3	H2W3	-----	-----	-----	-----	-----	-----	1	105	105	105.3	0.759	0.798	2	204	sp3		
d	H1W3	- 03W	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.759	0.759	1	41			
d	H2W3	- 03W	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.798	0.798	1	41			

 =====
 ***** Residue = 5 *****
 =====

										=A.N.G.L.E.S=				=B.O.N.D.S=							
Flag	Label	- Connected to (May be Incomplete for Polymeric Structures)								nra	min	max	Aver	min	max	nrb	tnr	Hyb	RS	Note	

d	O4W	-	H1W4	H2W4	-----	-----	-----	-----	-----	-----	1	102	102	101.9	0.788	0.843	2	204	sp3		
d	H1W4	-	O4W	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.788	0.788	1	41			
d	H2W4	-	O4W	-----	-----	-----	-----	-----	-----	-----	0	0	0	0.0	0.843	0.843	1	41			

Asymmetric Residue Unit (= ARU) Code List

=====														
ARU-CODE		Symmetry-Code		sym TX TY TZ Ires				x(cen)	y(cen)	z(cen)				
a	= [1465.01]	=	-1+x, 1+y, z	=	[	1	-1	1	0	1	]	-0.359	1.370	0.073
b	= [1645.01]	=	1+x, -1+y, z	=	[	1	1	-1	0	1	]	1.641	-0.630	0.073
c	= [2665.01]	=	1-x, 1-y, -z	=	[	2	1	1	0	1	]	0.359	0.630	-0.073
d	= [2756.01]	=	2-x, -y, 1-z	=	[	2	2	0	1	1	]	1.359	-0.370	0.927

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,

SYM - Number of the Symmetry Operator.
 Ires - Residue Number.
 TX, TY, TZ - Unit Cell Translations.

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Analysis of the IntraMolecular Geometry in Terms of Unique Molecule(s)/Ions, with Bond Criterium: d(i-j) < R(i) + R(j) + Tol

-- Tol = 0.40 Ang. for Normal Bonds + 0.70 for (Earth)alkali-NonMetal Contacts and adjusted by -.40 Ang. for Metal-Metal Distances

-- The Bond Distance and Angle su's have been Incremented to Include the Effect of the Unit-cell su.
(Rel.Error in Dist. 0.0002 Ang. , Abs. Angle Error 0.030 Deg.)

-- Bonds below with '>' or '<' Substituted for '-' have Distances that Deviate from Expected Values(Based on the hybridisations).

***** Residue = 1 *****

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Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

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Cu1 - O1	2.2745(16)	Cu1 - O11A	1.9637(13)	Cu1 - O11B	1.9690(14)	Cu1 - N1C	2.0135(17)
Cu1 - N1D	2.0144(17)	Cu2 - O2	2.2948(16)	Cu2 - O21A	1.9757(14)	Cu2 - N1E	1.9895(16)
Cu2 - N1F	2.0052(17)	Cu2 - O21B_b	1.9677(14)	O11A - C11A	1.267(2)	O11B - C11B	1.277(2)
O12A - C11A	1.242(2)	O12B - C11B	1.239(2)	O21A - C21A	1.265(2)	O21B - C21B	1.270(2)
O22A - C21A	1.248(2)	O22B - C21B	1.248(2)	N1C - C2C	1.344(2)	N1C - C6C	1.351(3)
N1D - C2D	1.346(3)	N1D - C6D	1.341(2)	N1E - C2E	1.340(3)	N1E - C6E	1.349(2)
N1F - C2F	1.341(3)	N1F - C6F	1.338(3)	C1A - C2A	1.401(3)	C1A - C6A	1.392(2)
C1A > C11A	1.514(3)	C1B - C2B	1.401(3)	C1B - C6B	1.395(3)	C1B > C11B	1.514(2)
C2A > C21A	1.512(3)	C2A - C6A_d	1.391(3)	C2B > C21B	1.509(2)	C2B - C6B_c	1.391(2)
C2C - C3C	1.382(3)	C2D - C3D	1.378(3)	C2E - C3E	1.378(3)	C2F - C3F	1.382(3)
C3C - C4C	1.380(3)	C3D - C4D	1.384(3)	C3E - C4E	1.388(3)	C3F - C4F	1.376(4)
C4C - C5C	1.381(3)	C4D - C5D	1.382(3)	C4E - C5E	1.382(3)	C4F - C5F	1.379(4)
C5C - C6C	1.379(3)	C5D - C6D	1.380(3)	C5E - C6E	1.375(3)	C5F - C6F	1.377(3)
O1 - H1	0.79(3)	O1 - H2	0.82(3)	O2 - H3	0.83(2)	O2 - H4	0.81(2)
C2C - H2C	0.95	C2D - H2D	0.95	C2E - H2E	0.95	C2F - H2F	0.95
C3C - H3C	0.95	C3D - H3D	0.95	C3E - H3E	0.95	C3F - H3F	0.95
C4C - H4C	0.95	C4D - H4D	0.95	C4E - H4E	0.95	C4F - H4F	0.95
C5C - H5C	0.95	C5D - H5D	0.95	C5E - H5E	0.95	C5F - H5F	0.95
C6A - H6A	0.95	C6B - H6B	0.95	C6C - H6C	0.95	C6D - H6D	0.95
C6E - H6E	0.95	C6F - H6F	0.95				

Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().

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O1 - Cu1 - O11A	92.07(6)	O1 - Cu1 - O11B	89.82(6)	O1 - Cu1 - N1C	92.00(7)
O1 - Cu1 - N1D	97.00(7)	O11A - Cu1 - O11B	177.78(6)	O11A - Cu1 - N1C	88.18(7)
O11A - Cu1 - N1D	91.33(7)	O11B - Cu1 - N1C	92.93(7)	O11B - Cu1 - N1D	87.27(7)
N1C - Cu1 - N1D	171.00(7)	O2 - Cu2 - O21A	92.84(6)	O2 - Cu2 - N1E	89.48(7)
O2 - Cu2 - N1F	102.22(7)	O2 - Cu2 - O21B_b	90.75(6)	O21A - Cu2 - N1E	90.67(7)
O21A - Cu2 - N1F	87.18(7)	O21A - Cu2 - O21B_b	175.41(6)	N1E - Cu2 - N1F	168.18(7)
N1E - Cu2 - O21B_b	92.22(7)	N1F - Cu2 - O21B_b	89.27(7)	Cu1 - O11A - C11A	121.10(12)
Cu1 - O11B - C11B	125.93(12)	Cu2 - O21A - C21A	121.58(12)	C21B - O21B - Cu2_a	122.31(12)
Cu1 - N1C - C2C	118.28(13)	Cu1 - N1C - C6C	123.62(13)	C2C - N1C - C6C	118.09(17)
Cu1 - N1D - C2D	122.38(13)	Cu1 - N1D - C6D	119.48(13)	C2D - N1D - C6D	117.68(17)

Cu2	-	N1E	-	C2E	121.30(13)	Cu2	-	N1E	-	C6E	120.20(13)	C2E	-	N1E	-	C6E	118.16(17)
Cu2	-	N1F	-	C2F	119.68(14)	Cu2	-	N1F	-	C6F	121.98(14)	C2F	-	N1F	-	C6F	118.16(17)
C2A	-	C1A	-	C6A	119.11(16)	C2A	-	C1A	-	C11A	122.77(16)	C6A	-	C1A	-	C11A	118.06(16)
C2B	-	C1B	-	C6B	118.70(16)	C2B	-	C1B	-	C11B	121.44(16)	C6B	-	C1B	-	C11B	119.84(16)
C1A	-	C2A	-	C21A	124.98(16)	C1A	-	C2A	-	C6A_d	118.79(16)	C21A	-	C2A	-	C6A_d	116.22(16)
C1B	-	C2B	-	C21B	124.27(16)	C1B	-	C2B	-	C6B_c	119.38(16)	C21B	-	C2B	-	C6B_c	116.34(16)
N1C	-	C2C	-	C3C	122.61(17)	N1D	-	C2D	-	C3D	122.94(19)	N1E	-	C2E	-	C3E	122.38(19)
N1F	-	C2F	-	C3F	122.3(2)	C2C	-	C3C	-	C4C	119.11(18)	C2D	-	C3D	-	C4D	118.65(19)
C2E	-	C3E	-	C4E	119.24(19)	C2F	-	C3F	-	C4F	119.1(2)	C3C	-	C4C	-	C5C	118.51(18)
C3D	-	C4D	-	C5D	119.02(19)	C3E	-	C4E	-	C5E	118.5(2)	C3F	-	C4F	-	C5F	118.9(2)
C4C	-	C5C	-	C6C	119.79(19)	C4D	-	C5D	-	C6D	118.87(19)	C4E	-	C5E	-	C6E	119.2(2)
C4F	-	C5F	-	C6F	118.9(2)	C1A	-	C6A	-	C2A_d	122.10(17)	C1B	-	C6B	-	C2B_c	121.92(17)
N1C	-	C6C	-	C5C	121.87(19)	N1D	-	C6D	-	C5D	122.80(18)	N1E	-	C6E	-	C5E	122.54(19)
N1F	-	C6F	-	C5F	122.66(19)	O11A	-	C11A	-	O12A	126.10(17)	O11A	-	C11A	-	C1A	115.60(16)
O12A	-	C11A	-	C1A	118.29(16)	O11B	-	C11B	-	O12B	126.42(17)	O11B	-	C11B	-	C1B	115.21(15)
O12B	-	C11B	-	C1B	118.37(17)	O21A	-	C21A	-	O22A	126.57(17)	O21A	-	C21A	-	C2A	116.03(16)
O22A	-	C21A	-	C2A	117.10(16)	O21B	-	C21B	-	O22B	126.37(17)	O21B	-	C21B	-	C2B	115.45(16)
O22B	-	C21B	-	C2B	117.83(16)												
Cu1	-	O1	-	H1	118.1(18)	Cu1	-	O1	-	H2	111.8(16)	H1	-	O1	-	H2	104(2)
Cu2	-	O2	-	H3	126.5(18)	Cu2	-	O2	-	H4	90.1(19)	H3	-	O2	-	H4	108(2)
N1C	-	C2C	-	H2C	119	C3C	-	C2C	-	H2C	119	N1D	-	C2D	-	H2D	119
C3D	-	C2D	-	H2D	119	N1E	-	C2E	-	H2E	119	C3E	-	C2E	-	H2E	119
N1F	-	C2F	-	H2F	119	C3F	-	C2F	-	H2F	119	C2C	-	C3C	-	H3C	120
C4C	-	C3C	-	H3C	120	C2D	-	C3D	-	H3D	121	C4D	-	C3D	-	H3D	121
C2E	-	C3E	-	H3E	120	C4E	-	C3E	-	H3E	120	C2F	-	C3F	-	H3F	120
C4F	-	C3F	-	H3F	120	C3C	-	C4C	-	H4C	121	C5C	-	C4C	-	H4C	121
C3D	-	C4D	-	H4D	120	C5D	-	C4D	-	H4D	121	C3E	-	C4E	-	H4E	121
C5E	-	C4E	-	H4E	121	C3F	-	C4F	-	H4F	121	C5F	-	C4F	-	H4F	121
C4C	-	C5C	-	H5C	120	C6C	-	C5C	-	H5C	120	C4D	-	C5D	-	H5D	121
C6D	-	C5D	-	H5D	121	C4E	-	C5E	-	H5E	120	C6E	-	C5E	-	H5E	120
C4F	-	C5F	-	H5F	121	C6F	-	C5F	-	H5F	121	C1A	-	C6A	-	H6A	119
H6A	-	C6A	-	C2A_d	119	C1B	-	C6B	-	H6B	119	H6B	-	C6B	-	C2B_c	119
N1C	-	C6C	-	H6C	119	C5C	-	C6C	-	H6C	119	N1D	-	C6D	-	H6D	119
C5D	-	C6D	-	H6D	119	N1E	-	C6E	-	H6E	119	C5E	-	C6E	-	H6E	119
N1F	-	C6F	-	H6F	119	C5F	-	C6F	-	H6F	119						

Torsion/Dihedral Angles (Deg.) - Klyne & Prelog Convention (Dunitz, p241) - (Excl. Minor Disorder & Embedded Bond Angl. > 160. Deg.)

O1	Cu1	O11A	C11A	-163.98(14)	N1C	Cu1	O11A	C11A	-72.04(14)	N1D	Cu1	O11A	C11A	98.97(14)
O1	Cu1	O11B	C11B	-177.74(15)	N1C	Cu1	O11B	C11B	90.27(15)	N1D	Cu1	O11B	C11B	-80.72(15)
O1	Cu1	N1C	C2C	52.12(14)	O1	Cu1	N1C	C6C	-126.55(16)	O11A	Cu1	N1C	C2C	-39.89(14)
O11A	Cu1	N1C	C6C	141.45(16)	O11B	Cu1	N1C	C2C	142.04(14)	O11B	Cu1	N1C	C6C	-36.62(16)
O1	Cu1	N1D	C2D	-140.65(16)	O1	Cu1	N1D	C6D	47.30(16)	O11A	Cu1	N1D	C2D	-48.40(16)
O11A	Cu1	N1D	C6D	139.54(16)	O11B	Cu1	N1D	C2D	129.87(16)	O11B	Cu1	N1D	C6D	-42.19(16)
O2	Cu2	O21A	C21A	40.33(14)	N1E	Cu2	O21A	C21A	129.85(14)	N1F	Cu2	O21A	C21A	-61.78(14)
O2	Cu2	N1E	C2E	135.63(15)	O2	Cu2	N1E	C6E	-51.31(15)	O21A	Cu2	N1E	C2E	42.80(15)
O21A	Cu2	N1E	C6E	-144.14(15)	O21B_b	Cu2	N1E	C2E	-133.64(15)	O21B_b	Cu2	N1E	C6E	39.43(15)

O2	Cu2	N1F	C2F	-152.68(15)	O2	Cu2	N1F	C6F	22.33(16)	O21A	Cu2	N1F	C2F	-60.39(15)
O21A	Cu2	N1F	C6F	114.62(16)	O21B_b	Cu2	N1F	C2F	116.70(15)	O21B_b	Cu2	N1F	C6F	-68.28(16)
O2	Cu2	O21B_b	C21B_b	154.51(14)	N1E	Cu2	O21B_b	C21B_b	64.99(14)	N1F	Cu2	O21B_b	C21B_b	-103.28(14)
Cu1	O11A	C11A	O12A	-23.4(3)	Cu1	O11A	C11A	C1A	155.15(12)	Cu1	O11B	C11B	O12B	-27.5(3)
Cu1	O11B	C11B	C1B	152.67(12)	Cu2	O21A	C21A	O22A	-13.2(3)	Cu2	O21A	C21A	C2A	160.18(12)
Cu2_a	O21B	C21B	O22B	0.2(2)	Cu2_a	O21B	C21B	C2B	-172.80(11)	C6A	C1A	C2A	C21A	-178.55(17)
C6A	C1A	C2A	C6A_d	0.0(3)	C11A	C1A	C2A	C21A	4.2(3)	C11A	C1A	C2A	C6A_d	-177.20(17)
C2A	C1A	C6A	C2A_d	0.0(3)	C11A	C1A	C6A	C2A_d	177.33(17)	C2A	C1A	C11A	O11A	4.6(3)
C2A	C1A	C11A	O12A	-176.73(18)	C6A	C1A	C11A	O11A	-172.61(17)	C6A	C1A	C11A	O12A	6.0(3)
C6B	C1B	C2B	C21B	-178.06(17)	C6B	C1B	C2B	C6B_c	0.5(3)	C11B	C1B	C2B	C21B	0.2(3)
C11B	C1B	C2B	C6B_c	178.76(17)	C2B	C1B	C6B	C2B_c	-0.5(3)	C11B	C1B	C6B	C2B_c	-178.80(17)
C2B	C1B	C11B	O11B	179.48(17)	C2B	C1B	C11B	O12B	-0.4(3)	C6B	C1B	C11B	O11B	-2.3(3)
C6B	C1B	C11B	O12B	177.82(18)	C1A	C2A	C21A	O21A	84.7(2)	C1A	C2A	C21A	O22A	-101.2(2)
C6A_d	C2A	C21A	O21A	-93.9(2)	C6A_d	C2A	C21A	O22A	80.2(2)	C1A	C2A	C6A_d	C1A_d	0.0(3)
C21A	C2A	C6A_d	C1A_d	178.68(17)	C1B	C2B	C21B	O21B	-97.7(2)	C1B	C2B	C21B	O22B	88.7(2)
C6B_c	C2B	C21B	O21B	83.7(2)	C6B_c	C2B	C21B	O22B	-89.9(2)	C1B	C2B	C6B_c	C1B_c	-0.5(3)
C21B	C2B	C6B_c	C1B_c	178.16(17)	C3C	C2C	N1C	Cu1	-179.08(14)	C3C	C2C	N1C	C6C	-0.3(3)
N1C	C2C	C3C	C4C	-1.1(3)	C3D	C2D	N1D	Cu1	-170.36(16)	C3D	C2D	N1D	C6D	1.8(3)
N1D	C2D	C3D	C4D	-0.6(3)	C3E	C2E	N1E	Cu2	171.58(15)	C3E	C2E	N1E	C6E	-1.6(3)
N1E	C2E	C3E	C4E	0.8(3)	C3F	C2F	N1F	Cu2	174.97(17)	C3F	C2F	N1F	C6F	-0.2(3)
N1F	C2F	C3F	C4F	-0.3(3)	C2C	C3C	C4C	C5C	2.0(3)	C2D	C3D	C4D	C5D	-1.1(3)
C2E	C3E	C4E	C5E	0.6(3)	C2F	C3F	C4F	C5F	0.1(4)	C3C	C4C	C5C	C6C	-1.5(3)
C3D	C4D	C5D	C6D	1.4(3)	C3E	C4E	C5E	C6E	-1.1(3)	C3F	C4F	C5F	C6F	0.6(3)
C4C	C5C	C6C	N1C	0.1(3)	C4D	C5D	C6D	N1D	-0.1(3)	C4E	C5E	C6E	N1E	0.3(3)
C4F	C5F	C6F	N1F	-1.3(3)	C5C	C6C	N1C	Cu1	179.50(15)	C5C	C6C	N1C	C2C	0.8(3)
C5D	C6D	N1D	Cu1	170.93(16)	C5D	C6D	N1D	C2D	-1.5(3)	C5E	C6E	N1E	Cu2	-172.19(17)
C5E	C6E	N1E	C2E	1.1(3)	C5F	C6F	N1F	Cu2	-174.05(17)	C5F	C6F	N1F	C2F	1.0(3)
O11A	Cu1	O1	H1	-29(2)	O11A	Cu1	O1	H2	91.6(19)	O11B	Cu1	O1	H1	150(2)
O11B	Cu1	O1	H2	-89.6(19)	N1C	Cu1	O1	H1	-117(2)	N1C	Cu1	O1	H2	3.4(19)
N1D	Cu1	O1	H1	63(2)	N1D	Cu1	O1	H2	-176.8(19)	O21A	Cu2	O2	H3	-148(2)
O21A	Cu2	O2	H4	-35.2(16)	N1E	Cu2	O2	H3	121(2)	N1E	Cu2	O2	H4	-125.9(16)
N1F	Cu2	O2	H3	-61(2)	N1F	Cu2	O2	H4	52.5(16)	O21B_b	Cu2	O2	H3	29(2)
O21B_b	Cu2	O2	H4	141.9(16)	C2A	C1A	C6A	H6A	180	C11A	C1A	C6A	H6A	-3
C2B	C1B	C6B	H6B	179	C11B	C1B	C6B	H6B	1	C1A	C2A	C6A_d	H6A_d	180
C21A	C2A	C6A_d	H6A_d	-1	C1B	C2B	C6B_c	H6B_c	179	C21B	C2B	C6B_c	H6B_c	-2
H2C	C2C	N1C	Cu1	1	H2C	C2C	N1C	C6C	180	N1C	C2C	C3C	H3C	179
H2C	C2C	C3C	C4C	179	H2C	C2C	C3C	H3C	-1	H2D	C2D	N1D	Cu1	10
H2D	C2D	N1D	C6D	-178	N1D	C2D	C3D	H3D	179	H2D	C2D	C3D	C4D	179
H2D	C2D	C3D	H3D	-1	H2E	C2E	N1E	Cu2	-8	H2E	C2E	N1E	C6E	178
N1E	C2E	C3E	H3E	-179	H2E	C2E	C3E	C4E	-179	H2E	C2E	C3E	H3E	1
H2F	C2F	N1F	Cu2	-5	H2F	C2F	N1F	C6F	180	N1F	C2F	C3F	H3F	180
H2F	C2F	C3F	C4F	180	H2F	C2F	C3F	H3F	0	C2C	C3C	C4C	H4C	-178
H3C	C3C	C4C	C5C	-178	H3C	C3C	C4C	H4C	2	C2D	C3D	C4D	H4D	179
H3D	C3D	C4D	C5D	179	H3D	C3D	C4D	H4D	-1	C2E	C3E	C4E	H4E	-179
H3E	C3E	C4E	C5E	-179	H3E	C3E	C4E	H4E	1	C2F	C3F	C4F	H4F	-180
H3F	C3F	C4F	C5F	-180	H3F	C3F	C4F	H4F	0	C3C	C4C	C5C	H5C	178
H4C	C4C	C5C	C6C	178	H4C	C4C	C5C	H5C	-2	C3D	C4D	C5D	H5D	-179

H4D	C4D	C5D	C6D	-179	H4D	C4D	C5D	H5D	1	C3E	C4E	C5E	H5E	179
H4E	C4E	C5E	C6E	179	H4E	C4E	C5E	H5E	-1	C3F	C4F	C5F	H5F	-180
H4F	C4F	C5F	C6F	-179	H4F	C4F	C5F	H5F	0	C4C	C5C	C6C	H6C	-180
H5C	C5C	C6C	N1C	-180	H5C	C5C	C6C	H6C	0	C4D	C5D	C6D	H6D	180
H5D	C5D	C6D	N1D	180	H5D	C5D	C6D	H6D	0	C4E	C5E	C6E	H6E	-180
H5E	C5E	C6E	N1E	-180	H5E	C5E	C6E	H6E	0	C4F	C5F	C6F	H6F	179
H5F	C5F	C6F	N1F	179	H5F	C5F	C6F	H6F	-1	H6C	C6C	N1C	Cu1	0
H6C	C6C	N1C	C2C	-179	H6D	C6D	N1D	Cu1	-9	H6D	C6D	N1D	C2D	178
H6E	C6E	N1E	Cu2	8	H6E	C6E	N1E	C2E	-179	H6F	C6F	N1F	Cu2	6
H6F	C6F	N1F	C2F	-179										

 =====
 ***** Residue = 2 *****
 =====

Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

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O1W	-	H1W1	0.78(2)	O1W	-	H2W1	0.87(3)

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Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().

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H1W1	-	O1W	-	H2W1	106(2)

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 =====
 ***** Residue = 3 *****
 =====

Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

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O2W	-	H1W2	0.76(3)	O2W	-	H2W2	0.81(2)

=====

Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().

=====

H1W2	-	O2W	-	H2W2	106(3)

=====

 =====
 ***** Residue = 4 *****
 =====

Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

=====

```
=====
03W   -  H1W3       0.76(2)   03W   -  H2W3       0.80(3)
=====
```

Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().

```
=====
H1W3   -  03W   -  H2W3       105(3)
=====
```

```
=====
***** Residue = 5 *****
=====
```

Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

```
=====
04W   -  H1W4       0.79(3)   04W   -  H2W4       0.84(2)
=====
```

Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().

```
=====
H1W4   -  04W   -  H2W4       102(2)
=====
```

[illegible]

Selected Bond Lengths (Angstrom) - see M.F.C. Ladd & R.A. Palmer, Structure Determination by X-Ray Crystallography (1985)

Formal single bonds

C4-C4	1.54	C4-C3	1.52	C4-C2	1.46	C4-N3	1.47	C4-N2	1.47	C4-O2	1.43	C3-C3	1.46	C3-C2	1.45	C3-N3	1.40	C3-N2	1.40
C3-O2	1.36	C2-C2	1.38	C2-N3	1.33	C2-N2	1.33	C2-O2	1.36	N3-N3	1.45	N3-N2	1.45	N3-O2	1.36	N2-N2	1.45	N2-O2	1.41

Formal double bonds

C3-C3 1.34 C3-C2 1.31 C3-N2 1.32 C3-O1 1.22 C2-C2 1.28 C2-N2 1.32 C2-O1 1.16 N3-O1 1.24 N2-N2 1.25 N2-O1 1.21

Formal triple bonds

Aromatic bonds

C2-C2 1.20 C2-N1 1.16 C3-C3 1.40 C2-N2 1.34 N2-N2 1.35

The notation in the table indicates the connectivity of the atoms

For more detailed standard bond distance tabulations see: J. Chem. Soc. Perkin II, (1987), S1-S19; J. Chem. Soc. Dalton Trans. (1989), S1 - S83 or International Tables C, (1992), 707-791.

Automatic Search for Rings (3 to 6-Membered) and Planes Determined by 4 or More Connected Atoms (with Deviation < 0.10 Ang.)

Least-Squares Planes - $P \cdot X + Q \cdot Y + R \cdot Z = S$:: First Line Orthogonal(X0,Y0,Z0), Second Line Fractional(X,Y,Z)
 Ring/Plan/Resd/Lspl N Indicates that the Ring/Plane/Residue Involves N Atoms
 Sigref - R.M.S-Error of the Contributing Atoms
 Sigpln - $\text{Sqrt}(\text{Sum}(j=1:N)(D(j)**2)/(N-3))$
 Chisq - Chi-Squared = $\text{Sum}(j=1:N)(D(j)**2)/\text{Sigref}**2$
 Pl.Hyp. - Result of the Chi.Sq. Test for Planarity (See Stout & Jensen, p424)

Calculated via Substitution in

$D = P \cdot X + Q \cdot Y + R \cdot Z - S$ (2nd Line)

**** - Atoms Deviating by More Than 1.5 Angstrom and Hydrogen Atoms are NOT Listed
 Note - Weights : UNIT
 **** - Maximum Metal Containing Ring Size: 6
 - Maximum Number of Bonds to Ring Metal: 6
 - Deviations from planes are in Angstrom Units
 - The Plane determining Atoms have been Marked #

Nr	1	P	Q	R	S	Sigref	0.002	Sigpln	0.009	Chisq	70.1	Pl.Hyp.	P<5
Ring		0.5237(7)	0.4794(7)	0.7043(6)	8.081(2)	#N1C	0.006(2)	#C2C	0.001(2)	#C3C	-0.009(2)	#C4C	0.010(2)
A 6		4.669(6)	6.066(8)	14.426(10)	8.081(2)	#C5C	-0.004(2)	#C6C	-0.005(2)	Cu1	-0.009(1)	Cu2	-0.397(1)
						O11A	1.237(1)	O11B	-1.206(1)	O12B	0.209(1)	O21A	1.122(1)
						O21B	-0.424(1)	O22A	0.200(1)	O22B	0.696(1)	N1D	0.230(2)
						N1E	-0.553(2)	N1F	0.072(2)	C2D	1.443(2)	C2E	0.532(2)
						C2F	1.280(2)	C3E	0.448(2)	C4D	0.526(2)	C4E	-0.803(2)
						C4F	0.849(2)	C5D	-0.729(2)	C5F	-0.393(2)	C6D	-0.835(2)
						C6F	-0.749(2)	C11B	-0.840(2)	C21A	1.153(2)	C21B	-0.299(2)
						Cu1_a	1.388(1)	Cu2_a	1.000(1)	O1_a	-0.419(1)	O2_a	-0.546(1)
						O11B_a	0.191(1)	O21B_a	0.973(1)	N1C_a	1.403(2)	N1E_a	0.843(2)
						N1F_a	1.469(2)	C1B_a	-0.411(2)	C2B_a	-0.146(2)	C2C_a	1.397(2)
						C3C_a	1.388(2)	C4C_a	1.407(2)	C4E_a	0.594(2)	C5C_a	1.393(2)
						C5D_a	0.668(2)	C5E_a	-0.528(2)	C5F_a	1.004(2)	C6C_a	1.392(2)
						C6D_a	0.561(2)	C6E_a	-0.370(2)	C6F_a	0.648(2)	C11B_a	0.557(2)
						C21B_a	1.098(2)	Cu1_b	-1.406(1)	O11A_b	-0.160(1)	O12B_b	-1.188(1)
						O21A_b	-0.275(1)	O22A_b	-1.197(1)	O22B_b	-0.701(1)	N1C_b	-1.391(2)
						N1D_b	-1.167(2)	N1F_b	-1.325(2)	C2A_b	1.119(2)	C2C_b	-1.396(2)
						C2D_b	0.047(2)	C2E_b	-0.865(2)	C2F_b	-0.117(2)	C3C_b	-1.405(2)
						C3D_b	0.236(2)	C3E_b	-0.949(2)	C3F_b	0.300(2)	C4C_b	-1.386(2)
						C4D_b	-0.871(2)	C4F_b	-0.548(2)	C5C_b	-1.400(2)	C6C_b	-1.401(2)
						C11A_b	1.049(2)	C21A_b	-0.244(2)				

Nr	2	P	Q	R	S	Sigref	0.002	Sigpln	0.010	Chisq	79.7	Pl.Hyp.	P<5
Ring		-0.5755(7)	0.8177(5)	-0.0102(9)	-2.593(9)	#N1D	0.011(2)	#C2D	-0.007(2)	#C3D	-0.003(2)	#C4D	0.009(2)
A 6		-5.132(6)	8.175(6)	-0.067(15)	-2.593(9)	#C5D	-0.006(2)	#C6D	-0.004(2)	Cu1	0.289(1)	O1	-1.213(2)
						O11A	-1.062(1)	O12A	0.339(1)	N1C	0.774(2)	C2C	-0.219(2)
						C3C	0.011(2)	C4C	1.309(2)	C6A	-1.340(2)	C11A	-0.726(2)

					Cu2_d	0.238(1)	O2_d	-1.054(2)	O21A_d	-1.030(1)	N1E_d	-0.718(2)	
					N1F_d	1.371(2)	C2E_d	-1.136(2)	C5E_d	-1.346(2)	C6E_d	-0.836(2)	
Nr	3	P	Q	R	S	Sigref	0.002	Sigpln	0.008	Chisq	52.1	Pl.Hyp.	P<5
Ring		0.8042(5)	-0.5608(7)	-0.1970(9)	8.963(7)	#N1E	0.009(2)	#C2E	-0.007(2)	#C3E	-0.001(2)	#C4E	0.007(2)
A	6	7.171(5)	-5.001(7)	-2.373(15)	8.963(7)	#C5E	-0.006(3)	#C6E	-0.002(2)	Cu2	0.247(1)	O2	-1.443(1)
						O21A	-0.994(1)	N1F	0.745(2)	C2F	1.275(2)	C4F	1.251(3)
						C5F	0.701(3)	C6F	0.475(2)	Cu1_d	-0.893(1)	O11B_d	0.324(1)
						O12A_d	-0.973(2)	N1C_d	0.303(2)	C2C_d	-0.270(2)	C3C_d	0.465(2)
						C6B_d	0.903(2)	C11B_d	1.275(2)				
Nr	4	P	Q	R	S	Sigref	0.002	Sigpln	0.005	Chisq	18.6	Pl.Hyp.	P<5
Ring		-0.5564(8)	0.6643(7)	0.4991(8)	-5.626(11)	#N1F	0.003(2)	#C2F	0.002(2)	#C3F	-0.003(2)	#C4F	0.000(2)
A	6	-4.961(7)	6.510(8)	8.421(13)	-5.626(11)	#C5F	0.005(2)	#C6F	-0.006(2)	Cu2	0.163(1)	O2	1.137(1)
						N1E	0.201(2)	C2E	0.592(2)	C3E	0.468(2)	C4E	-0.065(2)
						C5E	-0.442(2)	C6E	-0.300(2)	O21B_d	-0.091(1)	O22B_d	0.967(1)
						C5C_d	1.408(2)	C21B_d	0.936(2)				
Nr	5	P	Q	R	S	Sigref	0.002	Sigpln	0.001	Chisq	0.3	Pl.Hyp.	
Ring		0.9511(2)	0.1754(7)	-0.2542(7)	7.730(8)	#C1A	0.000(2)	#C2A	0.000(2)	#C6A	0.000(2)	#C1A_d	0.000(2)
A	6	8.481(2)	3.342(8)	-1.502(12)	7.730(8)	#C2A_d	0.000(2)	#C6A_d	0.000(2)	Cu1	-1.010(1)	Cu2	1.492(1)
						O1	-1.364(2)	O2	-0.492(1)	O11A	-0.207(1)	O12A	0.005(2)
						O21A	1.175(1)	O22A	-1.049(1)	O22B	-1.035(1)	N1D	0.807(2)
						N1F	0.944(2)	C3F	1.251(3)	C4F	0.107(3)	C5F	-0.616(3)
						C6D	0.998(2)	C6F	-0.161(2)	C11A	-0.062(2)	C21A	0.031(2)
						C3E_a	-1.111(2)	C4E_a	-1.251(2)	C3C_b	0.856(2)	C4C_b	-0.075(2)
						C5C_b	0.215(2)	C6C_b	1.426(2)	O21B_c	-0.367(1)	N1C_c	-0.849(2)
						C2C_c	-0.554(2)	C3C_c	0.646(2)	C5C_c	1.288(2)	C6C_c	0.077(2)
						Cu1_d	1.010(1)	Cu2_d	-1.492(1)	O1_d	1.364(2)	O2_d	0.492(1)
						O11A_d	0.207(1)	O12A_d	-0.005(2)	O21A_d	-1.175(1)	O22A_d	1.049(1)
						O22B_d	1.035(1)	N1D_d	-0.807(2)	N1F_d	-0.944(2)	C3F_d	-1.251(3)
						C4F_d	-0.107(3)	C5F_d	0.616(3)	C6D_d	-0.998(2)	C6F_d	0.161(2)
						C11A_d	0.062(2)	C21A_d	-0.031(2)				
Nr	6	P	Q	R	S	Sigref	0.002	Sigpln	0.003	Chisq	7.0	Pl.Hyp.	
Ring		0.9443(2)	0.2664(7)	-0.1933(7)	6.378(3)	#C1B	-0.002(2)	#C2B	0.002(2)	#C6B	0.002(2)	#C1B_c	0.002(2)
A	6	8.420(2)	4.336(8)	-0.294(13)	6.378(3)	#C2B_c	-0.002(2)	#C6B_c	-0.002(2)	Cu1	0.770(1)	O1	0.174(2)
						O2	0.835(1)	O11B	0.012(1)	O12B	0.067(2)	O21B	-1.083(1)
						O22A	0.502(1)	O22B	1.159(1)	N1C	-0.951(2)	C2C	-1.307(2)
						C4F	1.407(3)	C5F	0.623(3)	C6F	1.087(2)	C11B	0.030(2)
						C21B	0.041(2)	Cu2_a	-1.247(1)	O21A_a	-1.352(1)	N1E_a	-0.307(2)
						C2D_a	-0.432(2)	C2E_a	0.668(2)	C2F_a	-1.068(2)	C3D_a	0.747(2)
						C3E_a	1.448(2)	C3F_a	-1.463(3)	C4D_a	0.825(2)	C4E_a	1.214(2)
						C5D_a	-0.271(2)	C5E_a	0.191(3)	C6D_a	-1.419(2)	C6E_a	-0.542(2)

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					C4C_b	0.774(2)	C5C_b	1.126(2)	Cu1_c	-0.770(1)	O1_c	-0.174(2)	
					O2_c	-0.835(1)	O11B_c	-0.012(1)	O12B_c	-0.067(2)	O21B_c	1.083(1)	
					O22A_c	-0.502(1)	O22B_c	-1.159(1)	N1C_c	0.951(2)	C2C_c	1.307(2)	
					C4F_c	-1.407(3)	C5F_c	-0.623(3)	C6F_c	-1.087(2)	C11B_c	-0.030(2)	
					C21B_c	-0.041(2)	Cu2_d	0.954(1)	O21A_d	1.058(1)	N1D_d	1.225(2)	
					N1E_d	0.013(2)	C2D_d	0.139(2)	C2E_d	-0.961(2)	C2F_d	0.774(2)	
					C3D_d	-1.041(2)	C3F_d	1.170(3)	C4D_d	-1.119(2)	C5D_d	-0.023(2)	
					C5E_d	-0.484(3)	C6D_d	1.125(2)	C6E_d	0.248(2)			

Nr	7	P	Q	R	S	Sigref	0.002	Sigpln	1.958	Chisq	999999.9	Pl.Hyp.	

Resd		0.8161	0.5680	-0.1067	7.6726	#Cu1	-0.370(1)	#Cu2	-0.111(1)	#O1	-1.632(2)	#O2	-1.872(1)
A230		7.2766	7.4767	1.4543	7.6726	#O11A	0.165(1)	#O11B	-0.839(1)	#O12A	1.262(2)	#O12B	-0.049(1)
						#O21A	0.357(1)	#O21B	-0.342(1)	#O22A	-1.754(1)	#O22B	1.738(1)
						#N1C	-1.911(2)	#N1D	1.336(2)	#N1E	1.083(2)	#N1F	-0.963(2)
						#C1A	0.508(2)	#C1B	-0.362(2)	#C2A	-0.080(2)	#C2B	0.075(2)
						#C2C	-2.562(2)	#C2D	2.545(2)	#C2E	2.299(2)	#C2F	-0.218(2)
						#C3C	-3.642(2)	#C3D	3.727(2)	#C3E	3.209(2)	#C3F	-0.767(3)
						#C4C	-4.062(2)	#C4D	3.672(2)	#C4E	2.858(2)	#C4F	-2.126(3)
						#C5C	-3.409(2)	#C5D	2.438(2)	#C5E	1.594(3)	#C5F	-2.897(3)
						#C6A	0.907(2)	#C6B	-0.721(2)	#C6C	-2.343(2)	#C6D	1.300(2)
						#C6E	0.740(2)	#C6F	-2.282(2)	#C11A	0.674(2)	#C11B	-0.413(2)
						#C21A	-0.532(2)	#C21B	0.532(2)	#Cu1_a	-0.170(1)	#Cu2_a	0.089(1)
						#O1_a	-1.432(2)	#O2_a	-1.672(1)	#O11A_a	0.365(1)	#O11B_a	-0.639(1)
						#O12A_a	1.462(2)	#O12B_a	0.151(1)	#O21A_a	0.557(1)	#O21B_a	-0.142(1)
						#O22A_a	-1.554(1)	#O22B_a	1.938(1)	#N1C_a	-1.710(2)	#N1D_a	1.536(2)
						#N1E_a	1.283(2)	#N1F_a	-0.763(2)	#C1A_a	0.708(2)	#C1B_a	-0.162(2)
						#C2A_a	0.121(2)	#C2B_a	0.275(2)	#C2C_a	-2.362(2)	#C2D_a	2.745(2)
						#C2E_a	2.499(2)	#C2F_a	-0.018(2)	#C3C_a	-3.442(2)	#C3D_a	3.927(2)
						#C3E_a	3.409(2)	#C3F_a	-0.567(3)	#C4C_a	-3.862(2)	#C4D_a	3.872(2)
						#C4E_a	3.058(2)	#C4F_a	-1.926(3)	#C5C_a	-3.209(2)	#C5D_a	2.638(2)
						#C5E_a	1.794(3)	#C5F_a	-2.697(3)	#C6A_a	1.107(2)	#C6B_a	-0.520(2)
						#C6C_a	-2.143(2)	#C6D_a	1.500(2)	#C6E_a	0.940(2)	#C6F_a	-2.082(2)
						#C11A_a	0.874(2)	#C11B_a	-0.213(2)	#C21A_a	-0.332(2)	#C21B_a	0.732(2)
						#Cu1_b	-0.570(1)	#Cu2_b	-0.311(1)	#O1_b	-1.832(2)	#O2_b	-2.072(1)
						#O11A_b	-0.035(1)	#O11B_b	-1.039(1)	#O12A_b	1.062(2)	#O12B_b	-0.249(1)
						#O21A_b	0.157(1)	#O21B_b	-0.542(1)	#O22A_b	-1.954(1)	#O22B_b	1.538(1)
						#N1C_b	-2.111(2)	#N1D_b	1.136(2)	#N1E_b	0.883(2)	#N1F_b	-1.163(2)
						#C1A_b	0.307(2)	#C1B_b	-0.562(2)	#C2A_b	-0.280(2)	#C2B_b	-0.126(2)
						#C2C_b	-2.762(2)	#C2D_b	2.345(2)	#C2E_b	2.099(2)	#C2F_b	-0.418(2)
						#C3C_b	-3.842(2)	#C3D_b	3.527(2)	#C3E_b	3.009(2)	#C3F_b	-0.967(3)
						#C4C_b	-4.262(2)	#C4D_b	3.472(2)	#C4E_b	2.658(2)	#C4F_b	-2.326(3)
						#C5C_b	-3.609(2)	#C5D_b	2.238(2)	#C5E_b	1.394(3)	#C5F_b	-3.098(3)
						#C6A_b	0.707(2)	#C6B_b	-0.921(2)	#C6C_b	-2.543(2)	#C6D_b	1.099(2)
						#C6E_b	0.540(2)	#C6F_b	-2.482(2)	#C11A_b	0.474(2)	#C11B_b	-0.613(2)
						#C21A_b	-0.732(2)	#C21B_b	0.332(2)	#Cu1_c	-0.222(1)	#Cu2_c	-0.481(1)
						#O1_c	1.040(2)	#O2_c	1.280(1)	#O11A_c	-0.757(1)	#O11B_c	0.247(1)
						#O12A_c	-1.854(2)	#O12B_c	-0.543(1)	#O21A_c	-0.949(1)	#O21B_c	-0.250(1)

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					#022A_c	1.162(1)	#022B_c	-2.330(1)	#N1C_c	1.319(2)	#N1D_c	-1.928(2)
					#N1E_c	-1.675(2)	#N1F_c	0.371(2)	#C1A_c	-1.099(2)	#C1B_c	-0.230(2)
					#C2A_c	-0.512(2)	#C2B_c	-0.667(2)	#C2C_c	1.970(2)	#C2D_c	-3.137(2)
					#C2E_c	-2.891(2)	#C2F_c	-0.374(2)	#C3C_c	3.050(2)	#C3D_c	-4.319(2)
					#C3E_c	-3.801(2)	#C3F_c	0.175(3)	#C4C_c	3.470(2)	#C4D_c	-4.264(2)
					#C4E_c	-3.450(2)	#C4F_c	1.534(3)	#C5C_c	2.817(2)	#C5D_c	-3.030(2)
					#C5E_c	-2.186(3)	#C5F_c	2.306(3)	#C6A_c	-1.499(2)	#C6B_c	0.129(2)
					#C6C_c	1.751(2)	#C6D_c	-1.891(2)	#C6E_c	-1.332(2)	#C6F_c	1.690(2)
					#C11A_c	-1.266(2)	#C11B_c	-0.179(2)	#C21A_c	-0.060(2)	#C21B_c	-1.124(2)
					#Cu1_d	1.033(1)	#Cu2_d	0.773(1)	#O1_d	2.294(2)	#O2_d	2.534(1)
					#O11A_d	0.497(1)	#O11B_d	1.502(1)	#O12A_d	-0.600(2)	#O12B_d	0.712(1)
					#O21A_d	0.305(1)	#O21B_d	1.005(1)	#O22A_d	2.416(1)	#O22B_d	-1.076(1)
					#N1C_d	2.573(2)	#N1D_d	-0.674(2)	#N1E_d	-0.421(2)	#N1F_d	1.625(2)
					#C1A_d	0.155(2)	#C1B_d	1.024(2)	#C2A_d	0.742(2)	#C2B_d	0.588(2)
					#C2C_d	3.224(2)	#C2D_d	-1.883(2)	#C2E_d	-1.637(2)	#C2F_d	0.880(2)
					#C3C_d	4.304(2)	#C3D_d	-3.064(2)	#C3E_d	-2.547(2)	#C3F_d	1.429(3)
					#C4C_d	4.724(2)	#C4D_d	-3.010(2)	#C4E_d	-2.195(2)	#C4F_d	2.788(3)
					#C5C_d	4.071(2)	#C5D_d	-1.776(2)	#C5E_d	-0.932(3)	#C5F_d	3.560(3)
					#C6A_d	-0.245(2)	#C6B_d	1.383(2)	#C6C_d	3.006(2)	#C6D_d	-0.637(2)
					#C6E_d	-0.078(2)	#C6F_d	2.944(2)	#C11A_d	-0.012(2)	#C11B_d	1.075(2)
					#C21A_d	1.195(2)	#C21B_d	0.131(2)				

Nr	8	P	Q	R	S	Sigref	0.001	Sigpln	0.023	Chisq	612.8	Pl.Hyp.

Plan		0.7460(3)	0.1989(6)	-0.6356(4)	3.711(4)	#Cu1	-0.022(1)	#O1	0.008(2)	#O11A	0.010(1)	#O11B
A 5		6.652(3)	3.299(6)	-8.543(7)	3.711(4)	#C11B	0.017(2)	O1W	0.133(2)	O2	0.364(1)	O12A
						O12B	-0.414(1)	O21A	0.927(1)	O21B	-0.910(1)	O22A
						O22B	1.025(1)	N1F	0.516(2)	C1A	-0.797(2)	C1B
						C2A	-0.836(2)	C2B	0.737(2)	C2F	0.663(2)	C3F
						C4F	-1.210(3)	C5F	-1.369(3)	C6A	-1.292(2)	C6B
						C6F	-0.483(2)	C11A	-0.293(2)	C21A	-0.309(2)	C21B
						N1D_a	-1.380(2)	N1E_a	-0.265(2)	C2D_a	-0.753(2)	C2E_a
						C3D_a	0.573(2)	C3E_a	1.466(2)	C4D_a	1.297(2)	C5D_a
						C5E_a	1.229(2)	C6D_a	-0.658(2)	C6E_a	0.158(2)	N1C_b
						C2C_b	0.712(2)	C3C_b	-0.662(2)	C4C_b	-1.449(2)	C5C_b
						C6C_b	0.546(2)	Cu2_c	0.844(1)	N1D_c	0.557(2)	N1E_c
						C2D_c	-0.071(2)	C2E_c	-1.202(2)	C3D_c	-1.396(2)	C5D_c
						C6B_c	1.347(2)	C6D_c	-0.165(2)	C6E_c	-0.982(2)	N1C_d
						C2C_d	-0.021(2)	C3C_d	1.353(2)	C4F_d	-1.452(3)	C5F_d
						C6A_d	-1.370(2)	C6C_d	0.146(2)			

Nr	9	P	Q	R	S	Sigref	0.001	Sigpln	0.002	Chisq	2.4	Pl.Hyp.

Plan		-0.6877(4)	0.3879(7)	-0.6137(5)	-6.698(4)	#Cu1	0.002(1)	#O1	0.000(2)	#N1C	-0.001(2)	#N1D
A 4		-6.132(4)	3.265(7)	-11.579(9)	-6.698(4)	O1W	0.216(2)	C2C	-0.937(2)	C2D	-0.722(2)	C3C
						C3D	-0.588(2)	C4C	-0.103(2)	C4D	0.319(2)	C4E
						C5C	0.873(2)	C5D	1.042(2)	C5E	-1.171(2)	C6C
						C6D	0.856(2)					

Nr 10	P	Q	R	S	Sigref	0.001	Sigpln	0.027	Chisq	493.4	Pl.Hyp.	P<5
Plan	0.1189(7)	0.9055(2)	0.4073(6)	4.927(4)	#Cu1	-0.022(1)	#011A	0.011(1)	#011B	0.011(1)	#N1C	0.000(2)
A 4	1.061(6)	10.171(3)	9.109(11)	4.927(4)	N1D	0.271(2)	C1A	0.833(2)	C1B	0.878(2)	C2A	-0.430(2)
					C2C	-0.737(2)	C2D	1.232(2)	C3C	-0.802(2)	C3E	-1.413(2)
					C4C	-0.067(2)	C4D	0.887(2)	C5C	0.676(2)	C5D	-0.124(2)
					C6B	-0.354(2)	C6C	0.695(2)	C6D	-0.400(2)	C11A	1.057(2)
					C11B	1.057(2)	Cu1_c	1.400(1)	O11A_c	1.367(1)	O11B_c	1.367(1)
					O12A_c	-0.843(1)	O12B_c	-0.797(1)	N1C_c	1.378(2)	N1D_c	1.107(2)
					C1A_c	0.545(2)	C1B_c	0.500(2)	C2B_c	-0.560(2)	C2D_c	0.146(2)
					C3D_c	-0.193(2)	C4C_c	1.445(2)	C4D_c	0.490(2)	C5C_c	0.701(2)
					C6A_c	-0.549(2)	C6C_c	0.683(2)	C11A_c	0.321(2)	C11B_c	0.321(2)
					Cu1_d	1.398(1)	O11A_d	1.365(1)	O11B_d	1.366(1)	O12A_d	-0.845(1)
					O12B_d	-0.798(1)	N1C_d	1.376(2)	N1D_d	1.105(2)	C1A_d	0.543(2)
					C1B_d	0.498(2)	C2B_d	-0.561(2)	C2D_d	0.144(2)	C3D_d	-0.195(2)
					C4C_d	1.444(2)	C4D_d	0.489(2)	C5C_d	0.700(2)	C5D_d	1.500(2)
					C6A_d	-0.551(2)	C6C_d	0.681(2)	C11A_d	0.319(2)	C11B_d	0.319(2)
Nr 11	P	Q	R	S	Sigref	0.001	Sigpln	0.024	Chisq	400.6	Pl.Hyp.	P<5
Plan	0.0172(7)	0.8710(3)	0.4910(6)	4.390(5)	#Cu1	-0.020(1)	#011A	0.010(1)	#011B	0.010(1)	#N1D	0.000(2)
A 4	0.153(7)	9.640(4)	10.207(10)	4.390(5)	N1C	0.275(2)	C1A	0.937(2)	C1B	0.779(2)	C2A	-0.311(2)
					C2C	-0.373(2)	C2D	0.869(2)	C3C	-0.250(2)	C3D	1.025(2)
					C4C	0.585(2)	C4D	0.247(2)	C5C	1.238(2)	C5D	-0.672(2)
					C6B	-0.517(2)	C6C	1.069(2)	C6D	-0.765(2)	C11A	1.090(2)
					C11B	1.044(2)	Cu1_c	1.033(1)	O11A_c	1.003(1)	O11B_c	1.003(1)
					O12A_c	-1.224(1)	O12B_c	-1.198(1)	N1C_c	0.737(2)	N1D_c	1.013(2)
					C1A_c	0.076(2)	C1B_c	0.234(2)	C2A_c	1.323(2)	C2B_c	-0.804(2)
					C2C_c	1.385(2)	C2D_c	0.144(2)	C3C_c	1.263(2)	C3D_c	-0.012(2)
					C4C_c	0.428(2)	C4D_c	0.765(2)	C5C_c	-0.225(2)	C6A_c	-1.077(2)
					C6C_c	-0.056(2)	C11A_c	-0.077(2)	C11B_c	-0.031(2)	O12A_d	-0.503(1)
					O12B_d	-0.477(1)	N1C_d	1.458(2)	C1A_d	0.797(2)	C1B_d	0.955(2)
					C2B_d	-0.084(2)	C2D_d	0.865(2)	C3D_d	0.709(2)	C4C_d	1.149(2)
					C4D_d	1.486(2)	C5C_d	0.496(2)	C6A_d	-0.356(2)	C6C_d	0.664(2)
					C11A_d	0.644(2)	C11B_d	0.690(2)				
Nr 12	P	Q	R	S	Sigref	0.001	Sigpln	0.040	Chisq	1121.3	Pl.Hyp.	P<5
Plan	-0.1867(7)	-0.6824(3)	0.7068(3)	2.041(8)	#Cu2	-0.033(1)	#02	0.001(1)	#021A	0.016(1)	#021B_b	0.016(1)
A 4	-1.664(6)	-7.808(4)	10.280(6)	2.041(8)	O11A	-1.293(1)	O22A	1.313(1)	N1C	-0.933(2)	C1A	0.231(2)
					C2A	1.055(2)	C2C	0.327(2)	C3C	1.420(2)	C4C	1.222(2)
					C5C	-0.072(2)	C6A	0.626(2)	C6C	-1.125(2)	C11A	-1.053(2)
					C21A	0.742(2)	O22B_b	-0.968(1)	C1B_b	0.494(2)	C2B_b	-0.483(2)
					C3D_b	0.581(2)	C4D_b	-0.275(2)	C4E_b	1.360(2)	C5D_b	0.095(2)
					C6B_b	0.321(2)	C6D_b	1.296(2)	C21B_b	-0.444(2)	N1F_d	0.950(2)
					C2F_d	0.545(2)	C3C_d	1.450(2)	C3F_d	-0.792(2)	C5F_d	-1.333(2)
					C6F_d	0.016(2)						

=====												
Nr 13	P	Q	R	S	Sigref	0.001	Sigpln	0.022	Chisq	255.0	Pl.Hyp.	P<5
Plan	-0.1675(7)	0.7304(4)	0.6622(4)	-0.611(8)	#Cu2	-0.018(1)	#02	0.002(1)	#N1E	0.008(2)	#N1F	0.008(2)
A 4	-1.494(6)	7.814(4)	12.379(7)	-0.611(8)	C2E	0.811(2)	C2F	0.540(2)	C3E	0.729(2)	C3F	0.678(2)
					C4E	-0.206(2)	C4F	0.264(2)	C5E	-1.016(2)	C5F	-0.279(2)
					C6E	-0.887(2)	C6F	-0.402(2)	O12A_c	1.421(1)	O21B_c	0.220(1)
					O22B_c	0.460(1)	C5C_c	1.345(2)	C6A_c	1.145(2)	C21B_c	0.906(2)

Nr 14	P	Q	R	S	Sigref	0.001	Sigpln	0.042	Chisq	1143.1	Pl.Hyp.	P<5
Plan	0.9897(1)	0.1189(7)	0.0794(7)	11.107(4)	#Cu2	-0.034(1)	#021A	0.017(1)	#N1F	-0.001(2)	#O21B_b	0.017(1)
A 4	8.8251(6)	2.776(8)	4.214(13)	11.107(4)	O12A	-1.072(2)	N1D	-1.476(2)	N1E	0.337(2)	C1A	-0.607(2)
					C2A	-0.555(2)	C2D	-0.322(2)	C2E	1.255(2)	C2F	1.036(2)
					C3D	0.579(2)	C3F	1.067(3)	C4D	0.294(2)	C4E	1.074(2)
					C4F	-0.004(3)	C5D	-0.871(2)	C5E	0.107(3)	C5F	-1.076(3)
					C6A	-0.226(2)	C6E	-0.233(2)	C6F	-1.033(2)	C11A	-1.120(2)
					C21A	-0.907(2)	C1B_b	1.171(2)	C2B_b	0.903(2)	C3C_b	0.889(2)
					C4C_b	-0.047(2)	C5C_b	-0.073(2)	C6B_b	1.010(2)	C6C_b	0.847(2)
					C21B_b	1.075(2)	Cu2_d	-0.317(1)	O11A_d	1.238(1)	O12A_d	0.721(2)
					O21A_d	-0.368(1)	N1D_d	1.125(2)	N1E_d	-0.688(2)	N1F_d	-0.349(2)
					C1A_d	0.257(2)	C2A_d	0.205(2)	C2D_d	-0.028(2)	C2F_d	-1.387(2)
					C3D_d	-0.929(2)	C3F_d	-1.418(3)	C4D_d	-0.644(2)	C4E_d	-1.425(2)
					C4F_d	-0.346(3)	C5D_d	0.520(2)	C5E_d	-0.458(3)	C5F_d	0.726(3)
					C6A_d	-0.124(2)	C6D_d	1.375(2)	C6E_d	-0.117(2)	C6F_d	0.682(2)
					C11A_d	0.769(2)	C21A_d	0.557(2)				

Nr 15	P	Q	R	S	Sigref	0.001	Sigpln	0.023	Chisq	314.2	Pl.Hyp.	P<5
Plan	0.7446(4)	0.4390(18)	-0.5029(10)	4.854(7)	#Cu1	-0.018(1)	#011A	0.010(1)	#011B	0.009(1)	#C11A	0.000(2)
A 4	6.639(4)	5.947(19)	-5.792(18)	4.854(7)	Cu2	0.595(1)	O1	-0.608(2)	O1W	1.120(2)	O2	-0.794(1)
					O12A	0.372(1)	O12B	0.215(1)	O21A	0.356(1)	O21B	0.138(1)
					N1F	-0.691(2)	C1A	-0.553(2)	C1B	0.889(2)	C2A	-0.937(2)
					C2B	1.270(2)	C2F	-0.396(2)	C3F	-1.285(3)	C6A	-0.734(2)
					C6B	1.071(2)	C11B	0.327(2)	C21A	-0.772(2)	C21B	1.169(2)
					Cu1_a	-0.711(1)	Cu2_a	-0.097(1)	O1_a	-1.300(2)	O2_a	-1.486(1)
					O11A_a	-0.682(1)	O11B_a	-0.683(1)	O12A_a	-0.320(1)	O12B_a	-0.477(1)
					O21A_a	-0.336(1)	O21B_a	-0.554(1)	O22B_a	1.448(1)	N1D_a	1.283(2)
					N1E_a	1.450(2)	N1F_a	-1.383(2)	C1A_a	-1.245(2)	C1B_a	0.197(2)
					C2B_a	0.578(2)	C2F_a	-1.088(2)	C6A_a	-1.426(2)	C6B_a	0.379(2)
					C11A_a	-0.693(2)	C11B_a	-0.365(2)	C21A_a	-1.464(2)	C21B_a	0.477(2)
					Cu1_b	0.674(1)	Cu2_b	1.287(1)	O1_b	0.085(2)	O2_b	-0.102(1)
					O11A_b	0.702(1)	O11B_b	0.701(1)	O12A_b	1.064(1)	O12B_b	0.907(1)
					O21A_b	1.048(1)	O21B_b	0.831(1)	O22A_b	-1.093(1)	N1C_b	-1.251(2)
					N1F_b	0.001(2)	C1A_b	0.139(2)	C2A_b	-0.245(2)	C2F_b	0.296(2)
					C3F_b	-0.593(2)	C6A_b	-0.042(2)	C6F_b	-1.198(2)	C11A_b	0.692(2)
					C11B_b	1.019(2)	C21A_b	-0.080(2)	O22B_c	0.737(1)	N1D_c	0.902(2)
					N1E_c	0.735(2)	C2D_c	0.043(2)	C2E_c	-0.194(2)	C3D_c	-1.322(2)

Nr 19	P	Q	R	S	Sigref	0.002	Sigpln	0.029	Chisq	2464.2	Pl.Hyp.	P<5
Plan	0.9496(1)	0.1835(3)	-0.2542(3)	7.723(3)	#012A	0.029(2)	#C1A	0.007(2)	#C2A	-0.005(2)	#C6A	0.011(2)
A 12	8.4672(7)	3.430(4)	-1.489(5)	7.723(3)	#C11A	-0.048(2)	#C21A	0.020(2)	#012A_d	-0.029(2)	#C1A_d	-0.007(2)
					#C2A_d	0.005(2)	#C6A_d	-0.011(2)	#C11A_d	0.048(2)	#C21A_d	-0.020(2)
					Cu1	-0.993(1)	Cu2	1.467(1)	O1	-1.363(2)	O2	-0.514(1)
					O11A	-0.197(1)	O21A	1.162(1)	O22A	-1.065(1)	O22B	-0.971(1)
					N1D	0.827(2)	N1F	0.908(2)	C3F	1.208(3)	C4F	0.058(3)
					C5F	-0.664(3)	C6D	1.018(2)	C6F	-0.203(2)	C3E_a	-1.010(2)
					C4E_a	-1.151(2)	C3C_b	0.759(2)	C4C_b	-0.163(2)	C5C_b	0.136(2)
					C6C_b	1.348(2)	O21B_c	-0.343(1)	N1C_c	-0.776(2)	C2C_c	-0.472(2)
					C3C_c	0.730(2)	C5C_c	1.353(2)	C6C_c	0.141(2)	Cu1_d	0.993(1)
					Cu2_d	-1.467(1)	O1_d	1.363(2)	O2_d	0.514(1)	O11A_d	0.197(1)
					O21A_d	-1.162(1)	O22A_d	1.065(1)	O22B_d	0.971(1)	N1D_d	-0.827(2)
					N1F_d	-0.908(2)	C3F_d	-1.208(3)	C4F_d	-0.058(3)	C5F_d	0.664(3)
					C6D_d	-1.018(2)	C6F_d	0.203(2)				
Nr 20	P	Q	R	S	Sigref	0.002	Sigpln	0.036	Chisq	1361.9	Pl.Hyp.	P<5
Plan	0.9305(2)	0.1340(6)	-0.3408(7)	6.822(7)	#011A	-0.019(1)	#012A	0.006(2)	#C1A	-0.012(2)	#C2A	0.050(2)
A 6	8.2972(19)	2.855(7)	-3.126(12)	6.822(7)	#C11A	0.002(2)	#C6A_d	-0.028(2)	Cu1	-0.714(1)	O1	-0.893(2)
					O2	0.016(1)	O11B	-1.369(1)	O21A	1.419(1)	O22A	-0.793(1)
					O22B	-0.794(1)	N1D	1.150(2)	N1F	1.282(2)	C1B	-1.388(2)
					C3F	1.421(3)	C4F	0.321(3)	C5F	-0.294(3)	C6A	-0.148(2)
					C6B	-1.108(2)	C6D	1.464(2)	C6F	0.220(2)	C21A	0.228(2)
					C3E_a	-0.980(2)	C4E_a	-0.990(2)	C3C_b	1.322(2)	C4C_b	0.357(2)
					C5C_b	0.664(2)	O11B_c	-1.123(1)	O12B_c	-0.783(2)	O21B_c	0.502(1)
					N1C_c	0.072(2)	C1B_c	-1.105(2)	C2B_c	-0.971(2)	C2C_c	0.382(2)
					C6B_c	-1.384(2)	C6C_c	1.028(2)	C11B_c	-0.992(2)	C21B_c	-0.712(2)
					Cu1_d	0.539(1)	O1_d	0.717(2)	O2_d	-0.192(1)	O11A_d	-0.157(1)
					O11B_d	1.194(1)	O12A_d	-0.182(2)	O22A_d	0.618(1)	O22B_d	0.618(1)
					N1D_d	-1.326(2)	N1F_d	-1.458(2)	C1A_d	-0.164(2)	C1B_d	1.212(2)
					C2A_d	-0.226(2)	C2B_d	1.345(2)	C4F_d	-0.497(3)	C5F_d	0.119(3)
					C6B_d	0.932(2)	C6F_d	-0.396(2)	C11A_d	-0.178(2)	C11B_d	1.325(2)
					C21A_d	-0.403(2)						
Nr 21	P	Q	R	S	Sigref	0.002	Sigpln	0.015	Chisq	831.5	Pl.Hyp.	P<5
Plan	0.9434(1)	0.2597(3)	-0.2066(2)	6.3364(15)	#011B	-0.011(1)	#012B	0.020(2)	#C1B	-0.017(2)	#C2B	-0.018(2)
A 14	8.4115(7)	4.261(4)	-0.537(4)	6.3364(15)	#C6B	0.007(2)	#C11B	0.000(2)	#C21B	-0.001(2)	#O11B_c	0.011(1)
					#O12B_c	-0.020(2)	#C1B_c	0.017(2)	#C2B_c	0.018(2)	#C6B_c	-0.007(2)
					#C11B_c	0.000(2)	#C21B_c	0.001(2)	Cu1	0.734(1)	O1	0.165(2)
					O2	0.836(1)	O21B	-1.132(1)	O22A	0.463(1)	O22B	1.109(1)
					N1C	-1.001(2)	C2C	-1.359(2)	C4F	1.369(3)	C5F	0.599(3)
					C6F	1.072(2)	Cu2_a	-1.322(1)	O21A_a	-1.454(1)	N1E_a	-0.373(2)
					C2D_a	-0.536(2)	C2E_a	0.591(2)	C2F_a	-1.168(2)	C3D_a	0.649(2)
					C3E_a	1.378(2)	C4D_a	0.746(2)	C4E_a	1.163(2)	C5D_a	-0.337(2)

C5E_a	0.151(3)	C6D_a	-1.492(2)	C6E_a	-0.590(2)	C4C_b	0.772(2)
C5C_b	1.125(2)	Cu1_c	-0.734(1)	O1_c	-0.165(2)	O2_c	-0.836(1)
O21B_c	1.132(1)	O22A_c	-0.463(1)	O22B_c	-1.109(1)	N1C_c	1.001(2)
C2C_c	1.359(2)	C4F_c	-1.369(3)	C5F_c	-0.599(3)	C6F_c	-1.072(2)
Cu2_d	0.785(1)	O21A_d	0.917(1)	N1D_d	1.074(2)	N1E_d	-0.165(2)
N1F_d	1.373(2)	C2D_d	-0.001(2)	C2E_d	-1.128(2)	C2F_d	0.631(2)
C3D_d	-1.186(2)	C3F_d	1.036(3)	C4D_d	-1.283(2)	C5D_d	-0.200(2)
C5E_d	-0.688(3)	C6D_d	0.955(2)	C6E_d	0.053(2)		

(Acute) Angles (Degrees) Between Planes (Numbers I,J from List Above)

1, 2=	85.21(10)	1, 3=	89.22(9)	1, 4=	67.75(10)	1, 5=	66.23(9)	1, 6=	60.92(9)	1, 7=	51.36(7)	1, 8=	87.80(8)
1, 9=	52.67(8)	1, 10=	38.44(9)	1, 11=	39.44(9)	1, 12=	85.82(8)	1, 13=	43.22(8)	1, 14=	50.86(9)	1, 15=	75.75(14)
1, 16=	67.42(9)	1, 17=	0.10(8)	1, 18=	67.24(9)	1, 19=	66.03(7)	1, 20=	71.85(9)	1, 21=	61.77(7)	2, 3=	23.16(10)
2, 4=	30.87(10)	2, 5=	66.33(9)	2, 6=	71.11(9)	2, 7=	89.76(7)	2, 8=	74.92(8)	2, 9=	44.01(9)	2, 10=	48.10(9)
2, 11=	45.79(9)	2, 12=	62.76(8)	2, 13=	46.62(9)	2, 14=	61.76(9)	2, 15=	86.31(14)	2, 16=	49.95(9)	2, 17=	85.24(9)
2, 18=	32.75(9)	2, 19=	66.81(7)	2, 20=	65.01(9)	2, 21=	70.82(7)	3, 4=	23.33(10)	3, 5=	44.23(9)	3, 6=	49.60(9)
3, 7=	68.98(7)	3, 8=	52.16(8)	3, 9=	49.49(9)	3, 10=	60.50(9)	3, 11=	55.16(9)	3, 12=	84.64(8)	3, 13=	47.57(9)
3, 14=	44.47(9)	3, 15=	63.15(14)	3, 16=	66.96(9)	3, 17=	89.17(9)	3, 18=	24.22(9)	3, 19=	44.70(7)	3, 20=	42.24(9)
3, 21=	49.18(7)	4, 5=	57.35(10)	4, 6=	63.58(10)	4, 7=	82.53(7)	4, 8=	53.12(9)	4, 9=	70.49(9)	4, 10=	42.38(9)
4, 11=	35.50(9)	4, 12=	89.81(9)	4, 13=	24.64(9)	4, 14=	64.41(9)	4, 15=	68.06(14)	4, 16=	80.81(10)	4, 17=	67.81(9)
4, 18=	1.95(9)	4, 19=	57.78(8)	4, 20=	53.21(9)	4, 21=	62.91(8)	5, 6=	6.29(9)	5, 7=	25.46(6)	5, 8=	25.05(8)
5, 9=	64.53(8)	5, 10=	80.31(8)	5, 11=	87.46(8)	5, 12=	61.52(8)	5, 13=	78.49(8)	5, 14=	19.61(8)	5, 15=	24.08(13)
5, 16=	86.93(9)	5, 17=	66.14(8)	5, 18=	56.60(8)	5, 19=	0.48(7)	5, 20=	5.63(8)	5, 21=	5.57(7)	6, 7=	19.52(6)
6, 8=	28.33(8)	6, 9=	64.70(8)	6, 10=	74.05(8)	6, 11=	81.18(8)	6, 12=	60.36(8)	6, 13=	84.74(8)	6, 14=	18.03(8)
6, 15=	23.48(13)	6, 16=	86.37(9)	6, 17=	60.83(8)	6, 18=	62.86(8)	6, 19=	5.90(7)	6, 20=	11.40(8)	6, 21=	0.85(6)
7, 8=	37.85(4)	7, 9=	74.02(5)	7, 10=	55.39(5)	7, 11=	62.85(6)	7, 12=	52.02(5)	7, 13=	78.03(5)	7, 14=	29.92(6)
7, 15=	24.41(12)	7, 16=	77.85(6)	7, 17=	51.26(5)	7, 18=	81.65(6)	7, 19=	25.00(3)	7, 20=	29.33(6)	7, 21=	20.05(2)
8, 9=	87.38(7)	8, 10=	89.43(7)	8, 11=	82.77(7)	8, 12=	43.60(6)	8, 13=	66.39(7)	8, 14=	44.64(7)	8, 15=	15.77(13)
8, 16=	65.78(8)	8, 17=	87.70(7)	8, 18=	51.57(7)	8, 19=	24.99(5)	8, 20=	20.38(7)	8, 21=	27.54(5)	9, 10=	88.89(8)
9, 11=	88.59(8)	9, 12=	55.24(7)	9, 13=	89.55(7)	9, 14=	46.91(8)	9, 15=	88.11(13)	9, 16=	28.99(8)	9, 17=	52.67(7)
9, 18=	71.96(8)	9, 19=	64.80(6)	9, 20=	67.75(8)	9, 21=	65.09(6)	10, 11=	7.81(8)	10, 12=	69.38(7)	10, 13=	24.33(8)
10, 14=	75.06(8)	10, 15=	73.67(13)	10, 16=	78.46(8)	10, 17=	38.44(8)	10, 18=	43.09(8)	10, 19=	79.89(6)	10, 20=	84.66(8)
10, 21=	74.74(6)	11, 12=	75.49(7)	11, 13=	16.59(8)	11, 14=	80.82(8)	11, 15=	81.47(13)	11, 16=	81.84(8)	11, 17=	39.46(8)
11, 18=	36.03(8)	11, 19=	87.05(6)	11, 20=	88.02(8)	11, 21=	81.90(6)	12, 13=	89.95(7)	12, 14=	77.89(7)	12, 15=	37.44(13)
12, 16=	26.29(8)	12, 17=	85.89(7)	12, 18=	87.90(7)	12, 19=	61.18(5)	12, 20=	59.60(7)	12, 21=	60.05(5)	13, 14=	88.49(8)
13, 15=	82.12(13)	13, 16=	88.59(8)	13, 17=	43.27(7)	13, 18=	24.35(8)	13, 19=	78.85(6)	13, 20=	73.52(8)	13, 21=	83.97(6)
14, 15=	41.48(13)	14, 16=	75.90(9)	14, 17=	50.78(8)	14, 18=	64.35(8)	14, 19=	19.70(6)	14, 20=	24.52(8)	14, 21=	18.53(6)
15, 16=	63.06(13)	15, 17=	75.66(13)	15, 18=	66.63(13)	15, 19=	23.74(12)	15, 20=	22.62(13)	15, 21=	23.04(12)	16, 17=	67.47(8)
16, 18=	82.70(8)	16, 19=	86.63(7)	16, 20=	84.26(8)	16, 21=	86.01(7)	17, 18=	67.30(8)	17, 19=	65.94(6)	17, 20=	71.76(8)
17, 21=	61.68(6)	18, 19=	57.02(6)	18, 20=	52.33(8)	18, 21=	62.17(6)	19, 20=	5.83(6)	19, 21=	5.16(3)	20, 21=	10.58(6)

(Acute) Angles (Degrees) Between Axes, Lines, Bonds and L.S.-Plane

Bond / Plane NM --> M	1	2	3	4	5	6	7	8	9	10

Table 1. Crystallographic data for the studied compounds.																
Axes	0	---	a	/	0M	=	31.58(7),	35.14(7),	53.53(7),	33.80(7),	72.01(6),	70.79(6),	54.69,	48.24(4),	43.44(5),	6.83(5),
					1M	=	0.99(6),	10.76(5),	9.64(5),	81.78(6),	48.12(12),	14.88(6),	31.66(5),	33.84(6),	71.73(3),	68.52(6),
					2M	=	70.62(2),									
			b	/	0M	=	33.00(7),	47.23(7),	26.68(7),	35.77(7),	17.46(6),	22.92(6),	42.17,	17.23(4),	17.05(5),	65.96(5),
					1M	=	59.95(6),	44.52(5),	44.56(5),	14.44(6),	32.27(12),	33.87(6),	33.04(5),	34.30(6),	17.94(3),	14.85(6),
					2M	=	22.50(2),									
			c	/	0M	=	55.62(7),	0.22(7),	7.80(7),	28.80(7),	4.93(6),	0.96(6),	4.77,	29.26(4),	41.48(5),	31.41(5),
					1M	=	35.73(6),	36.02(5),	45.08(5),	13.95(6),	19.35(12),	45.84(6),	55.53(5),	30.35(6),	4.89(3),	10.30(6),
					2M	=	1.76(2),									
			a*	/	0M	=	20.82(7),	42.17(7),	62.90(7),	44.55(7),	70.98(6),	66.71(6),	47.83,	52.44(4),	40.01(5),	3.31(5),
					1M	=	9.46(6),	10.93(5),	20.52(5),	70.99(6),	47.88(12),	13.15(6),	20.90(5),	44.65(6),	70.53(3),	70.46(6),
					2M	=	66.96(2),									
			b*	/	0M	=	23.27(7),	54.43(7),	32.30(7),	37.04(7),	11.74(6),	16.67(6),	35.21,	15.71(4),	27.13(5),	58.49(5),
					1M	=	53.96(6),	49.40(5),	40.48(5),	6.26(6),	29.61(12),	42.87(6),	23.30(5),	35.33(6),	12.22(3),	9.93(6),
					2M	=	16.37(2),									
			c*	/	0M	=	44.77(7),	0.58(7),	11.36(7),	29.94(7),	14.73(6),	11.15(6),	6.13,	39.46(4),	37.86(5),	24.04(5),
					1M	=	29.41(6),	44.97(5),	41.47(5),	4.55(6),	30.19(12),	49.49(6),	44.68(5),	31.71(6),	14.72(3),	19.93(6),
					2M	=	11.92(2),									
Cu1	-01			/	0M	=	52.60(8),	41.30(8),	29.62(8),	48.29(8),	8.93(7),	15.20(7),	33.69(4),	0.74(6),	0.05(7),	88.27(7),
					1M	=	83.42(7),	18.89(6),	67.08(7),	14.73(7),	15.01(13),	9.96(7),	52.60(7),	47.65(7),	9.35(5),	4.49(7),
					2M	=	14.50(5),									
	-011A			/	0M	=	39.38(8),	43.45(8),	37.87(8),	16.81(8),	24.16(7),	24.29(7),	15.82(4),	0.92(6),	87.30(6),	0.96(7),
					1M	=	0.87(7),	35.43(6),	3.05(6),	42.21(7),	0.82(13),	61.72(7),	39.37(6),	15.35(7),	23.91(5),	20.75(7),
					2M	=	23.86(4),									
	-011B			/	0M	=	37.42(8),	44.82(8),	38.18(8),	17.57(8),	22.70(7),	22.64(7),	13.78(4),	0.23(6),	87.14(7),	0.96(7),
					1M	=	0.87(7),	37.28(6),	1.77(7),	40.49(7),	0.80(13),	63.57(7),	37.42(7),	16.06(7),	22.44(5),	19.43(7),
					2M	=	22.23(5),									
	-N1C			/	0M	=	0.43(8),	13.94(8),	36.45(8),	36.95(9),	61.98(8),	58.75(8),	49.90(5),	87.03(7),	0.07(7),	0.63(7),
					1M	=	8.43(7),	48.10(7),	24.92(7),	42.39(8),	72.87(13),	26.61(8),	0.34(7),	38.57(7),	62.04(5),	66.69(7),
					2M	=	59.52(5),									
	-N1D			/	0M	=	6.80(8),	7.93(8),	30.96(8),	28.75(9),	64.45(8),	63.02(8),	57.91(5),	81.85(7),	0.07(7),	8.36(7),
					1M	=	0.56(7),	52.03(7),	15.92(7),	45.33(8),	81.78(13),	28.01(8),	6.90(7),	30.29(7),	64.66(5),	67.72(7),
					2M	=	63.66(5),									
Cu2	-02			/	0M	=	42.34(8),	34.27(8),	47.42(8),	25.13(8),	59.84(7),	60.71(7),	50.12(4),	35.15(6),	54.40(7),	12.11(7),
					1M	=	7.51(7),	0.83(6),	0.49(7),	78.68(7),	37.23(13),	25.40(7),	42.41(7),	24.77(7),	59.67(5),	55.52(7),
					2M	=	60.24(5),									
	-021A			/	0M	=	50.24(8),	39.93(8),	38.94(8),	61.99(8),	9.24(7),	3.02(7),	13.70(4),	22.58(6),	3.97(7),	65.98(7),
					1M	=	73.43(7),	1.40(6),	86.39(7),	1.48(7),	6.95(13),	4.10(7),	50.18(7),	62.40(7),	8.89(5),	14.33(7),
					2M	=	3.82(5),									
	-N1E			/	0M	=	4.51(8),	28.72(8),	6.89(8),	1.11(9),	26.99(8),	28.22(8),	36.89(5),	44.84(6),	36.09(7),	21.10(7),
					1M	=	15.12(7),	88.43(7),	0.76(7),	10.74(7),	51.07(13),	64.99(8),	4.44(7),	0.81(7),	27.33(5),	28.86(7),
					2M	=	28.52(5),									
	-N1F			/	0M	=	13.52(8),	34.39(8),	14.37(8),	4.58(9),	15.87(8),	16.71(8),	25.15(5),	35.69(7),	47.82(7),	16.49(7),
					1M	=	11.64(7),	76.92(7),	0.76(7),	0.93(8),	39.88(13),	76.79(8),	13.46(7),	2.63(7),	16.19(5),	18.19(7),
					2M	=	17.05(5),									
	-021B_b			/	0M	=	46.33(8),	44.52(8),	42.89(8),	65.59(8),	11.05(7),	4.78(7),	12.67(4),	22.63(6),	0.61(7),	66.75(7),
					1M	=	74.54(7),	1.41(6),	88.51(7),	1.48(7),	6.88(13),	0.02(7),	46.27(7),	65.77(7),	10.68(5),	15.95(7),
					2M	=	5.55(5),									

011A	-C11A	/	0M =	72.54(11),	15.39(11),	14.43(11),	37.76(12),	6.55(11),	12.06(11),	23.71(9),	13.84(10),	28.60(10),	55.67(11),
		1M =	58.45(11),	10.96(10),	61.20(10),	21.72(11),	0.46(15),	22.78(11),	72.46(10),	38.56(11),	6.77(9),	0.95(11),	
		2M =	11.21(9),										
011B	-C11B	/	0M =	16.64(11),	70.25(11),	48.13(11),	49.73(12),	4.17(11),	0.79(11),	19.51(9),	1.37(10),	35.99(10),	55.02(11),
		1M =	54.01(11),	39.95(10),	45.61(10),	8.85(11),	14.40(15),	42.90(11),	16.64(10),	47.85(11),	3.69(9),	5.89(11),	
		2M =	0.47(9),										
012A	-C11A	/	0M =	31.30(11),	59.04(12),	40.69(12),	50.53(12),	3.09(11),	8.76(11),	28.24(9),	2.58(10),	21.30(11),	69.58(11),
		1M =	67.42(11),	34.26(10),	55.47(11),	2.23(11),	17.44(15),	30.74(11),	31.31(11),	48.99(11),	3.56(10),	0.19(11),	
		2M =	8.29(10),										
012B	-C11B	/	0M =	57.85(11),	31.89(12),	31.04(12),	54.28(12),	4.33(11),	1.73(11),	17.06(9),	20.36(10),	12.08(11),	64.40(11),
		1M =	70.41(11),	4.88(10),	78.17(11),	8.00(11),	5.18(15),	10.51(11),	57.78(11),	54.88(11),	4.02(10),	9.67(11),	
		2M =	0.91(10),										
021A	-C21A	/	0M =	1.41(11),	27.17(11),	49.59(11),	48.82(12),	64.78(11),	59.42(11),	44.70(9),	77.66(10),	9.77(10),	9.56(11),
		1M =	17.30(11),	35.04(10),	33.15(10),	46.96(11),	63.09(15),	14.96(11),	1.32(10),	50.28(11),	64.61(9),	70.41(11),	
		2M =	60.27(9),										
021B	-C21B	/	0M =	5.62(11),	39.35(11),	62.48(11),	53.97(12),	68.56(11),	62.28(11),	43.50(9),	64.81(10),	24.47(10),	11.71(11),
		1M =	18.90(11),	21.21(10),	32.69(10),	56.41(11),	54.22(15),	0.06(11),	5.71(10),	54.80(11),	68.15(9),	72.79(11),	
		2M =	62.99(9),										
022A	-C21A	/	0M =	49.79(11),	2.34(11),	20.55(11),	3.39(12),	60.00(11),	66.23(11),	78.26(9),	42.14(10),	25.08(11),	38.84(11),
		1M =	32.10(11),	27.23(10),	18.49(11),	64.09(11),	54.29(15),	2.02(11),	49.88(11),	3.93(11),	60.36(10),	54.90(11),	
		2M =	65.44(9),										
022B	-C21B	/	0M =	52.93(11),	1.86(11),	19.28(11),	1.39(12),	57.48(11),	63.65(11),	75.24(9),	39.04(10),	26.64(11),	40.63(11),
		1M =	34.11(11),	24.84(10),	20.93(11),	63.38(11),	51.16(15),	0.05(11),	53.03(11),	1.84(11),	57.82(10),	52.26(11),	
		2M =	62.83(9),										
N1C	-C2C	/	0M =	0.24(11),	47.57(11),	25.25(11),	19.88(11),	12.66(10),	15.37(10),	28.98(9),	26.89(10),	44.12(10),	33.25(10),
		1M =	28.81(10),	69.59(10),	16.56(10),	0.34(10),	35.94(15),	67.18(11),	0.29(10),	17.95(10),	13.07(9),	13.34(10),	
		2M =	15.45(9),										
	-C6C	/	0M =	0.45(14),	69.66(14),	87.15(14),	66.39(15),	43.24(14),	37.97(14),	18.68(13),	35.00(13),	41.97(14),	30.95(14),
		1M =	35.99(14),	8.16(14),	42.65(14),	43.89(14),	24.03(17),	25.49(14),	0.51(14),	65.30(14),	42.76(13),	45.07(14),	
		2M =	38.37(13),										
N1D	-C2D	/	0M =	64.37(14),	0.76(15),	14.85(15),	5.40(15),	47.96(14),	53.78(14),	63.87(13),	27.78(14),	32.38(14),	45.55(14),
		1M =	40.19(14),	15.44(14),	29.08(14),	58.94(14),	39.66(17),	8.11(14),	64.47(14),	5.25(14),	48.23(13),	42.46(14),	
		2M =	52.93(13),										
	-C6D	/	0M =	52.56(11),	0.62(11),	9.76(11),	30.19(11),	8.20(10),	4.26(10),	1.57(9),	32.56(10),	39.68(10),	30.04(10),
		1M =	34.77(10),	38.15(10),	45.12(10),	10.74(10),	22.60(15),	46.23(11),	52.47(10),	31.81(10),	8.16(9),	13.55(10),	
		2M =	5.06(9),										
N1E	-C2E	/	0M =	54.07(14),	18.19(15),	0.68(15),	16.96(15),	40.38(14),	46.63(14),	65.09(13),	28.67(14),	11.59(14),	59.31(14),
		1M =	52.01(14),	31.69(14),	36.81(14),	43.20(14),	43.86(18),	10.93(14),	54.15(14),	16.21(14),	40.81(13),	36.00(14),	
		2M =	45.95(13),										
	-C6E	/	0M =	64.06(11),	5.03(11),	0.44(11),	21.81(11),	6.16(10),	10.06(10),	14.75(8),	18.26(10),	48.41(10),	33.15(10),
		1M =	35.85(10),	29.96(10),	41.56(10),	25.03(10),	9.01(15),	45.26(11),	63.99(10),	23.15(10),	6.20(9),	0.80(10),	
		2M =	9.27(9),										
N1F	-C2F	/	0M =	64.29(14),	20.81(15),	23.32(15),	0.04(15),	31.29(14),	34.33(14),	33.76(13),	6.32(14),	62.57(14),	26.02(14),
		1M =	24.90(14),	17.59(14),	23.34(14),	50.70(14),	12.70(18),	41.60(14),	64.31(14),	0.90(14),	31.27(13),	26.19(14),	
		2M =	33.61(13),										
	-C6F	/	0M =	37.84(14),	9.51(15),	11.63(15),	0.38(15),	55.67(14),	61.23(14),	80.17(13),	48.27(14),	7.83(14),	41.53(14),
		1M =	33.81(14),	44.25(14),	17.83(14),	50.44(14),	63.59(18),	19.39(14),	37.93(14),	0.68(14),	56.14(13),	52.51(14),	
		2M =	60.80(13),										

C1A	-C2A	/	0M =	26.08(14),	63.75(14),	44.14(14),	51.34(14),	0.00(14),	5.46(14),	24.78(12),	1.60(13),	26.56(13),	64.45(13),
		1M =	62.99(14),	36.06(13),	52.67(13),	2.12(14),	15.92(17),	34.89(14),	26.08(13),	49.64(14),	0.47(13),	2.52(13),	
		2M =	5.03(12),										
	-C6A	/	0M =	66.23(11),	15.91(11),	17.77(11),	40.93(11),	0.00(10),	5.38(10),	16.68(8),	20.82(9),	27.89(10),	51.80(10),
		1M =	55.93(10),	16.49(9),	62.52(10),	15.87(10),	7.49(15),	25.90(10),	66.14(10),	41.97(10),	0.21(9),	5.62(10),	
		2M =	4.53(9),										
	-C11A	/	0M =	26.91(13),	41.14(13),	26.02(13),	10.38(14),	2.35(13),	1.99(13),	6.33(11),	19.44(12),	66.69(13),	8.51(13),
		1M =	5.79(13),	57.92(12),	2.43(12),	19.80(13),	21.39(16),	84.17(13),	26.87(12),	8.54(13),	2.06(12),	0.52(13),	
		2M =	1.61(12),										
C1B	-C2B	/	0M =	10.94(14),	70.46(14),	47.37(14),	45.56(14),	4.35(14),	0.15(14),	18.16(12),	3.75(13),	41.50(13),	49.16(13),
		1M =	47.83(14),	44.19(13),	39.54(13),	11.05(14),	15.77(17),	49.03(14),	10.95(13),	43.63(14),	3.88(13),	5.48(13),	
		2M =	0.08(12),										
	-C6B	/	0M =	56.90(14),	31.24(14),	31.52(14),	54.84(14),	6.16(14),	0.15(14),	14.90(12),	22.62(13),	12.62(13),	62.08(13),
		1M =	68.29(14),	7.12(13),	77.84(13),	6.64(14),	7.50(17),	12.13(14),	56.83(13),	55.57(14),	5.86(13),	11.55(14),	
		2M =	0.98(13),										
	-C11B	/	0M =	39.77(10),	25.84(10),	13.65(10),	4.44(11),	0.20(10),	1.20(10),	1.92(8),	24.55(9),	61.49(9),	6.80(9),
		1M =	10.06(9),	52.82(9),	18.59(9),	19.07(10),	21.82(14),	71.66(10),	39.71(9),	6.20(9),	0.37(8),	4.28(9),	
		2M =	0.62(8),										
C2A	-C21A	/	0M =	64.31(13),	21.74(13),	22.49(13),	45.79(14),	1.18(13),	4.50(13),	17.43(11),	20.41(12),	22.17(13),	57.04(13),
		1M =	61.65(13),	11.95(12),	68.28(12),	13.45(13),	6.26(16),	20.10(13),	64.23(12),	46.69(13),	0.94(12),	6.75(13),	
		2M =	3.65(12),										
	-C6A_d	/	0M =	29.45(14),	36.48(14),	21.66(14),	5.73(14),	0.00(14),	0.09(14),	6.82(12),	22.56(13),	64.52(13),	4.96(14),
		1M =	1.89(14),	58.82(13),	6.84(13),	18.06(14),	23.38(17),	83.12(14),	29.41(13),	3.89(14),	0.26(13),	3.20(14),	
		2M =	0.35(13),										
C2B	-C21B	/	0M =	55.45(10),	35.71(10),	33.76(10),	56.77(11),	4.69(10),	1.48(10),	17.64(8),	19.29(9),	8.30(9),	67.45(9),
		1M =	74.00(9),	1.48(9),	81.32(9),	6.56(10),	3.85(14),	6.46(10),	55.39(9),	57.18(9),	4.35(8),	9.89(9),	
		2M =	0.67(8),										
	-C6B_c	/	0M =	40.72(11),	23.54(11),	11.40(11),	6.76(11),	1.46(10),	0.15(10),	2.22(8),	26.00(9),	59.50(10),	8.50(10),
		1M =	11.94(10),	52.55(9),	20.75(10),	17.92(10),	22.67(15),	69.88(10),	40.66(10),	8.52(10),	1.61(9),	5.67(10),	
		2M =	0.45(9),										
C2C	-C3C	/	0M =	0.39(14),	9.56(14),	32.14(14),	32.73(14),	60.31(14),	57.89(14),	51.41(12),	84.01(13),	3.02(14),	2.70(14),
		1M =	5.08(14),	52.31(13),	21.63(13),	40.76(14),	75.42(17),	30.14(14),	0.48(13),	34.39(14),	60.44(13),	64.49(14),	
		2M =	58.61(13),										
C2D	-C3D	/	0M =	7.89(14),	0.19(14),	22.86(14),	21.17(15),	58.82(14),	58.87(14),	59.07(12),	74.14(13),	5.58(14),	14.26(14),
		1M =	6.52(14),	59.30(13),	10.06(13),	40.85(14),	82.22(17),	34.25(14),	7.99(14),	22.77(14),	59.12(13),	61.09(14),	
		2M =	59.35(13),										
C2E	-C3E	/	0M =	3.51(14),	21.73(14),	0.28(14),	5.16(15),	33.66(14),	34.49(14),	41.34(12),	52.07(13),	30.16(14),	18.29(14),
		1M =	11.76(14),	84.33(13),	3.42(13),	16.74(14),	57.70(17),	59.14(14),	3.43(14),	7.05(14),	33.99(13),	35.80(14),	
		2M =	34.85(13),										
C2F	-C3F	/	0M =	17.56(14),	30.39(14),	11.17(14),	0.20(14),	16.36(14),	16.63(14),	23.42(12),	37.55(13),	48.05(14),	11.57(14),
		1M =	6.63(14),	75.32(13),	5.76(13),	1.27(14),	40.06(17),	76.59(14),	17.50(13),	1.74(14),	16.64(13),	19.14(14),	
		2M =	17.03(13),										
C3C	-C4C	/	0M =	0.79(14),	70.13(14),	86.60(14),	67.54(14),	42.40(14),	37.06(14),	17.73(12),	34.76(13),	41.06(14),	32.16(14),
		1M =	37.23(14),	8.25(13),	43.88(13),	42.72(14),	23.52(17),	25.12(14),	0.74(13),	66.40(14),	41.92(13),	44.36(14),	
		2M =	37.48(13),										
C3D	-C4D	/	0M =	53.10(14),	0.50(14),	8.47(14),	28.97(14),	7.11(14),	3.24(14),	2.27(12),	31.55(13),	40.97(13),	29.62(14),
		1M =	34.19(14),	38.24(13),	44.23(13),	11.89(14),	21.83(17),	47.03(14),	53.01(13),	30.58(14),	7.07(13),	12.44(14),	
		2M =	4.03(13),										

C3E	-C4E	/	0M =	64.25(14),	4.26(14),	0.31(14),	22.58(14),	5.77(14),	9.73(14),	14.67(12),	18.58(13),	47.64(13),	33.76(14),
			1M =	36.53(14),	29.67(13),	42.32(13),	24.57(14),	9.16(17),	44.67(14),	64.17(13),	23.91(14),	5.82(13),	0.39(14),
			2M =	8.93(13),									
C3F	-C4F	/	0M =	38.02(18),	8.85(18),	12.26(18),	0.11(18),	56.27(18),	61.86(18),	80.86(17),	48.52(17),	8.44(17),	41.13(18),
			1M =	33.43(18),	43.78(17),	17.50(17),	51.13(18),	63.8(2),	18.84(18),	38.11(17),	1.16(18),	56.74(17),	53.06(18),
			2M =	61.43(17),									
C4C	-C5C	/	0M =	0.58(14),	47.71(14),	25.51(14),	19.78(14),	12.09(14),	14.74(14),	28.22(12),	26.60(13),	44.95(14),	32.57(14),
			1M =	28.21(14),	69.51(13),	16.10(13),	1.05(14),	35.45(17),	67.99(14),	0.54(13),	17.84(14),	12.50(13),	12.84(14),
			2M =	14.83(13),									
C4D	-C5D	/	0M =	65.27(14),	0.63(14),	13.33(14),	6.92(14),	46.63(14),	52.50(14),	63.23(12),	26.77(13),	31.53(14),	47.05(14),
			1M =	41.72(14),	15.55(13),	30.56(13),	57.41(14),	38.92(17),	7.68(14),	65.36(13),	6.76(14),	46.91(13),	41.15(14),
			2M =	51.65(13),									
C4E	-C5E	/	0M =	54.24(14),	17.00(14),	0.53(14),	15.85(14),	41.48(14),	47.73(14),	66.07(12),	29.42(13),	12.49(14),	58.21(14),
			1M =	50.96(14),	31.42(13),	35.88(13),	44.41(14),	44.51(17),	10.33(14),	54.32(13),	15.12(14),	41.90(13),	37.05(14),
			2M =	47.05(13),									
C4F	-C5F	/	0M =	64.26(18),	20.87(18),	23.50(18),	0.21(18),	31.60(18),	34.63(18),	34.03(17),	6.62(17),	62.52(17),	26.02(17),
			1M =	24.86(18),	17.34(17),	23.21(17),	50.99(18),	13.0(2),	41.39(18),	64.27(17),	0.72(18),	31.57(17),	26.49(18),
			2M =	33.91(17),									
C5C	-C6C	/	0M =	0.03(14),	12.16(14),	34.70(14),	35.21(14),	61.42(14),	58.52(14),	50.62(12),	86.15(13),	1.23(14),	0.77(14),
			1M =	7.02(14),	49.80(13),	23.54(13),	41.82(14),	74.06(17),	28.02(14),	0.06(13),	36.85(14),	61.51(13),	65.91(14),
			2M =	59.28(13),									
C5D	-C6D	/	0M =	4.44(14),	0.08(14),	22.95(14),	22.72(14),	56.77(14),	56.29(14),	55.63(12),	74.98(13),	7.76(14),	11.56(14),
			1M =	3.87(14),	60.47(13),	12.72(13),	38.30(14),	79.19(17),	36.16(14),	4.53(13),	24.39(14),	57.04(13),	59.55(14),
			2M =	56.83(13),									
C5E	-C6E	/	0M =	6.60(14),	21.75(14),	0.16(14),	5.93(15),	31.66(14),	32.20(14),	38.40(13),	51.14(13),	32.50(14),	15.87(14),
			1M =	9.50(14),	84.25(13),	5.39(14),	14.33(14),	55.56(17),	61.38(14),	6.53(14),	7.85(14),	31.97(13),	34.07(14),
			2M =	32.58(13),									
C5F	-C6F	/	0M =	14.99(14),	29.32(14),	9.45(14),	0.46(15),	19.27(14),	19.66(14),	26.56(12),	40.03(13),	45.03(14),	13.08(14),
			1M =	7.85(14),	78.41(13),	5.10(13),	1.79(14),	43.06(17),	73.79(14),	14.92(14),	2.41(14),	19.57(13),	21.93(14),
			2M =	20.06(13),									
Cu1_a	-01_a	/	0M =	52.60(8),	41.30(8),	29.62(8),	48.29(8),	8.93(7),	15.20(7),	33.69(4),	0.74(6),	0.05(7),	88.27(7),
			1M =	83.42(7),	18.89(6),	67.08(7),	14.73(7),	15.01(13),	9.96(7),	52.60(7),	47.65(7),	9.35(5),	4.49(7),
			2M =	14.50(5),									
	-011A_a	/	0M =	39.38(8),	43.45(8),	37.87(8),	16.81(8),	24.16(7),	24.29(7),	15.82(4),	0.92(6),	87.30(6),	0.96(7),
			1M =	0.87(7),	35.43(6),	3.05(6),	42.21(7),	0.82(13),	61.72(7),	39.37(6),	15.35(7),	23.91(5),	20.75(7),
			2M =	23.86(4),									
	-011B_a	/	0M =	37.42(8),	44.82(8),	38.18(8),	17.57(8),	22.70(7),	22.64(7),	13.78(4),	0.23(6),	87.14(7),	0.96(7),
			1M =	0.87(7),	37.28(6),	1.77(7),	40.49(7),	0.80(13),	63.57(7),	37.42(7),	16.06(7),	22.44(5),	19.43(7),
			2M =	22.23(5),									
	-N1C_a	/	0M =	0.43(8),	13.94(8),	36.45(8),	36.95(9),	61.98(8),	58.75(8),	49.90(5),	87.03(7),	0.07(7),	0.63(7),
			1M =	8.43(7),	48.10(7),	24.92(7),	42.39(8),	72.87(13),	26.61(8),	0.34(7),	38.57(7),	62.04(5),	66.69(7),
			2M =	59.52(5),									
	-N1D_a	/	0M =	6.80(8),	7.93(8),	30.96(8),	28.75(9),	64.45(8),	63.02(8),	57.91(5),	81.85(7),	0.07(7),	8.36(7),
			1M =	0.56(7),	52.03(7),	15.92(7),	45.33(8),	81.78(13),	28.01(8),	6.90(7),	30.29(7),	64.66(5),	67.72(7),
			2M =	63.66(5),									
Cu2_a	-021B	/	0M =	46.33(8),	44.52(8),	42.89(8),	65.59(8),	11.05(7),	4.78(7),	12.67(4),	22.63(6),	0.61(7),	66.75(7),
			1M =	74.54(7),	1.41(6),	88.51(7),	1.48(7),	6.88(13),	0.02(7),	46.27(7),	65.77(7),	10.68(5),	15.95(7),
			2M =	5.55(5),									

	-O2_a	/	0M =	42.34(8),	34.27(8),	47.42(8),	25.13(8),	59.84(7),	60.71(7),	50.12(4),	35.15(6),	54.40(7),	12.11(7),
			1M =	7.51(7),	0.83(6),	0.49(7),	78.68(7),	37.23(13),	25.40(7),	42.41(7),	24.77(7),	59.67(5),	55.52(7),
			2M =	60.24(5),									
	-O21A_a	/	0M =	50.24(8),	39.93(8),	38.94(8),	61.99(8),	9.24(7),	3.02(7),	13.70(4),	22.58(6),	3.97(7),	65.98(7),
			1M =	73.43(7),	1.40(6),	86.39(7),	1.48(7),	6.95(13),	4.10(7),	50.18(7),	62.40(7),	8.89(5),	14.33(7),
			2M =	3.82(5),									
	-N1E_a	/	0M =	4.51(8),	28.72(8),	6.89(8),	1.11(9),	26.99(8),	28.22(8),	36.89(5),	44.84(6),	36.09(7),	21.10(7),
			1M =	15.12(7),	88.43(7),	0.76(7),	10.74(7),	51.07(13),	64.99(8),	4.44(7),	0.81(7),	27.33(5),	28.86(7),
			2M =	28.52(5),									
	-N1F_a	/	0M =	13.52(8),	34.39(8),	14.37(8),	4.58(9),	15.87(8),	16.71(8),	25.15(5),	35.69(7),	47.82(7),	16.49(7),
			1M =	11.64(7),	76.92(7),	0.76(7),	0.93(8),	39.88(13),	76.79(8),	13.46(7),	2.63(7),	16.19(5),	18.19(7),
			2M =	17.05(5),									
011A_a-C11A_a	/	0M =	72.54(11),	15.39(11),	14.43(11),	37.76(12),	6.55(11),	12.06(11),	23.71(9),	13.84(10),	28.60(10),	55.67(11),	
		1M =	58.45(11),	10.96(10),	61.20(10),	21.72(11),	0.46(15),	22.78(11),	72.46(10),	38.56(11),	6.77(9),	0.95(11),	
		2M =	11.21(9),										
011B_a-C11B_a	/	0M =	16.64(11),	70.25(11),	48.13(11),	49.73(12),	4.17(11),	0.79(11),	19.51(9),	1.37(10),	35.99(10),	55.02(11),	
		1M =	54.01(11),	39.95(10),	45.61(10),	8.85(11),	14.40(15),	42.90(11),	16.64(10),	47.85(11),	3.69(9),	5.89(11),	
		2M =	0.47(9),										
012A_a-C11A_a	/	0M =	31.30(11),	59.04(12),	40.69(12),	50.53(12),	3.09(11),	8.76(11),	28.24(9),	2.58(10),	21.30(11),	69.58(11),	
		1M =	67.42(11),	34.26(10),	55.47(11),	2.23(11),	17.44(15),	30.74(11),	31.31(11),	48.99(11),	3.56(10),	0.19(11),	
		2M =	8.29(10),										
012B_a-C11B_a	/	0M =	57.85(11),	31.89(12),	31.04(12),	54.28(12),	4.33(11),	1.73(11),	17.06(9),	20.36(10),	12.08(11),	64.40(11),	
		1M =	70.41(11),	4.88(10),	78.17(11),	8.00(11),	5.18(15),	10.51(11),	57.78(11),	54.88(11),	4.02(10),	9.67(11),	
		2M =	0.91(10),										
021A_a-C21A_a	/	0M =	1.41(11),	27.17(11),	49.59(11),	48.82(12),	64.78(11),	59.42(11),	44.70(9),	77.66(10),	9.77(10),	9.56(11),	
		1M =	17.30(11),	35.04(10),	33.15(10),	46.96(11),	63.09(15),	14.96(11),	1.32(10),	50.28(11),	64.61(9),	70.41(11),	
		2M =	60.27(9),										
021B_a-C21B_a	/	0M =	5.62(11),	39.35(11),	62.48(11),	53.97(12),	68.56(11),	62.28(11),	43.50(9),	64.81(10),	24.47(10),	11.71(11),	
		1M =	18.90(11),	21.21(10),	32.69(10),	56.41(11),	54.22(15),	0.06(11),	5.71(10),	54.80(11),	68.15(9),	72.79(11),	
		2M =	62.99(9),										
022A_a-C21A_a	/	0M =	49.79(11),	2.34(11),	20.55(11),	3.39(12),	60.00(11),	66.23(11),	78.26(9),	42.14(10),	25.08(11),	38.84(11),	
		1M =	32.10(11),	27.23(10),	18.49(11),	64.09(11),	54.29(15),	2.02(11),	49.88(11),	3.93(11),	60.36(10),	54.90(11),	
		2M =	65.44(9),										
022B_a-C21B_a	/	0M =	52.93(11),	1.86(11),	19.28(11),	1.39(12),	57.48(11),	63.65(11),	75.24(9),	39.04(10),	26.64(11),	40.63(11),	
		1M =	34.11(11),	24.84(10),	20.93(11),	63.38(11),	51.16(15),	0.05(11),	53.03(11),	1.84(11),	57.82(10),	52.26(11),	
		2M =	62.83(9),										
N1C_a -C2C_a	/	0M =	0.24(11),	47.57(11),	25.25(11),	19.88(11),	12.66(10),	15.37(10),	28.98(9),	26.89(10),	44.12(10),	33.25(10),	
		1M =	28.81(10),	69.59(10),	16.56(10),	0.34(10),	35.94(15),	67.18(11),	0.29(10),	17.95(10),	13.07(9),	13.34(10),	
		2M =	15.45(9),										
	-C6C_a	/	0M =	0.45(14),	69.66(14),	87.15(14),	66.39(15),	43.24(14),	37.97(14),	18.68(13),	35.00(13),	41.97(14),	30.95(14),
		1M =	35.99(14),	8.16(14),	42.65(14),	43.89(14),	24.03(17),	25.49(14),	0.51(14),	65.30(14),	42.76(13),	45.07(14),	
		2M =	38.37(13),										
N1D_a -C2D_a	/	0M =	64.37(14),	0.76(15),	14.85(15),	5.40(15),	47.96(14),	53.78(14),	63.87(13),	27.78(14),	32.38(14),	45.55(14),	
		1M =	40.19(14),	15.44(14),	29.08(14),	58.94(14),	39.66(17),	8.11(14),	64.47(14),	5.25(14),	48.23(13),	42.46(14),	
		2M =	52.93(13),										
	-C6D_a	/	0M =	52.56(11),	0.62(11),	9.76(11),	30.19(11),	8.20(10),	4.26(10),	1.57(9),	32.56(10),	39.68(10),	30.04(10),
		1M =	34.77(10),	38.15(10),	45.12(10),	10.74(10),	22.60(15),	46.23(11),	52.47(10),	31.81(10),	8.16(9),	13.55(10),	
		2M =	5.06(9),										

N1E_a	-C2E_a	/	0M =	54.07(14),	18.19(15),	0.68(15),	16.96(15),	40.38(14),	46.63(14),	65.09(13),	28.67(14),	11.59(14),	59.31(14),
		1M =	52.01(14),	31.69(14),	36.81(14),	43.20(14),	43.86(18),	10.93(14),	54.15(14),	16.21(14),	40.81(13),	36.00(14),	
		2M =	45.95(13),										
	-C6E_a	/	0M =	64.06(11),	5.03(11),	0.44(11),	21.81(11),	6.16(10),	10.06(10),	14.75(8),	18.26(10),	48.41(10),	33.15(10),
		1M =	35.85(10),	29.96(10),	41.56(10),	25.03(10),	9.01(15),	45.26(11),	63.99(10),	23.15(10),	6.20(9),	0.80(10),	
		2M =	9.27(9),										
N1F_a	-C2F_a	/	0M =	64.29(14),	20.81(15),	23.32(15),	0.04(15),	31.29(14),	34.33(14),	33.76(13),	6.32(14),	62.57(14),	26.02(14),
		1M =	24.90(14),	17.59(14),	23.34(14),	50.70(14),	12.70(18),	41.60(14),	64.31(14),	0.90(14),	31.27(13),	26.19(14),	
		2M =	33.61(13),										
	-C6F_a	/	0M =	37.84(14),	9.51(15),	11.63(15),	0.38(15),	55.67(14),	61.23(14),	80.17(13),	48.27(14),	7.83(14),	41.53(14),
		1M =	33.81(14),	44.25(14),	17.83(14),	50.44(14),	63.59(18),	19.39(14),	37.93(14),	0.68(14),	56.14(13),	52.51(14),	
		2M =	60.80(13),										
C1A_a	-C2A_a	/	0M =	26.08(14),	63.75(14),	44.14(14),	51.34(14),	0.00(14),	5.46(14),	24.78(12),	1.60(13),	26.56(13),	64.45(13),
		1M =	62.99(14),	36.06(13),	52.67(13),	2.12(14),	15.92(17),	34.89(14),	26.08(13),	49.64(14),	0.47(13),	2.52(13),	
		2M =	5.03(12),										
	-C6A_a	/	0M =	66.23(11),	15.91(11),	17.77(11),	40.93(11),	0.00(10),	5.38(10),	16.68(8),	20.82(9),	27.89(10),	51.80(10),
		1M =	55.93(10),	16.49(9),	62.52(10),	15.87(10),	7.49(15),	25.90(10),	66.14(10),	41.97(10),	0.21(9),	5.62(10),	
		2M =	4.53(9),										
-C11A_a	/	0M =	26.91(13),	41.14(13),	26.02(13),	10.38(14),	2.35(13),	1.99(13),	6.33(11),	19.44(12),	66.69(13),	8.51(13),	
	1M =	5.79(13),	57.92(12),	2.43(12),	19.80(13),	21.39(16),	84.17(13),	26.87(12),	8.54(13),	2.06(12),	0.52(13),		
	2M =	1.61(12),											
C1B_a	-C2B_a	/	0M =	10.94(14),	70.46(14),	47.37(14),	45.56(14),	4.35(14),	0.15(14),	18.16(12),	3.75(13),	41.50(13),	49.16(13),
		1M =	47.83(14),	44.19(13),	39.54(13),	11.05(14),	15.77(17),	49.03(14),	10.95(13),	43.63(14),	3.88(13),	5.48(13),	
		2M =	0.08(12),										
	-C6B_a	/	0M =	56.90(14),	31.24(14),	31.52(14),	54.84(14),	6.16(14),	0.15(14),	14.90(12),	22.62(13),	12.62(13),	62.08(13),
		1M =	68.29(14),	7.12(13),	77.84(13),	6.64(14),	7.50(17),	12.13(14),	56.83(13),	55.57(14),	5.86(13),	11.55(14),	
		2M =	0.98(13),										
-C11B_a	/	0M =	39.77(10),	25.84(10),	13.65(10),	4.44(11),	0.20(10),	1.20(10),	1.92(8),	24.55(9),	61.49(9),	6.80(9),	
	1M =	10.06(9),	52.82(9),	18.59(9),	19.07(10),	21.82(14),	71.66(10),	39.71(9),	6.20(9),	0.37(8),	4.28(9),		
	2M =	0.62(8),											
C2A_a	-C21A_a	/	0M =	64.31(13),	21.74(13),	22.49(13),	45.79(14),	1.18(13),	4.50(13),	17.43(11),	20.41(12),	22.17(13),	57.04(13),
		1M =	61.65(13),	11.95(12),	68.28(12),	13.45(13),	6.26(16),	20.10(13),	64.23(12),	46.69(13),	0.94(12),	6.75(13),	
		2M =	3.65(12),										
C2B_a	-C21B_a	/	0M =	55.45(10),	35.71(10),	33.76(10),	56.77(11),	4.69(10),	1.48(10),	17.64(8),	19.29(9),	8.30(9),	67.45(9),
		1M =	74.00(9),	1.48(9),	81.32(9),	6.56(10),	3.85(14),	6.46(10),	55.39(9),	57.18(9),	4.35(8),	9.89(9),	
		2M =	0.67(8),										
C2C_a	-C3C_a	/	0M =	0.39(14),	9.56(14),	32.14(14),	32.73(14),	60.31(14),	57.89(14),	51.41(12),	84.01(13),	3.02(14),	2.70(14),
		1M =	5.08(14),	52.31(13),	21.63(13),	40.76(14),	75.42(17),	30.14(14),	0.48(13),	34.39(14),	60.44(13),	64.49(14),	
		2M =	58.61(13),										
C2D_a	-C3D_a	/	0M =	7.89(14),	0.19(14),	22.86(14),	21.17(15),	58.82(14),	58.87(14),	59.07(12),	74.14(13),	5.58(14),	14.26(14),
		1M =	6.52(14),	59.30(13),	10.06(13),	40.85(14),	82.22(17),	34.25(14),	7.99(14),	22.77(14),	59.12(13),	61.09(14),	
		2M =	59.35(13),										
C2E_a	-C3E_a	/	0M =	3.51(14),	21.73(14),	0.28(14),	5.16(15),	33.66(14),	34.49(14),	41.34(12),	52.07(13),	30.16(14),	18.29(14),
		1M =	11.76(14),	84.33(13),	3.42(13),	16.74(14),	57.70(17),	59.14(14),	3.43(14),	7.05(14),	33.99(13),	35.80(14),	
		2M =	34.85(13),										
C2F_a	-C3F_a	/	0M =	17.56(14),	30.39(14),	11.17(14),	0.20(14),	16.36(14),	16.63(14),	23.42(12),	37.55(13),	48.05(14),	11.57(14),
		1M =	6.63(14),	75.32(13),	5.76(13),	1.27(14),	40.06(17),	76.59(14),	17.50(13),	1.74(14),	16.64(13),	19.14(14),	
		2M =	17.03(13),										

[illegible]

Cu2_b	-N1D_b	/	0M =	6.80(8),	7.93(8),	30.96(8),	28.75(9),	64.45(8),	63.02(8),	57.91(5),	81.85(7),	0.07(7),	8.36(7),
			1M =	0.56(7),	52.03(7),	15.92(7),	45.33(8),	81.78(13),	28.01(8),	6.90(7),	30.29(7),	64.66(5),	67.72(7),
			2M =	63.66(5),									
	-O2_b	/	0M =	42.34(8),	34.27(8),	47.42(8),	25.13(8),	59.84(7),	60.71(7),	50.12(4),	35.15(6),	54.40(7),	12.11(7),
			1M =	7.51(7),	0.83(6),	0.49(7),	78.68(7),	37.23(13),	25.40(7),	42.41(7),	24.77(7),	59.67(5),	55.52(7),
			2M =	60.24(5),									
	-O21A_b	/	0M =	50.24(8),	39.93(8),	38.94(8),	61.99(8),	9.24(7),	3.02(7),	13.70(4),	22.58(6),	3.97(7),	65.98(7),
			1M =	73.43(7),	1.40(6),	86.39(7),	1.48(7),	6.95(13),	4.10(7),	50.18(7),	62.40(7),	8.89(5),	14.33(7),
			2M =	3.82(5),									
	-N1E_b	/	0M =	4.51(8),	28.72(8),	6.89(8),	1.11(9),	26.99(8),	28.22(8),	36.89(5),	44.84(6),	36.09(7),	21.10(7),
			1M =	15.12(7),	88.43(7),	0.76(7),	10.74(7),	51.07(13),	64.99(8),	4.44(7),	0.81(7),	27.33(5),	28.86(7),
			2M =	28.52(5),									
	-N1F_b	/	0M =	13.52(8),	34.39(8),	14.37(8),	4.58(9),	15.87(8),	16.71(8),	25.15(5),	35.69(7),	47.82(7),	16.49(7),
			1M =	11.64(7),	76.92(7),	0.76(7),	0.93(8),	39.88(13),	76.79(8),	13.46(7),	2.63(7),	16.19(5),	18.19(7),
			2M =	17.05(5),									
O11A_b-C11A_b	/	0M =	72.54(11),	15.39(11),	14.43(11),	37.76(12),	6.55(11),	12.06(11),	23.71(9),	13.84(10),	28.60(10),	55.67(11),	
			1M =	58.45(11),	10.96(10),	61.20(10),	21.72(11),	0.46(15),	22.78(11),	72.46(10),	38.56(11),	6.77(9),	0.95(11),
			2M =	11.21(9),									
O11B_b-C11B_b	/	0M =	16.64(11),	70.25(11),	48.13(11),	49.73(12),	4.17(11),	0.79(11),	19.51(9),	1.37(10),	35.99(10),	55.02(11),	
			1M =	54.01(11),	39.95(10),	45.61(10),	8.85(11),	14.40(15),	42.90(11),	16.64(10),	47.85(11),	3.69(9),	5.89(11),
			2M =	0.47(9),									
O12A_b-C11A_b	/	0M =	31.30(11),	59.04(12),	40.69(12),	50.53(12),	3.09(11),	8.76(11),	28.24(9),	2.58(10),	21.30(11),	69.58(11),	
			1M =	67.42(11),	34.26(10),	55.47(11),	2.23(11),	17.44(15),	30.74(11),	31.31(11),	48.99(11),	3.56(10),	0.19(11),
			2M =	8.29(10),									
O12B_b-C11B_b	/	0M =	57.85(11),	31.89(12),	31.04(12),	54.28(12),	4.33(11),	1.73(11),	17.06(9),	20.36(10),	12.08(11),	64.40(11),	
			1M =	70.41(11),	4.88(10),	78.17(11),	8.00(11),	5.18(15),	10.51(11),	57.78(11),	54.88(11),	4.02(10),	9.67(11),
			2M =	0.91(10),									
O21A_b-C21A_b	/	0M =	1.41(11),	27.17(11),	49.59(11),	48.82(12),	64.78(11),	59.42(11),	44.70(9),	77.66(10),	9.77(10),	9.56(11),	
			1M =	17.30(11),	35.04(10),	33.15(10),	46.96(11),	63.09(15),	14.96(11),	1.32(10),	50.28(11),	64.61(9),	70.41(11),
			2M =	60.27(9),									
O21B_b-C21B_b	/	0M =	5.62(11),	39.35(11),	62.48(11),	53.97(12),	68.56(11),	62.28(11),	43.50(9),	64.81(10),	24.47(10),	11.71(11),	
			1M =	18.90(11),	21.21(10),	32.69(10),	56.41(11),	54.22(15),	0.06(11),	5.71(10),	54.80(11),	68.15(9),	72.79(11),
			2M =	62.99(9),									
O22A_b-C21A_b	/	0M =	49.79(11),	2.34(11),	20.55(11),	3.39(12),	60.00(11),	66.23(11),	78.26(9),	42.14(10),	25.08(11),	38.84(11),	
			1M =	32.10(11),	27.23(10),	18.49(11),	64.09(11),	54.29(15),	2.02(11),	49.88(11),	3.93(11),	60.36(10),	54.90(11),
			2M =	65.44(9),									
O22B_b-C21B_b	/	0M =	52.93(11),	1.86(11),	19.28(11),	1.39(12),	57.48(11),	63.65(11),	75.24(9),	39.04(10),	26.64(11),	40.63(11),	
			1M =	34.11(11),	24.84(10),	20.93(11),	63.38(11),	51.16(15),	0.05(11),	53.03(11),	1.84(11),	57.82(10),	52.26(11),
			2M =	62.83(9),									
N1C_b	-C2C_b	/	0M =	0.24(11),	47.57(11),	25.25(11),	19.88(11),	12.66(10),	15.37(10),	28.98(9),	26.89(10),	44.12(10),	33.25(10),
			1M =	28.81(10),	69.59(10),	16.56(10),	0.34(10),	35.94(15),	67.18(11),	0.29(10),	17.95(10),	13.07(9),	13.34(10),
			2M =	15.45(9),									
	-C6C_b	/	0M =	0.45(14),	69.66(14),	87.15(14),	66.39(15),	43.24(14),	37.97(14),	18.68(13),	35.00(13),	41.97(14),	30.95(14),
			1M =	35.99(14),	8.16(14),	42.65(14),	43.89(14),	24.03(17),	25.49(14),	0.51(14),	65.30(14),	42.76(13),	45.07(14),
			2M =	38.37(13),									
N1D_b	-C2D_b	/	0M =	64.37(14),	0.76(15),	14.85(15),	5.40(15),	47.96(14),	53.78(14),	63.87(13),	27.78(14),	32.38(14),	45.55(14),
			1M =	40.19(14),	15.44(14),	29.08(14),	58.94(14),	39.66(17),	8.11(14),	64.47(14),	5.25(14),	48.23(13),	42.46(14),
			2M =	52.93(13),									

N1E_b	-C6D_b	/	0M =	52.56(11),	0.62(11),	9.76(11),	30.19(11),	8.20(10),	4.26(10),	1.57(9),	32.56(10),	39.68(10),	30.04(10),
			1M =	34.77(10),	38.15(10),	45.12(10),	10.74(10),	22.60(15),	46.23(11),	52.47(10),	31.81(10),	8.16(9),	13.55(10),
			2M =	5.06(9),									
	-C2E_b	/	0M =	54.07(14),	18.19(15),	0.68(15),	16.96(15),	40.38(14),	46.63(14),	65.09(13),	28.67(14),	11.59(14),	59.31(14),
			1M =	52.01(14),	31.69(14),	36.81(14),	43.20(14),	43.86(18),	10.93(14),	54.15(14),	16.21(14),	40.81(13),	36.00(14),
			2M =	45.95(13),									
N1F_b	-C6E_b	/	0M =	64.06(11),	5.03(11),	0.44(11),	21.81(11),	6.16(10),	10.06(10),	14.75(8),	18.26(10),	48.41(10),	33.15(10),
			1M =	35.85(10),	29.96(10),	41.56(10),	25.03(10),	9.01(15),	45.26(11),	63.99(10),	23.15(10),	6.20(9),	0.80(10),
			2M =	9.26(9),									
	-C2F_b	/	0M =	64.29(14),	20.81(15),	23.32(15),	0.04(15),	31.29(14),	34.33(14),	33.76(13),	6.32(14),	62.57(14),	26.02(14),
			1M =	24.90(14),	17.59(14),	23.34(14),	50.70(14),	12.70(18),	41.60(14),	64.31(14),	0.90(14),	31.27(13),	26.19(14),
			2M =	33.61(13),									
C1A_b	-C6F_b	/	0M =	37.84(14),	9.51(15),	11.63(15),	0.39(15),	55.67(14),	61.23(14),	80.17(13),	48.27(14),	7.83(14),	41.53(14),
			1M =	33.81(14),	44.25(14),	17.83(14),	50.44(14),	63.59(18),	19.39(14),	37.93(14),	0.68(14),	56.14(13),	52.51(14),
			2M =	60.80(13),									
	-C2A_b	/	0M =	26.08(14),	63.75(14),	44.14(14),	51.34(14),	0.00(14),	5.46(14),	24.78(12),	1.60(13),	26.56(13),	64.45(13),
			1M =	62.99(14),	36.06(13),	52.67(13),	2.12(14),	15.92(17),	34.89(14),	26.08(13),	49.64(14),	0.47(13),	2.52(13),
			2M =	5.03(12),									
C1B_b	-C6A_b	/	0M =	66.23(11),	15.91(11),	17.77(11),	40.93(11),	0.00(10),	5.38(10),	16.68(8),	20.82(9),	27.89(10),	51.80(10),
			1M =	55.93(10),	16.49(9),	62.52(10),	15.87(10),	7.49(15),	25.90(10),	66.14(10),	41.97(10),	0.21(9),	5.62(10),
			2M =	4.53(9),									
	-C11A_b	/	0M =	26.91(13),	41.14(13),	26.02(13),	10.38(14),	2.35(13),	1.99(13),	6.33(11),	19.44(12),	66.69(13),	8.51(13),
			1M =	5.79(13),	57.92(12),	2.43(12),	19.80(13),	21.39(16),	84.17(13),	26.87(12),	8.54(13),	2.06(12),	0.52(13),
			2M =	1.61(12),									
C2A_b	-C2B_b	/	0M =	10.94(14),	70.46(14),	47.37(14),	45.56(14),	4.35(14),	0.15(14),	18.16(12),	3.75(13),	41.50(13),	49.16(13),
			1M =	47.83(14),	44.19(13),	39.54(13),	11.05(14),	15.77(17),	49.03(14),	10.95(13),	43.63(14),	3.88(13),	5.48(13),
			2M =	0.08(12),									
	-C6B_b	/	0M =	56.90(14),	31.24(14),	31.52(14),	54.84(14),	6.16(14),	0.15(14),	14.90(12),	22.62(13),	12.62(13),	62.08(13),
			1M =	68.29(14),	7.12(13),	77.84(13),	6.64(14),	7.50(17),	12.13(14),	56.83(13),	55.57(14),	5.86(13),	11.55(14),
			2M =	0.98(13),									
C2B_b	-C11B_b	/	0M =	39.77(10),	25.84(10),	13.65(10),	4.44(11),	0.20(10),	1.20(10),	1.92(8),	24.55(9),	61.49(9),	6.80(9),
			1M =	10.06(9),	52.82(9),	18.59(9),	19.07(10),	21.82(14),	71.66(10),	39.71(9),	6.20(9),	0.37(8),	4.28(9),
			2M =	0.62(8),									
	-C21A_b	/	0M =	64.31(13),	21.74(13),	22.49(13),	45.79(14),	1.18(13),	4.50(13),	17.43(11),	20.41(12),	22.17(13),	57.04(13),
			1M =	61.65(13),	11.95(12),	68.28(12),	13.45(13),	6.26(16),	20.10(13),	64.23(12),	46.69(13),	0.94(12),	6.75(13),
			2M =	3.65(12),									
C2C_b	-C21B_b	/	0M =	55.45(10),	35.71(10),	33.76(10),	56.77(11),	4.69(10),	1.48(10),	17.64(8),	19.29(9),	8.30(9),	67.45(9),
			1M =	74.00(9),	1.48(9),	81.32(9),	6.56(10),	3.85(14),	6.46(10),	55.39(9),	57.18(9),	4.35(8),	9.89(9),
			2M =	0.67(8),									
	-C3C_b	/	0M =	0.39(14),	9.56(14),	32.14(14),	32.73(14),	60.31(14),	57.89(14),	51.41(12),	84.01(13),	3.02(14),	2.70(14),
			1M =	5.08(14),	52.31(13),	21.63(13),	40.76(14),	75.42(17),	30.14(14),	0.48(13),	34.39(14),	60.44(13),	64.49(14),
			2M =	58.61(13),									
C2D_b	-C3D_b	/	0M =	7.90(14),	0.19(14),	22.86(14),	21.17(15),	58.82(14),	58.87(14),	59.07(12),	74.14(13),	5.58(14),	14.26(14),
			1M =	6.52(14),	59.30(13),	10.06(13),	40.85(14),	82.22(17),	34.25(14),	7.99(14),	22.77(14),	59.12(13),	61.09(14),
			2M =	59.35(13),									
	-C3E_b	/	0M =	3.51(14),	21.73(14),	0.28(14),	5.16(15),	33.66(14),	34.49(14),	41.34(12),	52.07(13),	30.16(14),	18.29(14),
			1M =	11.76(14),	84.33(13),	3.42(13),	16.74(14),	57.70(17),	59.14(14),	3.43(14),	7.05(14),	33.99(13),	35.80(14),
			2M =	34.85(13),									

[illegible]

N1D_c	-C2D_c	/	0M =	64.37(14),	0.76(15),	14.85(15),	5.40(15),	47.96(14),	53.78(14),	63.87(13),	27.78(14),	32.38(14),	45.55(14),
		1M =	40.19(14),	15.44(14),	29.08(14),	58.94(14),	39.66(17),	8.11(14),	64.47(14),	5.25(14),	48.23(13),	42.46(14),	
		2M =	52.93(13),										
	-C6D_c	/	0M =	52.56(11),	0.62(11),	9.76(11),	30.19(11),	8.20(10),	4.26(10),	1.57(9),	32.56(10),	39.68(10),	30.04(10),
		1M =	34.77(10),	38.15(10),	45.12(10),	10.74(10),	22.60(15),	46.23(11),	52.47(10),	31.81(10),	8.16(9),	13.55(10),	
		2M =	5.06(9),										
N1E_c	-C2E_c	/	0M =	54.07(14),	18.19(15),	0.68(15),	16.96(15),	40.38(14),	46.63(14),	65.09(13),	28.67(14),	11.59(14),	59.31(14),
		1M =	52.01(14),	31.69(14),	36.81(14),	43.20(14),	43.86(18),	10.93(14),	54.15(14),	16.21(14),	40.81(13),	36.00(14),	
		2M =	45.95(13),										
	-C6E_c	/	0M =	64.06(11),	5.03(11),	0.44(11),	21.81(11),	6.16(10),	10.06(10),	14.75(8),	18.26(10),	48.41(10),	33.15(10),
		1M =	35.85(10),	29.96(10),	41.56(10),	25.03(10),	9.01(15),	45.26(11),	63.99(10),	23.15(10),	6.20(9),	0.80(10),	
		2M =	9.26(9),										
N1F_c	-C2F_c	/	0M =	64.29(14),	20.81(15),	23.32(15),	0.04(15),	31.29(14),	34.33(14),	33.76(13),	6.32(14),	62.57(14),	26.02(14),
		1M =	24.90(14),	17.59(14),	23.34(14),	50.70(14),	12.70(18),	41.60(14),	64.31(14),	0.90(14),	31.27(13),	26.19(14),	
		2M =	33.61(13),										
	-C6F_c	/	0M =	37.84(14),	9.51(15),	11.63(15),	0.38(15),	55.67(14),	61.23(14),	80.17(13),	48.27(14),	7.83(14),	41.53(14),
		1M =	33.81(14),	44.25(14),	17.83(14),	50.44(14),	63.59(18),	19.39(14),	37.93(14),	0.68(14),	56.14(13),	52.51(14),	
		2M =	60.80(13),										
C1A_c	-C2A_c	/	0M =	26.08(14),	63.75(14),	44.14(14),	51.34(14),	0.00(14),	5.46(14),	24.78(12),	1.60(13),	26.56(13),	64.45(13),
		1M =	62.99(14),	36.06(13),	52.67(13),	2.12(14),	15.92(17),	34.89(14),	26.08(13),	49.64(14),	0.47(13),	2.52(13),	
		2M =	5.03(12),										
	-C6A_c	/	0M =	66.23(11),	15.91(11),	17.77(11),	40.93(11),	0.00(10),	5.38(10),	16.68(8),	20.82(9),	27.89(10),	51.80(10),
		1M =	55.93(10),	16.49(9),	62.52(10),	15.87(10),	7.49(15),	25.90(10),	66.14(10),	41.97(10),	0.21(9),	5.62(10),	
		2M =	4.53(9),										
-C11A_c	/	0M =	26.91(13),	41.14(13),	26.02(13),	10.38(14),	2.35(13),	1.99(13),	6.33(11),	19.44(12),	66.69(13),	8.51(13),	
	1M =	5.79(13),	57.92(12),	2.43(12),	19.80(13),	21.39(16),	84.17(13),	26.87(12),	8.54(13),	2.06(12),	0.52(13),		
	2M =	1.61(12),											
C1B_c	-C2B_c	/	0M =	10.94(14),	70.46(14),	47.37(14),	45.56(14),	4.35(14),	0.15(14),	18.16(12),	3.75(13),	41.50(13),	49.16(13),
		1M =	47.83(14),	44.19(13),	39.54(13),	11.05(14),	15.77(17),	49.03(14),	10.95(13),	43.63(14),	3.88(13),	5.48(13),	
		2M =	0.08(12),										
	-C6B_c	/	0M =	56.90(14),	31.24(14),	31.52(14),	54.84(14),	6.16(14),	0.15(14),	14.90(12),	22.62(13),	12.62(13),	62.08(13),
		1M =	68.29(14),	7.12(13),	77.84(13),	6.64(14),	7.50(17),	12.13(14),	56.83(13),	55.57(14),	5.86(13),	11.55(14),	
		2M =	0.98(13),										
-C11B_c	/	0M =	39.77(10),	25.84(10),	13.65(10),	4.44(11),	0.20(10),	1.20(10),	1.92(8),	24.55(9),	61.49(9),	6.80(9),	
	1M =	10.06(9),	52.82(9),	18.59(9),	19.07(10),	21.82(14),	71.66(10),	39.71(9),	6.20(9),	0.37(8),	4.28(9),		
	2M =	0.62(8),											
C2A_c	-C21A_c	/	0M =	64.31(13),	21.74(13),	22.49(13),	45.79(14),	1.18(13),	4.50(13),	17.43(11),	20.41(12),	22.17(13),	57.04(13),
		1M =	61.65(13),	11.95(12),	68.28(12),	13.45(13),	6.26(16),	20.10(13),	64.23(12),	46.69(13),	0.94(12),	6.75(13),	
		2M =	3.65(12),										
C2B_c	-C6B	/	0M =	40.72(11),	23.54(11),	11.40(11),	6.76(11),	1.46(10),	0.15(10),	2.22(8),	26.00(9),	59.50(10),	8.50(10),
		1M =	11.94(10),	52.55(9),	20.75(10),	17.92(10),	22.67(15),	69.88(10),	40.66(10),	8.52(10),	1.61(9),	5.67(10),	
		2M =	0.45(9),										
	-C21B_c	/	0M =	55.45(10),	35.71(10),	33.76(10),	56.77(11),	4.69(10),	1.48(10),	17.64(8),	19.29(9),	8.30(9),	67.45(9),
		1M =	74.00(9),	1.48(9),	81.32(9),	6.56(10),	3.85(14),	6.46(10),	55.39(9),	57.18(9),	4.35(8),	9.89(9),	
		2M =	0.67(8),										
C2C_c	-C3C_c	/	0M =	0.39(14),	9.56(14),	32.14(14),	32.73(14),	60.31(14),	57.89(14),	51.41(12),	84.01(13),	3.02(14),	2.70(14),
		1M =	5.08(14),	52.31(13),	21.63(13),	40.76(14),	75.42(17),	30.14(14),	0.48(13),	34.39(14),	60.44(13),	64.49(14),	
		2M =	58.61(13),										

[illegible]

=====												
N1C_d	-C2C_d	/	0M =	0.24(11),	47.57(11),	25.25(11),	19.88(11),	12.66(10),	15.37(10),	28.98(9),	26.89(10),	44.12(10), 33.25(10),
			1M =	28.81(10),	69.59(10),	16.56(10),	0.34(10),	35.94(15),	67.18(11),	0.29(10),	17.95(10),	13.07(9), 13.34(10),
			2M =	15.45(9),								
	-C6C_d	/	0M =	0.45(14),	69.66(14),	87.15(14),	66.39(15),	43.24(14),	37.97(14),	18.68(13),	35.00(13),	41.97(14), 30.95(14),
			1M =	35.99(14),	8.16(14),	42.65(14),	43.89(14),	24.03(17),	25.49(14),	0.51(14),	65.30(14),	42.76(13), 45.07(14),
			2M =	38.37(13),								
N1D_d	-C2D_d	/	0M =	64.37(14),	0.76(15),	14.85(15),	5.40(15),	47.96(14),	53.78(14),	63.87(13),	27.78(14),	32.38(14), 45.55(14),
			1M =	40.19(14),	15.44(14),	29.08(14),	58.94(14),	39.66(17),	8.11(14),	64.47(14),	5.25(14),	48.23(13), 42.46(14),
			2M =	52.93(13),								
	-C6D_d	/	0M =	52.56(11),	0.62(11),	9.76(11),	30.19(11),	8.20(10),	4.26(10),	1.57(9),	32.56(10),	39.68(10), 30.04(10),
			1M =	34.77(10),	38.15(10),	45.12(10),	10.74(10),	22.60(15),	46.23(11),	52.47(10),	31.81(10),	8.16(9), 13.55(10),
			2M =	5.06(9),								
N1E_d	-C2E_d	/	0M =	54.07(14),	18.19(15),	0.68(15),	16.96(15),	40.38(14),	46.63(14),	65.09(13),	28.67(14),	11.59(14), 59.31(14),
			1M =	52.01(14),	31.69(14),	36.81(14),	43.20(14),	43.86(18),	10.93(14),	54.15(14),	16.21(14),	40.81(13), 36.00(14),
			2M =	45.95(13),								
	-C6E_d	/	0M =	64.06(11),	5.03(11),	0.44(11),	21.81(11),	6.16(10),	10.06(10),	14.75(8),	18.26(10),	48.41(10), 33.15(10),
			1M =	35.85(10),	29.96(10),	41.56(10),	25.03(10),	9.01(15),	45.26(11),	63.99(10),	23.15(10),	6.20(9), 0.80(10),
			2M =	9.27(9),								
N1F_d	-C2F_d	/	0M =	64.29(14),	20.81(15),	23.32(15),	0.04(15),	31.29(14),	34.33(14),	33.76(13),	6.32(14),	62.57(14), 26.02(14),
			1M =	24.90(14),	17.59(14),	23.34(14),	50.70(14),	12.70(18),	41.60(14),	64.31(14),	0.90(14),	31.27(13), 26.19(14),
			2M =	33.61(13),								
	-C6F_d	/	0M =	37.84(14),	9.51(15),	11.63(15),	0.38(15),	55.67(14),	61.23(14),	80.17(13),	48.27(14),	7.83(14), 41.53(14),
			1M =	33.81(14),	44.25(14),	17.83(14),	50.44(14),	63.59(18),	19.39(14),	37.93(14),	0.68(14),	56.14(13), 52.51(14),
			2M =	60.80(13),								
C1A_d	-C2A_d	/	0M =	26.08(14),	63.75(14),	44.14(14),	51.34(14),	0.00(14),	5.46(14),	24.78(12),	1.60(13),	26.56(13), 64.45(13),
			1M =	62.99(14),	36.06(13),	52.67(13),	2.12(14),	15.92(17),	34.89(14),	26.08(13),	49.64(14),	0.47(13), 2.52(13),
			2M =	5.03(12),								
	-C6A_d	/	0M =	66.23(11),	15.91(11),	17.77(11),	40.93(11),	0.00(10),	5.38(10),	16.68(8),	20.82(9),	27.89(10), 51.80(10),
			1M =	55.93(10),	16.49(9),	62.52(10),	15.87(10),	7.49(15),	25.90(10),	66.14(10),	41.97(10),	0.21(9), 5.62(10),
			2M =	4.53(9),								
	-C11A_d	/	0M =	26.91(13),	41.14(13),	26.02(13),	10.38(14),	2.35(13),	1.99(13),	6.33(11),	19.44(12),	66.69(13), 8.51(13),
			1M =	5.79(13),	57.92(12),	2.43(12),	19.80(13),	21.39(16),	84.17(13),	26.87(12),	8.54(13),	2.06(12), 0.52(13),
			2M =	1.61(12),								
C1B_d	-C2B_d	/	0M =	10.94(14),	70.46(14),	47.37(14),	45.56(14),	4.35(14),	0.15(14),	18.16(12),	3.75(13),	41.50(13), 49.16(13),
			1M =	47.83(14),	44.19(13),	39.54(13),	11.05(14),	15.77(17),	49.03(14),	10.95(13),	43.63(14),	3.88(13), 5.48(13),
			2M =	0.08(12),								
	-C6B_d	/	0M =	56.90(14),	31.24(14),	31.52(14),	54.84(14),	6.16(14),	0.15(14),	14.90(12),	22.62(13),	12.62(13), 62.08(13),
			1M =	68.29(14),	7.12(13),	77.84(13),	6.64(14),	7.50(17),	12.13(14),	56.83(13),	55.57(14),	5.86(13), 11.55(14),
			2M =	0.98(13),								
	-C11B_d	/	0M =	39.77(10),	25.84(10),	13.65(10),	4.44(11),	0.20(10),	1.20(10),	1.92(8),	24.55(9),	61.49(9), 6.80(9),
			1M =	10.06(9),	52.82(9),	18.59(9),	19.07(10),	21.82(14),	71.66(10),	39.71(9),	6.20(9),	0.37(8), 4.28(9),
			2M =	0.62(8),								
C2A_d	-C6A	/	0M =	29.45(14),	36.48(14),	21.66(14),	5.73(14),	0.00(14),	0.09(14),	6.82(12),	22.56(13),	64.52(13), 4.96(14),
			1M =	1.89(14),	58.82(13),	6.84(13),	18.06(14),	23.38(17),	83.12(14),	29.41(13),	3.89(14),	0.26(13), 3.20(14),
			2M =	0.35(13),								
	-C21A_d	/	0M =	64.31(13),	21.74(13),	22.49(13),	45.79(14),	1.18(13),	4.50(13),	17.43(11),	20.41(12),	22.17(13), 57.04(13),
			1M =	61.65(13),	11.95(12),	68.28(12),	13.45(13),	6.26(16),	20.10(13),	64.23(12),	46.69(13),	0.94(12), 6.75(13),
			2M =	3.65(12),								

C2B_d -C21B_d	/	0M =	55.45(10),	35.71(10),	33.76(10),	56.77(11),	4.69(10),	1.48(10),	17.64(8),	19.29(9),	8.30(9),	67.45(9),
		1M =	74.00(9),	1.48(9),	81.32(9),	6.56(10),	3.85(14),	6.46(10),	55.39(9),	57.18(9),	4.35(8),	9.89(9),
		2M =	0.67(8),									
C2C_d -C3C_d	/	0M =	0.39(14),	9.56(14),	32.14(14),	32.73(14),	60.31(14),	57.89(14),	51.41(12),	84.01(13),	3.02(14),	2.70(14),
		1M =	5.08(14),	52.31(13),	21.63(13),	40.76(14),	75.42(17),	30.14(14),	0.48(13),	34.39(14),	60.44(13),	64.49(14),
		2M =	58.61(13),									
C2D_d -C3D_d	/	0M =	7.89(14),	0.19(14),	22.86(14),	21.17(15),	58.82(14),	58.87(14),	59.07(12),	74.14(13),	5.58(14),	14.26(14),
		1M =	6.52(14),	59.30(13),	10.06(13),	40.85(14),	82.22(17),	34.25(14),	7.99(14),	22.77(14),	59.12(13),	61.09(14),
		2M =	59.35(13),									
C2E_d -C3E_d	/	0M =	3.51(14),	21.73(14),	0.28(14),	5.16(15),	33.66(14),	34.49(14),	41.34(12),	52.07(13),	30.16(14),	18.29(14),
		1M =	11.76(14),	84.33(13),	3.42(13),	16.74(14),	57.70(17),	59.14(14),	3.43(14),	7.05(14),	33.99(13),	35.80(14),
		2M =	34.85(13),									
C2F_d -C3F_d	/	0M =	17.56(14),	30.39(14),	11.17(14),	0.20(14),	16.36(14),	16.63(14),	23.42(12),	37.55(13),	48.05(14),	11.57(14),
		1M =	6.63(14),	75.32(13),	5.76(13),	1.27(14),	40.06(17),	76.59(14),	17.50(13),	1.74(14),	16.64(13),	19.14(14),
		2M =	17.03(13),									
C3C_d -C4C_d	/	0M =	0.79(14),	70.13(14),	86.60(14),	67.54(14),	42.40(14),	37.06(14),	17.73(12),	34.76(13),	41.06(14),	32.16(14),
		1M =	37.23(14),	8.25(13),	43.88(13),	42.72(14),	23.52(17),	25.12(14),	0.74(13),	66.40(14),	41.92(13),	44.36(14),
		2M =	37.48(13),									
C3D_d -C4D_d	/	0M =	53.10(14),	0.50(14),	8.47(14),	28.97(14),	7.11(14),	3.24(14),	2.27(12),	31.55(13),	40.97(13),	29.62(14),
		1M =	34.19(14),	38.24(13),	44.23(13),	11.89(14),	21.83(17),	47.03(14),	53.01(13),	30.58(14),	7.07(13),	12.44(14),
		2M =	4.03(13),									
C3E_d -C4E_d	/	0M =	64.25(14),	4.26(14),	0.31(14),	22.58(14),	5.77(14),	9.73(14),	14.67(12),	18.58(13),	47.64(13),	33.76(14),
		1M =	36.53(14),	29.67(13),	42.32(13),	24.57(14),	9.16(17),	44.67(14),	64.17(13),	23.91(14),	5.82(13),	0.39(14),
		2M =	8.93(13),									
C3F_d -C4F_d	/	0M =	38.02(18),	8.85(18),	12.26(18),	0.11(18),	56.27(18),	61.86(18),	80.86(17),	48.52(17),	8.44(17),	41.13(18),
		1M =	33.43(18),	43.78(17),	17.50(17),	51.13(18),	63.8(2),	18.84(18),	38.11(17),	1.16(18),	56.74(17),	53.06(18),
		2M =	61.43(17),									
C4C_d -C5C_d	/	0M =	0.58(14),	47.71(14),	25.51(14),	19.78(14),	12.09(14),	14.74(14),	28.22(12),	26.60(13),	44.95(14),	32.57(14),
		1M =	28.21(14),	69.51(13),	16.10(13),	1.05(14),	35.45(17),	67.99(14),	0.54(13),	17.84(14),	12.50(13),	12.84(14),
		2M =	14.83(13),									
C4D_d -C5D_d	/	0M =	65.27(14),	0.63(14),	13.33(14),	6.92(14),	46.63(14),	52.50(14),	63.23(12),	26.77(13),	31.53(14),	47.05(14),
		1M =	41.72(14),	15.55(13),	30.56(13),	57.41(14),	38.92(17),	7.68(14),	65.36(13),	6.76(14),	46.91(13),	41.15(14),
		2M =	51.65(13),									
C4E_d -C5E_d	/	0M =	54.24(14),	17.00(14),	0.53(14),	15.85(14),	41.48(14),	47.73(14),	66.07(12),	29.42(13),	12.49(14),	58.21(14),
		1M =	50.96(14),	31.42(13),	35.88(13),	44.41(14),	44.51(17),	10.33(14),	54.32(13),	15.12(14),	41.90(13),	37.05(14),
		2M =	47.05(13),									
C4F_d -C5F_d	/	0M =	64.26(18),	20.87(18),	23.50(18),	0.21(18),	31.60(18),	34.63(18),	34.03(17),	6.62(17),	62.52(17),	26.02(17),
		1M =	24.86(18),	17.34(17),	23.21(17),	50.99(18),	13.0(2),	41.39(18),	64.27(17),	0.72(18),	31.57(17),	26.49(18),
		2M =	33.91(17),									
C5C_d -C6C_d	/	0M =	0.03(14),	12.16(14),	34.70(14),	35.21(14),	61.42(14),	58.52(14),	50.62(12),	86.15(13),	1.23(14),	0.77(14),
		1M =	7.02(14),	49.80(13),	23.54(13),	41.82(14),	74.06(17),	28.02(14),	0.06(13),	36.85(14),	61.51(13),	65.92(14),
		2M =	59.28(13),									
C5D_d -C6D_d	/	0M =	4.44(14),	0.08(14),	22.95(14),	22.72(14),	56.77(14),	56.29(14),	55.63(12),	74.98(13),	7.76(14),	11.56(14),
		1M =	3.87(14),	60.47(13),	12.72(13),	38.30(14),	79.19(17),	36.16(14),	4.53(13),	24.39(14),	57.04(13),	59.55(14),
		2M =	56.83(13),									
C5E_d -C6E_d	/	0M =	6.60(14),	21.75(14),	0.16(14),	5.93(15),	31.66(14),	32.20(14),	38.40(13),	51.14(13),	32.50(14),	15.87(14),
		1M =	9.50(14),	84.25(13),	5.39(14),	14.33(14),	55.56(17),	61.38(14),	6.53(14),	7.85(14),	31.97(13),	34.07(14),
		2M =	32.58(13),									

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C5F_d -C6F_d / 0M = 14.99(14), 29.32(14), 9.45(14), 0.46(15), 19.27(14), 19.66(14), 26.56(12), 40.03(13), 45.03(14), 13.08(14),
                  1M = 7.85(14), 78.41(13), 5.10(13), 1.79(14), 43.06(17), 73.79(14), 14.92(14), 2.41(14), 19.57(13), 21.93(14),
                  2M = 20.06(13),
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Ring Puckering Analysis (Cremer & Pople) - (e.s.d. following Norrestam, Acta Cryst. (1981), A37, 764-765)

Symmetrical Forms

References

6-Membered Rings : C : Chair - Th = 0.0
 H : Half-Chair- Th = 50.8; Phi = k X 60 + 30
 E : Envelope - Th = 54.7; Phi = k X 60
 S : Screw-Boat- Th = 67.5; Phi = k X 60 + 30
 B : Boat - Th = 90.0; Phi = k X 60
 T : Twist-Boat- Th = 90.0; Phi = k X 60 + 30

J.C.A. Boeyens, J.Cryst.Mol.Struct. 8,(1978),317-320

Definitions (All Values Rounded on Esd)

Dev - Deviation of Atom I from Cremer&Pople Plane (Defined Differently from Least-Squares Plane)
 Cs(I),C2(I) - Mirror Plane and 2-Axis Asym. Par. for Atom I (See Duax et al., Topics in Stereochemistry,V-9, (1976) pp.271-383)
 Cs(I-J),C2(I-J)- Asymmetry Parameters for Bond I-J
 Tors(I-J) - Torsion Angle for Bond I-J

Descriptors for Torsion Angles

Descriptors for Ring Substituents (J.Appl.Cryst.,1983,16,431)

Torsion Angle Range	Full Descriptor	Short Descriptor
0 0 to 30 Deg	+ Syn-Periplanar	+sp
30 to 90	+ Syn-Clinal	+sc
90 to 150	+ Anti-Clinal	+ac
150 to 180	+ Anti-Periplanar	+ap
0 to -30	- Syn-Periplanar	-sp
-30 to -90	- Syn-Clinal	-sc
-90 to -150	- Anti-Clinal	-ac
-150 to -180	- Anti-Periplanar	-ap

Angle Range of Subst.	Full Descriptor	Short Descriptor
0 0 to 30 Deg.	Axial	ax
30 to 60	Bisectional	bi
60 to 90	Equatorial	eq

*** NOTE *** - For Ring Puckering Comparisons: Make Sure that the Absolute Configuration, Pivot Atom and Cyclic Sense Agree.
 - The "RING AT1 AT2 AT3 ... ATn" Instruction Gives the User Explicit Choice of Pivot Atom (AT1) and Sense (AT2).
 - Use TRNS Instructions to Obtain the Required Absolute Configuration.
 - The Values of Theta and Phi [= Phi(2)] Depend on the Abs. Conf. and the Choice of the First and Second Ring Atom.
 - Alternatively, Appropriate Phase Shifts may be Applied to the Same Effect (see Below)

For Correct Usage of C&P Puckering Parameters see also: D. Cremer, Acta Cryst. (1984). B40, 498-500.

6-Membered Ring (1)	N1C	-->	C2C	-->	C3C	-->	C4C	-->	C5C	-->	C6C	-->
			sp2		sp2		sp2		sp2		sp2	
Dev. (Ang)	0.0061(18)		0.001(2)		-0.009(2)		0.010(2)		-0.004(2)		-0.005(2)	
Cs(I)-Asym-Par (Deg)	0.7(2)		2.0(2)		1.3(2)		0.7(2)		2.0(2)		1.3(2)	
C2(I)-Asym-Par (Deg)	2.2(2)		1.2(2)		2.0(2)		2.2(2)		1.2(2)		2.0(2)	
Ring Bond Angle(Deg)	118.09(17)		122.61(17)		119.11(18)		118.51(18)		119.79(19)		121.87(19)	
Tors(I-J) (Deg)		-0.3(3)		-1.1(3)		2.0(3)		-1.5(3)		0.1(3)		0.8(3)
Cs(I-J)-Asym-Par (Deg)		1.5(3)		1.3(3)		1.8(3)		1.5(3)		1.3(3)		1.8(3)
C2(I-J)-Asym-Par (Deg)		1.9(3)		2.3(3)		0.4(3)		1.9(3)		2.3(3)		0.4(3)
Ring Bond Distance (Ang)		1.344(2)		1.382(3)		1.380(3)		1.381(3)		1.379(3)		1.351(3)

Weighted Average Ring Bond Distance = 1.3651(11, 77) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.97(12, 29) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 1.0 < 5.0 Deg.

Centroid Cg1	: x ,y ,z	0.46353(8)	0.10419(7)	0.36629(5)
	X0,Y0,Z0	5.2547(7)	1.8793(8)	6.2874(8)

6-Membered Ring (2)	N1D	-->	C2D	-->	C3D	-->	C4D	-->	C5D	-->	C6D	-->
			sp2		sp2		sp2		sp2		sp2	
Dev. (Ang)	-0.0106(18)		0.007(2)		0.003(2)		-0.009(2)		0.006(2)		0.004(2)	
Cs(I)-Asym-Par (Deg)	0.5(2)		1.8(2)		2.3(2)		0.5(2)		1.8(2)		2.3(2)	
C2(I)-Asym-Par (Deg)	2.4(2)		1.7(2)		0.9(2)		2.4(2)		1.7(2)		0.9(2)	
Ring Bond Angle(Deg)	117.68(17)		122.94(19)		118.65(19)		119.02(19)		118.87(19)		122.80(18)	
Tors(I-J) (Deg)		1.8(3)		-0.6(3)		-1.1(3)		1.4(3)		-0.1(3)		-1.5(3)
Cs(I-J)-Asym-Par (Deg)		1.7(3)		0.5(3)		1.3(3)		1.7(3)		0.5(3)		1.3(3)
C2(I-J)-Asym-Par (Deg)		1.0(3)		2.9(3)		2.0(3)		1.0(3)		2.9(3)		2.0(3)
Ring Bond Distance (Ang)		1.346(3)		1.378(3)		1.384(3)		1.382(3)		1.380(3)		1.341(2)

Weighted Average Ring Bond Distance = 1.3638(11, 86) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 1.08(12, 26) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 1.1 < 5.0 Deg.

Centroid Cg2	: x ,y ,z	1.03403(8)	0.33289(8)	0.11168(5)
	X0,Y0,Z0	10.0073(7)	3.8969(9)	1.9170(8)

6-Membered Ring (3)	N1E	-->	C2E	-->	C3E	-->	C4E	-->	C5E	-->	C6E	-->
			sp2		sp2		sp2		sp2		sp2	
Dev. (Ang)	0.0085(18)		-0.007(2)		0.000(2)		0.007(2)		-0.006(2)		-0.002(2)	
Cs(I)-Asym-Par (Deg)	0.8(2)		1.2(2)		1.9(2)		0.8(2)		1.2(2)		1.9(2)	
C2(I)-Asym-Par (Deg)	1.9(2)		1.6(2)		0.6(2)		1.9(2)		1.6(2)		0.6(2)	
Ring Bond Angle(Deg)	118.16(17)		122.38(19)		119.24(19)		118.5(2)		119.2(2)		122.54(19)	
Tors(I-J) (Deg)		-1.6(3)		0.8(3)		0.6(3)		-1.1(3)		0.3(3)		1.1(3)
Cs(I-J)-Asym-Par (Deg)		1.5(3)		0.7(3)		0.9(3)		1.5(3)		0.7(3)		0.9(3)
C2(I-J)-Asym-Par (Deg)		0.3(3)		2.2(3)		1.9(3)		0.3(3)		2.2(3)		1.9(3)
Ring Bond Distance (Ang)		1.340(3)		1.378(3)		1.388(3)		1.382(3)		1.375(3)		1.349(2)

Weighted Average Ring Bond Distance = 1.3653(11, 79) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.92(12, 19) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 0.9 < 5.0 Deg.

Centroid Cg3	: x ,y ,z	1.29036(9)	0.01575(8)	0.08887(5)
	X0,Y0,Z0	11.7638(8)	0.3508(8)	1.5254(8)

6-Membered Ring (4)	N1F	-->	C2F	-->	C3F	-->	C4F	-->	C5F	-->	C6F	-->
			sp2		sp2		sp2		sp2		sp2	
Dev. (Ang)	0.0028(18)		0.002(2)		-0.003(3)		0.000(3)		0.005(3)		-0.006(2)	
Cs(I)-Asym-Par (Deg)	1.1(3)		0.8(3)		0.3(3)		1.1(3)		0.8(3)		0.3(3)	
C2(I)-Asym-Par (Deg)	1.0(2)		1.2(3)		1.4(2)		1.0(2)		1.2(3)		1.4(2)	
Ring Bond Angle(Deg)	118.16(17)		122.3(2)		119.1(2)		118.9(2)		118.9(2)		122.66(19)	
Tors(I-J) (Deg)		-0.2(3)		-0.3(3)		0.1(4)		0.6(3)		-1.3(3)		1.0(3)
Cs(I-J)-Asym-Par (Deg)		1.0(3)		1.1(3)		1.1(3)		1.0(3)		1.1(3)		1.1(3)
C2(I-J)-Asym-Par (Deg)		1.4(3)		0.4(3)		1.0(3)		1.4(3)		0.4(3)		1.0(3)
Ring Bond Distance (Ang)		1.341(3)		1.382(3)		1.376(4)		1.379(4)		1.377(3)		1.338(3)

Weighted Average Ring Bond Distance = 1.3635(13, 86) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.62(13, 19) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 0.6 < 5.0 Deg.

Centroid Cg4	: x ,y ,z	1.21261(10)	-0.43455(8)	0.38219(5)
	X0,Y0,Z0	11.1793(9)	-4.0358(9)	6.5604(8)

=====												
6-Membered Ring (5)	C1A	-->	C2A	-->	C6A_d	-->	C1A_d	-->	C2A_d	-->	C6A	-->

	sp2		sp2		sp2		sp2		sp2		sp2	
Dev. (Ang)	0.0000(19)		0.000(2)		0.000(2)		0.0000(19)		0.000(2)		0.000(2)	
Cs(I)-Asym-Par (Deg)	0.00		0.00		0.00		0.00		0.00		0.00	
C2(I)-Asym-Par (Deg)	0.00		0.00		0.00		0.00		0.00		0.00	
Ring Bond Angle(Deg)	119.11(16)		118.79(16)		122.10(17)		119.11(16)		118.79(16)		122.10(17)	
Tors(I-J) (Deg)		0.0(3)		0.0(3)		0.0(3)		0.0(3)		0.0(3)		0.0(3)
Cs(I-J)-Asym-Par (Deg)		0.00		0.00		0.00		0.00		0.00		0.00
C2(I-J)-Asym-Par (Deg)		0.00		0.00		0.00		0.00		0.00		0.00
Ring Bond Distance (Ang)		1.401(3)		1.391(3)		1.392(2)		1.401(3)		1.391(3)		1.392(2)

Weighted Average Ring Bond Distance = 1.3939(10, 18) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.00(12, 0) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 0.0 < 5.0 Deg.

Centroid Cg5	: x ,y ,z	1.00000(8)	0.00000(7)	0.50000(4)
	X0,Y0,Z0	10.2373(7)	0.9955(8)	8.5826(7)

=====												
6-Membered Ring (6)	C1B	-->	C2B	-->	C6B_c	-->	C1B_c	-->	C2B_c	-->	C6B	-->

	sp2		sp2		sp2		sp2		sp2		sp2	
Dev. (Ang)	-0.0019(19)		0.0019(19)		-0.002(2)		0.0019(19)		-0.0019(19)		0.002(2)	
Cs(I)-Asym-Par (Deg)	0.00		0.00		0.00		0.00		0.00		0.00	
C2(I)-Asym-Par (Deg)	1.0(2)		1.0(2)		1.0(2)		1.0(2)		1.0(2)		1.0(2)	
Ring Bond Angle(Deg)	118.70(16)		119.38(16)		121.92(17)		118.70(16)		119.38(16)		121.92(17)	
Tors(I-J) (Deg)	0.5(3)		-0.5(3)		0.5(3)		-0.5(3)		0.5(3)		-0.5(3)	
Cs(I-J)-Asym-Par (Deg)	1.0(3)		1.0(3)		1.0(3)		1.0(3)		1.0(3)		1.0(3)	
C2(I-J)-Asym-Par (Deg)	0.00		0.00		0.00		0.00		0.00		0.00	
Ring Bond Distance (Ang)	1.401(3)		1.391(2)		1.395(3)		1.401(3)		1.391(2)		1.395(3)	

Weighted Average Ring Bond Distance = 1.3943(10, 18) Ang. - NOTE: 1st esd. Internal, 2nd esd External.

Weighted Average Abs. Torsion Angl. = 0.50(12, 0) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 0.5 < 5.0 Deg.

Centroid Cg6	: x ,y ,z	0.50000(8)	0.50000(7)	0.00000(4)
	X0,Y0,Z0	5.1977(7)	5.5192(7)	0.0000(7)

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	[1] ->	Cg1	[2656.01]	5.0295(16)	-0.5236-0.4794-0.7043 -11.0151	0.03	54.31	54.31	2.935	2.935	4.085
Cg1	[1] ->	Cg3	[1455.01]	5.5506(17)	0.8042-0.5608-0.1970 1.7924	89.22	15.56	88.54	0.141	5.347	
Cg1	[1] ->	Cg5	[1555.01]	5.5566(16)	0.9511 0.1754-0.2542 7.7297	66.23	46.83	43.95	4.001	3.802	
Cg1	[1] ->	Cg5	[2756.01]	5.5566(16)	-0.9511-0.1754 0.2542 -7.7297	66.23	46.83	43.95	4.001	3.802	
Cg2	[1] ->	Cg2	[2765.01]	5.0715(17)	0.5755-0.8177 0.0102 -0.5039	0.00	52.37	52.37	3.096	3.096	4.016
Cg2	[1] ->	Cg3	[1555.01]	3.9766(15)	0.8042-0.5608-0.1970 8.9631	23.16	10.77	28.99	3.478	3.907	
Cg2	[1] ->	Cg6	[1555.01]	5.4258(16)	0.9443 0.2663-0.1933 6.3782	71.11	40.69	46.44	3.739	4.114	
Cg2	[1] ->	Cg6	[2665.01]	5.4258(16)	-0.9443-0.2663 0.1933 -6.3782	71.11	40.69	46.44	3.739	4.114	
Cg3	[1] ->	Cg2	[1555.01]	3.9766(15)	-0.5755 0.8177-0.0102 -2.5926	23.16	28.99	10.77	3.907	3.478	
Cg3	[1] ->	Cg3	[2855.01]	4.4928(15)	-0.8042 0.5608 0.1970 -12.5490	0.02	37.05	37.05	3.586	3.586	2.707
Cg4	[1] ->	Cg1	[1645.01]	5.3490(17)	0.5236 0.4794 0.7043 6.6838	67.75	35.00	69.70	1.856	4.382	
Cg4	[1] ->	Cg4	[2746.01]	5.3496(17)	0.5564-0.6643-0.4991 2.3848	0.00	52.70	52.70	3.241	3.241	4.256
Cg4	[1] ->	Cg5	[1555.01]	5.5037(17)	0.9511 0.1754-0.2542 7.7297	57.35	27.63	84.50	0.528	4.876	
Cg4	[1] ->	Cg5	[2756.01]	5.5037(17)	-0.9511-0.1754 0.2542 -7.7297	57.35	27.63	84.50	0.528	4.876	
Cg5	[1] ->	Cg1	[1555.01]	5.5566(16)	0.5236 0.4794 0.7043 8.0805	66.23	43.95	46.83	3.802	4.001	
Cg5	[1] ->	Cg1	[1655.01]	4.6396(15)	0.5236 0.4794 0.7043 12.7497	66.23	15.06	79.23	0.867	4.480	
Cg5	[1] ->	Cg1	[2656.01]	4.6396(15)	-0.5236-0.4794-0.7043 -11.0151	66.23	15.06	79.23	0.867	4.480	
Cg5	[1] ->	Cg1	[2756.01]	5.5566(16)	-0.5236-0.4794-0.7043 -15.6843	66.23	43.95	46.83	3.802	4.001	
Cg6	[1] ->	Cg2	[1455.01]	4.8140(15)	-0.5755 0.8177-0.0102 2.5393	71.11	13.50	77.80	1.018	4.681	
Cg6	[1] ->	Cg2	[1555.01]	5.4258(16)	-0.5755 0.8177-0.0102 -2.5926	71.11	46.44	40.69	4.114	3.739	
Cg6	[1] ->	Cg2	[2665.01]	5.4258(16)	0.5755-0.8177 0.0102 -5.6358	71.11	46.44	40.69	4.114	3.739	
Cg6	[1] ->	Cg2	[2765.01]	4.8140(15)	0.5755-0.8177 0.0102 -0.5039	71.11	13.50	77.80	1.018	4.681	
Cg6	[1] ->	Cg3	[1455.01]	5.8792(17)	0.8042-0.5608-0.1970 1.7924	49.60	48.56	83.09	0.708	3.891	
Cg6	[1] ->	Cg3	[2765.01]	5.8792(17)	-0.8042 0.5608 0.1970 -0.3772	49.60	48.56	83.09	0.708	3.891	
-----						0.00	10.77	88.54	0.141	2.935	
Min or Max						3.977					

- [2656] = 1-X, -Y, 1-Z
- [1455] = -1+X, Y, Z
- [1555] = X, Y, Z
- [2756] = 2-X, -Y, 1-Z
- [2765] = 2-X, 1-Y, -Z
- [2665] = 1-X, 1-Y, -Z
- [2855] = 3-X, -Y, -Z

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[ 1645] = 1+X, -1+Y, Z
[ 2746] = 2-X, -1-Y, 1-Z
[ 1655] = 1+X, Y, Z
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Analysis of X-H...Cg(Pi-Ring) Interactions (H...Cg < 3.0 Ang. - Gamma < 30.0 Deg)

X--H(I)	Res(I)	Cg(J)	[ARU(J)]	H...Cg	Transformed J-Plane P, Q, R, S	H-Perp	Gamma	X-H...Cg	X...Cg	X-H, Pi
C4C	-H4C	[1] -> Cg5	[1455.01]	2.45	0.9511 0.1754-0.2542 -0.7512	2.45	2.67	151	3.310(2)	60
C4C	-H4C	[1] -> Cg5	[2656.01]	2.45	-0.9511-0.1754 0.2542 0.7512	2.45	2.67	151	3.310(2)	60
C4D	-H4D	[1] -> Cg6	[1655.01]	2.72	0.9443 0.2663-0.1933 14.7982	2.72	3.95	144	3.532(2)	57
C4D	-H4D	[1] -> Cg6	[2765.01]	2.72	-0.9443-0.2663 0.1933 -14.7982	2.72	3.95	144	3.532(2)	57
				-----		-----				
				Min or Max	2.450			2.447 2.67	151.00	3.310 60.00

[1455] = -1+X,Y,Z
 [2656] = 1-X,-Y,1-Z
 [1655] = 1+X,Y,Z
 [2765] = 2-X,1-Y,-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg1	0.46353(8)	0.10419(7)	0.36629(5)	5.2547(7)	1.8793(8)	6.2874(8)
Cg2	1.03403(8)	0.33289(8)	0.11168(5)	10.0073(7)	3.8969(9)	1.9170(8)
Cg3	1.29036(9)	0.01575(8)	0.08887(5)	11.7638(8)	0.3508(8)	1.5254(8)
Cg4	1.21261(10)	-0.43455(8)	0.38219(5)	11.1793(9)	-4.0358(9)	6.5604(8)
Cg5	1.00000(8)	0.00000(7)	0.50000(4)	10.2373(7)	0.9955(8)	8.5826(7)
Cg6	0.50000(8)	0.50000(7)	0.00000(4)	5.1977(7)	5.5192(7)	0.0000(7)

=====

Analysis of Short Intra- and Inter-molecular Contacts , $d(I-J) < R(I) + R(J) + \text{Tolr}$, With Tolr = 0.2 Ang. (X - I...J) > 100. Deg.

Contact Radii : C H Cu N O
(Angstrom) 1.70 1.20 2.32 1.55 1.52

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

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ARU = 1555.01 *****

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At(I)[1555.01]	At(J)	[ARU(J)]		D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
Cu1	 01W	[]		3.6461(18) <	3.84	-0.19		0.7566	0.1950	0.2326	0.7331	0.4871	0.3089	01	175.30(5)
Cu1	 012A	[]		3.1330(16) <<	3.84	-0.71	Intra	0.7566	0.1950	0.2326	0.8708	0.2741	0.3773	01	136.97(6)
														011B	133.02(6)
Cu1	 012B	[]		3.2788(16) <<	3.84	-0.56	Intra	0.7566	0.1950	0.2326	0.5386	0.4548	0.2091	01	131.15(6)
														011A	136.24(5)
Cu1	 H1W1	[]		3.32(2) <<	3.52	-0.20		0.7566	0.1950	0.2326	0.7670	0.4270	0.3321	01	172.0(5)
Cu1	 H2W1	[]		3.29(2) <<	3.52	-0.23		0.7566	0.1950	0.2326	0.6580	0.4680	0.2885	01	164.8(5)
														011A	102.8(5)
Cu2	 04W	[1645.05]		3.3821(19) <<	3.84	-0.46		1.2120-0.2129	0.2298		1.5631-0.1422	0.2445		02	163.37(6)
Cu2	 022A	[]		3.1320(15) <<	3.84	-0.71	Intra	1.2120-0.2129	0.2298		0.9149-0.1665	0.3479		N1E	113.98(6)
Cu2	 022B	[1645.01]		3.1313(16) <<	3.84	-0.71	Intra	1.2120-0.2129	0.2298		1.5317-0.2852	0.1357		02	130.84(5)
														021A	132.30(6)
Cu2	 H1W4	[1645.05]		3.67(3)	3.52	0.15		1.2120-0.2129	0.2298		1.5910-0.1870	0.2797		02	173.9(4)
Cu2	 H2W4	[1645.05]		3.05(3) <<	3.52	-0.47		1.2120-0.2129	0.2298		1.5530-0.1910	0.2132		02	160.6(5)
01	 02	[]		2.911(2) <	3.04	-0.13	Intra	0.7732	0.0214	0.1750	0.9701-0.2069	0.1985		Cu1	129.84(7)
01	 04W	[1545.05]		2.817(2) <<	3.04	-0.22		0.7732	0.0214	0.1750	0.5631-0.1422	0.2445		Cu1	115.04(7)
01	 011A	[]		3.058(2)	3.04	0.02	Intra	0.7732	0.0214	0.1750	0.8951	0.1174	0.3068	H2	107.5(17)
01	 011B	[]		3.004(2) <	3.04	-0.04	Intra	0.7732	0.0214	0.1750	0.6208	0.2789	0.1583	H1	149.0(18)
														H2	106.0(17)
01	 N1C	[]		3.090(2)	3.07	0.02	Intra	0.7732	0.0214	0.1750	0.5809	0.1447	0.3117	H1	128.2(18)
01	 N1D	[]		3.217(2)	3.07	0.15	Intra	0.7732	0.0214	0.1750	0.9294	0.2689	0.1622	H2	150.1(16)
01	 C2C	[]		3.273(2)	3.22	0.05	Intra	0.7732	0.0214	0.1750	0.5971	0.0338	0.3527	H1	109.8(17)
01	 C6D	[]		3.405(3)	3.22	0.18	Intra	0.7732	0.0214	0.1750	0.9372	0.2714	0.0848	H2	159.0(17)
01	 H2C	[]		2.92	2.72	0.20	Intra	0.7732	0.0214	0.1750	0.6911-0.0166	0.3436			
01	 H4	[]		2.91(2)	2.72	0.19	Intra	0.7732	0.0214	0.1750	0.9350-0.2020	0.2434		Cu1	119.2(5)
01	 H5E	[2755.01]		2.50 <<	2.72	-0.22		0.7732	0.0214	0.1750	0.7615-0.0043	0.0362		Cu1	130
02	 01	[]		2.911(2) <	3.04	-0.13	Intra	0.9701-0.2069	0.1985		0.7732	0.0214	0.1750	Cu2	121.88(7)

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02		03W	[1545.04]	2.735(2)<< 3.04 -0.31	0.9701-0.2069 0.1985	0.8281-0.3855 0.1555				H3	110.4(18)	
										H4	104.6(18)	
02		021A	[]	3.101(2) 3.04 0.06 Intra	0.9701-0.2069 0.1985	1.1442-0.0997 0.3095				H3	153.4(17)	
02		021B	[1645.01]	3.043(2) 3.04 0.00 Intra	0.9701-0.2069 0.1985	1.2907-0.3329 0.1562				H4	120.7(19)	
02		022A	[]	2.6705(19)<< 3.04 -0.37 Intra	0.9701-0.2069 0.1985	0.9149-0.1665 0.3479				H3	120.8(17)	
02		N1E	[]	3.024(2) < 3.07 -0.05 Intra	0.9701-0.2069 0.1985	1.2491-0.0734 0.1484				H3	136.1(18)	
										H4	112.8(18)	
02		C6E	[]	3.208(2) < 3.22 -0.01 Intra	0.9701-0.2069 0.1985	1.2206-0.0774 0.0752				H3	115.7(17)	
										H4	135.8(18)	
02		C21A	[]	3.197(2) < 3.22 -0.02 Intra	0.9701-0.2069 0.1985	1.0200-0.1067 0.3548				H3	141.2(17)	
02		H1	[]	2.19(2)<< 2.72 -0.53 Intra	0.9701-0.2069 0.1985	0.8490-0.0240 0.1756				Cu2	115.4(7)	
										H3	115.8(19)	
02		H6E	[]	2.79 2.72 0.07 Intra	0.9701-0.2069 0.1985	1.1710-0.1429 0.0650				H4	152	
02		H6F	[]	2.90 2.72 0.18 Intra	0.9701-0.2069 0.1985	1.0575-0.4357 0.2893						
011A		01	[]	3.058(2) 3.04 0.02 Intra	0.8951 0.1174 0.3068	0.7732 0.0214 0.1750				C11A	163.19(12)	
011A		021A	[]	3.059(2) 3.04 0.02 Intra	0.8951 0.1174 0.3068	1.1442-0.0997 0.3095				Cu1	135.24(7)	
										C11A	103.36(11)	
011A		022A	[]	3.135(2) 3.04 0.10 Intra	0.8951 0.1174 0.3068	0.9149-0.1665 0.3479				Cu1	117.95(7)	
										C11A	108.66(11)	
011A		N1C	[]	2.768(2)<< 3.07 -0.30 Intra	0.8951 0.1174 0.3068	0.5809 0.1447 0.3117						
011A		N1D	[]	2.846(2)<< 3.07 -0.22 Intra	0.8951 0.1174 0.3068	0.9294 0.2689 0.1622				C11A	117.35(12)	
011A		C2C	[]	2.896(2)<< 3.22 -0.32 Intra	0.8951 0.1174 0.3068	0.5971 0.0338 0.3527						
011A		C2D	[]	3.149(3) < 3.22 -0.07 Intra	0.8951 0.1174 0.3068	1.0283 0.3290 0.1890						
011A		C21A	[]	2.676(2)<< 3.22 -0.54 Intra	0.8951 0.1174 0.3068	1.0200-0.1067 0.3548				Cu1	138.44(8)	
011A		H2C	[]	2.46<< 2.72 -0.26 Intra	0.8951 0.1174 0.3068	0.6911-0.0166 0.3436				C11A	106	
011A		H2D	[]	2.76 2.72 0.04 Intra	0.8951 0.1174 0.3068	1.0259 0.3260 0.2437						
011B		01	[]	3.004(2) < 3.04 -0.04 Intra	0.6208 0.2789 0.1583	0.7732 0.0214 0.1750				C11B	174.83(12)	
011B		N1C	[]	2.887(2) < 3.07 -0.18 Intra	0.6208 0.2789 0.1583	0.5809 0.1447 0.3117				C11B	115.07(11)	
011B		N1D	[]	2.749(2)<< 3.07 -0.32 Intra	0.6208 0.2789 0.1583	0.9294 0.2689 0.1622				C11B	107.71(12)	
011B		C6C	[]	3.126(2) < 3.22 -0.09 Intra	0.6208 0.2789 0.1583	0.4463 0.2153 0.3248						
011B		C6D	[]	2.913(2)<< 3.22 -0.31 Intra	0.6208 0.2789 0.1583	0.9372 0.2714 0.0848				C11B	107.10(12)	
011B		H3E	[1455.01]	2.58 < 2.72 -0.14	0.6208 0.2789 0.1583	0.4104 0.1752 0.1157				Cu1	122	
										C11B	103	
011B		H6B	[]	2.42<< 2.72 -0.30 Intra	0.6208 0.2789 0.1583	0.6057 0.2977 0.0200				Cu1	139	
011B		H6C	[]	2.73 2.72 0.01 Intra	0.6208 0.2789 0.1583	0.4326 0.2934 0.2958						
011B		H6D	[]	2.59 < 2.72 -0.13 Intra	0.6208 0.2789 0.1583	0.8697 0.2277 0.0650				C11B	116	
012A		Cu1	[]	3.1330(16)<< 3.84 -0.71 Intra	0.8708 0.2741 0.3773	0.7566 0.1950 0.2326						
012A		01W	[]	2.735(2)<< 3.04 -0.31	0.8708 0.2741 0.3773	0.7331 0.4871 0.3089				C11A	141.13(13)	
012A		C2D	[]	3.387(3) 3.22 0.17 Intra	0.8708 0.2741 0.3773	1.0283 0.3290 0.1890						
012A		C5F	[1565.01]	3.401(3) 3.22 0.18	0.8708 0.2741 0.3773	1.1137 0.4786 0.3916				C11A	127.36(13)	
012A		H1W1	[]	1.96(2)<< 2.72 -0.76	0.8708 0.2741 0.3773	0.7670 0.4270 0.3321				C11A	142.3(7)	
012A		H2D	[]	2.56 < 2.72 -0.16 Intra	0.8708 0.2741 0.3773	1.0259 0.3260 0.2437						
012A		H5F	[1565.01]	2.47<< 2.72 -0.25	0.8708 0.2741 0.3773	1.0440 0.4194 0.3974				C11A	128	
012A		H6A	[]	2.43<< 2.72 -0.29 Intra	0.8708 0.2741 0.3773	0.9208 0.2054 0.5098						
012B		Cu1	[]	3.2788(16)<< 3.84 -0.56 Intra	0.5386 0.4548 0.2091	0.7566 0.1950 0.2326						
012B		01W	[]	2.727(2)<< 3.04 -0.31	0.5386 0.4548 0.2091	0.7331 0.4871 0.3089				C11B	127.52(13)	
012B		021B	[]	3.159(2) 3.04 0.12 Intra	0.5386 0.4548 0.2091	0.2907 0.6671 0.1562				C11B	104.32(12)	

012B		O22B	[		]	3.004(2)	<	3.04	-0.04	Intra	0.5386	0.4548	0.2091	0.5317	0.7148	0.1357	C11B	106.21(11)
012B		C6C	[		]	3.246(3)		3.22	0.03	Intra	0.5386	0.4548	0.2091	0.4463	0.2153	0.3248		
012B		C21B	[		]	2.662(2)	<<	3.22	-0.56	Intra	0.5386	0.4548	0.2091	0.4292	0.6553	0.1249		
012B		H2W1	[		]	1.90(3)	<<	2.72	-0.82		0.5386	0.4548	0.2091	0.6580	0.4680	0.2885	C11B	130.2(7)
012B		H1W3	[		]	2.92(3)		2.72	0.20		0.5386	0.4548	0.2091	0.8170	0.5720	0.1931	C11B	102.4(5)
012B		H6C	[		]	2.39	<<	2.72	-0.33	Intra	0.5386	0.4548	0.2091	0.4326	0.2934	0.2958		
021A		O2	[		]	3.101(2)		3.04	0.06	Intra	1.1442	-0.0997	0.3095	0.9701	-0.2069	0.1985		
021A		O11A	[		]	3.059(2)		3.04	0.02	Intra	1.1442	-0.0997	0.3095	0.8951	0.1174	0.3068	Cu2	128.19(7)
021A		N1E	[		]	2.820(2)	<<	3.07	-0.25	Intra	1.1442	-0.0997	0.3095	1.2491	-0.0734	0.1484	C21A	139.13(12)
021A		N1F	[		]	2.745(2)	<<	3.07	-0.33	Intra	1.1442	-0.0997	0.3095	1.2162	-0.3481	0.3178		
021A		C2E	[		]	3.039(2)	<	3.22	-0.18	Intra	1.1442	-0.0997	0.3095	1.3169	0.0205	0.1621	C21A	148.52(12)
021A		C2F	[		]	3.097(3)	<	3.22	-0.12	Intra	1.1442	-0.0997	0.3095	1.3080	-0.3483	0.3719		
021A		H2E	[		]	2.60	<	2.72	-0.12	Intra	1.1442	-0.0997	0.3095	1.3350	0.0253	0.2138	C21A	151
021A		H2F	[		]	2.92		2.72	0.20	Intra	1.1442	-0.0997	0.3095	1.3759	-0.2877	0.3653	C21A	109
021A		H4	[		]	2.77(3)		2.72	0.05	Intra	1.1442	-0.0997	0.3095	0.9350	-0.2020	0.2434		
021B		O2	[	1465.01	]	3.043(2)		3.04	0.00	Intra	0.2907	0.6671	0.1562	-0.0299	0.7931	0.1985	C21B	157.87(12)
021B		O12B	[		]	3.159(2)		3.04	0.12	Intra	0.2907	0.6671	0.1562	0.5386	0.4548	0.2091		
021B		N1E	[	1465.01	]	2.852(2)	<<	3.07	-0.22	Intra	0.2907	0.6671	0.1562	0.2491	0.9266	0.1484		
021B		N1F	[	1465.01	]	2.791(2)	<<	3.07	-0.28	Intra	0.2907	0.6671	0.1562	0.2162	0.6519	0.3178	C21B	120.75(12)
021B		C6E	[	1465.01	]	3.036(3)	<	3.22	-0.18	Intra	0.2907	0.6671	0.1562	0.2206	0.9226	0.0752		
021B		C6F	[	1465.01	]	3.277(2)		3.22	0.06	Intra	0.2907	0.6671	0.1562	0.1217	0.5656	0.3278	C21B	132.22(12)
021B		H3D	[	1455.01	]	2.78		2.72	0.06		0.2907	0.6671	0.1562	0.2003	0.4367	0.1616	C21B	104
021B		H6E	[	1465.01	]	2.68	<	2.72	-0.04	Intra	0.2907	0.6671	0.1562	0.1710	0.8571	0.0650	C21B	102
022A		Cu2	[		]	3.1320(15)	<<	3.84	-0.71	Intra	0.9149	-0.1665	0.3479	1.2120	-0.2129	0.2298		
022A		O2	[		]	2.6705(19)	<<	3.04	-0.37	Intra	0.9149	-0.1665	0.3479	0.9701	-0.2069	0.1985	C21A	103.28(11)
022A		O2W	[		]	2.794(2)	<<	3.04	-0.25		0.9149	-0.1665	0.3479	0.6616	-0.2971	0.3787	C21A	163.42(12)
022A		O11A	[		]	3.135(2)		3.04	0.10	Intra	0.9149	-0.1665	0.3479	0.8951	0.1174	0.3068		
022A		N1F	[		]	3.162(2)		3.07	0.09	Intra	0.9149	-0.1665	0.3479	1.2162	-0.3481	0.3178		
022A		C2C	[		]	3.364(2)		3.22	0.14	Intra	0.9149	-0.1665	0.3479	0.5971	0.0338	0.3527	C21A	105.60(12)
022A		C6F	[		]	3.324(3)		3.22	0.10	Intra	0.9149	-0.1665	0.3479	1.1217	-0.4344	0.3278		
022A		H2C	[		]	2.43	<<	2.72	-0.29	Intra	0.9149	-0.1665	0.3479	0.6911	-0.0166	0.3436	C21A	105
022A		H1W2	[		]	2.06(3)	<<	2.72	-0.66		0.9149	-0.1665	0.3479	0.7350	-0.2690	0.3777	C21A	160.1(8)
022A		H4	[		]	1.90(2)	<<	2.72	-0.82	Intra	0.9149	-0.1665	0.3479	0.9350	-0.2020	0.2434	C21A	109.1(8)
022B		Cu2	[	1465.01	]	3.1313(16)	<<	3.84	-0.71	Intra	0.5317	0.7148	0.1357	0.2120	0.7871	0.2298		
022B		O3W	[		]	2.782(2)	<<	3.04	-0.26		0.5317	0.7148	0.1357	0.8281	0.6145	0.1555	C21B	124.43(12)
022B		O4W	[		]	2.705(2)	<<	3.04	-0.34		0.5317	0.7148	0.1357	0.5631	0.8578	0.2445	C21B	134.54(13)
022B		O12B	[		]	3.004(2)	<	3.04	-0.04	Intra	0.5317	0.7148	0.1357	0.5386	0.4548	0.2091		
022B		N1E	[	1465.01	]	3.218(2)		3.07	0.15	Intra	0.5317	0.7148	0.1357	0.2491	0.9266	0.1484		
022B		H2W3	[		]	1.99(3)	<<	2.72	-0.73		0.5317	0.7148	0.1357	0.7440	0.6400	0.1463	C21B	123.1(7)
022B		H2W4	[		]	1.87(2)	<<	2.72	-0.85		0.5317	0.7148	0.1357	0.5530	0.8090	0.2132	C21B	133.7(8)
022B		H4E	[	2765.01	]	2.50	<<	2.72	-0.22		0.5317	0.7148	0.1357	0.6360	0.8347	0.0123	C21B	111
N1C		O1	[		]	3.090(2)		3.07	0.02	Intra	0.5809	0.1447	0.3117	0.7732	0.0214	0.1750	C6C	137.72(13)
N1C		O11A	[		]	2.768(2)	<<	3.07	-0.30	Intra	0.5809	0.1447	0.3117	0.8951	0.1174	0.3068	C6C	148.45(13)
N1C		O11B	[		]	2.887(2)	<	3.07	-0.18	Intra	0.5809	0.1447	0.3117	0.6208	0.2789	0.1583	C2C	145.07(13)
N1C		C11A	[		]	3.226(3)	<	3.25	-0.02	Intra	0.5809	0.1447	0.3117	0.9043	0.1648	0.3677	C6C	129.35(13)
N1C		H2	[		]	2.93(2)		2.75	0.18	Intra	0.5809	0.1447	0.3117	0.7060	-0.0210	0.1949	C6C	133.2(5)
N1D		O1	[		]	3.217(2)		3.07	0.15	Intra	0.9294	0.2689	0.1622	0.7732	0.0214	0.1750	C2D	147.12(13)
N1D		O11A	[		]	2.846(2)	<<	3.07	-0.22	Intra	0.9294	0.2689	0.1622	0.8951	0.1174	0.3068	C6D	144.41(14)

N1D		O11B	[		]	2.749(2)<<	3.07	-0.32	Intra	0.9294	0.2689	0.1622	0.6208	0.2789	0.1583	C2D	139.60(14)
N1D		C11B	[		]	3.365(3)	3.25	0.12	Intra	0.9294	0.2689	0.1622	0.5651	0.3910	0.1546	C2D	120.82(13)
N1E		O2	[		]	3.024(2) <	3.07	-0.05	Intra	1.2491-0.0734	0.1484		0.9701-0.2069	0.1985		C2E	143.31(13)
N1E		O21A	[		]	2.820(2)<<	3.07	-0.25	Intra	1.2491-0.0734	0.1484		1.1442-0.0997	0.3095		C6E	148.17(13)
N1E		O21B	[	1645.01]		2.852(2)<<	3.07	-0.22	Intra	1.2491-0.0734	0.1484		1.2907-0.3329	0.1562		C2E	141.52(13)
N1E		O22B	[	1645.01]		3.218(2)	3.07	0.15	Intra	1.2491-0.0734	0.1484		1.5317-0.2852	0.1357		C2E	101.63(12)
N1E		C21B	[	1645.01]		3.274(2)	3.25	0.02	Intra	1.2491-0.0734	0.1484		1.4292-0.3447	0.1249		C2E	123.76(13)
N1F		O21A	[		]	2.745(2)<<	3.07	-0.33	Intra	1.2162-0.3481	0.3178		1.1442-0.0997	0.3095		C6F	128.48(13)
N1F		O21B	[	1645.01]		2.791(2)<<	3.07	-0.28	Intra	1.2162-0.3481	0.3178		1.2907-0.3329	0.1562		C2F	128.79(13)
N1F		O22A	[		]	3.162(2)	3.07	0.09	Intra	1.2162-0.3481	0.3178		0.9149-0.1665	0.3479		C2F	111.45(13)
N1F		C21A	[		]	3.095(3) <	3.25	-0.15	Intra	1.2162-0.3481	0.3178		1.0200-0.1067	0.3548		C6F	107.18(13)
C1A		C4C	[	1655.01]		3.420(3)	3.40	0.02		0.9580	0.0772	0.4346	1.3463	0.0638	0.4219	C11A	109.01(12)
C1A		C5C	[	1655.01]		3.577(3)	3.40	0.18		0.9580	0.0772	0.4346	1.3282	0.1771	0.3792		
C1A		H4C	[	1655.01]		2.83 <	2.90	-0.07		0.9580	0.0772	0.4346	1.2669	0.0371	0.4604	C11A	122
C1A		H4C	[	2656.01]		2.82 <	2.90	-0.08		0.9580	0.0772	0.4346	0.7331-0.0371	0.5396		C11A	117
C1B		H3D	[	1455.01]		3.10	2.90	0.20		0.5290	0.4484	0.0751	0.2003	0.4367	0.1616	C6B	114
C1B		H4D	[	2765.01]		3.00	2.90	0.10		0.5290	0.4484	0.0751	0.7929	0.5557-0.0262		C11B	114
C2A		C4C	[	1655.01]		3.405(3)	3.40	0.00		1.0057-0.0466	0.4286		1.3463	0.0638	0.4219	C21A	104.97(12)
C2A		H4C	[	1655.01]		2.78 <	2.90	-0.12		1.0057-0.0466	0.4286		1.2669	0.0371	0.4604	C21A	117
C2A		H4C	[	2656.01]		2.87 <	2.90	-0.03		1.0057-0.0466	0.4286		0.7331-0.0371	0.5396		C21A	123
C2B		H4D	[	1455.01]		3.04	2.90	0.14		0.4662	0.5703	0.0625	0.2071	0.4443	0.0262	C21B	118
C2B		H4D	[	2765.01]		3.08	2.90	0.18		0.4662	0.5703	0.0625	0.7929	0.5557-0.0262		C21B	117
C2C		O4W	[	1545.05]		2.971(3)<<	3.22	-0.25		0.5971	0.0338	0.3527	0.5631-0.1422	0.2445		N1C	105.75(12)
C2C		O22A	[		]	3.364(2)	3.22	0.14	Intra	0.5971	0.0338	0.3527	0.9149-0.1665	0.3479		N1C	126.71(13)
																C3C	110.58(13)
C2C		C11A	[		]	3.328(3) <	3.40	-0.07	Intra	0.5971	0.0338	0.3527	0.9043	0.1648	0.3677	C3C	132.49(13)
C2C		H2	[		]	2.90(2)	2.90	0.00	Intra	0.5971	0.0338	0.3527	0.7060-0.0210	0.1949		C3C	131.4(5)
C2C		H1W4	[	1545.05]		2.93(2)	2.90	0.03		0.5971	0.0338	0.3527	0.5910-0.1870	0.2797		N1C	120.9(5)
C2D		O12A	[		]	3.387(3)	3.22	0.17	Intra	1.0283	0.3290	0.1890	0.8708	0.2741	0.3773	C3D	142.84(15)
C2D		C11A	[		]	3.507(3)	3.40	0.11	Intra	1.0283	0.3290	0.1890	0.9043	0.1648	0.3677	C3D	151.70(14)
C2D		H1W3	[		]	3.09(2)	2.90	0.19		1.0283	0.3290	0.1890	0.8170	0.5720	0.1931		
C2E		O4W	[	1645.05]		3.063(3) <	3.22	-0.16		1.3169	0.0205	0.1621	1.5631-0.1422	0.2445		C3E	118.60(13)
C2E		H2W4	[	1645.05]		3.08(2)	2.90	0.18		1.3169	0.0205	0.1621	1.5530-0.1910	0.2132		C3E	119.8(5)
C2F		O2W	[	1655.03]		3.300(3)	3.22	0.08		1.3080-0.3483	0.3719		1.6616-0.2972	0.3787		N1F	138.03(14)
C2F		C21A	[		]	3.480(3)	3.40	0.08	Intra	1.3080-0.3483	0.3719		1.0200-0.1067	0.3548		C3F	122.15(15)
C3C		O4W	[	1545.05]		3.320(3)	3.22	0.10		0.4824-0.0096	0.4074		0.5631-0.1422	0.2445		C4C	120.07(14)
C3C		C3C	[	2656.01]		3.336(3) <	3.40	-0.06		0.4824-0.0096	0.4074		0.5176	0.0096	0.5926	C2C	115.55(13)
C3C		C4C	[	2656.01]		3.500(3)	3.40	0.10		0.4824-0.0096	0.4074		0.6537-0.0638	0.5781		C2C	102.67(12)
																C4C	108.25(13)
C3D		O3W	[		]	3.410(3)	3.22	0.19		1.1328	0.3948	0.1407	0.8281	0.6145	0.1555		
C4C		C1A	[	1455.01]		3.420(3)	3.40	0.02		0.3463	0.0638	0.4219	-0.0420	0.0772	0.4346	C3C	144.35(15)
C4C		C2A	[	1455.01]		3.405(3)	3.40	0.00		0.3463	0.0638	0.4219	0.0057-0.0466	0.4286		C3C	120.88(14)
																C5C	104.13(13)
C4C		C6A	[	1455.01]		3.599(3)	3.40	0.20		0.3463	0.0638	0.4219	-0.0468	0.1214	0.5059	C3C	153.49(15)
C4C		C3C	[	2656.01]		3.500(3)	3.40	0.10		0.3463	0.0638	0.4219	0.5176	0.0096	0.5926	C5C	123.28(14)
C4C		C6A	[	2656.01]		3.568(3)	3.40	0.17		0.3463	0.0638	0.4219	0.0468-0.1214	0.4941		C3C	109.58(14)
																C5C	125.05(13)
C4D		C4E	[		]	3.570(3)	3.40	0.17	Intra	1.1374	0.3985	0.0609	1.3336	0.1049	0.0287	C3D	101.02(14)

C4D		C5D	[2765.01]	3.496(3)	3.40	0.10		1.1374	0.3985	0.0609	0.9609	0.6653-0.0326	C3D	115.80(15)
C4E		C4D	[]	3.570(3)	3.40	0.17	Intra	1.3336	0.1049	0.0287	1.1374	0.3985 0.0609	C5E	122.96(15)
C4E		C5D	[]	3.414(3)	3.40	0.01	Intra	1.3336	0.1049	0.0287	1.0391	0.3347 0.0326	C5E	100.73(15)
C4F		H5C	[1645.01]	3.07	2.90	0.17	Intra	1.2087-0.5214	0.4470		1.2346-0.7715	0.3872	C3F	132
C5C		C1A	[1455.01]	3.577(3)	3.40	0.18		0.3282	0.1771	0.3792	-0.0420	0.0772 0.4346	C6C	152.85(15)
C5D		C4E	[]	3.414(3)	3.40	0.01	Intra	1.0391	0.3347	0.0326	1.3336	0.1049 0.0287		
C5D		O3W	[2765.04]	3.322(3)	3.22	0.10		1.0391	0.3347	0.0326	1.1719	0.3855-0.1555	C6D	143.04(15)
C5D		C4D	[2765.01]	3.496(3)	3.40	0.10		1.0391	0.3347	0.0326	0.8626	0.6015-0.0609	C6D	112.50(14)
C5F		O12A	[1545.01]	3.401(3)	3.22	0.18		1.1137-0.5214	0.3916		0.8708-0.7259	0.3773	C4F	129.38(16)
													C6F	111.45(15)
C5F		H5C	[1645.01]	2.86 < 2.90	-0.04	Intra		1.1137-0.5214	0.3916		1.2346-0.7715	0.3872	C6F	124
C6A		C4C	[1655.01]	3.599(3)	3.40	0.20		0.9532	0.1214	0.5059	1.3463	0.0638 0.4219	H6A	113
C6A		H4C	[1655.01]	2.86 < 2.90	-0.04			0.9532	0.1214	0.5059	1.2669	0.0371 0.4604	H6A	121
C6A		C4C	[2656.01]	3.568(3)	3.40	0.17		0.9532	0.1214	0.5059	0.6537-0.0638	0.5781	H6A	112
C6A		H4C	[2656.01]	2.76 < 2.90	-0.14			0.9532	0.1214	0.5059	0.7331-0.0371	0.5396	H6A	117
C6B		H3E	[1455.01]	3.05	2.90	0.15		0.5623	0.3803	0.0119	0.4104	0.1752 0.1157		
C6B		H4D	[2765.01]	2.97	2.90	0.07		0.5623	0.3803	0.0119	0.7929	0.5557-0.0262	H6B	113
C6C		O12B	[]	3.246(3)	3.22	0.03	Intra	0.4463	0.2153	0.3248	0.5386	0.4548 0.2091	C5C	140.46(15)
C6C		C11B	[]	3.443(3)	3.40	0.04	Intra	0.4463	0.2153	0.3248	0.5651	0.3910 0.1546	C5C	148.93(15)
C6D		C11B	[]	3.508(3)	3.40	0.11	Intra	0.9372	0.2714	0.0848	0.5651	0.3910 0.1546	C5D	124.80(15)
C6E		C21B	[1645.01]	3.378(3) < 3.40	-0.02	Intra		1.2206-0.0774	0.0752		1.4292-0.3447	0.1249	C5E	126.47(15)
C6F		O22A	[]	3.324(3)	3.22	0.10	Intra	1.1217-0.4344	0.3278		0.9149-0.1665	0.3479	C5F	116.98(15)
C11A		C2C	[]	3.328(3) < 3.40	-0.07	Intra		0.9043	0.1648	0.3677	0.5971	0.0338 0.3527	O12A	111.56(13)
C11A		C2D	[]	3.507(3)	3.40	0.11	Intra	0.9043	0.1648	0.3677	1.0283	0.3290 0.1890	C1A	143.68(12)
C11A		H1W1	[]	3.04(2)	2.90	0.14		0.9043	0.1648	0.3677	0.7670	0.4270 0.3321	O11A	103.4(5)
													C1A	140.5(5)
C11A		H2C	[]	3.06	2.90	0.16	Intra	0.9043	0.1648	0.3677	0.6911-0.0166	0.3436	O12A	128
C11A		H2D	[]	2.81 < 2.90	-0.09	Intra		0.9043	0.1648	0.3677	1.0259	0.3260 0.2437	C1A	139
C11B		C6C	[]	3.443(3)	3.40	0.04	Intra	0.5651	0.3910	0.1546	0.4463	0.2153 0.3248	C1B	146.83(13)
C11B		C6D	[]	3.508(3)	3.40	0.11	Intra	0.5651	0.3910	0.1546	0.9372	0.2714 0.0848	O12B	121.98(13)
C11B		H2W1	[]	2.87(3) < 2.90	-0.03			0.5651	0.3910	0.1546	0.6580	0.4680 0.2885	O11B	102.4(5)
													C1B	137.3(5)
C11B		H6C	[]	2.72 < 2.90	-0.18	Intra		0.5651	0.3910	0.1546	0.4326	0.2934 0.2958	C1B	142
C21A		O11A	[]	2.676(2)<< 3.22	-0.54	Intra		1.0200-0.1067	0.3548		0.8951	0.1174 0.3068		
C21A		C2F	[]	3.480(3)	3.40	0.08	Intra	1.0200-0.1067	0.3548		1.3080-0.3483	0.3719	C2A	105.53(12)
C21A		H2C	[]	3.00	2.90	0.10	Intra	1.0200-0.1067	0.3548		0.6911-0.0166	0.3436	O21A	135
C21A		H4	[]	2.59(2)<< 2.90	-0.31	Intra		1.0200-0.1067	0.3548		0.9350-0.2020	0.2434	C2A	158.5(6)
C21B		O12B	[]	2.662(2)<< 3.22	-0.56	Intra		0.4292	0.6553	0.1249	0.5386	0.4548 0.2091	O21B	100.95(12)
C21B		C6E	[1465.01]	3.378(3) < 3.40	-0.02	Intra		0.4292	0.6553	0.1249	0.2206	0.9226 0.0752	C2B	115.30(12)
C21B		H2W3	[]	2.87(3) < 2.90	-0.03			0.4292	0.6553	0.1249	0.7440	0.6400 0.1463	O21B	146.9(5)
C21B		H2W4	[]	2.87(2) < 2.90	-0.03			0.4292	0.6553	0.1249	0.5530	0.8090 0.2132	C2B	145.0(5)
H1		O2	[]	2.19(2)<< 2.72	-0.53	Intra		0.8490-0.0240	0.1756		0.9701-0.2069	0.1985	O1	152(2)
H1		H4	[]	2.27(3) < 2.40	-0.13	Intra		0.8490-0.0240	0.1756		0.9350-0.2020	0.2434	O1	139(2)
H2		O4W	[1545.05]	2.00(2)<< 2.72	-0.72			0.7060-0.0210	0.1949		0.5631-0.1422	0.2445	O1	173(2)
H2		C2C	[]	2.90(2)	2.90	0.00	Intra	0.7060-0.0210	0.1949		0.5971	0.0338 0.3527	O1	110.2(18)
H2		H2C	[]	2.59	2.40	0.19	Intra	0.7060-0.0210	0.1949		0.6911-0.0166	0.3436	O1	105
H2		H1W4	[1545.05]	2.45(3)	2.40	0.05		0.7060-0.0210	0.1949		0.5910-0.1870	0.2797	O1	157(2)
H2		H2W4	[1545.05]	2.44(3)	2.40	0.04		0.7060-0.0210	0.1949		0.5530-0.1910	0.2132	O1	158(2)

H2C		01	[			2.92	2.72	0.20	Intra	0.6911-0.0166	0.3436	0.7732	0.0214	0.1750	C2C	104	
H2C		04W	[	1545.05]		2.82	2.72	0.10		0.6911-0.0166	0.3436	0.5631-0.1422	0.2445				
H2C		011A	[			2.46<<	2.72	-0.26	Intra	0.6911-0.0166	0.3436	0.8951	0.1174	0.3068	C2C	108	
H2C		022A	[			2.43<<	2.72	-0.29	Intra	0.6911-0.0166	0.3436	0.9149-0.1665	0.3479		C2C	168	
H2C		C11A	[			3.06	2.90	0.16	Intra	0.6911-0.0166	0.3436	0.9043	0.1648	0.3677			
H2C		C21A	[			3.00	2.90	0.10	Intra	0.6911-0.0166	0.3436	1.0200-0.1067	0.3548		C2C	157	
H2C		H2	[			2.59	2.40	0.19	Intra	0.6911-0.0166	0.3436	0.7060-0.0210	0.1949				
H2D		011A	[			2.76	2.72	0.04	Intra	1.0259	0.3260	0.2437	0.8951	0.1174	0.3068	C2D	105
H2D		012A	[			2.56 <	2.72	-0.16	Intra	1.0259	0.3260	0.2437	0.8708	0.2741	0.3773	C2D	145
H2D		C11A	[			2.81 <	2.90	-0.09	Intra	1.0259	0.3260	0.2437	0.9043	0.1648	0.3677	C2D	131
H2E		04W	[	1645.05]		2.64 <	2.72	-0.08		1.3350	0.0253	0.2138	1.5631-0.1422	0.2445		C2E	108
H2E		021A	[			2.60 <	2.72	-0.12	Intra	1.3350	0.0253	0.2138	1.1442-0.0997	0.3095		C2E	108
H2F		02W	[	1655.03]		2.58 <	2.72	-0.14		1.3759-0.2877	0.3653	1.6616-0.2972	0.3787		C2F	133	
H2F		021A	[			2.92	2.72	0.20	Intra	1.3759-0.2877	0.3653	1.1442-0.0997	0.3095				
H2F		H1W4	[	1645.05]		2.54	2.40	0.14		1.3759-0.2877	0.3653	1.5910-0.1870	0.2797		C2F	147	
H3		03W	[	1545.04]		1.91(2)<<	2.72	-0.81		0.9340-0.2630	0.1833	0.8281-0.3855	0.1555		02	173(2)	
H3		H1W3	[	1545.04]		2.21(3) <	2.40	-0.19		0.9340-0.2630	0.1833	0.8170-0.4280	0.1931		02	157(2)	
H3		H2W3	[	1545.04]		2.34(4) <	2.40	-0.06		0.9340-0.2630	0.1833	0.7440-0.3600	0.1463		02	156(2)	
H3C		02W	[			2.78	2.72	0.06		0.4971-0.0890	0.4347	0.6616-0.2971	0.3787		C3C	128	
H3D		021B	[	1655.01]		2.78	2.72	0.06		1.2003	0.4367	0.1616	1.2907	0.6671	0.1562	C3D	141
H3D		C1B	[	1655.01]		3.10	2.90	0.20		1.2003	0.4367	0.1616	1.5290	0.4484	0.0751	C3D	118
H3E		011B	[	1655.01]		2.58 <	2.72	-0.14		1.4104	0.1752	0.1157	1.6208	0.2789	0.1583	C3E	157
H3E		C6B	[	1655.01]		3.05	2.90	0.15		1.4104	0.1752	0.1157	1.5623	0.3803	0.0119	C3E	132
H4		01	[			2.91(2)	2.72	0.19	Intra	0.9350-0.2020	0.2434	0.7732	0.0214	0.1750			
H4		022A	[			1.90(2)<<	2.72	-0.82	Intra	0.9350-0.2020	0.2434	0.9149-0.1665	0.3479		02	160(3)	
H4		C21A	[			2.59(2)<<	2.90	-0.31	Intra	0.9350-0.2020	0.2434	1.0200-0.1067	0.3548		02	133(2)	
H4		H1	[			2.27(3) <	2.40	-0.13	Intra	0.9350-0.2020	0.2434	0.8490-0.0240	0.1756				
H4C		C1A	[	1455.01]		2.83 <	2.90	-0.07		0.2669	0.0371	0.4604	-0.0420	0.0772	0.4346	C4C	122
H4C		C2A	[	1455.01]		2.78 <	2.90	-0.12		0.2669	0.0371	0.4604	0.0057-0.0466	0.4286		C4C	124
H4C		C6A	[	1455.01]		2.86 <	2.90	-0.04		0.2669	0.0371	0.4604	-0.0468	0.1214	0.5059	C4C	136
H4C		C1A	[	2656.01]		2.82 <	2.90	-0.08		0.2669	0.0371	0.4604	0.0420-0.0772	0.5654		C4C	171
H4C		C2A	[	2656.01]		2.87 <	2.90	-0.03		0.2669	0.0371	0.4604	-0.0057	0.0466	0.5714	C4C	160
H4C		C6A	[	2656.01]		2.76 <	2.90	-0.14		0.2669	0.0371	0.4604	0.0468-0.1214	0.4941		C4C	144
H4D		C2B	[	1655.01]		3.04	2.90	0.14		1.2071	0.4443	0.0262	1.4662	0.5703	0.0625	C4D	129
H4D		C1B	[	2765.01]		3.00	2.90	0.10		1.2071	0.4443	0.0262	1.4710	0.5516-0.0751		C4D	169
H4D		C2B	[	2765.01]		3.08	2.90	0.18		1.2071	0.4443	0.0262	1.5338	0.4297-0.0625		C4D	143
H4D		C6B	[	2765.01]		2.97	2.90	0.07		1.2071	0.4443	0.0262	1.4377	0.6197-0.0119		C4D	154
H4E		022B	[	2765.01]		2.50<<	2.72	-0.22		1.3640	0.1653-0.0123	1.4683	0.2852-0.1357		C4E	167	
H4F		02W	[	2746.03]		2.82	2.72	0.10		1.2060-0.5809	0.4913	1.3384-0.7028	0.6213		C4F	150	
H5C		C4F	[	1465.01]		3.07	2.90	0.17	Intra	0.2346	0.2285	0.3872	0.2087	0.4786	0.4470	C5C	123
H5C		C5F	[	1465.01]		2.86 <	2.90	-0.04	Intra	0.2346	0.2285	0.3872	0.1137	0.4786	0.3916	C5C	142
H5C		H5F	[	1465.01]		2.55	2.40	0.15	Intra	0.2346	0.2285	0.3872	0.0440	0.4194	0.3974	C5C	161
H5D		03W	[	2765.04]		2.48<<	2.72	-0.24		1.0417	0.3343-0.0219	1.1719	0.3855-0.1555		C5D	148	
H5E		01	[	2755.01]		2.50<<	2.72	-0.22		1.2385	0.0043-0.0362	1.2268-0.0214-0.1750			C5E	170	
H5F		012A	[	1545.01]		2.47<<	2.72	-0.25		1.0440-0.5806	0.3974	0.8708-0.7259	0.3773		C5F	166	
H5F		H5C	[	1645.01]		2.55	2.40	0.15	Intra	1.0440-0.5806	0.3974	1.2346-0.7715	0.3872				
H6A		012A	[			2.43<<	2.72	-0.29	Intra	0.9208	0.2054	0.5098	0.8708	0.2741	0.3773	C6A	100
H6B		011B	[			2.42<<	2.72	-0.30	Intra	0.6057	0.2977	0.0200	0.6208	0.2789	0.1583	C6B	100

H6B		H6D	[	]	2.58	2.40	0.18	Intra	0.6057	0.2977	0.0200	0.8697	0.2277	0.0650	C6B	125
H6C		011B	[	]	2.73	2.72	0.01	Intra	0.4326	0.2934	0.2958	0.6208	0.2789	0.1583	C6C	106
H6C		012B	[	]	2.39<<	2.72	-0.33	Intra	0.4326	0.2934	0.2958	0.5386	0.4548	0.2091	C6C	149
H6C		C11B	[	]	2.72 <	2.90	-0.18	Intra	0.4326	0.2934	0.2958	0.5651	0.3910	0.1546	C6C	133
H6D		011B	[	]	2.59 <	2.72	-0.13	Intra	0.8697	0.2277	0.0650	0.6208	0.2789	0.1583	C6D	100
H6D		H6B	[	]	2.58	2.40	0.18	Intra	0.8697	0.2277	0.0650	0.6057	0.2977	0.0200	C6D	131
H6E		02	[	]	2.79	2.72	0.07	Intra	1.1710	-0.1429	0.0650	0.9701	-0.2069	0.1985	C6E	107
H6E		021B	[	1645.01]	2.68 <	2.72	-0.04	Intra	1.1710	-0.1429	0.0650	1.2907	-0.3329	0.1562	C6E	103
H6F		02	[	]	2.90	2.72	0.18	Intra	1.0575	-0.4357	0.2893	0.9701	-0.2069	0.1985	C6F	118

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 1 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact Resd.			
1	[1555.02]	9	1.9000	-0.82	0 C11B	- 012B	... H2W1	-01W	2	<<	1555.02			
2	[1645.05]	7	2.5400	0.14	1 C2F	- H2F	... H1W4	-04W	2		1645.05			
3	[1545.05]	8	2.0000	-0.72	2 01	- H2	... 04W	-H1W4	0	<<	1545.05			
4	[2755.01]	2	2.5000	-0.22	1 C5E	- H5E	... 01	-Cu1	0	<<	1554.01	1645.01	2665.01	2755.01
5	[1545.04]	4	1.9100	-0.81	2 02	- H3	... 03W	-H1W3	0	<<	1545.04			
6	[1455.01]	12	2.5800	-0.14	0 Cu1	- 011B	... H3E	-C3E	1	<	1365.01	1455.01	1545.01	2565.01
7	[1565.01]	2	2.4700	-0.25	0 C11A	- 012A	... H5F	-C5F	1	<<	1475.01	1565.01	1655.01	2675.01
8	[1555.04]	6	1.9900	-0.73	0 C21B	- 022B	... H2W3	-03W	2	<<	1555.04			
9	[1555.03]	3	2.0600	-0.66	0 C21A	- 022A	... H1W2	-02W	2	<<	1555.03			
10	[1555.05]	3	1.8700	-0.85	0 C21B	- 022B	... H2W4	-04W	2	<<	1555.05			
11	[2765.01]	10	2.5000	-0.22	1 C4E	- H4E	... 022B	-C21B	0	<<	1564.01	1655.01	2675.01	2765.01
12	[1655.01]	12	2.5800	-0.14	1 C3E	- H3E	... 011B	-Cu1	0	<	1565.01	1655.01	1745.01	2765.01
13	[2656.01]	11	2.7600	-0.14	1 C4C	- H4C	... C6A	-C1A	0	<	1455.01	1546.01	2566.01	2656.01
14	[1655.03]	2	2.5800	-0.14	1 C2F	- H2F	... 02W	-H1W2	0	<	1655.03			
15	[2765.04]	2	2.4800	-0.24	1 C5D	- H5D	... 03W	-H1W3	0	<<	2765.04			
16	[2746.03]	1	2.8200	0.10	1 C4F	- H4F	... 02W	-H1W2	0		2746.03			
17	[1465.02]	9	1.9000	-0.82	0 C11B	- 012B	... H2W1	-01W	2	<<	1465.02			
18	[1455.05]	8	2.0000	-0.72	2 01	- H2	... 04W	-H1W4	0	<<	1455.05			
19	[2665.01]	2	2.5000	-0.22	1 C5E	- H5E	... 01	-Cu1	0	<<	1464.01	1555.01	2575.01	2665.01
20	[1455.04]	4	1.9100	-0.81	2 02	- H3	... 03W	-H1W3	0	<<	1455.04			
21	[1365.01]	12	2.5800	-0.14	0 Cu1	- 011B	... H3E	-C3E	1	<	1275.01	1365.01	1455.01	2475.01
22	[1475.01]	2	2.4700	-0.25	0 C11A	- 012A	... H5F	-C5F	1	<<	1385.01	1475.01	1565.01	2585.01
23	[1465.04]	6	1.9900	-0.73	0 C21B	- 022B	... H2W3	-03W	2	<<	1465.04			
24	[1465.03]	3	2.0600	-0.66	0 C21A	- 022A	... H1W2	-02W	2	<<	1465.03			
25	[1465.05]	3	1.8700	-0.85	0 C21B	- 022B	... H2W4	-04W	2	<<	1465.05			
26	[2675.01]	10	2.5000	-0.22	1 C4E	- H4E	... 022B	-C21B	0	<<	1474.01	1565.01	2585.01	2675.01
27	[1565.03]	2	2.5800	-0.14	1 C2F	- H2F	... 02W	-H1W2	0	<	1565.03			
28	[2675.04]	2	2.4800	-0.24	1 C5D	- H5D	... 03W	-H1W3	0	<<	2675.04			
29	[2656.03]	1	2.8200	0.10	1 C4F	- H4F	... 02W	-H1W2	0		2656.03			
30	[1645.02]	9	1.9000	-0.82	0 C11B	- 012B	... H2W1	-01W	2	<<	1645.02			
31	[1735.05]	7	2.5400	0.14	1 C2F	- H2F	... H1W4	-04W	2		1735.05			

O1W		O3W	[		]	2.924(2) < 3.04	-0.12	0.7331	0.4871	0.3089	0.8281	0.6145	0.1555	H1W1	132.7(19)	
O1W		O12A	[		]	2.735(2)<< 3.04	-0.31	0.7331	0.4871	0.3089	0.8708	0.2741	0.3773	H2W1	106.6(15)	
O1W		O12B	[		]	2.727(2)<< 3.04	-0.31	0.7331	0.4871	0.3089	0.5386	0.4548	0.2091	H1W1	114.9(18)	
O1W		H2W2	[	1565.03]		1.99(2)<< 2.72	-0.73	0.7331	0.4871	0.3089	0.6870	0.6380	0.3617	H1W1	119(2)	
														H2W1	114.9(18)	
O1W		H1W3	[		]	2.19(3)<< 2.72	-0.53	0.7331	0.4871	0.3089	0.8170	0.5720	0.1931	H1W1	129(2)	
H1W1		Cu1	[		]	3.32(2)<< 3.52	-0.20	0.7670	0.4270	0.3321	0.7566	0.1950	0.2326	O1W	109(2)	
H1W1		O12A	[		]	1.96(2)<< 2.72	-0.76	0.7670	0.4270	0.3321	0.8708	0.2741	0.3773	O1W	172(3)	
H1W1		C11A	[		]	3.04(2)	2.90	0.14	0.7670	0.4270	0.3321	0.9043	0.1648	0.3677	O1W	160(2)
H1W1		H2W2	[	1565.03]		2.46(3)	2.40	0.06	0.7670	0.4270	0.3321	0.6870	0.6380	0.3617		
H2W1		Cu1	[		]	3.29(2)<< 3.52	-0.23	0.6580	0.4680	0.2885	0.7566	0.1950	0.2326	O1W	107.9(18)	
H2W1		O12B	[		]	1.90(3)<< 2.72	-0.82	0.6580	0.4680	0.2885	0.5386	0.4548	0.2091	O1W	158(2)	
H2W1		C11B	[		]	2.87(3) < 2.90	-0.03	0.6580	0.4680	0.2885	0.5651	0.3910	0.1546	O1W	146(2)	
H2W1		H2W2	[	1565.03]		2.48(3)	2.40	0.08	0.6580	0.4680	0.2885	0.6870	0.6380	0.3617		
H2W1		H1W3	[		]	2.31(4) < 2.40	-0.09	0.6580	0.4680	0.2885	0.8170	0.5720	0.1931			

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 2 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn	X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact Resd.			
1	[1555.01]	9	1.9000	-0.82	2	O1W	- H2W1	... O12B	-C11B	0	<<	1465.01	1555.01	1645.01	2665.01
2	[1565.03]	4	1.9900	-0.73	0	H1W1	- O1W	... H2W2	-O2W	2	<<	1565.03			
3	[1555.04]	3	2.1900	-0.53	0	H1W1	- O1W	... H1W3	-O3W	2	<<	1555.04			

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 =====
 ARU = 1555.03
 =====

At(I)[1555.03]	At(J)	[	ARU(J)	]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
O2W		O1W	[	1545.02]	2.794(2) << 3.04	-0.25			0.6616	-0.2971	0.3787	0.7331	-0.5129	0.3089	H1W2	108(2)
O2W		O4W	[	1545.05]	2.898(2) < 3.04	-0.14			0.6616	-0.2971	0.3787	0.5631	-0.1422	0.2445	H2W2	102.2(19)
O2W		O22A	[		2.794(2) << 3.04	-0.25			0.6616	-0.2971	0.3787	0.9149	-0.1665	0.3479	H2W2	107.5(19)
O2W		C2F	[	1455.01]	3.300(3)	3.22	0.08		0.6616	-0.2971	0.3787	0.3080	-0.3483	0.3719	H1W2	166(2)
O2W		H2F	[	1455.01]	2.58	< 2.72	-0.14		0.6616	-0.2971	0.3787	0.3759	-0.2877	0.3653	H1W2	154
O2W		H3C	[		2.78	2.72	0.06		0.6616	-0.2971	0.3787	0.4971	-0.0890	0.4347	H2W2	165
O2W		H1W4	[	1545.05]	2.11(3) << 2.72	-0.61			0.6616	-0.2971	0.3787	0.5910	-0.1870	0.2797	H2W2	101(2)
O2W		H4F	[	2746.01]	2.82	2.72	0.10		0.6616	-0.2971	0.3787	0.7940	-0.4191	0.5087		
H1W2		O22A	[		2.06(3) << 2.72	-0.66			0.7350	-0.2690	0.3777	0.9149	-0.1665	0.3479	O2W	164(3)

H1W2		H1W4	[1545.05]	2.31(4)	< 2.40	-0.09	0.7350-0.2690	0.3777	0.5910-0.1870	0.2797		
H2W2		O1W	[1545.02]	1.99(2)	<< 2.72	-0.73	0.6870-0.3620	0.3617	0.7331-0.5129	0.3089	02W	173(3)
H2W2		H1W1	[1545.02]	2.46(3)	2.40	0.06	0.6870-0.3620	0.3617	0.7670-0.5730	0.3321	02W	171(3)
H2W2		H2W1	[1545.02]	2.48(3)	2.40	0.08	0.6870-0.3620	0.3617	0.6580-0.5320	0.2885	02W	155(3)
H2W2		H1W4	[1545.05]	2.40(3)	2.40	0.00	0.6870-0.3620	0.3617	0.5910-0.1870	0.2797		

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 3 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn	X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact Resd.			
1	[1545.02]	4	1.9900	-0.73	2	O2W	- H2W2	... O1W	-H1W1	0	<<	1545.02			
2	[1545.05]	4	2.1100	-0.61	0	H1W2	- O2W	... H1W4	-O4W	2	<<	1545.05			
3	[1555.01]	3	2.0600	-0.66	2	O2W	- H1W2	... O22A	-C21A	0	<<	1465.01	1555.01	1645.01	2665.01
4	[1455.01]	2	2.5800	-0.14	0	H1W2	- O2W	... H2F	-C2F	1	<	1365.01	1455.01	1545.01	2565.01
5	[2746.01]	1	2.8200	0.10	0	H1W2	- O2W	... H4F	-C4F	1		1545.01	1636.01	2656.01	2746.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

===== ARU = 1555.04 *****
=====

At(I)[1555.04]	At(J)	[ARU(J)]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
O3W		O1W	[]	2.924(2)	< 3.04	-0.12	0.8281	0.6145	0.1555	0.7331	0.4871	0.3089		
O3W		O2	[1565.01]	2.735(2)	<< 3.04	-0.31	0.8281	0.6145	0.1555	0.9701	0.7931	0.1985	H1W3	102.1(19)
													H2W3	111.1(16)
O3W		O22B	[]	2.782(2)	<< 3.04	-0.26	0.8281	0.6145	0.1555	0.5317	0.7148	0.1357	H1W3	103(2)
O3W		C3D	[]	3.410(3)	3.22	0.19	0.8281	0.6145	0.1555	1.1328	0.3948	0.1407	H2W3	149.3(17)
O3W		H3	[1565.01]	1.91(2)	<< 2.72	-0.81	0.8281	0.6145	0.1555	0.9340	0.7370	0.1833	H1W3	103(2)
													H2W3	112.7(18)
O3W		C5D	[2765.01]	3.322(3)	3.22	0.10	0.8281	0.6145	0.1555	0.9609	0.6653	-0.0326	H1W3	151.0(18)
O3W		H5D	[2765.01]	2.48	<< 2.72	-0.24	0.8281	0.6145	0.1555	0.9583	0.6657	0.0219	H1W3	152
H1W3		O1W	[]	2.19(3)	<< 2.72	-0.53	0.8170	0.5720	0.1931	0.7331	0.4871	0.3089	O3W	164(3)
H1W3		O12B	[]	2.92(3)	2.72	0.20	0.8170	0.5720	0.1931	0.5386	0.4548	0.2091	O3W	112(2)
H1W3		C2D	[]	3.09(2)	2.90	0.19	0.8170	0.5720	0.1931	1.0283	0.3290	0.1890	O3W	113(2)
H1W3		H2W1	[]	2.31(4)	< 2.40	-0.09	0.8170	0.5720	0.1931	0.6580	0.4680	0.2885	O3W	150(3)
H1W3		H3	[1565.01]	2.21(3)	< 2.40	-0.19	0.8170	0.5720	0.1931	0.9340	0.7370	0.1833		
H2W3		O22B	[]	1.99(3)	<< 2.72	-0.73	0.7440	0.6400	0.1463	0.5317	0.7148	0.1357	O3W	173(2)
H2W3		C21B	[]	2.87(3)	< 2.90	-0.03	0.7440	0.6400	0.1463	0.4292	0.6553	0.1249	O3W	163(2)
H2W3		H3	[1565.01]	2.34(4)	< 2.40	-0.06	0.7440	0.6400	0.1463	0.9340	0.7370	0.1833		

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 4 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact Resd.			
1	[1555.02]	3	2.1900	-0.53	2 03W	- H1W3	... 01W	-H1W1	0	<<	1555.02			
2	[1565.01]	4	1.9100	-0.81	0 H1W3	- 03W	... H3	-02	2	<<	1475.01	1565.01	1655.01	2675.01
3	[1555.01]	6	1.9900	-0.73	2 03W	- H2W3	... 022B	-C21B	0	<<	1465.01	1555.01	1645.01	2665.01
4	[2765.01]	2	2.4800	-0.24	0 H1W3	- 03W	... H5D	-C5D	1	<<	1564.01	1655.01	2675.01	2765.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

 =====
 ARU = 1555.05
 =====

At(I)[1555.05]	At(J)	[ARU(J)]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
04W	 Cu2	[1465.01]	3.3821(19)<<	3.84	-0.46		0.5631	0.8578	0.2445	0.2120	0.7871	0.2298	H1W4	105.5(19)
04W	 01	[1565.01]	2.817(2)<<	3.04	-0.22		0.5631	0.8578	0.2445	0.7732	1.0214	0.1750	H1W4	113.8(19)
													H2W4	110.6(18)
04W	 02W	[1565.03]	2.898(2) <	3.04	-0.14		0.5631	0.8578	0.2445	0.6616	0.7028	0.3787	H2W4	104.6(17)
04W	 022B	[]	2.705(2)<<	3.04	-0.34		0.5631	0.8578	0.2445	0.5317	0.7148	0.1357	H1W4	105.8(17)
04W	 C2C	[1565.01]	2.971(3)<<	3.22	-0.25		0.5631	0.8578	0.2445	0.5971	1.0338	0.3527	H2W4	179(2)
04W	 C2E	[1465.01]	3.063(3) <	3.22	-0.16		0.5631	0.8578	0.2445	0.3169	1.0205	0.1621	H1W4	152.7(19)
04W	 C3C	[1565.01]	3.320(3)	3.22	0.10		0.5631	0.8578	0.2445	0.4824	0.9904	0.4074	H2W4	155.9(18)
04W	 H2	[1565.01]	2.00(2)<<	2.72	-0.72		0.5631	0.8578	0.2445	0.7060	0.9790	0.1949	H1W4	115(2)
													H2W4	111.2(19)
04W	 H2C	[1565.01]	2.82	2.72	0.10		0.5631	0.8578	0.2445	0.6911	0.9834	0.3436	H2W4	162
04W	 H2E	[1465.01]	2.64 <	2.72	-0.08		0.5631	0.8578	0.2445	0.3350	1.0253	0.2138	H1W4	140
H1W4	 Cu2	[1465.01]	3.67(3)	3.52	0.15		0.5910	0.8130	0.2797	0.2120	0.7871	0.2298		
H1W4	 02W	[1565.03]	2.11(3)<<	2.72	-0.61		0.5910	0.8130	0.2797	0.6616	0.7028	0.3787	04W	176(2)
H1W4	 C2C	[1565.01]	2.93(2)	2.90	0.03		0.5910	0.8130	0.2797	0.5971	1.0338	0.3527		
H1W4	 H2	[1565.01]	2.45(3)	2.40	0.05		0.5910	0.8130	0.2797	0.7060	0.9790	0.1949		
H1W4	 H2F	[1465.01]	2.54	2.40	0.14		0.5910	0.8130	0.2797	0.3759	0.7123	0.3653	04W	113
H1W4	 H1W2	[1565.03]	2.31(4) <	2.40	-0.09		0.5910	0.8130	0.2797	0.7350	0.7310	0.3777	04W	160(3)
H1W4	 H2W2	[1565.03]	2.40(3)	2.40	0.00		0.5910	0.8130	0.2797	0.6870	0.6380	0.3617	04W	165(2)
H2W4	 Cu2	[1465.01]	3.05(3)<<	3.52	-0.47		0.5530	0.8090	0.2132	0.2120	0.7871	0.2298	04W	106(2)
H2W4	 022B	[]	1.87(2)<<	2.72	-0.85		0.5530	0.8090	0.2132	0.5317	0.7148	0.1357	04W	174(2)
H2W4	 C2E	[1465.01]	3.08(2)	2.90	0.18		0.5530	0.8090	0.2132	0.3169	1.0205	0.1621		
H2W4	 C21B	[]	2.87(2) <	2.90	-0.03		0.5530	0.8090	0.2132	0.4292	0.6553	0.1249	04W	164(2)

H2W4 H2 [1565.01] 2.44(3) 2.40 0.04 0.5530 0.8090 0.2132 0.7060 0.9790 0.1949

Summary of Shortest Inter Contacts with $d(I-J) < R(I) + R(J) + 0.2$ of Residue # 5 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn X	- At(I)	At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact Resd.			
1	[1465.01]	7	2.5400	0.14	2 04W	- H1W4 ...	H2F	-C2F	1		1375.01	1465.01	1555.01	2575.01
2	[1565.01]	8	2.0000	-0.72	0 H1W4	- 04W ...	H2	-01	2	<<	1475.01	1565.01	1655.01	2675.01
3	[1565.03]	4	2.1100	-0.61	2 04W	- H1W4 ...	02W	-H1W2	0	<<	1565.03			
4	[1555.01]	3	1.8700	-0.85	2 04W	- H2W4 ...	022B	-C21B	0	<<	1465.01	1555.01	1645.01	2665.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.

Nr.Cont. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)
[1465.01]	= -1+x,1+y,z	= [	1	-1	1	0 1]	-0.359	1.370	0.073
[1645.01]	= 1+x,-1+y,z	= [	1	1	-1	0 1]	1.641	-0.630	0.073
[2665.01]	= 1-x,1-y,-z	= [	2	1	1	0 1]	0.359	0.630	-0.073
[2756.01]	= 2-x,-y,1-z	= [	2	2	0	1 1]	1.359	-0.370	0.927
[1645.05]	= 1+x,-1+y,z	= [	1	1	-1	0 5]	1.564	-0.147	0.245
[1545.05]	= x,-1+y,z	= [	1	0	-1	0 5]	0.564	-0.147	0.245
[2755.01]	= 2-x,-y,-z	= [	2	2	0	0 1]	1.359	-0.370	-0.073
[1545.04]	= x,-1+y,z	= [	1	0	-1	0 4]	0.823	-0.386	0.157
[1455.01]	= -1+x,y,z	= [	1	-1	0	0 1]	-0.359	0.370	0.073
[1565.01]	= x,1+y,z	= [	1	0	1	0 1]	0.641	1.370	0.073
[2765.01]	= 2-x,1-y,-z	= [	2	2	1	0 1]	1.359	0.630	-0.073
[1655.01]	= 1+x,y,z	= [	1	1	0	0 1]	1.641	0.370	0.073
[2656.01]	= 1-x,-y,1-z	= [	2	1	0	1 1]	0.359	-0.370	0.927
[1655.03]	= 1+x,y,z	= [	1	1	0	0 3]	5/3	-0.299	0.378
[2765.04]	= 2-x,1-y,-z	= [	2	2	1	0 4]	1.177	0.386	-0.157
[1545.01]	= x,-1+y,z	= [	1	0	-1	0 1]	0.641	-0.630	0.073
[2746.03]	= 2-x,-1-y,1-z	= [	2	2	-1	1 3]	4/3	-0.701	0.622
[1565.03]	= x,1+y,z	= [	1	0	1	0 3]	2/3	0.701	0.378
[1545.02]	= x,-1+y,z	= [	1	0	-1	0 2]	0.731	-0.517	0.309
[2746.01]	= 2-x,-1-y,1-z	= [	2	2	-1	1 1]	1.359	-1.370	0.927

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Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

$X(J) = X(\text{sym}) + TX$, $Y(J) = Y(\text{sym}) + TY$, $Z(J) = Z(\text{sym}) + TZ$,

SYM	-	Number of the Symmetry Operator.
Ires	-	Residue Number.
TX, TY, TZ	-	Unit Cell Translations.

Analysis of Short Non-Hydrogen Inter-Molecular Contacts For Inter-Molecular Clusters and/or Networks (Minor Disorder Excluded)

Contact-Nr	Atom I[	ARU	]	Atom J[	ARU	]	d(I-J)	Del
1	Cu2	[	1555.01]	...	04W	[	1645.05]	= 3.382 -0.46
2	01	[	1555.01]	...	04W	[	1545.05]	= 2.817 -0.22
3	02	[	1555.01]	...	03W	[	1545.04]	= 2.735 -0.31
4	012A	[	1555.01]	...	01W	[	1555.02]	= 2.735 -0.31
5	012B	[	1555.01]	...	01W	[	1555.02]	= 2.727 -0.31
6	022A	[	1555.01]	...	02W	[	1555.03]	= 2.794 -0.25
7	022B	[	1555.01]	...	03W	[	1555.04]	= 2.782 -0.26
8	022B	[	1555.01]	...	04W	[	1555.05]	= 2.705 -0.34
9	C2C	[	1555.01]	...	04W	[	1545.05]	= 2.971 -0.25
10	01W	[	1555.02]	...	02W	[	1565.03]	= 2.794 -0.25
11	01W	[	1555.02]	...	012A	[	1555.01]	= 2.735 -0.31
12	01W	[	1555.02]	...	012B	[	1555.01]	= 2.727 -0.31
13	02W	[	1555.03]	...	01W	[	1545.02]	= 2.794 -0.25
14	02W	[	1555.03]	...	022A	[	1555.01]	= 2.794 -0.25
15	03W	[	1555.04]	...	02	[	1565.01]	= 2.735 -0.31
16	03W	[	1555.04]	...	022B	[	1555.01]	= 2.782 -0.26
17	04W	[	1555.05]	...	Cu2	[	1465.01]	= 3.382 -0.46
18	04W	[	1555.05]	...	01	[	1565.01]	= 2.817 -0.22
19	04W	[	1555.05]	...	022B	[	1555.01]	= 2.705 -0.34
20	04W	[	1555.05]	...	C2C	[	1565.01]	= 2.971 -0.25

***** Cluster = 1 *****

(N:M)	:	ARU	--	Connected	with (N)	Interactions	to/from (M)	ARU(S).	T = Translated Molecule (Infinite chain etc.)
9	11	1555.01	--	1465.01*	1645.01*	2665.01*	2756.01*	1645.05	1545.05T 1545.04 1555.02 1555.03 1555.04T 1555.05T
9	11	2665.01	--	2755.01*	2575.01*	1555.01*	1464.01*	2575.05	2675.05T 2675.04 2665.02 2665.03 2665.04T 2665.05T
4	3	1645.05	--	1555.01	1655.01T	1645.01T			
2	2	1545.04	--	1555.01	1545.01T				
3	2	1555.02	--	1565.03T	1555.01				
2	2	1555.03	--	1545.02T	1555.01				
4	3	2575.05	--	2665.01	2565.01T	2575.01T			
2	2	2675.04	--	2665.01	2675.01T				
3	2	2665.02	--	2655.03T	2665.01				
2	2	2665.03	--	2675.02T	2665.01				

:: Starred ARUs belong (chemically) to the previous ARU

:: Analysis of Polymeric Structure(s)

:: Resd # 0 - Infinite Two-Dimensional Network :: Base Vectors: #1 = [1 0 0], #2 = [0 1 0], - Plane: (0 0 1)

Analysis of Potential Hydrogen Bonds and Schemes with $d(D...A) < R(D)+R(A)+0.50$, $d(H...A) < R(H)+R(A)-0.12$ Ang., $D-H...A > 100.0$ Deg

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)

Nr	Typ	Res	Donor	---	H...Acceptor	[ARU]	D - H	H...A	D...A	D - H...A	A...H...A* A'...H...A"	Sum(XY,YZ)	Sum(XZ)
1	Intra	1	O1	--H1	..02	[]	0.79(3)	2.19(2)	2.911(2)	152(2)			
2		2	O1W	--H1W1	..012A	[]	0.78(2)	1.96(2)	2.735(2)	172(3)			
3		1	O1	--H2	..04W	[1545.05]	0.82(3)	2.00(2)	2.817(2)	173(2)			
4		2	O1W	--H2W1	..012B	[]	0.87(3)	1.90(3)	2.727(2)	158(2)			
5		1	O2	--H3	..03W	[1545.04]	0.83(2)	1.91(2)	2.735(2)	173(2)			
6		3	O2W	--H1W2	..022A	[]	0.76(3)	2.06(3)	2.794(2)	164(3)			
7	Intra	1	O2	--H4	..022A	[]	0.81(2)	1.90(2)	2.6705(19)	160(3)			
8		3	O2W	--H2W2	..01W	[1545.02]	0.81(2)	1.99(2)	2.794(2)	173(3)			
9		4	O3W	--H1W3	..01W	[]	0.76(2)	2.19(3)	2.924(2)	164(3)			
10		4	O3W	--H2W3	..022B	[]	0.80(3)	1.99(3)	2.782(2)	173(2)			
11		5	O4W	--H1W4	..02W	[1565.03]	0.79(3)	2.11(3)	2.898(2)	176(2)			
12		5	O4W	--H2W4	..022B	[]	0.84(2)	1.87(2)	2.705(2)	174(2)			
13	Intra	1	C2C	--H2C	..011A	[]	0.95	2.46	2.896(2)	108			
14	Intra	1	C2C	--H2C	..022A	[]	0.95	2.43	3.364(2)	168'	80'	356.00	
15	Intra	1	C2D	--H2D	..012A	[]	0.95	2.56	3.387(3)	145			
16		1	C2F	--H2F	..02W	[1655.03]	0.95	2.58	3.300(3)	133			
17		1	C3E	--H3E	..011B	[1655.01]	0.95	2.58	3.474(3)	157			
18		1	C4E	--H4E	..022B	[2765.01]	0.95	2.50	3.435(3)	167			
19		1	C5D	--H5D	..03W	[2765.04]	0.95	2.48	3.322(3)	148			
20		1	C5E	--H5E	..01	[2755.01]	0.95	2.50	3.440(3)	170			
21		1	C5F	--H5F	..012A	[1545.01]	0.95	2.47	3.401(3)	166			
22	Intra	1	C6A	--H6A	..012A	[]	0.95	2.43	2.763(2)	100			
23	Intra	1	C6B	--H6B	..011B	[]	0.95	2.42	2.752(2)	100			
24	Intra	1	C6C	--H6C	..012B	[]	0.95	2.39	3.246(3)	149			
25	Intra	1	C6D	--H6D	..011B	[]	0.95	2.59	2.913(2)	100			

Translation of ARU-code to Equivalent Position Code

```

[ 1545. ] = x, -1+y, z
[ 2755. ] = 2-x, -y, -z
[ 2765. ] = 2-x, 1-y, -z
[ 1655. ] = 1+x, y, z
[ 1565. ] = x, 1+y, z

```

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

 2-Centre (linear) D-H...X most prob. angle 160 deg - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
 3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg Springer-Verlag, Berlin, 1991, pp 20.
 4-Centre (trifurcated)

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)

At.Nr	D/A	#Cov.Bonds	# H	#D-H..A	#A..H	#A..H-C	Sum(A-H)	Sum(A-X)
1	Cu1	5	-	0	0	0	0	5
2	Cu2	5	-	0	0	0	0	5
3	O1	3	2 H	2	0	1	3	4
4	O1W	2	2 H	2	2	0	4	4
5	O2	3	2 H	2	1	0	3	4
6	O2W	2	2 H	2	1	1	4	4
7	O3W	2	2 H	2	1	1	4	4
8	O4W	2	2 H	2	1	0	3	3
9	O11A	2	-	0	0	1	1	3
10	O11B	2	-	0	0	3	3	5
11	O12A	1	-	0	1	3	4	5
12	O12B	1	-	0	1	1	2	3
13	O21A	2	-	0	0	0	0	2
14	O21B	2	-	0	0	0	0	2
15	O22A	1	-	0	2	1	3	4
16	O22B	1	-	0	2	1	3	4
17	N1C	3	-	0	0	0	0	3
18	N1D	3	-	0	0	0	0	3
19	N1E	3	-	0	0	0	0	3
20	N1F	3	-	0	0	0	0	3

Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)

Coordinates of Donor and Acceptor Atoms												Coordinates of D/A-Bonded Atom(s)							
=====												=====							
D/A I	[	ARU	]	X	Y	Z	--	D/A J	[	ARU	]	X	Y	Z	Atom K	X	Y	Z	I..J--K Angle
01	[	1555.01],	0.7732	0.0214	0.1750	>>	02	[	1555.01],	0.9701-0.2069	0.1985	Cu2	1.2120-0.2129	0.2298	121.88(9)				
												H3	0.9340-0.2630	0.1833	110.41(18)				
												H4	0.9350-0.2020	0.2434	82.09(17)				
02	[	1555.01],	0.9701-0.2069	0.1985	<<	01	[	1555.01],	0.7732	0.0214	0.1750	Cu1	0.7566	0.1950	0.2326	129.84(9)			
												H1	0.8490-0.0240	0.1756	20.99(16)				
												H2	0.7060-0.0210	0.1949	82.92(17)				
01W	[	1555.02],	0.7331	0.4871	0.3089	>>	012A	[	1555.01],	0.8708	0.2741	0.3773	C11A	0.9043	0.1648	0.3677	141.13(14)		
012A	[	1555.01],	0.8708	0.2741	0.3773	<<	01W	[	1555.02],	0.7331	0.4871	0.3089	H1W1	0.7670	0.4270	0.3321	5.46(16)		
													H2W1	0.6580	0.4680	0.2885	106.57(17)		
01	[	1555.01],	0.7732	0.0214	0.1750	>>	04W	[	1545.05],	0.5631-0.1422	0.2445	H1W4	0.5910-0.1870	0.2797	113.83(19)				
												H2W4	0.5530-0.1910	0.2132	110.57(17)				
04W	[	1555.05],	0.5631	0.8578	0.2445	<<	01	[	1565.01],	0.7732	1.0214	0.1750	Cu1	0.7566	1.1950	0.2326	115.04(9)		
													H1	0.8490	0.9760	0.1756	98.63(18)		
													H2	0.7060	0.9790	0.1949	5.21(15)		
01W	[	1555.02],	0.7331	0.4871	0.3089	>>	012B	[	1555.01],	0.5386	0.4548	0.2091	C11B	0.5651	0.3910	0.1546	127.52(14)		
012B	[	1555.01],	0.5386	0.4548	0.2091	<<	01W	[	1555.02],	0.7331	0.4871	0.3089	H1W1	0.7670	0.4270	0.3321	114.91(19)		
													H2W1	0.6580	0.4680	0.2885	15.35(14)		
02	[	1555.01],	0.9701-0.2069	0.1985	>>	03W	[	1545.04],	0.8281-0.3855	0.1555	H1W3	0.8170-0.4280	0.1931	102.11(19)					
											H2W3	0.7440-0.3600	0.1463	111.09(19)					
03W	[	1555.04],	0.8281	0.6145	0.1555	<<	02	[	1565.01],	0.9701	0.7931	0.1985	Cu2	1.2120	0.7871	0.2298	130.29(9)		
													H3	0.9340	0.7370	0.1833	4.80(15)		
													H4	0.9350	0.7980	0.2434	104.63(18)		
02W	[	1555.03],	0.6616-0.2971	0.3787	>>	022A	[	1555.01],	0.9149-0.1665	0.3479	C21A	1.0200-0.1067	0.3548	163.42(14)					
022A	[	1555.01],	0.9149-0.1665	0.3479	<<	02W	[	1555.03],	0.6616-0.2971	0.3787	H1W2	0.7350-0.2690	0.3777	11.43(16)					
													H2W2	0.6870-0.3620	0.3617	107.46(18)			
02	[	1555.01],	0.9701-0.2069	0.1985	>>	022A	[	1555.01],	0.9149-0.1665	0.3479	C21A	1.0200-0.1067	0.3548	103.28(13)					
022A	[	1555.01],	0.9149-0.1665	0.3479	<<	02	[	1555.01],	0.9701-0.2069	0.1985	Cu2	1.2120-0.2129	0.2298	77.81(8)					
												H3	0.9340-0.2630	0.1833	120.80(18)				
												H4	0.9350-0.2020	0.2434	13.79(15)				
02W	[	1555.03],	0.6616-0.2971	0.3787	>>	01W	[	1545.02],	0.7331-0.5129	0.3089	H1W1	0.7670-0.5730	0.3321	120.66(19)					
											H2W1	0.6580-0.5320	0.2885	113.19(18)					
01W	[	1555.02],	0.7331	0.4871	0.3089	<<	02W	[	1565.03],	0.6616	0.7028	0.3787	H1W2	0.7350	0.7310	0.3777	108.26(19)		
													H2W2	0.6870	0.6380	0.3617	5.29(15)		
03W	[	1555.04],	0.8281	0.6145	0.1555	>>	01W	[	1555.02],	0.7331	0.4871	0.3089	H1W1	0.7670	0.4270	0.3321	132.68(19)		
													H2W1	0.6580	0.4680	0.2885	86.07(16)		
01W	[	1555.02],	0.7331	0.4871	0.3089	<<	03W	[	1555.04],	0.8281	0.6145	0.1555	H1W3	0.8170	0.5720	0.1931	11.57(16)		
													H2W3	0.7440	0.6400	0.1463	95.92(18)		
03W	[	1555.04],	0.8281	0.6145	0.1555	>>	022B	[	1555.01],	0.5317	0.7148	0.1357	C21B	0.4292	0.6553	0.1249	124.43(13)		

022B	[1555.01],	0.5317	0.7148	0.1357	<<	03W	[1555.04],	0.8281	0.6145	0.1555	H1W3	0.8170	0.5720	0.1931	103.17(19)
											H2W3	0.7440	0.6400	0.1463	5.32(15)
04W	[1555.05],	0.5631	0.8578	0.2445	>>	02W	[1565.03],	0.6616	0.7028	0.3787	H1W2	0.7350	0.7310	0.3777	95.49(19)
											H2W2	0.6870	0.6380	0.3617	102.19(18)
02W	[1555.03],	0.6616-0.2971	0.3787	<<	04W	[1545.05],	0.5631-0.1422	0.2445	H1W4	0.5910-0.1870	0.2797	2.85(16)			
									H2W4	0.5530-0.1910	0.2132	104.64(17)			
04W	[1555.05],	0.5631	0.8578	0.2445	>>	022B	[1555.01],	0.5317	0.7148	0.1357	C21B	0.4292	0.6553	0.1249	134.54(14)
022B	[1555.01],	0.5317	0.7148	0.1357	<<	04W	[1555.05],	0.5631	0.8578	0.2445	H1W4	0.5910	0.8130	0.2797	105.81(19)
											H2W4	0.5530	0.8090	0.2132	4.14(14)

 =====
 ***** Aggregate = 1 *****
 =====

(N:M) : ARU -- Connected with N Hydrogen Bonds to/from M ARU(S). T = Translated Molecule (Infinite chain etc.)

7	10	1555.01	--	1465.01*	1645.01*	2665.01*	2756.01*	1545.05	1545.04	1555.02	1555.03	1555.04T	1555.05T
7	10	2665.01	--	2755.01*	2575.01*	1555.01*	1464.01*	2675.05	2675.04	2665.02	2665.03	2665.04T	2665.05T
3	3	1545.05	--	1555.03	1545.01T	1555.01							
3	3	1545.04	--	1545.02T	1545.01T	1555.01							
4	3	1555.02	--	1555.01	1565.03T	1555.04T							
3	3	1555.03	--	1555.01	1545.02T	1545.05							
3	3	2675.05	--	2665.03	2675.01T	2665.01							
3	3	2675.04	--	2675.02T	2675.01T	2665.01							
4	3	2665.02	--	2665.01	2655.03T	2665.04T							
3	3	2665.03	--	2665.01	2675.02T	2675.05							

:: Starred ARUs belong (chemically) to the previous ARU

:: Analysis of Polymeric Structure(s)

:: Resd # 0 - Infinite One-Dimensional Chain :: Base Vector: [0 1 0]

Search for ARU-Circuits (Max = 6) and Infinite ARU-Chains (Max = 4)

=====

6-Membered ARU-Circuit

1555.01 1465.01 1375.01 2485.01 2575.01 2665.01 1555.01

6-Membered ARU-Circuit

1555.01 1465.01 1375.01 2485.01 2575.01 1465.01 1555.01

6-Membered ARU-Circuit

1555.01 1465.01 1375.01 2576.01 2666.01 2756.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1375.01 2576.01 2666.01 1465.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 2575.01 2665.01 2755.01 1645.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 2575.01 1374.01 1464.01 2665.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 2666.01 2756.01 2846.01 1645.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 2666.01 1556.01 1646.01 2756.01 1555.01

5-Membered ARU-Circuit
1555.01 1465.01 1455.05 1465.03 1465.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1455.05 1455.01 1545.01 1545.04 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1455.05 1455.01 1545.01 1545.05 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1455.05 1455.01 1455.04 1465.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1455.04 1455.02 1465.03 1465.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1455.04 1455.01 1545.01 1545.04 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1455.04 1455.01 1545.01 1545.05 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1465.02 1475.03 1465.05 1465.01 1555.01

5-Membered ARU-Circuit
1555.01 1465.01 1465.02 1465.04 1465.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1465.04 1475.01 1565.01 1555.05 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1465.04 1475.01 1565.01 1555.04 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1465.04 1475.01 1465.05 1465.01 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1465.05 1475.01 1565.01 1555.05 1555.01

6-Membered ARU-Circuit
1555.01 1465.01 1465.05 1475.01 1565.01 1555.04 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 1735.01 2845.01 2755.01 2665.01 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 1735.01 2845.01 2755.01 1645.01 1555.01

4-Membered ARU-Circuit
1555.01 1645.01 2755.01 2665.01 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 2755.01 1554.01 1464.01 2665.01 1555.01

4-Membered ARU-Circuit
1555.01 1645.01 2846.01 2756.01 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 2846.01 1736.01 1646.01 2756.01 1555.01

5-Membered ARU-Circuit
1555.01 1645.01 1635.05 1645.03 1645.01 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 1635.05 1635.01 1545.01 1545.04 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 1635.05 1635.01 1545.01 1545.05 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 1635.05 1635.01 1635.04 1645.01 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 1635.04 1635.02 1645.03 1645.01 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 1635.04 1635.01 1545.01 1545.04 1555.01

6-Membered ARU-Circuit
1555.01 1645.01 1635.04 1635.01 1545.01 1545.05 1555.01

6-Membered ARU-Circuit
 1555.01 1645.01 1645.02 1655.03 1645.05 1645.01 1555.01

5-Membered ARU-Circuit
 1555.01 1645.01 1645.02 1645.04 1645.01 1555.01

6-Membered ARU-Circuit
 1555.01 1645.01 1645.04 1655.01 1565.01 1555.05 1555.01

6-Membered ARU-Circuit
 1555.01 1645.01 1645.04 1655.01 1565.01 1555.04 1555.01

6-Membered ARU-Circuit
 1555.01 1645.01 1645.04 1655.01 1645.05 1645.01 1555.01

6-Membered ARU-Circuit
 1555.01 1645.01 1645.05 1655.01 1565.01 1555.05 1555.01

6-Membered ARU-Circuit
 1555.01 1645.01 1645.05 1655.01 1565.01 1555.04 1555.01

6-Membered ARU-Circuit
 1555.01 2665.01 2755.01 1554.01 1464.01 2665.01 1555.01

6-Membered ARU-Circuit
 1555.02 1555.01 1465.01 2575.01 2665.01 1555.01 1555.02

6-Membered ARU-Circuit
 1555.02 1555.01 1465.01 2666.01 2756.01 1555.01 1555.02

6-Membered ARU-Circuit
 1555.02 1555.01 1645.01 2755.01 2665.01 1555.01 1555.02

6-Membered ARU-Circuit
 1555.02 1555.01 1645.01 2846.01 2756.01 1555.01 1555.02

5-Membered ARU-Circuit
 1555.02 1555.01 1545.05 1555.03 1555.01 1555.02

6-Membered ARU-Circuit
 1555.02 1555.01 1545.05 1545.01 1545.04 1555.01 1555.02

6-Membered ARU-Circuit
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6-Membered ARU-Circuit
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1-Membered Infinite ARU-Chain (Translation [-1 1 0])
1555.01 1465.01

4-Membered Infinite ARU-Chain (Translation [-2 2 0])
1555.02 1555.01 1465.01 1375.01 1375.02

4-Membered Infinite ARU-Chain (Translation [-1 0 0])
1555.02 1555.01 1465.01 1455.04 1455.02

4-Membered Infinite ARU-Chain (Translation [2 -2 0])
1555.02 1555.01 1645.01 1735.01 1735.02

4-Membered Infinite ARU-Chain (Translation [1 -2 0])
1555.02 1555.01 1645.01 1635.04 1635.02

4-Membered Infinite ARU-Chain (Translation [-1 1 -1])
1555.02 1555.01 2665.01 1464.01 1464.02

4-Membered Infinite ARU-Chain (Translation [1 -1 1])
1555.02 1555.01 2756.01 1646.01 1646.02

4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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3-Membered Infinite ARU-Chain (Translation [0 -1 0])
1555.02 1555.01 1545.04 1545.02

3-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [0 1 0])
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4-Membered Infinite ARU-Chain (Translation [0 1 0])
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4-Membered Infinite ARU-Chain (Translation [-1 2 0])
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4-Membered Infinite ARU-Chain (Translation [1 0 0])
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4-Membered Infinite ARU-Chain (Translation [0 1 0])
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4-Membered Infinite ARU-Chain (Translation [-1 1 0])
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4-Membered Infinite ARU-Chain (Translation [1 -1 0])
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4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [-1 2 0])
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4-Membered Infinite ARU-Chain (Translation [1 0 0])
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4-Membered Infinite ARU-Chain (Translation [-2 2 0])
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4-Membered Infinite ARU-Chain (Translation [-1 1 0])
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4-Membered Infinite ARU-Chain (Translation [-1 2 0])
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4-Membered Infinite ARU-Chain (Translation [2 -2 0])
1555.03 1555.01 1645.01 1735.01 1735.03

4-Membered Infinite ARU-Chain (Translation [1 -1 0])
1555.03 1555.01 1645.01 1635.05 1645.03

4-Membered Infinite ARU-Chain (Translation [1 0 0])
1555.03 1555.01 1645.01 1645.02 1655.03

4-Membered Infinite ARU-Chain (Translation [-1 1 -1])
1555.03 1555.01 2665.01 1464.01 1464.03

4-Membered Infinite ARU-Chain (Translation [1 -1 1])
1555.03 1555.01 2756.01 1646.01 1646.03

4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [0 1 0])
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3-Membered Infinite ARU-Chain (Translation [0 1 0])
1555.03 1555.01 1555.05 1565.03

4-Membered Infinite ARU-Chain (Translation [-1 0 0])
1555.03 1545.02 1545.01 1455.01 1455.03

4-Membered Infinite ARU-Chain (Translation [1 -2 0])
1555.03 1545.02 1545.01 1635.01 1635.03

4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [-1 0 0])
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4-Membered Infinite ARU-Chain (Translation [1 -2 0])
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4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [-1 1 0])
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4-Membered Infinite ARU-Chain (Translation [1 -1 0])
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4-Membered Infinite ARU-Chain (Translation [0 1 0])
1555.03 1545.05 1555.01 1555.05 1565.03

4-Membered Infinite ARU-Chain (Translation [-1 0 0])
1545.04 1545.02 1545.01 1455.01 1445.04

4-Membered Infinite ARU-Chain (Translation [1 -2 0])
1545.04 1545.02 1545.01 1635.01 1625.04

4-Membered Infinite ARU-Chain (Translation [0 1 0])
1545.04 1545.02 1555.03 1555.01 1555.04

4-Membered Infinite ARU-Chain (Translation [-2 1 0])
1545.04 1545.01 1455.01 1365.01 1355.04

4-Membered Infinite ARU-Chain (Translation [2 -3 0])
1545.04 1545.01 1635.01 1725.01 1715.04

4-Membered Infinite ARU-Chain (Translation [-1 0 -1])
1545.04 1545.01 2655.01 1454.01 1444.04

4-Membered Infinite ARU-Chain (Translation [1 -2 1])
1545.04 1545.01 2746.01 1636.01 1626.04

4-Membered Infinite ARU-Chain (Translation [0 -2 0])
1545.04 1545.01 1535.05 1535.01 1525.04

4-Membered Infinite ARU-Chain (Translation [-2 2 0])
1545.04 1555.01 1465.01 1375.01 1365.04

4-Membered Infinite ARU-Chain (Translation [2 -2 0])
1545.04 1555.01 1645.01 1735.01 1725.04

4-Membered Infinite ARU-Chain (Translation [-1 1 -1])
1545.04 1555.01 2665.01 1464.01 1454.04

4-Membered Infinite ARU-Chain (Translation [1 -1 1])
1545.04 1555.01 2756.01 1646.01 1636.04

4-Membered Infinite ARU-Chain (Translation [0 -1 0])
1545.04 1555.01 1545.05 1545.01 1535.04

4-Membered Infinite ARU-Chain (Translation [-1 1 0])
1545.05 1555.03 1555.01 1465.01 1455.05

4-Membered Infinite ARU-Chain (Translation [1 -1 0])
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4-Membered Infinite ARU-Chain (Translation [0 -1 0])
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4-Membered Infinite ARU-Chain (Translation [-2 1 0])
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4-Membered Infinite ARU-Chain (Translation [2 -3 0])
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4-Membered Infinite ARU-Chain (Translation [-1 0 -1])
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4-Membered Infinite ARU-Chain (Translation [1 -2 1])
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4-Membered Infinite ARU-Chain (Translation [-2 2 0])
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4-Membered Infinite ARU-Chain (Translation [2 -2 0])
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4-Membered Infinite ARU-Chain (Translation [-1 1 -1])
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4-Membered Infinite ARU-Chain (Translation [1 -1 1])
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4-Membered Infinite ARU-Chain (Translation [0 1 0])
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4-Membered Infinite ARU-Chain (Translation [0 1 0])
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Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))

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=====
 NetworkK = 1
 =====

Code	Acc	Donor Atom	X	Y	Z	Acceptor Atom	X	Y	Z up to	BondCode(s) of Forward Link(s)
1.555		O1 [1555.01]	0.7732	0.0214	0.1750	O2 [1555.01]	0.9701	-0.2069	0.1985	3.555 4.555
		H1	0.8490	-0.0240	0.1756					
2.555		O1 [1555.01]	0.7732	0.0214	0.1750	O4W [1545.05]	0.5631	-0.1422	0.2445	5.555 6.555
		H2	0.7060	-0.0210	0.1949					
3.555	A	O2 [1555.01]	0.9701	-0.2069	0.1985	O3W [1545.04]	0.8281	-0.3855	0.1555	7.555 8.555
		H3	0.9340	-0.2630	0.1833					
4.555	A	O2 [1555.01]	0.9701	-0.2069	0.1985	O22A [1555.01]	0.9149	-0.1665	0.3479	
		H4	0.9350	-0.2020	0.2434					
5.555	A	O4W [1545.05]	0.5631	-0.1422	0.2445	O2W [1555.03]	0.6616	-0.2971	0.3787	9.555R 10.555
		H1W4	0.5910	-0.1870	0.2797					
6.555	A	O4W [1545.05]	0.5631	-0.1422	0.2445	O22B [1545.01]	0.5317	-0.2852	0.1357	
		H2W4	0.5530	-0.1910	0.2132					
7.555	A	O3W [1545.04]	0.8281	-0.3855	0.1555	O1W [1545.02]	0.7331	-0.5129	0.3089	11.555 12.555
		H1W3	0.8170	-0.4280	0.1931					
8.555	A	O3W [1545.04]	0.8281	-0.3855	0.1555	O22B [1545.01]	0.5317	-0.2852	0.1357	
		H2W3	0.7440	-0.3600	0.1463					
9.555	A	O2W [1555.03]	0.6616	-0.2971	0.3787	O22A [1555.01]	0.9149	-0.1665	0.3479	
		H1W2	0.7350	-0.2690	0.3777					
10.555	A	O2W [1555.03]	0.6616	-0.2971	0.3787	O1W [1545.02]	0.7331	-0.5129	0.3089	11.555R 12.555R
		H2W2	0.6870	-0.3620	0.3617					
11.555	A	O1W [1545.02]	0.7331	-0.5129	0.3089	O12A [1545.01]	0.8708	-0.7259	0.3773	
		H1W1	0.7670	-0.5730	0.3321					
12.555	A	O1W [1545.02]	0.7331	-0.5129	0.3089	O12B [1545.01]	0.5386	-0.5452	0.2091	
		H2W1	0.6580	-0.5320	0.2885					

Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)

I - 5 = Nr of Translation Units Along A-Axis

J - 5 = Nr of Translation Units Along B-Axis

K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with 'R' and Infinite Chain Links With 'T'

Analysis of the Coordination Geometry

Distances are calculated from atom I of Unique Molecule Coordinate List to atom J in Asymmetric Residue Unit: ARU.

Phi = Azimuth angle(counter clockwise from X0 in X0,Y0-Plane), Mu = Angle between D and X0,Y0-plane.

'To-Code' : '--' = Bonded atoms, '<<' = .LT. sum vdW-radii - 0.2, '<' = .LT. sum vdW-radii, '..' = .GT. sum vdW-radii.

>>>> NOTICE >>>> : The Symmetry Code Character Added to the Atom Label Applies to the Current Coordination Sphere Only.

>>>>>>>>>>>> : Symmetry operations refer to the coordinates listed in the fractional coordinate table given above

The List May be Limited to the Shortest Distances.

=====															
3.6 Angstrom Coordination Sphere Around Atom I = Cu1						[ARU = 1555.01]			0.75664	0.19504	0.23260	7.6495	2.6160	3.9926	

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	1.9637(13)	--	O11A	[	=	]	Intra	-28.32	40.42	0.89514	0.11740	0.30677	8.9655	1.9067	5.2658
2	1.9690(14)	--	O11B	[	=	]	Intra	148.76	-40.35	0.62084	0.27894	0.15833	6.3665	3.3943	2.7178
3	2.0135(17)	--	N1C	[	=	]	Intra	-164.47	42.40	0.58089	0.14471	0.31169	6.2168	2.2179	5.3502
4	2.0144(17)	--	N1D	[	=	]	Intra	24.76	-36.87	0.92935	0.26889	0.16218	9.1127	3.2910	2.7839
5	2.2745(16)	--	O1	[	=	]	Intra	-97.32	-25.76	0.77323	0.02137	0.17500	7.3885	0.5843	3.0039
6	2.8342(19)	<<	C11A	[	=	]	Intra	-2.29	54.89	0.90430	0.16478	0.36767	9.2781	2.5509	6.3111
7	2.9028(19)	<<	C2C	[	=	]	Intra	-131.10	45.24	0.59710	0.03385	0.35267	6.3057	1.0758	6.0537
8	2.908(2)	<<	C11B	[	=	]	Intra	128.98	-27.40	0.56510	0.39096	0.15462	6.0253	4.6234	2.6541
9	2.918(2)	<<	C6D	[	=	]	Intra	22.38	-60.41	0.93720	0.27140	0.08477	8.9819	3.1646	1.4551
10	2.962(2)	<<	C2D	[	=	]	Intra	29.06	-14.63	1.02830	0.32903	0.18901	10.1548	4.0083	3.2444
11	2.982(2)	<<	C6C	[	=	]	Intra	170.73	32.07	0.44630	0.21527	0.32484	5.1558	3.0230	5.5760
12	3.1330(16)	<<	O12A	[	=	]	Intra	37.42	52.43	0.87081	0.27409	0.37727	9.1665	3.7767	6.4759
13	3.2788(16)	<<	O12B	[	=	]	Intra	119.91	-7.08	0.53857	0.45479	0.20906	6.0269	5.4364	3.5886
14	2.69(2)	<<	H2	[	=	]	Intra	-109.49	-13.93	0.70600	-0.02100	0.19490	6.7789	0.1562	3.3455
15	2.74(2)	<<	H1	[	=	]	Intra	-82.15	-20.95	0.84900	-0.02400	0.17560	7.9986	0.0847	3.0142
16	2.91	<<	H2C	[	=	]	Intra	-105.94	40.90	0.69110	-0.01660	0.34360	7.0453	0.5009	5.8980
17	2.94	<<	H6D	[	=	]	Intra	2.50	-77.95	0.86970	0.22770	0.06500	8.2632	2.6429	1.1157
18	3.01	<<	H2D	[	=	]	Intra	29.22	3.63	1.02590	0.32600	0.24370	10.2734	4.0837	4.1832
19	3.05	<<	H6C	[	=	]	Intra	154.82	20.86	0.43260	0.29340	0.29580	5.0725	3.8276	5.0775
20	3.29(2)	<<	H2W1	[	=	02]		96.00	16.99	0.65800	0.46800	0.28850	7.3212	5.7404	4.9522
21	3.32(2)	<<	H1W1	[	=	02]		75.80	30.97	0.76700	0.42700	0.33210	8.3477	5.3746	5.7006

Bond Valence Analysis

N.E. Brese & M. O'Keeffe (1991) Acta Cryst. B47, 192-197.

I.D. Brown (2002). The Chemical Bond in Inorganic Chemistry: The Bond Valence Model. Oxford University Press.

Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 1 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu1 O11A	1.9637	1.6100	0.37	0.384	0.384	0.616	
2	Cu1 O11B	1.9690	1.6100	0.37	0.379	0.763	0.237	
3	Cu1 N1C	2.0135	1.5200	0.37	0.263	1.027	0.027	
4	Cu1 N1D	2.0144	1.5200	0.37	0.263	1.290	0.290	
5	Cu1 O1	2.2745	1.6100	0.37	0.166	1.456	0.456	
	Cu1 C11A	2.8342						(Contribution below Minimum, Skipped)
	Cu1 C2C	2.9028						(Contribution below Minimum, Skipped)
	Cu1 C11B	2.9080						(Contribution below Minimum, Skipped)
	Cu1 C6D	2.9180						(Contribution below Minimum, Skipped)
	Cu1 C2D	2.9620						(Contribution below Minimum, Skipped)
	Cu1 C6C	2.9820						(Contribution below Minimum, Skipped)
	Cu1 O12A	3.1330						(Contribution below Minimum, Skipped)
	Cu1 O12B	3.2788						(Contribution below Minimum, Skipped)
	Cu1 H2	2.6900						(Contribution not Tabulated, Result Dubious !)
	Cu1 H1	2.7400						(Contribution not Tabulated, Result Dubious !)
	Cu1 H2C	2.9100						(Contribution not Tabulated, Result Dubious !)
	Cu1 H6D	2.9400						(Contribution not Tabulated, Result Dubious !)
	Cu1 H2D	3.0100						(Contribution not Tabulated, Result Dubious !)
	Cu1 H6C	3.0500						(Contribution not Tabulated, Result Dubious !)
	Cu1 H2W1	3.2900						(Contribution not Tabulated, Result Dubious !)
	Cu1 H1W1	3.3200						(Contribution not Tabulated, Result Dubious !)

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Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 2 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu1 O11A	1.9637	1.6790	0.37	0.463	0.463	1.537	
2	Cu1 O11B	1.9690	1.6790	0.37	0.457	0.920	1.080	
3	Cu1 N1C	2.0135	1.7510	0.37	0.492	1.412	0.588	
4	Cu1 N1D	2.0144	1.7510	0.37	0.491	1.903	0.097	
5	Cu1 O1	2.2745	1.6790	0.37	0.200	2.103	0.103	
	Cu1 C11A	2.8342						(Contribution below Minimum, Skipped)
	Cu1 C2C	2.9028						(Contribution below Minimum, Skipped)
	Cu1 C11B	2.9080						(Contribution below Minimum, Skipped)
	Cu1 C6D	2.9180						(Contribution below Minimum, Skipped)
	Cu1 C2D	2.9620						(Contribution below Minimum, Skipped)
	Cu1 C6C	2.9820						(Contribution below Minimum, Skipped)
	Cu1 O12A	3.1330						(Contribution below Minimum, Skipped)
	Cu1 O12B	3.2788						(Contribution below Minimum, Skipped)
	Cu1 H2	2.6900						(Contribution below Minimum, Skipped)
	Cu1 H1	2.7400						(Contribution below Minimum, Skipped)
	Cu1 H2C	2.9100						(Contribution below Minimum, Skipped)
	Cu1 H6D	2.9400						(Contribution below Minimum, Skipped)
	Cu1 H2D	3.0100						(Contribution below Minimum, Skipped)
	Cu1 H6C	3.0500						(Contribution below Minimum, Skipped)
	Cu1 H2W1	3.2900						(Contribution below Minimum, Skipped)
	Cu1 H1W1	3.3200						(Contribution below Minimum, Skipped)

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Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 3 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu1 O11A	1.9637	1.7350	0.37	0.539	0.539	2.461	
2	Cu1 O11B	1.9690	1.7350	0.37	0.531	1.070	1.930	
3	Cu1 N1C	2.0135	1.7680	0.37	0.515	1.585	1.415	
4	Cu1 N1D	2.0144	1.7680	0.37	0.514	2.099	0.901	
5	Cu1 O1	2.2745	1.7350	0.37	0.233	2.332	0.668	
	Cu1 C11A	2.8342						(Contribution below Minimum, Skipped)
	Cu1 C2C	2.9028						(Contribution below Minimum, Skipped)
	Cu1 C11B	2.9080						(Contribution below Minimum, Skipped)
	Cu1 C6D	2.9180						(Contribution below Minimum, Skipped)
	Cu1 C2D	2.9620						(Contribution below Minimum, Skipped)
	Cu1 C6C	2.9820						(Contribution below Minimum, Skipped)
	Cu1 O12A	3.1330						(Contribution below Minimum, Skipped)
	Cu1 O12B	3.2788						(Contribution below Minimum, Skipped)
	Cu1 H2	2.6900						(Contribution not Tabulated, Result Dubious !)
	Cu1 H1	2.7400						(Contribution not Tabulated, Result Dubious !)
	Cu1 H2C	2.9100						(Contribution not Tabulated, Result Dubious !)
	Cu1 H6D	2.9400						(Contribution not Tabulated, Result Dubious !)
	Cu1 H2D	3.0100						(Contribution not Tabulated, Result Dubious !)
	Cu1 H6C	3.0500						(Contribution not Tabulated, Result Dubious !)
	Cu1 H2W1	3.2900						(Contribution not Tabulated, Result Dubious !)
	Cu1 H1W1	3.3200						(Contribution not Tabulated, Result Dubious !)

Polyhedral Volume 6.389 Ang**3

Angles (Degrees) At1...V...At2 with Vertex V = Cu1

O11A	,	C11A	22.51(6)	O11A	,	C2C	70.02(6)	O11A	,	C11B	157.21(6)	O11A	,	C6D	109.01(6)
O11A	,	C2D	76.51(6)	O11A	,	C6C	105.40(6)	O11A	,	O12A	45.20(6)	O11A	,	O12B	136.24(5)
O11B	,	C11A	155.95(6)	O11B	,	C2C	111.58(6)	O11B	,	C11B	20.83(6)	O11B	,	C6D	70.14(6)
O11B	,	C2D	101.64(6)	O11B	,	C6C	75.22(6)	O11B	,	O12A	133.02(6)	O11B	,	O12B	42.08(5)
N1C	,	C11A	81.53(7)	N1C	,	C2C	24.07(7)	N1C	,	C11B	92.83(6)	N1C	,	C6D	161.51(7)
N1C	,	C2D	149.88(7)	N1C	,	C6C	22.16(7)	N1C	,	O12A	83.30(6)	N1C	,	O12B	84.32(6)
N1D	,	C11A	94.66(7)	N1D	,	C2C	160.07(7)	N1D	,	C11B	84.16(7)	N1D	,	C6D	23.58(7)
N1D	,	C2D	22.57(7)	N1D	,	C6C	151.69(7)	N1D	,	O12A	89.99(6)	N1D	,	O12B	89.85(6)
O1	,	C11A	113.64(6)	O1	,	C2C	77.38(6)	O1	,	C11B	110.64(6)	O1	,	C6D	80.93(6)
O1	,	C2D	114.02(6)	O1	,	C6C	104.88(6)	O1	,	O12A	136.97(6)	O1	,	O12B	131.15(6)
C11A	,	C2C	70.91(6)	C11A	,	C11B	135.50(6)	C11A	,	C6D	116.96(6)	C11A	,	C2D	74.42(6)
C11A	,	C6C	92.83(6)	C11A	,	O12A	23.34(6)	C11A	,	O12B	113.89(5)	C2C	,	C11B	115.75(6)
C2C	,	C6D	158.21(6)	C2C	,	C2D	145.11(6)	C2C	,	C6C	46.23(6)	C2C	,	O12A	81.83(5)
C2C	,	O12B	108.35(5)	C11B	,	C6D	74.04(6)	C11B	,	C2D	91.82(6)	C11B	,	C6C	71.53(6)
C11B	,	O12A	112.30(5)	C11B	,	O12B	22.07(5)	C6D	,	C2D	46.04(6)	C6D	,	C6C	144.88(6)
C6D	,	O12A	113.49(6)	C6D	,	O12B	87.54(6)	C2D	,	C6C	141.01(6)	C2D	,	O12A	67.45(6)
C2D	,	O12B	89.03(6)	C6C	,	O12A	86.19(6)	C6C	,	O12B	62.24(6)	O12A	,	O12B	91.07(5)

Dist. Cu1 - Polyh_C.G.:0.3789(7) Ang, C.G.: 0.75989(7) 0.16626(6) 0.22279(4) 7.6100(7) 2.2789(7) 3.8243(6)

Real Angles I - Cu1		- J	Real Edge I - J	Unit Polyhedron Dihedral Angles			Norm. IJK:IJL	K	L	
O11A	,	O11B	177.78(6)	3.932(2)	172.83(4)	-90.42(4)	-96.75(4)	-7.17(4)	N1C	N1D
O11A	,	N1C	88.18(7)	2.768(2)	58.72(3)	4.94(3)	53.79(3)	121.27(3)	N1D	O1
O11A	,	N1D	91.33(7)	2.846(2)	-57.14(3)	-5.19(4)	-51.95(3)	122.86(3)	N1C	O1
O11A	,	O1	92.07(6)	3.058(2)	106.28(3)	55.95(3)	50.33(3)	73.72(3)	N1C	N1D
O11B	,	N1C	92.93(7)	2.887(2)	-61.04(3)	-5.12(3)	-55.92(3)	118.96(3)	N1D	O1
O11B	,	N1D	87.27(7)	2.749(2)	57.12(3)	4.98(3)	52.14(3)	122.88(3)	N1C	O1
O11B	,	O1	89.82(6)	3.004(2)	-104.90(3)	-53.21(3)	-51.69(3)	75.10(3)	N1C	N1D
N1C	,	N1D	171.00(7)	4.015(2)	172.86(4)	87.71(4)	85.15(4)	7.14(4)	O11A	O11B
N1C	,	O1	92.00(7)	3.090(2)	-108.93(3)	-54.96(3)	-53.97(3)	71.07(3)	O11A	O11B
N1D	,	O1	97.00(7)	3.217(2)	112.69(3)	54.59(3)	58.10(3)	67.31(3)	O11A	O11B

Tau-Descriptor for 5-Coordination (A.W.Addison,T.N.Rao,J.Reedijk,J.van Rijn,G.C.Verschoor, J.Chem.Soc.Dalton Trans.(1984),1349-1356)

Tau = (Beta - Alpha) / 60 = (177.78-171.00) / 60 = 0.11 : (Extreme forms: Tau = 0.00 for SP and 1.00 for TP)

=====

Analysis of Five-Coordination (See R.R. Holmes in Progress in Inorg. Chem. Vol. 32 (1984),119-235 and References Therein)

Idealized Dihedral Angles for Trans Basal Angle : 150.0
 Del(13) & Del(23) Trigonal Bipyramid (TP): 101.5 53.1
 Del(12) & Del(13) Square Pyramid (SP): 118.5 76.9
 Distance Between TP and SP Along Berry Coordinate: 217.7

Pivot(3)	Sum(/Del:C - Del:TP/)	Sum(/Del:C - Del:SP/)	217.7 - Sum(/Del:C - Del:SP/)	Del(24)	Th(24)	Th(15)
N1C	212.2 Deg.	326.2 Deg.	-108.5 Deg.	67.31	97.00	177.78
N1D	212.2 Deg.	333.8 Deg.	-116.0 Deg.	71.07	92.00	177.78
01	212.2 Deg.	39.4 Deg.	178.3 Deg.	7.14	171.00	177.78

Trigonal Bipyramid (TP) to Square Pyramid (SP) ::: Perc. Along Berry Pseudorotation Coordinate: 89.7 ::: D3h ---> C2v ---> C4v

NOTE: This Analysis Depends on the Value of the Trans Basal Angle that is used (Default Value = 150 Deg.).

The Pivot Atom that Best Describes a Berry Pseudo Rotation is: 01

The Percentage has been Calculated for the Average value, 195.3 Deg., of the Second and Fourth Table Entry.

The Difference, 33.8 Deg., Between the Second and Fourth Table Entry (for pivot) should be Zero for a True Berry Rotation.

>> Distance to SP square base plane defined by: 011A 011B N1C N1D
 011A -0.0634(13), 011B -0.0629(13), N1C 0.0625(16), N1D 0.0638(16), Cu1 -0.0947(2), 01 -2.3665(15)

3.6 Angstrom Coordination Sphere Around Atom I = Cu2														[ARU = 1555.01]		1.21202	-0.21291	0.22984	11.0994	-1.8926	3.9452
Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0						
1	1.9677(14)	--	O21B_b	[1+x, -1+y, z	=	1645.01]	Intra	-77.37	-39.99	1.29071	-0.33288	0.15616	11.4291	-3.3635	2.6805						
2	1.9757(14)	--	O21A	[	=	]	Intra	99.18	43.80	1.14415	-0.09975	0.30950	10.8720	-0.4849	5.3126						
3	1.9895(16)	--	N1E	[	=	]	Intra	76.87	-44.67	1.24906	-0.07339	0.14835	11.4208	-0.5147	2.5465						
4	2.0052(17)	--	N1F	[	=	]	Intra	-86.96	48.87	1.21623	-0.34810	0.31782	11.1694	-3.2097	5.4555						
5	2.2948(16)	--	O2	[	=	]	Intra	179.91	-13.57	0.97015	-0.20694	0.19846	8.8687	-1.8891	3.4066						
6	2.8494(19)	<<	C21A	[	=	]	Intra	130.76	48.81	1.02000	-0.10669	0.35476	9.8743	-0.4714	6.0895						
7	2.8557(19)	<<	C21B_b	[1+x, -1+y, z	=	1645.01]	Intra	-48.64	-39.10	1.42920	-0.34468	0.12492	12.5640	-3.5560	2.1443						
8	2.912(2)	<<	C6E	[	=	]	Intra	96.32	-65.77	1.22060	-0.07740	0.07516	10.9678	-0.7047	1.2901						
9	2.912(2)	<<	C2F	[	=	]	Intra	-49.61	56.89	1.30800	-0.34830	0.37193	12.1303	-3.1042	6.3843						
10	2.920(2)	<<	C2E	[	=	]	Intra	65.72	-23.45	1.31690	0.02049	0.16215	12.2010	0.5490	2.7833						
11	2.942(2)	<<	C6F	[	=	]	Intra	-111.23	34.86	1.12170	-0.43442	0.32780	10.2253	-4.1426	5.6268						
12	3.1313(16)	<<	O22B_b	[1+x, -1+y, z	=	1645.01]	Intra	-21.55	-31.05	1.53170	-0.28519	0.13573	13.5945	-2.8778	2.3298						
13	3.1320(15)	<<	O22A	[	=	]	Intra	161.76	40.30	0.91494	-0.16648	0.34786	8.8308	-1.1451	5.9711						
14	3.3821(19)	<<	O4W_e	[1+x, -1+y, z	=	1645.05]		13.89	4.27	1.56313	-0.14221	0.24452	14.3735	-1.0829	4.1972						
15	2.43(3)	<<	H4	[	=	]	Intra	176.51	5.49	0.93500	-0.20200	0.24340	8.6813	-1.7451	4.1780						
16	2.87(3)	<<	H3	[	=	]	Intra	-166.44	-16.18	0.93400	-0.26300	0.18330	8.4234	-2.5381	3.1464						
17	2.94	<<	H2F	[	=	]	Intra	-18.02	52.31	1.37590	-0.28770	0.36530	12.8079	-2.4484	6.2705						
18	2.95	<<	H6E	[	=	]	Intra	147.49	-73.70	1.17100	-0.14290	0.06500	10.4018	-1.4480	1.1157						
19	2.97	<<	H2E	[	=	]	Intra	61.57	-5.32	1.33500	0.02530	0.21380	12.5059	0.7050	3.6699						
20	2.99	<<	H6F	[	=	]	Intra	-123.51	19.98	1.05750	-0.43570	0.28930	9.5492	-4.2334	4.9659						
21	3.05(3)	<<	H2W4_e	[1+x, -1+y, z	=	1645.05]		3.94	-5.37	1.55300	-0.19100	0.21320	14.1283	-1.6838	3.6596						

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Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 1 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu2 O21B_b	1.9677	1.6100	0.37	0.380	0.380	0.620	
2	Cu2 O21A	1.9757	1.6100	0.37	0.372	0.752	0.248	
3	Cu2 N1E	1.9895	1.5200	0.37	0.281	1.034	0.034	
4	Cu2 N1F	2.0052	1.5200	0.37	0.269	1.303	0.303	
5	Cu2 O2	2.2948	1.6100	0.37	0.157	1.460	0.460	
	Cu2 C21A	2.8494						(Contribution below Minimum, Skipped)
	Cu2 C21B_b	2.8557						(Contribution below Minimum, Skipped)
	Cu2 C6E	2.9120						(Contribution below Minimum, Skipped)
	Cu2 C2F	2.9120						(Contribution below Minimum, Skipped)
	Cu2 C2E	2.9200						(Contribution below Minimum, Skipped)
	Cu2 C6F	2.9420						(Contribution below Minimum, Skipped)
	Cu2 O22B_b	3.1313						(Contribution below Minimum, Skipped)
	Cu2 O22A	3.1320						(Contribution below Minimum, Skipped)
	Cu2 O4W_e	3.3821						(Contribution below Minimum, Skipped)
	Cu2 H4	2.4300						(Contribution not Tabulated, Result Dubious !)
	Cu2 H3	2.8700						(Contribution not Tabulated, Result Dubious !)
	Cu2 H2F	2.9400						(Contribution not Tabulated, Result Dubious !)
	Cu2 H6E	2.9500						(Contribution not Tabulated, Result Dubious !)
	Cu2 H2E	2.9700						(Contribution not Tabulated, Result Dubious !)
	Cu2 H6F	2.9900						(Contribution not Tabulated, Result Dubious !)
	Cu2 H2W4_e	3.0500						(Contribution not Tabulated, Result Dubious !)

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Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 2 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu2 O21B_b	1.9677	1.6790	0.37	0.458	0.458	1.542	
2	Cu2 O21A	1.9757	1.6790	0.37	0.448	0.907	1.093	
3	Cu2 N1E	1.9895	1.7510	0.37	0.525	1.432	0.568	
4	Cu2 N1F	2.0052	1.7510	0.37	0.503	1.935	0.065	
5	Cu2 O2	2.2948	1.6790	0.37	0.189	2.124	0.124	
	Cu2 C21A	2.8494						(Contribution below Minimum, Skipped)
	Cu2 C21B_b	2.8557						(Contribution below Minimum, Skipped)
	Cu2 C6E	2.9120						(Contribution below Minimum, Skipped)
	Cu2 C2F	2.9120						(Contribution below Minimum, Skipped)
	Cu2 C2E	2.9200						(Contribution below Minimum, Skipped)
	Cu2 C6F	2.9420						(Contribution below Minimum, Skipped)
	Cu2 O22B_b	3.1313						(Contribution below Minimum, Skipped)
	Cu2 O22A	3.1320						(Contribution below Minimum, Skipped)
	Cu2 O4W_e	3.3821						(Contribution below Minimum, Skipped)
	Cu2 H4	2.4300						(Contribution below Minimum, Skipped)
	Cu2 H3	2.8700						(Contribution below Minimum, Skipped)
	Cu2 H2F	2.9400						(Contribution below Minimum, Skipped)
	Cu2 H6E	2.9500						(Contribution below Minimum, Skipped)
	Cu2 H2E	2.9700						(Contribution below Minimum, Skipped)
	Cu2 H6F	2.9900						(Contribution below Minimum, Skipped)
	Cu2 H2W4_e	3.0500						(Contribution below Minimum, Skipped)

Bond Valence Analysis

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Nr	Bond	Dist	R	B	BVal	Sum	Diff	- Assume Valence = 3 -- Min. BondVal Contribution = 0.04 * Cation Val.
1	Cu2 O21B_b	1.9677	1.7350	0.37	0.533	0.533	2.467	
2	Cu2 O21A	1.9757	1.7350	0.37	0.522	1.055	1.945	
3	Cu2 N1E	1.9895	1.7680	0.37	0.550	1.604	1.396	
4	Cu2 N1F	2.0052	1.7680	0.37	0.527	2.131	0.869	
5	Cu2 O2	2.2948	1.7350	0.37	0.220	2.351	0.649	
	Cu2 C21A	2.8494						(Contribution below Minimum, Skipped)
	Cu2 C21B_b	2.8557						(Contribution below Minimum, Skipped)
	Cu2 C6E	2.9120						(Contribution below Minimum, Skipped)
	Cu2 C2F	2.9120						(Contribution below Minimum, Skipped)
	Cu2 C2E	2.9200						(Contribution below Minimum, Skipped)
	Cu2 C6F	2.9420						(Contribution below Minimum, Skipped)
	Cu2 O22B_b	3.1313						(Contribution below Minimum, Skipped)
	Cu2 O22A	3.1320						(Contribution below Minimum, Skipped)
	Cu2 O4W_e	3.3821						(Contribution below Minimum, Skipped)
	Cu2 H4	2.4300						(Contribution not Tabulated, Result Dubious !)
	Cu2 H3	2.8700						(Contribution not Tabulated, Result Dubious !)
	Cu2 H2F	2.9400						(Contribution not Tabulated, Result Dubious !)
	Cu2 H6E	2.9500						(Contribution not Tabulated, Result Dubious !)
	Cu2 H2E	2.9700						(Contribution not Tabulated, Result Dubious !)
	Cu2 H6F	2.9900						(Contribution not Tabulated, Result Dubious !)
	Cu2 H2W4_e	3.0500						(Contribution not Tabulated, Result Dubious !)

Polyhedral Volume 6.480 Ang**3

Angles (Degrees) At1...V...At2 with Vertex V = Cu2

021B_b , C21A	158.22(6)	021B_b , C21B_b	22.08(6)	021B_b , C6E	74.13(6)	021B_b , C2F	99.67(6)
021B_b , C2E	107.83(6)	021B_b , C6F	81.11(6)	021B_b , 022B_b	45.55(6)	021B_b , 022A	135.68(6)
021B_b , 04W_e	93.71(6)	021A , C21A	22.22(6)	021A , C21B_b	155.58(6)	021A , C6E	109.59(6)
021A , C2F	75.96(6)	021A , C2E	73.92(6)	021A , C6F	96.61(6)	021A , 022B_b	132.30(6)
021A , 022A	45.48(6)	021A , 04W_e	83.64(6)	N1E , C21A	104.66(7)	N1E , C21B_b	82.95(7)
N1E , C6E	23.61(7)	N1E , C2F	145.07(7)	N1E , C2E	23.10(7)	N1E , C6F	168.39(7)
N1E , 022B_b	74.13(6)	N1E , 022A	113.98(6)	N1E , 04W_e	74.35(6)	N1F , C21A	77.05(7)
N1F , C21B_b	94.27(7)	N1F , C6E	163.02(7)	N1F , C2F	23.58(7)	N1F , C2E	146.70(7)
N1F , C6F	22.70(7)	N1F , 022B_b	98.86(6)	N1F , 022A	72.23(6)	N1F , 04W_e	93.86(6)
O2 , C21A	75.99(6)	O2 , C21B_b	110.57(6)	O2 , C6E	75.02(6)	O2 , C2F	122.77(6)
O2 , C2E	105.79(6)	O2 , C6F	81.17(6)	O2 , 022B_b	130.84(5)	O2 , 022A	56.45(5)
O2 , 04W_e	163.37(6)	C21A , C21B_b	170.27(6)	C21A , C6E	117.60(6)	C21A , C2F	74.30(6)
C21A , C2E	92.56(6)	C21A , C6F	79.84(6)	C21A , 022B_b	152.59(5)	C21A , 022A	23.47(5)
C21A , 04W_e	103.93(5)	C21B_b , C6E	71.69(6)	C21B_b , C2F	95.99(6)	C21B_b , C2E	92.45(6)
C21B_b , C6F	93.86(6)	C21B_b , 022B_b	23.48(5)	C21B_b , 022A	156.69(5)	C21B_b , 04W_e	71.94(5)
C6E , C2F	161.72(6)	C6E , C2E	46.61(6)	C6E , C6F	145.07(6)	C6E , 022B_b	72.18(5)
C6E , 022A	117.37(5)	C6E , 04W_e	90.81(5)	C2F , C2E	123.21(6)	C2F , C6F	46.23(6)
C2F , 022B_b	91.09(5)	C2F , 022A	79.28(5)	C2F , 04W_e	72.21(6)	C2E , C6F	168.28(6)
C2E , 022B_b	75.95(5)	C2E , 022A	109.34(5)	C2E , 04W_e	57.60(6)	C6F , 022B_b	106.92(5)
C6F , 022A	66.27(5)	C6F , 04W_e	115.35(5)	022B_b , 022A	170.37(5)	022B_b , 04W_e	48.88(5)
022A , 04W_e	126.57(5)						

Dist. Cu2 - Polyh_C.G.:0.3534(7) Ang, C.G.: 1.17406(7) -0.21221(6) 0.22606(4) 10.7520(7) -1.8924(7) 3.8803(6)

Real Angles I - Cu2 - J	Real Edge I - J	Unit Polyhedron	Dihedral Angles	Norm. IJK:IJL	K	L
021B_b , 021A	175.41(6)	3.940(2)	-171.56(4)	86.35(4)	102.10(4)	-8.45(4) N1E N1F
021B_b , N1E	92.22(7)	2.852(2)	-63.47(4)	-5.81(4)	-57.66(3)	116.53(3) N1F O2
021B_b , N1F	89.27(7)	2.791(2)	56.44(3)	6.00(4)	50.44(4)	123.56(4) N1E O2
021B_b , O2	90.75(6)	3.043(2)	-103.27(4)	-56.06(3)	-47.21(3)	76.73(3) N1E N1F
021A , N1E	90.67(7)	2.820(2)	62.17(4)	5.92(4)	56.24(4)	117.84(4) N1F O2
021A , N1F	87.18(7)	2.745(2)	-55.33(3)	-6.08(4)	-49.26(4)	124.66(4) N1E O2
021A , O2	92.84(6)	3.101(2)	105.76(4)	57.35(3)	48.41(3)	74.24(3) N1E N1F
N1E , N1F	168.18(7)	3.973(2)	-171.60(4)	-84.10(4)	-87.50(4)	8.40(4) 021B_b 021A
N1E , O2	89.48(7)	3.024(2)	106.19(4)	54.25(3)	51.94(3)	73.81(3) 021B_b 021A
N1F , O2	102.22(7)	3.352(2)	-115.68(4)	-59.03(3)	-56.66(3)	64.31(3) 021B_b 021A

Tau-Descriptor for 5-Coordination (A.W.Addison,T.N.Rao,J.Reedijk,J.van Rijn,G.C.Verschoor, J.Chem.Soc.Dalton Trans.(1984),1349-1356)

Tau = (Beta - Alpha) / 60 = (175.41-168.18) / 60 = 0.12 : (Extreme forms: Tau = 0.00 for SP and 1.00 for TP)

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Analysis of Five-Coordination (See R.R. Holmes in Progress in Inorg. Chem. Vol. 32 (1984),119-235 and References Therein)

Idealized Dihedral Angles for Trans Basal Angle : 150.0
 Del(13) & Del(23) Trigonal Bipyramid (TP): 101.5 53.1
 Del(12) & Del(13) Square Pyramid (SP): 118.5 76.9
 Distance Between TP and SP Along Berry Coordinate: 217.7

Pivot(3)	Sum(/Del:C - Del:TP/)	Sum(/Del:C - Del:SP/)	217.7 - Sum(/Del:C - Del:SP/)	Del(24)	Th(24)	Th(15)
N1E	205.1 Deg.	313.7 Deg.	-96.0 Deg.	64.32	102.22	175.41
N1F	205.1 Deg.	337.9 Deg.	-120.2 Deg.	73.81	89.48	175.41
O2	205.1 Deg.	40.6 Deg.	177.2 Deg.	8.40	168.18	175.41

Trigonal Bipyramid (TP) to Square Pyramid (SP) ::: Perc. Along Berry Pseudorotation Coordinate: 87.8 ::: D3h ---> C2v ---> C4v

NOTE: This Analysis Depends on the Value of the Trans Basal Angle that is used (Default Value = 150 Deg.).

The Pivot Atom that Best Describes a Berry Pseudo Rotation is: O2

The Percentage has been Calculated for the Average value, 191.1 Deg., of the Second and Fourth Table Entry.

The Difference, 28.0 Deg., Between the Second and Fourth Table Entry (for pivot) should be Zero for a True Berry Rotation.

>> Distance to SP square base plane defined by: O21A N1E N1F O21B_b
 O21A 0.0746(14), N1E -0.0718(16), N1F -0.0754(16), O21B_b 0.0726(14), Cu2 0.1295(3), O2 2.4099(15)

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3.6 Angstrom Coordination Sphere Around Atom I = 01      [ARU = 1555.01]      0.77323  0.02137  0.17500      7.3885  0.5843  3.0039
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Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	0.79(3)	--	H1	[	=	]	Intra	-39.31	0.75	0.84900	-0.02400	0.17560	7.9986	0.0847	3.0142
2	0.82(3)	--	H2	[	=	]	Intra	-144.92	24.64	0.70600	-0.02100	0.19490	6.7789	0.1562	3.3455
3	2.2745(16)	--	Cu1	[	=	]	Intra	82.68	25.76	0.75664	0.19504	0.23260	7.6495	2.6160	3.9926
4	2.817(2)	<<	O4W_e	[x, -1+y, z	=	1545.05]		-139.20	25.06	0.56313	-0.14221	0.24452	5.4568	-1.0829	4.1972
5	2.911(2)	<.	O2	[	=	]	Intra	-59.10	7.95	0.97015	-0.20694	0.19846	8.8687	-1.8891	3.4066
6	3.004(2)	<.	O11B	[	=	]	Intra	109.99	-5.47	0.62084	0.27894	0.15833	6.3665	3.3943	2.7178
7	3.058(2)	..	O11A	[	=	]	Intra	39.98	47.70	0.89514	0.11740	0.30677	8.9655	1.9067	5.2658
8	3.090(2)	..	N1C	[	=	]	Intra	125.65	49.41	0.58089	0.14471	0.31169	6.2168	2.2179	5.3502
9	3.217(2)	..	N1D	[	=	]	Intra	57.50	-3.92	0.92935	0.26889	0.16218	9.1127	3.2910	2.7839
10	3.273(2)	..	C2C	[	=	]	Intra	155.59	68.70	0.59710	0.03385	0.35267	6.3057	1.0758	6.0537
11	3.405(3)	..	C6D	[	=	]	Intra	58.30	-27.05	0.93720	0.27140	0.08477	8.9819	3.1646	1.4551
12	3.440(3)	..	C5E_f	[2-x, -y, -z	=	2755.01]		-139.73	-71.12	0.73930	-0.00960	-0.01464	6.5393	-0.1351	-0.2513
13	2.50	<<	H5E_f	[2-x, -y, -z	=	2755.01]		-132.29	-72.38	0.76150	-0.00430	0.03620	6.8793	0.0246	0.6214
14	2.91(2)	..	H4	[	=	]	Intra	-60.97	23.78	0.93500	-0.20200	0.24340	8.6813	-1.7451	4.1780
15	2.92	..	H2C	[	=	]	Intra	-166.33	83.04	0.69110	-0.01660	0.34360	7.0453	0.5009	5.8980
16	2.93	..	H6D	[	=	]	Intra	66.98	-40.17	0.86970	0.22770	0.06500	8.2632	2.6429	1.1157
17	3.21(2)	..	H2W4_e	[x, -1+y, z	=	1545.05]		-133.82	11.78	0.55300	-0.19100	0.21320	5.2116	-1.6838	3.6596
18	3.22(2)	..	H1W4_e	[x, -1+y, z	=	1545.05]		-128.38	33.96	0.59100	-0.18700	0.27970	5.7320	-1.5073	4.8011
19	3.29(2)	..	H3	[	=	]	Intra	-71.66	2.48	0.93400	-0.26300	0.18330	8.4234	-2.5381	3.1464

Angles (Degrees) At1...V...At2 with Vertex V = 01

Cu1	, 04W_e	115.04(7)	Cu1	, 02	129.84(7)	Cu1	, 011B	40.96(5)	Cu1	, 011A	39.92(5)
Cu1	, N1C	40.64(5)	Cu1	, N1D	38.43(5)	Cu1	, C2C	59.93(5)	Cu1	, C6D	57.80(6)
Cu1	, C5E_f	128.79(7)	04W_e	, 02	77.71(7)	04W_e	, 011B	111.15(7)	04W_e	, 011A	107.23(7)
04W_e	, N1C	74.41(6)	04W_e	, N1D	153.45(8)	04W_e	, C2C	57.82(6)	04W_e	, C6D	164.16(8)
04W_e	, C5E_f	96.19(7)	02	, 011B	168.88(8)	02	, 011A	90.17(6)	02	, N1C	122.49(7)
02	, N1D	116.87(7)	02	, C2C	99.61(7)	02	, C6D	117.96(7)	02	, C5E_f	94.52(7)
011B	, 011A	80.87(6)	011B	, N1C	56.54(5)	011B	, N1D	52.32(6)	011B	, C2C	80.55(6)
011B	, C6D	53.63(6)	011B	, C5E_f	91.23(7)	011A	, N1C	53.51(5)	011A	, N1D	53.87(5)
011A	, C2C	54.31(5)	011A	, C6D	76.55(6)	011A	, C5E_f	156.58(8)	N1C	, N1D	79.07(6)
N1C	, C2C	24.17(5)	N1C	, C6D	97.02(7)	N1C	, C5E_f	137.35(8)	N1D	, C2C	96.59(7)
N1D	, C6D	23.14(5)	N1D	, C5E_f	104.10(7)	C2C	, C6D	117.70(7)	C2C	, C5E_f	146.24(8)
C6D	, C5E_f	81.00(7)									

3.6 Angstrom Coordination Sphere Around Atom I = O1W	[ARU = 1555.02]	0.73310	0.48711	0.30894	8.0731	5.9920	5.3030

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	0.78(2)	--	H1W1	[	=		Intra	-66.03	30.47	0.76700	0.42700	0.33210	8.3477	5.3746	5.7006
2	0.87(3)	--	H2W1	[	=		Intra	-161.50	-23.87	0.65800	0.46800	0.28850	7.3212	5.7404	4.9522
3	2.727(2)	<<	O12B	[	=	01]		-164.81	-38.96	0.53857	0.45479	0.20906	6.0269	5.4364	3.5886
4	2.735(2)	<<	O12A	[	=	01]		-63.73	25.40	0.87081	0.27409	0.37727	9.1665	3.7767	6.4759
5	2.794(2)	<<	O2W_e	[x,1+y,z	=	1565.03]		93.04	25.38	0.66163	0.70285	0.37871	7.9391	8.5124	6.5006
6	2.924(2)	<	O3W	[	=	04]		60.21	-64.30	0.82808	0.61448	0.15546	8.7030	7.0924	2.6685
7	3.537(3)	..	C2D	[	=	01]		-43.62	-35.60	1.02830	0.32903	0.18901	10.1548	4.0083	3.2444
8	1.99(2)	<<	H2W2_e	[x,1+y,z	=	1565.03]		91.57	27.08	0.68700	0.63800	0.36170	8.0245	7.7626	6.2087
9	2.19(3)	<<	H1W3	[	=	04]		51.21	-65.50	0.81700	0.57200	0.19310	8.6408	6.6984	3.3146
10	3.08	..	H6F_f	[x,1+y,z	=	1565.01]		15.38	-6.28	1.05750	0.56430	0.28930	11.0279	6.8050	4.9659
11	3.11(3)	..	H2W3	[	=	04]		94.46	-63.89	0.74400	0.64000	0.14630	7.9668	7.3559	2.5113
12	3.12(3)	..	H1W2_e	[x,1+y,z	=	1565.03]		78.82	22.26	0.73500	0.73100	0.37770	8.6323	8.8211	6.4833
13	3.12	..	H2D	[	=	01]		-40.94	-21.03	1.02590	0.32600	0.24370	10.2734	4.0837	4.1832
14	3.33	..	H5F_f	[x,1+y,z	=	1565.01]		-11.12	27.15	1.04400	0.41940	0.39740	10.9788	5.4207	6.8215

Angles (Degrees) At1...V...At2 with Vertex V = 01W

012B	,	012A	113.87(8)	012B	,	02W_e	114.67(8)	012B	,	03W	70.84(6)	012B	,	C2D	87.79(7)
012A	,	02W_e	124.48(8)	012A	,	03W	127.24(8)	012A	,	C2D	63.89(6)	02W_e	,	03W	93.27(7)
02W_e	,	C2D	141.61(8)	03W	,	C2D	63.88(6)								

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3.6 Angstrom Coordination Sphere Around Atom I = 02 [ARU = 1555.01] 0.97015 -0.20694 0.19846 8.8687 -1.8891 3.4066

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	0.81(2)	--	H4	[	=		Intra	142.46	72.97	0.93500	-0.20200	0.24340	8.6813	-1.7451	4.1780
2	0.83(2)	--	H3	[	=		Intra	-124.45	-18.30	0.93400	-0.26300	0.18330	8.4234	-2.5381	3.1464
3	2.2948(16)	--	Cu2	[	=		Intra	-0.09	13.57	1.21202	-0.21291	0.22984	11.0994	-1.8926	3.9452

4	2.6705(19)	<<	O22A	[	=		Intra	92.91	73.80	0.91494	-0.16648	0.34786	8.8308	-1.1451	5.9711
5	2.735(2)	<<	O3W_e	[x, -1+y, z	=	1545.04]		-128.64	-15.66	0.82808	-0.38552	0.15546	7.2243	-3.9460	2.6685
6	2.911(2)	.<	O1	[	=		Intra	120.90	-7.95	0.77323	0.02137	0.17500	7.3885	0.5843	3.0039
7	3.024(2)	.<	N1E	[	=		Intra	28.30	-16.53	1.24906	-0.07339	0.14835	11.4208	-0.5147	2.5465
8	3.043(2)	..	O21B_b	[1+x, -1+y, z	=	1645.01]	Intra	-29.94	-13.81	1.29071	-0.33288	0.15616	11.4291	-3.3635	2.6805
9	3.101(2)	..	O21A	[	=		Intra	35.03	37.92	1.14415	-0.09975	0.30950	10.8720	-0.4849	5.3126
10	3.197(2)	.<	C21A	[	=		Intra	54.65	57.06	1.02000	-0.10669	0.35476	9.8743	-0.4714	6.0895
11	3.208(2)	.<	C6E	[	=		Intra	29.43	-41.29	1.22060	-0.07740	0.07516	10.9678	-0.7047	1.2901
12	3.352(2)	..	N1F	[	=		Intra	-29.85	37.68	1.21623	-0.34810	0.31782	11.1694	-3.2097	5.4555
13	3.442(3)	..	C6F	[	=		Intra	-58.95	40.17	1.12170	-0.43442	0.32780	10.2253	-4.1426	5.6268
14	3.594(2)	..	O4W_f	[x, -1+y, z	=	1545.05]		166.71	12.71	0.56313	-0.14221	0.24452	5.4568	-1.0829	4.1972

15	2.19(2)	<<	H1	[	=		Intra	113.79	-10.31	0.84900	-0.02400	0.17560	7.9986	0.0847	3.0142
16	2.79	..	H6E	[	=		Intra	16.05	-55.15	1.17100	-0.14290	0.06500	10.4018	-1.4480	1.1157
17	2.90	..	H6F	[	=		Intra	-73.81	32.57	1.05750	-0.43570	0.28930	9.5492	-4.2334	4.9659
18	2.93(2)	..	H2	[	=		Intra	135.62	-1.20	0.70600	-0.02100	0.19490	6.7789	0.1562	3.3455
19	2.99(2)	..	H1W3_e	[x, -1+y, z	=	1545.04]		-124.85	-1.76	0.81700	-0.42800	0.19310	7.1621	-4.3400	3.3146
20	3.11(3)	..	H2W3_e	[x, -1+y, z	=	1545.04]		-143.01	-16.72	0.74400	-0.36000	0.14630	6.4881	-3.6825	2.5113
21	3.45(3)	..	H1W4_f	[x, -1+y, z	=	1545.05]		173.06	23.81	0.59100	-0.18700	0.27970	5.7320	-1.5073	4.8011
22	3.54(3)	..	H1W2	[	=	03]		-169.17	60.42	0.73500	-0.26900	0.37770	7.1536	-2.2173	6.4833
23	3.58	..	H5D_g	[2-x, -y, -z	=	2755.01]		-113.40	-57.72	0.95830	-0.33430	0.02190	8.1084	-3.6465	0.3759

Angles (Degrees) At1...V...At2 with Vertex V = 02

Cu2	,	O22A	77.81(6)	Cu2	,	O3W_e	130.29(8)	Cu2	,	O1	121.88(7)	Cu2	,	N1E	41.15(5)
Cu2	,	O21B_b	40.29(5)	Cu2	,	O21A	39.51(5)	Cu2	,	C21A	59.86(5)	Cu2	,	C6E	61.27(6)
Cu2	,	N1F	35.78(5)	Cu2	,	C6F	57.63(5)	Cu2	,	O4W_f	150.64(7)	O22A	,	O3W_e	117.40(7)
O22A	,	O1	83.62(6)	O22A	,	N1E	99.12(7)	O22A	,	O21B_b	112.09(7)	O22A	,	O21A	44.99(5)
O22A	,	C21A	22.32(5)	O22A	,	C6E	122.69(7)	O22A	,	N1F	62.13(6)	O22A	,	C6F	64.44(6)
O22A	,	O4W_f	73.31(6)	O3W_e	,	O1	107.22(7)	O3W_e	,	N1E	140.59(8)	O3W_e	,	O21B_b	94.42(7)
O3W_e	,	O21A	153.48(8)	O3W_e	,	C21A	138.52(8)	O3W_e	,	C6E	119.55(7)	O3W_e	,	N1F	106.34(7)
O3W_e	,	C6F	85.34(7)	O3W_e	,	O4W_f	69.96(6)	O1	,	N1E	90.21(7)	O1	,	O21B_b	143.79(7)
O1	,	O21A	91.65(6)	O1	,	C21A	84.21(6)	O1	,	C6E	85.86(7)	O1	,	N1F	140.22(7)
O1	,	C6F	147.79(7)	O1	,	O4W_f	49.98(6)	N1E	,	O21B_b	56.09(6)	N1E	,	O21A	54.82(5)
N1E	,	C21A	76.80(6)	N1E	,	C6E	24.78(6)	N1E	,	N1F	76.92(6)	N1E	,	C6F	98.54(7)
N1E	,	O4W_f	139.64(7)	O21B_b	,	O21A	79.78(6)	O21B_b	,	C21A	98.66(6)	O21B_b	,	C6E	58.05(6)
O21B_b	,	N1F	51.49(5)	O21B_b	,	C6F	60.33(6)	O21B_b	,	O4W_f	163.77(7)	O21A	,	C21A	23.10(5)
O21A	,	C6E	79.37(6)	O21A	,	N1F	50.16(5)	O21A	,	C6F	69.23(6)	O21A	,	O4W_f	112.11(6)
C21A	,	C6E	100.61(7)	C21A	,	N1F	56.35(6)	C21A	,	C6F	67.98(6)	C21A	,	O4W_f	90.83(6)

C6E	,	N1F	95.72(6)	C6E	,	C6F	114.17(7)	C6E	,	O4W_f	133.13(7)	N1F	,	C6F	22.67(5)
N1F	,	O4W_f	127.27(6)	C6F	,	O4W_f	112.28(6)								

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3.6 Angstrom Coordination Sphere Around Atom I = O2W [ARU = 1555.03] 0.66163 -0.29715 0.37871 6.4604 -2.5260 6.5006

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	0.76(3)	--	H1W2	[	=		Intra	24.01	-1.31	0.73500	-0.26900	0.37770	7.1536	-2.2173	6.4833
2	0.81(2)	--	H2W2	[	=		Intra	-83.50	-21.15	0.68700	-0.36200	0.36170	6.5458	-3.2757	6.2087
3	2.794(2)	<<	O1W_e	[x, -1+y, z	=	1545.02]		-86.96	-25.38	0.73310	-0.51289	0.30894	6.5944	-5.0464	5.3030
4	2.794(2)	<<	O22A	[	=	01]		30.22	-10.93	0.91494	-0.16648	0.34786	8.8308	-1.1451	5.9711
5	2.898(2)	.<	O4W_f	[x, -1+y, z	=	1545.05]		124.82	-52.65	0.56313	-0.14221	0.24452	5.4568	-1.0829	4.1972
6	3.300(3)	..	C2F_g	[-1+x, y, z	=	1455.01]		-169.90	-2.02	0.30800	-0.34830	0.37193	3.2136	-3.1042	6.3843
7	3.448(3)	..	C3C	[	=	01]		108.76	8.22	0.48240	-0.00963	0.40743	5.3633	0.7049	6.9936
8	2.11(3)	<<	H1W4_f	[x, -1+y, z	=	1545.05]		125.56	-53.61	0.59100	-0.18700	0.27970	5.7320	-1.5073	4.8011
9	2.58	.<	H2F_g	[-1+x, y, z	=	1455.01]		178.27	-5.12	0.37590	-0.28770	0.36530	3.8912	-2.4484	6.2705
10	2.78	..	H3C	[	=	01]		112.77	20.20	0.49710	-0.08900	0.43470	5.4490	-0.1169	7.4617
11	2.82	..	H4F_h	[2-x, -1-y, 1-z	=	2746.01]		-38.99	52.24	0.79400	-0.41910	0.50870	7.8037	-3.6134	8.7320
12	3.14	..	H2C	[	=	01]		79.06	-11.06	0.69110	-0.01660	0.34360	7.0453	0.5009	5.8980
13	3.22(3)	..	H2W4_f	[x, -1+y, z	=	1545.05]		146.00	-62.07	0.55300	-0.19100	0.21320	5.2116	-1.6838	3.6596
14	3.24(2)	..	H2W1_e	[x, -1+y, z	=	1545.02]		-102.57	-28.60	0.65800	-0.53200	0.28850	5.8425	-5.2980	4.9522
15	3.26(2)	..	H1W1_e	[x, -1+y, z	=	1545.02]		-82.58	-14.19	0.76700	-0.57300	0.33210	6.8689	-5.6638	5.7006
16	3.27	..	H3F_g	[-1+x, y, z	=	1455.01]		-152.67	30.10	0.37400	-0.43200	0.47420	3.9485	-3.8244	8.1398
17	3.31(3)	..	H4	[	=	01]		19.37	-44.61	0.93500	-0.20200	0.24340	8.6813	-1.7451	4.1780

Angles (Degrees) At1...V...At2 with Vertex V = O2W

O1W_e , O22A	108.90(8)	O1W_e , O4W_f	97.19(8)	O1W_e , C2F_g	82.76(7)	O1W_e , C3C	157.23(8)
O22A , O4W_f	84.09(7)	O22A , C2F_g	156.16(8)	O22A , C3C	80.44(6)	O4W_f , C2F_g	73.65(7)
O4W_f , C3C	62.40(6)	C2F_g , C3C	81.73(7)				

3.6 Angstrom Coordination Sphere Around Atom I = O3W	[ARU = 1555.04]	0.82808	0.61448	0.15546	8.7030	7.0924	2.6685

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	0.76(2)	--	H1W3	[	=	]	Intra	-98.97	58.31	0.81700	0.57200	0.19310	8.6408	6.6984	3.3146
2	0.80(3)	--	H2W3	[	=	]	Intra	160.31	-11.37	0.74400	0.64000	0.14630	7.9668	7.3559	2.5113
3	2.735(2)	<<	O2_e	[x,1+y,z	=	1565.01]		51.36	15.66	0.97015	0.79306	0.19846	10.3474	9.1492	3.4066
4	2.782(2)	<<	O22B	[	=	01]		157.24	-6.99	0.53170	0.71481	0.13573	6.1565	8.1606	2.3298
5	2.924(2)	<.	O1W	[	=	02]		-119.79	64.30	0.73310	0.48711	0.30894	8.0731	5.9920	5.3030
6	3.279(2)	..	O12B	[	=	01]		-148.25	16.30	0.53857	0.45479	0.20906	6.0269	5.4364	3.5886
7	3.322(3)	..	C5D_f	[2-x,1-y,-z	=	2765.01]		13.75	-76.32	0.96090	0.66530	-0.03257	9.4658	7.2790	-0.5591
8	3.410(3)	..	C3D	[	=	01]		-46.21	-4.28	1.13280	0.39480	0.14065	11.0561	4.6380	2.4143
9	3.457(3)	..	C2D	[	=	01]		-64.79	9.59	1.02830	0.32903	0.18901	10.1548	4.0083	3.2444
10	1.91(2)	<<	H3_e	[x,1+y,z	=	1565.01]		49.58	14.49	0.93400	0.73700	0.18330	9.9021	8.5002	3.1464
11	2.48	<<	H5D_f	[2-x,1-y,-z	=	2765.01]		18.71	-67.85	0.95830	0.66570	0.02190	9.5871	7.3919	0.3759
12	2.99(3)	..	H2W1	[	=	02]		-135.62	49.75	0.65800	0.46800	0.28850	7.3212	5.7404	4.9522
13	3.04(2)	..	H4_e	[x,1+y,z	=	1565.01]		56.49	29.77	0.93500	0.79800	0.24340	10.1600	9.2933	4.1780
14	3.19(2)	..	H2W4	[	=	05]		131.66	18.12	0.55300	0.80900	0.21320	6.6903	9.3545	3.6596
15	3.28	..	H6F_e	[x,1+y,z	=	1565.01]		-7.05	44.44	1.05750	0.56430	0.28930	11.0279	6.8050	4.9659
16	3.39	..	H4D_f	[2-x,1-y,-z	=	2765.01]		-131.06	-66.74	0.79290	0.55570	-0.02620	7.8226	6.0819	-0.4497
17	3.50(3)	..	H1W1	[	=	02]		-101.69	59.95	0.76700	0.42700	0.33210	8.3477	5.3746	5.7006
18	3.57(2)	..	H1W4	[	=	05]		121.46	36.72	0.59100	0.81300	0.27970	7.2107	9.5311	4.8011

Angles (Degrees) At1...V...At2 with Vertex V = 03W

[illegible]

3.6 Angstrom Coordination Sphere Around Atom I = O4W	[ARU = 1555.05]	0.56313	0.85779	0.24452	6.9355	9.9555	4.1972

Nr	d(I, J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	0.79(3)	--	H1W4	[	=		Intra	-57.04	50.05	0.59100	0.81300	0.27970	7.2107	9.5311	4.8011
2	0.84(2)	--	H2W4	[	=		Intra	-112.20	-39.64	0.55300	0.80900	0.21320	6.6903	9.3545	3.6596
3	2.705(2)	<<	O22B	[	=	01]		-113.46	-43.66	0.53170	0.71481	0.13573	6.1565	8.1606	2.3298
4	2.817(2)	<<	O1_e	[x,1+y,z	=	1565.01]		40.80	-25.06	0.77323	1.02137	0.17500	8.8672	11.6227	3.0039
5	2.898(2)	.<	O2W_f	[x,1+y,z	=	1565.03]		-55.18	52.65	0.66163	0.70285	0.37871	7.9391	8.5124	6.5006
6	2.971(3)	<<	C2C_e	[x,1+y,z	=	1565.01]		68.53	38.67	0.59710	1.03385	0.35267	7.7844	12.1142	6.0537
7	3.063(3)	.<	C2E_a	[-1+x,1+y,z	=	1465.01]		143.09	-27.49	0.31690	1.02049	0.16215	4.7630	11.5874	2.7833
8	3.320(3)	..	C3C_e	[x,1+y,z	=	1565.01]		92.99	57.37	0.48240	0.99037	0.40743	6.8420	11.7433	6.9936
9	3.3821(19)	<<	Cu2_a	[-1+x,1+y,z	=	1465.01]		-166.11	-4.27	0.21202	0.78709	0.22984	3.6614	9.1458	3.9452
10	3.430(2)	..	N1E_a	[-1+x,1+y,z	=	1465.01]		169.11	-28.77	0.24906	0.92661	0.14835	3.9828	10.5237	2.5465
11	3.578(2)	..	N1C_e	[x,1+y,z	=	1565.01]		77.03	18.80	0.58089	1.14471	0.31169	7.6956	13.2563	5.3502
12	3.594(2)	..	O2_e	[x,1+y,z	=	1565.01]		-13.29	-12.71	0.97015	0.79306	0.19846	10.3474	9.1492	3.4066
13	2.00(2)	<<	H2_e	[x,1+y,z	=	1565.01]		43.15	-25.18	0.70600	0.97900	0.19490	8.2576	11.1946	3.3455
14	2.64	.<	H2E_a	[-1+x,1+y,z	=	1465.01]		136.25	-11.53	0.33500	1.02530	0.21380	5.0679	11.7433	3.6699
15	2.82	..	H2C_e	[x,1+y,z	=	1565.01]		44.92	37.17	0.69110	0.98340	0.34360	8.5240	11.5393	5.8980
16	2.93	..	H2F_a	[-1+x,1+y,z	=	1465.01]		-138.91	44.94	0.37590	0.71230	0.36530	5.3699	8.5900	6.2705
17	3.04(3)	..	H1_e	[x,1+y,z	=	1565.01]		24.67	-22.93	0.84900	0.97600	0.17560	9.4773	11.1231	3.0142
18	3.07(3)	..	H1W2_f	[x,1+y,z	=	1565.03]		-33.77	48.24	0.73500	0.73100	0.37770	8.6323	8.8211	6.4833
19	3.17(3)	..	H2W2_f	[x,1+y,z	=	1565.03]		-63.59	39.40	0.68700	0.63800	0.36170	8.0245	7.7626	6.2087
20	3.27(2)	..	H2W3	[	=	04]		-68.36	-31.08	0.74400	0.64000	0.14630	7.9668	7.3559	2.5113
21	3.29(3)	..	H4_e	[x,1+y,z	=	1565.01]		-11.61	-0.33	0.93500	0.79800	0.24340	10.1600	9.2933	4.1780
22	3.40	..	H3C_e	[x,1+y,z	=	1565.01]		90.46	73.52	0.49710	0.91100	0.43470	6.9277	10.9215	7.4617
23	3.47(3)	..	H3_e	[x,1+y,z	=	1565.01]		-26.13	-17.64	0.93400	0.73700	0.18330	9.9021	8.5002	3.1464

Angles (Degrees) At1...V...At2 with Vertex V = 04W

022B	, 01_e	107.33(7)	022B	, 02W_f	108.55(8)	022B	, C2C_e	174.79(8)	022B	, C2E_a	80.25(7)
022B	, C3C_e	158.54(8)	022B	, Cu2_a	60.72(5)	022B	, N1E_a	61.95(6)	022B	, N1C_e	153.62(8)
022B	, 02_e	88.43(6)	01_e	, 02W_f	113.21(8)	01_e	, C2C_e	68.82(7)	01_e	, C2E_a	88.60(7)
01_e	, C3C_e	93.29(7)	01_e	, Cu2_a	140.71(7)	01_e	, N1E_a	106.76(7)	01_e	, N1C_e	56.28(6)
01_e	, 02_e	52.31(6)	02W_f	, C2C_e	76.48(7)	02W_f	, C2E_a	151.40(8)	02W_f	, C3C_e	66.95(6)
02W_f	, Cu2_a	105.98(7)	02W_f	, N1E_a	139.75(8)	02W_f	, N1C_e	97.45(7)	02W_f	, 02_e	74.59(6)
C2C_e	, C2E_a	95.97(8)	C2C_e	, C3C_e	24.58(6)	C2C_e	, Cu2_a	119.81(7)	C2C_e	, N1E_a	115.23(7)
C2C_e	, N1C_e	21.20(5)	C2C_e	, 02_e	91.67(7)	C2E_a	, C3C_e	94.70(7)	C2E_a	, Cu2_a	53.60(5)
C2E_a	, N1E_a	22.94(6)	C2E_a	, N1C_e	78.92(7)	C2E_a	, 02_e	133.74(7)	C3C_e	, Cu2_a	99.46(6)
C3C_e	, N1E_a	106.97(7)	C3C_e	, N1C_e	40.35(5)	C3C_e	, 02_e	109.44(7)	Cu2_a	, N1E_a	33.95(4)
Cu2_a	, N1C_e	116.78(6)	Cu2_a	, 02_e	148.10(6)	N1E_a	, N1C_e	100.67(6)	N1E_a	, 02_e	138.46(7)
N1C_e	, 02_e	94.37(6)									

C11A	,	Cu1	121.10(12)	C11A	,	O12A	26.66(10)	C11A	,	C1A	35.41(11)	C11A	,	C21A	96.55(12)
C11A	,	N1C	99.36(11)	C11A	,	C2A	65.05(11)	C11A	,	N1D	117.35(12)	C11A	,	C2C	98.51(11)
C11A	,	O1	163.19(12)	C11A	,	O21A	103.36(11)	C11A	,	O22A	108.66(11)	C11A	,	C2D	95.57(12)
Cu1	,	O12A	96.26(7)	Cu1	,	C1A	150.60(8)	Cu1	,	C21A	138.44(8)	Cu1	,	N1C	46.65(5)
Cu1	,	C2A	159.07(8)	Cu1	,	N1D	45.05(5)	Cu1	,	C2C	70.40(6)	Cu1	,	O1	48.01(5)
Cu1	,	O21A	135.24(7)	Cu1	,	O22A	117.95(7)	Cu1	,	C2D	66.16(6)	O12A	,	C1A	62.06(7)
O12A	,	C21A	123.09(8)	O12A	,	N1C	88.78(7)	O12A	,	C2A	91.70(7)	O12A	,	N1D	93.47(7)
O12A	,	C2C	100.09(8)	O12A	,	O1	143.91(8)	O12A	,	O21A	126.12(7)	O12A	,	O22A	134.11(7)
O12A	,	C2D	75.84(7)	C1A	,	C21A	61.39(7)	C1A	,	N1C	109.51(8)	C1A	,	C2A	29.69(7)
C1A	,	N1D	146.38(8)	C1A	,	C2C	92.89(7)	C1A	,	O1	146.87(8)	C1A	,	O21A	72.61(7)
C1A	,	O22A	74.19(7)	C1A	,	C2D	121.13(8)	C21A	,	N1C	115.33(7)	C21A	,	C2A	31.79(6)
C21A	,	N1D	133.10(8)	C21A	,	C2C	88.46(7)	C21A	,	O1	91.06(7)	C21A	,	O21A	24.32(6)
C21A	,	O22A	23.10(6)	C21A	,	C2D	131.49(8)	N1C	,	C2A	114.50(7)	N1C	,	N1D	91.33(7)
N1C	,	C2C	27.34(6)	N1C	,	O1	63.83(6)	N1C	,	O21A	134.95(7)	N1C	,	O22A	93.44(6)
N1C	,	C2D	108.64(7)	C2A	,	N1D	153.75(8)	C2A	,	C2C	89.18(7)	C2A	,	O1	120.16(7)
C2A	,	O21A	47.08(6)	C2A	,	O22A	46.27(6)	C2A	,	C2D	134.73(7)	N1D	,	C2C	115.11(7)
N1D	,	O1	65.92(6)	N1D	,	O21A	111.19(6)	N1D	,	O22A	132.22(7)	N1D	,	C2D	25.31(6)
C2C	,	O1	66.64(6)	C2C	,	O21A	110.12(7)	C2C	,	O22A	67.67(6)	C2C	,	C2D	135.48(7)
O1	,	O21A	89.69(6)	O1	,	O22A	73.94(6)	O1	,	C2D	90.49(6)	O21A	,	O22A	42.46(5)
O21A	,	C2D	107.23(6)	O22A	,	C2D	144.12(7)								

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3.6 Angstrom Coordination Sphere Around Atom I = 011B [ARU = 1555.01] 0.62084 0.27894 0.15833 6.3665 3.3943 2.7178

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	1.277(2)	--	C11B	[	=		Intra	105.51	-2.86	0.56510	0.39096	0.15462	6.0253	4.6234	2.6541
2	1.9690(14)	--	Cu1	[	=		Intra	-31.24	40.35	0.75664	0.19504	0.23260	7.6495	2.6160	3.9926

3	2.2458(19)	<<	O12B	[	=		Intra	99.44	22.81	0.53857	0.45479	0.20906	6.0269	5.4364	3.5886
4	2.360(2)	<<	C1B	[	=		Intra	114.82	-37.28	0.52900	0.44835	0.07506	5.5782	5.0985	1.2884
5	2.749(2)	<<	N1D	[	=		Intra	-2.15	1.38	0.92935	0.26889	0.16218	9.1127	3.2910	2.7839
6	2.752(2)	<<	C6B	[	=		Intra	132.54	-65.93	0.56230	0.38027	0.01192	5.6077	4.2213	0.2046
7	2.887(2)	.<	N1C	[	=		Intra	-97.25	65.75	0.58089	0.14471	0.31169	6.2168	2.2179	5.3502
8	2.913(2)	<<	C6D	[	=		Intra	-5.02	-25.68	0.93720	0.27140	0.08477	8.9819	3.1646	1.4551
9	3.004(2)	.<	O1	[	=		Intra	-70.01	5.47	0.77323	0.02137	0.17500	7.3885	0.5843	3.0039
10	3.126(2)	.<	C6C	[	=		Intra	-162.95	66.10	0.44630	0.21527	0.32484	5.1558	3.0230	5.5760
11	3.474(3)	..	C3E_e	[-1+x,y,z	=	1455.01]		-143.96	-15.52	0.36130	0.11030	0.10417	3.6598	1.4249	1.7881

12	2.42	<<	H6B	[	=		Intra	-171.77	-78.63	0.60570	0.29770	0.02000	5.8939	3.3260	0.3433
13	2.58	.<	H3E_e	[-1+x,y,z	=	1455.01]		-150.14	-16.50	0.41040	0.17520	0.11570	4.2241	2.1643	1.9860
14	2.59	.<	H6D	[	=		Intra	-21.61	-38.14	0.86970	0.22770	0.06500	8.2632	2.6429	1.1157
15	2.73	..	H6C	[	=		Intra	161.49	59.96	0.43260	0.29340	0.29580	5.0725	3.8276	5.0775
16	3.32(2)	..	H2	[	=		Intra	-82.74	10.89	0.70600	-0.02100	0.19490	6.7789	0.1562	3.3455
17	3.38(2)	..	H2W1	[	=	02]		67.86	41.42	0.65800	0.46800	0.28850	7.3212	5.7404	4.9522

Angles (Degrees) At1...V...At2 with Vertex V = 011B

C11B	,	Cu1	125.93(12)	C11B	,	O12B	26.35(9)	C11B	,	C1B	35.47(10)	C11B	,	N1D	107.71(12)
C11B	,	C6B	65.90(10)	C11B	,	N1C	115.07(11)	C11B	,	C6D	107.10(12)	C11B	,	O1	174.83(12)
C11B	,	C6C	93.24(11)	C11B	,	C3E_e	108.91(12)	Cu1	,	O12B	101.94(7)	Cu1	,	C1B	153.54(9)
Cu1	,	N1D	47.05(5)	Cu1	,	C6B	152.82(8)	Cu1	,	N1C	44.15(5)	Cu1	,	C6D	70.40(6)
Cu1	,	O1	49.22(5)	Cu1	,	C6C	67.26(6)	Cu1	,	C3E_e	117.19(7)	O12B	,	C1B	61.82(7)
O12B	,	N1D	100.13(8)	O12B	,	C6B	92.24(7)	O12B	,	N1C	90.52(7)	O12B	,	C6D	112.05(8)
O12B	,	O1	149.90(7)	O12B	,	C6C	72.24(7)	O12B	,	C3E_e	120.09(8)	C1B	,	N1D	112.05(8)
C1B	,	C6B	30.44(7)	C1B	,	N1C	146.01(8)	C1B	,	C6D	95.41(8)	C1B	,	O1	147.88(8)
C1B	,	C6C	120.68(8)	C1B	,	C3E_e	89.26(7)	N1D	,	C6B	107.98(7)	N1D	,	N1C	90.83(7)
N1D	,	C6D	27.20(6)	N1D	,	O1	67.83(6)	N1D	,	C6C	111.13(7)	N1D	,	C3E_e	139.77(7)
C6B	,	N1C	160.16(8)	C6B	,	C6D	82.85(7)	C6B	,	O1	117.51(7)	C6B	,	C6C	139.79(8)
C6B	,	C3E_e	73.21(7)	N1C	,	C6D	114.18(7)	N1C	,	O1	63.23(6)	N1C	,	C6C	25.57(6)
N1C	,	C3E_e	88.43(7)	C6D	,	O1	70.25(7)	C6D	,	C6C	137.27(7)	C6D	,	C3E_e	122.60(7)
O1	,	C6C	86.19(6)	O1	,	C3E_e	76.13(6)	C6C	,	C3E_e	82.85(7)				

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3.6 Angstrom Coordination Sphere Around Atom I = 012A [ARU = 1555.01] 0.87081 0.27409 0.37727 9.1665 3.7767 6.4759

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	1.242(2)	--	C11A	[	=		Intra	-84.80	-7.63	0.90430	0.16478	0.36767	9.2781	2.5509	6.3111

2	2.236(2)	<<	011A	[	=		Intra	-96.13	-32.76	0.89514	0.11740	0.30677	8.9655	1.9067	5.2658
3	2.370(2)	<<	C1A	[	=		Intra	-72.79	24.55	0.95800	0.07718	0.43463	9.8043	1.7173	7.4605
4	2.735(2)	<<	01W	[	=	02]		116.27	-25.40	0.73310	0.48711	0.30894	8.0731	5.9920	5.3030
5	2.763(2)	<<	C6A	[	=		Intra	-59.30	53.02	0.95320	0.12141	0.50587	10.0150	2.3474	8.6834
6	3.1330(16)	<<	Cu1	[	=		Intra	-142.58	-52.43	0.75664	0.19504	0.23260	7.6495	2.6160	3.9926
7	3.387(3)	..	C2D	[	=		Intra	13.19	-72.56	1.02830	0.32903	0.18901	10.1548	4.0083	3.2444
8	3.401(3)	..	C5F_e	[x,1+y,z	=	1565.01]		42.37	4.16	1.11370	0.47860	0.39164	11.6726	6.0627	6.7226
9	3.521(2)	..	N1C	[	=		Intra	-152.15	-18.65	0.58089	0.14471	0.31169	6.2168	2.2179	5.3502

10	1.96(2)	<<	H1W1	[	=	02]		117.13	-23.36	0.76700	0.42700	0.33210	8.3477	5.3746	5.7006
11	2.43	<<	H6A	[	=		Intra	-35.46	69.46	0.92080	0.20540	0.50980	9.8607	3.2823	8.7508
12	2.47	<<	H5F_e	[x,1+y,z	=	1565.01]		42.21	8.04	1.04400	0.41940	0.39740	10.9788	5.4207	6.8215
13	2.56	.<	H2D	[	=		Intra	15.50	-63.39	1.02590	0.32600	0.24370	10.2734	4.0837	4.1832
14	3.10(2)	..	H2W1	[	=	02]		133.22	-29.49	0.65800	0.46800	0.28850	7.3212	5.7404	4.9522
15	3.24	..	H5C_f	[1+x,y,z	=	1655.01]		-8.58	3.01	1.23460	0.22850	0.38720	12.3691	3.2932	6.6464

Angles (Degrees) At1...V...At2 with Vertex V = 012A

C11A	,	011A	27.25(10)	C11A	,	C1A	34.24(10)	C11A	,	01W	141.13(13)	C11A	,	C6A	64.40(11)
C11A	,	Cu1	64.70(10)	C11A	,	C2D	85.11(11)	C11A	,	C5F_e	127.36(13)	C11A	,	N1C	66.17(11)
011A	,	C1A	61.47(7)	011A	,	01W	114.16(8)	011A	,	C6A	91.57(8)	011A	,	Cu1	38.54(5)
011A	,	C2D	64.35(7)	011A	,	C5F_e	131.87(8)	011A	,	N1C	51.80(6)	C1A	,	01W	171.74(9)
C1A	,	C6A	30.24(7)	C1A	,	Cu1	97.92(7)	C1A	,	C2D	112.16(8)	C1A	,	C5F_e	110.83(8)
C1A	,	N1C	88.49(7)	01W	,	C6A	152.18(8)	01W	,	Cu1	76.50(6)	01W	,	C2D	69.64(6)
01W	,	C5F_e	77.36(7)	01W	,	N1C	83.49(7)	C6A	,	Cu1	126.18(7)	C6A	,	C2D	135.07(8)
C6A	,	C5F_e	93.64(7)	C6A	,	N1C	106.48(7)	Cu1	,	C2D	53.87(5)	Cu1	,	C5F_e	131.55(7)
Cu1	,	N1C	34.61(4)	C2D	,	C5F_e	78.94(7)	C2D	,	N1C	88.26(6)	C5F_e	,	N1C	159.72(7)

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3.6 Angstrom Coordination Sphere Around Atom I = 012B [ARU = 1555.01] 0.53857 0.45479 0.20906 6.0269 5.4364 3.5886

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.239(2)	--	C11B	[	=	]	Intra	-90.11	-48.98	0.56510	0.39096	0.15462	6.0253	4.6234	2.6541
2	2.2458(19)	<<	011B	[	=	]	Intra	-80.56	-22.81	0.62084	0.27894	0.15833	6.3665	3.3943	2.7178
3	2.368(2)	<<	C1B	[	=	]	Intra	-143.02	-76.28	0.52900	0.44835	0.07506	5.5782	5.0985	1.2884
4	2.662(2)	<<	C21B	[	=	]	Intra	113.77	-32.86	0.42920	0.65532	0.12492	5.1260	7.4824	2.1443
5	2.727(2)	<<	01W	[	=	02]		15.19	38.96	0.73310	0.48711	0.30894	8.0731	5.9920	5.3030
6	2.835(2)	<<	C2B	[	=	]	Intra	131.22	-62.54	0.46620	0.57029	0.06254	5.1654	6.4196	1.0735
7	3.004(2)	<.	022B	[	=	]	Intra	87.28	-24.77	0.53170	0.71481	0.13573	6.1565	8.1606	2.3298
8	3.159(2)	..	021B	[	=	]	Intra	132.29	-16.70	0.29071	0.66712	0.15616	3.9911	7.6749	2.6805
9	3.246(3)	..	C6C	[	=	]	Intra	-109.85	37.76	0.44630	0.21527	0.32484	5.1558	3.0230	5.5760
10	3.279(2)	..	03W	[	=	04]		31.75	-16.30	0.82808	0.61448	0.15546	8.7030	7.0924	2.6685
11	3.2788(16)	<<	Cu1	[	=	]	Intra	-60.09	7.08	0.75664	0.19504	0.23260	7.6495	2.6160	3.9926
12	1.90(3)	<<	H2W1	[	=	02]		13.22	45.73	0.65800	0.46800	0.28850	7.3212	5.7404	4.9522
13	2.39	<<	H6C	[	=	]	Intra	-120.68	38.52	0.43260	0.29340	0.29580	5.0725	3.8276	5.0775
14	2.92(3)	..	H1W3	[	=	04]		25.77	-5.39	0.81700	0.57200	0.19310	8.6408	6.6984	3.3146
15	2.93(3)	..	H2W3	[	=	04]		44.70	-21.54	0.74400	0.64000	0.14630	7.9668	7.3559	2.5113
16	3.14(3)	..	H1W1	[	=	02]		-1.52	42.29	0.76700	0.42700	0.33210	8.3477	5.3746	5.7006
17	3.28	..	H3D_e	[-1+x,y,z	=	1455.01]		-174.70	-14.36	0.20030	0.43670	0.16160	2.8586	5.1422	2.7739

Angles (Degrees) At1...V...At2 with Vertex V = 012B

C11B	,	011B	27.23(10)	C11B	,	C1B	34.23(11)	C11B	,	C21B	95.44(12)	C11B	,	01W	127.52(13)
C11B	,	C2B	63.76(11)	C11B	,	022B	106.21(11)	C11B	,	021B	104.32(12)	C11B	,	C6C	88.49(12)
C11B	,	03W	96.94(12)	C11B	,	Cu1	61.90(11)	011B	,	C1B	61.46(7)	011B	,	C21B	122.67(8)
011B	,	01W	108.40(8)	011B	,	C2B	90.99(7)	011B	,	022B	130.97(7)	011B	,	021B	129.07(7)
011B	,	C6C	66.54(7)	011B	,	03W	103.12(7)	011B	,	Cu1	35.98(5)	C1B	,	C21B	61.21(7)
C1B	,	01W	141.46(9)	C1B	,	C2B	29.53(7)	C1B	,	022B	74.37(7)	C1B	,	021B	72.53(7)
C1B	,	C6C	115.97(8)	C1B	,	03W	87.37(7)	C1B	,	Cu1	95.21(7)	C21B	,	01W	116.01(8)
C21B	,	C2B	31.68(6)	C21B	,	022B	24.50(6)	C21B	,	021B	23.25(6)	C21B	,	C6C	144.40(8)
C21B	,	03W	74.68(7)	C21B	,	Cu1	153.59(7)	01W	,	C2B	135.67(8)	01W	,	022B	92.65(7)
01W	,	021B	121.33(7)	01W	,	C6C	88.16(7)	01W	,	03W	57.39(6)	01W	,	Cu1	74.13(6)
C2B	,	022B	47.68(6)	C2B	,	021B	45.84(6)	C2B	,	C6C	136.03(8)	C2B	,	03W	79.86(6)
C2B	,	Cu1	123.93(6)	022B	,	021B	42.67(5)	022B	,	C6C	160.49(7)	022B	,	03W	52.35(5)
022B	,	Cu1	144.14(6)	021B	,	C6C	122.00(7)	021B	,	03W	95.02(6)	021B	,	Cu1	164.54(6)
C6C	,	03W	140.04(7)	C6C	,	Cu1	54.39(5)	03W	,	Cu1	93.74(6)				

Angles (Degrees) At1...V...At2 with Vertex V = 021A

C21A	, Cu2	121.58(12)	C21A	, O22A	26.52(10)	C21A	, C2A	35.17(10)	C21A	, N1F	93.68(11)
C21A	, N1E	139.13(12)	C21A	, C2E	148.52(12)	C21A	, O11A	60.62(10)	C21A	, C2F	96.72(11)
C21A	, O2	82.69(11)	C21A	, C6A_d	44.69(10)	C21A	, C1A	47.84(10)	C21A	, C11A	57.79(10)
Cu2	, O22A	95.63(7)	Cu2	, C2A	152.83(9)	Cu2	, N1F	46.86(5)	Cu2	, N1E	44.86(5)
Cu2	, C2E	67.41(6)	Cu2	, O11A	128.19(7)	Cu2	, C2F	65.80(6)	Cu2	, O2	47.65(5)
Cu2	, C6A_d	136.83(7)	Cu2	, C1A	167.47(8)	Cu2	, C11A	148.28(7)	O22A	, C2A	61.58(7)
O22A	, N1F	77.95(7)	O22A	, N1E	117.50(7)	O22A	, C2E	137.92(8)	O22A	, O11A	70.59(6)
O22A	, C2F	91.10(7)	O22A	, O2	57.29(6)	O22A	, C6A_d	66.66(6)	O22A	, C1A	72.97(6)
O22A	, C11A	76.24(6)	C2A	, N1F	109.90(8)	C2A	, N1E	157.36(9)	C2A	, C2E	139.32(9)
C2A	, O11A	61.17(7)	C2A	, C2F	98.09(8)	C2A	, O2	117.40(8)	C2A	, C6A_d	23.29(6)
C2A	, C1A	22.37(6)	C2A	, C11A	45.70(7)	N1F	, N1E	91.11(7)	N1F	, C2E	109.49(7)
N1F	, O11A	147.62(7)	N1F	, C2F	25.63(6)	N1F	, O2	69.66(6)	N1F	, C6A_d	90.13(7)
N1F	, C1A	132.27(7)	N1F	, C11A	151.37(7)	N1E	, C2E	26.11(6)	N1E	, O11A	96.58(6)
N1E	, C2F	104.56(7)	N1E	, O2	61.19(6)	N1E	, C6A_d	175.83(8)	N1E	, C1A	135.89(7)
N1E	, C11A	111.72(6)	C2E	, O11A	89.65(6)	C2E	, C2F	113.46(7)	C2E	, O2	85.70(6)
C2E	, C6A_d	150.17(8)	C2E	, C1A	117.54(7)	C2E	, C11A	97.97(7)	O11A	, C2F	156.89(7)
O11A	, O2	86.68(6)	O11A	, C6A_d	84.46(6)	O11A	, C1A	43.70(5)	O11A	, C11A	20.19(5)
C2F	, O2	95.29(7)	C2F	, C6A_d	75.14(7)	C2F	, C1A	118.49(7)	C2F	, C11A	143.47(7)
O2	, C6A_d	122.95(7)	O2	, C1A	119.99(7)	O2	, C11A	105.57(6)	C6A_d	, C1A	43.69(6)
C6A_d	, C11A	68.36(6)	C1A	, C11A	25.09(5)						

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3.6 Angstrom Coordination Sphere Around Atom I = 021B [ARU = 1555.01] 0.29071 0.66712 0.15616 3.9911 7.6749 2.6805

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	1.270(2)	--	C21B	[	=		Intra	-9.62	-24.98	0.42920	0.65532	0.12492	5.1260	7.4824	2.1443
2	1.9677(14)	--	Cu2_a	[-1+x,1+y,z	=	1465.01]	Intra	102.63	39.99	0.21202	0.78709	0.22984	3.6614	9.1458	3.9452

3	2.247(2)	<<	022B	[	=		Intra	12.64	-8.98	0.53170	0.71481	0.13573	6.1565	8.1606	2.3298
4	2.353(2)	<<	C2B	[	=		Intra	-46.91	-43.07	0.46620	0.57029	0.06254	5.1654	6.4196	1.0735
5	2.791(2)	<<	N1F_a	[-1+x,1+y,z	=	1465.01]	Intra	149.35	83.79	0.21623	0.65190	0.31782	3.7315	7.8287	5.4555
6	2.852(2)	<<	N1E_a	[-1+x,1+y,z	=	1465.01]	Intra	90.17	-2.69	0.24906	0.92661	0.14835	3.9828	10.5237	2.5465
7	3.036(3)	<	C6E_a	[-1+x,1+y,z	=	1465.01]	Intra	99.84	-27.26	0.22060	0.92260	0.07516	3.5298	10.3337	1.2901
8	3.043(2)	..	02_a	[-1+x,1+y,z	=	1465.01]	Intra	150.06	13.81	-0.02985	0.79306	0.19846	1.4307	9.1492	3.4066
9	3.114(2)	<	C6B_c	[1-x,1-y,-z	=	2665.01]	Intra	-47.12	-67.92	0.43770	0.61973	-0.01192	4.7878	6.8171	-0.2046
10	3.159(2)	..	012B	[	=		Intra	-47.71	16.70	0.53857	0.45479	0.20906	6.0269	5.4364	3.5886
11	3.277(2)	..	C6F_a	[-1+x,1+y,z	=	1465.01]	Intra	-147.09	64.05	0.12170	0.56558	0.32780	2.7873	6.8958	5.6268
12	3.331(2)	..	C1B	[	=		Intra	-58.37	-24.71	0.52900	0.44835	0.07506	5.5782	5.0985	1.2884
13	3.567(3)	..	C3D_e	[-1+x,y,z	=	1455.01]		-121.37	-4.28	0.13280	0.39480	0.14065	2.1394	4.6380	2.4143

14	2.68	<	H6E_a	[-1+x,1+y,z	=	1465.01]	Intra	118.20	-35.75	0.17100	0.85710	0.06500	2.9638	9.5904	1.1157
15	2.78	..	H3D_e	[-1+x,y,z	=	1455.01]		-114.09	1.93	0.20030	0.43670	0.16160	2.8586	5.1422	2.7739
16	3.07	..	H6B_c	[1-x,1-y,-z	=	2665.01]	Intra	4.21	-80.39	0.39430	0.70230	-0.02000	4.5015	7.7124	-0.3433
17	3.08	..	H6F_a	[-1+x,1+y,z	=	1465.01]	Intra	-155.17	47.81	0.05750	0.56430	0.28930	2.1112	6.8050	4.9659
18	3.15(3)	..	H3_a	[-1+x,1+y,z	=	1465.01]	Intra	164.64	8.50	-0.06600	0.73700	0.18330	0.9854	8.5002	3.1464
19	3.33(3)	..	H2W4	[	=	05]		31.89	17.12	0.55300	0.80900	0.21320	6.6903	9.3545	3.6596
20	3.52(3)	..	H4_a	[-1+x,1+y,z	=	1465.01]	Intra	149.50	25.15	-0.06500	0.79800	0.24340	1.2433	9.2933	4.1780

Angles (Degrees) At1...V...At2 with Vertex V = 021B

C21B	,	Cu2_a	122.31(12)	C21B	,	022B	26.56(10)	C21B	,	C2B	35.39(10)	C21B	,	N1F_a	120.75(12)
C21B	,	N1E_a	97.71(11)	C21B	,	C6E_a	94.31(11)	C21B	,	02_a	157.87(12)	C21B	,	C6B_c	48.57(10)
C21B	,	012B	55.81(10)	C21B	,	C6F_a	132.22(12)	C21B	,	C1B	43.98(10)	C21B	,	C3D_e	107.66(11)
Cu2_a	,	022B	95.75(7)	Cu2_a	,	C2B	157.12(9)	Cu2_a	,	N1F_a	45.91(5)	Cu2_a	,	N1E_a	44.19(5)
Cu2_a	,	C6E_a	67.30(6)	Cu2_a	,	02_a	48.96(5)	Cu2_a	,	C6B_c	147.60(8)	Cu2_a	,	012B	116.93(6)
Cu2_a	,	C6F_a	62.50(6)	Cu2_a	,	C1B	157.92(7)	Cu2_a	,	C3D_e	126.69(7)	022B	,	C2B	61.82(7)
022B	,	N1F_a	103.47(7)	022B	,	N1E_a	77.26(7)	022B	,	C6E_a	83.43(7)	022B	,	02_a	138.04(8)
022B	,	C6B_c	70.63(7)	022B	,	012B	64.97(6)	022B	,	C6F_a	123.08(7)	022B	,	C1B	69.07(6)
022B	,	C3D_e	132.28(8)	C2B	,	N1F_a	139.00(8)	C2B	,	N1E_a	120.15(8)	C2B	,	C6E_a	103.31(8)
C2B	,	02_a	147.30(8)	C2B	,	C6B_c	24.84(6)	C2B	,	012B	59.78(6)	C2B	,	C6F_a	132.11(8)
C2B	,	C1B	20.64(6)	C2B	,	C3D_e	75.76(7)	N1F_a	,	N1E_a	89.51(7)	N1F_a	,	C6E_a	113.14(7)
N1F_a	,	02_a	69.99(6)	N1F_a	,	C6B_c	163.78(8)	N1F_a	,	012B	79.24(6)	N1F_a	,	C6F_a	23.80(6)
N1F_a	,	C1B	120.16(7)	N1F_a	,	C3D_e	94.18(7)	N1E_a	,	C6E_a	26.25(6)	N1E_a	,	02_a	61.62(6)
N1E_a	,	C6B_c	103.44(7)	N1E_a	,	012B	136.32(7)	N1E_a	,	C6F_a	106.18(7)	N1E_a	,	C1B	138.97(7)
N1E_a	,	C3D_e	147.72(7)	C6E_a	,	02_a	63.70(6)	C6E_a	,	C6B_c	81.71(7)	C6E_a	,	012B	148.23(7)
C6E_a	,	C6F_a	124.35(7)	C6E_a	,	C1B	123.95(7)	C6E_a	,	C3D_e	129.25(7)	02_a	,	C6B_c	124.75(7)
02_a	,	012B	144.80(6)	02_a	,	C6F_a	65.89(6)	02_a	,	C1B	151.11(7)	02_a	,	C3D_e	89.63(6)
C6B_c	,	012B	84.62(6)	C6B_c	,	C6F_a	149.51(7)	C6B_c	,	C1B	43.76(6)	C6B_c	,	C3D_e	80.16(6)

012B	,	C6F_a	79.04(6)	012B	,	C1B	42.69(5)	012B	,	C3D_e	75.68(6)	C6F_a	,	C1B	111.53(7)
C6F_a	,	C3D_e	70.97(6)	C1B	,	C3D_e	63.74(6)								

3.6 Angstrom Coordination Sphere Around Atom I = 022A [ARU = 1555.01]													
0.91494 -0.16648 0.34786 8.8308 -1.1451 5.9711													
Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0 Y0 Z0
1	1.248(2)	--	C21A	[	=	]	Intra	32.85	5.45	1.02000	-0.10669	0.35476	9.8743 -0.4714 6.0895
2	2.244(2)	<<	021A	[	=	]	Intra	17.92	-17.06	1.14415	-0.09975	0.30950	10.8720 -0.4849 5.3126
3	2.358(2)	<<	C2A	[	=	]	Intra	51.05	35.97	1.00570	-0.04657	0.42855	10.0305 0.3392 7.3562
4	2.6705(19)	<<	O2	[	=	]	Intra	-87.09	-73.80	0.97015	-0.20694	0.19846	8.8687 -1.8891 3.4066
5	2.794(2)	<<	O2W	[	=	03]		-149.78	10.93	0.66163	-0.29715	0.37871	6.4604 -2.5260 6.5006
6	3.095(2)	.<	C6A_d	[2-x, -y, 1-z	=	2756.01]	Intra	25.84	54.22	1.04680	-0.12141	0.49413	10.4596 -0.3564 8.4819
7	3.1320(15)	<<	Cu2	[	=	]	Intra	-18.24	-40.30	1.21202	-0.21291	0.22984	11.0994 -1.8926 3.9452
8	3.135(2)	..	O11A	[	=	]	Intra	87.47	-13.00	0.89514	0.11740	0.30677	8.9655 1.9067 5.2658
9	3.162(2)	..	N1F	[	=	]	Intra	-41.44	-9.39	1.21623	-0.34810	0.31782	11.1694 -3.2097 5.4555
10	3.324(3)	..	C6F	[	=	]	Intra	-65.05	-5.95	1.12170	-0.43442	0.32780	10.2253 -4.1426 5.6268
11	3.364(2)	..	C2C	[	=	]	Intra	138.67	1.41	0.59710	0.03385	0.35267	6.3057 1.0758 6.0537
12	3.370(2)	..	C1A	[	=	]	Intra	71.22	26.23	0.95800	0.07718	0.43463	9.8043 1.7173 7.4605
13	1.90(2)	<<	H4	[	=	]	Intra	-103.99	-70.97	0.93500	-0.20200	0.24340	8.6813 -1.7451 4.1780
14	2.06(3)	<<	H1W2	[	=	03]		-147.41	14.43	0.73500	-0.26900	0.37770	7.1536 -2.2173 6.4833
15	2.43	<<	H2C	[	=	]	Intra	137.33	-1.72	0.69110	-0.01660	0.34360	7.0453 0.5009 5.8980
16	3.03	..	H6A_d	[2-x, -y, 1-z	=	2756.01]	Intra	-4.69	53.79	1.07920	-0.20540	0.49020	10.6139 -1.2913 8.4144
17	3.13(3)	..	H2W2	[	=	03]		-137.00	4.35	0.68700	-0.36200	0.36170	6.5458 -3.2757 6.2087
18	3.18(2)	..	H3	[	=	]	Intra	-106.30	-62.80	0.93400	-0.26300	0.18330	8.4234 -2.5381 3.1464
19	3.31(2)	..	H1	[	=	]	Intra	124.09	-63.33	0.84900	-0.02400	0.17560	7.9986 0.0847 3.0142
20	3.33	..	H6F	[	=	]	Intra	-76.90	-17.59	1.05750	-0.43570	0.28930	9.5492 -4.2334 4.9659
21	3.33(3)	..	H1W4_e	[x, -1+y, z	=	1545.05]		-173.33	-20.56	0.59100	-0.18700	0.27970	5.7320 -1.5073 4.8011
22	3.58(2)	..	H2	[	=	]	Intra	147.62	-47.22	0.70600	-0.02100	0.19490	6.7789 0.1562 3.3455

Angles (Degrees) At1...V...At2 with Vertex V = 022A

C21A	,	021A	26.91(10)	C21A	,	C2A	34.80(10)	C21A	,	O2	103.28(11)	C21A	,	O2W	163.42(12)
C21A	,	C6A_d	49.10(10)	C21A	,	Cu2	65.45(10)	C21A	,	O11A	57.30(10)	C21A	,	N1F	75.49(11)
C21A	,	C6F	98.39(12)	C21A	,	C2C	105.60(12)	C21A	,	C1A	42.09(10)	O21A	,	C2A	61.60(7)
O21A	,	O2	77.72(7)	O21A	,	O2W	166.59(8)	O21A	,	C6A_d	71.60(6)	O21A	,	Cu2	38.89(5)
O21A	,	O11A	66.95(6)	O21A	,	N1F	58.10(6)	O21A	,	C6F	81.57(7)	O21A	,	C2C	119.72(7)
O21A	,	C1A	67.49(6)	C2A	,	O2	137.07(8)	C2A	,	O2W	129.15(8)	C2A	,	C6A_d	25.23(6)
C2A	,	Cu2	99.30(7)	C2A	,	O11A	59.84(6)	C2A	,	N1F	97.50(8)	C2A	,	C6F	114.52(8)
C2A	,	C2C	87.25(7)	C2A	,	C1A	19.77(6)	O2	,	O2W	93.23(7)	O2	,	C6A_d	147.41(8)
O2	,	Cu2	45.74(5)	O2	,	O11A	93.13(6)	O2	,	N1F	69.57(6)	O2	,	C6F	69.10(6)
O2	,	C2C	102.60(7)	O2	,	C1A	131.07(7)	O2W	,	C6A_d	114.75(7)	O2W	,	Cu2	128.25(6)
O2W	,	O11A	124.07(7)	O2W	,	N1F	109.61(7)	O2W	,	C6F	85.98(7)	O2W	,	C2C	71.63(6)
O2W	,	C1A	125.52(7)	C6A_d	,	Cu2	101.79(6)	C6A_d	,	O11A	84.94(6)	C6A_d	,	N1F	84.81(6)
C6A_d	,	C6F	95.34(7)	C6A_d	,	C2C	101.94(7)	C6A_d	,	C1A	43.37(6)	Cu2	,	O11A	93.19(5)
Cu2	,	N1F	37.15(4)	Cu2	,	C6F	54.12(5)	Cu2	,	C2C	135.82(6)	Cu2	,	C1A	106.22(6)
O11A	,	N1F	124.55(6)	O11A	,	C6F	146.77(7)	O11A	,	C2C	52.78(5)	O11A	,	C1A	42.29(5)
N1F	,	C6F	23.65(5)	N1F	,	C2C	172.02(7)	N1F	,	C1A	114.39(7)	C6F	,	C2C	155.90(7)

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C6F	,	C1A	133.67(7)	C2C	,	C1A	69.22(6)

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3.6 Angstrom Coordination Sphere Around Atom I = 022B [ARU = 1555.01] 0.53170 0.71481 0.13573 6.1565 8.1606 2.3298

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	1.248(2)	--	C21B	[	=		Intra	-146.65	-8.55	0.42920	0.65532	0.12492	5.1260	7.4824	2.1443

2	2.247(2)	<<	021B	[	=		Intra	-167.36	8.98	0.29071	0.66712	0.15616	3.9911	7.6749	2.6805
3	2.365(2)	<<	C2B	[	=		Intra	-119.65	-32.09	0.46620	0.57029	0.06254	5.1654	6.4196	1.0735
4	2.705(2)	<<	04W	[	=	05]		66.54	43.66	0.56313	0.85779	0.24452	6.9355	9.9555	4.1972
5	2.782(2)	<<	03W	[	=	04]		-22.76	6.99	0.82808	0.61448	0.15546	8.7030	7.0924	2.6685
6	3.004(2)	.<	012B	[	=		Intra	-92.72	24.77	0.53857	0.45479	0.20906	6.0269	5.4364	3.5886
7	3.1313(16)	<<	Cu2_a	[	=	1465.01]	Intra	158.45	31.05	0.21202	0.78709	0.22984	3.6614	9.1458	3.9452
8	3.178(2)	.<	C6B_c	[	=	2665.01]	Intra	-135.53	-52.88	0.43770	0.61973	-0.01192	4.7878	6.8171	-0.2046
9	3.218(2)	..	N1E_a	[	=	1465.01]	Intra	132.61	3.86	0.24906	0.92661	0.14835	3.9828	10.5237	2.5465
10	3.286(2)	..	C1B	[	=		Intra	-100.70	-18.48	0.52900	0.44835	0.07506	5.5782	5.0985	1.2884
11	3.435(3)	..	C4E_e	[	=	2765.01]		58.14	-55.26	0.66640	0.89510	-0.02873	7.1898	9.8233	-0.4932
12	3.554(2)	..	C11B	[	=		Intra	-92.12	5.23	0.56510	0.39096	0.15462	6.0253	4.6234	2.6541
13	3.564(3)	..	C6E_a	[	=	1465.01]	Intra	140.40	-16.96	0.22060	0.92260	0.07516	3.5298	10.3337	1.2901

14	1.87(2)	<<	H2W4	[	=	05]		65.91	45.48	0.55300	0.80900	0.21320	6.6903	9.3545	3.6596
15	1.99(3)	<<	H2W3	[	=	04]		-23.97	5.23	0.74400	0.64000	0.14630	7.9668	7.3559	2.5113
16	2.50	<<	H4E_e	[	=	2765.01]		54.06	-57.86	0.63600	0.83470	0.01230	6.9378	9.2382	0.2111
17	3.02(3)	..	H1W4	[	=	05]		52.43	55.02	0.59100	0.81300	0.27970	7.2107	9.5311	4.8011
18	3.05(3)	..	H1W3	[	=	04]		-30.48	18.86	0.81700	0.57200	0.19310	8.6408	6.6984	3.3146
19	3.18	..	H6B_c	[	=	2665.01]	Intra	-164.85	-57.32	0.39430	0.70230	-0.02000	4.5015	7.7124	-0.3433

Angles (Degrees) At1...V...At2 with Vertex V = 022B

C21B	,	021B	27.07(10)	C21B	,	C2B	34.36(10)	C21B	,	04W	134.54(13)	C21B	,	03W	124.43(12)
C21B	,	012B	62.20(11)	C21B	,	Cu2_a	65.77(10)	C21B	,	C6B_c	45.24(10)	C21B	,	N1E_a	81.45(11)
C21B	,	C1B	45.64(10)	C21B	,	C4E_e	112.91(12)	C21B	,	C11B	56.09(11)	C21B	,	C6E_a	71.30(11)
021B	,	C2B	61.30(7)	021B	,	04W	108.26(8)	021B	,	03W	141.27(8)	021B	,	012B	72.36(6)
021B	,	Cu2_a	38.70(5)	021B	,	C6B_c	67.54(6)	021B	,	N1E_a	59.82(6)	021B	,	C1B	71.24(7)
021B	,	C4E_e	121.52(7)	021B	,	C11B	74.64(6)	021B	,	C6E_a	57.80(6)	C2B	,	04W	167.45(9)
C2B	,	03W	99.53(8)	C2B	,	012B	62.41(7)	C2B	,	Cu2_a	99.89(7)	C2B	,	C6B_c	23.74(6)
C2B	,	N1E_a	107.06(8)	C2B	,	C1B	21.82(6)	C2B	,	C4E_e	92.63(7)	C2B	,	C11B	45.60(6)
C2B	,	C6E_a	89.14(7)	04W	,	03W	84.67(7)	04W	,	012B	108.96(7)	04W	,	Cu2_a	70.40(6)
04W	,	C6B_c	162.76(8)	04W	,	N1E_a	70.17(6)	04W	,	C1B	152.62(7)	04W	,	C4E_e	99.18(7)
04W	,	C11B	127.45(7)	04W	,	C6E_a	90.52(7)	03W	,	012B	68.92(6)	03W	,	Cu2_a	141.94(7)
03W	,	C6B_c	109.20(7)	03W	,	N1E_a	153.13(7)	03W	,	C1B	80.90(6)	03W	,	C4E_e	90.60(7)
03W	,	C11B	68.94(6)	03W	,	C6E_a	160.76(7)	012B	,	Cu2_a	92.00(5)	012B	,	C6B_c	86.11(6)
012B	,	N1E_a	127.49(7)	012B	,	C1B	43.95(5)	012B	,	C4E_e	142.78(7)	012B	,	C11B	19.55(5)
012B	,	C6E_a	130.05(7)	Cu2_a	,	C6B_c	101.61(6)	Cu2_a	,	N1E_a	36.49(4)	Cu2_a	,	C1B	108.45(6)
Cu2_a	,	C4E_e	120.75(6)	Cu2_a	,	C11B	103.69(6)	Cu2_a	,	C6E_a	51.05(5)	C6B_c	,	N1E_a	94.20(6)
C6B_c	,	C1B	43.74(6)	C6B_c	,	C4E_e	71.27(6)	C6B_c	,	C11B	68.67(6)	C6B_c	,	C6E_a	73.01(6)
N1E_a	,	C1B	125.93(7)	N1E_a	,	C4E_e	84.44(6)	N1E_a	,	C11B	134.40(7)	N1E_a	,	C6E_a	22.20(5)
C1B	,	C4E_e	104.10(7)	C1B	,	C11B	25.17(5)	C1B	,	C6E_a	110.25(7)	C4E_e	,	C11B	124.59(7)

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C4E_e	,	C6E_a	71.75(6)	C11B	,	C6E_a	127.31(7)

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3.6 Angstrom Coordination Sphere Around Atom I = N1C [ARU = 1555.01] 0.58089 0.14471 0.31169 6.2168 2.2179 5.3502

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.344(2)	--	C2C	[	=	]	Intra	-85.55	31.55	0.59710	0.03385	0.35267	6.3057	1.0758	6.0537
2	1.351(3)	--	C6C	[	=	]	Intra	142.81	9.62	0.44630	0.21527	0.32484	5.1558	3.0230	5.5760
3	2.0135(17)	--	Cu1	[	=	]	Intra	15.53	-42.40	0.75664	0.19504	0.23260	7.6495	2.6160	3.9926
4	2.386(3)	<<	C5C	[	=	]	Intra	166.36	29.04	0.32820	0.17710	0.37917	4.1898	2.7098	6.5085
5	2.391(3)	<<	C3C	[	=	]	Intra	-119.43	43.41	0.48240	-0.00963	0.40743	5.3633	0.7049	6.9936
6	2.768(2)	<<	O11A	[	=	]	Intra	-6.46	-1.75	0.89514	0.11740	0.30677	8.9655	1.9067	5.2658
7	2.779(3)	<<	C4C	[	=	]	Intra	-160.67	42.92	0.34630	0.06381	0.42192	4.2966	1.5444	7.2424
8	2.887(2)	<	O11B	[	=	]	Intra	82.75	-65.75	0.62084	0.27894	0.15833	6.3665	3.3943	2.7178
9	3.090(2)	..	O1	[	=	]	Intra	-54.35	-49.41	0.77323	0.02137	0.17500	7.3885	0.5843	3.0039
10	3.226(3)	<	C11A	[	=	]	Intra	6.21	17.33	0.90430	0.16478	0.36767	9.2781	2.5509	6.3111
11	3.521(2)	..	O12A	[	=	]	Intra	27.85	18.65	0.87081	0.27409	0.37727	9.1665	3.7767	6.4759
12	3.578(2)	..	O4W_e	[x, -1+y, z	=	1545.05]		-102.97	-18.80	0.56313	-0.14221	0.24452	5.4568	-1.0829	4.1972
13	1.98	<<	H2C	[	=	]	Intra	-64.24	16.03	0.69110	-0.01660	0.34360	7.0453	0.5009	5.8980
14	1.99	<<	H6C	[	=	]	Intra	125.41	-7.86	0.43260	0.29340	0.29580	5.0725	3.8276	5.0775
15	2.93(2)	..	H2	[	=	]	Intra	-74.75	-43.17	0.70600	-0.02100	0.19490	6.7789	0.1562	3.3455
16	3.24	..	H5C	[	=	]	Intra	158.75	23.60	0.23460	0.22850	0.38720	3.4524	3.2932	6.6464
17	3.24	..	H3C	[	=	]	Intra	-108.20	40.66	0.49710	-0.08900	0.43470	5.4490	-0.1169	7.4617
18	3.47	..	H2E_f	[-1+x, y, z	=	1455.01]		-150.07	-28.99	0.33500	0.02530	0.21380	3.5892	0.7050	3.6699

Angles (Degrees) At1...V...At2 with Vertex V = N1C

C2C	,	C6C	118.09(17)	C2C	,	Cu1	118.28(13)	C2C	,	C5C	88.70(12)	C2C	,	C3C	29.13(10)
C2C	,	O11A	81.65(11)	C2C	,	C4C	58.90(11)	C2C	,	O11B	145.07(13)	C2C	,	O1	85.59(11)
C2C	,	C11A	82.48(11)	C2C	,	O12A	98.83(12)	C2C	,	O4W_e	53.05(10)	C6C	,	Cu1	123.62(13)
C6C	,	C5C	29.39(11)	C6C	,	C3C	88.96(13)	C6C	,	O11A	148.45(13)	C6C	,	C4C	59.20(12)
C6C	,	O11B	87.15(12)	C6C	,	O1	137.72(13)	C6C	,	C11A	129.35(13)	C6C	,	O12A	109.92(12)
C6C	,	O4W_e	115.90(13)	Cu1	,	C5C	153.01(10)	Cu1	,	C3C	147.40(10)	Cu1	,	O11A	45.17(5)
Cu1	,	C4C	177.16(9)	Cu1	,	O11B	42.93(5)	Cu1	,	O1	47.37(5)	Cu1	,	C11A	60.35(6)
Cu1	,	O12A	62.10(6)	Cu1	,	O4W_e	96.68(7)	C5C	,	C3C	59.57(9)	C5C	,	O11A	151.86(9)
C5C	,	C4C	29.80(8)	C5C	,	O11B	113.75(9)	C5C	,	O1	143.11(9)	C5C	,	C11A	129.82(9)
C5C	,	O12A	117.73(8)	C5C	,	O4W_e	99.57(8)	C3C	,	O11A	107.72(8)	C3C	,	C4C	29.78(7)
C3C	,	O11B	154.54(9)	C3C	,	O1	108.83(8)	C3C	,	C11A	101.50(8)	C3C	,	O12A	111.06(8)
C3C	,	O4W_e	64.02(7)	O11A	,	C4C	132.83(8)	O11A	,	O11B	88.08(7)	O11A	,	O1	62.66(6)
O11A	,	C11A	22.80(5)	O11A	,	O12A	39.42(5)	O11A	,	O4W_e	95.59(7)	C4C	,	O11B	139.06(8)
C4C	,	O1	130.62(8)	C4C	,	C11A	118.56(8)	C4C	,	O12A	117.94(7)	C4C	,	O4W_e	81.32(7)
O11B	,	O1	60.22(6)	O11B	,	C11A	100.39(7)	O11B	,	O12A	93.88(6)	O11B	,	O4W_e	95.34(6)
O1	,	C11A	85.47(7)	O1	,	O12A	99.16(6)	O1	,	O4W_e	49.31(5)	C11A	,	O12A	20.62(5)
C11A	,	O4W_e	113.13(7)	O12A	,	O4W_e	133.58(7)								


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3.6 Angstrom Coordination Sphere Around Atom I = N1E      [ARU = 1555.01]      1.24906 -0.07339  0.14835   11.4208 -0.5147  2.5465
```

Nr	d(I, J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0
1	1.340(3)	--	C2E	[	=	]	Intra	53.74	10.18	1.31690	0.02049	0.16215	12.2010	0.5490	2.7833
2	1.349(2)	--	C6E	[	=	]	Intra	157.25	-68.64	1.22060	-0.07740	0.07516	10.9678	-0.7047	1.2901
3	1.9895(16)	--	Cu2	[	=	]	Intra	103.13	44.67	1.21202	-0.21291	0.22984	11.0994	-1.8926	3.9452
4	2.382(3)	<<	C3E	[	=	]	Intra	59.21	-18.57	1.36130	0.11030	0.10417	12.5765	1.4249	1.7881
5	2.389(3)	<<	C5E	[	=	]	Intra	101.03	-73.91	1.26070	0.00960	0.01464	11.2941	0.1351	0.2513
6	2.775(3)	<<	C4E	[	=	]	Intra	67.93	-47.73	1.33360	0.10490	0.02873	12.1223	1.2151	0.4932
7	2.820(2)	<<	021A	[	=	]	Intra	176.88	78.76	1.14415	-0.09975	0.30950	10.8720	-0.4849	5.3126
8	2.852(2)	<<	021B_b	[1+x, -1+y, z	=	1645.01]	Intra	-89.83	2.69	1.29071	-0.33288	0.15616	11.4291	-3.3635	2.6805
9	3.024(2)	<	02	[	=	]	Intra	-151.70	16.53	0.97015	-0.20694	0.19846	8.8687	-1.8891	3.4066
10	3.218(2)	..	022B_b	[1+x, -1+y, z	=	1645.01]	Intra	-47.39	-3.86	1.53170	-0.28519	0.13573	13.5945	-2.8778	2.3298
11	3.274(2)	..	C21B_b	[1+x, -1+y, z	=	1645.01]	Intra	-69.40	-7.06	1.42920	-0.34468	0.12492	12.5640	-3.5560	2.1443
12	3.430(2)	..	04W_e	[1+x, -1+y, z	=	1645.05]		-10.89	28.77	1.56313	-0.14221	0.24452	14.3735	-1.0829	4.1972
13	1.98	<<	H2E	[	=	]	Intra	48.34	34.54	1.33500	0.02530	0.21380	12.5059	0.7050	3.6699
14	1.99	<<	H6E	[	=	]	Intra	137.51	-46.00	1.17100	-0.14290	0.06500	10.4018	-1.4480	1.1157
15	3.15(3)	..	H2W4_e	[1+x, -1+y, z	=	1645.05]		-23.35	20.68	1.55300	-0.19100	0.21320	14.1283	-1.6838	3.6596
16	3.23	..	H3E	[	=	]	Intra	57.30	-9.98	1.41040	0.17520	0.11570	13.1408	2.1643	1.9860
17	3.24	..	H5E	[	=	]	Intra	133.60	-77.94	1.23850	0.00430	-0.03620	10.9541	-0.0246	-0.6214
18	3.42(3)	..	H4	[	=	]	Intra	155.81	28.51	0.93500	-0.20200	0.24340	8.6813	-1.7451	4.1780
19	3.51(3)	..	H1	[	=	]	Intra	170.06	7.67	0.84900	-0.02400	0.17560	7.9986	0.0847	3.0142

Angles (Degrees) At1...V...At2 with Vertex V = N1E

C2E	, C6E	118.16(17)	C2E	, Cu2	121.30(13)	C2E	, C3E	29.25(11)	C2E	, C5E	89.13(13)
C2E	, C4E	59.26(12)	C2E	, O21A	86.07(12)	C2E	, O21B_b	141.52(13)	C2E	, O2	143.31(13)
C2E	, O22B_b	101.63(12)	C2E	, C21B_b	123.76(13)	C2E	, O4W_e	62.96(11)	C6E	, Cu2	120.20(13)
C6E	, C3E	88.92(13)	C6E	, C5E	29.03(11)	C6E	, C4E	58.91(12)	C6E	, O21A	148.17(13)
C6E	, O21B_b	84.50(12)	C6E	, O2	85.27(12)	C6E	, O22B_b	93.48(12)	C6E	, C21B_b	82.65(12)
C6E	, O4W_e	135.56(13)	Cu2	, C3E	150.02(10)	Cu2	, C5E	148.80(10)	Cu2	, C4E	173.10(9)
Cu2	, O21A	44.47(5)	Cu2	, O21B_b	43.58(5)	Cu2	, O2	49.37(5)	Cu2	, O22B_b	69.38(6)
Cu2	, C21B_b	59.96(6)	Cu2	, O4W_e	71.70(6)	C3E	, C5E	59.89(9)	C3E	, C4E	30.01(8)
C3E	, O21A	113.46(9)	C3E	, O21B_b	145.79(9)	C3E	, O2	150.50(9)	C3E	, O22B_b	104.41(8)
C3E	, C21B_b	123.23(9)	C3E	, O4W_e	82.56(8)	C5E	, C4E	29.87(8)	C5E	, O21A	158.31(10)
C5E	, O21B_b	108.49(9)	C5E	, O2	110.63(9)	C5E	, O22B_b	99.84(9)	C5E	, C21B_b	98.81(8)
C5E	, O4W_e	123.58(10)	C4E	, O21A	140.20(8)	C4E	, O21B_b	131.05(8)	C4E	, O2	135.01(8)
C4E	, O22B_b	103.72(7)	C4E	, C21B_b	113.57(8)	C4E	, O4W_e	103.99(7)	O21A	, O21B_b	88.00(6)
O21A	, O2	63.99(6)	O21A	, O22B_b	101.84(7)	O21A	, C21B_b	101.44(7)	O21A	, O4W_e	72.38(6)
O21B_b	, O2	62.29(6)	O21B_b	, O22B_b	42.92(5)	O21B_b	, C21B_b	22.61(5)	O21B_b	, O4W_e	79.01(6)
O2	, O22B_b	104.80(7)	O2	, C21B_b	84.69(6)	O2	, O4W_e	120.96(7)	O22B_b	, C21B_b	22.14(5)
O22B_b	, O4W_e	47.88(5)	C21B_b	, O4W_e	66.71(6)						

=====

3.6 Angstrom Coordination Sphere Around Atom I = N1F [ARU = 1555.01] 1.21623 -0.34810 0.31782 11.1694 -3.2097 5.4555

Nr	d(I,J)	To	Atom J	Symm_Oper.	on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	X0	Y0	Z0

1	1.338(3)	--	C6F	[	=	]	Intra	-135.34	7.35	1.12170	-0.43442	0.32780	10.2253	-4.1426	5.6268
2	1.341(3)	--	C2F	[	=	]	Intra	6.27	43.86	1.30800	-0.34830	0.37193	12.1303	-3.1042	6.3843
3	2.0052(17)	--	Cu2	[	=	]	Intra	93.04	-48.87	1.21202	-0.21291	0.22984	11.0994	-1.8926	3.9452

4	2.382(3)	<<	C5F	[	=	]	Intra	-118.92	32.13	1.11370	-0.52140	0.39164	10.1939	-4.9757	6.7226
5	2.384(3)	<<	C3F	[	=	]	Intra	-35.28	59.07	1.30730	-0.43370	0.43696	12.1696	-3.9174	7.5005
6	2.745(2)	<<	O21A	[	=	]	Intra	96.23	-2.98	1.14415	-0.09975	0.30950	10.8720	-0.4849	5.3126
7	2.767(3)	<<	C4F	[	=	]	Intra	-89.38	53.25	1.20870	-0.52140	0.44700	11.1872	-4.8654	7.6729
8	2.791(2)	<<	O21B_b	[1+x, -1+y, z	=	1645.01]	Intra	-30.65	-83.79	1.29071	-0.33288	0.15616	11.4291	-3.3635	2.6805
9	3.095(3)	<	C21A	[	=	]	Intra	115.31	11.82	1.02000	-0.10669	0.35476	9.8743	-0.4714	6.0895
10	3.162(2)	..	O22A	[	=	]	Intra	138.56	9.39	0.91494	-0.16648	0.34786	8.8308	-1.1451	5.9711
11	3.352(2)	..	O2	[	=	]	Intra	150.15	-37.68	0.97015	-0.20694	0.19846	8.8687	-1.8891	3.4066

12	1.98	<<	H6F	[	=	]	Intra	-147.71	-14.33	1.05750	-0.43570	0.28930	9.5492	-4.2334	4.9659
13	1.98	<<	H2F	[	=	]	Intra	24.92	24.28	1.37590	-0.28770	0.36530	12.8079	-2.4484	6.2705
14	3.16(3)	..	H4	[	=	]	Intra	149.52	-23.87	0.93500	-0.20200	0.24340	8.6813	-1.7451	4.1780
15	3.23	..	H5F	[	=	]	Intra	-124.73	25.00	1.04400	-0.58060	0.39740	9.5001	-5.6177	6.8215
16	3.23	..	H3F	[	=	]	Intra	-19.93	56.10	1.37400	-0.43200	0.47420	12.8652	-3.8244	8.1398
17	3.57	..	H6A_d	[2-x, -y, 1-z	=	2756.01]	Intra	106.15	55.98	1.07920	-0.20540	0.49020	10.6139	-1.2913	8.4144

Angles (Degrees) At1...V...At2 with Vertex V = N1F

C6F	,	C2F	118.16(17)	C6F	,	Cu2	121.98(14)	C6F	,	C5F	29.11(12)	C6F	,	C3F	88.81(13)
C6F	,	O21A	128.48(13)	C6F	,	C4F	59.00(12)	C6F	,	O21B_b	98.89(13)	C6F	,	C21A	107.18(13)
C6F	,	O22A	84.98(12)	C6F	,	O2	82.45(12)	C2F	,	Cu2	119.68(14)	C2F	,	C5F	89.05(14)
C2F	,	C3F	29.35(12)	C2F	,	O21A	92.04(13)	C2F	,	C4F	59.16(12)	C2F	,	O21B_b	128.79(13)
C2F	,	C21A	95.07(13)	C2F	,	O22A	111.45(13)	C2F	,	O2	152.19(14)	Cu2	,	C5F	150.83(11)
Cu2	,	C3F	148.84(11)	Cu2	,	O21A	45.97(5)	Cu2	,	C4F	175.36(10)	Cu2	,	O21B_b	44.82(5)
Cu2	,	C21A	63.80(6)	Cu2	,	O22A	70.62(6)	Cu2	,	O2	42.00(5)	C5F	,	C3F	59.70(10)
C5F	,	O21A	135.99(10)	C5F	,	C4F	29.89(9)	C5F	,	O21B_b	121.73(9)	C5F	,	C21A	112.06(9)
C5F	,	O22A	95.42(9)	C5F	,	O2	109.64(9)	C3F	,	O21A	112.63(9)	C3F	,	C4F	29.82(9)
C3F	,	O21B_b	142.88(10)	C3F	,	C21A	105.22(9)	C3F	,	O22A	111.36(9)	C3F	,	O2	158.32(10)
O21A	,	C4F	129.52(8)	O21A	,	O21B_b	90.75(7)	O21A	,	C21A	24.07(5)	O21A	,	O22A	43.95(5)
O21A	,	O2	60.18(6)	C4F	,	O21B_b	139.73(9)	C4F	,	C21A	111.59(8)	C4F	,	O22A	105.35(8)
C4F	,	O2	136.88(9)	O21B_b	,	C21A	106.94(7)	O21B_b	,	O22A	105.48(7)	O21B_b	,	O2	58.53(6)
C21A	,	O22A	22.97(5)	C21A	,	O2	59.30(6)	O22A	,	O2	48.30(5)				

Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6

van der Waals (or ion) Radii used in the Analysis

C	H	Cu	N	O
1.70	1.20	2.32	1.55	1.52

:: Grid: X-Axis Step = 0.0208 = Points 48, Angstrom Step = 0.19
 :: Grid: Y-Axis Step = 0.0167 = Points 60, Angstrom Step = 0.19
 :: Grid: Z-Axis Step = 0.0119 = Points 84, Angstrom Step = 0.21

:: Total Potential Solvent Area Vol 21.9 Ang^3
 per Unit Cell Vol 1689.5 Ang^3 [1.3%]

Note: Expected volumes for solvent molecules are:
 A hydrogen bonded H2O-molecule 40 Ang^3
 Small molecules (e.g. Toluene) 100-300 Ang^3

Values below for gridpoints and volumes in []
 refer to areas where atom centers may reside.

:: Use the CALC SQUEEZE instruction to calculate and optionally correct for
 :: Density identified in solvent accessible areas (Reflection data required)

Area	#GridPoint	VolPerc.	Vol(A^3)	X(av)	Y(av)	Z(av)	Eigenvector(frac)	Sig(Ang)
1	1570[	3]	1	11[	0.0]	0.458	0.732	0.530
						1	1.000-0.396-0.136	0.75
						2	0.555 1.000-0.001	0.56
						3	0.189-0.377 1.000	0.56
2	1570[	3]	1	11[	0.0]	0.542	0.268	0.470
						1	1.000-0.396-0.136	0.75
						2	0.539 1.000-0.043	0.56
						3	0.233-0.295 1.000	0.56

x	y	z	Shortest Contacts within 4.5 Angstrom (Excl. H)																		
1	0.458	0.732	0.530	C6C	2.94;	C5C	3.00;	O2W	3.01;	O12A	3.13;	C3F	3.16;	N1C	3.20;	C4C	3.30;	C3C	3.36;	C2C	3.46;
2	0.542	0.268	0.470	C6C	2.94;	C5C	3.00;	O2W	3.01;	O12A	3.13;	C3F	3.16;	N1C	3.20;	C4C	3.30;	C3C	3.36;	C2C	3.46;

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

Report the Distance from VOID-CG to Boundary in EV-Directions

Nr MinEV1 MaxEV1 MinEV2 MaxEV2 MinEV3 MaxEV3 MaxDist (Ang)

1	-1.57	1.58	-1.27	1.25	-1.17	1.22	1.58
2	-1.58	1.58	-1.18	1.28	-1.22	1.17	1.58

Report Expected Number of Independent Reflections for given Symmetry and Resolution.

:: Hmax = 11 Kmax = 14 Lmax= 23 , Sorting Order : Fast H, Medium K, Slow L

:: Actual Theta-Max: 28.277 Deg. (Applied Theta Limit: 28.280 Deg.)

Space Group P-1 No: 2, Laue: -1 [Hall: -P 1]

Lattice Type aP, Centric, Triclinic, Order 2(1) [Schoenflies: Ci¹]

Nr ***** Symmetry Operation(s) *****

1	H ,	K ,	L
2	- H ,	- K ,	- L

:: Number of Independent Type H, K, L Reflections = 8378

Table 0 - Crystal Data and Details of the Structure Determination
for: C:xtalRUP-1no3pyrcunR = 0.03F

Crystal Data

Formula			[(C10
Formula Weight			801.69
Crystal System			Triclinic
Space group		P-1	(No. 2)
a, b, c [Angstrom]	8.9167(18)	11.137(2)	17.481(4)
alpha, beta, gamma [deg]	82.36(3)	81.31(3)	82.37(3)
V [Ang**3]			1689.5(6)
Z			2
D(calc) [g/cm**3]			1.576
Mu(MoKa) [/mm]			1.333
F(000)			824
Crystal Size [mm]		0.10 x 0.25 x 0.25	

Data Collection

Temperature (K)			113
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			2.4, 28.3
Dataset		-11: 11 ; -14: 14 ; -22: 23	
Tot., Uniq. Data, R(int)		27065, 8330, 0.050	
Observed data [I > 2.0 sigma(I)]			6690

Refinement

Nref, Npar		8330, 487
R, wR2, S		0.0324, 0.0830, 1.02
w = 1/[s^2^(Fo^2^)+(0.0398P)^2^+0.6001P]		where P=(Fo^2^+2Fc^2^)/3
Max. and Av. Shift/Error		0.03, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]		-0.65, 0.48

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***** N O T I C E *****

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- PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13
- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow
- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)
- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.
- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.
- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@chem.uu.nl
- Recent versions of PLATON may be obtained by Anonymous FTP from xraysoft.chem.uu.nl
- More INFO can be found on <http://www.cryst.chem.uu.nl/platon/>

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Page - Index
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Page 1 --- GENERAL
Page 2 --- ADDSYM
Page 3 --- GEOMETRY
Page 15 --- ADP-Anal
Page 23 --- GEOMETRY
Page 78 --- INTER
Page 93 --- H-BONDS
Page 110 --- COORDN
Page 145 --- VOIDS
Page 147 --- EXPECT
Page 148 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

W: NOMOVE option used.

:: >>> WARNING: 'CONNECTED INPUT SET' is assumed 'TRUE'

:: >>> Network Analysis may be INCORRECT when FALSE

N: Number of modified (= #) ATOM labels 8

N: Total Potential Solvent Accessible Void Vol 21.9 Ang^3
=====

:: Input Xtal Data from File CUN03PYR.CIF - Data Type CIF

:: NORMAL END of PLATON : 150 Pages on:

:: CUN03PYR.lis (ASCII, 132 Characters Wide)

:: CUN03PYR.lps (PostScript Version of .lis)

::

:: SPF File on :CUN03PYR.eld

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README.TXT

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This CD-ROM contains supplementary material relating to the Ph. D. thesis of Emmanuel Lamprecht (Department of Chemistry, Rhodes University, 2008).

The folder, 'PLATON-listings', contains complete PLATON calculation outputs for the crystal structures referred to in the thesis as xut-cu-b4c-acet-xtals, xst-cu-b4c-cl-rhombi, xut-cu-b4c-pyr2-no3-xtals. These are in PDF format, and can be read with Adobe Acrobat Reader.

The folder, 'source-code/working-prototype', contains the complete C source for the digital part of the prototype X-ray detector system described in the thesis. It can be compiled using earlier versions of AVR-GCC for Windows (those based on GCC 2.95.2), but will need minor modifications to compile on later versions. See the README file in this folder for more details.

The folder, 'source-code/ratemeter-development', contains a modified version of the file ratemeter.h, together with a simple test program, which attempts to overcome some defects in the prototype version. See the file 'ratemeter.h' for details. It should compile on GNU C, but will need slight modification to run on a microcontroller. It is included for demonstration purposes only.

The folder, 'stoichiometry-solver', contains a very rough python program for working out stoichiometric decomposition routes given a starting material and stated decomposition products. This program was written for the sole use of the author, and is not ready for general use. It is included for demonstration purposes only. It should run on any current version of python.

THIS MATERIAL IS DISTRIBUTED TO YOU ON CONDITION THAT YOU DO NOT REDISTRIBUTE IT TO ANYONE ELSE OR MAKE ANY COPIES EXCEPT TO MAKE BACK-UPS FOR YOURSELF.

This distribution contains the C source files for the microcontroller program currently resident in the XRPD-DS Prototype Version 0.1 . They will compile without change on earlier versions of AVR-GCC, but will require small changes on more modern versions of AVR-GCC.

Some day I'll make the conversion!

HISTORY

Version 0.1/2004-07-15:

- a. First working version, currently resident in prototype.
- b. TODO:

There are small bugs in this version which aren't significant for normal every-day use in the current application, but should it be important to have greater accuracy especially at low count-rates, these should be fixed:

- i. RUN-TIME MISBEHAVIOUR AT LOW COUNT-RATES

At low count rates, there is a baseline offset arising from roundoff error in the RateMeter_tick(...) function. There is a comprehensive discussion in the Notes (Sep. 2003-*) on p. 135, BUT THE REMEDY PROVIDED UP TO P. 139 WILL NOT WORK EXACTLY AS PROPOSED. I might move to floating-point arithmetic, although it bloats the code big-time and may prove too slow; or I might modify the remedy in the Notes, which will (when corrected) fix the problem by means of a few shifting operations.

- ii. COMPILE-TIME PROBLEM ON MODERN AVR-GCC

The current implementation won't compile on modern AVR-GCC implementations because the TCCNT1 macro doesn't exist on modern versions. The new macro is TCCNT1L for the lower half of the word and TCCNT1H for the upper one. This is easy to fix, but there's no point just now.