Facile Synthesis of a Chiral Urea Bridged Bisoxazoline Ligand and Structural Characterization of its Bis-Copper(II)-Chloride Complex

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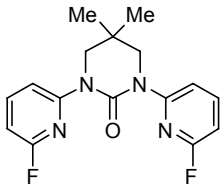
Electronic Supplementary Information

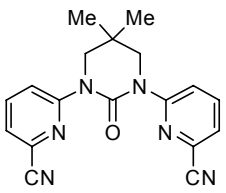
General information: Starting materials, reagents and solvents were purchased from commercial sources and were used as received. Methanol was distilled over magnesium methoxide prior to use. Tetrahydrofuran was distilled over sodium/benzophenone prior to use. Chlorobenzene and anhydrous DMSO were purchased from commercial sources and were used without further purification. Reactions were run under an atmosphere of dry nitrogen unless mentioned otherwise. Purification of the reaction products was carried out by flash chromatography using EM Reagent silica gel 60 (230-400 mesh). Analytical thin layer chromatography was performed on EM Reagent 0.25 mm silica gel 60 F_{254} plates. Visualization was accomplished with UV light, iodine stain or permanganate stain followed by heating. Melting points were recorded on an open end Thomas Hoover capillary melting point apparatus and are uncorrected. Infrared (IR) spectra were recorded on an ATI Mattson Genesis Series FT-Infrared spectrophotometer. Proton nuclear magnetic resonance spectra (^{1}H-NMR) were recorded on a Varian VNMRS-500 MHz instrument and chemical shifts are reported in parts per million (ppm) downfield from TMS, using residual $CDCl_3$ (7.26 ppm) as an internal standard. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, comp = complex, app = apparent), coupling constant(s) in Hz and integration. Proton-decoupled carbon nuclear magnetic resonance spectra (^{13}C-NMR) spectra were recorded on a Varian VNMRS-500 MHz instrument and are reported in ppm using solvent as an internal standard ($CDCl_3$ at 77.0 ppm). Mass spectra were recorded on a Finnigan LCQ-DUO mass spectrometer. Optical rotations were recorded on a Perkin-Elmer 343 polarimeter at 589 nm and 293 K. The starting material 5,5-dimethyltetrahydropyrimidin-2(1H)-one (**7**) was prepared according to a published method[1].

Preparation of 1,3-difluoro-5,5-dimethyltetrahydropyrimidin-2(1H)-one (8). To a slurry of NaH (11.02 mmol, 0.441g, 60 weight % in mineral oil) in 8 mL of THF was added 5,5-dimethyltetrahydropyrimidin-2(1H)-one[1] (**7**) (5.01 mmol, 0.642 g). The reaction mixture was subsequently heated under reflux for 30 min. To the resulting thick slurry was added 2,6-difluoropyridine (11.02 mmol, 1 mL) in 3 mL of THF and heating under reflux was continued for 24 h. After completion, the reaction mixture was allowed to cool to room temperature and the volatiles were removed under reduced pressure. Ethyl acetate (100 mL) was added to the residue and the resulting solution was washed with saturated $NaHCO_3$ (100 mL) followed by brine, then dried over $NaSO_4$, filtered and concentrated under reduced pressure. The crude material was purified by silica gel column chromatography (4:1 v/v Hexanes/ EtOAc) to provide

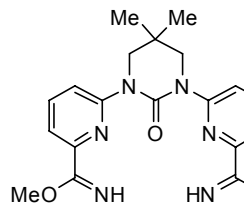


the title compound (61%) as a white crystalline solid; R_f = 0.35 (4:1 Hexanes/EtOAc); mp: 120 °C; IR (KBr) 3080, 2967, 2895, 1668, 1579, 1305, 1246, 1205 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.84-7.79 (m, 2H), 7.76-7.69 (m, 2H), 6.66-6.62 (m, 2H), 3.77 (s, 4H), 1.20 (s, 6H) ^{13}C NMR (126 MHz, $CDCl_3$) 161.91 (d_{C-F}, J = 238.6 Hz), 153.68, 153.33 (d_{C-F}, J = 13.2 Hz), 141.74 (d_{C-F}, J = 7.4 Hz), 116.45 (d_{C-F}, J = 4.6 Hz), 104.08 (d_{C-F}, J = 35.9 Hz), 56.8, 29.7, 24.5; *m/z* (ESIMS) 319.5 $[M + H]^+$.

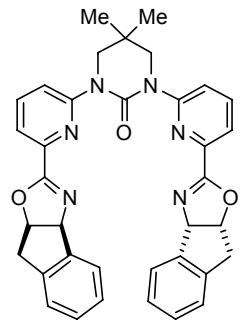
Preparation of 1,3-dicyano-5, 5-dimethyltetrahydropyrimidin-2(1H)-one (9). To a mixture of compound **8** (2.80 mmol, 0.890 g) and KCN (8.77 mmol, 0.571 g) was added 30 mL of anhydrous DMSO. The resulting mixture was heated at 130 °C for 40 h. Subsequently, the reaction mixture was allowed to cool to room temperature and water (200 mL) was added. The mixture was extracted with EtOAc (3 x 100 mL). The combined organic layers were washed with brine and dried over Na_2SO_4. The crude material was purified by silica gel column chromatography (1:1 v/v Hexanes/ EtOAc) to give the title compound (66%) as white crystalline solid with R_f = 0.40 (1:1 Hexanes/ EtOAc); mp: 208-210 °C; IR (KBr) 3131, 2976, 2235, 1672, 1582 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 8.19 (dd, J = 8.6, 0.7 Hz, 2H), 7.76 (dd, J = 8.6, 7.4 Hz, 2H), 7.45 (dd, J = 7.4, 0.8 Hz, 2H), 3.85 (s, 4H), 1.24 (s, 6H) ^{13}C NMR (125 MHz, $CDCl_3$) 155.5, 153.6, 137.5, 131.0, 124.3, 123.4, 117.0, 56.7, 29.5, 24. 4 ; *m/z* (ESIMS) 333.3 $[M+H]^+$.



Preparation of Dimethyl 6,6'-(5,5-dimethyl-2-oxodihydropyrimidine-1,3(2H,4H)-diyl) dipicolinimidate (10). Compound **9** (1.77 mmol, 0.589 g) was suspended in methanol (10 mL). Freshly prepared 1.1 M NaOMe (0.354 mmol, 0.322 mL) was added to the reaction mixture. After 36 h of stirring at room temperature, a clear solution was obtained. Acetic acid (0.372 mmol, 0.021 mL) was added and the solvent was removed under reduced pressure to give the title compound which was used directly in the next step without further purification. ^1H NMR (500 MHz, $CDCl_3$) δ 8.95 (s, 2H), 7.92 (app d, J = 8.3 Hz, 2H), 7.70-7.63 (m, 2H), 7.51 (app d, J = 7.5 Hz, 2H), 3.93 (s, 6H), 3.82 (s, 4H), 1.18 (s, 6H) ^{13}C NMR (125 MHz, $CDCl_3$) 166.6, 154.1, 153.6, 144.9, 137.8, 121.6, 116.6, 56.6, 53.6, 29.4, 24.4.



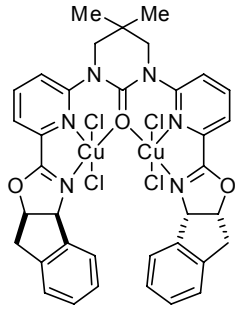
Preparation of 1,3-bis(6-((3aS,8aR)-8,8a-dihydro-3aH-indeno[1,2-d]oxazol-2-yl)-pyridin-2-yl)-5,5-dimethyltetrahydropyrimidin-2(1H)-one (11). Compound **10** (0.926 mmol, 0.367 g) was mixed with (1S, 2R)-1-amino-2,3-dihydro-1H-inden-2-ol (2.03 mmol 0.304 g) in 5 mL of anhydrous dichloromethane. The resulting mixture was heated at 70 °C in a sealed tube for 48 h. The crude material was purified by silica gel column chromatography which provided the title compound as a pale yellow solid in 84% yield. (R_f = 0.25, EtOAc). mp = 125–130 °C; $[\alpha]_D^{20}$ – 74.8 (C 1, EtOH); IR (KBr) 3069 , 2959, 1666, 1576, 1201 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.89 (app d, J = 7.89 Hz, 2H), 7.75-7.71 (m, 2H), 7.69 – 7.62 (m, 2H), 7.61-7.56



(m, 2H), 7.29 – 7.26 (comp, 6H), 5.81 (d, J = 8.0 Hz, 2H), 5.58 – 5.53 (m, 2H), 3.89-3.80 (comp, 4H), 3.52 (dd, J = 11.3, 6.8 Hz, 2H), 3.47-3.40 (m, 2H), 1.20 (s, 6H) ^{13}C NMR (125 MHz, $CDCl_3$) 163.3, 155.1, 154.2, 145.0, 141.9, 140.0, 137.3, 128.8, 127.8. 126.0, 125.5, 122.4, 120.47, 83.9, 77.5, 57.0, 40.0, 30.0, 24.9; *m/z* (ESIMS) 597.4 $[M + H]^+$, 619.5 $[M + Na]^+$.

Alternative route for 1,3-bis(6-((3aS,8aR)-8,8a-dihydro-3aH-indeno[1,2-d]oxazol-2-yl)pyridin-2-yl)-5, 5-dimethyltetrahydropyrimidin-2(1H)-one (11). Compound **9** (0.602 mmol, 0.2 g), (1S, 2R)-1-amino-2, 3-dihydro-1H-inden-2-ol (1.324 mmol, 0.198 g) and $ZnBr_2$ (1.324 mmol, 0.298 g) were mixed in 2 mL of chlorobenzene. The resulting mixture was heated under reflux for 12 h. Once cooled to room temperature, EtOAc (50 mL), water (20 mL), saturated NH_4Cl (10 mL) and 2 mL of aqueous ammonia were added. The resulting biphasic mixture was stirred rapidly for 15 min. The organic layer was separated and then washed with water (50 mL) followed by brine. It was dried over Na_2SO_4 and the volatiles were removed under reduced pressure. The crude material was purified by silica gel column chromatography (R_f = 0.25, EtOAc), to provide the title compound with 80% yield. The crude material can also be purified by recrystallization (Hexanes/EtOAc) to provide the title compound in 72% yield.

Preparation of 11•2CuCl$_2$.



Compound **11** (0.05 mmol, 0.03 g) was dissolved in 2 mL of anhydrous dichloromethane. Anhydrous $CuCl_2$ (0.106 mol, 0.014 g) was added and the resulting mixture was stirred for 3 h at room temperature. The resulting green solution was filtered and subsequently layered with hexanes. Crystals suitable for single X-ray crystallographic analysis were obtained after several days.

X-ray crystallographic analysis of 11•2CuCl$_2$.

We have modeled the disordered water molecules, to conform with assigning 4 partially-occupied water sites to the 4 peaks on the final difference-Fourier map (1.2 – 2.9 e/Å^3). Other peaks in the region are less than 1 e/Å^3 and are not significant. The result includes arbitrary positions for the partially-occupied H atoms sites, fixed to a typical water geometry in each case. Because of the degree of site disorder and the lack of nearby H bonding donor or acceptor atoms, the H bonding that the water molecules may engage in is not known with any degree of confidence, and any discussion of H bonding in this crystal structure cannot be substantiated and is left out of this paper. That the water molecules are partially-occupied and disordered in a cavity between molecules in this crystal structure is consistent with a presumed lack of importance of H bonding in this case. Extinction is not a major correction, and is likely anisotropic, since the sample was a thin plate, but the isotropic treatment in SHELXL[2] appears to help a little, and its value of 0.0029(4) is consistent with the idea that the value is not large, but statistically significant (e.g., > 3*σ). The ESD values for two of the C-C bonds in the outer region

aromatic ring systems are 0.03 Å and are twice the ESD value of C-C bonds closer to the molecular center-of-mass, where the latter appear to be more rigid and closer to the more electron dense Cu and Cl atoms. No attempt at a libration correction was made, as it was estimated to be statistically insignificant. More importantly, the two aromatic ring systems in question are adjacent to the region of disordered partially-occupied water molecules (and its symmetry equivalent region on the other end of the molecule), and that ring itself has much more spatial ambiguity (and higher ESDs are calculated in SHELXL for the coordinates of its C atoms). This situation is identical to countless other structures in the literature with partially filled voids adjacent to phenyl group substituents, and is evident from the large thermal ellipsoids in Figure 2 (manuscript).

References:

1. G. S. Skinner, R. H. Hall, and P. V. Susi, *J. Am. Chem. Soc.*, 1957, **79**, 3786.
2. G. M. Sheldrick, *SHELXS97* and *SHELXL97*. University of Göttingen, Germany, 1997.

Table 1. Crystal data and structure refinement for **11**•2$CuCl_2$.

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Identification code	DS109	
Empirical formula	C36 H35 Cl4 Cu2 N6 O4.50	
Formula weight	892.58	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.9797(8) Å	α= 90°.
	b = 15.387(1) Å	β= 90°.
	c = 29.293(3) Å	γ = 90°.
Volume	4047.5(6) $Å^3$	
Z	4	
Density (calculated)	1.465 Mg/m^3	
Absorption coefficient	1.361 mm^{-1}	
F(000)	1820	
Crystal size	0.41 x 0.21 x 0.01 mm^3	
Theta range for data collection	1.92 to 25.34°.	
Index ranges	-10<=h<=10, -18<=k<=18, -35<=l<=35	
Reflections collected	31080	
Independent reflections	7406 [R(int) = 0.0891]	
Completeness to theta = 25.34°	99.5 %	
Absorption correction	Numerical	
Max. and min. transmission	0.986 and 0.605	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7406 / 793 / 477	
Goodness-of-fit on F^2	1.000	
Final R indices [I>2sigma(I)]	R1 = 0.0800, wR2 = 0.1722	
R indices (all data)	R1 = 0.1014, wR2 = 0.1830	
Absolute structure parameter	0.02(3)	
Extinction coefficient	0.0029(4)	
Largest diff. peak and hole	1.096 and -1.132 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For **11**•2$CuCl_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2069(1)	7734(1)	8007(1)	20(1)
Cu(2)	2007(1)	7864(1)	6544(1)	22(1)
Cl(1)	3027(3)	6504(1)	7711(1)	33(1)
Cl(2)	4014(3)	8609(2)	8362(1)	49(1)
Cl(3)	63(3)	6986(2)	6579(1)	39(1)
Cl(4)	827(3)	9126(2)	6407(1)	25(1)
O(1)	2205(7)	8336(3)	7412(2)	19(1)
O(2)	-957(8)	7130(5)	8967(2)	38(2)
O(3)	5647(8)	6558(4)	6104(2)	32(2)
N(1)	1116(8)	9653(4)	7585(2)	17(1)
N(2)	3306(7)	9560(4)	7146(2)	17(1)
N(3)	349(8)	8593(5)	8108(2)	19(1)
N(4)	1049(9)	7136(5)	8518(3)	30(2)
N(5)	4084(8)	8354(5)	6698(2)	19(1)
N(6)	3302(8)	6952(5)	6268(3)	24(2)
C(1)	2198(9)	9143(5)	7385(3)	17(2)
C(2)	1017(10)	10591(5)	7492(3)	21(2)
C(3)	2588(9)	10986(5)	7443(3)	21(2)
C(4)	3331(10)	10499(6)	7061(3)	25(2)
C(5)	3480(10)	10909(6)	7887(3)	26(2)
C(6)	2444(11)	11944(6)	7306(4)	33(2)
C(7)	40(9)	9297(5)	7871(3)	19(2)
C(8)	-1356(10)	9706(6)	7903(3)	25(2)
C(9)	-2383(10)	9381(6)	8216(3)	26(2)
C(10)	-2020(11)	8689(6)	8481(3)	27(2)
C(11)	-658(10)	8304(6)	8420(3)	24(2)
C(12)	-167(11)	7505(6)	8637(3)	28(2)
C(13)	-168(16)	6305(8)	9072(4)	49(2)
C(14)	1247(14)	6339(7)	8798(4)	41(2)
C(15)	2467(17)	6420(9)	9150(5)	61(2)
C(16)	1860(20)	6372(10)	9578(5)	74(3)

C(17)	241(19)	6256(11)	9572(5)	73(3)
C(18)	3928(19)	6589(11)	9074(6)	76(3)
C(19)	4940(20)	6658(13)	9443(7)	97(3)
C(20)	4310(20)	6620(14)	9857(7)	104(4)
C(21)	2840(20)	6504(12)	9965(6)	94(3)
C(22)	4435(9)	9048(5)	6947(3)	17(2)
C(23)	5945(10)	9303(6)	7024(4)	28(2)
C(24)	7064(12)	8827(6)	6841(3)	29(2)
C(25)	6716(10)	8101(6)	6594(3)	26(2)
C(26)	5224(9)	7872(6)	6527(3)	22(2)
C(27)	4677(10)	7107(6)	6296(3)	26(2)
C(28)	4721(12)	5809(7)	5957(4)	37(2)
C(29)	3137(13)	6180(7)	5988(4)	37(2)
C(30)	2755(17)	6390(9)	5510(4)	56(2)
C(31)	3880(17)	6060(9)	5213(5)	59(2)
C(32)	5033(16)	5585(8)	5467(4)	52(2)
C(33)	1600(20)	6831(11)	5351(6)	81(3)
C(34)	1630(20)	7031(14)	4887(6)	101(4)
C(35)	2790(20)	6818(13)	4585(7)	103(4)
C(36)	3880(20)	6245(12)	4744(6)	85(3)
O(4WA)	8410(20)	4027(12)	5787(6)	55(4)
O(4WB)	8870(20)	4984(12)	5940(6)	61(5)
O(5WA)	9010(40)	5380(20)	5204(12)	57(9)
O(5WB)	8800(60)	5660(30)	4532(18)	98(16)

Table 3. Bond lengths [Å] and angles [°] for **11**•2$CuCl_2$.

Cu(1)-O(1)	1.978(6)	C(3)-C(5)	1.530(13)
Cu(1)-N(4)	1.981(8)	C(3)-C(6)	1.534(12)
Cu(1)-N(3)	2.055(7)	C(4)-H(4A)	0.9900
Cu(1)-Cl(1)	2.252(2)	C(4)-H(4B)	0.9900
Cu(1)-Cl(2)	2.438(3)	C(5)-H(5A)	0.9800
Cu(2)-N(6)	1.992(7)	C(5)-H(5B)	0.9800
Cu(2)-N(5)	2.062(8)	C(5)-H(5C)	0.9800
Cu(2)-Cl(3)	2.210(3)	C(6)-H(6A)	0.9800
Cu(2)-Cl(4)	2.250(2)	C(6)-H(6B)	0.9800
Cu(2)-O(1)	2.651(6)	C(6)-H(6C)	0.9800
Cu(1)-Cu(2)	4.291(2)	C(7)-C(8)	1.406(13)
O(1)-C(1)	1.244(10)	C(8)-C(9)	1.392(13)
O(2)-C(12)	1.330(12)	C(8)-H(8)	0.9500
O(2)-C(13)	1.485(14)	C(9)-C(10)	1.359(14)
O(3)-C(27)	1.338(11)	C(9)-H(9)	0.9500
O(3)-C(28)	1.485(12)	C(10)-C(11)	1.371(13)
N(1)-C(1)	1.379(11)	C(10)-H(10)	0.9500
N(1)-C(7)	1.391(11)	C(11)-C(12)	1.454(13)
N(1)-C(2)	1.472(10)	C(13)-C(14)	1.505(17)
N(2)-C(1)	1.376(11)	C(13)-C(17)	1.512(19)
N(2)-C(22)	1.411(11)	C(13)-H(13)	1.0000
N(2)-C(4)	1.467(11)	C(14)-C(15)	1.508(18)
N(3)-C(7)	1.315(11)	C(14)-H(14)	1.0000
N(3)-C(11)	1.359(12)	C(15)-C(18)	1.36(2)
N(4)-C(12)	1.280(13)	C(15)-C(16)	1.37(2)
N(4)-C(14)	1.487(13)	C(16)-C(21)	1.45(2)
N(5)-C(22)	1.330(11)	C(16)-C(17)	1.47(2)
N(5)-C(26)	1.361(11)	C(17)-H(17A)	0.9900
N(6)-C(27)	1.261(12)	C(17)-H(17B)	0.9900
N(6)-C(29)	1.451(12)	C(18)-C(19)	1.42(2)
C(2)-C(3)	1.543(12)	C(18)-H(18)	0.9500
C(2)-H(2A)	0.9900	C(19)-C(20)	1.34(3)
C(2)-H(2B)	0.9900	C(19)-H(19)	0.9500
C(3)-C(4)	1.504(13)	C(20)-C(21)	1.37(3)

C(20)-H(20)	0.9500	C(31)-C(32)	1.470(19)
C(21)-H(21)	0.9500	C(32)-H(32A)	0.9900
C(22)-C(23)	1.429(12)	C(32)-H(32B)	0.9900
C(23)-C(24)	1.353(14)	C(33)-C(34)	1.39(2)
C(23)-H(23)	0.9500	C(33)-H(33)	0.9500
C(24)-C(25)	1.367(13)	C(34)-C(35)	1.41(3)
C(24)-H(24)	0.9500	C(34)-H(34)	0.9500
C(25)-C(26)	1.399(12)	C(35)-C(36)	1.40(2)
C(25)-H(25)	0.9500	C(35)-H(35)	0.9500
C(26)-C(27)	1.443(13)	C(36)-H(36)	0.9500
C(28)-C(32)	1.503(16)	O(4WA)-H(4WA)	0.84
C(28)-C(29)	1.535(15)	O(4WA)-H(4WB)	0.85
C(28)-H(28)	1.0000	O(4WB)-H(4WC)	0.84
C(29)-C(30)	1.479(17)	O(4WB)-H(4WD)	0.85
C(29)-H(29)	1.0000	O(5WA)-H(5WA)	0.90
C(30)-C(33)	1.325(19)	O(5WA)-H(5WB)	0.93
C(30)-C(31)	1.425(19)	O(5WB)-H(5WC)	0.99
C(31)-C(36)	1.40(2)	O(5WB)-H(5WD)	0.89

O(1)-Cu(1)-N(4)	155.8(3)	N(5)-Cu(2)-O(1)	68.2(2)
O(1)-Cu(1)-N(3)	82.6(3)	Cl(3)-Cu(2)-O(1)	100.12(16)
N(4)-Cu(1)-N(3)	80.9(3)	Cl(4)-Cu(2)-O(1)	88.07(14)
O(1)-Cu(1)-Cl(1)	91.77(17)	O(1)-Cu(1)-Cu(2)	25.68(16)
N(4)-Cu(1)-Cl(1)	94.4(2)	N(4)-Cu(1)-Cu(2)	140.4(2)
N(3)-Cu(1)-Cl(1)	152.1(2)	N(3)-Cu(1)-Cu(2)	96.0(2)
O(1)-Cu(1)-Cl(2)	94.16(19)	Cl(1)-Cu(1)-Cu(2)	70.11(7)
N(4)-Cu(1)-Cl(2)	105.4(3)	Cl(2)-Cu(1)-Cu(2)	114.16(9)
N(3)-Cu(1)-Cl(2)	97.0(2)	N(6)-Cu(2)-Cu(1)	111.4(2)
Cl(1)-Cu(1)-Cl(2)	110.76(11)	N(5)-Cu(2)-Cu(1)	77.6(2)
N(6)-Cu(2)-N(5)	79.6(3)	Cl(3)-Cu(2)-Cu(1)	86.28(9)
N(6)-Cu(2)-Cl(3)	92.9(2)	Cl(4)-Cu(2)-Cu(1)	103.00(7)
N(5)-Cu(2)-Cl(3)	158.2(2)	O(1)-Cu(2)-Cu(1)	18.86(12)
N(6)-Cu(2)-Cl(4)	144.1(2)	C(1)-O(1)-Cu(1)	121.5(5)
N(5)-Cu(2)-Cl(4)	98.6(2)	C(1)-O(1)-Cu(1)	121.5(5)
Cl(3)-Cu(2)-Cl(4)	99.41(10)	C(1)-O(1)-Cu(2)	102.3(5)
N(6)-Cu(2)-O(1)	122.9(3)	Cu(1)-O(1)-Cu(2)	135.5(2)

C(12)-O(2)-C(13)	105.5(8)	N(2)-C(4)-H(4A)	109.5
C(27)-O(3)-C(28)	104.3(7)	C(3)-C(4)-H(4A)	109.5
C(1)-N(1)-C(7)	121.4(7)	N(2)-C(4)-H(4B)	109.5
C(1)-N(1)-C(2)	121.5(7)	C(3)-C(4)-H(4B)	109.5
C(7)-N(1)-C(2)	117.1(7)	H(4A)-C(4)-H(4B)	108.1
C(1)-N(2)-C(22)	118.1(7)	C(3)-C(5)-H(5A)	109.5
C(1)-N(2)-C(4)	123.9(7)	C(3)-C(5)-H(5B)	109.5
C(22)-N(2)-C(4)	117.9(7)	H(5A)-C(5)-H(5B)	109.5
C(7)-N(3)-C(11)	118.9(8)	C(3)-C(5)-H(5C)	109.5
C(7)-N(3)-Cu(1)	127.7(6)	H(5A)-C(5)-H(5C)	109.5
C(11)-N(3)-Cu(1)	112.7(6)	H(5B)-C(5)-H(5C)	109.5
C(12)-N(4)-C(14)	108.5(8)	C(3)-C(6)-H(6A)	109.5
C(12)-N(4)-Cu(1)	113.3(7)	C(3)-C(6)-H(6B)	109.5
C(14)-N(4)-Cu(1)	138.1(7)	H(6A)-C(6)-H(6B)	109.5
C(22)-N(5)-C(26)	117.5(8)	C(3)-C(6)-H(6C)	109.5
C(22)-N(5)-Cu(2)	128.9(6)	H(6A)-C(6)-H(6C)	109.5
C(26)-N(5)-Cu(2)	113.5(6)	H(6B)-C(6)-H(6C)	109.5
C(27)-N(6)-C(29)	106.9(8)	N(3)-C(7)-N(1)	119.7(8)
C(27)-N(6)-Cu(2)	114.3(7)	N(3)-C(7)-C(8)	121.4(8)
C(29)-N(6)-Cu(2)	138.2(7)	N(1)-C(7)-C(8)	118.9(8)
O(1)-C(1)-N(2)	119.6(7)	C(9)-C(8)-C(7)	118.3(9)
O(1)-C(1)-N(1)	123.0(8)	C(9)-C(8)-H(8)	120.9
N(2)-C(1)-N(1)	117.4(7)	C(7)-C(8)-H(8)	120.9
N(1)-C(2)-C(3)	110.3(7)	C(10)-C(9)-C(8)	119.9(9)
N(1)-C(2)-H(2A)	109.6	C(10)-C(9)-H(9)	120.0
C(3)-C(2)-H(2A)	109.6	C(8)-C(9)-H(9)	120.0
N(1)-C(2)-H(2B)	109.6	C(9)-C(10)-C(11)	118.5(9)
C(3)-C(2)-H(2B)	109.6	C(9)-C(10)-H(10)	120.8
H(2A)-C(2)-H(2B)	108.1	C(11)-C(10)-H(10)	120.8
C(4)-C(3)-C(5)	111.2(7)	N(3)-C(11)-C(10)	122.8(9)
C(4)-C(3)-C(6)	108.7(8)	N(3)-C(11)-C(12)	111.7(8)
C(5)-C(3)-C(6)	109.9(8)	C(10)-C(11)-C(12)	125.3(9)
C(4)-C(3)-C(2)	106.2(7)	N(4)-C(12)-O(2)	117.5(9)
C(5)-C(3)-C(2)	111.7(8)	N(4)-C(12)-C(11)	120.9(9)
C(6)-C(3)-C(2)	109.0(7)	O(2)-C(12)-C(11)	121.6(9)
N(2)-C(4)-C(3)	110.9(7)	O(2)-C(13)-C(14)	105.2(9)

O(2)-C(13)-C(17)	111.1(11)	N(5)-C(22)-C(23)	122.1(8)
C(14)-C(13)-C(17)	108.2(12)	N(2)-C(22)-C(23)	117.6(8)
O(2)-C(13)-H(13)	110.7	C(24)-C(23)-C(22)	119.6(9)
C(14)-C(13)-H(13)	110.7	C(24)-C(23)-H(23)	120.2
C(17)-C(13)-H(13)	110.7	C(22)-C(23)-H(23)	120.2
N(4)-C(14)-C(13)	102.8(9)	C(23)-C(24)-C(25)	118.8(9)
N(4)-C(14)-C(15)	113.3(10)	C(23)-C(24)-H(24)	120.6
C(13)-C(14)-C(15)	104.6(10)	C(25)-C(24)-H(24)	120.6
N(4)-C(14)-H(14)	111.8	C(24)-C(25)-C(26)	120.0(9)
C(13)-C(14)-H(14)	111.8	C(24)-C(25)-H(25)	120.0
C(15)-C(14)-H(14)	111.8	C(26)-C(25)-H(25)	120.0
C(18)-C(15)-C(16)	123.0(16)	N(5)-C(26)-C(25)	122.0(8)
C(18)-C(15)-C(14)	127.4(14)	N(5)-C(26)-C(27)	111.2(8)
C(16)-C(15)-C(14)	109.4(14)	C(25)-C(26)-C(27)	126.7(8)
C(15)-C(16)-C(21)	117.8(18)	N(6)-C(27)-O(3)	119.4(9)
C(15)-C(16)-C(17)	113.0(14)	N(6)-C(27)-C(26)	121.2(9)
C(21)-C(16)-C(17)	129.0(17)	O(3)-C(27)-C(26)	119.3(8)
C(16)-C(17)-C(13)	104.3(12)	O(3)-C(28)-C(32)	110.5(10)
C(16)-C(17)-H(17A)	110.9	O(3)-C(28)-C(29)	102.3(8)
C(13)-C(17)-H(17A)	110.9	C(32)-C(28)-C(29)	108.4(10)
C(16)-C(17)-H(17B)	110.9	O(3)-C(28)-H(28)	111.8
C(13)-C(17)-H(17B)	110.9	C(32)-C(28)-H(28)	111.8
H(17A)-C(17)-H(17B)	108.9	C(29)-C(28)-H(28)	111.8
C(15)-C(18)-C(19)	120.8(18)	N(6)-C(29)-C(30)	112.4(9)
C(15)-C(18)-H(18)	119.6	N(6)-C(29)-C(28)	104.1(8)
C(19)-C(18)-H(18)	119.6	C(30)-C(29)-C(28)	103.9(10)
C(20)-C(19)-C(18)	114(2)	N(6)-C(29)-H(29)	112.0
C(20)-C(19)-H(19)	122.8	C(30)-C(29)-H(29)	112.0
C(18)-C(19)-H(19)	122.8	C(28)-C(29)-H(29)	112.0
C(19)-C(20)-C(21)	129(2)	C(33)-C(30)-C(31)	121.6(14)
C(19)-C(20)-H(20)	115.7	C(33)-C(30)-C(29)	128.8(14)
C(21)-C(20)-H(20)	115.7	C(31)-C(30)-C(29)	109.6(12)
C(20)-C(21)-C(16)	115.1(19)	C(36)-C(31)-C(30)	121.7(14)
C(20)-C(21)-H(21)	122.4	C(36)-C(31)-C(32)	126.5(14)
C(16)-C(21)-H(21)	122.4	C(30)-C(31)-C(32)	111.6(12)
N(5)-C(22)-N(2)	120.3(7)	C(31)-C(32)-C(28)	103.7(11)

C(31)-C(32)-H(32A)	111.0	C(36)-C(35)-C(34)	117.2(18)
C(28)-C(32)-H(32A)	111.0	C(36)-C(35)-H(35)	121.4
C(31)-C(32)-H(32B)	111.0	C(34)-C(35)-H(35)	121.4
C(28)-C(32)-H(32B)	111.0	C(35)-C(36)-C(31)	116.9(17)
H(32A)-C(32)-H(32B)	109.0	C(35)-C(36)-H(36)	121.5
C(30)-C(33)-C(34)	116.0(17)	C(31)-C(36)-H(36)	121.5
C(30)-C(33)-H(33)	122.0	H(4WA)-O(4WA)-H(4WB)	116
C(34)-C(33)-H(33)	122.0	H(4WC)-O(4WB)-H(4WD)	116
C(33)-C(34)-C(35)	125.3(19)	H(5WA)-O(5WA)-H(5WB)	104
C(33)-C(34)-H(34)	117.4	H(5WC)-O(5WB)-H(5WD)	100
C(35)-C(34)-H(34)	117.4		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **11**•2$CuCl_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	14(1)	12(1)	36(1)	2(1)	1(1)	2(1)
Cu(2)	13(1)	18(1)	35(1)	1(1)	2(1)	0(1)
Cl(1)	26(1)	14(1)	60(2)	0(1)	2(1)	6(1)
Cl(2)	28(1)	29(1)	90(2)	18(1)	-27(2)	-13(1)
Cl(3)	16(1)	25(1)	76(2)	10(1)	2(1)	-2(1)
Cl(4)	19(1)	21(1)	35(1)	1(1)	-4(1)	2(1)
O(1)	20(3)	6(2)	31(3)	-4(2)	9(2)	1(2)
O(2)	45(3)	28(3)	42(3)	4(3)	9(3)	-9(3)
O(3)	28(3)	28(3)	39(3)	-6(3)	5(3)	5(3)
N(1)	14(3)	16(3)	22(3)	-2(2)	1(2)	2(2)
N(2)	12(3)	15(3)	24(3)	3(2)	3(2)	1(2)
N(3)	15(3)	20(3)	22(3)	-6(2)	3(2)	2(2)
N(4)	32(3)	26(3)	32(3)	5(3)	2(3)	-1(3)
N(5)	13(3)	13(3)	30(3)	3(2)	7(3)	6(2)
N(6)	22(3)	16(3)	33(3)	2(3)	-1(3)	3(2)
C(1)	13(3)	15(3)	23(3)	0(3)	2(3)	3(3)
C(2)	19(3)	12(3)	32(4)	1(3)	-3(3)	5(3)
C(3)	17(4)	13(3)	32(4)	3(3)	-1(3)	1(3)
C(4)	25(4)	19(3)	29(4)	2(3)	2(3)	-4(3)
C(5)	25(4)	20(4)	34(4)	-4(4)	-7(3)	2(4)
C(6)	33(5)	20(4)	47(5)	5(4)	0(4)	0(3)
C(7)	12(3)	15(3)	29(4)	-5(3)	1(3)	-1(3)
C(8)	14(3)	25(4)	36(4)	-7(3)	-3(3)	-8(3)
C(9)	15(4)	20(4)	43(4)	-13(3)	6(3)	-4(3)
C(10)	19(3)	25(3)	38(4)	-7(3)	7(4)	-11(3)
C(11)	19(3)	25(3)	30(4)	-5(3)	2(3)	-3(3)
C(12)	28(4)	28(4)	28(4)	-1(3)	6(3)	-5(3)
C(13)	62(4)	37(4)	49(4)	9(4)	13(4)	-3(4)
C(14)	47(4)	31(4)	45(4)	8(3)	5(3)	-3(3)
C(15)	68(4)	57(5)	57(4)	14(4)	-12(4)	10(4)
C(16)	95(5)	68(5)	59(4)	15(4)	-10(4)	4(5)

C(17)	88(5)	72(5)	58(5)	16(5)	7(4)	9(5)
C(18)	72(5)	78(6)	80(5)	14(5)	-21(4)	7(5)
C(19)	88(5)	107(6)	95(6)	8(6)	-27(5)	8(6)
C(20)	107(6)	111(6)	93(5)	8(6)	-23(5)	8(6)
C(21)	110(6)	98(6)	74(5)	12(5)	-19(5)	14(6)
C(22)	12(3)	9(3)	29(4)	5(3)	5(3)	-2(3)
C(23)	20(3)	29(4)	37(4)	1(3)	1(3)	-6(3)
C(24)	17(3)	29(4)	42(4)	2(3)	-4(4)	-6(3)
C(25)	15(3)	26(4)	36(4)	5(3)	4(3)	4(3)
C(26)	18(3)	16(3)	30(4)	4(3)	8(3)	1(3)
C(27)	26(3)	24(3)	27(4)	-3(3)	5(3)	0(3)
C(28)	38(4)	30(4)	43(4)	-15(3)	0(3)	1(3)
C(29)	38(4)	30(4)	44(4)	-10(3)	-2(3)	2(3)
C(30)	61(5)	56(5)	50(4)	-9(4)	-12(4)	6(4)
C(31)	68(5)	60(5)	51(4)	-16(4)	-4(4)	2(4)
C(32)	53(5)	52(5)	52(4)	-23(4)	0(4)	1(4)
C(33)	82(6)	92(6)	69(5)	-10(5)	-24(5)	28(5)
C(34)	104(6)	118(6)	80(5)	1(5)	-16(5)	27(5)
C(35)	110(6)	115(6)	83(5)	3(5)	-9(5)	21(6)
C(36)	94(6)	93(6)	68(5)	-6(5)	-2(5)	9(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **11**•2$CuCl_2$.

	x	y	z	U(eq)
H(2A)	481	10883	7745	25
H(2B)	447	10688	7207	25
H(4A)	2811	10626	6770	30
H(4B)	4375	10698	7031	30
H(5A)	2964	11224	8131	39
H(5B)	4473	11159	7842	39
H(5C)	3574	10296	7971	39
H(6A)	1945	12266	7551	50
H(6B)	1858	11989	7025	50
H(6C)	3437	12189	7255	50
H(8)	-1593	10191	7716	30
H(9)	-3336	9643	8243	31
H(10)	-2695	8476	8705	32
H(13)	-786	5793	8981	59
H(14)	1375	5810	8604	49
H(17A)	-260	6721	9748	87
H(17B)	-40	5685	9703	87
H(18)	4277	6662	8770	92
H(19)	5985	6726	9400	116
H(20)	4969	6682	10109	125
H(21)	2494	6510	10271	113
H(23)	6162	9803	7202	34
H(24)	8073	8995	6883	35
H(25)	7487	7752	6469	31
H(28)	4856	5296	6163	44
H(29)	2423	5755	6125	45
H(32A)	6042	5778	5376	63
H(32B)	4948	4951	5415	63
H(33)	794	7000	5542	97
H(34)	803	7337	4765	121

H(35)	2837	7055	4286	123
H(36)	4593	5992	4544	102
H(4WA)	7647	3795	5672	82
H(4WB)	8263	4385	6003	82
H(4WC)	8525	4971	5672	91
H(4WD)	8468	5347	6122	91
H(5WA)	9442	5335	4929	86
H(5WB)	8901	5978	5245	86
H(5WC)	8380	5668	4845	148
H(5WD)	8035	5869	4377	148

Table 6. Torsion angles [°] for **11**•2$CuCl_2$.

N(4)-Cu(1)-O(1)-C(1)	95.2(9)	C(22)-N(2)-C(1)-O(1)	-1.3(12)
N(3)-Cu(1)-O(1)-C(1)	47.6(7)	C(4)-N(2)-C(1)-O(1)	174.6(8)
Cl(1)-Cu(1)-O(1)-C(1)	-159.9(7)	C(22)-N(2)-C(1)-N(1)	178.8(7)
Cl(2)-Cu(1)-O(1)-C(1)	-48.9(7)	C(4)-N(2)-C(1)-N(1)	-5.3(12)
O(1)-Cu(1)-N(3)-C(7)	-14.6(7)	C(7)-N(1)-C(1)-O(1)	6.7(13)
N(4)-Cu(1)-N(3)-C(7)	-176.7(8)	C(2)-N(1)-C(1)-O(1)	-171.0(8)
Cl(1)-Cu(1)-N(3)-C(7)	-94.4(8)	C(7)-N(1)-C(1)-N(2)	-173.5(7)
Cl(2)-Cu(1)-N(3)-C(7)	78.7(7)	C(2)-N(1)-C(1)-N(2)	8.9(11)
O(1)-Cu(1)-N(3)-C(11)	156.0(6)	C(1)-N(1)-C(2)-C(3)	-36.7(11)
N(4)-Cu(1)-N(3)-C(11)	-6.2(6)	C(7)-N(1)-C(2)-C(3)	145.5(8)
Cl(1)-Cu(1)-N(3)-C(11)	76.2(8)	N(1)-C(2)-C(3)-C(4)	58.3(9)
Cl(2)-Cu(1)-N(3)-C(11)	-110.7(6)	N(1)-C(2)-C(3)-C(5)	-63.2(10)
O(1)-Cu(1)-N(4)-C(12)	-43.3(11)	N(1)-C(2)-C(3)-C(6)	175.2(8)
N(3)-Cu(1)-N(4)-C(12)	4.6(7)	C(1)-N(2)-C(4)-C(3)	30.7(11)
Cl(1)-Cu(1)-N(4)-C(12)	-147.6(7)	C(22)-N(2)-C(4)-C(3)	-153.4(8)
Cl(2)-Cu(1)-N(4)-C(12)	99.4(7)	C(5)-C(3)-C(4)-N(2)	66.9(9)
O(1)-Cu(1)-N(4)-C(14)	133.0(10)	C(6)-C(3)-C(4)-N(2)	-171.9(7)
N(3)-Cu(1)-N(4)-C(14)	-179.1(11)	C(2)-C(3)-C(4)-N(2)	-54.8(9)
Cl(1)-Cu(1)-N(4)-C(14)	28.6(10)	C(11)-N(3)-C(7)-N(1)	173.4(8)
Cl(2)-Cu(1)-N(4)-C(14)	-84.4(10)	Cu(1)-N(3)-C(7)-N(1)	-16.5(12)
N(6)-Cu(2)-N(5)-C(22)	-175.0(8)	C(11)-N(3)-C(7)-C(8)	-5.9(13)
Cl(3)-Cu(2)-N(5)-C(22)	-103.8(8)	Cu(1)-N(3)-C(7)-C(8)	164.1(6)
Cl(4)-Cu(2)-N(5)-C(22)	41.3(7)	C(1)-N(1)-C(7)-N(3)	28.7(12)
N(6)-Cu(2)-N(5)-C(26)	3.1(6)	C(2)-N(1)-C(7)-N(3)	-153.5(8)
Cl(3)-Cu(2)-N(5)-C(26)	74.3(9)	C(1)-N(1)-C(7)-C(8)	-151.9(8)
Cl(4)-Cu(2)-N(5)-C(26)	-140.5(6)	C(2)-N(1)-C(7)-C(8)	25.9(11)
N(5)-Cu(2)-N(6)-C(27)	-2.8(7)	N(3)-C(7)-C(8)-C(9)	4.1(13)
Cl(3)-Cu(2)-N(6)-C(27)	-162.2(7)	N(1)-C(7)-C(8)-C(9)	-175.3(8)
Cl(4)-Cu(2)-N(6)-C(27)	87.5(8)	C(7)-C(8)-C(9)-C(10)	0.3(13)
N(5)-Cu(2)-N(6)-C(29)	-173.4(10)	C(8)-C(9)-C(10)-C(11)	-2.6(13)
Cl(3)-Cu(2)-N(6)-C(29)	27.3(10)	C(7)-N(3)-C(11)-C(10)	3.5(13)
Cl(4)-Cu(2)-N(6)-C(29)	-83.1(10)	Cu(1)-N(3)-C(11)-C(10)	-167.9(7)
Cu(1)-O(1)-C(1)-N(2)	127.8(7)	C(7)-N(3)-C(11)-C(12)	177.8(8)
Cu(1)-O(1)-C(1)-N(1)	-52.4(11)	Cu(1)-N(3)-C(11)-C(12)	6.4(9)

C(9)-C(10)-C(11)-N(3)	0.8(14)	C(15)-C(18)-C(19)-C(20)	-6(3)
C(9)-C(10)-C(11)-C(12)	-172.7(9)	C(18)-C(19)-C(20)-C(21)	2(3)
C(14)-N(4)-C(12)-O(2)	0.2(13)	C(19)-C(20)-C(21)-C(16)	3(3)
Cu(1)-N(4)-C(12)-O(2)	177.6(7)	C(15)-C(16)-C(21)-C(20)	-3(3)
C(14)-N(4)-C(12)-C(11)	-179.9(9)	C(17)-C(16)-C(21)-C(20)	-178.0(19)
Cu(1)-N(4)-C(12)-C(11)	-2.5(12)	C(26)-N(5)-C(22)-N(2)	-178.1(8)
C(13)-O(2)-C(12)-N(4)	-4.7(13)	Cu(2)-N(5)-C(22)-N(2)	0.0(12)
C(13)-O(2)-C(12)-C(11)	175.4(9)	C(26)-N(5)-C(22)-C(23)	1.7(13)
N(3)-C(11)-C(12)-N(4)	-2.8(13)	Cu(2)-N(5)-C(22)-C(23)	179.8(7)
C(10)-C(11)-C(12)-N(4)	171.4(10)	C(1)-N(2)-C(22)-N(5)	48.5(11)
N(3)-C(11)-C(12)-O(2)	177.1(9)	C(4)-N(2)-C(22)-N(5)	-127.6(9)
C(10)-C(11)-C(12)-O(2)	-8.8(15)	C(1)-N(2)-C(22)-C(23)	-131.3(8)
C(12)-O(2)-C(13)-C(14)	6.9(12)	C(4)-N(2)-C(22)-C(23)	52.6(11)
C(12)-O(2)-C(13)-C(17)	123.8(11)	N(5)-C(22)-C(23)-C(24)	-0.2(14)
C(12)-N(4)-C(14)-C(13)	4.2(12)	N(2)-C(22)-C(23)-C(24)	179.6(8)
Cu(1)-N(4)-C(14)-C(13)	-172.2(8)	C(22)-C(23)-C(24)-C(25)	-1.4(14)
C(12)-N(4)-C(14)-C(15)	-108.1(12)	C(23)-C(24)-C(25)-C(26)	1.4(14)
Cu(1)-N(4)-C(14)-C(15)	75.5(14)	C(22)-N(5)-C(26)-C(25)	-1.7(13)
O(2)-C(13)-C(14)-N(4)	-6.6(12)	Cu(2)-N(5)-C(26)-C(25)	179.9(7)
C(17)-C(13)-C(14)-N(4)	-125.4(11)	C(22)-N(5)-C(26)-C(27)	175.5(8)
O(2)-C(13)-C(14)-C(15)	112.0(11)	Cu(2)-N(5)-C(26)-C(27)	-2.9(9)
C(17)-C(13)-C(14)-C(15)	-6.8(14)	C(24)-C(25)-C(26)-N(5)	0.2(14)
N(4)-C(14)-C(15)-C(18)	-59(2)	C(24)-C(25)-C(26)-C(27)	-176.6(9)
C(13)-C(14)-C(15)-C(18)	-170.5(16)	C(29)-N(6)-C(27)-O(3)	-3.5(12)
N(4)-C(14)-C(15)-C(16)	115.4(13)	Cu(2)-N(6)-C(27)-O(3)	-176.9(7)
C(13)-C(14)-C(15)-C(16)	4.2(15)	C(29)-N(6)-C(27)-C(26)	175.6(9)
C(18)-C(15)-C(16)-C(21)	0(2)	Cu(2)-N(6)-C(27)-C(26)	2.2(12)
C(14)-C(15)-C(16)-C(21)	-175.3(13)	C(28)-O(3)-C(27)-N(6)	-8.0(12)
C(18)-C(15)-C(16)-C(17)	175.1(16)	C(28)-O(3)-C(27)-C(26)	172.9(8)
C(14)-C(15)-C(16)-C(17)	0.2(19)	N(5)-C(26)-C(27)-N(6)	0.6(13)
C(15)-C(16)-C(17)-C(13)	-4.4(19)	C(25)-C(26)-C(27)-N(6)	177.6(10)
C(21)-C(16)-C(17)-C(13)	170.5(16)	N(5)-C(26)-C(27)-O(3)	179.7(8)
O(2)-C(13)-C(17)-C(16)	-108.2(13)	C(25)-C(26)-C(27)-O(3)	-3.3(15)
C(14)-C(13)-C(17)-C(16)	6.8(16)	C(27)-O(3)-C(28)-C(32)	129.9(10)
C(16)-C(15)-C(18)-C(19)	5(3)	C(27)-O(3)-C(28)-C(29)	14.7(10)
C(14)-C(15)-C(18)-C(19)	179.1(15)	C(27)-N(6)-C(29)-C(30)	-98.9(11)

Cu(2)-N(6)-C(29)-C(30)	72.1(14)
C(27)-N(6)-C(29)-C(28)	12.9(11)
Cu(2)-N(6)-C(29)-C(28)	-176.1(7)
O(3)-C(28)-C(29)-N(6)	-16.7(11)
C(32)-C(28)-C(29)-N(6)	-133.4(10)
O(3)-C(28)-C(29)-C(30)	101.2(10)
C(32)-C(28)-C(29)-C(30)	-15.5(12)
N(6)-C(29)-C(30)-C(33)	-58(2)
C(28)-C(29)-C(30)-C(33)	-170.1(15)
N(6)-C(29)-C(30)-C(31)	120.0(12)
C(28)-C(29)-C(30)-C(31)	8.1(14)
C(33)-C(30)-C(31)-C(36)	5(2)
C(29)-C(30)-C(31)-C(36)	-173.2(14)
C(33)-C(30)-C(31)-C(32)	-179.2(14)
C(29)-C(30)-C(31)-C(32)	2.4(17)
C(36)-C(31)-C(32)-C(28)	163.3(15)
C(30)-C(31)-C(32)-C(28)	-12.0(16)
O(3)-C(28)-C(32)-C(31)	-94.5(12)
C(29)-C(28)-C(32)-C(31)	16.8(13)
C(31)-C(30)-C(33)-C(34)	-7(2)
C(29)-C(30)-C(33)-C(34)	171.4(15)
C(30)-C(33)-C(34)-C(35)	-1(3)
C(33)-C(34)-C(35)-C(36)	11(3)
C(34)-C(35)-C(36)-C(31)	-12(3)
C(30)-C(31)-C(36)-C(35)	4(3)
C(32)-C(31)-C(36)-C(35)	-170.4(16)