CHAPTER-V

CRYSTAL AND MOLECULAR STRUCTURE OF DICHLOROBIS(4-CYANOPYRIDINE)COPPER(II)

$CuC_{12}H_8N_4Cl_2$

5.1 INTRODUCTION :

Nitriles are organic compounds that contain a triple bond between a carbon and nitrogen atom. The functional group in nitriles is the cyano group, C ≡ N. The carbon atom of the cyano group is bonded to nitrogen and to one other atom.

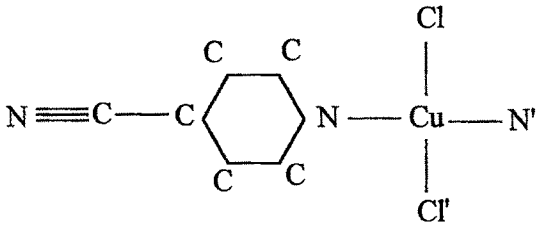
The carbon and the nitrogen atom in the cyano group are sp-hybridized and the carbon nitrogen triple bond is formed in the same way as that of C ≡ C triple bond.

The cyano triple bond consists of a σ bond , formed by the overlap of one sp hybrid orbital from carbon and one from nitrogen, and two π bonds, formed by the overlap of two p orbitals on each atom. One of the sp orbitals of carbon overlaps with the sp^3 orbital of the tetrahedral carbon atom to which it is bonded. The non bonding electrons of nitrogen occupy its second sp orbitals.

The complex compounds of the type CuX_2L_2 where L is pyridine or a substituted pyridine and X is halide are the subject of many structural, magnetic and spectroscopic studies[1,2,3,4,5,6,7]. In the field of inorganic and coordination polymers, B. F. Hoskins and R. Robsons[8] have proposed a strategy in the design of new 3D phases, which are assembled by using suitable metal centres and have potential utility in host-guest chemistry, ion exchange and catalysis. The structure determination of the title compound has been undertaken in order to find the relationship between the structure and the properties of the complexes, particularly the magnetic interactions between copper atoms.

The synthesis of the title compound was done by Dr. B. K. Das and R. K. Barman of Department of Chemistry, Gauhati University, Guwahati.

The present work comprises of the determination of the crystal and molecular structure of dichlorobis(4-cyanopyridine)copper(II), by X-ray diffraction method. The structural formula of the title compound (I) is as follows :



(I)

5.2 EXPERIMENTAL :

The needle shaped light blue crystals of the title compound were grown by the reaction of 1mmol. cupric chloride dihydrate and 2 mmol. of 4-cyanopyridine ligand in water solution in presence of 2 mmol. of sodium maleate salt when kept for several days.

Preliminary crystal data were determined from oscillation and Weissenberg photographs using CuKα radiation. The crystals were found to be monoclinic. The systematic absences h 0 l for h + l = 2n + 1 and 0 k 0 for k = 2n + 1 uniquely establishes that the space group is $P\ 2_1/n$, with the general equivalent positions ± x, y, z and ± (0.5 + x, 0.5 – y, 0.5 + z) The number of the molecules per unit cell was found to be 2.

A single crystal of size 0.20 X 0.31 X 0.13 mm^3 was chosen for collection of intensity data. The three dimensional intensity data were collected in CAD 4 Enraf - Nonius 4 - circle automatic diffractometer using graphite monochromated CuKα radiation, in Bio-physics Department, All India Institute of Medical Sciences, New Delhi.

The unit cell parameters were refined by the least-square refinement method on the basis of 25 high angle reflections with the setting angles lying in the range $10° \leq \theta \leq 20°$. Altogether 3310 independent reflections were recorded up to 75° in 2θ

by the ω - 2θ scan technique, in the h k l range $0 \leq h \leq 4, -32 \leq k \leq 32, -8 \leq l \leq 8$ with the scan speed of 4°/ min.

Three standard reflections (–1, 5, 1), (0, 5, –5) and (1, 3, –5) were monitored after every 100 reflections showed no significant variation in intensity and this ensured stability of the crystal in the data collection time.

Out of 3310 reflections measured, 1423 were found unique and the value of R_{int} = 0.1146; 1272 [$F_o > 4\sigma (F_o)$] were considered observed, and used in the structure determination. The_intensities were corrected for the Lorentz and polarization factors and also for absorption correction.

DETAILS OF CRYSTAL AND EXPERIMENTAL DATA

Molecular formula	$C_{12}H_8N_4Cl_2Cu$
Molecular weight (M_r)	342.66
Colour	Blue
Crystal system	Monoclinic
Space group	P $2_1/n$
Unit cell dimensions	a = 3.589(3)Å
	b = 25.903(6)Å
	c = 7.116(1)Å
	β = 96.05(4)°
Volume	657.9(6)Å^3
Z	2
Calculated density D_x	1.730 Mg / m^3
Radiation	Cu Kα
Wavelength	1.5418Å
Absorption coefficient	5.997 mm^{-1}
F (000)	342
Temperature	293(2) K
Goodness-of-fit 'S '	1.068
R	0.0591

$\Delta\rho_{max.}$	0.76 eÅ^{-3}
$\Delta\rho_{min}$	–1.53 eÅ^{-3}
$(\Delta / \sigma)_{max.}$	0.000

5.3 STRUCTURE SOLUTION AND REFINEMENT :

The structure was solved by direct methods using the program SHELXS-97 (Sheldrick, 1997)[9]. In this program the E-values are calculated by modified K-curve method[10].

The E-statistics $< |E^2 - 1| > = 0.893$ imply clearly that the crystal is centrosymmetric. Initial phase refinement was performed using 124 subset reflections; 1393 unique TPRs were used for filter.

188 large E-values refined using 3660 unique TPRs. 199 reflections and 3973 unique TPR for R_α. The number of negative quartets found was 1491, of which 1274 were used for phase refinement. The strongest negative quartets included in FILTER was 179. Multisolution tangent refinement was carried out using 372 E - values with $E > 1.2$.

A total of 250 parallel correct phase sets were refined with the best solution having an absolute figure of merit, Mobs = 1.237 (range 0.420 – 1.237) and combined figure of merit CFOM = 0.0536, which is the minimum value.

An E - map drawn with the correct set of phases revealed all the 10 non hydrogen atoms of the structure. The R factor based on the 372 E - values was found to be $R_E = 0.219$. The Cu atom sits on special position (0.5, 0.5, 0.5) with an occupancy of 0.5.

The structure refinement based on F was carried out using the program SHELXL-97 (Sheldrick, 1997)[11]. Full matrix least squares refinement first isotropic and then with anisotropic thermal parameter were carried out. All the hydrogen atoms were located on difference synthesis and their positional and thermal parameters were refined. The final agreement residual arrived at is R = 0.0591 for 1272 $F_o > 4\,\sigma(F_o)$ and wR=

0.1643. The function was minimized with weight w =1/ [sigma^2 (F_o^2) + (0.0950 * P)^2 + 0.31* P] where P = [Max (F_o^2, 0)+ 2 * Fc ^{2}] / 3.

The final difference Fourier map showed that peaks are lying in the range of 0.76 to – 1.54 eÅ^{-3}. The occupancy sum of the asymmetric unit = 9.50 for non hydrogen and = 4.00 for hydrogen atoms. The atomic scattering factors used were taken from the International Tables for X-ray Crystallography Vol. IV[12].

The molecular geometry calculations for the present structure were carried out using the program PARST (Nardelli, 1983)[13].

5.4 RESULTS AND DISCUSSIONS :

The ORTEP (Johnson, 1976)[14] diagram showing the conformation of the molecules and the atom numbering scheme with thermal ellipsoids is given in the Fig. 5.1. The positional parameters of the atoms are given in the Table 5.1 and the anisotropic temperature factors for the non-H atoms are given in the Table 5.2. The bond lengths and bond angles of the molecule are given in Table 5.3. The list of structure factors are given in Appendix - IV.

The important structural geometry of the title compound is now discussed in detail :

5.4 (a) THE PYRIDINE RING :

A comparison of average bond lengths and bond angles of pyridine ring of the title compound, with the corresponding values in some other compounds are given in the Table 5.7.

The compounds selected for comparison are as follows :–

2. 1DPED → 1,2-di-(2-pyridyl)-ethane-1,2-diol (Ashida et al., 1965)[15].
3. PL → Picolinamide (Takano et al., 1966)[16].
4. 2DBP → 2-(2′,4′-dinitrobenzyl)-pyridine (Seff et al., 1968)[17].
5. 2TP → 2-thioamidopyridine (Downie et al., 1972)[18].
6. DCPCP → Diaquachlorobis(pyridinioacetato)copper(II) perchlorate (Yu-Lung et al., 1998)[19].

7. IBBCT → (Isocyanato)bis(2,2'bypyridine)copper(II) tricyanomethanide (Potocnak et al., 1998)[20].

From the analysis of the structure, it is found that the bond lengths and bond angles of the pyridine ring are in good agreement with those of the other compounds (Table 5.7).

In the pyridine part of the present structure, the C – N – C angles are less than 120° [117.9(3)°], the adjacent N – C – C angles are larger than 120° [123.1(3)° and 122.9(3)°] with the average C – C bond length [1.378(5)Å] larger than the average N – C bond length [1.330(4)Å]. Thus it appears that the pyridine ring has distorted to some extent similar to that found in case of other reported substituted pyridine[2,7,17,18,19,20].

5.4(b) <u>THE Cu(II) MOIETY</u> :

The Cu atom sits on a special position (0.5, 0.5, 0.5) with an occupancy of 0.5 and are linked by two closely bonded [2.23(1)Å] chlorine atoms as also found by W. E. Marsh et al., (1981)[7] in the structure of bis(4-methylpyridine)dichloro -copper(II) and X. M. Chen et al., (1998)[19] in the structure of diaquachlorobis-(pyridinioacetato)copper(II) perchlorate. The Cu – Cu distance is found to be 3.59(3)Å. The coordination geometry at copper(II) is commonly-observed square planar arrangement. In the plane containing Cu, N and Cl atoms, the trans – nitrogen and trans – chlorine atoms with Cu – N and Cu – Cl distances are of 2.03(3)Å and 2.23(1)Å respectively[7,19,20]. The cis N – Cu – Cl angles are 89.81(7)° and 90.19(7)°, while trans angles are constrained to be 180° by the inversion symmetry at copper and are in good agreement with the values reported in the literature. The metal ligand bonding arrangement is very similar to those in $Cu(pyridine)_2Cl_2$[1], $Cu(4\text{-}Ethylpyridine)_2Cl_2$[5], $Cu(4\text{-}vinylpyridine)_2Cl_2$[6] and other related structures.

5.4 (c) CONFORMATION OF THE MOLECULE :

The weighted least squares planes through the various sets of atoms, together with their displacements from the respective planes and the dihedral angle between the LSQ planes is given in the Table 5.5. Weighted least squares plane is described by the equation

$$Ax + By + Cz - D = 0$$

where x, y, z are the orthogonal coordinates in Å and A, B, C and D are constants.

From the analysis of the least squares plane, it appears that the pyridine ring plane is almost planar with the maximum deviation of atoms lying in the range – 0.006(5)Å to + 0.004(3)Å. The individual deviation of Cu1, C6 and N2 from the pyridine mean plane are found to be – 0.064(1)Å, – 0.023(4)Å and – 0.064(5)Å respectively which shows that the metal atom copper is deviated from the pyridine ring plane by – 0.064(1)Å.

The molecular conformation can be described by the torsion angles about the various bonds; and the least squares planes, together with their e.s.d.'s from the respective planes.

The torsion angles of the molecule are given in the Table 5.4. The torsion angles Cl1 – Cu1 – N1 – C4 and Cl1 – Cu1 – N1 – C5 about the central bond Cu1 – N1 are given by 57.4(2)° and – 123.9(2)° respectively. The dihedral angle between the least square planes through the pyridine and that through the nitrogen – nearest halide atom [N1– Cu1 – Cl1] is 56.8(1)° which shows clearly that the pyridine ring plane is tilted away from the nitrogen–nearest halide atom plane [N1– Cu1 – Cl1]. The same type of tilt was also found in the structure of bis(4-methylpyridine)dichlorocopper(II) [59.7°] by W. E. Marsh et al.,(1981)[7] and in the structure of dichloro- and dibromobis(pyridine)copper(II) complexes [58.2° and 58.7°] by B. Morosin (1975)[2].

The dihedral angle between the pyridine ring plane and the plane containing the cyano group and the C1 atom of the pyridine ring is found to be 27.9(8)°, which shows that the plane C1 – C6 – N2 is tilted out of the pyridine ring plane by an amount of 27.9(8)°. From the consideration of torsion angles also, it is seen that torsion angles

N2 – C6 – C1 – C2 and N2 – C6 – C1 – C3 about the central bond C6 – C1 are 151.9(12)° and – 27.9(12)° respectively. The C ≡ N bond distance is 1.140(7)Å which is of the same order as the normal C ≡ N bond distance. The same value of C ≡ N bond distance is also reported by others in the structure of various cyano derivatives[21,22,23].

5.4 (d) MOLECULAR PACKING :

The packing diagram of the molecule as viewed down the a-axis and c-axis of the unit cell are shown in the Fig. 5.2 and Fig. 5.3 respectively.

There is no intra or intermolecular hydrogen bond. In the packing configuration of the structure under consideration, it is observed that the molecules are stabilized by van der Waals interactions only, as no permitted hydrogen bond is possible by the stereochemistry of the molecule. There are considerable number of shortened non-bonded intermolecular contacts, the values [less than 3.2Å] of which are listed in the Table 5.6.

From the study of the packing diagrams, it is clear that the molecules arrange themselves into the distinct regions in the crystalline space. It can be easily understood that the structural features of the title compound investigated fit well with the pattern observed in all other cyanopyridine derivatives.

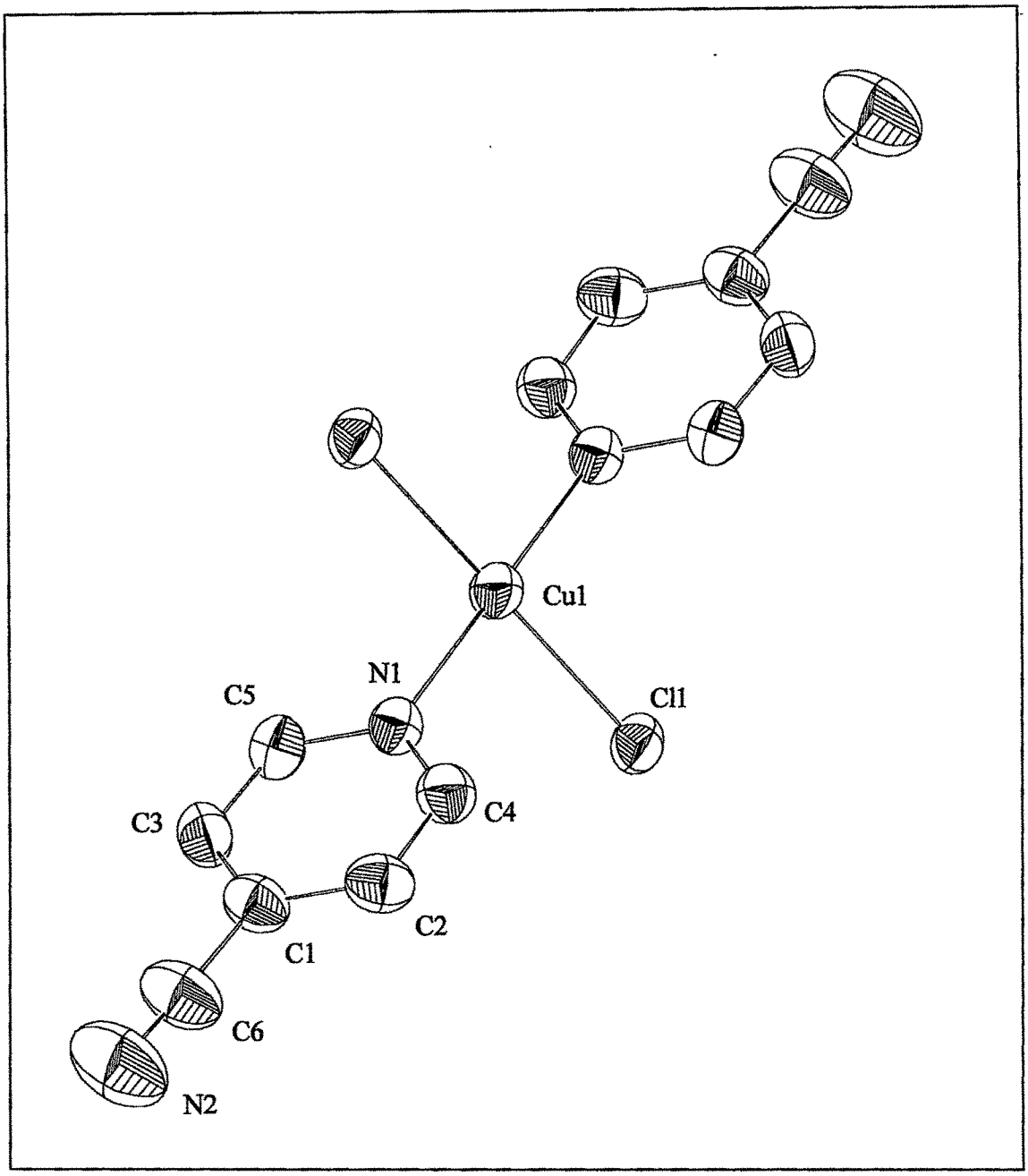


Fig. 5.1 A view of the molecule with 50% probability anisotropic displacement ellipsoids for the non-H atoms and atomic numbering scheme.

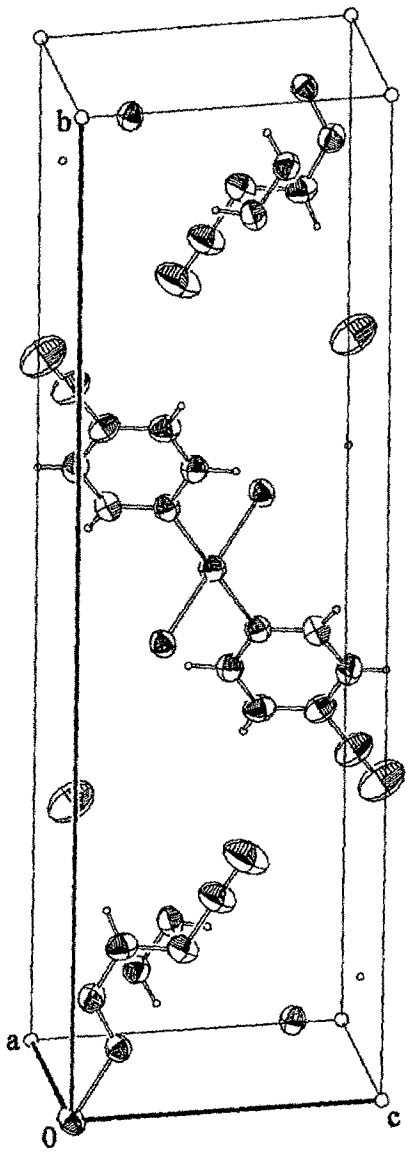


Fig. 5.2 Packing of the molecules in the unit cell as viewed down the a-axis.

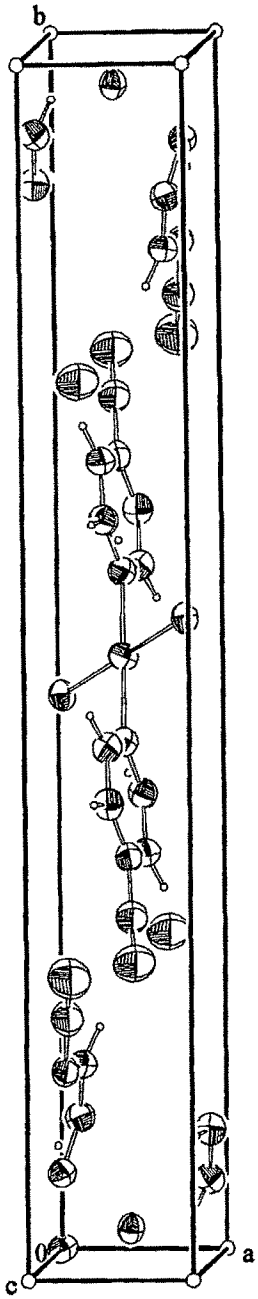


Fig. 5.3 Packing of the molecules in the unit cell as viewed down the c-axis.

Table 5.1

Fractional atomic coordinates and equivalent isotropic temperature factors in $Å^2$ with e. s. d.'s in parenthesis.

$U_{eq} = \frac{1}{3}\Sigma i \ \Sigma j \ U_{ij} a_i^* a_j^* a_i a_j$ where U_{ij} are defined by the expression,

$$\exp\left[-2\pi^2\left(U_{11}a^{*2}h^2 + U_{22}b^{*2}k^2 + U_{33}c^{*2}l^2 + 2U_{23}b^*c^*kl + 2U_{13}a^*c^*hl + 2U_{12}a^*b^*hk\right)\right]$$

Atom	*x*	*y*	*z*	U_{eq}
Cu1	0.5000(0)	0.5000(0)	0.5000(0)	0.0387(4)
Cl1	0.0817(2)	0.4629(1)	0.2873(1)	0.0384(4)
N1	0.5324(7)	0.4338(1)	0.6528(3)	0.0371(6)
N2	0.6712(13)	0.2626(2)	1.0748(7)	0.0915(15)
C1	0.5984(8)	0.3446(1)	0.8659(5)	0.0433(7)
C2	0.6648(9)	0.3436(1)	0.6782(5)	0.0459(8)
C3	0.4953(9)	0.3902(2)	0.9436(4)	0.0436(8)
C4	0.6275(9)	0.3894(1)	0.5773(5)	0.0422(7)
C5	0.4659(9)	0.4338(1)	0.8333(4)	0.0413(7)
C6	0.6376(11)	0.2982(2)	0.9800(6)	0.0611(10)
Atom	***x***	***y***	***z***	**U11**
H1	0.4304(123)	0.3926(18)	1.0553(65)	0.0567(118)
H2	0.6762(103)	0.3901(15)	0.4500(53)	0.0403(88)
H3	0.3746(120)	0.4612(17)	0.8858(57)	0.0466(104)
H4	0.7619(126)	0.3139(19)	0.6402(65)	0.0636(132)

Table 5.2

Anisotropic temperature factors in $Å^2$ for the non-H atoms,

Displacement parameters U_{ij},

$$\exp\left[-2\pi^2\left(U_{11}h^2a^{*2}+\cdots\cdots\cdots+2U_{12}a^*b^*hk\right)+\cdots\cdots\cdots\right]$$

Atom	U11	U22	U33	U23	U13	U12
Cu1	0.0425(4)	0.0370(6)	0.0348(4)	0.0036(2)	-0.0048(3)	-0.0043(2)
Cl1	0.0351(5)	0.0453(6)	0.0346(5)	-0.0034(3)	0.0019(3)	-0.0022(3)
N1	0.0375(12)	0.0381(14)	0.0353(11)	0.0002(9)	0.0013(9)	-0.0010(9)
N2	0.0884(30)	0.0707(31)	0.1158(34)	0.0430(27)	0.0128(26)	0.0095(23)
C1	0.0338(13)	0.0434(17)	0.0530(17)	0.0095(15)	0.0056(11)	-0.0001(12)
C2	0.0432(16)	0.0360(17)	0.0599(19)	-0.0016(15)	0.0119(13)	0.0000(13)
C3	0.0448(15)	0.0498(19)	0.0361(15)	0.0049(14)	0.0047(11)	-0.0001(14)
C4	0.0438(15)	0.0414(18)	0.0427(16)	-0.0023(13)	0.0099(12)	-0.0018(13)
C5	0.0427(17)	0.0434(18)	0.0376(14)	-0.0033(13)	0.0031(11)	0.0024(13)
C6	0.0503(19)	0.0537(23)	0.0802(26)	0.0222(21)	0.0108(17)	0.0038(17)

Table 5.3

Bond lengths (Å) and bond angles (°) of the molecule, with e.s.d.'s in parenthesis.

Cu1— Cl1	2.233(1)	Cu1— N1	2.026(1)
N1 — C4	1.330(4)	N1 — C5	1.330(4)
N2 — C6	1.140(6)	C1 — C2	1.382(5)
C1 — C3	1.372(5)	C1 — C6	1.450(6)
C2 — C4	1.386(5)	C3 — C5	1.372(5)
C2 — H2	0.896(49)	C3 — H3	0.854(47)
C4 — H4	0.941(38)	C5 — H5	0.882(43)

Cl1 — Cu1— N1	89.8(1)	Cu1— N1 — C5	120.9(2)
Cu1— N1 — C4	121.2(2)	C4 — N1 — C5	117.9(3)
C3 — C1 — C6	120.2(4)	C2 — C1 — C6	120.6(3)
C2 — C1 — C3	119.2(3)	C1 — C2 — C4	117.9(3)
C1 — C3 — C5	119.1(4)	N1— C4 — C2	123.1(3)
N1 — C5 — C3	122.9(3)	N2 — C6 — C1	177.8(5)
C1 — C2 — H2	114.8(3)	C4 — C2 — H4	126.6(3)
C1 — C3 — H3	123.3(3)	C5 — C3 — H3	117.5(3)
C2 — C4 — H4	119.9(2)	N1 — C4 — H4	116.9(2)
C3 — C5 — H5	115.5(2)	N1 — C5 — H5	121.3(2)

Table 5.4

Some of the selected torsion angles (°) with e.s.d.'s in parenthesis.

Cl1— Cu1— N1 — C4	57.4(2)
Cl1— Cu1— N1 — C5	-123.9(2)
Cu1— N1 — C5 — C3	-178.1(1)
Cu1— N1 — C4 — C2	177.9(3)
C4 — N1 — C5 — C3	-0.7(5)
C5 — N1 — C4 — C2	-0.9(5)
C3 — C1 — C6 — N2	-27.9(12)
C2 — C1 — C6 — N2	151.9(12)
C2 — C1 — C3 — C5	-0.9(5)
C3 — C1 — C2 — C4	0.7(5)
C6 — C1— C2 — C4	-179.1(3)
C6 — C1— C3 — C5	178.9(3)
C1 — C2 — C4 — N1	0.2(5)
C1 — C3 — C5 — N1	0.2(5)

Table 5.5

Weighted least squares plane through the starred atoms and atomic deviations (Å) with e.s.d.'s in parenthesis.

Plane 1

$-0.9403(5)X - 0.2069(12)Y - 0.2703(13)Z + 4.9064(142) = 0$, $\chi^2 = 7.81$

* C1	–0.005(3)	* C2	0.002(3)	* C3	0.004(3)
* C4	0.004(3)	* C5	0.003(3)	* N1	–0.004(2)
Cu1	–0.064(1)	C6	– 0.023(4)	N2	–0.064(5)

Plane 2

$-0.7994(2)X + 0.3199(10)Y + 0.5085(6)Z - 4.8091(114) = 0$

Cu1	0.000(0)	Cl1	0.000(1)	N1	0.000(2)

Plane 3

$-0.9895(280)X + 0.0467(1145)Y + 0.1370(1336)Z + 0.2264(469) = 0$

C1	0.000(3)	C6	0.000(4)	N2	0.000(5)

Dihedral angles (°) formed by LSQ - planes

Plane	—	Plane	Angle
1		2	56.8(1)
1		3	27.9(8)
2		3	28.9(8)

Table 5.6

Intermolecular contacts less than 3.2Å for the non-hydrogen atoms.

ATOMS	SYMMETRY CODE	DISTANCE(Å)
Cu1 — Cl1	$-x, -y+1, -z+1$	2.870(2)
Cu1 — Cl1	$x+1, +y, +z$	2.970(2)
Cu1 — Cl1	$-x+1, -y+1, -z+1$	2.233(1)
Cu1 — N1	$-x+1, -y+1, -z+1$	2.027(3)
Cu1 — C4	$-x+1, -y+1, -z+1$	2.945(4)
Cu1 — C5	$-x+1, -y+1, -z+1$	2.940(3)
Cl1 — Cu1	$x-1, +y, +z$	2.870(2)
Cl1 — N1	$-x+1, -y+1, -z+1$	3.021(3)

Table 5.7

A comparison of some average distances (Å) and angles (°) in pyridine rings with the corresponding values in related structures.

The compounds	C — C	N — C	C — N — C	N — C — C	C — C — C
1. DBCPCO	1.378(5)	1.330(4)	117.9(3)	123.0(3)	118.7(3)
2. 1DPED	1.393	1.342	119.0	123.6	118.9
3. PL	1.373	1.379	117.3	123.5	118.6
4. 2DBP	1.383	1.346	117.0	123.5	118.6
5. 2TP	1.383(8)	1.336(6)	117.0(4)	123.6(4)	118.5
6. DCPCP	1.367(9)	1.343(7)	121.1(5)	119.8(5)	119.8(5)
7. IBBCT	1.370(6)	1.343(5)	117.4(4)	122.6(4)	119.2(4)

References to Chapter -V

1. Dunitz, J. D.(1957). *Acta Cryst.* **10**, 307 – 313.
2. Morosin, B. (1975). *Acta Cryst.* **B31**, 632 – 634.
3. Ooijen, J. A. C. V. and Reedijk, J. (1977). *Inorg. Chim. Acta.* **25**, 131 – 140.
4. Crawford, V. H. and Hatfield, W. E. (1977). *Inorg. Chem.* **16(6)**, 1336 – 1341.
5. Liang, M. and Carr, G. (1971). *J. Chem. Soc. (A).* 1141 – 1144.
6. Liang, M. and Horsfield, E. (1961). *Chem. Comm.* 9735.
7. Marsh, W. E., Valente, E. J. and Hodgson, D. J.(1981). *Inorg.Chim.Acta.* **51**,49 – 53.
8. Hoskins, B. F. and Robsons, R. (1990). *J. Am. Chem. Soc.* **112**, 154 – 156.
9. Sheldrick, G. M. (1997). *SHELXS97. Program for the solution of Crystal Structure.* University of Gottingen, Germany.
10. Karle, J. , Hauptman, H. and Christ, C. L. (1958). *Acta Cryst.* **11** , 757 – 761.
11. Sheldrick, G. M. (1997). *SHELXL97. Program for the refinement of Crystal Structures.* University of Gottingen, Germany.
12. *International Tables for X-ray Crystallography,* **Vol. IV**. Kynoch Press, Birmingham (present distributor: Kluwer Academic Publisherrs: Dordrecht).
13. Nardelli, M. (1983). *Comput. Chem.* **7** , 95 – 98.
14. Johnson, C. K.(1976). *ORTEPII. Report ORNL - 5138.* Oak Ridge National Laboratory, Tennessee, USA.
15. Ashida, T. , Hirokawa, S. and Okaya, Y. (1965). *Acta Cryst.* **18**, 122 – 127.
16. Takanoi, T., Sasada, Y. and Kakudo, M. (1966). *Acta Cryst.* **21**, 514 – 522.
17. Seff, K. and Trueblood, K. N. (1968). *Acta Cryst.* **B24**, 1406 – 1415.
18. Downie, T. C., Harrison, W and Raper, E. S. (1972). *Acta Cryst.* **B28**, 283 – 290.
19. Chen, X. M., Yu-Lung, W., Ye-Xiang, T., Mak, T. C. W. and Kong. (1998). *Acta Cryst.* **C54**, 606 – 608.
20. Potocnak, I., Michal, D. J., San, M. D. and Lothar, J. (1998). *Acta Cryst.* **C54**, 313 – 315.
21. Nayak, N. P., Mukherjee, A. K., Mondal, A. and Choudhury, N. R. (1998). *Acta*

Cryst. **C54**, 208 – 210.

22. Tao, Y., Song, G., Xiong-Wei, C., Chun-Hua, Y. and Biao-Guo., L. (1998). *Acta Cryst.* **C54**, 41 – 43.

23. Tainyan, N., Gerardo, C., Jian, L. and Allan, J. J. (1998). *Acta Cryst.* **C54**, 565 – 567.

Calculated and observed structure factors for dichlorobis(4-cyanopyridine)copper(II)

h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2
2	0	0	4039.18	3345.44	1	16	0	8.45	6.89	4	2	1	10.89	10.57
4	0	0	0.38	1.73	2	16	0	258.81	332.38	-4	3	1	3.46	3.08
1	1	0	5636.41	4607.11	3	16	0	70.87	78.46	-3	3	1	1.34	5.53
2	1	0	1474.34	1294.84	4	16	0	139.31	54.61	-2	3	1	7.65	2.45
3	1	0	326.09	296.16	1	17	0	2136.08	2263.82	-1	3	1	1363.45	1483.10
4	1	0	0.92	1.75	2	17	0	277.19	352.36	0	3	1	6891.46	7770.43
0	2	0	9069.14	9033.18	3	17	0	235.87	279.91	1	3	1	9091.761	0780.61
1	2	0	1153.32	965.40	0	18	0	768.62	668.61	2	3	1	4705.74	4805.62
2	2	0	3991.76	3284.28	1	18	0	27.66	27.35	3	3	1	53.99	58.76
3	2	0	2.66	3.33	2	18	0	245.12	332.92	4	3	1	174.85	139.26
4	2	0	54.75	40.59	3	18	0	59.61	73.69	-4	4	1	18.10	11.84
1	3	0	578.10	624.99	1	19	0	1310.51	1317.28	-3	4	1	1061.79	992.79
2	3	0	294.93	242.52	2	19	0	195.63	247.99	-2	4	1	400.01	378.11
3	3	0	621.01	546.76	3	19	0	36.11	51.81	-1	4	1	546.58	501.19
4	3	0	61.74	46.40	0	20	0	774.57	657.63	0	4	1	733.74	689.63
0	4	0	1679.51	1675.62	1	20	0	232.00	231.16	1	4	1	1679.95	1633.99
1	4	0	2511.96	2586.67	2	20	0	83.04	101.86	2	4	1	564.93	586.54
2	4	0	669.02	521.55	3	20	0	213.29	201.15	3	4	1	251.16	233.58
3	4	0	360.71	313.57	1	21	0	23.35	20.36	4	4	1	173.90	130.76
4	4	0	26.09	16.94	2	21	0	1.28	1.14	-4	5	1	57.43	41.33
1	5	0	3.18	7.15	3	21	0	17.62	20.28	-3	5	1	108.43	101.57
2	5	0	218.00	176.83	0	22	0	12.42	15.89	-2	5	1	586.40	597.61
3	5	0	24.37	24.00	1	22	0	220.02	208.05	-1	5	1	3234.45	3810.09
4	5	0	95.25	64.87	2	22	0	30.22	38.22	0	5	1	733.01	590.86
0	6	0	509.30	410.99	3	22	0	116.17	158.40	1	5	1	559.78	513.90
1	6	0	501.53	503.70	1	23	0	188.19	166.78	2	5	1	2191.49	2095.64
2	6	0	206.44	155.44	2	23	0	143.13	173.79	3	5	1	120.73	114.14
3	6	0	415.83	331.24	3	23	0	38.49	51.01	4	5	1	232.18	151.61
4	6	0	0.41	0.73	0	24	0	207.81	180.89	-4	6	1	6.68	6.96
1	7	0	382.73	335.95	1	24	0	30.98	28.86	-3	6	1	389.36	348.72
2	7	0	586.41	591.71	2	24	0	57.85	64.50	-2	6	1	9.76	6.60
3	7	0	37.86	31.77	3	24	0	6.82	6.77	-1	6	1	3580.45	4078.07
4	7	0	120.63	85.73	1	25	0	11.23	13.67	0	6	1	2889.56	2412.41
0	8	0	435.26	333.32	2	25	0	58.88	53.78	1	6	1	282.52	239.09
1	8	0	482.36	477.11	3	25	0	0.11	0.18	2	6	1	150.29	137.91
2	8	0	105.48	90.36	0	26	0	1087.17	1021.17	3	6	1	97.72	91.79
3	8	0	230.42	212.09	1	26	0	18.31	20.85	4	6	1	155.74	90.03
4	8	0	33.74	29.89	2	26	0	126.70	93.50	-4	7	1	21.81	18.82
1	9	0	2163.97	2255.18	1	27	0	17.86	15.17	-3	7	1	44.16	40.96
2	9	0	640.76	649.47	2	27	0	25.21	9.93	-2	7	1	802.32	863.16
3	9	0	92.97	94.91	0	28	0	458.40	448.16	-1	7	1	2774.74	3275.71
4	9	0	72.87	41.11	1	28	0	0.60	0.81	0	7	1	3324.70	2522.38
0	10	0	31.37	34.73	2	28	0	214.30	237.96	1	7	1	1329.23	1424.19
1	10	0	53.18	62.76	1	29	0	16.17	14.60	2	7	1	52.08	40.88
2	10	0	165.66	166.32	2	29	0	10.70	7.15	3	7	1	81.15	81.01
3	10	0	151.78	149.72	0	30	0	308.55	292.03	4	7	1	30.86	11.30
4	10	0	91.42	54.19	1	30	0	9.21	8.65	-4	8	1	5.61	5.04
1	11	0	2792.54	3065.84	1	31	0	19.23	9.28	-3	8	1	8.50	9.88
2	11	0	73.45	69.87	0	32	0	107.19	89.46	-2	8	1	635.36	686.54
3	11	0	185.72	185.83	-3	0	1	1497.91	1174.49	-1	8	1	618.57	580.68
4	11	0	23.04	15.05	-1	0	1	2465.55	2390.00	0	8	1	763.69	563.74
0	12	0	55.14	38.39	1	0	1	1237.03	1430.04	1	8	1	1757.61	1700.94
1	12	0	126.77	141.63	3	0	1	106.93	105.13	2	8	1	188.74	189.54
2	12	0	84.03	102.77	-4	1	1	38.71	30.32	3	8	1	149.85	156.05
3	12	0	31.82	35.66	-3	1	1	2.64	6.02	4	8	1	3.60	4.82
4	12	0	99.90	54.75	-2	1	1	62.62	48.74	-4	9	1	60.28	61.95
1	13	0	4033.65	4666.15	-1	1	1	2990.88	3157.01	-3	9	1	0.21	1.06
2	13	0	21.04	25.57	0	1	1	3115.68	3191.94	-2	9	1	526.65	535.83
3	13	0	121.37	130.10	1	1	1	580.10	561.62	-1	9	1	744.01	795.58
4	13	0	1.32	2.09	2	1	1	1790.25	1488.79	0	9	1	398.80	282.34
0	14	0	7.43	7.83	3	1	1	4.67	8.71	1	9	1	239.46	238.71
1	14	0	132.55	125.14	4	1	1	206.35	175.91	2	9	1	170.43	172.12
2	14	0	165.38	200.39	-4	2	1	0.07	0.36	3	9	1	67.13	63.31
3	14	0	12.77	16.93	-3	2	1	675.53	563.17	4	9	1	1.02	0.21
4	14	0	102.57	60.06	-2	2	1	16.51	12.92	-4	10	1	0.12	1.12
1	15	0	2620.72	2886.71	-1	2	1	4870.77	5306.09	-3	10	1	16.33	18.94
2	15	0	4.62	7.38	0	2	1	2519.38	2376.68	-2	10	1	367.15	452.54
3	15	0	282.86	332.55	1	2	1	953.06	846.62	-1	10	1	319.23	272.83
4	15	0	2.11	1.75	2	2	1	140.62	144.26	0	10	1	3260.23	2981.05
0	16	0	73.46	60.33	3	2	1	32.94	29.06	1	10	1	2604.76	2773.20

Calculated and observed structure factors for dichlorobis(4-cyanopyridine)copper(II)

h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2
2	10	1	149.43	160.36	3	18	1	56.58	69.78	1	30	1	16.45	13.29
3	10	1	501.78	474.08	-3	19	1	10.87	18.06	-1	31	1	29.57	9.96
4	10	1	8.47	7.59	-2	19	1	345.59	449.63	0	31	1	68.78	50.52
-4	11	1	156.56	102.42	-1	19	1	279.94	282.21	1	31	1	10.96	2.82
-3	11	1	1.09	1.73	0	19	1	405.13	362.11	0	32	1	21.63	18.81
-2	11	1	1100.56	1340.74	1	19	1	3.48	4.50	-4	0	2	18.59	18.79
-1	11	1	43.54	72.97	2	19	1	12.68	14.15	-2	0	2	116.03	132.25
0	11	1	1300.79	1071.44	3	19	1	113.09	146.31	0	0	2	474.11	363.84
1	11	1	0.83	2.28	-3	20	1	66.17	82.83	2	0	2	105.69	91.41
2	11	1	2.19	3.07	-2	20	1	83.79	113.24	4	0	2	194.43	156.76
3	11	1	4.61	7.82	-1	20	1	274.28	272.98	-4	1	2	5.29	6.27
4	11	1	0.54	0.54	0	20	1	1461.45	1347.31	-3	1	2	632.86	685.84
-4	12	1	0.37	2.17	1	20	1	56.14	54.23	-2	1	2	201.27	230.78
-3	12	1	1.93	1.34	2	20	1	219.75	269.04	-1	1	2	9683.831	1946.74
-2	12	1	390.68	484.77	3	20	1	43.19	44.11	0	1	2	66.15	58.41
-1	12	1	771.74	828.51	-3	21	1	14.90	13.54	1	1	2	2626.82	2509.49
0	12	1	947.09	890.77	-2	21	1	68.68	80.44	2	1	2	60.52	57.59
1	12	1	2266.40	2310.78	-1	21	1	38.96	37.21	3	1	2	2.96	4.58
2	12	1	44.68	48.80	0	21	1	171.69	155.43	4	1	2	4.03	3.88
3	12	1	630.48	651.16	1	21	1	0.96	0.33	-4	2	2	113.68	89.68
4	12	1	0.74	1.70	2	21	1	311.04	375.79	-3	2	2	226.84	262.39
-4	13	1	289.73	282.14	3	21	1	2.75	3.97	-2	2	2	22.91	23.88
-3	13	1	15.19	18.08	-3	22	1	85.27	119.52	-1	2	2	73.94	75.58
-2	13	1	1952.28	2532.06	-2	22	1	109.49	122.89	0	2	2	438.16	465.31
-1	13	1	81.75	86.55	-1	22	1	143.25	131.03	1	2	2	296.99	298.95
0	13	1	484.23	392.20	0	22	1	380.87	327.91	2	2	2	333.57	303.77
1	13	1	16.60	16.88	1	22	1	333.90	329.85	3	2	2	19.46	18.50
2	13	1	3.01	5.11	2	22	1	27.17	29.47	4	2	2	131.48	90.90
3	13	1	7.74	10.79	3	22	1	41.82	53.18	-4	3	2	20.58	18.73
4	13	1	1.65	1.74	-3	23	1	4.29	6.20	-3	3	2	585.54	623.83
-4	14	1	3.68	3.47	-2	23	1	2.61	6.02	-2	3	2	221.12	230.07
-3	14	1	4.82	5.24	-1	23	1	264.32	259.77	-1	3	2	2909.03	3109.81
-2	14	1	2.01	9.29	0	23	1	433.88	391.33	0	3	2	522.58	420.88
-1	14	1	572.41	610.64	1	23	1	149.35	138.69	1	3	2	2228.21	2165.57
0	14	1	1.99	5.26	2	23	1	492.19	556.52	2	3	2	437.22	467.19
1	14	1	2049.65	2136.42	3	23	1	12.47	10.80	3	3	2	4.80	5.01
2	14	1	24.59	38.24	-3	24	1	146.92	136.08	4	3	2	23.48	16.24
3	14	1	781.32	828.94	-2	24	1	2.48	3.59	-4	4	2	37.03	31.00
4	14	1	23.46	10.41	-1	24	1	201.74	189.20	-3	4	2	148.12	162.66
-4	15	1	236.02	156.65	0	24	1	3.51	3.78	-2	4	2	1.42	0.27
-3	15	1	2.27	3.37	1	24	1	15.10	17.63	-1	4	2	41.51	49.74
-2	15	1	986.86	1296.63	2	24	1	1.60	2.15	0	4	2	289.79	244.04
-1	15	1	11.44	7.87	3	24	1	3.05	1.61	1	4	2	1020.55	1033.05
0	15	1	616.46	531.73	-3	25	1	1.73	2.67	2	4	2	282.38	269.96
1	15	1	47.30	45.39	-2	25	1	15.15	17.83	3	4	2	180.63	179.03
2	15	1	31.34	40.29	-1	25	1	120.20	89.08	4	4	2	86.48	58.99
3	15	1	15.61	21.19	0	25	1	105.80	77.88	-4	5	2	131.50	105.99
4	15	1	1.73	0.84	1	25	1	195.98	179.37	-3	5	2	73.51	80.46
-4	16	1	3.22	3.04	2	25	1	188.36	148.71	-2	5	2	176.35	201.36
-3	16	1	3.99	3.96	-2	26	1	2.21	2.36	-1	5	2	2124.91	2272.05
-2	16	1	147.85	187.68	-1	26	1	216.12	187.12	0	5	2	42.42	32.37
-1	16	1	168.14	176.66	0	26	1	7.76	7.84	1	5	2	2091.59	2166.62
0	16	1	320.41	293.58	1	26	1	3.49	3.12	2	5	2	187.91	169.73
1	16	1	2017.42	2130.90	2	26	1	46.64	37.35	3	5	2	196.03	200.29
2	16	1	2.03	1.87	-2	27	1	0.11	0.78	4	5	2	34.54	28.42
3	16	1	541.62	615.43	-1	27	1	1.37	0.78	-4	6	2	6.51	7.11
-4	17	1	48.90	74.72	0	27	1	248.64	221.24	-3	6	2	146.38	157.37
-3	17	1	2.35	2.15	1	27	1	14.59	11.76	-2	6	2	140.43	145.15
-2	17	1	395.76	521.52	2	27	1	120.73	105.21	-1	6	2	33.56	38.59
-1	17	1	153.02	150.94	-2	28	1	35.44	43.50	0	6	2	278.18	196.32
0	17	1	549.43	487.51	-1	28	1	110.59	76.19	1	6	2	1756.85	1884.57
1	17	1	263.35	233.14	0	28	1	3.61	5.85	2	6	2	1415.81	1481.30
2	17	1	49.83	57.77	1	28	1	13.39	14.82	3	6	2	433.11	429.51
3	17	1	75.13	79.90	2	28	1	0.33	1.82	4	6	2	173.25	53.13
-3	18	1	1.32	0.77	-2	29	1	0.28	0.82	-4	7	2	185.26	134.81
-2	18	1	182.49	232.89	-1	29	1	0.12	0.53	-3	7	2	167.31	173.65
-1	18	1	479.74	485.51	0	29	1	73.30	55.34	-2	7	2	505.23	577.72
0	18	1	295.65	278.98	1	29	1	20.68	16.30	-1	7	2	684.20	718.75
1	18	1	605.59	598.95	-1	30	1	40.28	29.62	0	7	2	1072.52	866.11
2	18	1	200.73	262.12	0	30	1	57.28	44.66	1	7	2	1656.73	1644.66

Calculated and observed structure factors for dichlorobis(4-cyanopyridine)copper(II)

h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2
2	7	2	738.18	790.42	1	15	2	61.61	52.12	2	25	2	41.55	33.76
3	7	2	671.71	680.91	2	15	2	6.21	9.83	-2	26	2	5.79	3.82
4	7	2	2.80	2.37	3	15	2	41.73	45.54	-1	26	2	3.57	3.11
-4	8	2	18.94	19.22	-4	16	2	42.56	23.01	0	26	2	1.34	1.86
-3	8	2	135.17	148.25	-3	16	2	89.11	113.78	1	26	2	2.27	2.35
-2	8	2	1400.92	1643.63	-2	16	2	748.66	990.20	2	26	2	41.92	27.01
-1	8	2	46.33	50.35	-1	16	2	4.51	5.80	-2	27	2	3.50	2.60
0	8	2	5222.12	4755.42	0	16	2	2019.61	1830.96	-1	27	2	416.07	384.06
1	8	2	66.76	46.71	1	16	2	172.13	169.46	0	27	2	0.11	0.78
2	8	2	787.79	837.77	2	16	2	50.93	53.02	1	27	2	168.34	161.53
3	8	2	207.66	201.49	3	16	2	0.39	0.27	2	27	2	7.66	7.68
4	8	2	75.23	44.91	-3	17	2	56.52	79.76	-2	28	2	1.76	0.99
-4	9	2	61.75	18.11	-2	17	2	43.20	62.75	-1	28	2	0.05	1.39
-3	9	2	71.26	92.78	-1	17	2	156.13	151.88	0	28	2	3.13	3.79
-2	9	2	116.78	127.34	0	17	2	95.38	72.10	1	28	2	0.98	1.28
-1	9	2	1852.17	2194.19	1	17	2	14.90	17.40	2	28	2	13.03	9.83
0	9	2	192.71	180.88	2	17	2	380.89	440.82	-1	29	2	254.16	221.51
1	9	2	1833.66	1912.18	3	17	2	33.67	45.06	0	29	2	11.57	9.78
2	9	2	797.65	868.76	-3	18	2	75.50	95.51	1	29	2	134.54	98.74
3	9	2	237.50	243.03	-2	18	2	662.03	824.96	-1	30	2	10.05	6.12
4	9	2	17.19	15.98	-1	18	2	9.88	8.59	0	30	2	0.51	0.40
-4	10	2	31.41	18.18	0	18	2	858.90	757.75	1	30	2	49.50	25.36
-3	10	2	238.22	272.87	1	18	2	41.29	41.01	0	31	2	5.12	3.88
-2	10	2	1475.08	1729.49	2	18	2	167.15	205.96	-3	0	3	49.17	56.95
-1	10	2	106.47	109.83	3	18	2	58.29	31.96	-1	0	3	978.49	1043.00
0	10	2	7177.15	7174.83	-3	19	2	34.12	43.37	1	0	3	2910.02	2725.39
1	10	2	645.91	656.58	-2	19	2	53.02	60.04	3	0	3	480.61	504.51
2	10	2	702.60	732.82	-1	19	2	170.22	152.79	-4	1	3	253.15	227.50
3	10	2	71.91	69.42	0	19	2	168.56	142.04	-3	1	3	0.50	1.19
4	10	2	1.99	1.96	1	19	2	298.41	287.34	-2	1	3	1251.45	1394.81
-4	11	2	8.18	7.33	2	19	2	171.82	199.46	-1	1	3	215.20	262.44
-3	11	2	36.56	41.92	3	19	2	119.16	92.99	0	1	3	2.15	1.20
-2	11	2	12.29	18.52	-3	20	2	27.52	23.02	1	1	3	7.91	8.05
-1	11	2	4.54	3.58	-2	20	2	134.57	161.17	2	1	3	69.95	78.36
0	11	2	248.63	191.40	-1	20	2	0.03	0.52	3	1	3	12.77	14.55
1	11	2	481.04	464.61	0	20	2	617.50	554.13	4	1	3	0.45	0.23
2	11	2	22.57	22.22	1	20	2	272.48	260.62	-4	2	3	1.02	1.51
3	11	2	271.65	285.72	2	20	2	262.61	332.63	-3	2	3	25.21	26.40
4	11	2	47.54	23.98	3	20	2	77.25	87.13	-2	2	3	665.99	750.76
-4	12	2	25.44	28.80	-3	21	2	20.64	25.50	-1	2	3	2180.81	2236.99
-3	12	2	74.60	91.64	-2	21	2	159.32	197.22	0	2	3	1653.22	1571.25
-2	12	2	1238.68	1446.52	-1	21	2	384.84	367.91	1	2	3	3362.40	3508.42
-1	12	2	114.57	135.97	0	21	2	43.71	36.45	2	2	3	0.39	0.40
0	12	2	1903.96	1513.23	1	21	2	325.56	327.05	3	2	3	446.90	459.49
1	12	2	99.05	105.52	2	21	2	161.89	185.00	4	2	3	21.46	13.41
2	12	2	306.76	332.76	3	21	2	49.05	53.68	-4	3	3	154.14	152.69
3	12	2	22.19	19.64	-3	22	2	15.02	19.82	-3	3	3	27.84	27.27
4	12	2	0.34	0.74	-2	22	2	8.13	11.81	-2	3	3	314.51	307.93
-4	13	2	1.40	3.45	-1	22	2	3.26	8.84	-1	3	3	38.33	26.46
-3	13	2	2.61	3.70	0	22	2	58.67	52.86	0	3	3	754.31	603.55
-2	13	2	5.30	6.08	1	22	2	67.81	62.46	1	3	3	114.10	118.08
-1	13	2	242.59	283.69	2	22	2	168.14	196.25	2	3	3	19.45	23.75
0	13	2	2.04	1.85	3	22	2	55.96	46.70	3	3	3	23.36	27.81
1	13	2	54.20	62.67	-3	23	2	49.91	68.80	4	3	3	16.30	7.28
2	13	2	36.81	38.82	-2	23	2	18.51	20.62	-4	4	3	73.77	64.03
3	13	2	345.39	348.56	-1	23	2	205.19	189.40	-3	4	3	2.30	2.55
4	13	2	4.34	2.35	0	23	2	40.34	38.70	-2	4	3	494.92	561.87
-4	14	2	21.28	27.34	1	23	2	372.42	371.97	-1	4	3	487.23	447.08
-3	14	2	0.09	0.78	2	23	2	80.25	87.52	0	4	3	1065.42	913.91
-2	14	2	639.73	815.70	3	23	2	28.79	43.28	1	4	3	3840.83	4000.40
-1	14	2	20.20	21.36	-3	24	2	42.12	31.28	2	4	3	7.10	7.51
0	14	2	1139.81	875.07	-2	24	2	1.97	1.89	3	4	3	564.32	585.59
1	14	2	78.41	89.54	-1	24	2	1.89	0.50	4	4	3	110.07	42.88
2	14	2	235.60	250.16	0	24	2	16.24	18.90	-4	5	3	150.75	128.39
3	14	2	14.65	20.27	1	24	2	64.62	58.98	-3	5	3	4.61	5.77
-4	15	2	2.51	2.23	2	24	2	135.19	127.71	-2	5	3	588.01	630.59
-3	15	2	1.96	3.44	-2	25	2	0.77	1.05	-1	5	3	1374.42	1413.31
-2	15	2	0.13	2.60	-1	25	2	557.93	526.13	0	5	3	453.48	380.23
-1	15	2	142.26	138.49	0	25	2	1.12	1.94	1	5	3	380.43	384.43
0	15	2	0.94	2.26	1	25	2	283.76	283.93	2	5	3	421.20	436.95

Calculated and observed structure factors for dichlorobis(4-cyanopyridine)copper(II)

h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2
3	5	3	22.13	24.12	-4	14	3	12.45	10.19	-2	24	3	154.90	137.57
4	5	3	36.29	17.12	-3	14	3	402.47	500.44	-1	24	3	134.20	106.63
-4	6	3	25.45	21.22	-2	14	3	32.18	35.80	0	24	3	123.35	86.33
-3	6	3	178.31	209.11	-1	14	3	305.34	271.04	1	24	3	354.48	338.11
-2	6	3	808.51	886.92	0	14	3	122.89	105.15	2	24	3	0.20	0.41
-1	6	3	1606.69	1661.95	1	14	3	0.88	2.32	-2	25	3	123.20	82.83
0	6	3	201.91	166.59	2	14	3	39.38	44.39	-1	25	3	1.04	0.50
1	6	3	1295.49	1300.10	3	14	3	0.53	0.71	0	25	3	0.37	0.80
2	6	3	172.79	190.51	-4	15	3	4.54	2.73	1	25	3	2.02	1.63
3	6	3	298.96	301.30	-3	15	3	0.07	1.61	2	25	3	1.84	1.40
4	6	3	105.36	72.38	-2	15	3	80.85	103.55	-2	26	3	12.38	5.07
-4	7	3	14.06	12.19	-1	15	3	13.96	12.24	-1	26	3	112.17	77.50
-3	7	3	170.82	191.69	0	15	3	1018.95	827.29	0	26	3	54.91	43.34
-2	7	3	642.88	720.61	1	15	3	2.08	6.42	1	26	3	296.91	268.30
-1	7	3	1036.42	1080.13	2	15	3	767.56	866.66	2	26	3	2.53	1.97
0	7	3	1771.48	1538.20	3	15	3	5.52	6.79	-2	27	3	84.95	102.21
1	7	3	473.78	447.50	-3	16	3	145.37	195.76	-1	27	3	2.11	1.10
2	7	3	517.93	556.98	-2	16	3	83.18	91.19	0	27	3	10.85	11.94
3	7	3	58.26	62.91	-1	16	3	129.03	123.11	1	27	3	0.17	0.55
4	7	3	20.15	11.85	0	16	3	124.88	91.48	-1	28	3	91.63	59.37
-4	8	3	3.32	2.90	1	16	3	0.55	1.82	0	28	3	10.08	13.34
-3	8	3	172.87	188.30	2	16	3	20.55	26.04	1	28	3	140.41	111.12
-2	8	3	245.01	284.75	3	16	3	0.39	1.91	-1	29	3	6.50	4.57
-1	8	3	632.98	626.43	-3	17	3	79.56	112.10	0	29	3	1.04	0.43
0	8	3	462.33	403.06	-2	17	3	18.50	24.50	1	29	3	9.03	4.78
1	8	3	554.71	532.83	-1	17	3	123.75	127.26	0	30	3	30.23	25.41
2	8	3	13.63	16.70	0	17	3	849.11	730.87	-4	0	4	75.93	74.20
3	8	3	36.17	41.42	1	17	3	16.16	15.63	-2	0	4	1084.16	1144.86
4	8	3	33.76	22.82	2	17	3	432.17	508.59	0	0	4	795.62	552.80
-4	9	3	1.04	0.81	3	17	3	65.83	38.60	2	0	4	28.42	26.42
-3	9	3	185.03	198.84	-3	18	3	106.31	130.21	-4	1	4	5.06	5.59
-2	9	3	142.85	152.03	-2	18	3	134.70	158.58	-3	1	4	31.09	32.24
-1	9	3	1133.69	1109.77	-1	18	3	303.06	276.77	-2	1	4	1.05	3.28
0	9	3	1607.68	1354.21	0	18	3	376.36	311.08	-1	1	4	286.30	351.69
1	9	3	76.46	71.14	1	18	3	35.04	37.83	0	1	4	17.15	13.44
2	9	3	543.98	573.40	2	18	3	4.33	3.39	1	1	4	158.14	118.41
3	9	3	154.47	167.66	3	18	3	0.18	0.26	2	1	4	0.18	1.07
4	9	3	61.25	29.92	-3	19	3	70.93	80.91	3	1	4	432.82	448.27
-4	10	3	0.93	1.03	-2	19	3	244.03	278.62	-4	2	4	34.51	30.99
-3	10	3	252.94	258.74	-1	19	3	260.40	206.11	-3	2	4	29.97	32.30
-2	10	3	143.72	171.29	0	19	3	276.05	248.04	-2	2	4	1064.69	1161.40
-1	10	3	585.71	585.19	1	19	3	100.02	90.22	-1	2	4	24.45	23.46
0	10	3	334.96	289.64	2	19	3	107.08	141.00	0	2	4	1514.36	1236.25
1	10	3	18.07	22.91	3	19	3	41.48	46.49	1	2	4	475.35	464.28
2	10	3	16.28	20.84	-3	20	3	96.17	93.50	2	2	4	71.60	67.00
3	10	3	4.96	5.47	-2	20	3	81.87	106.21	3	2	4	74.21	79.91
-4	11	3	11.77	8.74	-1	20	3	183.77	159.93	-4	3	4	69.64	57.35
-3	11	3	85.01	96.08	0	20	3	5.84	11.30	-3	3	4	19.77	27.18
-2	11	3	160.87	177.72	1	20	3	90.67	95.07	-2	3	4	1.26	2.43
-1	11	3	137.76	122.96	2	20	3	7.67	8.82	-1	3	4	60.72	57.31
0	11	3	1659.64	1460.10	3	20	3	35.36	31.89	0	3	4	119.54	106.20
1	11	3	27.21	36.85	-3	21	3	25.28	36.65	1	3	4	446.19	425.72
2	11	3	975.82	1028.38	-2	21	3	56.45	57.48	2	3	4	43.15	38.50
3	11	3	14.24	13.00	-1	21	3	605.43	539.29	3	3	4	359.90	375.40
-4	12	3	1.10	1.10	0	21	3	137.78	94.71	-4	4	4	10.67	10.91
-3	12	3	388.96	455.05	1	21	3	53.17	46.42	-3	4	4	6.49	7.90
-2	12	3	2.80	3.51	2	21	3	112.99	133.03	-2	4	4	1006.19	1114.56
-1	12	3	250.65	239.40	3	21	3	21.25	10.87	-1	4	4	96.25	97.20
0	12	3	358.83	330.66	-3	22	3	1.35	1.14	0	4	4	2335.15	2178.68
1	12	3	64.69	66.73	-2	22	3	57.36	62.89	1	4	4	415.47	398.09
2	12	3	5.05	9.03	-1	22	3	152.14	126.77	2	4	4	207.97	220.87
3	12	3	1.06	1.99	0	22	3	105.98	82.36	3	4	4	89.08	91.19
-4	13	3	6.01	6.43	1	22	3	543.19	532.16	-4	5	4	65.23	49.23
-3	13	3	23.71	27.75	2	22	3	5.27	5.82	-3	5	4	7.63	10.25
-2	13	3	75.17	81.77	-3	23	3	12.17	10.19	-2	5	4	97.39	113.44
-1	13	3	52.31	46.11	-2	23	3	44.60	49.73	-1	5	4	291.22	304.65
0	13	3	2123.70	1826.56	-1	23	3	15.58	16.77	0	5	4	1061.36	926.82
1	13	3	0.11	0.28	0	23	3	114.61	80.12	1	5	4	1023.75	1034.85
2	13	3	1562.73	1823.82	1	23	3	18.26	17.68	2	5	4	381.86	426.82
3	13	3	25.16	23.59	2	23	3	16.95	15.13	3	5	4	212.21	222.82

Calculated and observed structure factors for dichlorobis(4-cyanopyridine)copper(II)

h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2
-4	6	4	123.05	84.81	-3	15	4	33.98	44.73	0	27	4	0.69	1.17
-3	6	4	78.65	89.17	-2	15	4	36.04	42.85	1	27	4	9.43	8.90
-2	6	4	370.33	410.85	-1	15	4	668.44	625.35	-1	28	4	0.35	0.54
-1	6	4	238.47	229.85	0	15	4	150.44	116.88	0	28	4	105.03	94.36
0	6	4	1205.87	1057.74	1	15	4	437.38	445.55	-3	0	5	131.84	141.00
1	6	4	404.93	394.00	2	15	4	7.84	9.56	-1	0	5	0.44	1.59
2	6	4	484.03	531.34	3	15	4	1.31	1.65	1	0	5	1.16	0.08
3	6	4	10.11	10.43	-3	16	4	0.12	0.81	3	0	5	21.76	23.31
-4	7	4	12.91	13.55	-2	16	4	14.35	13.89	-4	1	5	7.95	6.65
-3	7	4	390.87	416.54	-1	16	4	2.19	1.40	-3	1	5	15.81	18.51
-2	7	4	10.08	10.72	0	16	4	55.16	49.71	-2	1	5	214.49	226.08
-1	7	4	701.51	688.05	1	16	4	131.23	122.84	-1	1	5	1.66	1.75
0	7	4	236.22	209.68	2	16	4	116.33	134.18	0	1	5	2005.87	1779.32
1	7	4	682.43	664.44	3	16	4	48.31	36.47	1	1	5	8.75	10.00
2	7	4	600.80	659.31	-3	17	4	120.23	133.29	2	1	5	819.57	900.91
3	7	4	100.54	101.00	-2	17	4	20.53	24.63	3	1	5	5.00	5.98
-4	8	4	63.52	18.22	-1	17	4	706.06	660.25	-4	2	5	6.77	4.48
-3	8	4	252.10	276.86	0	17	4	66.79	58.88	-3	2	5	162.27	172.05
-2	8	4	625.91	707.15	1	17	4	65.32	69.07	-2	2	5	117.30	116.61
-1	8	4	67.05	64.17	2	17	4	18.01	22.45	-1	2	5	55.16	49.75
0	8	4	722.75	598.21	3	17	4	2.42	4.06	0	2	5	146.69	132.05
1	8	4	705.05	706.17	-3	18	4	84.60	34.82	1	2	5	19.54	18.45
2	8	4	315.83	338.72	-2	18	4	16.49	28.01	2	2	5	10.35	14.11
3	8	4	33.89	35.55	-1	18	4	68.70	60.21	3	2	5	16.62	18.32
-4	9	4	52.57	26.67	0	18	4	5.67	8.23	-4	3	5	1.79	1.52
-3	9	4	404.34	454.13	1	18	4	259.34	251.19	-3	3	5	25.06	28.50
-2	9	4	6.89	7.17	2	18	4	98.24	116.03	-2	3	5	329.66	341.02
-1	9	4	2860.62	2850.64	3	18	4	11.79	7.15	-1	3	5	65.21	58.65
0	9	4	462.42	381.36	-3	19	4	98.27	79.08	0	3	5	1383.62	1205.90
1	9	4	613.26	595.52	-2	19	4	1.00	1.58	1	3	5	71.95	74.36
2	9	4	121.96	134.94	-1	19	4	138.27	124.94	2	3	5	510.78	561.51
3	9	4	14.71	15.33	0	19	4	144.42	101.26	3	3	5	74.84	72.27
-4	10	4	0.23	0.28	1	19	4	233.71	233.51	-4	4	5	66.12	43.28
-3	10	4	0.27	0.47	2	19	4	172.16	206.89	-3	4	5	120.41	131.88
-2	10	4	83.76	101.39	-3	20	4	16.38	20.40	-2	4	5	408.96	430.29
-1	10	4	64.10	57.17	-2	20	4	61.86	64.11	-1	4	5	118.37	111.05
0	10	4	807.11	661.28	-1	20	4	17.05	17.08	0	4	5	183.12	175.96
1	10	4	305.73	298.59	0	20	4	217.37	185.43	1	4	5	28.72	25.66
2	10	4	440.03	497.21	1	20	4	82.90	82.48	2	4	5	3.71	6.87
3	10	4	54.54	52.88	2	20	4	75.19	82.79	3	4	5	17.41	19.24
-4	11	4	67.29	51.44	-3	21	4	27.11	30.65	-4	5	5	0.26	0.55
-3	11	4	300.54	331.49	-2	21	4	1.71	0.41	-3	5	5	26.69	28.33
-2	11	4	171.20	202.02	-1	21	4	218.19	180.72	-2	5	5	144.80	158.30
-1	11	4	1706.93	1671.93	0	21	4	214.86	153.84	-1	5	5	93.76	86.33
0	11	4	56.82	49.52	1	21	4	174.03	163.19	0	5	5	1118.61	960.83
1	11	4	685.00	674.60	2	21	4	123.02	122.79	1	5	5	120.60	123.97
2	11	4	100.81	104.71	-2	22	4	263.18	245.67	2	5	5	412.80	463.08
3	11	4	0.32	0.87	-1	22	4	19.59	19.45	3	5	5	204.79	195.86
-4	12	4	3.66	2.44	0	22	4	321.66	258.83	-4	6	5	76.26	15.21
-3	12	4	30.42	34.63	1	22	4	93.48	98.66	-3	6	5	18.57	24.33
-2	12	4	44.76	51.24	2	22	4	51.05	46.35	-2	6	5	679.87	750.90
-1	12	4	108.22	100.82	-2	23	4	0.34	0.58	-1	6	5	296.73	280.61
0	12	4	1.20	1.07	-1	23	4	57.81	40.96	0	6	5	378.15	326.45
1	12	4	21.30	21.53	0	23	4	39.58	39.03	1	6	5	468.19	477.02
2	12	4	366.76	402.41	1	23	4	202.12	200.23	2	6	5	11.10	12.91
3	12	4	16.42	19.87	2	23	4	49.94	14.94	3	6	5	60.01	58.41
-3	13	4	210.75	249.50	-2	24	4	182.44	125.33	-4	7	5	10.17	5.86
-2	13	4	3.04	4.65	-1	24	4	0.62	1.39	-3	7	5	59.31	62.41
-1	13	4	518.13	494.94	0	24	4	358.24	323.01	-2	7	5	80.73	93.38
0	13	4	17.54	14.20	1	24	4	61.43	49.24	-1	7	5	22.18	20.90
1	13	4	214.25	211.40	2	24	4	26.99	25.18	0	7	5	671.20	581.12
2	13	4	0.19	1.29	-2	25	4	4.11	1.83	1	7	5	96.31	99.29
3	13	4	1.77	1.00	-1	25	4	0.29	0.42	2	7	5	303.22	338.11
-3	14	4	6.48	8.91	0	25	4	15.65	18.85	3	7	5	110.64	105.67
-2	14	4	312.42	348.10	1	25	4	61.14	50.11	-3	8	5	59.77	67.81
-1	14	4	48.55	45.62	-2	26	4	174.59	217.43	-2	8	5	590.66	636.32
0	14	4	1.60	1.90	-1	26	4	1.93	0.82	-1	8	5	576.58	543.66
1	14	4	4.13	3.26	0	26	4	95.57	77.32	0	8	5	399.81	354.83
2	14	4	417.25	465.34	1	26	4	9.88	8.78	1	8	5	710.08	766.81
3	14	4	0.05	0.11	-1	27	4	8.96	5.74	2	8	5	136.32	147.86

Calculated and observed structure factors for dichlorobis(4-cyanopyridine)copper(II)

h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2
3	8	5	78.52	64.95	0	19	5	62.37	52.98	-1	6	6	104.18	99.88
-3	9	5	160.50	171.55	1	19	5	1.85	1.84	0	6	6	277.46	263.69
-2	9	5	377.14	414.94	2	19	5	28.30	28.41	1	6	6	253.77	265.05
-1	9	5	94.66	84.82	-2	20	5	46.46	46.30	2	6	6	31.08	33.97
0	9	5	24.05	23.36	-1	20	5	62.99	50.25	3	6	6	15.67	5.04
1	9	5	8.30	13.86	0	20	5	5.39	6.92	-3	7	6	9.94	10.29
2	9	5	9.70	10.99	1	20	5	136.18	131.70	-2	7	6	96.77	97.67
3	9	5	17.29	16.19	2	20	5	59.18	56.26	-1	7	6	111.17	101.76
-3	10	5	157.84	158.70	-2	21	5	38.26	38.11	0	7	6	250.83	233.62
-2	10	5	5.94	9.92	-1	21	5	128.06	94.68	1	7	6	23.83	25.89
-1	10	5	773.01	734.96	0	21	5	177.07	134.35	2	7	6	6.18	6.64
0	10	5	63.18	51.07	1	21	5	2.94	3.29	3	7	6	2.68	2.85
1	10	5	343.13	360.94	2	21	5	63.68	39.82	-3	8	6	12.99	11.68
2	10	5	109.76	116.01	-2	22	5	46.54	38.61	-2	8	6	88.35	93.35
3	10	5	114.11	113.40	-1	22	5	48.19	42.05	-1	8	6	179.88	162.41
-3	11	5	107.05	106.55	0	22	5	2.06	2.36	0	8	6	0.39	1.65
-2	11	5	135.32	149.13	1	22	5	19.91	21.96	1	8	6	568.77	631.48
-1	11	5	1338.42	1211.73	-2	23	5	72.33	18.27	2	8	6	0.12	0.57
0	11	5	9.96	14.18	-1	23	5	50.31	42.06	-3	9	6	0.62	0.81
1	11	5	103.41	116.11	0	23	5	205.83	173.34	-2	9	6	15.49	15.73
2	11	5	3.39	5.69	1	23	5	2.24	2.28	-1	9	6	51.57	46.27
3	11	5	24.36	16.62	-2	24	5	19.52	11.92	0	9	6	90.40	77.29
-3	12	5	10.03	9.20	-1	24	5	7.24	5.73	1	9	6	50.10	50.27
-2	12	5	103.56	115.04	0	24	5	33.61	31.28	2	9	6	44.79	48.39
-1	12	5	506.31	440.96	1	24	5	0.50	1.16	-3	10	6	0.02	0.83
0	12	5	234.98	215.70	-1	25	5	1.55	0.73	-2	10	6	100.55	109.99
1	12	5	1549.55	1701.78	0	25	5	247.89	212.12	-1	10	6	125.73	109.86
2	12	5	14.26	14.75	1	25	5	0.27	0.37	0	10	6	40.64	36.69
3	12	5	99.02	50.34	-1	26	5	1.19	0.71	1	10	6	42.23	46.22
-3	13	5	34.12	40.39	0	26	5	1.86	1.23	2	10	6	4.15	6.11
-2	13	5	4.05	5.36	-2	0	6	4.13	4.68	-3	11	6	14.79	15.21
-1	13	5	46.12	45.75	0	0	6	413.21	378.48	-2	11	6	0.14	0.42
0	13	5	61.38	56.21	2	0	6	576.43	632.89	-1	11	6	6.91	6.78
1	13	5	37.95	39.52	-3	1	6	409.65	408.83	0	11	6	239.20	217.07
2	13	5	9.73	11.72	-2	1	6	20.94	21.60	1	11	6	261.42	280.91
3	13	5	7.07	5.68	-1	1	6	1083.68	1020.14	2	11	6	59.00	66.03
-3	14	5	3.97	4.52	0	1	6	25.02	26.59	-3	12	6	0.03	0.49
-2	14	5	8.02	8.73	1	1	6	181.52	195.08	-2	12	6	571.60	591.04
-1	14	5	561.24	497.58	2	1	6	8.93	12.76	-1	12	6	5.40	5.78
0	14	5	27.14	28.85	3	1	6	0.36	0.53	0	12	6	411.75	384.62
1	14	5	958.10	1041.50	-3	2	6	18.13	15.73	1	12	6	1.60	1.51
2	14	5	18.81	19.46	-2	2	6	0.44	0.67	2	12	6	0.09	0.18
3	14	5	87.88	61.39	-1	2	6	13.76	14.12	-3	13	6	5.47	7.36
-3	15	5	29.71	31.65	0	2	6	292.80	276.15	-2	13	6	0.10	0.21
-2	15	5	95.17	101.83	1	2	6	37.85	37.95	-1	13	6	148.28	111.44
-1	15	5	221.55	188.75	2	2	6	620.82	682.83	0	13	6	0.81	1.13
0	15	5	39.52	36.38	3	2	6	4.68	4.46	1	13	6	447.43	481.93
1	15	5	0.61	1.29	-3	3	6	252.81	256.87	2	13	6	5.32	5.50
2	15	5	1.99	3.13	-2	3	6	34.57	36.58	-3	14	6	3.95	2.63
-3	16	5	30.83	33.12	-1	3	6	558.47	546.57	-2	14	6	466.96	448.50
-2	16	5	0.33	0.37	0	3	6	268.52	250.83	-1	14	6	0.36	1.71
-1	16	5	282.69	242.97	1	3	6	207.48	233.23	0	14	6	647.33	592.79
0	16	5	12.14	14.78	2	3	6	109.05	131.98	1	14	6	6.94	6.54
1	16	5	379.68	379.70	3	3	6	12.89	10.72	2	14	6	27.95	28.44
2	16	5	65.28	72.64	-3	4	6	2.21	3.09	-3	15	6	7.00	5.74
-3	17	5	114.81	33.49	-2	4	6	0.13	1.32	-2	15	6	0.31	0.62
-2	17	5	57.29	63.83	-1	4	6	120.06	113.85	-1	15	6	47.52	40.77
-1	17	5	169.71	128.77	0	4	6	237.83	234.89	0	15	6	49.44	44.14
0	17	5	2.47	2.69	1	4	6	32.76	38.71	1	15	6	518.03	542.69
1	17	5	31.94	32.97	2	4	6	438.20	490.49	2	15	6	31.49	32.04
2	17	5	0.81	1.73	3	4	6	0.85	0.39	-2	16	6	281.32	302.69
-3	18	5	6.63	3.48	-3	5	6	43.63	47.94	-1	16	6	86.58	68.24
-2	18	5	24.42	25.80	-2	5	6	18.76	17.64	0	16	6	232.17	205.65
-1	18	5	221.92	190.58	-1	5	6	397.33	380.00	1	16	6	7.59	8.67
0	18	5	3.87	2.60	0	5	6	543.25	518.34	2	16	6	46.01	44.98
1	18	5	284.64	292.41	1	5	6	222.20	251.81	-2	17	6	5.00	5.49
2	18	5	91.78	98.82	2	5	6	122.33	136.16	-1	17	6	6.55	7.81
-3	19	5	102.90	142.24	3	5	6	1.19	1.31	0	17	6	49.37	44.57
-2	19	5	44.64	46.62	-3	6	6	0.80	0.96	1	17	6	122.97	132.33
-1	19	5	206.42	171.66	-2	6	6	24.79	26.52	2	17	6	14.65	15.83

Calculated and observed structure factors for dichlorobis(4-cyanopyridine)copper(II)

h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2	h	k	l	Fc^2	Fo^2
2	17	6	14.65	15.83	-3	6	7	10.14	9.22	0	17	7	278.99	262.14
-2	18	6	137.13	147.10	-2	6	7	45.09	44.56	1	17	7	5.32	5.61
-1	18	6	62.85	47.53	-1	6	7	103.45	99.61	-1	18	7	10.85	10.33
0	18	6	84.49	72.43	0	6	7	2.05	2.45	0	18	7	1.62	2.03
1	18	6	177.19	186.10	1	6	7	60.34	68.84	-1	19	7	25.35	23.37
-2	19	6	8.31	9.08	2	6	7	38.52	39.92	0	19	7	48.26	37.30
-1	19	6	36.56	35.41	-3	7	7	130.33	122.59	-2	0	8	95.17	99.27
0	19	6	42.05	39.24	-2	7	7	37.69	38.03	0	0	8	0.23	1.28
1	19	6	43.24	45.97	-1	7	7	47.44	42.61	-2	1	8	2.64	1.90
-2	20	6	28.14	22.04	0	7	7	74.50	72.06	-1	1	8	4.00	4.60
-1	20	6	125.45	94.47	1	7	7	57.71	62.70	0	1	8	0.27	0.47
0	20	6	79.28	67.77	2	7	7	43.30	44.05	1	1	8	171.03	184.24
1	20	6	114.21	110.62	-3	8	7	15.14	12.23	-2	2	8	132.30	124.91
-2	21	6	1.16	0.31	-2	8	7	38.74	35.19	-1	2	8	37.69	34.99
-1	21	6	25.86	21.98	-1	8	7	18.62	17.23	0	2	8	15.86	16.63
0	21	6	74.75	63.37	0	8	7	8.95	10.88	1	2	8	27.22	28.84
1	21	6	6.23	6.34	1	8	7	58.43	62.67	-2	3	8	24.40	23.42
-1	22	6	46.54	34.02	2	8	7	117.69	122.30	-1	3	8	54.61	45.63
0	22	6	8.40	7.07	-3	9	7	53.43	57.74	0	3	8	43.07	38.56
1	22	6	62.12	52.24	-2	9	7	114.65	117.63	1	3	8	175.14	187.02
-1	23	6	18.05	12.07	-1	9	7	80.12	65.02	-2	4	8	120.75	111.88
0	23	6	27.27	27.24	0	9	7	312.45	295.61	-1	4	8	67.90	66.92
-3	0	7	79.24	68.85	1	9	7	6.52	7.92	0	4	8	95.42	91.77
-1	0	7	690.65	635.52	2	9	7	104.22	105.23	1	4	8	28.06	33.27
1	0	7	513.21	557.96	-2	10	7	37.31	41.30	-2	5	8	49.20	45.52
-3	1	7	0.12	0.15	-1	10	7	0.14	0.80	-1	5	8	95.49	81.37
-2	1	7	9.53	9.07	0	10	7	13.99	12.84	0	5	8	120.73	105.76
-1	1	7	17.27	14.83	1	10	7	10.19	11.46	1	5	8	194.10	203.44
0	1	7	10.11	11.58	2	10	7	74.28	76.10	-2	6	8	59.36	59.47
1	1	7	11.04	14.04	-2	11	7	133.84	139.27	-1	6	8	122.83	111.29
2	1	7	35.32	34.73	-1	11	7	12.56	8.79	0	6	8	125.39	110.91
-3	2	7	32.14	30.29	0	11	7	379.71	365.11	1	6	8	23.06	24.92
-2	2	7	119.38	110.10	1	11	7	2.16	3.13	-2	7	8	23.81	23.16
-1	2	7	543.52	500.64	2	11	7	109.25	109.47	-1	7	8	48.03	41.83
0	2	7	28.52	26.71	-2	12	7	26.53	31.74	0	7	8	152.86	148.30
1	2	7	619.14	687.34	-1	12	7	5.47	3.67	1	7	8	55.93	55.50
2	2	7	17.80	19.64	0	12	7	12.00	11.92	-2	8	8	0.80	0.70
-3	3	7	7.36	7.45	1	12	7	0.43	1.11	-1	8	8	84.72	68.46
-2	3	7	0.34	0.84	-2	13	7	106.68	111.27	0	8	8	39.59	37.65
-1	3	7	4.07	2.84	-1	13	7	10.12	10.70	1	8	8	28.69	31.06
0	3	7	11.81	11.98	0	13	7	463.12	451.04	-2	9	8	29.04	27.40
1	3	7	66.18	75.05	1	13	7	10.48	11.25	-1	9	8	3.32	3.93
2	3	7	25.97	27.41	-2	14	7	11.18	12.39	0	9	8	79.17	72.38
-3	4	7	7.01	7.79	-1	14	7	1.00	1.69	1	9	8	5.67	6.55
-2	4	7	102.03	101.29	0	14	7	0.12	0.77	-1	10	8	62.11	47.99
-1	4	7	377.13	342.59	1	14	7	2.70	2.78	0	10	8	59.90	54.28
0	4	7	1.82	2.28	-2	15	7	104.45	102.90	1	10	8	51.07	54.50
1	4	7	328.54	361.70	-1	15	7	0.24	0.29	-1	11	8	47.36	36.76
2	4	7	4.05	3.96	0	15	7	380.28	350.30	0	11	8	4.00	3.73
-3	5	7	82.26	73.97	1	15	7	8.37	9.79	-1	12	8	23.24	20.10
-2	5	7	17.86	18.89	-2	16	7	40.65	37.60	0	12	8	107.36	95.89
-1	5	7	42.88	38.56	-1	16	7	0.11	0.35	-1	13	8	125.87	105.68
0	5	7	15.33	16.74	0	16	7	0.88	0.58	0	13	8	0.07	0.43
1	5	7	163.13	177.40	1	16	7	16.16	16.26					
2	5	7	4.24	5.28	-1	17	7	0.06	0.43					