

## Dichloro[6-methyl-2-(2-pyridylmethyl)-pyridine-*N,N'*]copper(II)

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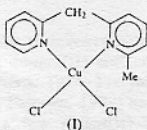
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### Abstract

The crystal structure of  $[\text{CuCl}_2(\text{C}_{12}\text{H}_{12}\text{N}_2)]$  is reported. The complex is monomeric, with the Cu atom coordinated to two N atoms and two  $\text{Cl}^-$  ions. The compound displays simple paramagnetic behaviour.

### Comment

Copper(II) shows a great 'plasticity' in its coordination geometries, as expected for an ion with Jahn–Teller active ground states (Bersuker, 1984). This fact has permitted the magneto-structural studies of  $\text{Cu}^{\text{II}}$  complexes with heterocyclic amines. Continuing the characterization of complexes with di(2-pyridyl)methane ligands, we have prepared  $[\text{Cu}(\text{MeDPM})_2\text{Cl}_2]$ , (I), where MeDPM is 6-methyl-2-(2-pyridylmethyl)pyridine. While the chloro and bromo di(2-pyridyl)copper(II) complexes are dimeric in nature and show a ferromagnetically coupled ground state (Spodine, Manzur, Peña & Garland, 1986; Spodine *et al.*, 1993), the title complex is found to be monomeric, with simple paramagnetic behaviour.



The Cu atom is coordinated to two N atoms from the bidentate MeDPM ligand and to two Cl<sup>-</sup> ions [Cu—N 2.010 (4) and 2.013 (4) Å, Cu—Cl 2.224 (2) and 2.242 (2) Å]. The dihedral angle between the N—Cu—N and Cl—Cu—Cl planes is 48°, half-way between that characterizing a square-planar arrangement (0°) and that of a regular tetrahedron (90°). Inspection of Fig. 1 suggests that the driving force for this distortion is the steric repulsion between the methyl group attached to C11 and the chloro ligand. This argument is supported by comparison with the closely related structure of dichloro- $\mu$ -chloro-bis(dipyridylmethane)dycopper(II) (Spodine *et al.*, 1993), which differs from (I) only in the absence of the methyl substituent; in this complex the homologous dihedral angle spans 29° and is much closer to that of a planar arrangement. This fact in turn seems to enable the inclusion of a fifth ligand in the Cu coordination sphere (a symmetry-related Cl atom), leading to the formation of a dimer. The monomeric nature of (I) then seems to be a direct consequence of the presence of the methyl group in the organic chelate. Another interesting difference between these two structures is the dihedral angle between the two pyridyl rings of the organic ligand, which in the dimeric complex is 64.8° (one of the largest found), while in (I) it has a value of 56.2 (2)°, the smallest reported (Garland, Grandjean, Spodine & Manzur, 1987; Garland, Le Marouille, Spodine & Manzur, 1986; Spodine *et al.*, 1993; Spodine *et al.*, 1991).

There are three short non-bonding H...Cl contacts below 3.0 Å in the structure: C4—H4A...Cl2' ca 2.95 Å, C6—H6B...Cl1' ca 2.91 Å and C8—H8A...Cl1' ca 2.97 Å [symmetry code: (i)  $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$ ] (Fig. 2).

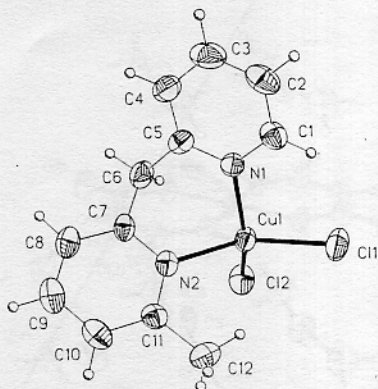


Fig. 1. View of the molecule showing the labelling of the non-H atoms. Displacement ellipsoids are plotted at the 50% probability level.

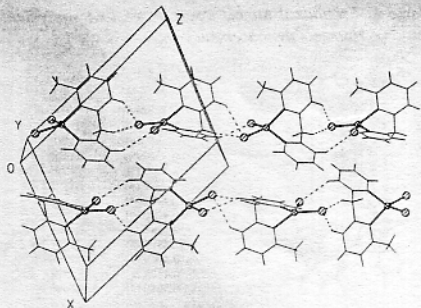


Fig. 2. Packing of the molecules showing the short non-bonding intermolecular contacts.

## Experimental

### Crystal data

[CuCl<sub>2</sub>(C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>)]

*M<sub>r</sub>* = 318.68

Monoclinic

*P*2<sub>1</sub>/*n*

*a* = 12.125 (2) Å

*b* = 7.593 (2) Å

*c* = 15.216 (3) Å

$\beta$  = 112.86 (3)°

*V* = 1290.8 (5) Å<sup>3</sup>

*Z* = 4

*D<sub>x</sub>* = 1.640 Mg m<sup>-3</sup>

Mo *K*α radiation

$\lambda$  = 0.71073 Å

Cell parameters from 25

reflections

$\theta$  = 7.5–12.5°

$\mu$  = 2.083 mm<sup>-1</sup>

*T* = 293 (2) K

Plate

0.42 × 0.32 × 0.06 mm

Green

### Data collection

Siemens R3m diffractometer

$\theta/2\theta$  scans (4.19–29.3°

min<sup>-1</sup>)

Absorption correction:

none

1793 measured reflections

1702 independent reflections

1387 observed reflections

[*I* > 2 $\sigma$ (*I*)]

*R*<sub>int</sub> = 0.0263

$\theta_{\max}$  = 22.76°

*h* = 0 → 13

*k* = 0 → 8

*l* = -16 → 15

2 standard reflections

monitored every 98

reflections

intensity variation: none

### Refinement

Refinement on *F*<sup>2</sup>

$R[F^2 > 2\sigma(F^2)] = 0.0476$

*wR*(*F*<sup>2</sup>) = 0.1137

*S* = 1.163

1702 reflections

154 parameters

H-atom parameters not

refined

$w = 1/[\sigma^2(F_o^2) + (0.0812P)^2$

+ 0.1467P]

where  $P = (F_o^2 + 2F_c^2)/3$

( $\Delta/\sigma$ )<sub>max</sub> = 0.094

$\Delta\rho_{\max} = 0.715 \text{ e } \text{Å}^{-3}$

$\Delta\rho_{\min} = -0.846 \text{ e } \text{Å}^{-3}$

Extinction correction: none

Atomic scattering factors

from *International Tables*

for *Crystallography* (1992,

Vol. C, Tables 4.2.6.8 and

6.1.1.4)

**Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ )**

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	$U_{\text{eq}}$
Cu1	0.02025 (5)	0.13736 (8)	0.27088 (4)	0.0348 (3)
C11	-0.06963 (12)	-0.0144 (2)	0.13690 (9)	0.0525 (4)
C12	-0.02378 (13)	0.4119 (2)	0.21378 (9)	0.0506 (4)
N1	0.1573 (3)	-0.0303 (6)	0.3314 (3)	0.0350 (10)
N2	0.0250 (3)	0.1991 (5)	0.4009 (3)	0.0332 (10)
C1	0.1621 (5)	-0.1945 (7)	0.2977 (4)	0.0412 (13)
C2	0.2583 (5)	-0.3027 (8)	0.3413 (4)	0.051 (2)
C3	0.3487 (5)	-0.2486 (9)	0.4220 (4)	0.056 (2)
C4	0.3433 (5)	-0.0819 (9)	0.4591 (4)	0.050 (2)
C5	0.2471 (4)	0.0254 (7)	0.4113 (3)	0.0376 (13)
C6	0.2378 (5)	0.2084 (7)	0.4463 (4)	0.0445 (13)
C7	0.1316 (4)	0.2298 (7)	0.4722 (3)	0.0351 (12)
C8	0.1399 (5)	0.2790 (7)	0.5618 (4)	0.0448 (14)
C9	0.0397 (6)	0.2996 (8)	0.5802 (4)	0.0513 (15)
C10	-0.0690 (5)	0.2687 (7)	0.5076 (4)	0.0465 (14)
C11	-0.0751 (4)	0.2173 (7)	0.4181 (3)	0.0378 (12)
C12	-0.1897 (5)	0.1826 (9)	0.3371 (4)	0.053 (2)

**Table 2. Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ )**

Cu1—N1	2.010 (4)	C3—C4	1.397 (9)
Cu1—N2	2.013 (4)	C4—C5	1.376 (7)
Cu1—C11	2.224 (2)	C5—C6	1.508 (8)
Cu1—C12	2.242 (2)	C6—C7	1.496 (7)
N1—C5	1.346 (6)	C7—C8	1.379 (7)
N1—C1	1.359 (7)	C8—C9	1.358 (8)
N2—C11	1.345 (6)	C9—C10	1.371 (8)
N2—C7	1.346 (6)	C10—C11	1.391 (7)
C1—C2	1.370 (8)	C11—C12	1.479 (7)
C2—C3	1.353 (8)		
N1—Cu1—N2	89.7 (2)	C5—C4—C3	119.0 (5)
N1—Cu1—C11	96.64 (12)	N1—C5—C4	120.9 (5)
N2—Cu1—C11	146.99 (13)	N1—C5—C6	117.6 (4)
N1—Cu1—C12	142.80 (12)	C4—C5—C6	121.5 (5)
N2—Cu1—C12	94.36 (12)	C7—C6—C5	112.5 (4)
C11—Cu1—C12	99.70 (6)	N2—C7—C8	121.5 (5)
C5—N1—C1	119.4 (4)	N2—C7—C6	115.1 (4)
C5—N1—Cu1	116.7 (3)	C8—C7—C6	123.4 (4)
C1—N1—Cu1	123.9 (3)	C9—C8—C7	120.5 (5)
C11—N2—C7	118.8 (4)	C8—C9—C10	118.1 (5)
C11—N2—Cu1	122.2 (3)	C9—C10—C11	120.4 (5)
C7—N2—Cu1	119.0 (3)	N2—C11—C10	120.7 (5)
N1—C1—C2	121.4 (5)	N2—C11—C12	116.5 (4)
C3—C2—C1	119.6 (6)	C10—C11—C12	122.8 (5)
C2—C3—C4	119.6 (5)		

Data collection and cell refinement: *P3/P4-PC Diffractometer Program* (Siemens, 1991). Data reduction: *SHELXTL/PC XDISK* (Sheldrick, 1991). Program(s) used to solve structure: *SHELXTL/PC XS*. Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1994). Molecular graphics: *SHELXTL/PC XP*. Software used to prepare material for publication: *SHELXL93 CIFTAB*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, least-squares-planes data and torsion angles have been deposited with the IUCr (Reference: BK1029). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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