{4,6-Dichloro-2-[(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)iminomethyl]phenolato-κ²*N*,*O*}copper(II)

Guo-Bing Yan, Ming-Hua Yang* and Yun-Fa Zheng

Department of Chemistry, Lishui College, 323000 Lishui, ZheJiang, People's Republic of China

Correspondence e-mail: zjls05@56.com

In the mononuclear title complex, [Cu(C$_{18}$H$_{14}$Cl$_2$N$_3$O$_2$)$_2$], the Cu^{II} atom is coordinated by two N atoms and two O atoms from the Schiff base ligands in a square-planar geometry, with a dihedral angle between the two chelate NCuO planes of 31.57 (3)°. The Cu atom is located on a twofold axis.

Comment

There has been continuous interest in bis-bidentate Schiff base Cu^{II} complexes because, in the solid state, the ligands display a wide range of geometric arrangements around copper, from ideal *trans*-square-planar to deformed tetrahedral geometry (Bluhm *et al.*, 2003; Lacroix *et al.*, 2004). In investigations of these complexes based on bis-bidentate Schiff base ligands, both electronic effects (Maslen & Waters, 1975) and crystal packing (Panova *et al.*, 1980) have been invoked as the driving forces responsible for the distortion. In this paper, we report the synthesis and crystal structure of the title complex, (I).

(I)
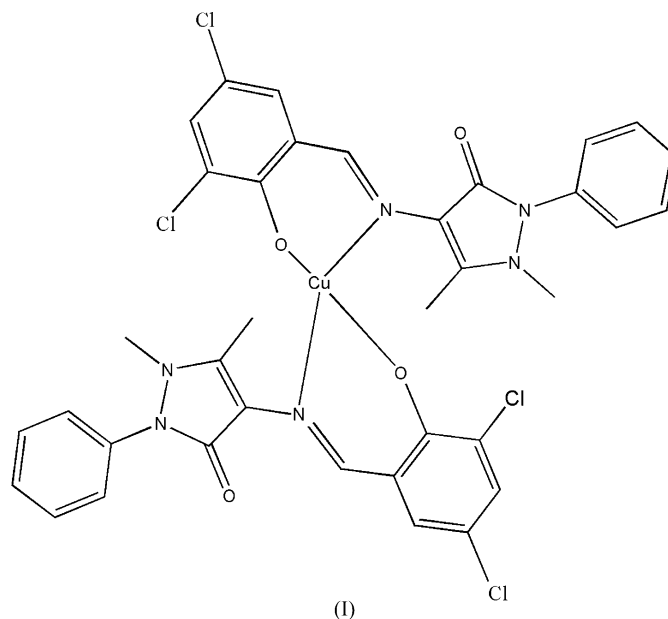
The Cu atom is located on a twofold axis, and it is coordinated in a square-planar geometry, defined by two O atoms and two N atoms from the ligands (Fig. 1). The dihedral angle between the two ligand coordination planes [Cu1/N1/O1 and Cu1/N1*A*/O1*A*; symmetry code: (*A*) −*x*, *y*, ½ − *z*] is 31.57 (3)°. The bond lengths and angles at the Cu^{II} atom are given in Table 1 and the torsion angle C17—C18—N1—C1 is 177.95 (2)°. The packing is governed by weak hydrogen bonds (Table 2 and Fig. 2).

Experimental

The title compound was prepared by the addition of $[Cu(OAc)_2]$ (0.5 mmol) and 4-(3,5-dichloro-2-hydroxylbenzylideneamino)-1,5-dimethyl-2-phenyl-1,2-dihydropyrazol-3-one (1 mmol) to a hot aqueous ethanol solution (50%, 30 ml). The mixture was stirred for 10 h and filtered. The filtrate was then added to a mixed solvent (EtOH–CH$_2$Cl$_2$ = 1:1, 10 ml), and dark-blue single crystals were obtained at room temperature over a period of days.

Crystal data

$[Cu(C_{18}H_{14}Cl_2N_3O_2)_2]$	$Z = 4$
$M_r = 813.98$	$D_x = 1.514$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 23.4341$ (17) Å	$\mu = 0.96$ mm^{-1}
$b = 6.7434$ (5) Å	$T = 273$ (2) K
$c = 22.6048$ (16) Å	Prism, blue
$\beta = 91.570$ (1)°	$0.34 \times 0.16 \times 0.13$ mm
$V = 3570.8$ (4) Å^3	

Data collection

Bruker APEX-II area-detector diffractometer	10369 measured reflections
φ and ω scans	3172 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2660 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.031$
$T_{min} = 0.736$, $T_{max} = 0.885$	$\theta_{max} = 25.2°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0692P)^2 + 0.3862P]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.105$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.08$	$\Delta\rho_{max} = 0.55$ e Å^{-3}
3172 reflections	$\Delta\rho_{min} = -0.37$ e Å^{-3}
233 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.8835 (15)	Cu1—N1	1.9587 (17)
O1^i—Cu1—O1	154.58 (11)	O1—Cu1—N1	93.73 (7)
O1^i—Cu1—N1	90.65 (7)	N1—Cu1—N1^i	159.96 (11)

Symmetry code: (i) $-x, y, -z + \frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C11—H11$\cdots$O2	0.93	2.49	2.950 (3)	111
C5—H5$A\cdots$O2^{ii}	0.96	2.46	3.352 (3)	154

Symmetry code: (ii) $-x, -y, -z$.

H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) and 0.96 Å (methyl), and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic and $1.5U_{eq}(C)$ for methyl H atoms.

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2; data reduction: APEX2; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: APEX2; software used to prepare material for publication: APEX2.
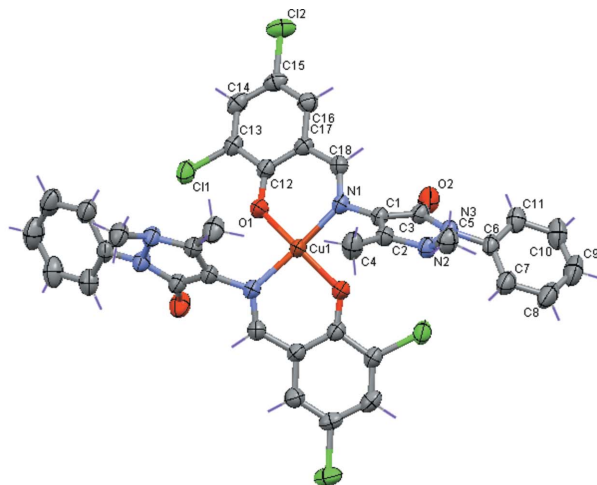

Figure 1
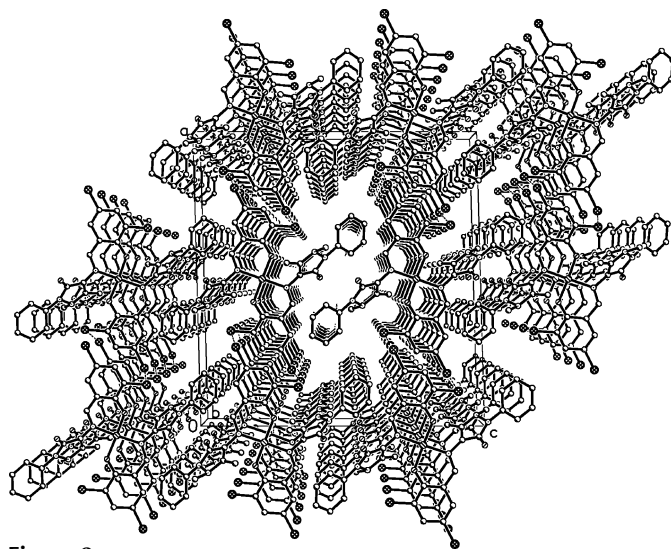The molecular structure of (I), showing 50% probability displacement ellipsoids. [Symmetry code: (A) $-x, y, \frac{1}{2} - z$.]

Figure 2
A packing diagram of the title complex.

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