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Methanol[4-nitro-2-(pyridin-2-ylmethyliminomethyl)phenolato](thiocyanato)copper(II)

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Key indicators

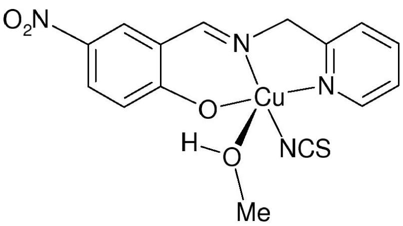
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.043
wR factor = 0.120
Data-to-parameter ratio = 16.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[Cu(C_{13}H_{10}N_3O_3)(NCS)(CH_4O)]$, is a mononuclear copper(II) complex. The Cu^{II} atom has a square-pyramidal geometry. In the basal plane, the Cu atom is coordinated by two N atoms and one O atom of the Schiff base, and by the N atom of a thiocyanate anion. The apical position is occupied by the O atom of a coordinated MeOH molecule. In the crystal structure, the molecules are linked *via* intermolecular O—H$\cdots$O hydrogen bonds, forming chains parallel to the *b* axis.

Comment

Over the last few years, there has been a burgeoning effort to identify the biological role of copper, primarily through techniques associated with the interface of biology, biochemistry and coordination chemistry (Collinson & Fenton, 1996; Hossain *et al.*, 1996; Tarafder *et al.*, 2002). It appears that the biological role of copper is primarily in redox reactions and as a biological catalyst, although much remains to be understood (Musie *et al.*, 2003; García-Raso *et al.*, 2003). An extensive effort has been made to prepare and characterize a variety of copper(II) coordination complexes in an attempt to model the physical and chemical behaviour of copper-containing enzymes (Reddy *et al.*, 2000). The peculiarity of copper lies in its ability to form complexes with coordination numbers of four, five and six (Ray *et al.*, 2003; Arnold *et al.*, 2003; Raptopoulou *et al.*, 1998). As part of our investigation in this area, we report here the title mononuclear copper(II) complex, (I) (Fig. 1.)



(I)

The Cu atom in (I) has a square-pyramidal coordination geometry. In the basal plane, the Cu^{II} atom is coordinated by the pyridine and imine N atoms and the phenolate O atom of the Schiff base ligand, together with one N atom from a thiocyanate anion. The apical position is occupied by an O atom of a coordinated MeOH molecule. A slight distortion of the square pyramid is revealed by the bond angles between the apical and basal donor atoms (Table 1). The bond angles between the donor atoms in the basal positions show less distortion. The apical bond of the square pyramid is longer

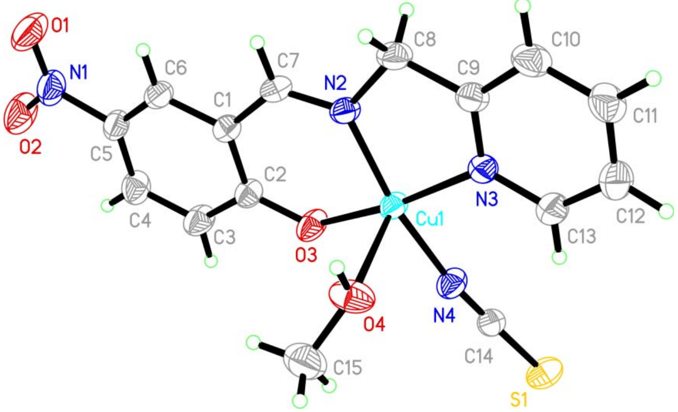


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

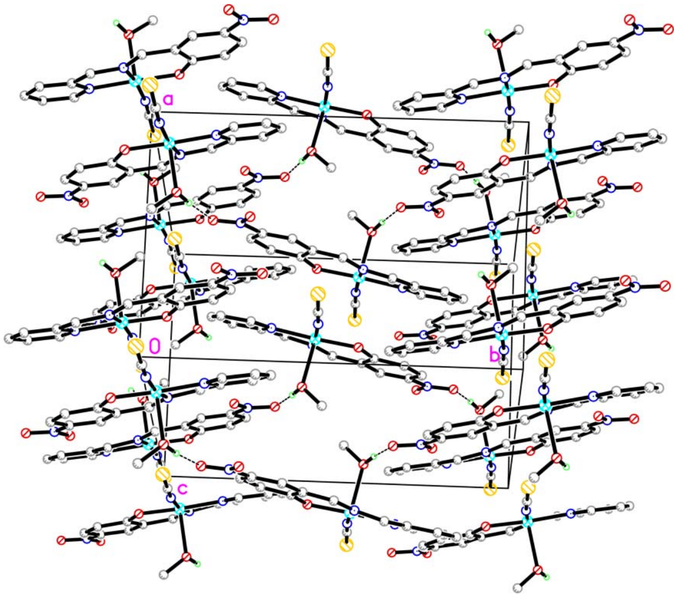


Figure 2
The crystal packing of (I). Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

than the basal bonds (Table 1), which is probably due to the formation of an intermolecular O4—H4*A*···O2 hydrogen bond. The N2—Cu1—N3 bond angle deviates from 90° by 8.07 (10)°, due to the strain created by the Cu1/N2/C8/C9/N3 five-membered chelate ring. The dihedral angle between the O1/N1/O2 plane and the C1–C6 benzene ring is 5.1 (3)°.

In the crystal structure of (I), the molecules are linked *via* intermolecular O—H···O hydrogen bonds, forming chains parallel to the *b* axis (Fig. 2 and Table 2).

Experimental

5-Nitrosalicylaldehyde (0.1 mmol, 16.7 mg) and 2-aminomethylpyridine (0.1 mmol, 10.8 mg) were dissolved in MeOH (10 ml). The mixture was stirred for 1 h to give a yellow solution, which was added to a stirred aqueous solution of NH_4NCS (0.1 mmol, 7.6 mg, 3 ml) and a solution of $Cu(CH_3COO)_2\cdot H_2O$ (0.1 mmol, 19.9 mg) in MeOH (5 ml). The mixture was stirred at room temperature for 30 min and then filtered. The filtrate was kept in air for 8 d, forming blue block-shaped crystals of (I).

Crystal data

$[Cu(C_{13}H_{10}N_3O_3)(NCS)(CH_4O)]$
$M_r = 409.90$
Monoclinic, $P2_1/n$
$a = 10.539$ (2) Å
$b = 15.986$ (2) Å
$c = 10.905$ (2) Å
$\beta = 113.480$ (2)°
$V = 1685.1$ (5) Å^3
$Z = 4$
$D_x = 1.616$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3174 reflections
$\theta = 2.3$–24.4°
$\mu = 1.45$ mm^{-1}
$T = 298$ (2) K
Block, blue
0.25 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.714$, $T_{max} = 0.845$
14081 measured reflections
3837 independent reflections
2734 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 27.5°$
$h = -13 \rightarrow 13$
$k = -20 \rightarrow 20$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.120$
$S = 1.03$
3837 reflections
230 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2 + 0.2163P]$
where = $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.78$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.931 (2)	Cu1—N3	2.013 (2)
Cu1—N4	1.939 (3)	Cu1—O4	2.304 (3)
Cu1—N2	1.943 (2)		
O3—Cu1—N4	90.51 (10)	N2—Cu1—N3	81.93 (10)
O3—Cu1—N2	91.92 (9)	O3—Cu1—O4	94.29 (11)
N4—Cu1—N2	168.94 (11)	N4—Cu1—O4	90.08 (11)
O3—Cu1—N3	172.83 (10)	N2—Cu1—O4	100.49 (10)
N4—Cu1—N3	94.85 (11)	N3—Cu1—O4	90.46 (10)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O2^i	0.88 (3)	1.94 (1)	2.818 (3)	169 (3)

Symmetry code: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$.

Atom H4*A* was located in a difference Fourier map and refined isotropically, with the O—H distance restrained to 0.90 (1) Å. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics:

SHELXTL (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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