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Methanol[4-nitro-2-(2-pyridylmethyliminomethyl)phenolato]copper(II) perchlorate

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In the title mononuclear copper(II) complex, [Cu($C_{13}H_{10}N_3O_3$)(CH_4O)]ClO_4, the Cu^{II} atom is four-coordinated by one N and two O atoms of the Schiff base ligand and by one O atom of the methanol molecule, forming a slightly distorted square-planar coordination. In the crystal structure, pairs of cations are linked into a centrosymmetric dimer *via* intermolecular O—H···O hydrogen bonds.

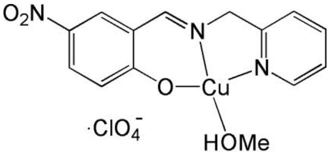
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.010 Å
Disorder in solvent or counterion
R factor = 0.087
wR factor = 0.160
Data-to-parameter ratio = 11.8

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

Comment

Recently, the author has reported the structures of a few Schiff base metal complexes (You, 2006*a*,*b*; You & Zhu, 2006). As an extension of the work on the structural characterization of these complexes, the crystal structure of the title copper(II) complex, (I), is reported here.



(I)

Complex (I) is a mononuclear copper(II) compound (Fig. 1), which consists of a methanol[4-nitro-2-(2-pyridylmethyliminomethyl)phenolato]copper(II) cation and a disordered perchlorate anion. The Cu^{II} atom is four-coordinated in a square-planar coordination by one O and two N atoms of the Schiff base ligand and by one O atom of the methanol molecule. The *trans* angles in the CuO_2N_2 square plane are 176.0 (2) and 175.7 (2)°, indicating a slightly distorted square-planar coordination. However, the Cu1—O5 [2.527 (13)Å] and Cu1—O6^i [2.469 (13) Å; symmetry code: (i) 1 + *x*, *y*, *z*] distances are appreciably less than the sum of the corresponding van der Waals radii (3.84 Å). If this bonding is considered to be significant, then the coordination around the Cu^{II} atom may be alternatively described as elongated octahedral with the O5 and O6^i atoms in axial positions. The Cu—O and Cu—N bond lengths (Table 1) are comparable to the corresponding values observed in other Schiff base copper(II) complexes (You *et al.*, 2006; You, 2006*c*,*d*; MacLachlan *et al.*, 1996; Colacio *et al.*, 2000). The dihedral angle between the C1–C6 benzene ring and the C9–C13/N3 pyridine ring is 13.6 (2)°.

In the crystal structure, adjacent cations are linked through intermolecular O—H···O hydrogen bonds (Table 2), forming dimers. If the longer Cu···O(perchlorate) coordination is taken into account, then the dimers are further linked by the perchlorate anions, forming chains running along the *a* axis (Fig. 2).

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Experimental

All reagents were of commercially available grade and were used without further purification. 5-Nitrosalicylaldehyde (0.1 mmol, 16.5 mg) and pyridin-2-ylmethylamine (0.1 mmol, 10.8 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added a MeOH solution (10 ml) of $Cu(ClO_4)_2\cdot 7H_2O$ (0.1 mmol, 38.9 mg) with stirring. The mixture was stirred for another 10 min at room temperature. After leaving the filtrate to stand in air for 5 d, blue needle-shaped crystals of (I) were formed. Analysis found: C 37.11, H 3.23, N 9.17%; calculated for $C_{14}H_{14}ClCuN_3O_8$: C 37.26, H 3.13, N 9.31%.

Crystal data

$[Cu(C_{13}H_{10}N_3O_3)(CH_4O)]ClO_4$
$M_r = 451.27$
Monoclinic, $P2_1/n$
$a = 7.166\ (2)$ Å
$b = 19.295\ (4)$ Å
$c = 12.544\ (2)$ Å
$\beta = 98.186\ (3)^\circ$
$V = 1716.8\ (7)$ Å^3
$Z = 4$
$D_x = 1.746$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.48$ mm^{-1}
$T = 298\ (2)$ K
Needle, blue
0.15 × 0.06 × 0.03 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.809$, $T_{max} = 0.957$
13255 measured reflections
3373 independent reflections
2378 reflections with $I > 2\sigma(I)$
$R_{int} = 0.105$
$\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.087$
$wR(F^2) = 0.160$
$S = 1.14$
3373 reflections
285 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 2.3878P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.58$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.907 (4)	Cu1—N3	1.980 (6)
Cu1—N2	1.944 (6)	Cu1—O4	1.982 (5)
O3—Cu1—N2	93.2 (2)	O3—Cu1—O4	89.5 (2)
O3—Cu1—N3	176.0 (2)	N2—Cu1—O4	175.7 (2)
N2—Cu1—N3	83.4 (2)	N3—Cu1—O4	94.0 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3^{i}	0.86 (6)	1.85 (6)	2.701 (6)	170 (9)

Symmetry code: (i) $-x+1, -y, -z$.

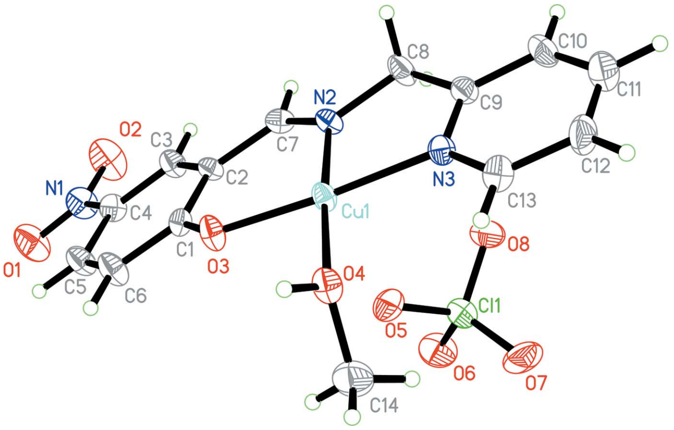

Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

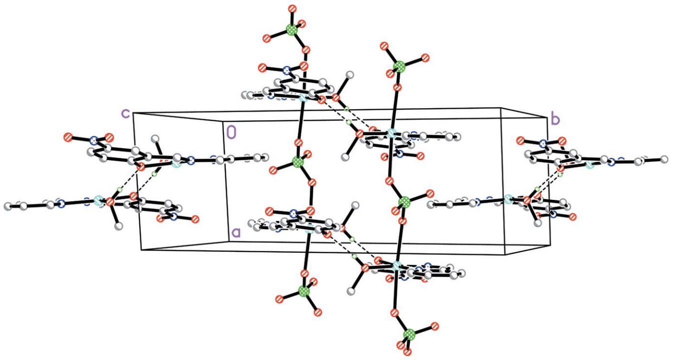

Figure 2
The crystal packing of (I), showing the long Cu···O(perchlorate) coordination. Intermolecular O—H···O hydrogen bonds are shown as dashed lines.

The O atoms of the perchlorate anion are disordered over two sites, with occupancies of 0.55 (2) and 0.45 (2). The Cl—O and O···O distances in the disordered components were restrained to be equal. Atom H4 was located in a difference Fourier map and refined isotropically, with the O—H distance restrained to 0.85 (1)Å and with $U_{iso}(H) = 0.08$Å^2. All other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96Å, and with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$. The high R_{int} and R values may be due to the poor diffraction quality of the crystal.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); 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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