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trans-Bis{2-[3-(cyclohexylammonio)propylimino-methyl]phenolato}dithiocyanatocopper(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.049
wR factor = 0.155
Data-to-parameter ratio = 15.0

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

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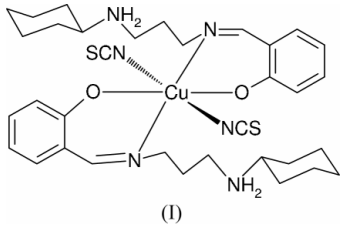
The title compound, $[Cu(NCS)_2(C_{16}H_{24}N_2O)_2]$, is a mononuclear copper(II) complex. The Cu atom lies on an inversion centre and is coordinated by two N atoms and two O atoms from two Schiff base ligands, and two N atoms from two thiocyanate anions. The six atoms around the metal constitute a slightly distorted octahedral geometry.

Comment

Transition metal compounds containing Schiff base ligands have been of great interest for many years. As an extension of work on the structural characterization of Schiff base compounds, the title copper(II) complex, (I), is reported here.



(I)

Compound (I) (Fig. 1) is a mononuclear copper(II) complex. The Cu^{II} atom, lying on an inversion center, has octahedral geometry and is coordinated by two 2-[(3-cyclohexylaminopropylimino)methyl]phenolate Schiff base ligands and two thiocyanate anions. The Schiff base acts as a bidentate ligand and coordinates to the Cu atom through the phenolate O atoms and the imine N atoms. The cyanate ligands are monodentate and coordinate to Cu *via* N. The three *trans*

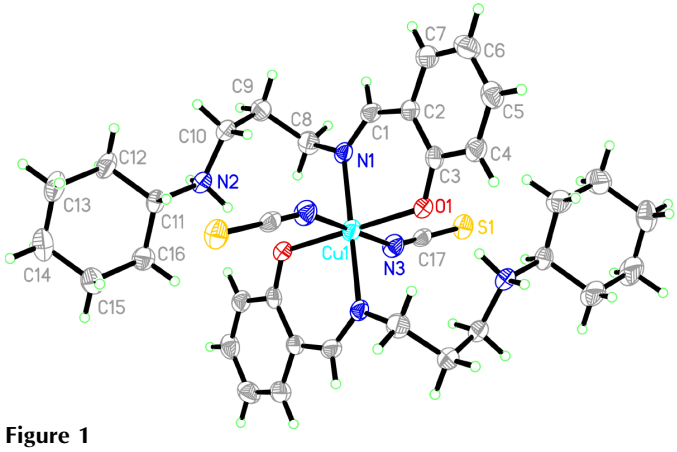


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are generated by the symmetry operation $1-x, 1-y, -z$. H atoms are represented by small spheres.

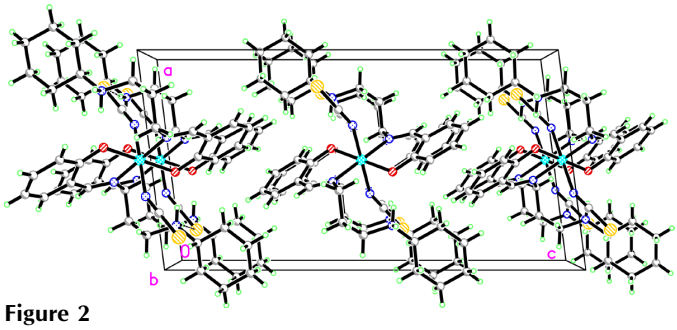


Figure 2
The packing of (I), viewed along the *b* axis.

angles at Cu are, by symmetry, exactly 180°; the other angles are close to 90°, varying from 87.34 (14) to 92.66 (14)°, which indicates a distorted octahedral geometry of the Cu atom. The Cu—O bond length of 2.027 (3) Å (Table 1) is longer than the value of 1.875 (2) Å observed in a related Schiff base copper(II) compound (You & Zhu, 2004). The Cu—N(imine) bond length of 2.079 (4) is longer than the value of 1.916 (2) Å observed in the same compound. As expected, the cyclohexyl groups adopt chair conformations to minimize steric effects.

Experimental

Salicylaldehyde (0.1 mmol, 12.1 mg) and *N*-cyclohexyl-1,3-diamine (0.1 mmol, 15.7 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 10 min, and a methanol solution (10 ml) of $Cu(NO_3)_2{\cdot}4H_2O$ (0.1 mmol, 26.0 mg) and ammonium thiocyanate (0.1 mmol, 7.6 mg) was added. The mixture was stirred for another 10 min at room temperature and then filtered. After leaving the filtrate to stand in air for 7 d, blue block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent. Analysis found: C 58.0, H 7.0 N 11.9%; calculated for $C_{34}H_{48}CuN_6O_2S_2$: C 58.3, H 6.9, N 12.0%. IR data: 3022 (*w*); 2924 (*m*); 2847 (*w*); 2093 (*s*); 1634 (*s*); 1591 (*w*); 1547 (*m*); 1482 (*s*); 1443 (*s*); 1301 (*m*); 1187 (*w*); 1148 (*w*); 771 (*s*); 586 (*w*); 515 (*w*) cm^{-1}.

Crystal data

$[Cu(NCS)_2(C_{16}H_{24}N_2O)_2]$
M_r = 700.44
Monoclinic, $P2_1/c$
a = 10.901 (2) Å
b = 7.789 (2) Å
c = 20.719 (4) Å
β = 97.07 (3)°
V = 1745.8 (7) $Å^3$
Z = 2
D_x = 1.332 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1027 reflections
θ = 2.5–25.0°
μ = 0.78 mm^{-1}
T = 293 (2) K
Block, blue
0.27 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.816, T_{max} = 0.872
8924 measured reflections
3085 independent reflections
1857 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.0°
$h = -12 \rightarrow 12$
$k = -9 \rightarrow 9$
$l = -14 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.155
S = 0.96
3085 reflections
205 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0783P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.54 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.56 e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	2.027 (3)	Cu1—N3	2.113 (4)
Cu1—N1	2.079 (4)		
$O1^i$—Cu1—N1	91.35 (13)	O1—Cu1—N3	88.44 (14)
O1—Cu1—N1	88.65 (13)	N1—Cu1—N3	87.34 (14)
$O1^i$—Cu1—N3	91.56 (14)	$N1^i$—Cu1—N3	92.66 (14)

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

All H atoms were placed in geometrically idealized positions, with C—H = 0.93–0.97 Å and N—H = 0.90 Å. They were refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C/N)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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References

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Systems Inc., Madison, Wisconsin, USA.
You, Z.-L. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, m1079–m1080.