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## Key indicators

Single-crystal X-ray study  
T = 298 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
R factor = 0.043  
wR factor = 0.117  
Data-to-parameter ratio = 19.7

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

## Bis[4-bromo-2-(cyclohexyliminomethyl)-phenolato]copper(II)

The title compound,  $[\text{Cu}(\text{C}_{13}\text{H}_{15}\text{BrNO})_2]$ , is a mononuclear copper(II) complex. The Cu atom is four-coordinated by two N atoms and two O atoms from two Schiff base ligands in a slightly distorted tetrahedral geometry.

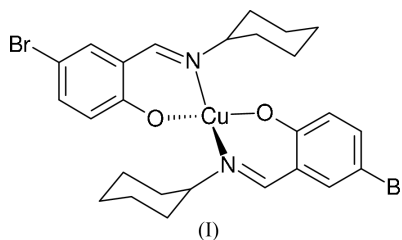
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## Comment

Transition metal compounds containing Schiff base ligands have been of interest for a long time (Archer & Wang, 1990; Chang *et al.*, 1998). These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). As an extension of work on the structural characterization of Schiff base  $\text{Cu}^{\text{II}}$  compounds, the crystal structure of the title compound, (I), is reported here.



Compound (I) is a mononuclear  $\text{Cu}^{\text{II}}$  complex (Fig. 1). The Cu atom is coordinated by two O and two N atoms from two Schiff base ligands. This  $\text{CuO}_2\text{N}_2$  coordination forms a distorted tetrahedral geometry, with angles subtended at the  $\text{Cu}^{\text{II}}$  atom in the range  $93.69(11)$ – $122.65(12)^\circ$  (Table 1). The average Cu–O bond length [ $1.919(3) \text{ \AA}$ ] is a little longer than the value of  $1.888(3) \text{ \AA}$  observed in a similar Schiff base  $\text{Cu}^{\text{II}}$  compound, (II), bis(*N*-octylsalicylideneiminato-*N,O*)-copper(II) (Zhang *et al.*, 2001). The mean Cu–N bond length [ $2.026(3) \text{ \AA}$ ] is also a little longer than the value of  $2.009(3) \text{ \AA}$  observed in (II). As expected, the cyclohexyl groups in the ligands adopt a chair form to minimize steric effects. There are no short molecular contacts ( $< 3.2 \text{ \AA}$ ) in the crystal structure (Fig. 2).

## Experimental

Cyclohexylamine (0.2 mmol, 11.4 mg) and 5-bromosalicylaldehyde (0.2 mmol, 40.4 mg) were dissolved in MeOH (10 ml). The mixture was stirred for 10 min to give a clear yellow solution. To this solution was added an MeOH solution (10 ml) of  $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$  (1.0 mmol, 25.4 mg), with stirring. After keeping the resulting solution at room temperature in air for 11 d, blue block-shaped crystals of (I) were formed on slow evaporation of the solvent. The crystals were

collected, washed three times with MeOH and dried in a vacuum desiccator using anhydrous CaCl<sub>2</sub> (yield 61.3%). Analysis found: C 49.7, H 4.9, N 4.6%; calculated for C<sub>26</sub>H<sub>30</sub>Br<sub>2</sub>CuN<sub>2</sub>O<sub>2</sub>: C 49.9, H 4.8, N 4.5%.

Crystal data

[Cu(C<sub>13</sub>H<sub>15</sub>BrNO)<sub>2</sub>]  
*M<sub>r</sub>* = 625.88  
 Orthorhombic, *Pbca*  
*a* = 14.996 (1) Å  
*b* = 13.597 (1) Å  
*c* = 25.156 (2) Å  
*V* = 5129.3 (7) Å<sup>3</sup>  
*Z* = 8  
*D<sub>x</sub>* = 1.621 Mg m<sup>-3</sup>

Mo *K*α radiation  
 Cell parameters from 10 170 reflections  
 $\theta$  = 2.6–22.8°  
 $\mu$  = 3.99 mm<sup>-1</sup>  
*T* = 298 (2) K  
 Block, blue  
 0.22 × 0.21 × 0.18 mm

Data collection

Bruker APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.433, *T<sub>max</sub>* = 0.487  
 56 364 measured reflections

5866 independent reflections  
 4083 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.046  
 $\theta_{max}$  = 27.5°  
*h* = -19 → 19  
*k* = -17 → 17  
*l* = -32 → 32

Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.043  
*wR*(*F*<sup>2</sup>) = 0.117  
*S* = 1.03  
 5866 reflections  
 298 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 4.6248P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 (Δ/σ)<sub>max</sub> < 0.001  
 Δρ<sub>max</sub> = 0.71 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.36 e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Cu1—O2	1.918 (3)	Cu1—N2	2.024 (3)
Cu1—O1	1.920 (3)	Cu1—N1	2.027 (3)
O2—Cu1—O1	119.73 (12)	O2—Cu1—N1	113.83 (11)
O2—Cu1—N2	93.69 (11)	O1—Cu1—N1	95.32 (11)
O1—Cu1—N2	113.74 (12)	N2—Cu1—N1	122.65 (12)

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C).

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXL97.

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References

Archer, R. D. & Wang, B. (1990). *Inorg. Chem.* **29**, 39–43.  
 Bhatia, S. C., Bindlish, J. M., Saini, A. R. & Jain, P. C. (1981). *J. Chem. Soc. Dalton Trans.* pp. 1773–1779.

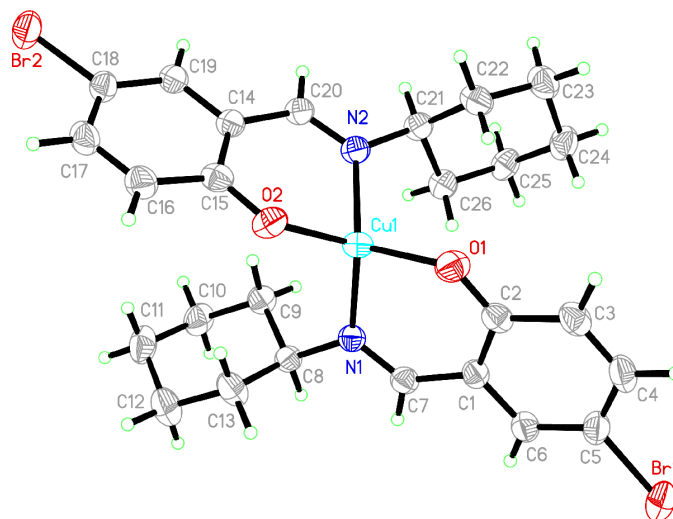


Figure 1

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

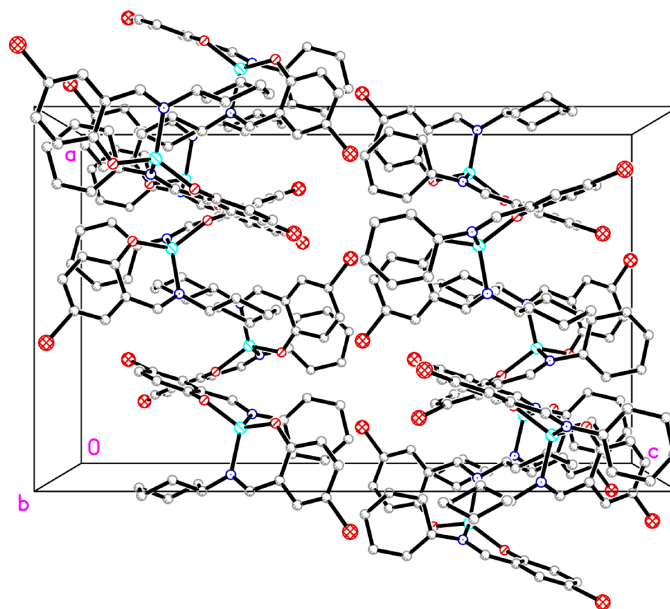


Figure 2

The crystal packing of (I), viewed along the *b* axis. H atoms have been omitted.

Bruker (2002). SAINT (Version 6.02) and SMART (Version 5.0). Bruker AXS Inc., Madison, Wisconsin, USA.  
 Chang, S., Jones, L., Wang, C. M., Henling, L. M. & Grubbs, R. H. (1998). *Organometallics*, **17**, 3460–3465.  
 Costamagna, J., Vargas, J., Latorre, R., Alvarado, A. & Mena, G. (1992). *Coord. Chem. Rev.* **119**, 67–88.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997b). SHELXTL. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Zhang, L. Z., Bu, P.-Y., Wang, L.-J. & Cheng, P. (2001). *Acta Cryst.* **C57**, 1166–1167.