Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

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Key indicators

Single-crystal X-ray study T = 298 KMean σ (C–C) = 0.011 Å R factor = 0.060 wR factor = 0.197 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.

Bis[2-(o-tolyliminomethyl)phenolato]copper(II)

The title compound, $[Cu(C_{14}H_{12}NO)_2]$, is a mononuclear copper(II) compound. The Cu^{II} atom, lying on a centre of symmetry, is four-coordinated by two N atoms and two O atoms from two Schiff base ligands, giving a square-planar geometry.

Received 9 March 2005 Accepted 21 March 2005 Online 31 March 2005

Comment

Transition metal compounds containing Schiff base ligands have been of great interest for many years. 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 the work on this series, a mononuclear copper(II) complex, (I), is reported here.



The title complex is a mononuclear copper(II) compound (Fig. 1). The Schiff base acts as a bidentate ligand and ligates



displacement ellipsoids and the atom-numbering scheme. Unlabelled

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atoms are related to labelled atoms by -x, 2 - y, -z.

metal-organic papers

to the Cu^{II} atom through the phenolate O and imine N atoms. The two *trans* angles are both 180° , by crystallographic symmetry, as the Cu atom lies on an inversion centre. All other angles around the Cu^{II} atom are close to 90° (Table 1), which indicates a slightly distorted square-planar geometry of the Cu^{II} atom. The Cu1—N1 bond length of 1.998 (4) Å is a little longer than the corresponding bond distance of 1.927 (3) Å observed in a Schiff base copper(II) complex reported recently (You *et al.*, 2004). The Cu–O bond distance of 1.877 (3) Å is shorter than the corresponding value of 1.975 (3) Å observed in another Schiff base complex (You & Zhu, 2004). The C7—N1 bond distance of 1.300 (6) Å conforms to the value for a double bond, while the C8–N1 bond distance of 1.469 (6) Å conforms to the value for a single bond.

Experimental

o-Toluidine and salicylaldehyde were available commercially and were used without further purification. *o*-Toluidine (2.0 mmol, 214 mg) and salicylaldehyde (2.0 mmol, 244 mg) were dissolved in methanol (100 ml). The mixture was stirred for 1 h to give a clear yellow solution. To this solution was added a methanol solution (30 ml) of Cu(NO₃)₂·3H₂O (1.0 mmol, 241 mg) with stirring. After keeping the resulting solution in air for 15 d, black block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using P₄O₁₀ (yield 92.7%). Analysis found: C 69.3, H 5.0, N 5.8%; calculated for C₂₈H₂₄CuN₂O₂: C 69.5, H 5.0, N 5.7%.

Crystal data

| $[Cu(C_{14}H_{12}NO)_2]$ | $D_x = 1.374 \text{ Mg m}^{-3}$ | |
|--|---|--|
| $M_r = 484.03$ | Mo $K\alpha$ radiation | |
| Monoclinic, $P2_1/n$ | Cell parameters from 1213 | |
| a = 10.931 (2) Å | reflections | |
| b = 9.149(2) Å | $\theta = 2.8 - 21.8^{\circ}$ | |
| c = 12.522(1) Å | $\mu = 0.96 \text{ mm}^{-1}$ | |
| $\beta = 110.94(2)^{\circ}$ | T = 298 (2) K | |
| V = 1169.6 (4) Å ³ | Block, black | |
| Z = 2 | $0.25 \times 0.15 \times 0.11 \ \mathrm{mm}$ | |
| Data collection | | |
| Bruker SMART CCD area-detector | 2541 independent reflections | |
| diffractometer | 1393 reflections with $I > 2\sigma(I)$ | |
| ω scans | $R_{\rm int} = 0.054$ | |
| Absorption correction: multi-scan | $\theta_{\rm max} = 27.0^{\circ}$ | |
| (SADABS; Sheldrick, 1996) | $h = -13 \rightarrow 13$ | |
| $T_{\rm min} = 0.795, T_{\rm max} = 0.902$ | $k = -11 \rightarrow 11$ | |
| 11859 measured reflections | $l = -15 \rightarrow 15$ | |
| Refinement | | |
| Refinement on F^2 | $w = 1/[\sigma^2(F_o^2) + (0.0887P)^2]$ | |
| $R[F^2 > 2\sigma(F^2)] = 0.060$ | + 0.8345P] | |
| $wR(F^2) = 0.197$ | where $P = (F_o^2 + 2F_c^2)/3$ | |
| S = 1.08 | $(\Delta/\sigma)_{\rm max} < 0.001$ | |
| 2541 reflections | $\Delta \rho_{\rm max} = 0.53 \ {\rm e} \ {\rm \AA}^{-3}$ | |
| 152 parameters | $\Delta \rho_{\rm min} = -0.26 \text{ e} \text{ Å}^{-3}$ | |



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

Table 1 Selected geometric parameters (Å, $^{\circ}$).

| Cu1-O1 | 1.877 (4) | Cu1-N1 | 1.999 (4) |
|-------------------------|------------|------------------------|------------|
| $O1^{i}$ -Cu1-O1 | 180 | O1-Cu1-N1 | 91.65 (15) |
| O1 ⁱ -Cu1-N1 | 88.35 (15) | N1-Cu1-N1 ⁱ | 180 |

Symmetry code: (i) -x, 2 - y, -z.

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.96 Å, and with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

This project is sponsored by the Scientific Research Foundation for Returned Overseas Chinese Scholars.

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H-atom parameters constrained