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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.034
 wR factor = 0.098
Data-to-parameter ratio = 13.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis[2,4-dichloro-6-(piperidin-1-ylmethyl)-
phenolato- $\kappa^2\text{N},\text{O}$]copper(II)

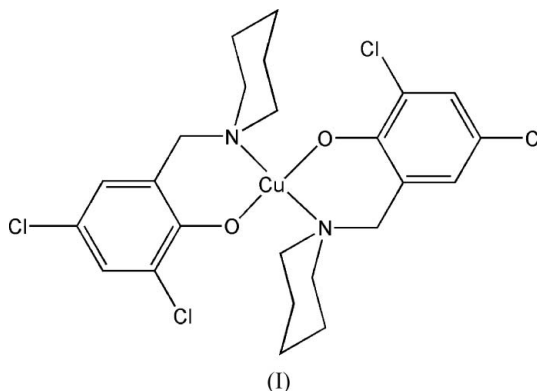
In the title compound, $[\text{Cu}(\text{C}_{12}\text{H}_{14}\text{Cl}_2\text{NO})_2]$, the Cu^{II} atom is four-coordinated in a distorted square-planar geometry by two N atoms and two O atoms from two 2,4-dichloro-6-(piperidin-1-ylmethyl)phenolate ligands. The dihedral angle between the N/Cu/O coordination planes is $16.53(9)^\circ$.

Received 26 September 2006

Accepted 29 September 2006

Comment

Piperidine compounds can act as complexing reagents with metallic ions, but few metal complexes with piperidine derivatives have been reported (Näther & Beck, 2004). Recently, we determined the crystal structure of 2,4-dichloro-6-(piperidin-1-ylmethyl)phenol (HCl_2bpipe) in which intermolecular $\text{C}\cdots\text{C}$ and $\text{Cl}\cdots\text{Cl}$ contacts were observed (Kubono *et al.*, 2005). The present paper describes the crystal structure of the Cu^{II} complex with HCl_2bpipe , (I).



The molecular structure of (I) is shown in Fig. 1. The Cu^{II} atom is four-coordinated by two amine N atoms and two phenolate O atoms derived from two bidentate 2,4-dichloro-6-(piperidin-1-ylmethyl)phenolate ligands. The geometry of the coordination is distorted square-planar. The dihedral angle between the N/Cu/O coordination planes is $16.53(9)^\circ$. The Cu—O and Cu—N bond lengths are comparable to those of other aminophenol Cu^{II} complexes (You, 2005; Chen *et al.*, 2005). In the crystal structure, no significant intermolecular interactions are observed.

Experimental

HCl_2bpipe (0.104 g, 0.4 mmol) was dissolved in 20 ml of hot chloroform and 30 ml of a methanol solution of copper(II) acetate monohydrate (0.040 g, 0.2 mmol) were then added to this solution. The mixture was stirred for 20 min at 340 K. After a few days at room temperature, brown crystals of (I) were obtained. Yield 86.9%; m.p. 465.0–465.7 K. Analysis calculated for $\text{C}_{24}\text{H}_{28}\text{Cl}_4\text{CuN}_2\text{O}_2$: C 49.54, H 4.85, N 4.81%; found: C 49.45, H 4.89, N 4.79%.

Crystal data

[Cu(C₁₂H₁₄Cl₂NO)₂] $M_r = 581.83$ Monoclinic, $P2_1/n$ $a = 12.602$ (6) Å $b = 18.049$ (16) Å $c = 11.123$ (4) Å $\beta = 95.07$ (4)° $V = 2520$ (3) Å³ $Z = 4$ $D_x = 1.534$ Mg m⁻³Mo $K\alpha$ radiation $\mu = 1.32$ mm⁻¹ $T = 298.1$ K

Prism, brown

 $0.23 \times 0.20 \times 0.18$ mm

Data collection

Rigaku AFC7R diffractometer

 ω -2 θ scansAbsorption correction: ψ scan(North *et al.*, 1968) $T_{\min} = 0.733$, $T_{\max} = 0.789$

6951 measured reflections

5790 independent reflections

4342 reflections with $F^2 > 2\sigma(F^2)$ $R_{\text{int}} = 0.021$ $\theta_{\max} = 27.5^\circ$

3 standard reflections

every 150 reflections

intensity decay: 0.2%

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.034$ $wR(F^2) = 0.098$ $S = 1.00$

4342 reflections

326 parameters

H-atom parameters constrained

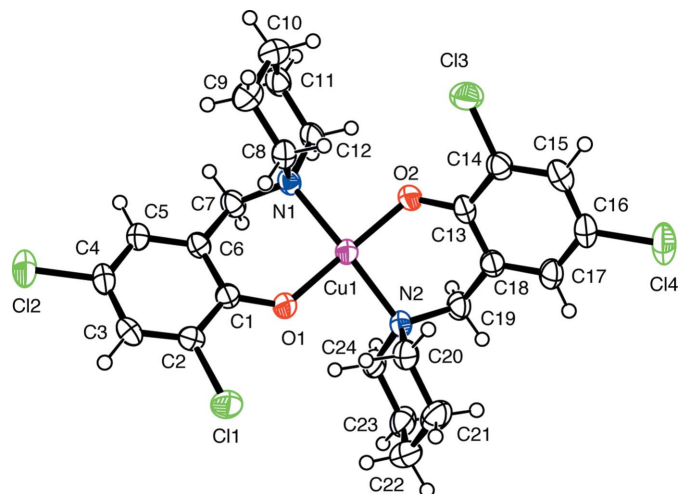
 $w = 1/[0.0011F_o^2 + \sigma(F_o^2)]/(4F_o^2)$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.42$ e Å⁻³ $\Delta\rho_{\min} = -0.48$ e Å⁻³

Figure 1

The molecular structure of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

This study was financially supported in part by Grants-in-Aid for Scientific Research (Nos. 16750061 and 18550070) from the Japan Society for the Promotion of Science.

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.894 (2)	Cu1—N1	2.074 (2)
Cu1—O2	1.895 (2)	Cu1—N2	2.072 (2)
O1—Cu1—O2	166.02 (9)	O2—Cu1—N1	88.97 (9)
O1—Cu1—N1	92.60 (9)	O2—Cu1—N2	93.76 (9)
O1—Cu1—N2	86.99 (9)	N1—Cu1—N2	170.32 (9)

All H atoms were placed at idealized positions and refined as riding atoms, with C—H distance of 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *WinAFC* (Rigaku/MS, 2004); cell refinement: *WinAFC*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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