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Bis{μ-2-[3-(cyclohexylammonio)-propyliminomethyl]phenolato}-bis[dichlorocopper(II)]

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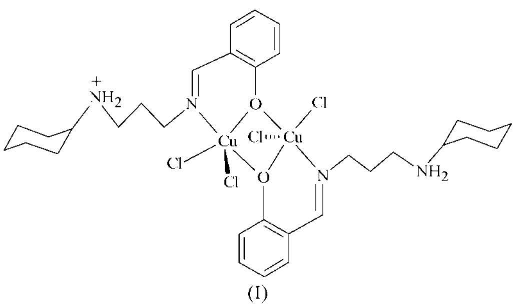
The title compound, $[Cu_2(C_{16}H_{24}N_2O)_2Cl_4]$, is a dinuclear copper(II) complex with inversion symmetry. Each Cu^{II} atom is five-coordinated by two O and one N atom from two Schiff base ligands, and by two Cl atoms, giving an approximately trigonal–bipyramidal coordination environment.

Comment

Investigations into the magnetic properties of molecule-based materials containing a polymetallic assembly have become a fascinating subject in the field of condensed matter physics and materials chemistry (Dalai *et al.*, 2002; Bhaduri *et al.*, 2003). Much attention has been focused on coordination complexes with novel magnetic properties, which may have potentially useful applications in materials science (Ray *et al.*, 2003). The prime strategy for designing these molecular materials is to use a suitable bridging ligand that determines the nature of the magnetic interactions (Koner *et al.*, 2003). Recently, we have reported a few Schiff base complexes (You *et al.*, 2003; You, Xiong *et al.*, 2004; You, Zhu & Liu, 2004). As an extension of this work, the title dinuclear copper(II) complex, (I), is reported here.



(I)

Complex (I) exhibits inversion symmetry (Fig. 1). Each copper(II) ion in the complex is five-coordinated by one imine N atom from a Schiff base ligand, two terminal Cl^- ions and two bridging phenolate O atoms; the Cu$\cdots$Cu separation is 3.141 (2) Å. The mean Cu—Cl bond length [2.398 (2) Å; Table 1] is a little shorter than the corresponding bond distance [2.421 (2) Å] observed in a similar copper(II) complex (Kani *et al.*, 2000). The fact that the Cu1—O1 distances [2.013 (3) Å] is longer than the Cu1—O1($-x$, $1 - y$, $-z$) distance [1.974 (3) Å] indicates that the *trans* influence of the Cl^- ion is greater than that of the Schiff base imine N atom. The Cu1—N1 bond length is a little longer than the corresponding bond distance [1.927 (3) Å] observed in a Schiff base copper(II) complex reported recently by us (You, Chen *et al.*, 2004). This difference is probably caused by the two Cl atoms in (I) having a larger hindrance than the water molecule in the related complex. The Cu—O(phenolate) bond distances exhibit the same pattern in each complex. The C7=N1 bond distance in (I) [1.277 (6) Å] conforms to the value for a double bond, while the C8—N1 bond distance [1.491 (6) Å] conforms to the value for a single bond. The six-membered chelate ring in the complex is nearly planar, with a deviation of 0.0349 Å. The C1–C6 phenyl ring and the Cu1/O1/Cu1^i/O1^i four-membered chelate ring are nearly coplanar, with a dihedral angle of 8.5 (3)° [symmetry code: (i) $-x$, $1 - y$, $-z$].

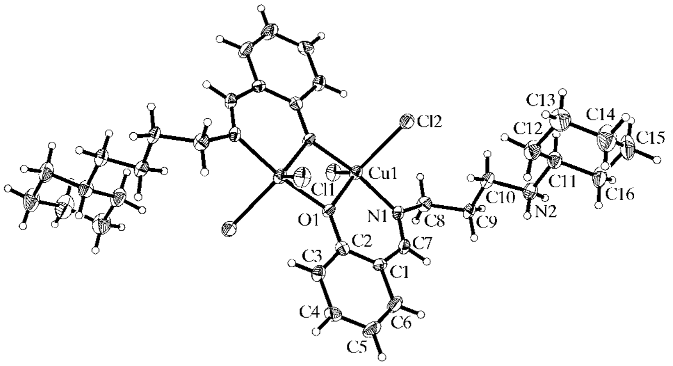


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

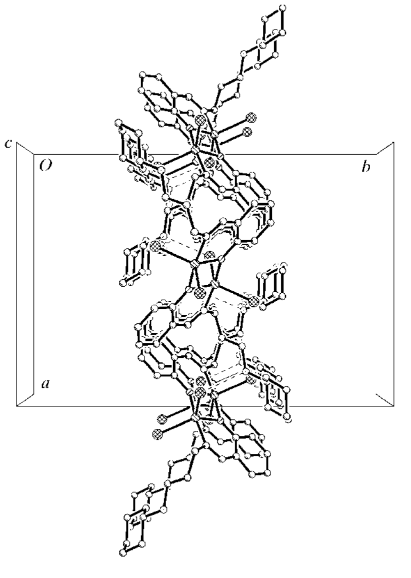


Figure 2
A view of part of the crystal packing of (I), viewed along the *c* axis. All H atoms have been omitted for clarity.

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The stereochemistry around the Cu^{II} atom in (I) can be described as a slightly distorted trigonal–bipyramidal geometry. Taking atoms N1 and $O1^{i}$ as the axial donors, an angle of 168.18 (17)° is subtended at the copper(II) ion, which is a little smaller than the theoretical value of 180°. The angles between the two axial donors and the three equatorial donor atoms O1, Cl1 and Cl2 range from 76.04 (16)° for the $O1^{i}$—Cu1—O1 angle to 94.12 (11)° for the $O1^{i}$—Cu1—Cl1 angle. The three equatorial angles range from 116.17 (6)° for Cl1—Cu1—Cl2 to 122.72 (11)° for O1—Cu1—Cl2, showing only slight differences from the ideal value of 120°.

In the crystal structure, all the Cl and amine N atoms contribute to hydrogen bonds, leading to the formation of sheets parallel to the *ac* plane (Table 2 and Fig. 2). As expected, the cyclohexyl groups in the complex adopt chair conformations to minimize steric effects.

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.950 (4)	Cu1—Cl1	2.386 (2)
Cu1—$O1^{i}$	1.974 (3)	Cu1—Cl2	2.410 (2)
Cu1—O1	2.013 (3)		
N1—Cu1—$O1^{i}$	168.18 (17)	O1—Cu1—Cl1	120.67 (11)
N1—Cu1—O1	92.22 (17)	N1—Cu1—Cl2	91.31 (13)
$O1^{i}$—Cu1—O1	76.04 (16)	$O1^{i}$—Cu1—Cl2	93.92 (11)
N1—Cu1—Cl1	93.07 (13)	O1—Cu1—Cl2	122.72 (11)
$O1^{i}$—Cu1—Cl1	94.12 (11)	Cl1—Cu1—Cl2	116.17 (6)

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

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N2—H2*A*⋯$Cl2^{ii}$	0.93 (3)	2.20 (3)	3.118 (5)	170 (4)
N2—H2*B*⋯$Cl1^{iii}$	0.93 (4)	2.19 (4)	3.120 (5)	178 (5)

Symmetry codes: (ii) $\frac{1}{2}-x, y, \frac{1}{2}+z$; (iii) $\frac{1}{2}+x, 1-y, \frac{1}{2}-z$.

Experimental

Salicylaldehyde and *N*-cyclohexylpropane-1,3-diamine were available commercially and were used without further purification. Salicylaldehyde (0.2 mmol, 24.4 mg) and *N*-cyclohexylpropane-1,3-diamine (0.2 mmol, 31.2 mg) were dissolved in ethanol (20 ml). The mixture was stirred for 1 h to give a clear orange solution of *L* (0.2 mmol), where *L* is 2-[3-(cyclohexylamino)propyliminomethyl]-phenol. To the solution of *L* was added an ethanol solution (10 ml) of $CuCl_2\cdot 2H_2O$ (0.1 mmol, 17.0 mg) with stirring. After keeping the resulting solution in air for 15 d, blue block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvents. The crystals were isolated, washed three times with ethanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 63.2%). Analysis found: C 48.8, H 6.3, N 7.2%; calculated for $C_{32}H_{48}Cl_4Cu_2N_4O_2$: C 48.7, H 6.1, N 7.1%.

Crystal data

$[Cu_2(C_{16}H_{24}N_2O)_2Cl_4]$
$M_r = 789.62$
Orthorhombic, Pc_cn
$a = 15.487$ (3) Å
$b = 22.117$ (4) Å
$c = 10.442$ (2) Å
$V = 3576.7$ (12) $Å^3$
$Z = 4$
$D_x = 1.466$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3328 reflections
$\theta = 2.2$–23.2°
$\mu = 1.52$ mm^{-1}
$T = 293$ (2) K
Block, blue
0.23 × 0.18 × 0.12 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.721$, $T_{max} = 0.838$
11 330 measured reflections
3402 independent reflections
1917 reflections with $I > 2\sigma(I)$
$R_{int} = 0.096$
$\theta_{max} = 26.0°$
$h = -17 \rightarrow 18$
$k = -24 \rightarrow 27$
$l = -12 \rightarrow 1$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.104$
$S = 0.96$
3402 reflections
205 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0216P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.63$ e $Å^{-3}$
$\Delta\rho_{min} = -0.44$ e $Å^{-3}$

Atoms H2*A* and H2*B* were located in a difference Fourier map and refined isotropically, with the N—H and H⋯H distances restrained to 0.93 (1) and 1.51 (2) Å, respectively, and with U_{iso}(H) values fixed at 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 of 0.93–0.98 Å, and with U_{iso}(H) values of $1.2U_{eq}$(C).

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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Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1192). Services for accessing these data are described at the back of the journal.

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