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Bis(*trans*-(*E*)-2-{[4-(4-acetylphenylsulfanyl)phenylimino-κ*N*]methyl}phenolato-κ*O*)copper(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.119
Data-to-parameter ratio = 14.6

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

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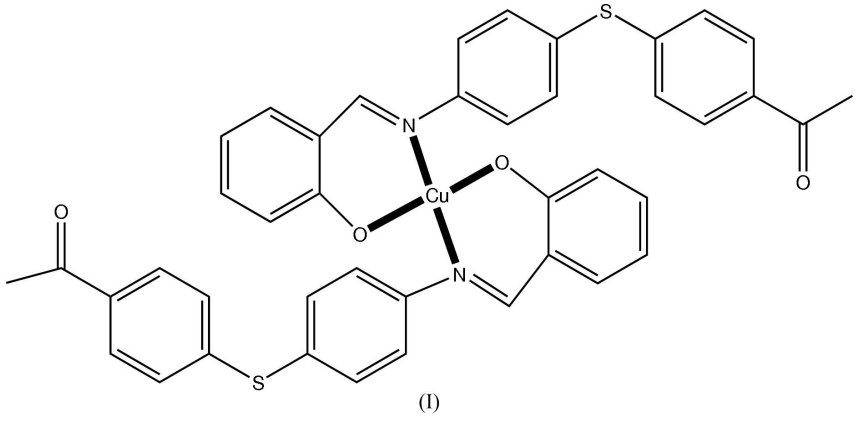
In the structure of the mononuclear title complex, $[Cu(C_{21}H_{16}NO_2S)_2]$, the Cu^{II} atom, which lies on an inversion centre, displays approximately square-planar coordination geometry. The bidentate ligands coordinate through their phenolate O and imine N atoms in a mutually *trans* orientation. The structure is stabilized by a three-dimensional network of C—H···O hydrogen bonds.

Comment

Great interest is shown in complexes with N-donor ligands due to the diversity of their chemical and catalytic properties (Togni & Venanzi, 1994; Fache *et al.*, 2000; Kalyanasundaram, 1982). Schiff bases have been used as ligands in coordination chemistry for many years (Pfeiffer *et al.*, 1933), and copper and cobalt Schiff base complexes were among the first whose structures were determined by X-ray diffraction methods (Martell & Calvin, 1958). Research on new Schiff base complexes of copper continues (Losada *et al.*, 2001; Santos *et al.*, 2001). This work is a continuation of our research on the synthesis and structure of transition metal complexes of new polydentate ligands containing N- and O-donor atoms (Benali-Cherif *et al.*, 1995; Champloy *et al.*, 1998; Laifa & Benali-Cherif, 2003; Laifa *et al.*, 2003; Harek *et al.*, 2005) and describes the structure of the title mononuclear Schiff base complex, (I).



(I)

The Schiff base loses an H atom from the hydroxyl group and acts as a singly charged bidentate ligand coordinating to copper(II) through the phenolate O and imine N atoms to give a square-planar complex. The Cu atom lies on an inversion centre so that the two ligands adopt a *trans* configuration with equivalent Cu—N and Cu—O bonds. Bond distances, angles and torsion angles around the Cu atom confirm a slightly distorted square-planar coordination environment, similar to that observed previously in copper Schiff base complexes

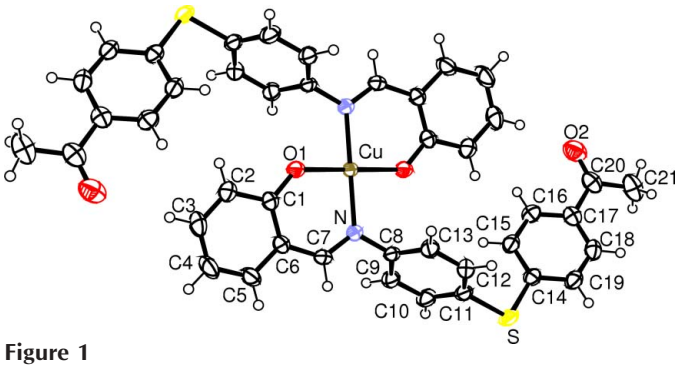


Figure 1
The molecular structure of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator $(-x, 1-y, -z)$.

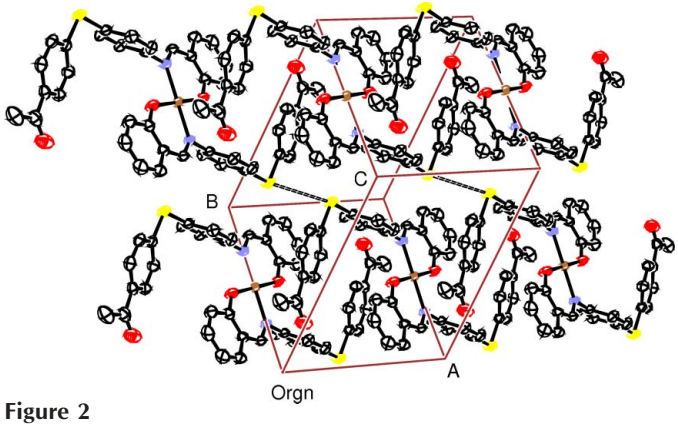


Figure 2
The crystal packing, showing the zig-zag layers and S···S van der Waals interactions (double dashed lines). H atoms have been omitted.

(Külcü *et al.*, 2005; Xu *et al.*, 2001; Baker *et al.*, 1967; Bombieri *et al.*, 1969). The Cu atom is located at the centre of the coordination plane *P*1 (Table 3), with a deviation of 0.089 (2) Å. The planes, *P*2, of the benzene rings of the iminomethylphenolate sections of the ligands are almost coplanar with the Cu coordination plane [dihedral angle 6.21 (7)°], suggesting a degree of delocalization in this portion of the molecule. The benzene ring planes, *P*3 and *P*4, of the diphenylsulfane fragment are almost orthogonal [dihedral angle = 84.12 (8)°], which may minimize steric interactions in the system. The structure is stabilized by non-classical intermolecular C—H···O hydrogen bonds (Table 2) (Steiner, 1996; Nardelli, 1995) to form zigzag chains running along the *c* axis. A short van der Waals interaction is also observed between the S atoms in adjacent chains [S···S = 3.439 (2) Å] (Fig. 2). This zig-zag arrangement, has been noted previously in other Schiff base complexes of copper(II) (Marinovich *et al.*, 1999).

Experimental

The bidentate ligand (*E*)-2-{[4-(4-acetylphenylthio)phenylimino]-methyl}phenol was synthesized according to literature methods (Abbady & Hebbachi, 1993). The ligand was precipitated from ethanol as very light amorphous flakes. The title compound, (I), was prepared by condensation of the ligand with copper(II) acetate in a 2:1 stoichiometric ratio, in refluxing absolute ethanol over 3 h. The resulting precipitate of (I) was filtered off and recrystallized by slow evaporation of a chloroform–hexane (1:1) solution.

Crystal data

$[Cu(C_{21}H_{16}NO_2S)_2]$	$Z = 1$
$M_r = 756.40$	$D_x = 1.422$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.172$ (3) Å	Cell parameters from 6926 reflections
$b = 11.032$ (3) Å	$\theta = 2.2$–$26.0°$
$c = 11.106$ (3) Å	$\mu = 0.78$ mm^{-1}
$\alpha = 60.825$ (2)°	$T = 293$ (2) K
$\beta = 67.219$ (2)°	Prism, brown
$\gamma = 89.136$ (3)°	0.3 × 0.1 × 0.1 mm
$V = 883.4$ (4) Å^3	

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.031$
φ scans	$\theta_{max} = 26.0°$
Absorption correction: none	$h = -11 \rightarrow 11$
6940 measured reflections	$k = -13 \rightarrow 13$
3396 independent reflections	$l = -11 \rightarrow 13$
2921 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.2786P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.034$	
$wR(F^2) = 0.119$	
$S = 1.21$	$(\Delta/\sigma)_{max} < 0.001$
3396 reflections	$\Delta\rho_{max} = 0.30$ e Å^{-3}
232 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.302 (3)	N—Cu	2.019 (2)
C8—N	1.436 (3)	O1—Cu	1.8817 (18)
N—C7	1.297 (3)		
O1—Cu—O1^{i}	180	O1^{i}—Cu—N	88.62 (8)
O1—Cu—N	91.38 (8)	N—Cu—N^{i}	180
C1—O1—Cu—N^{i}	169.7 (2)	C8—N—C7—C6	−179.9 (2)
C8—N—Cu—O1	−177.48 (17)	C5—C6—C7—N	179.2 (2)
C7—N—Cu—O1^{i}	−168.9 (2)	C1—C6—C7—N	−0.4 (4)
C8—N—Cu—O1^{i}	2.52 (17)		

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*
C5—H5···O2^{ii}	0.93	2.60	3.462 (5)	154
C9—H9···O2^{iii}	0.93	2.73	3.550 (3)	147

Symmetry codes: (ii) $1+x, 1+y, z$; (iii) $-1-x, 1-y, -z$.

Table 3
Dihedral angles (°) between the four planes present in (I).

Planes	*P*1	*P*2	*P*3	*P*4
*P*1	0	—	—	—
*P*2	6.21 (7)	0	—	—
*P*3	65.10 (6)	58.91 (8)	0	—
*P*4	30.13 (7)	33.78 (9)	84.12 (8)	0

Notes: *P*1 = Cu/O1/C1/C6/C7/N, coordination plane; *P*2 = C1—C6, benzene ring of the iminomethylphenolate; P3 = C8–C13, benzene ring (4) of the diphenylsulfane; *P*4 = C14–C19, benzene ring (4′) of the diphenylsulfane.

The H atoms attached to C7 and aromatic C atoms were placed in calculated positions, with C—H = 0.93 Å, and were refined using a riding model, with $U_{iso} = 1.2U_{eq}$ of the parent atoms. Methyl H atoms were refined as an idealized methyl group, with C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C21)$.

Data collection: *KappaCCD* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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