

{2,2'-[1,2-Phenylenebis(nitrilomethylidyne)]-diphenolato}copper(II) dichloromethane solvate

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Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.016\text{ \AA}$

R factor = 0.048

w R factor = 0.108

Data-to-parameter ratio = 6.6

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

The title compound, $[\text{Cu}(\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_2)] \cdot \text{CH}_2\text{Cl}_2$, crystallizes as a monomer, with the copper ion in a square-planar environment provided by the tetradentate 2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato (L18) ligand. The planar molecules pack parallel to the (101) crystallographic planes.

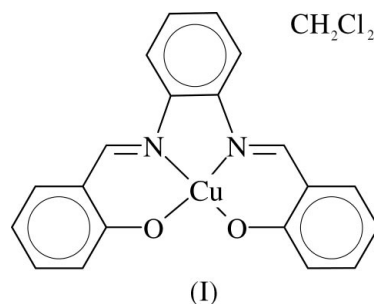
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Comment

2,2'-[1,2-Phenylenebis(nitrilomethylidyne)]diphenol (L18) is a well known Schiff base which can act as a tetradentate ligand, and its square-planar copper complex has been described as an isolated molecule in a number of crystalline forms, both on its own (Suresh *et al.*, 1996), (1), as well as stabilized by a variety of different solvates, *e.g.* water [(2); Yao *et al.*, 1997], thiourea [(3); Ferrari *et al.*, 1976] and tetracyanoquinodimethane [(4); Cassoux & Gleizes, 1980]. During the synthesis of a heteronuclear Cu–Gd(L18) complex, we obtained some crystals which happened to be a new unreported form of the Cu(L18) complex, (I), this time stabilized by a molecule of CH_2Cl_2 , and which we report herein.



The molecular structure of (I) is quite similar to those described previously (Fig. 1), in spite of the very different crystalline forms, and a least-squares fit showed that the extreme differences were found when comparing it with the two independent moieties in (2), with a minimum mean-squares deviation of 0.079 \AA and a maximum of 0.158 \AA . The largest misfit appeared as deviations of the ligand from its planar character, rather than from the intrinsic bond lengths and angles, which remained fairly stable.

The planar molecules pack parallel to each other and to the (101) planes (Fig. 2), with no obvious interaction besides the usual van der Waals forces.

The CH_2Cl_2 solvate molecule attaches to the complex through a medium strength $\text{C}-\text{H}\cdots\text{O}$ interaction [$\text{H1XB}\cdots\text{O1}$ $2.313(3)\text{ \AA}$ and $\text{C1X}-\text{H1XB}\cdots\text{O1}$ $171(3)^\circ$].

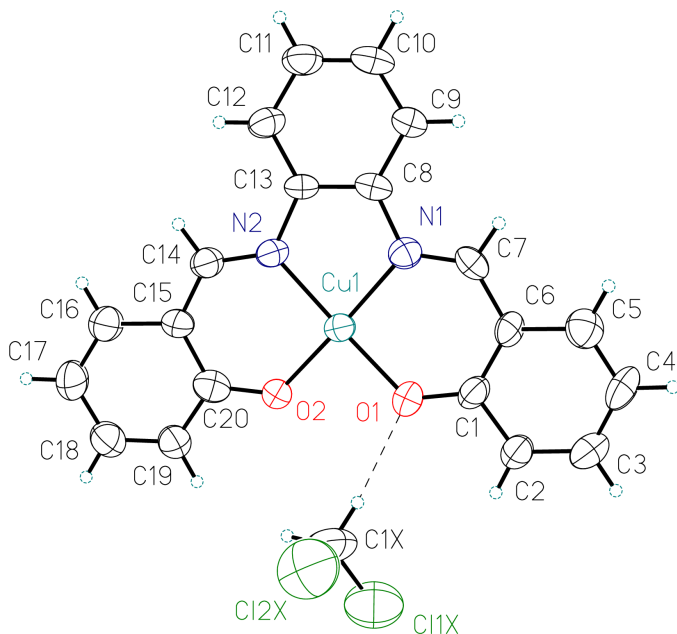


Figure 1
The molecular structure of (I) showing the atom numbering and displacement ellipsoids at the 50% probability level.

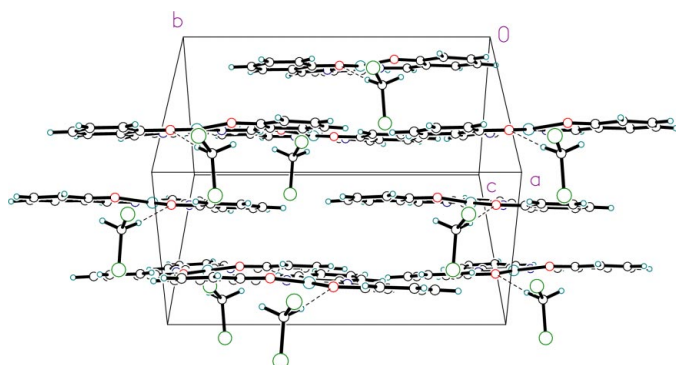


Figure 2
Packing diagram showing the way in which the molecules organize parallel to (101).

Experimental

To a solution containing 1 mmol of $\text{Cu}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ in CH_2Cl_2 , 1 mmol of $\text{Gd}(\text{NO}_3)_2$ and 1 mmol of L18 were added. The $\text{Cu}(\text{L18}) \cdot \text{CH}_2\text{Cl}_2$ complex precipitated as a polycrystalline brown powder, which by filtering was separated from the solution containing the heteronuclear species.

Crystal data

$[\text{Cu}(\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_2)] \cdot \text{CH}_2\text{Cl}_2$
 $M_r = 462.80$
 Monoclinic, C_c
 $a = 15.787(3) \text{ \AA}$
 $b = 14.359(3) \text{ \AA}$
 $c = 9.1630(15) \text{ \AA}$
 $\beta = 111.59(2)^\circ$
 $V = 1931.5(6) \text{ \AA}^3$
 $Z = 4$

$D_x = 1.591 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 25 reflections
 $\theta = 7.5\text{--}12.5^\circ$
 $\mu = 1.43 \text{ mm}^{-1}$
 $T = 293(2) \text{ K}$
 Prism, red–brown
 $0.15 \times 0.12 \times 0.10 \text{ mm}$

Data collection

Siemens R3m diffractometer
 $\omega/2\theta$ scans
 Absorption correction: ψ scan
 (SHELXTL/PC; Sheldrick, 1994)
 $T_{\min} = 0.80, T_{\max} = 0.84$
 3419 measured reflections
 1718 independent reflections
 1308 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$
 $\theta_{\max} = 25^\circ$
 $h = -18 \rightarrow 18$
 $k = -17 \rightarrow 17$
 $l = 0 \rightarrow 10$
 2 standard reflections
 every 98 reflections
 intensity decay: 4.8%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.108$
 $S = 1.02$
 1718 reflections
 262 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.061P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.49 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.34 \text{ e \AA}^{-3}$
 Absolute structure: Flack (1983);
 119 Friedel pairs
 Flack parameter = $-0.01(3)$

Table 1

Hydrogen-bonding geometry ($\text{\AA}, ^\circ$).

$D\text{--}H \cdots A$	$D\text{--}H$	$H \cdots A$	$D \cdots A$	$D\text{--}H \cdots A$
$\text{Cl1X--H1XB} \cdots \text{O1}$	0.89 (4)	2.32 (4)	3.20 (2)	171 (3)

H atoms attached to C atoms were included in idealized positions and refined using a riding scheme ($\text{C--H} = 0.93 \text{ \AA}$), both for the coordinates and the displacement parameters. The H atoms of the CH_2Cl_2 molecule were found in the difference Fourier map and refined with similarity restraints in the C--H distances ($\text{C--H} = 0.90 \text{ \AA}$).

Data collection: P3/P4-PC (Siemens, 1991); cell refinement: P3/P4-PC; data reduction: XDISK in SHELXTL/PC (Sheldrick, 1994); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL/PC (Sheldrick, 1994); software used to prepare material for publication: SHELXTL and PARST (Nardelli, 1983).

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