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[*N*,*N*′-Bis(1-benzoylisopropylidene)propane-1,3-diamine(2−)]copper(II)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.102
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.

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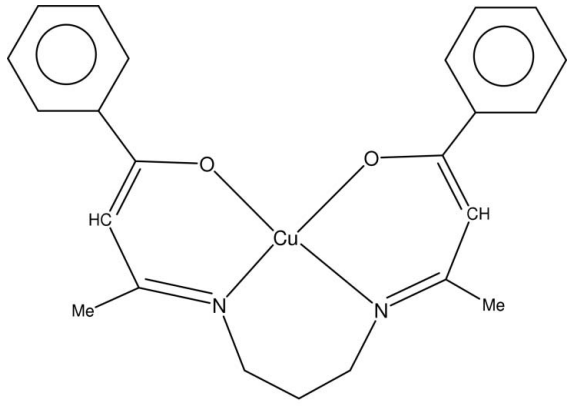
In the title compound, $[Cu(C_{23}H_{24}N_2O_2)]$, the Cu^{II} atom is coordinated by two imine N and two phenol O atoms of the ligand. The geometry of the coordination is distorted tetrahedral. The dihedral angle between the N/Cu/O coordination planes is 7.37 (7)°.

Comment

The Schiff base reactions of aldehydes with a symmetrical diamino group such as 1,3-propanediamine or ethylenediamine are of interest because of their metal-complexing behaviour. The chemistry of the metal complexes with Schiff base ligands and their applications have aroused considerable attention mainly because of their structural variability, preparative accesibility and diversity. There has been interest in copper(II) imine–phenols because of their colour isomerism (Yao *et al.*, 1997). The copper complexes of diamine Schiff bases generally display square-planar coordination (Akhtar, 1981; Drew *et al.*,1985).

In the structure of the title compound, (I) (Fig.1), the Cu atom has a distorted tetrahedral coordination geometry involving the two O- and two N-atom donors of the tetradentate ligand (Table 1). The Cu atom is located 0.0023 (3) Å from the mean coordination plane consisting of atoms O1, O2, N1 and N2. The dihedral angle between the N/Cu/O planes is 7.37 (7)°. This angle between planes is less than that of other similar Cu^{II} complexes, for example 21.0 (1)° (Drew *et al.*, 1985) and 35.13 (7)° (Arıcı *et al.*, 2001). The dihedral angle between the C12–C17 and C18–C23 phenol rings is 11.15 (9)°.



(I)

The six-membered Cu/N1/C5–C7/N2 chelate ring has a boat conformation. The distances of atoms Cu and C6, from the least-squares plane defined by atoms N1, C5, C7 and N2 are 0.0071 (2) and 0.644 (2) Å, respectively.

There is an intramolecular close contact between C17/H17 and O2 [H17···O2 = 2.40 Å, C17···O2 = 2.728 (3) Å and C17—H17···O3 = 100.1°].

Experimental

The complex was prepared by a template synthesis. 1-Phenyl-1,3-butanedione (0.325 g, 0.002 mol), 1,3-propanediamine (0.74 g, 0.001 mol) and $CuCl_2{\cdot}2H_2O$ (0.171 g, 0.001 mol) were dissolved in CH_3OH (70 ml) by heating. Et_3N (0.5 ml) was added to this mixture, which was heated under reflux for two hours. The resulting mixture was set aside for 2 d and the dark-green crystals that formed were filtered off and dried in air.

Crystal data

$[Cu(C_{23}H_{24}N_2O_2)]$
M_r = 423.99
Monoclinic, $C2/c$
a = 24.2385 (12) Å
b = 8.3306 (13) Å
c = 20.1928 (14) Å
β = 102.113 (3)°
V = 3986.6 (7) Å^3
Z = 8
D_x = 1.413 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.12 mm^{-1}
T = 100 (2) K
Prism, dark green
0.30 × 0.25 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (*MolEN*; Fair, 1990)
T_{min} = 0.723, T_{max} = 0.800
4331 measured reflections
4228 independent reflections
3509 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.8°
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.102
S = 1.04
4228 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2 + 1.7129P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Cu	1.9740 (18)	O1—Cu	1.9196 (15)
N2—Cu	1.9735 (18)	O2—Cu	1.9285 (16)
O1—Cu—O2	81.40 (7)	O1—Cu—N1	91.29 (7)
O1—Cu—N2	170.07 (7)	O2—Cu—N1	170.53 (7)
O2—Cu—N2	90.14 (8)	N2—Cu—N1	97.64 (8)

H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 Å and U_{eq}(H) = 1.2–1.5U_{eq}(C).

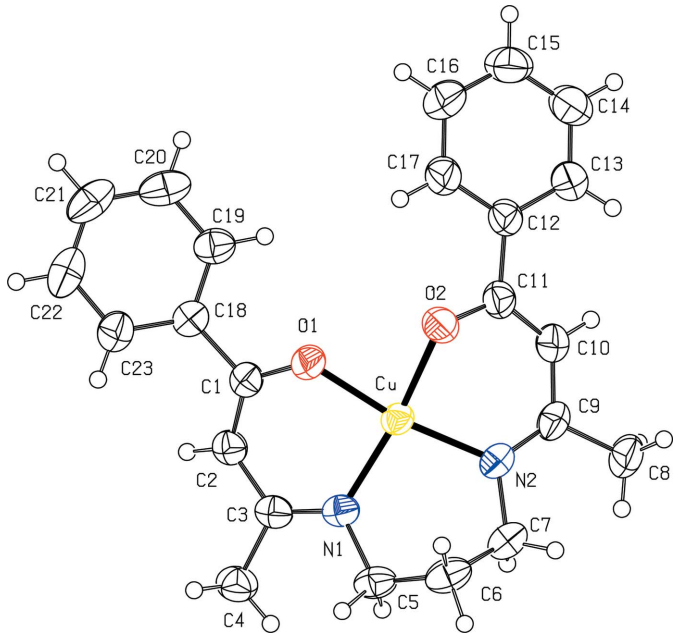


Figure 1
PLATON (Spek, 2003) plot of the title compound, with the atom-numbering scheme. The displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small circles of arbitrary radii.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1993); cell refinement: *CAD-4 EXPRESS*; data reduction: *CAD-4 EXPRESS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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