

**{Benzil bis[(2-oxidobenzylidene)hydrazone]}-
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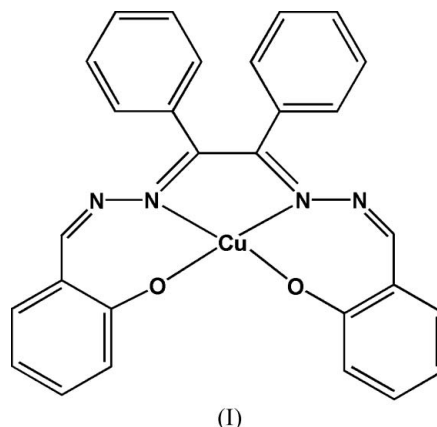
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Key indicatorsSingle-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$
 R factor = 0.056
 wR factor = 0.128
Data-to-parameter ratio = 12.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title complex, $[\text{Cu}(\text{C}_{28}\text{H}_{20}\text{N}_4\text{O}_2)]$, can be described as a single-stranded helix with the Cu^{II} atom having a distorted square-planar coordination. Face-to-face and edge-to-face $\pi-\pi$ stacking interactions and a $\text{C}-\text{H}\cdots\pi$ interaction between the aromatic rings lead to a three-dimensional network in the crystal structure.

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It is well established that self-assembly processes driven by metal–ligand interactions may generate a considerable variety of molecular architectures in a spontaneous and directed manner (Lehn, 1995; Su *et al.*, 2003). Within the field of modern supramolecular chemistry, construction of coordination complexes *via* self-assembly of predesigned ligands with appropriate metal ions is a subject of current interest because of their unusual structures and special functional properties such as luminescence, redox activity and magnetism (Bai *et al.*, 2004; Leininger *et al.*, 2000). Bis-bidentate Schiff base ligands with two symmetrically related coordination capabilities derived from benzil dihydrazone are excellent ligands, which are easy to prepare and inexpensive, allowing us to probe systematically the effect of modifications to the ligand backbone through which we are attempting to control the precise topography, or microarchitecture, of the arrays (Bai *et al.*, 2005; Chowdhury *et al.*, 2003). In the present paper, a structural study of the title compound, (I), is presented.



The title complex, which contains one copper center and one ligand, forms a single-stranded helix (Fig. 1). The Cu^{II} atom has a highly distorted square-planar coordination, formed by two imine N atoms and two phenolate O atoms; angles at Cu are given in Table 1. The Cu–O and Cu–N distances agree well with those of related compounds (Fang *et al.*, 2001). The ligand is twisted, the C7–N1–N2–C8, C15–

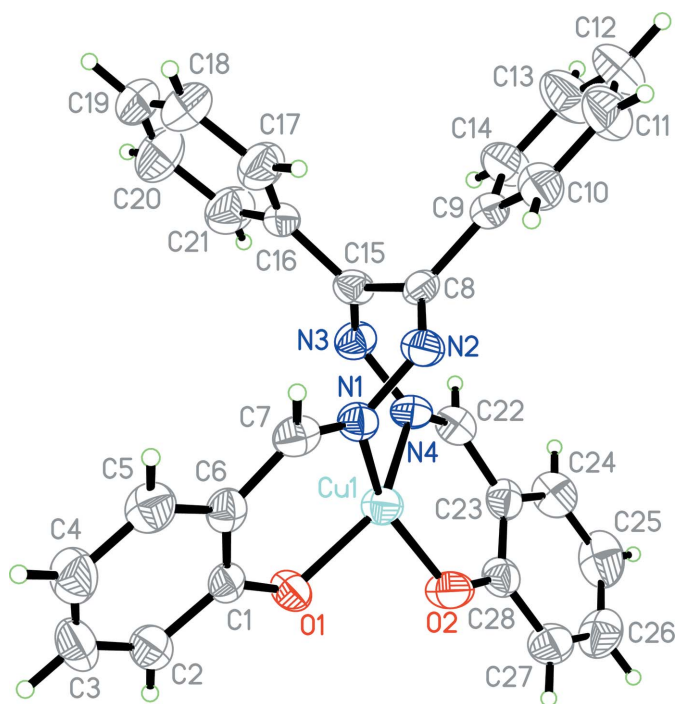


Figure 1
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

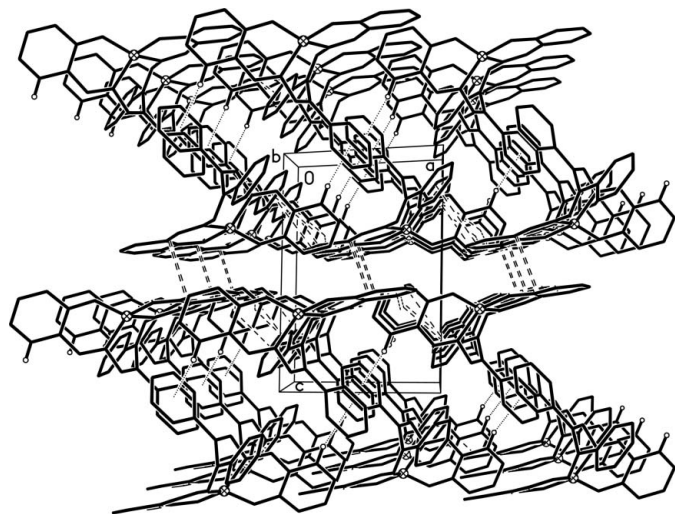


Figure 2
Intermolecular face-to-face π - π stacking (dashed open lines), edge-to-face π - π stacking (dashed lines) and C-H... π (dotted lines) interactions in (I), viewed along the b axis. H atoms, except that involved in the C-H... π interaction, have been omitted for clarity.

N3-N4-C22 and N2-C8-C15-N3 torsion angles being -122.7 (4), -134.9 (4) and -74.9 (6) $^\circ$, respectively. The dihedral angle between the C9-C14 and C16-C21 phenyl rings is 88.9 (2) $^\circ$. These results are similar to those found in a related compound (Chowdhury *et al.*, 2003).

In the crystal structure of (I), the molecules further interact with each other, forming a three-dimensional network through face-to-face and edge-to-face π - π interactions and a C-H... π interaction (Fig. 2 and Table 2). The intermolecular face-to-face π - π interaction between parallel salicylidenehy-

drazone groups, O1/C1-C7/N1/N2, related by an inversion center is characterized by a shortest contact distance of 3.281 (6) \AA for C1...C7ⁱⁱ [symmetry code: (ii) $1 - x, 2 - y, 1 - z$] and a centroid-centroid distance of 3.43 (6) \AA . There are also extensive edge-to-face π - π interactions between the benzene rings of adjacent molecules. The shortest contact distances are 3.482 (7) \AA for C3...C23ⁱⁱⁱ [symmetry code: (iii) $-1 + x, y, z$], 3.594 (7) \AA for C4...C10ⁱⁱⁱ and 3.581 (7) \AA for C11...C28^{iv} [symmetry code: (iv) $x, 1 + y, z$]. The dihedral angles between the two corresponding benzene rings are 55.3 (2) $^\circ$ for C1-C6 and C23ⁱⁱⁱ-C28ⁱⁱⁱ, 52.3 (2) $^\circ$ for C1-C6 and C9ⁱⁱⁱ-C14ⁱⁱⁱ and 82.2 (2) $^\circ$ for C9-C14 and C23^{iv}-C28^{iv}.

Experimental

All chemicals were of reagent grade quality obtained from commercial sources and used without further purification. Benzil bis(salicylidenehydrazone) (H_2L) was readily prepared by the reaction of benzil dihydrazone with salicylaldehyde in a 1:2 ratio. The ligand H_2L (0.2 mmol, 0.088 g) and $Cu(ClO_4)_2 \cdot 6H_2O$ (0.2 mmol, 0.074 g) were mixed in methanol (40 ml). The solution was left for 10 d at room temperature to afford green crystals (yield 80%). Analysis calculated for $C_{28}H_{20}CuN_4O_2$: C 66.2, H 4.0, N 11.0%; found: C 66.3, H 4.1, N 10.9%.

Crystal data

$[Cu(C_{28}H_{20}N_4O_2)]$	$V = 1153.3$ (4) \AA^3
$M_r = 508.02$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.463$ Mg m $^{-3}$
$a = 9.223$ (2) \AA	Mo $K\alpha$ radiation
$b = 10.702$ (2) \AA	$\mu = 0.98$ mm $^{-1}$
$c = 12.720$ (3) \AA	$T = 293$ (2) K
$\alpha = 85.132$ (5) $^\circ$	Block, green
$\beta = 89.749$ (5) $^\circ$	$0.20 \times 0.15 \times 0.15$ mm
$\gamma = 67.273$ (4) $^\circ$	

Data collection

Bruker SMART CCD area-detector diffractometer	5694 measured reflections
φ and ω scans	3934 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	2605 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.668, T_{\max} = 0.863$	$R_{\text{int}} = 0.048$
	$\theta_{\max} = 25.0^\circ$

Refinement

Refinement on F^2	$[\exp\{2(\sin\theta/\lambda)^2\}]/[\sigma^2(F_o^2) + (0.045P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.057$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.128$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.02$	$\Delta\rho_{\max} = 0.64$ e \AA^{-3}
3934 reflections	$\Delta\rho_{\min} = -0.27$ e \AA^{-3}
316 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cu1-O1	1.891 (3)	Cu1-N1	1.939 (4)
Cu1-O2	1.876 (3)	Cu1-N4	1.976 (4)
O1-Cu1-O2	94.49 (15)	O2-Cu1-N1	152.98 (16)
O1-Cu1-N1	93.45 (15)	O2-Cu1-N4	92.74 (17)
O1-Cu1-N4	144.66 (14)	N1-Cu1-N4	95.59 (16)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C24–H24A \cdots Cg ⁱ	0.93	3.05	3.93 (2)	152

Symmetry code: (i) $-x + 2, -y + 2, -z$.

All H atoms were positioned geometrically (C–H = 0.93 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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