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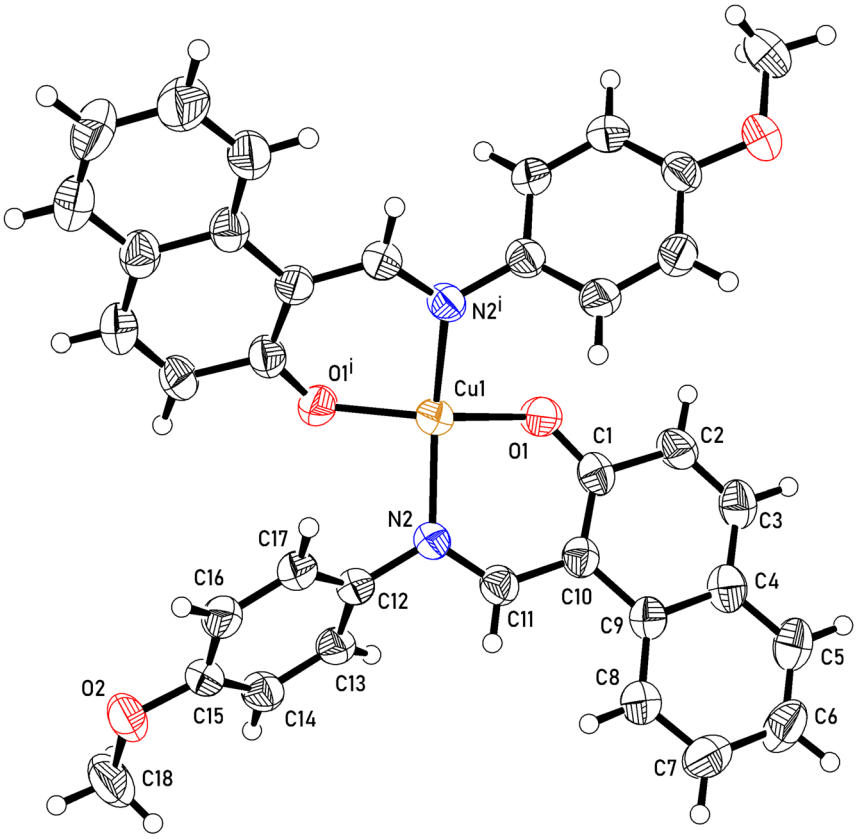
Crystal structure of *bis* ((1-((*E*)-((4-methoxyphenyl) imino)methyl)naphthalen-2-yl)oxy) copper(II), $C_{36}H_{28}CuN_2O_4$



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Abstract

$C_{36}H_{28}CuN_2O_4$, tetragonal, $P\bar{4}2_1c$ (no. 114), a = 18.9249(5) Å, c = 7.9571(5) Å, V = 2,849.9(2) Å^3, Z = 4, $R_{gt}(F)$ = 0.0538, $wR_{ref}(F^2)$ = 0.1336, T = 293 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Orange needle
Size:	0.29 × 0.01 × 0.01 mm
Wavelength:	CuKα radiation (1.54184 Å)
μ:	1.44 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	73.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7,201, 2679, 0.081
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1800
$N(param)_{refined}$:	196
Programs:	CrysAlis^{PRO},[1] SHELX,[2,3] WinGX/ORTEP[4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5947 (3)	0.1191 (3)	0.6115 (10)	0.0436 (16)
C2	0.6671 (3)	0.1405 (4)	0.6309 (12)	0.0495 (19)
H2	0.700116	0.108776	0.673211	0.059*
C3	0.6874 (3)	0.2062 (4)	0.5881 (11)	0.0526 (18)
H3	0.734152	0.219291	0.605449	0.063*
C4	0.6403 (3)	0.2561 (4)	0.5178 (10)	0.0489 (17)
C5	0.6637 (4)	0.3229 (4)	0.4670 (13)	0.061 (2)
H5	0.710623	0.335427	0.485207	0.073*
C6	0.6199 (4)	0.3698 (4)	0.3921 (14)	0.069 (3)
H6	0.637013	0.413248	0.355436	0.082*
C7	0.5490 (4)	0.3526 (4)	0.3703 (14)	0.072 (3)
H7	0.518103	0.385356	0.323291	0.087*
C8	0.5247 (4)	0.2874 (4)	0.4180 (12)	0.057 (2)
H8	0.477452	0.276234	0.399430	0.069*
C9	0.5682 (3)	0.2376 (3)	0.4933 (9)	0.0423 (15)
C10	0.5455 (3)	0.1661 (3)	0.5417 (10)	0.0403 (15)
C11	0.4734 (3)	0.1474 (3)	0.5255 (10)	0.0437 (17)
H11	0.443057	0.183400	0.491955	0.052*
C12	0.3686 (3)	0.0846 (3)	0.5432 (10)	0.0412 (15)
C13	0.3273 (3)	0.1328 (3)	0.6298 (12)	0.0441 (18)
H13	0.348912	0.166367	0.698076	0.053*
C14	0.2538 (3)	0.1319 (3)	0.6163 (11)	0.0470 (17)
H14	0.226798	0.165491	0.672578	0.056*
C15	0.2213 (3)	0.0812 (3)	0.5193 (11)	0.0456 (17)
C16	0.2623 (3)	0.0321 (3)	0.4323 (10)	0.0472 (18)
H16	0.240567	−0.001512	0.364734	0.057*
C17	0.3352 (3)	0.0332 (3)	0.4458 (11)	0.0458 (17)
H17	0.362019	−0.000551	0.389685	0.055*
C18	0.1062 (4)	0.1246 (5)	0.5782 (16)	0.080 (3)
H18A	0.113401	0.123166	0.697543	0.121*
H18B	0.057574	0.114595	0.553427	0.121*
H18C	0.118132	0.170668	0.536531	0.121*
N2	0.4441 (2)	0.0860 (3)	0.5516 (8)	0.0400 (13)
O1	0.5797 (2)	0.0554 (2)	0.6580 (7)	0.0493 (12)
O2	0.1498 (2)	0.0734 (3)	0.5000 (9)	0.0616 (16)
Cu1	0.500000	0.000000	0.60260 (16)	0.0420 (3)

1 Source of material

In a three-neck round-bottom flask fitted with a thermometer and condenser, a solution of (*E*)-1-(((4-methoxy-phenyl) imino)methyl)naphthalene-2-ol (0.28 g, 1.0 mmol) in dry EtOH (20 mL) was stirred. The solution was heated under reflux while a solution of NaOH (10 % w/v) was added dropwise. Subsequently, a solution of copper nitrate trihydrate (0.24 g, 1.0 mmol) in EtOH (10 mL) was added dropwise. The mixture was maintained under reflux for 5 h, and the progress of the reaction was monitored using thin-layer chromatography. The mixture was allowed to cool, and the solid produced was collected by filtration, washed with EtOH (3 × 10 mL), and dried in a vacuum oven to give the title compound in 82 % yield as orange crystals, mp 340–341 °C. **IR** (KBr; cm^{-1}): 1607 (C=N), 1501 (C=C), 3017 (C–H).

2 Experimental details

All hydrogen atoms were identified by difference Fourier syntheses. The methyl group was refined with idealized geometry as a rigid group and allowed to rotate about the O–C bond (AFIX 137 option of the SHELXL program[3]). The U_{iso} values of the hydrogen atoms of methyl groups were set to 1.5 U_{eq} (C) and the U_{iso} values of all other hydrogen atoms were set to 1.2 U_{eq} (C, N).

3 Comment

Schiff bases are cost-effective, easily synthesized, and environmentally friendly compounds used as ligands in various applications, including the development of new anti-corrosion agents.[5–7] Schiff bases of 2-hydroxynaphthaldehyde act as multidentate ligands with important potential applications.[8] The strong chelation affinity of these Schiff bases for transition metals can be used to produce useful complexes.[9–11] Copper complexes containing O and N donor systems show interesting biological activities.[12] The synthesis of such complexes is therefore of wide interest.

The asymmetric unit of the crystal structure of the title compound consists of one [(4-methoxyphenyl)imino]-methylnaphthalenolate ligand and a Cu ion located on a 2-fold rotation axis (Figure). The ligand has two planar fragments, namely (iminomethyl)naphthalen-2-olate (C1–C11, N2, O1) and 4-methoxyaniline (C12–C18, O2) groups. The twist angle between the planes of the two fragments of one ligand is 58.8 (1)°.

The Cu ion is coordinated by two nitrogen and two oxygen atoms in trans geometry. Atoms O1, Cu1 and N2 form a triangle and a second triangle is generated by twofold rotation to complete the Cu coordination. The twist angle between the planes through the triangles is 35.8 (1)°, leading to distortion from perfect planarity. Similar distortion is also observed in, for example, bis(N-menthyl-2-amino-5,5,5-trifluoro-4-trifluoromethyl-4-hydroxy-pentane–N, O)-copper(II)[13] with an angle of 14.77° and in bis(N-(5,5,5-trifluoro-4-trifluoromethylpentan-2-yl-4-olato)methylamine)-copper(II)[14] with an angle of 33.34°.

In the crystal structure, complex units related by glide symmetry are stacked along the *c* axis. In a stack, the distance between the copper ions of neighbouring complex units is 3.979 Å. Adjacent stacks are linked by C–H···O contacts with a C18···O2 distance of 3.49(1) Å and a C18–H18B···O2 angle of 153.7°. Bond lengths and angles are all in the expected ranges.[15]

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