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Crystal structure of bis{4-methyl-2-((*E*)-((4-((*E*)-1-(ethoxyimino)ethyl)phenyl)imino)methyl)phenolato- $\kappa^2 N, O$ }copper(II), $C_{36}H_{38}CuN_4O_4$

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.28 × 0.25 × 0.22 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.72 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II CCD, φ and ω
$\theta_{\max}$, completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5943, 2842, 0.031
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2452
$N(\text{param})_{\text{refined}}$:	208
Programs:	Bruker [17], SHELX [18]

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Abstract

$C_{36}H_{38}CuN_4O_4$, triclinic, $P\bar{1}$, $a = 8.492(2)$ Å, $b = 9.574(2)$ Å, $c = 10.512(2)$ Å, $\alpha = 100.170(7)^\circ$, $\beta = 103.421(7)^\circ$, $\gamma = 95.055(8)^\circ$, $Z = 1$, $V = 810.8(3)$ Å³, $R_{\text{gt}}(F) = 0.0418$, $wR_{\text{ref}}(F^2) = 0.1193$, $T = 296(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Synthesis of the ligand: 4-Amino acetophenone ethoxy oxime was prepared by a similar method reported earlier [1, 2], refluxing a mixture of a solution of 2-hydroxy-5-methylbenzaldehyde (544.7 mg, 4 mmol) in ethanol (10 mL) and a solution of 4-amino acetophenone ethoxy oxime (712.9 mg, 4 mmol) in ethanol (10 mL) at 328 K. Nine hours later, the

mixture was filtered at room temperature. The product was dried under vacuum and a yellow solid was obtained (yield 76.5%, m.p. 401–408 K). Elemental analysis: Anal. Calcd. for $C_{18}H_{20}N_2O_2$: C, 72.95%; H, 6.80%; N, 9.45%; Found: C, 72.92%; H, 6.87%; N, 9.40%.

Synthesis of the copper(II) complex: Copper(II) acetate monohydrate (2.0 mg, 10 mmol) in ethanol (2 mL) was added dropwise to a solution of the ligand (5.9 mg, 20 mmol) in trichloromethane (4 mL) at room temperature. The color of the solution turned to brown, immediately. The mixture was filtered after being stirred for 2 h at room temperature and the filtrate was allowed to stand for 22 days at room temperature. The solvent was partially evaporated and several clear dark brown crystals were obtained. Anal. Calcd. for $C_{36}H_{38}CuN_4O_4$: C, 66.09%; H, 5.85%; Cu, 9.71%; N, 8.56%. Found: C, 66.14%; H, 5.82%; Cu, 9.75%; N, 8.51%.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Oximes are an important class of ligands due to the presence of several coordination sites [3–5]. Thus oxime-type compound and their metal complexes have been widely studied [6–8]. For example: it has been used as analytical reagents for the detection and determination of some metal ions [9, 10], in nonlinear optic [11–13] and supramolecular architectures [14–16] etc.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C1	0.3023(5)	1.0995(4)	−0.0563(3)	0.0682(10)
H1A	0.3946	1.1730	−0.0323	0.102*
H1B	0.2239	1.1155	−0.1324	0.102*
H1C	0.3378	1.0077	−0.0779	0.102*
C2	0.2243(4)	1.1027(3)	0.0603(3)	0.0474(7)
C3	0.1139(4)	1.1972(3)	0.0823(3)	0.0518(8)
H3	0.0888	1.2597	0.0244	0.062*
C4	0.0404(4)	1.2023(3)	0.1858(3)	0.0528(8)
H4	−0.0311	1.2690	0.1972	0.063*
C5	0.0711(4)	1.1083(3)	0.2752(3)	0.0417(7)
C6	0.1835(3)	1.0115(3)	0.2549(3)	0.0382(6)
C7	0.2581(4)	1.0118(3)	0.1470(3)	0.0449(7)
H7	0.3325	0.9481	0.1350	0.054*
C8	0.2236(4)	0.9094(3)	0.3370(3)	0.0416(7)
H8	0.3002	0.8513	0.3164	0.050*
C9	0.2274(3)	0.7736(3)	0.4981(3)	0.0381(6)
C10	0.1622(4)	0.6345(3)	0.4439(3)	0.0578(9)
H10	0.0746	0.6134	0.3685	0.069*
C11	0.2253(4)	0.5241(3)	0.5000(3)	0.0561(9)
H11	0.1792	0.4301	0.4613	0.067*
C12	0.3542(3)	0.5505(3)	0.6114(3)	0.0376(6)
C13	0.4167(4)	0.6922(3)	0.6662(3)	0.0608(9)
H13	0.5033	0.7140	0.7423	0.073*
C14	0.3539(4)	0.8020(3)	0.6109(3)	0.0608(9)
H14	0.3979	0.8963	0.6505	0.073*
C15	0.4236(4)	0.4331(3)	0.6710(3)	0.0402(6)
C16	0.3409(5)	0.2817(3)	0.6212(4)	0.0665(10)
H16A	0.3596	0.2448	0.5357	0.100*
H16B	0.2256	0.2796	0.6127	0.100*
H16C	0.3846	0.2240	0.6834	0.100*
C17	0.7637(4)	0.4035(4)	0.9170(3)	0.0637(9)
H17A	0.8278	0.4736	0.8866	0.076*
H17B	0.8258	0.3244	0.9287	0.076*
C18	0.7362(5)	0.4694(5)	1.0464(4)	0.0789(12)
H18A	0.6806	0.5514	1.0364	0.118*
H18B	0.8394	0.4986	1.1111	0.118*
H18C	0.6707	0.4010	1.0759	0.118*
Cu1	0.0000	1.0000	0.5000	0.03844(19)
N1	0.1657(3)	0.8878(2)	0.4372(2)	0.0388(5)
N2	0.5538(3)	0.4700(3)	0.7656(2)	0.0494(6)
O1	−0.0041(3)	1.1145(2)	0.3714(2)	0.0537(6)
O2	0.6117(3)	0.3517(2)	0.8164(2)	0.0570(6)

In the title complex, Cu1 atom is four-coordinate, with a N₂O₂ coordination sphere, and a planar arrangement. The Cu1–N1 bond lengths are both 2.004(2) Å and the Cu1–O1 bond lengths are both 1.881(2) Å. The angles of N1–Cu1–O1 and N1–Cu1–O1ⁱ are 92.52(9) and 87.48(9), respectively. All geometric parameters are in the typical ranges.

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