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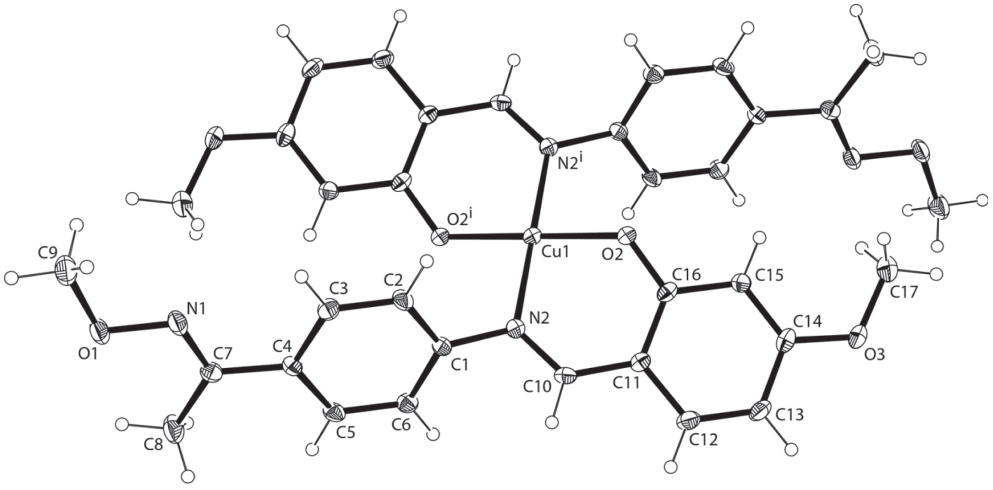
Crystal structure of bis{5-methoxy-2-((*E*)-((4-((*E*)-1-(methoxyimino)ethyl)phenyl)imino)methyl) phenolato-κ^2*N*,*O*)}copper(II), $C_{34}H_{34}CuN_4O_6$



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Abstract

$C_{34}H_{34}CuN_4O_6$, Monoclinic, $P2_1/c$, $a = 10.4018(4)$ Å, $b = 6.1634(2)$ Å, $c = 24.2227(15)$ Å, $\beta = 101.820(5)°$, $Z = 2$, $V = 1520.01(13)$ Å^3, $R_{gt}(F) = 0.0565$, $wR_{ref}(F^2) = 0.1455$, $T = 292$ K.

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The crystal title 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.

Table 1: Data collection and handling.

Crystal:	Clear light red block
Size:	0.24 × 0.21 × 0.16 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.77 mm^{-1}
Diffractometer, scan mode:	SuperNova, *ω*
θ_{max}, completeness:	26.0°, 99.7%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5769, 2976, 0.039
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2206
$N(param)_{refined}$:	208
Programs:	Olex2 [25], CrysAlis PRO [26], SHEL [24]

Source of material

All reagents and starting materials were obtained from commercial suppliers and used as received. Synthesis of the ligand was prepared by a similar method reported earlier [1–5]. A solution of copper(II) acetate monohydrate (2.0 mg, 10 mmol) in ethanol (2 mL) was added dropwise to a solution of ligand (*E*)-1-(4-(((*E*)-2-hydroxy-4-methoxybenzylidene)amino)phenyl)ethan-1-one *O*-methyl oxime (6.0 mg, 20 mmol) in ethanol (5 mL) at room temperature. Immediately, the color of the solution turned brown, and the solution was stirred for 1 h. The solution was filtered and the filtrate was allowed to stand at room temperature for about six weeks, and we got several clear light red block crystals. Elemental analysis: Anal. calcd for $C_{34}H_{34}CuN_4O_6$: C, 62.04%; H, 5.21%; N, 8.51%; Found: C, 62.09%; H, 5.20%; N, 8.46%.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cu1	1.0000	0.0000	0.5000	0.0247(2)
O1	0.3629(3)	0.3197(5)	0.65238(12)	0.0356(7)
O2	1.0320(3)	−0.0707(4)	0.42829(11)	0.0312(7)
O3	1.2118(3)	0.1246(5)	0.27022(11)	0.0325(7)
N1	0.4417(3)	0.2707(6)	0.61350(14)	0.0311(8)
N2	0.8768(3)	0.2317(5)	0.46522(12)	0.0236(7)
C1	0.7781(3)	0.2979(6)	0.49570(15)	0.0221(8)
C2	0.6921(4)	0.1419(6)	0.50698(17)	0.0283(9)
H2	0.6928	0.0043	0.4913	0.034*
C3	0.6056(4)	0.1880(7)	0.54112(17)	0.0289(9)
H3	0.5483	0.0807	0.5483	0.035*
C4	0.6018(3)	0.3928(6)	0.56541(15)	0.0228(8)
C5	0.6863(3)	0.5500(6)	0.55223(16)	0.0267(9)
H5	0.6846	0.6888	0.5671	0.032*
C6	0.7731(3)	0.5045(6)	0.51729(16)	0.0252(8)
H6	0.8278	0.6127	0.5084	0.030*
C7	0.5134(3)	0.4341(7)	0.60514(16)	0.0253(9)
C8	0.5133(4)	0.6493(7)	0.6334(2)	0.0437(12)
H8A	0.4864	0.7596	0.6054	0.066*
H8B	0.6001	0.6811	0.6542	0.066*
H8C	0.4533	0.6457	0.6586	0.066*
C9	0.2949(5)	0.1265(8)	0.6611(2)	0.0492(13)
H9A	0.2519	0.0682	0.6253	0.074*
H9B	0.2307	0.1588	0.6833	0.074*
H9C	0.3563	0.0221	0.6806	0.074*
C10	0.8904(3)	0.3362(6)	0.42059(15)	0.0245(8)
H10	0.8403	0.4609	0.4113	0.029*
C11	0.9770(3)	0.2742(6)	0.38423(15)	0.0228(8)
C12	0.9939(4)	0.4171(7)	0.34096(16)	0.0296(9)
H12	0.9513	0.5506	0.3376	0.036*
C13	1.0715(4)	0.3637(7)	0.30390(16)	0.0315(9)
H13	1.0825	0.4603	0.2757	0.038*
C14	1.1347(3)	0.1607(7)	0.30881(15)	0.0267(9)
C15	1.1186(4)	0.0163(6)	0.34978(15)	0.0252(8)
H15	1.1590	−0.1188	0.3516	0.030*
C16	1.0413(3)	0.0708(6)	0.38914(15)	0.0235(8)
C17	1.2808(4)	−0.0752(8)	0.27302(19)	0.0411(11)
H17A	1.3351	−0.0757	0.2454	0.062*
H17B	1.2191	−0.1928	0.2656	0.062*
H17C	1.3349	−0.0923	0.3100	0.062*

Experimental details

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

Discussion

Oxime-type compounds, a unique family of organic compounds with a wide spectrum of practical applications, can act as chelating agents with various metal ions [6–11]. Owing to their unique chemical reactivity, oxime derivatives have found their ways into a wide range of industrial practices and engineering applications, including photophysical properties [12–16], molecular recognition [17, 18] and supramolecular architectures [19–23] and so on.

We have designed and synthesized a new copper(II) complex, which is built up by the $C_{34}H_{34}CuN_4O_6$ complexes. Cu1 is four-coordinated by two O atoms and two N atoms from two different ligands. The Cu1–N2 bond lengths are both 1.987(3) Å and the Cu1–O2 bond lengths are both 1.885(3) Å . The angles of N2–Cu1–O2 and N2–Cu1–O2^i are 89.76(12) and 90.25(12), respectively. All geometric parameters are in the typical ranges.

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