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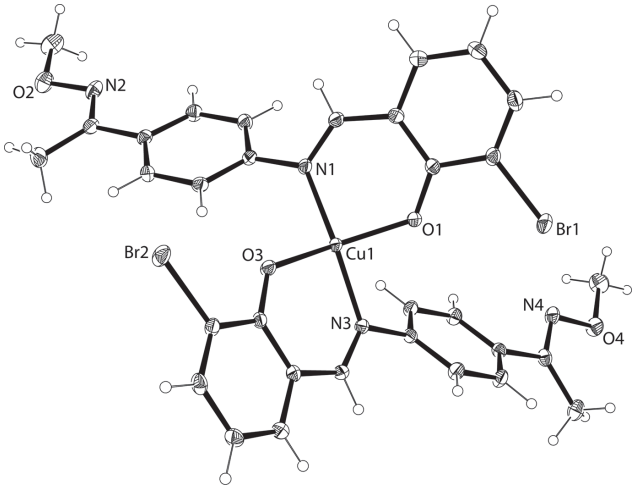
Crystal structure of bis{2-bromo-6-(((4-(1-(methoxyimino)ethyl)phenyl)imino)methyl) phenolato-κ²*N*,*O*}copper(II), $C_{32}H_{28}Br_2CuN_4O_4$



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Abstract

$C_{32}H_{28}Br_2CuN_4O_4$, triclinic, $P\bar{1}$ (no. 2), $a = 8.6466(2)$ Å, $b = 13.4901(4)$ Å, $c = 14.5322(4)$ Å, $\alpha = 115.997(1)°$, $\beta = 90.645(1)°$, $\gamma = 100.083(1)°$, $Z = 2$, $V = 1492.61(7)$ Å^3, $R_{gt}(F) = 0.0282$, $wR_{ref}(F^2) = 0.0660$, $T = 173(2)$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title complex was prepared by a similar method reported previously [4]. Copper(II) acetate tetrahydrate (2.00 mg,

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Table 1: Data collection and handling.

Crystal:	Brown block
Size:	0.19 × 0.17 × 0.14 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	3.45 mm^{-1}
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
θ_{max}, completeness:	27.9°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	31737, 7121, 0.035
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 6160
$N(param)_{refined}$:	409
Programs:	Bruker [1], SHELX [2], Olex2 [3]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.28079(4)	0.51674(2)	0.73366(2)	0.04486(8)
Br2	0.00757(3)	−0.17278(2)	0.24531(2)	0.03321(7)
Cu1	0.36609(3)	0.16755(2)	0.47474(2)	0.02016(6)
O1	0.37557(18)	0.32345(12)	0.55742(11)	0.0253(3)
O2	0.8174(2)	−0.14128(16)	−0.13359(13)	0.0418(4)
O3	0.24777(18)	0.01852(12)	0.40255(11)	0.0257(3)
O4[a]	0.9797(2)	0.67866(16)	0.99864(14)	0.0376(5)
O4A[b]	0.9106(18)	0.6082(12)	0.8620(12)	0.0376(5)
N1	0.4121(2)	0.19014(14)	0.35000(13)	0.0212(3)
N2	0.7638(2)	−0.06325(18)	−0.04610(14)	0.0326(4)
N3	0.4088(2)	0.15045(14)	0.60000(13)	0.0208(3)
N4[a]	0.8894(5)	0.5899(3)	0.9102(2)	0.0316(7)
N4A[b]	0.893(3)	0.598(2)	0.9487(19)	0.034(4)
C1	0.3279(2)	0.38910(16)	0.52441(15)	0.0220(4)
C2	0.2736(3)	0.48603(17)	0.59315(16)	0.0260(4)
C3	0.2142(3)	0.55500(18)	0.56162(18)	0.0306(5)
H3	0.174880	0.617221	0.610020	0.037*
C4	0.2111(3)	0.53419(19)	0.45867(19)	0.0335(5)
H4	0.169733	0.581800	0.436566	0.040*
C5	0.2688(3)	0.44394(19)	0.38956(18)	0.0311(5)
H5	0.270607	0.431138	0.319915	0.037*
C6	0.3250(2)	0.37029(17)	0.42032(16)	0.0229(4)
C7	0.3823(3)	0.27781(17)	0.34298(16)	0.0238(4)
H7	0.400225	0.281113	0.279919	0.029*
C8	0.4788(2)	0.11376(17)	0.26314(15)	0.0219(4)
C9	0.5981(3)	0.15495(18)	0.21740(16)	0.0261(4)
H9	0.638140	0.233686	0.245477	0.031*

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
C10	0.6583(3)	0.08222(18)	0.13177(17)	0.0276(5)
H10	0.739220	0.111706	0.101564	0.033*
C11	0.6024(2)	−0.03394(18)	0.08879(15)	0.0233(4)
C12	0.4855(3)	−0.07404(17)	0.13601(16)	0.0256(4)
H12	0.446259	−0.152823	0.108385	0.031*
C13	0.4248(2)	−0.00161(17)	0.22263(16)	0.0240(4)
H13	0.346126	−0.031158	0.254112	0.029*
C14	0.6659(3)	−0.11170(19)	−0.00443(16)	0.0262(4)
C15	0.6156(3)	−0.2361(2)	−0.0425(2)	0.0401(6)
H15A	0.502167	−0.258787	−0.064642	0.060*
H15B	0.637604	−0.255902	0.012977	0.060*
H15C	0.673970	−0.275114	−0.100724	0.060*
C16	0.9266(3)	−0.0806(3)	−0.1737(2)	0.0469(7)
H16A	0.976564	−0.133560	−0.229342	0.070*
H16B	1.007835	−0.026514	−0.118722	0.070*
H16C	0.870025	−0.040235	−0.200391	0.070*
C17	0.1827(2)	−0.04624(16)	0.44213(15)	0.0206(4)
C18	0.2240(2)	−0.02905(16)	0.54376(16)	0.0226(4)
C19	0.1506(3)	−0.10523(17)	0.57968(17)	0.0267(4)
H19	0.181867	−0.093282	0.647218	0.032*
C20	0.0350(3)	−0.19634(18)	0.51952(18)	0.0292(5)
H20	−0.014055	−0.246566	0.545193	0.035*
C21	−0.0096(3)	−0.21411(17)	0.41980(17)	0.0275(5)
H21	−0.090742	−0.276079	0.377604	0.033*
C22	0.0638(2)	−0.14208(17)	0.38286(15)	0.0234(4)
C23	0.3380(2)	0.06630(17)	0.61472(15)	0.0224(4)
H23	0.364250	0.067938	0.679088	0.027*
C24	0.5077(2)	0.24150(16)	0.68528(15)	0.0209(4)
C25	0.4613(3)	0.28170(18)	0.78410(16)	0.0268(4)
H25	0.362146	0.248885	0.796359	0.032*
C26	0.5601(3)	0.36990(18)	0.86494(16)	0.0273(5)
H26	0.529008	0.395636	0.932744	0.033*
C27	0.7040(2)	0.42146(17)	0.84857(16)	0.0225(4)
C28	0.7481(3)	0.38039(18)	0.74852(16)	0.0258(4)
H28	0.846260	0.413994	0.735746	0.031*
C29	0.6514(3)	0.29170(17)	0.66787(16)	0.0247(4)
H29	0.683105	0.264875	0.600190	0.030*
C30	0.8043(3)	0.51803(17)	0.93588(17)	0.0255(4)
C31	0.8027(3)	0.5260(2)	1.04140(18)	0.0359(5)
H31A	0.908794	0.559769	1.077872	0.054*
H31B	0.770021	0.450539	1.036787	0.054*
H31C	0.728398	0.573031	1.078957	0.054*
C32[a]	1.0769(4)	0.7524(3)	0.9665(3)	0.0446(8)
H32A[a]	1.146757	0.711130	0.917687	0.067*
H32B[a]	1.140497	0.815333	1.026561	0.067*
H32C[a]	1.010061	0.781543	0.933285	0.067*
C32A[b]	1.030(3)	0.7042(18)	0.8725(18)	0.0446(8)
H32D[b]	1.034884	0.706374	0.806097	0.067*
H32E[b]	1.133083	0.697009	0.894975	0.067*
H32F[b]	1.002612	0.773808	0.923652	0.067*

[a]Occupancy: 0.878(3), [b]Occupancy: 0.122(3).

10 mmol) was dissolved in ethanol (2 mL) and was added dropwise to 3-bromo-2-(((4-(1-(ethoxy-imino)ethyl)phenyl) imino)methyl)phenole (6.95 mg, 20 mmol) dissolved in chloroform (4 mL) at room temperature. One hour later, the mixture was filtered. The filtrate was allowed to stand for 16 days at a quiet environment. Several clear light brown crystals were obtained. **Anal. Calcd.** for $C_{32}H_{28}Br_2CuN_4O_4$: C, 50.84%; H, 3.73%; N, 7.41%. Found: C, 50.66%; H, 3.96%; N, 7.22%.

Experimental details

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

Comment

Transition metal complexes are obtained by reacting inorganic transition metal ions with organic ligands [5, 6]. The complexes containing different transition metal ions have found their ways into a wide range of applications, including luminescence materials [7] and supramolecular projects [8–11] and so on. Therefore, we designed and prepared various transition metal complexes, and predicted their properties [12, 13].

In the title complex, Cu1 is four-coordinated by two O atoms and two N atoms from two ligands. The Cu1—N1 bond length is 1.9989(17) Å and the Cu1—N3 is 1.9713(17) Å. The Cu1—O1 and Cu1—O3 bond lengths are both 1.8962(14) Å. The angle of N1—Cu1—O1 is 92.25(6)°, N1—Cu1—O3 is 96.01(6)°, N3—Cu1—O1 is 89.44(7)° and O1—Cu1—O3 is 150.39(7)°, respectively. All geometric parameters are in the typical ranges [14].

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