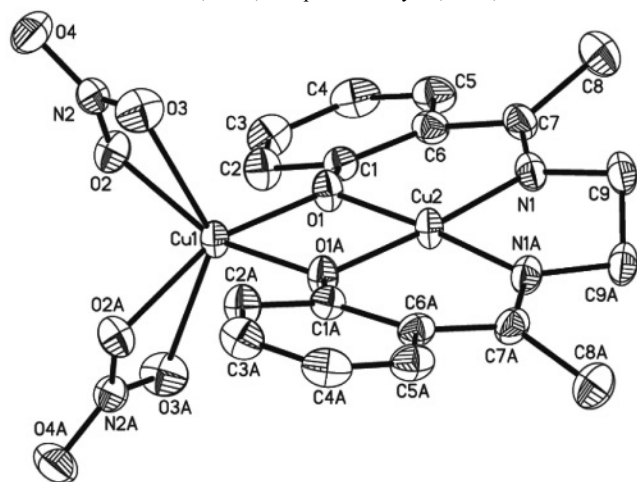


Crystal structure of *N,N'*-ethylene-bis(*o*-hydroxyacetophenone-iminato- $\kappa^6O,O',N,N':O,O'$ -bis(nitrato- κ^2O,O')-dicopper(II), $C_{18}H_{18}Cu_2N_4O_8$

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Abstract

$C_{18}H_{18}Cu_2N_4O_8$, monoclinic, $C2/c$ (no. 15), $a = 11.488(2)$ Å, $b = 10.475(2)$ Å, $c = 16.942(3)$ Å, $\beta = 106.769(3)^\circ$, $V = 1952.1$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0247$, $wR_{\text{ref}}(F^2) = 0.0866$, $T = 296$ K.

Table 1. Data collection and handling.

Crystal:	black blocks, size 0.12×0.13×0.16 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	22.37 cm ⁻¹
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{\text{max}}$:	55.6°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	8663, 2293
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1956
$N(\text{param})_{\text{refined}}$:	147
Programs:	SHELX [5]

Source of material

A solution of $Cu(NO_3)_2 \cdot 3H_2O$ (24.2 mg, 0.10 mmol) in 1 ml methanol was slowly added to a solution of *N,N*-bis(*o*-hydroxyacetophenone)-1,2-diaminoethane (H_2L) (14.8 mg, 0.05 mmol) in 3 ml methanol with general stirring. The resulting mixture was placed in the dark, and black well shaped crystals were obtained after one day, in a yield of 46% (based on Cu).

Experimental details

H atoms were included in the refinement at calculated positions [$C-H_{\text{aromatic}} = 0.93$ Å with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$; $C-H_{\text{methyl}} = 0.96$ Å with $U_{\text{iso}} = 1.5 U_{\text{eq}}(C)$].

Discussion

Schiff bases complexes are an important and popular area of research due to their simple synthesis, versatility, and diverse range

of applications [1]. In particularly, a large number of copper(II)-Schiff bases complexes have been synthesized and characterized due to their interesting properties and novel topologies [2,3]. Herein, the title compound has been synthesized and its crystal structure has also been determined. The molecular structure of the title structure is made up of discrete neutral $[Cu_2(L)(NO_3)_2]$. The metal center Cu(1) is sixfold coordinated by two phenoxo oxygen atoms and four oxygen atoms from two NO_3^- . The second metal center Cu(2) is coordinated to two phenoxo oxygen atoms and two imine nitrogen atoms from one ligand to exhibit a square plane geometry. In the title complex, the bond lengths of Cu–O are in the range of 1.892(1) Å to 2.426(2) Å, and the Cu–N bond distance is 1.910(2) Å, which are normally observed in Cu(II) complexes [4].

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}
H(2)	8f	0.0352	0.0847	0.4272	0.057
H(3)	8f	0.0877	0.0920	0.5687	0.065
H(4)	8f	0.1534	0.2806	0.6374	0.067
H(5)	8f	0.1595	0.4622	0.5639	0.062
H(8A)	8f	0.2193	0.6659	0.4206	0.108
H(8B)	8f	0.2528	0.5789	0.4993	0.108
H(8C)	8f	0.1376	0.6667	0.4804	0.108
H(9A)	8f	0.1281	0.6601	0.2730	0.058
H(9B)	8f	0.0461	0.7179	0.3241	0.058

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(1)	8 <i>f</i>	0.0689(2)	0.2691(2)	0.4079(1)	0.0381(9)	0.0405(9)	0.0328(9)	0.0006(7)	0.0097(7)	−0.0030(7)
C(2)	8 <i>f</i>	0.0616(2)	0.1614(2)	0.4541(1)	0.060(1)	0.045(1)	0.0388(9)	−0.0002(9)	0.0160(9)	0.0036(8)
C(3)	8 <i>f</i>	0.0927(2)	0.1656(2)	0.5391(1)	0.060(1)	0.064(1)	0.042(1)	0.005(1)	0.0189(9)	0.009(1)
C(4)	8 <i>f</i>	0.1309(2)	0.2780(3)	0.5801(1)	0.051(1)	0.084(2)	0.033(1)	0.006(1)	0.0108(9)	−0.002(1)
C(5)	8 <i>f</i>	0.1354(2)	0.3861(2)	0.5357(1)	0.045(1)	0.065(2)	0.041(1)	−0.0027(9)	0.0068(9)	−0.0148(9)
C(6)	8 <i>f</i>	0.1048(2)	0.3864(2)	0.4487(1)	0.037(1)	0.045(1)	0.0387(9)	−0.0032(7)	0.0095(7)	−0.0075(7)
C(7)	8 <i>f</i>	0.1111(2)	0.5084(2)	0.4075(1)	0.043(1)	0.039(1)	0.051(1)	−0.0068(8)	0.0144(8)	−0.0128(8)
C(8)	8 <i>f</i>	0.1871(3)	0.6146(2)	0.4564(2)	0.071(2)	0.057(2)	0.079(2)	−0.012(1)	0.006(1)	−0.019(1)
C(9)	8 <i>f</i>	0.0534(2)	0.6484(2)	0.2880(1)	0.059(1)	0.0280(9)	0.066(1)	−0.0052(8)	0.030(1)	−0.0044(8)
Cu(1)	4 <i>e</i>	0	0.11154(3)		0.0458(2)	0.0260(2)	0.0348(2)	0	0.0098(1)	0
Cu(2)	4 <i>e</i>	0	0.39411(3)		0.0555(2)	0.0252(2)	0.0351(2)	0	0.0127(2)	0
N(1)	8 <i>f</i>	0.0561(2)	0.5250(2)	0.3305(1)	0.0479(9)	0.0311(8)	0.0478(8)	−0.0050(6)	0.0194(7)	−0.0063(6)
N(2)	8 <i>f</i>	0.1883(2)	−0.0372(2)	0.2766(1)	0.0440(9)	0.0374(8)	0.0492(9)	−0.0019(7)	0.0062(7)	−0.0105(7)
O(1)	8 <i>f</i>	0.0454(2)	0.2572(1)	0.32545(9)	0.0585(9)	0.0299(7)	0.0318(7)	−0.0015(5)	0.0100(6)	−0.0008(4)
O(2)	8 <i>f</i>	0.1105(1)	−0.0208(1)	0.31670(9)	0.0568(9)	0.0434(8)	0.0478(7)	0.0094(6)	0.0168(7)	0.0070(6)
O(3)	8 <i>f</i>	0.1748(2)	0.0286(2)	0.2135(1)	0.062(1)	0.078(1)	0.0573(9)	0.0029(9)	0.0235(8)	0.0088(8)
O(4)	8 <i>f</i>	0.2708(2)	−0.1139(2)	0.3016(1)	0.057(1)	0.059(1)	0.086(1)	0.0209(8)	0.0081(9)	−0.0063(8)

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