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Crystal structure of bis((*E*)-2-ethoxy-6-(((2-hydroxyethyl)imino)methyl)phenolato- $\kappa^2 N,O$) copper(II), $C_{22}H_{28}N_2CuO_6$

Table 1: Data collection and handling.

Crystal:	Blue block
Size:	0.13 × 0.11 × 0.09 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	1.07 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	15460, 1865, 0.018
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1814
$N(\text{param})_{\text{refined}}$:	144
Programs:	Bruker [1], SHELX [2, 3]

structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

<https://doi.org/10.1515/ncrs-2018-0367>

Received September 12, 2018; accepted November 12, 2018;
available online December 5, 2018

Abstract

$C_{22}H_{28}N_2CuO_6$, monoclinic, $P2_1/c$ (no. 14), $a = 8.5942(7)$ Å, $b = 25.888(2)$ Å, $c = 4.8204(4)$ Å, $\beta = 97.785(3)^\circ$, $V = 1062.60(15)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0313$, $wR_{\text{ref}}(F^2) = 0.0878$, $T = 296(2)$ K.

CCDC no.: 1878496

The crystal structure is shown in the figure. The asymmetric unit is labelled. Tables 1 and 2 contain details on crystal

Source of material

The Schiff base ligand was purchased from Acros Ltd. and used without further purification; also other reagents were commercially available and used as purchased. A mixture of $CuCl_2$ (53.78 mg, 0.4 mmol), Schiff base ligand (49.64 mg, 0.4 mmol) and distilled water (10 mL) was sealed in a 23 mL Teflon-lined steel vessel and heated at 140 °C for 72 h, and then cooled to room temperature at a rate of 0.05 °C min⁻¹. The resulting light turquoise block crystals of the compound were obtained and washed with distilled water. The yield is ca. 22%. IR(KBr): 3226(s), 1527(s), 1518(s), 1492(s), 1441(s), 1352(s), 1242(s), 1171(s), 1112(s), 1071(s), 1001(s), 921(s), 891(s), 831(m), 771(m), 712(m), 611(m), 491(m) cm⁻¹.

Experimental details

All H atoms were placed geometrically and treated as riding on their parent atoms, with C–H 0.96, with $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$.

Comment

Schiff bases are able to form the coordination bonds with many transition metal ions via phenolic or azomethine groups accordingly, they have been used for synthesis of metal complexes because of their easy formation and strong metal binding ability [4–8]. Transition elements are the

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

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cu1	0.5000	0.5000	0.5000	0.03140(15)
N1	0.3245(2)	0.52338(7)	0.7057(4)	0.0330(4)
O1	0.5958(2)	0.64550(7)	0.0678(4)	0.0501(5)
O2	0.52984(18)	0.56843(6)	0.3773(4)	0.0416(4)
O3	0.1441(2)	0.43089(8)	0.5498(4)	0.0574(5)
H3	0.2300	0.4166	0.5777	0.086*
C1	0.8001(4)	0.67862(13)	−0.1606(8)	0.0751(10)
H1A	0.8705	0.6730	0.0089	0.113*
H1B	0.8345	0.7080	−0.2571	0.113*
H1C	0.7991	0.6487	−0.2782	0.113*
C2	0.6384(3)	0.68826(10)	−0.0912(6)	0.0526(7)
H2A	0.6364	0.7199	0.0163	0.063*
H2B	0.5650	0.6918	−0.2616	0.063*
C3	0.4573(3)	0.64877(9)	0.1764(5)	0.0392(5)
C4	0.3519(3)	0.68908(10)	0.1344(6)	0.0479(6)
H4	0.3725	0.7166	0.0212	0.057*
C5	0.2152(3)	0.68903(10)	0.2592(7)	0.0540(7)
H5	0.1449	0.7164	0.2286	0.065*
C6	0.1843(3)	0.64900(10)	0.4259(6)	0.0490(6)
H6	0.0934	0.6494	0.5107	0.059*
C7	0.2890(3)	0.60676(9)	0.4718(5)	0.0374(5)
C8	0.4270(3)	0.60597(8)	0.3454(5)	0.0346(5)
C9	0.2536(3)	0.56683(9)	0.6606(5)	0.0370(5)
H9	0.1704	0.5731	0.7608	0.044*
C10	0.2631(3)	0.48976(9)	0.9147(5)	0.0381(5)
H10A	0.2362	0.5109	1.0674	0.046*
H10B	0.3446	0.4658	0.9911	0.046*
C11	0.1196(3)	0.45955(10)	0.7896(5)	0.0445(6)
H11A	0.0896	0.4361	0.9299	0.053*
H11B	0.0332	0.4834	0.7396	0.053*

essential elements for human beings with their bio essential, enzymatic activity and oxidative nature has attracted numerous inorganic chemists to address medicinal applications of Cu, Ni and Co cationic complexes. Now, we synthesized a new copper complex.

The compound crystallizes in the monoclinic space group *P*2₁/*c* with two formula units in the unit cell. As shown in the figure, one formula unit consists of two Schiff base ligands and one Cu atom, located on an inversion center. The Cu1 ion is in a slightly distorted square coordination environment, with two nitrogen atoms and two oxygen atoms from two

Schiff base ligands. The bond length of Cu1–N1 is 2.007 Å, while the bond length of Cu1–O2 is 1.896 Å. The structure is closely related to a literature known Cu(II) complex [9].

Acknowledgements: This work was supported by Henan science and technology project (Nos. 172102210161, 172102310166), the Key Scientific Research Projects of Colleges and Universities, Henan Province (Nos. 18A150020) and the Research Fund of Anyang Institute of Technology (Nos. YJJ2016014).

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