Baiying Wei and Chenzhong Cao*

Crystal structure of [6,6'-((1*E*,1'*E*)-(propane-1,3-diylbis(azaneylylidene))bis(methaneylylidene))bis(3-chlorophenol)- $\kappa^4 N,N',O,O'$] copper(II), $C_{17}H_{14}Cl_2CuN_2O_2$

Table 1: Data collection and handling.

Crystal:	Black block
Size:	0.22 × 0.18 × 0.14 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.68 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} :	4151, 1449, 0.023
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1154
$N(\text{param})_{\text{refined}}$:	123
Programs:	Bruker [1], SHELX [2], Olex2 [3]

Source of material

The title salen-type Schiff base ligand was prepared according to the literature method [4, 5] and the title complex was prepared according to the literature reported earlier [6]. The ethanol solution (20 ml) of the copper(II) acetate monohydrate (2 mmol) was slowly added into the ethanol solution (10 ml) of the title Schiff base ligand (2 mmol). The resulting mixture was kept being stirred for 1 h at room temperature until precipitation occurs. The product was collected by filtration and washed with ethanol solution. Then the product was dissolved in anhydrous ethanol and allowed to stand at room temperature 30 days in a quiet environment. Several block crystals were obtained.

Experimental details

H atoms were geometrically added and isotropically refined by the riding model. The propan-diyl moiety is disordered (see the Figure).

Comment

Some salen-type Schiff base complexes show photophysical properties, extensive attention has been attracted and were

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Abstract

$C_{17}H_{14}Cl_2CuN_2O_2$, monoclinic, $C2/c$ (no. 15), $a = 22.743(4)$ Å, $b = 8.0434(15)$ Å, $c = 8.9388(17)$ Å, $V = 1630.8(5)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0376$, $wR_{\text{ref}}(F^2) = 0.0997$, $T = 296(2)$ 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.

*Corresponding author: **Chenzhong Cao**, School of Resource Environment and Safety Engineering, School of Chemistry and Chemical Engineering, Key Laboratory of Theoretical Organic Chemistry and Function Molecule, Ministry of Education, Hunan University of Science and Technology, Xiangtan, 411201, P. R. China, E-mail: czcao@hnust.edu.cn

Baiying Wei, School of Resource Environment and Safety Engineering, Hunan University of Science and Technology, Xiangtan, 411201, P. R. China. <https://orcid.org/0000-0003-1694-1449>

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	U_{iso}^*/U_{eq}
Cu1	0.500000	0.46495 (6)	0.750000	0.0615 (2)
Cl1	0.28741 (5)	−0.06158 (17)	0.44459 (13)	0.1018 (4)
O1	0.44328 (10)	0.2942 (3)	0.7093 (3)	0.0628 (6)
N1	0.45644 (15)	0.6245 (3)	0.6191 (4)	0.0748 (9)
C1	0.40053 (13)	0.2882 (4)	0.6034 (4)	0.0580 (8)
C2	0.36714 (13)	0.1414 (5)	0.5848 (4)	0.0629 (9)
H2	0.373861	0.053845	0.651793	0.075*
C3	0.32476 (14)	0.1267 (6)	0.4684 (4)	0.0737 (10)
C4	0.31140 (18)	0.2532 (7)	0.3696 (5)	0.0928 (13)
H4	0.283212	0.239169	0.289861	0.111*
C5	0.34051 (19)	0.4007 (7)	0.3910 (4)	0.0899 (13)
H5	0.330381	0.488990	0.327046	0.108*
C6	0.38572 (15)	0.4242 (5)	0.5072 (4)	0.0668 (9)
C7	0.41233 (19)	0.5829 (5)	0.5270 (5)	0.0768 (10)
H7	0.396109	0.667446	0.466207	0.092*
C8 ^a	0.4630 (11)	0.8084 (12)	0.618 (3)	0.125 (9)
H8A ^a	0.427850	0.859470	0.652911	0.150*
H8B ^a	0.467233	0.846092	0.516234	0.150*
C9 ^a	0.5166 (5)	0.8622 (9)	0.7182 (16)	0.100 (4)
H9A ^a	0.551721	0.827456	0.671390	0.120*
H9B ^a	0.517028	0.982707	0.722659	0.120*
C10 ^a	0.5200 (10)	0.7979 (13)	0.872 (2)	0.103 (9)
H10A ^a	0.481044	0.799724	0.909843	0.123*
H10B ^a	0.545369	0.869600	0.936092	0.123*

^aOccupancy: 0.5.

applied to many fields [7, 8]. And copper salen-type Schiff base complexes are amongst the most versatile catalysts known for oxygenation reactions [9]. So, a variety of salen-type complexes have been synthesized and investigated [10–13].

In the crystal structure of the title compound the Cu atom is four-coordinated by two O atoms and two N atoms of the corresponding salen-type Schiff base ligand forming a tetrahedral N_2O_2 coordination mode. The bond lengths of Cu1–O1 is 1.901(2) Å and the Cu1–N1 is 1.957(3) Å. The angles of N1–Cu1–O1, N1–Cu1–N1', O1–N1–O1' and N1–Cu1–O1' are 93.00(2), 98.0(2), 87.50(13) and 153.53(11)°, respectively.

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References

1. Bruker. APEX2, Saint and SADABS; Bruker AXS Inc.: Madison, WI, USA, 2012.
2. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* 2015, C71, 3–8.
3. Dolomanov O. V., Bourhis L. J., Gildea R. J., Howard J. A. K., Puschmann H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* 2009, 42, 339–341.
4. Shi L., Ge H., Tan S., Li H., Song Y., Zhu H., Tan R. Synthesis and antimicrobial activities of Schiff bases derived from 5-chloro-salicylaldehyde. *Eur. J. Med. Chem.* 2007, 42, 558–564.
5. Asadi Z., Shorkaei M. R. Synthesis, X-ray crystallography, thermal studies, spectroscopic and electrochemistry investigations of uranyl Schiff base complexes. *Spectrochim. Acta, Part A* 2013, 105, 344–351.
6. Kargar H., Ardakani A. A., Tahir M. N., Ashfaq M., Munawar K. S. Synthesis, spectral characterization, crystal structure and antibacterial activity of nickel(II), copper(II) and zinc(II) complexes containing ONNO donor Schiff base ligands. *J. Mol. Struct.* 2021, 1233, 130112.
7. Andruh M. Compartmental Schiff-base ligands—a rich library of tectons in designing magnetic and luminescent materials. *Chem. Commun.* 2011, 47, 3025–3042.
8. Chen L., Ding L., Chu Z., Yong L., Lü X., Song J., Fan D., Jin W. Bulk solvent-free melt ring-opening polymerization of L-lactide catalyzed by Cu(II) and Cu(II)—Nd(III) complexes of the Salen-type Schiff-base ligand. *J. Appl. Organomet. Chem.* 2011, 25, 310–316.
9. Rayati S., Zakavi S., Koliaei M., Kozakiewicz A. Electron-rich salen-type Schiff base complexes of Cu(II) as catalysts for oxidation of cyclooctene and styrene with tert-butylhydroperoxide: a comparison with electron-deficient ones. *Inorg. Chem. Commun.* 2010, 13, 203–207.
10. Nathan L. C., Koehne J. E., Gilmore J. M., Hannibal K. A., Dewhurst W. E., Mai T. D. The X-ray structures of a series of copper(II) complexes with tetradentate Schiff base ligands derived from salicylaldehyde and polymethylenediamines of varying chain length. *Polyhedron* 2003, 22, 887–894.
11. You Z. L., Lu Y., Zhang N., Ding B. W., Sun H., Hou P., Wang C. Preparation and structural characterization of hetero-dinuclear Schiff base copper(II)-zinc(II) complexes and their inhibition studies on *Helicobacter pylori* urease. *Polyhedron* 2011, 30, 2186–2194.
12. Tella S., Bekiari V., Kessler V. G., Papaefstathiou G. S. Gallium(III) complexes based on *N,N'*-bis(salicylidene)propane-1,3-diamine and its derivatives. *Polyhedron* 2013, 64, 77–83.
13. Xiao J. C., Zhou C., Huang M. F., Tan H., Wu Q. Crystal structure of aqua-azido- κ^3N -(6,6'-((propane-1,3-diylbis(azanylylidene)) bis(methanylylidene)) bis(3-bromophenolato)- κ^4N,N',O,O' iron(III), $C_{17}H_{16}Br_2FeN_5O_3$. *Z. Kristallogr. NCS* 2020, 235, 903–904.