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Crystal structure of 6,6'-((pentane-1,3-diylbis(azaneylylidene))bis(methaneylylidene))bis(2,4-dibromophenolato- $\kappa^4 N, N', O, O'$)copper(II), $C_{19}H_{16}Br_4CuN_2O_2$

Table 1: Data collection and handling.

Crystal:	Block, clear brownish brown
Size:	0.20 × 0.18 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	8.33 mm ⁻¹
Diffractometer, scan mode:	CCD area detector, φ and ω -scans
$\theta_{\max}$, completeness:	26.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	24444, 4468, 0.078
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3154
$N(\text{param})_{\text{refined}}$:	254
Programs:	CrysAlis ^{PRO} [1], OLEX2 [2], SHELX [3, 4]

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Abstract

$C_{19}H_{16}Br_4CuN_2O_2$: monoclinic, $P2_1/c$ (no. 14), $a = 10.2649(3)$ Å, $b = 10.1903(3)$ Å, $c = 21.2494(6)$ Å, $\beta = 100.522(1)^\circ$, $V = 2185.36(11)$ Å³, $Z = 4$, $wR^2 = 0.0730$, $T = 169.0$ 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 structure was solved with the OLEX2 program [2] as an interface together with the SHELXT and SHELXL programs

[3, 4]. All H atoms were placed in geometrically idealized positions and refined using a riding model, with C–H = 0.98 (methylene), 0.95 Å (benzene), and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for H atoms.

Experimental details

3,5-dibromosalicylaldehyde (0.0279 g, 0.10 mmol) was dissolved in methanol (30 mL) with stirring, adding 1,3-diaminopentane (0.05 mmol). The mixture was stirred and refluxed at 80 °C for 3 h. The solvent was removed by rotary evaporator to give yellow the powdered was dissolved in a mixture containing 20 mL metanol and 10 mL ethanol. Then, 0.1 g copper nitrate was add to the above solution and the resulting dark green mixture was further stirred at room temperature overnight. Dark brown crystals of the title compound were isolated after two weeks.

Comment

Schiff base is a kind of excellent ligand for 3d and 4f metal ion owing to its characteristic –C=N– group, in which the N atom has a lone pair of electrons, creating an electron-rich chemical environment [5, 6]. The introduction of electron-

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

Atom	x	y	z	U _{iso} */U _{eq}
Br1	0.02669 (6)	0.12909 (5)	0.08882 (2)	0.03108 (15)
Br2	−0.35796 (6)	0.20353 (5)	−0.13526 (2)	0.03574 (16)
Br3	0.43141 (5)	0.42199 (5)	0.22468 (2)	0.02917 (14)
Br4	0.46623 (6)	0.78530 (7)	0.42967 (3)	0.04799 (19)
Cu1	0.00102 (6)	0.58628 (5)	0.13835 (3)	0.02068 (15)
O1	−0.0103 (3)	0.4156 (3)	0.10207 (14)	0.0236 (8)
O2	0.1621 (3)	0.5360 (3)	0.19085 (15)	0.0247 (8)
N1	−0.1228 (4)	0.6607 (4)	0.06701 (18)	0.0229 (10)
N2	−0.0379 (4)	0.7205 (4)	0.19815 (18)	0.0211 (9)
C1	−0.1694 (5)	0.4589 (4)	0.0059 (2)	0.0204 (11)
C2	−0.0856 (5)	0.3770 (4)	0.0497 (2)	0.0194 (11)
C3	−0.0888 (5)	0.2409 (4)	0.0333 (2)	0.0212 (11)
C4	−0.1684 (5)	0.1904 (5)	−0.0197 (2)	0.0246 (12)
H4	−0.169288	0.098751	−0.027989	0.029*
C5	−0.2480 (5)	0.2752 (5)	−0.0614 (2)	0.0264 (12)
C6	−0.2477 (5)	0.4078 (5)	−0.0500 (2)	0.0239 (12)
H6	−0.300209	0.464881	−0.079703	0.029*
C7	−0.1786 (5)	0.5984 (4)	0.0164 (2)	0.0216 (11)
H7	−0.230127	0.648477	−0.016824	0.026*
C8	−0.1428 (5)	0.8025 (4)	0.0716 (2)	0.0274 (12)
H8A	−0.192169	0.835288	0.030184	0.033*
H8B	−0.055531	0.846820	0.080081	0.033*
C9	−0.2190 (6)	0.8376 (5)	0.1245 (2)	0.0329 (13)
H9A	−0.314071	0.819609	0.108566	0.039*
H9B	−0.209715	0.933084	0.132519	0.039*
C10	−0.1772 (5)	0.7656 (5)	0.1888 (2)	0.0255 (12)
H10	−0.186081	0.827901	0.224071	0.031*
C11	0.0407 (5)	0.7512 (5)	0.2511 (2)	0.0243 (12)
H11	0.008057	0.811626	0.278566	0.029*
C12	0.1727 (5)	0.7017 (5)	0.2720 (2)	0.0206 (11)
C13	0.2243 (5)	0.5969 (5)	0.2409 (2)	0.0208 (11)
C14	0.3558 (5)	0.5579 (5)	0.2672 (2)	0.0231 (11)
C15	0.4286 (5)	0.6130 (5)	0.3218 (2)	0.0266 (12)
H15	0.516021	0.583692	0.338205	0.032*
C16	0.3709 (5)	0.7127 (5)	0.3524 (2)	0.0266 (12)
C17	0.2465 (5)	0.7571 (5)	0.3282 (2)	0.0292 (13)
H17	0.209287	0.825860	0.349379	0.035*
C18	−0.2653 (5)	0.6457 (5)	0.1940 (2)	0.0274 (12)
H18A	−0.358945	0.674274	0.187774	0.033*
H18B	−0.256729	0.582909	0.159458	0.033*
C19	−0.2294 (6)	0.5766 (6)	0.2583 (2)	0.0398 (15)
H19A	−0.289962	0.502773	0.259780	0.060*
H19B	−0.236802	0.638477	0.292742	0.060*
H19C	−0.138210	0.543872	0.263744	0.060*

rich atoms such as O, N and S that favorable to the space environment of −C=N− structure into Schiff base can create more favorable electron-rich chemical environment for coordination between Schiff base and metal ions. As a part of our current research on the exploration of the regulating effect of Schiff base ligands on transition metal complexes [7, 8], we report herein a new.

Single-crystal X-ray diffraction reveals that there is one crystallography independent Cu(II) complex in the asymmetric unit. The central Cu(II) exhibits tetra-coordinated environment which is defined by N₂O₂ from the Schiff-base ligand. The bond lengths of Cu–O(N) are in the range of 1.889(3)–1.957(4) Å and bond angles of O(N)–Cu–O varies from 88.47(23) to 160.54(26)°, which is compared favorably with the corresponding values observed in salen-type Cu(II) analogous [9, 10].

The dihedral angle calculated between the planes of the two benzene rings is 38.135(16)°.

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