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Synthesis and crystal structure of bis{2-bromo-6-(((4-(1-(methoxyimino)ethyl)phenyl)imino)methyl)phenolato- κ^2N,O }cobalt(II)–dichloromethane(1/1), C₃₄H₃₂Br₂Cl₄CoN₄O₄

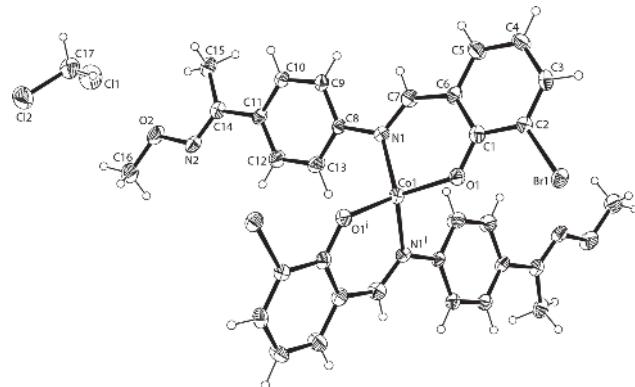


Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.19 × 0.18 × 0.14 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.02 mm $^{-1}$
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	26.1°, >99%
N(hkl) _{measured} , N(hkl) _{unique} , R _{int} :	19893, 3588, 0.172
Criterion for I_{obs} , N(hkl) _{gt} :	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2148
N($param$) _{refined} :	224
Programs:	Bruker [1], SHELX [2]

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Abstract

C₃₄H₃₂Br₂Cl₄CoN₄O₄, monoclinic, C2/c (no. 15), $a = 30.281(3)$ Å, $b = 8.9971(8)$ Å, $c = 13.9050(13)$ Å, $\beta = 107.053(5)$ °, $Z = 4$, $V = 3621.7(6)$ Å³, $R_{\text{gt}}(F) = 0.0648$, $wR_{\text{ref}}(F^2) = 0.1629$, $T = 173(2)$ K.

CCDC no.: 1951375

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

Synthesis of the title complex was prepared by a similar method reported earlier [3]. A methanol solution (3 mL) of cobalt(II) acetate tetrahydrate (2.5 mg, 10 mmol) was added dropwise to a dichloromethane solution (6 mL) of 1-(4-((3-bromo-2-hydroxybenzylidene)amino)phenyl)ethan-1-one

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

Atom	x	y	z	U_{iso}^* / U_{eq}
Br1	0.62802(3)	-0.29725(7)	0.19180(6)	0.0415(3)
Co1	0.500000	-0.01772(13)	0.250000	0.0322(3)
Cl1	0.32079(10)	0.8358(2)	0.7111(2)	0.0834(9)
O1	0.55592(16)	-0.1171(5)	0.2524(4)	0.0355(11)
N1	0.52599(19)	0.0874(5)	0.3816(4)	0.0300(13)
C1	0.5956(3)	-0.1144(7)	0.3227(5)	0.0354(17)
Cl2	0.25159(9)	0.6112(3)	0.7096(2)	0.0899(9)
O2	0.3426(2)	0.5612(6)	0.5312(4)	0.0589(16)
N2	0.3689(2)	0.4722(6)	0.4852(5)	0.0433(16)
C2	0.6345(2)	-0.1932(6)	0.3132(5)	0.0327(16)
C3	0.6758(3)	-0.1963(7)	0.3871(6)	0.0409(18)
H3	0.700830	-0.251175	0.376772	0.049*
C4	0.6817(3)	-0.1208(8)	0.4767(6)	0.0463(19)
H4	0.710084	-0.126901	0.529004	0.056*
C5	0.6459(3)	-0.0371(8)	0.4885(6)	0.049(2)
H5	0.650235	0.017655	0.548976	0.059*
C6	0.6028(2)	-0.0295(7)	0.4137(5)	0.0354(17)
C8	0.4979(2)	0.1815(6)	0.4243(5)	0.0297(15)
C7	0.5686(3)	0.0642(7)	0.4357(6)	0.0404(18)
H7	0.578316	0.116345	0.497754	0.048*
C9	0.5100(3)	0.2141(8)	0.5267(6)	0.0410(18)
H9	0.537064	0.173064	0.571962	0.049*
C10	0.4813(2)	0.3083(7)	0.5613(6)	0.0397(17)
H10	0.489769	0.333188	0.630752	0.048*
C11	0.4414(3)	0.3660(7)	0.4983(5)	0.0346(16)
C12	0.4301(3)	0.3318(8)	0.3964(6)	0.048(2)
H12	0.402769	0.371882	0.351418	0.057*
C13	0.4583(3)	0.2397(8)	0.3595(6)	0.047(2)
H13	0.450207	0.217070	0.289771	0.057*
C14	0.4106(3)	0.4593(7)	0.5408(6)	0.0369(17)
C15	0.4295(3)	0.5291(8)	0.6420(6)	0.048(2)

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Table 2 (continued)

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
H15A	0.461103	0.563339	0.650276	0.071*
H15B	0.429611	0.455860	0.694280	0.071*
H15C	0.410127	0.613860	0.647942	0.071*
C16	0.2966(3)	0.5699(10)	0.4673(7)	0.064(3)
H16A	0.296310	0.619094	0.404290	0.096*
H16B	0.277756	0.627262	0.500726	0.096*
H16C	0.283786	0.469537	0.452875	0.096*
C17	0.3098(3)	0.6544(9)	0.7415(7)	0.063(3)
H17A	0.325221	0.584679	0.706563	0.076*
H17B	0.323581	0.639610	0.814813	0.076*

O-methyl oxime (HL) (8.3 mg, 20 mmol) at room temperature. The mixture solution turns light red, immediately. The mixture was kept being stirred for 1 h. The filtrate was allowed to stand for 11 days at quite environment. The solvent was partially evaporated and several clear light red crystals were obtained. Anal. Calcd. for $C_{34}H_{32}Br_2Cl_4CoN_4O_4$: C, 44.33%; H, 3.50%; N, 6.08%. Found: C, 44.65%; H, 3.72%; N, 5.54%.

Experimental details

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

Comment

Schiff base molecules form an important class of ligands in the field of coordination chemistry [3]. The Schiff base ligands can form stable complexes with transition metal ions [4–6]. So far, we have designed and synthesized a variety of Schiff base N_2O_2 type complexes [7–9].

The single crystal structure of the title complex was determined by X-ray crystallography. In the title complex, Co1 is four-coordinated by two O atoms and two N atoms from two

Schiff base ligands L^{-1} . The Co1–N1 bond lengths are both 2.004(5) Å and the Co1–O1 bond lengths are both 1.907(4) Å. The angles of N1–Co1–O1 and N1–Co1–O1ⁱ are 95.5(2) $^\circ$ and 110.2(2) $^\circ$, respectively. All geometric parameters are in the typical ranges.

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