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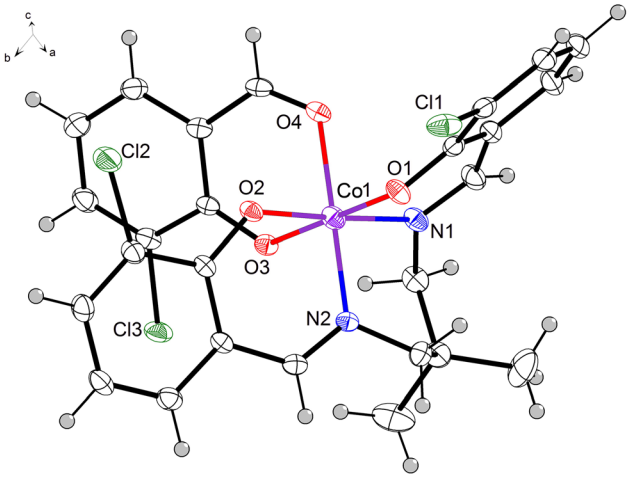
Crystal structure of 2-chloro-6-formylphenolato-κ^2O,O′-(6,6′-(((2,2-dimethylpropane-1,3-diyl)bis(azaneylylidene))bis(methaneylylidene))bis(2-chlorophenolato)κ^4*N*,*N*,*O*,*O*′)cobalt(III), $C_{26}H_{22}Cl_3CoN_2O_4$



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Abstract

$C_{26}H_{22}Cl_3CoN_2O_4$, triclinic, $P\bar{1}$ (no. 2), a = 11.1835(5) Å, b = 11.6782(5) Å, c = 11.9295(5) Å, α = 83.900(3)°, β = 66.911(4)°, γ = 64.232(4)°, V = 1286.83(11) Å^3, Z = 2, $R_{gt}(F)$ = 0375, $wR_{ref}(F^2)$ = 0.0899, T = 213.0 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.

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Table 1: Data collection and handling.

Crystal:	Black block
Size:	0.18 × 0.16 × 0.16 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	8.40 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy, ω
θ_{max}, completeness:	76.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14,183, 4954, 0.041
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4515
$N(param)_{refined}$:	327
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

Source of material

3-Chlorosalicylaldehyde (0.157 g, 1.0 mmol) and 2,2-dimethyl-1,3-propanediamine (0.052 g, 0.5 mmol) were dissolved in a mixture 20 mL ethanol, the Schiff base solution was stirred at room temperature for 2 h. After this, $CoCl_2{\cdot}6H_2O$ (0.120 g, 0.5 mmol) was added and the obtained green mixture was further stirred for another 2 h and filtered. The acquired green filtrate was sealed in a beaker with parafilm and kept undisturbed at room temperature. Black block crystals of the title compound were afforded after two days by slow evaporation.

Experimental details

X-ray single crystal data was collected on a Bruker SMART APEX II diffractometer. Data reduction was performed using the program SAINT and empirical absorption corrections were made using SADABS [1]. 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 0.97 Å (methyl); U_{iso}(H) values were set 1.2 times for H atoms on methylene and benzene, and 1.5 times for methyl.

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

Atom	x	y	z	U_{iso}*/U_{eq}
Co1	0.36015 (4)	0.49529 (3)	0.28411 (3)	0.02518 (10)
Cl1	0.32305 (8)	0.20055 (7)	0.07343 (6)	0.04810 (18)
Cl2	−0.11658 (7)	0.75288 (7)	0.31895 (9)	0.0645 (2)
Cl3	0.28492 (7)	0.88694 (6)	0.43409 (6)	0.04186 (15)
O1	0.39269 (18)	0.35796 (15)	0.18783 (15)	0.0342 (4)
O2	0.19007 (17)	0.59492 (14)	0.25649 (15)	0.0301 (3)
O3	0.32329 (17)	0.63653 (14)	0.37694 (14)	0.0291 (3)
O4	0.24152 (18)	0.43812 (15)	0.42205 (15)	0.0328 (4)
N1	0.5276 (2)	0.39147 (18)	0.31854 (19)	0.0334 (4)
N2	0.4757 (2)	0.55223 (17)	0.14905 (17)	0.0273 (4)
C1	0.5198 (3)	0.1926 (2)	0.2928 (3)	0.0382 (6)
C2	0.4392 (2)	0.2407 (2)	0.2185 (2)	0.0328 (5)
C3	0.4154 (3)	0.1499 (2)	0.1710 (2)	0.0378 (6)
C4	0.4644 (3)	0.0235 (3)	0.1980 (3)	0.0484 (7)
H4	0.4459	−0.0336	0.1650	0.058*
C5	0.5407 (3)	−0.0193 (3)	0.2734 (3)	0.0566 (8)
H5	0.5724	−0.1048	0.2929	0.068*
C6	0.5693 (3)	0.0639 (3)	0.3191 (3)	0.0509 (7)
H6	0.6228	0.0348	0.3688	0.061*
C7	0.5729 (3)	0.2708 (2)	0.3265 (3)	0.0396 (6)
H7	0.6462	0.2300	0.3566	0.047*
C8	0.6163 (3)	0.4542 (2)	0.3191 (2)	0.0379 (6)
H8A	0.6815	0.4026	0.3596	0.046*
H8B	0.5542	0.5378	0.3649	0.046*
C9	0.7049 (3)	0.4708 (3)	0.1861 (3)	0.0401 (6)
C10	0.6318 (3)	0.4738 (2)	0.0992 (2)	0.0343 (5)
H10A	0.6752	0.5067	0.0225	0.041*
H10B	0.6508	0.3864	0.0803	0.041*
C11	0.4238 (3)	0.6589 (2)	0.1035 (2)	0.0301 (5)
H11	0.4904	0.6837	0.0429	0.036*
C12	0.2743 (2)	0.7434 (2)	0.1359 (2)	0.0284 (5)
C13	0.1650 (2)	0.7048 (2)	0.2094 (2)	0.0276 (4)
C14	0.0229 (3)	0.7921 (2)	0.2258 (2)	0.0349 (5)
C15	−0.0095 (3)	0.9070 (2)	0.1730 (3)	0.0410 (6)
H15	−0.1056	0.9616	0.1853	0.049*
C16	0.0998 (3)	0.9423 (2)	0.1015 (3)	0.0410 (6)
H16	0.0781	1.0208	0.0661	0.049*
C17	0.2389 (3)	0.8616 (2)	0.0836 (2)	0.0370 (5)
H17	0.3127	0.8854	0.0352	0.044*
C18	0.8539 (3)	0.3571 (4)	0.1364 (4)	0.0707 (10)
H18A	0.8428	0.2783	0.1475	0.106*
H18B	0.9106	0.3577	0.1803	0.106*
H18C	0.9024	0.3636	0.0501	0.106*
C19	0.7187 (4)	0.5956 (4)	0.1862 (3)	0.0660 (10)
H19A	0.7808	0.6044	0.1052	0.099*
H19B	0.7597	0.5946	0.2446	0.099*
H19C	0.6243	0.6668	0.2088	0.099*
C20	0.1386 (3)	0.5134 (2)	0.5085 (2)	0.0325 (5)
H20	0.0765	0.4808	0.5641	0.039*
C21	0.1035 (3)	0.6433 (2)	0.5335 (2)	0.0306 (5)
C22	−0.0260 (3)	0.7147 (3)	0.6311 (2)	0.0393 (6)
H22	−0.0900	0.6784	0.6736	0.047*
C23	−0.0591 (3)	0.8372 (3)	0.6646 (3)	0.0454 (6)
H23	−0.1465	0.8853	0.7288	0.054*
C24	0.0371 (3)	0.8895 (2)	0.6033 (2)	0.0409 (6)
H24	0.0148	0.9730	0.6270	0.049*
C25	0.1643 (3)	0.8211 (2)	0.5085 (2)	0.0326 (5)
C26	0.2022 (2)	0.6959 (2)	0.4670 (2)	0.0268 (4)

Comment

Cobalt containing complexes have applications in the field of molecular based photocatalysis, nonlinear optics and magnetic materials. The variety of structures of coordination complex can be enriched by connecting copper ions with different organic and inorganic ligands [5–9]. As a part of our current research interest on the exploration of the regulating effect of Schiff base ligands on transition metal complexes [10–12], herein we report a new Co(II) complex based on halogenated Schiff base ligand.

The molecular structure is shown in the figure. The complex is a Co(III) complex constructed from 2-chloro-6-formylphenolate ligand and halogenated salen-type Schiff base mixed ligands. It is worth noting that the bidentate coordination of the 2-chloro-6-formylphenolate is usually regarded as metastable coordination mode, which is promising for catalytic applications. The bond length and bond angles are range from 1.886(2) to 1.933(2) Å and 85.97(7)° to 177.79(7)°, respectively, which are consistent with those previously found in similar complexes [13].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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