Crystal structure of diaquabis(5-chlorosalicylaldehydato)cobalt(II), $\text{Co}(\text{H}_2\text{O})_2(\text{C}_7\text{H}_4\text{ClO}_2)_2$

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Abstract

$\text{C}_{14}\text{H}_{12}\text{Cl}_2\text{CoO}_6$, monoclinic, $P12_1/c1$ (no. 14), $a = 15.412(2)$ Å, $b = 7.474(2)$ Å, $c = 14.733(2)$ Å, $\beta = 116.703(2)^\circ$, $V = 1516.1$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.039$, $wR_{\text{ref}}(F^2) = 0.101$, $T = 298$ K.

Source of material

5-Chlorosalicylaldehyde (0.1 mmol, 15.7 mg) and cobalt(II) acetate tetrahydrate (0.1 mmol, 24.9 mg) were dissolved in methanol (10 ml). The mixture was stirred for 30 min at room temperature to give a clear brown solution. After allowing the resulting solution to stand in air for 11 d, brown block-shaped crystals were formed at the bottom of the vessel by slow evaporation of the solvent. The crystals were isolated by filtration, washed with methanol and dried in a vacuum desiccator using anhydrous CaCl_2 (yield 54 %). Elemental analysis: found – C, 41.3 %; H, 3.1 %; calc. for $\text{C}_{14}\text{H}_{12}\text{Cl}_2\text{CoO}_6$ – C, 41.4 %; H, 3.0 %.

Experimental details

The hydrogen atoms bound to oxygen atoms were located from Fourier difference maps and refined with the O—H and H...H distances restrained to 0.84(1) Å and 1.37(2) Å, respectively. The other H atom were calculated and refined using riding rigid-body approximation.

Discussion

Cobalt complexes are of great interest in coordination chemistry in relation to catalysis and enzymatic reactions, magnetism and molecular architectures [1–2]. The complex reported here is an extension of the work on structural characterization of such cobalt complexes.

The title compound is a mononuclear cobalt(II) complex being structurally similar to the nickel(II) and zinc(II) complexes derived from other Schiff base ligands [3,4]. The Co(II) ion is in an octahedral coordination by four O atoms from two 5-chloro-

salicylaldehydato ligands defining the basal plane, and by two O atoms from two coordinated water molecules occupying the axial positions. The three *trans* angles at Co1 are all close to 180°. The other angles are close to 90°, varying from 84.79(8)° to 95.96(8)°, which indicates a slightly distorted octahedral geometry of the Co1 atom. The bond lengths around the Co1 atom are ranging from 2.025(2) Å to 2.112(2) Å. The dihedral angle between the two benzene rings is 20.4(3)°.

Table 1. Data collection and handling.

Crystal:	brown block, size 0.04 × 0.09 × 0.11 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	15.12 cm ^{−1}
Diffractometer, scan mode:	Siemens SMART CCD, ω/ϕ
$2\theta_{\text{max}}$:	53°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	11892, 3150
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2178
$N(\text{param})_{\text{refined}}$:	224
Program:	SHELXTL [5]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(3)	4e	0.6835	0.1691	0.4635	0.046
H(4)	4e	0.8491	0.1752	0.5571	0.053
H(6)	4e	0.8788	0.3210	0.3130	0.047
H(7)	4e	0.7530	0.3251	0.1543	0.045
H(10)	4e	0.3203	0.2195	−0.2184	0.041
H(11)	4e	0.1641	0.1181	−0.3087	0.045
H(13)	4e	0.1300	0.1023	−0.0569	0.042
H(14)	4e	0.2470	0.1814	0.0975	0.044
H(5A)	4e	0.474(2)	−0.087(3)	0.152(2)	0.04(1)
H(6A)	4e	0.530(2)	0.588(3)	0.102(2)	0.037(9)
H(5B)	4e	0.515(2)	−0.092(3)	0.088(2)	0.05(1)
H(6B)	4e	0.481(2)	0.590(3)	0.160(2)	0.035(9)

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Co(1)	4e	0.49956(3)	0.25352(5)	0.12423(2)	0.0277(2)	0.0259(2)	0.0195(2)	0.0002(2)	0.0128(2)	0.0004(2)
Cl(1)	4e	1.00406(6)	0.2587(1)	0.51670(7)	0.0267(4)	0.123(1)	0.0518(6)	−0.0057(5)	0.0087(4)	0.0187(6)
Cl(2)	4e	0.01735(6)	0.0061(1)	−0.25793(6)	0.0317(4)	0.0716(6)	0.0498(5)	−0.0121(4)	0.0121(4)	−0.0066(5)
O(1)	4e	0.5805(1)	0.2321(2)	0.2766(1)	0.025(1)	0.042(1)	0.021(1)	−0.0024(8)	0.0124(9)	0.0019(8)
O(2)	4e	0.6235(2)	0.2720(3)	0.1033(1)	0.033(1)	0.052(1)	0.024(1)	0.003(1)	0.016(1)	0.0035(9)
O(3)	4e	0.4188(1)	0.2578(2)	−0.0287(1)	0.028(1)	0.038(1)	0.021(1)	−0.0031(9)	0.0131(9)	0.0018(8)
O(4)	4e	0.3753(2)	0.2454(2)	0.1449(2)	0.034(1)	0.049(1)	0.028(1)	0.001(1)	0.020(1)	−0.002(1)
O(5)	4e	0.4892(2)	−0.0282(3)	0.1147(2)	0.060(2)	0.026(1)	0.044(1)	0.004(1)	0.037(1)	0.002(1)
O(6)	4e	0.5082(2)	0.5277(3)	0.1342(2)	0.059(2)	0.024(1)	0.045(1)	−0.001(1)	0.039(1)	−0.000(1)
C(1)	4e	0.7375(2)	0.2776(4)	0.2811(2)	0.028(2)	0.037(2)	0.028(2)	0.000(1)	0.016(1)	0.001(1)
C(2)	4e	0.6758(2)	0.2359(3)	0.3268(2)	0.032(2)	0.027(2)	0.027(2)	0.001(1)	0.016(1)	−0.001(1)
C(3)	4e	0.7216(2)	0.1983(4)	0.4315(2)	0.030(2)	0.064(2)	0.025(2)	−0.004(2)	0.016(1)	0.005(2)
C(4)	4e	0.8210(2)	0.2031(5)	0.4882(2)	0.032(2)	0.074(2)	0.026(2)	−0.001(2)	0.012(1)	0.008(2)
C(5)	4e	0.8790(2)	0.2493(4)	0.4426(2)	0.022(2)	0.058(2)	0.037(2)	−0.000(1)	0.010(1)	0.002(2)
C(6)	4e	0.8389(2)	0.2876(4)	0.3422(2)	0.031(2)	0.057(2)	0.038(2)	−0.002(2)	0.023(2)	0.003(2)
C(7)	4e	0.7052(2)	0.2938(4)	0.1735(2)	0.032(2)	0.056(2)	0.031(2)	0.003(2)	0.019(2)	0.006(2)
C(8)	4e	0.2660(2)	0.1803(4)	−0.0300(2)	0.029(2)	0.035(2)	0.026(2)	0.000(1)	0.015(1)	−0.001(1)
C(9)	4e	0.3265(2)	0.2130(3)	−0.0780(2)	0.026(2)	0.029(2)	0.025(2)	0.004(1)	0.012(1)	0.001(1)
C(10)	4e	0.2839(2)	0.1924(4)	−0.1841(2)	0.031(2)	0.051(2)	0.023(2)	−0.002(2)	0.013(1)	0.004(1)
C(11)	4e	0.1899(2)	0.1331(4)	−0.2387(2)	0.036(2)	0.049(2)	0.021(2)	−0.002(2)	0.007(1)	0.000(1)
C(12)	4e	0.1337(2)	0.0959(4)	−0.1894(2)	0.026(2)	0.041(2)	0.035(2)	−0.001(1)	0.010(1)	0.001(1)
C(13)	4e	0.1695(2)	0.1224(4)	−0.0885(2)	0.033(2)	0.043(2)	0.037(2)	0.000(1)	0.022(2)	−0.002(1)
C(14)	4e	0.2950(2)	0.2024(4)	0.0770(2)	0.033(2)	0.051(2)	0.036(2)	−0.001(2)	0.024(2)	−0.001(2)

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