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Diaquabis(5-chloro-2-formylphenolato-κ^2O,O')-cobalt(II)

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Key indicators

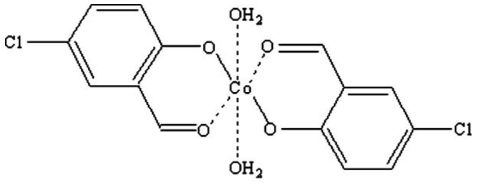
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.099
Data-to-parameter ratio = 14.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the mononuclear title compound, $[Co(C_7H_4ClO_2)_2(H_2O)_2]$, the Co^{II} atom is six-coordinated by four O atoms from two 5-chlorosalicylaldehyde ligands and two O atoms from two coordinated water molecules in a slightly distorted octahedral geometry.

Comment

Cobalt complexes are of great interest in coordination chemistry in relation to catalysis and enzymatic reactions, magnetism, and molecular architectures (Billson *et al.*, 2000; Fritsky *et al.*, 2003; Kotera *et al.*, 2003). As an extension of work on the structural characterization of cobalt(II) compounds, the crystal structure of the title compound, (I), is reported here.



(I)

Compound (I) is a mononuclear Co^{II} complex (Fig. 1). The Co^{II} ion is six-coordinated in an octahedral geometry by four O atoms from two 5-chlorosalicylaldehyde ligands defining the equatorial plane and by two O atoms from two coordinated water molecules occupying the axial positions. The three *trans* angles at the Co^{II} centre are close to 180°. All other angles subtended at the Co^{II} atom are close to 90°, ranging from 84.78 (8) to 95.96 (8)° (Table 1), which indicates a slightly distorted octahedral geometry of atom Co1. The Co—O bond lengths lie in the range 2.0274 (18)–2.110 (2) Å. In the crystal structure, O—H$\cdots$O hydrogen bonds (Table 2) link the molecules into a sheet parallel to the *bc* plane (Fig. 2).

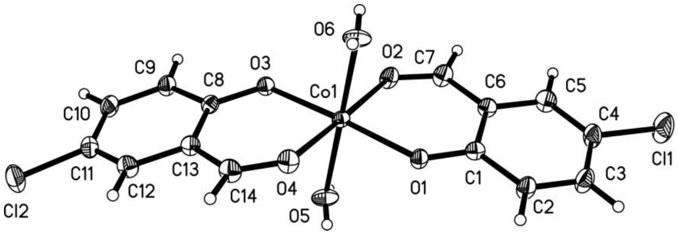


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

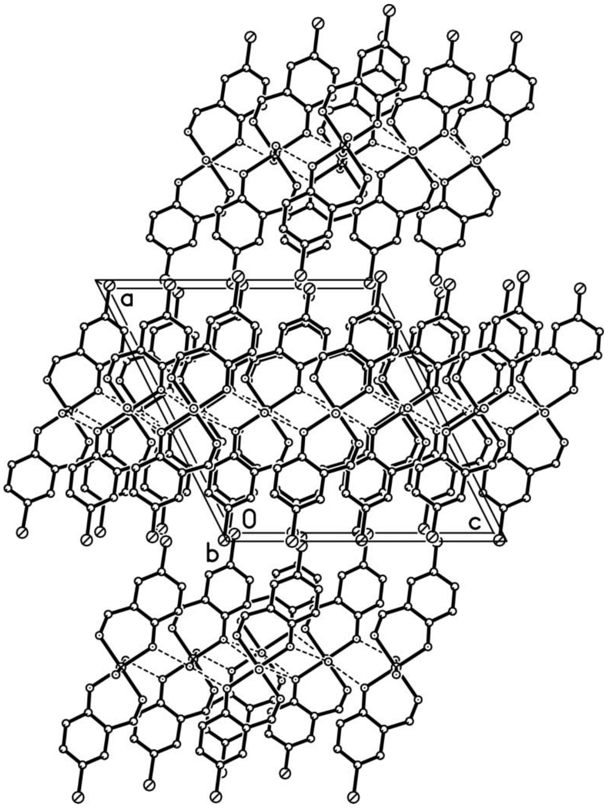


Figure 2
The crystal packing of (I), viewed along the *b* axis. H atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.7 mg) and cyclohexylamine (0.1 mmol, 9.3 mg) were dissolved in methanol (10 ml). Almost immediately, $Co(CH_3COO)_2\cdot 4H_2O$ (0.1 mmol, 24.9 mg) was added to the solution. The mixture was stirred for 30 min at room temperature to give a clear brown solution. After allowing the solution to stand in air for 11 d, brown block-shaped crystals of (I) were formed on slow evaporation of the solvent. The crystals were collected, washed with methanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 54%). Analysis found: C 41.4, H 3.0%; calculated for $C_{14}H_{12}Cl_2CoO_6$: C 4.13, H 3.1%.

Crystal data

$[Co(C_7H_4ClO_2)_2(H_2O)_2]$
$M_r = 406.07$
Monoclinic, $P2_1/c$
$a = 15.4115\ (17)$ Å
$b = 7.4744\ (8)$ Å
$c = 14.7332\ (16)$ Å
$\beta = 116.703\ (2)^\circ$
$V = 1516.1\ (3)$ Å^3
$Z = 4$
$D_x = 1.779$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1679 reflections
$\theta = 2.6$–24.9°
$\mu = 1.51$ mm^{-1}
$T = 295\ (2)$ K
Block, brown
$0.11 \times 0.09 \times 0.04$ mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.851$, $T_{max} = 0.942$
11886 measured reflections
3149 independent reflections
2177 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 26.5^\circ$
$h = -19 \rightarrow 19$
$k = -9 \rightarrow 9$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.099$
$S = 1.02$
3149 reflections
224 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.0274 (18)	Co1—O4	2.0716 (19)
Co1—O3	2.0287 (18)	Co1—O2	2.0721 (19)
Co1—O6	2.053 (2)	Co1—O5	2.110 (2)
O1—Co1—O3	176.38 (7)	O6—Co1—O2	84.78 (8)
O1—Co1—O6	90.66 (8)	O4—Co1—O2	177.84 (7)
O3—Co1—O6	92.95 (8)	O1—Co1—O5	89.17 (8)
O1—Co1—O4	89.18 (8)	O3—Co1—O5	87.23 (8)
O3—Co1—O4	90.92 (8)	O6—Co1—O5	179.24 (9)
O6—Co1—O4	93.08 (8)	O4—Co1—O5	86.18 (8)
O1—Co1—O2	91.11 (7)	O2—Co1—O5	95.96 (8)
O3—Co1—O2	88.92 (8)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O1^{i}	0.82 (3)	2.10 (3)	2.912 (3)	172 (3)
O5—H5B···O3^{ii}	0.82 (3)	2.04 (3)	2.860 (3)	178 (3)
O6—H6A···O3^{iii}	0.83 (3)	1.97 (3)	2.798 (3)	178 (3)
O6—H6B···O1^{iv}	0.83 (3)	1.92 (3)	2.750 (3)	177 (2)

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y, -z$; (iii) $-x+1, -y+1, -z$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

The C-bound H atoms were placed in idealized positions (C—H = 0.93 Å) and allowed to ride on their parent atoms, with U_{iso}(H) set to $1.2U_{eq}$(C). The water H atoms were located in a difference Fourier map and were refined with distance restraints of O—H = 0.84 (1) Å and H···H = 1.37 (2) Å.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

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