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Bis(*N*-(2-(2-hydroxyethylamino)ethyl)-salicylideneimine)cobalt(III) chloride

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Key indicators

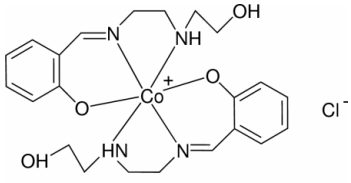
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.041
wR factor = 0.113
Data-to-parameter ratio = 14.0

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

In the title compound, $[Co(C_{11}H_{15}N_2O_2)_2]Cl$, the Co^{III} atom is six-coordinated by four N atoms and two O atoms from two Schiff base ligands, and is in a distorted octahedral geometry. The alcohol O atoms and the amine N atoms in the Schiff base and the chloride anions contribute to the formation of intermolecular hydrogen bonds.

Comment

Recently we reported (Zhu *et al.*, 2003) a cobalt(III) nitrate complex with a Schiff base *L*, where *L* is bis(N-(2-(2-hydroxyethylamino)ethyl)salicylideneimine). As a subsequent part of our research on this series, we now report the crystal structure of the title compound, (I), which has a similar cation structure to the previously reported complex.



(I)

The title compound consists of a $[CoL_2]^+$ cation and a chloride anion. The cobalt(III) atom in the cation is in a distorted octahedral geometry, being coordinated by four N atoms and two phenoxy O atoms from two chelating Schiff base ligands (*L*). The average Co(III)—N(imine) bond length is 1.904 (3) Å and the average Co(III)—N(amine) contact is 2.010 (3) Å, both of which are slightly shorter than the corresponding bonds in $[CoL_2]NO_3$ (*L* is the same Schiff base ligand as in the title complex) (Zhu *et al.*, 2003). The mean Co—O distance is 1.889 (3) Å, also shorter than that [1.904 (4) Å] in the $[CoL_2]NO_3$ complex. The dihedral angle between the two aromatic rings in the cation is 77.2 (2) °.

All the alcohol O atoms and all the amine N atoms in the Schiff base, together with the chloride atoms, contribute to the formation of intermolecular hydrogen bonds N2—H2···Cl1^{i}, N4—H4···Cl1^{i}, O2—H2*A*···Cl1^{i} and O4—H4*B*···Cl1^{i} (Fig. 2; for symmetry codes, see Table 1).

Experimental

Salicylaldehyde, 2-hydroxylaminoethylamine, and $CoCl_2{\cdot}6H_2O$ were available commercially and were used without further purification. Equimolar salicylaldehyde (1 mmol, 122 mg) and 2-hydroxylaminoethylamine (1 mmol, 104 mg) were dissolved in anhydrous ethanol (5 ml). The mixture was stirred to give a clear solution of *L*, where *L* is *N*-(2-(2-hydroxyethylamino)ethyl)salicylideneimine. To this solu-

tion was added $CoCl_2·6H_2O$ (1 mmol, 238 mg) in anhydrous ethanol (5 ml). After keeping the resulting solution in air to evaporate about half of the solvent, dark red prisms of the title compound were formed. The crystals were isolated, washed with ethanol three times and dried in a vacuum desiccator using silica gel (Yield 55%). Elemental analysis: found: C, 51.70; H, 5.82; N, 10.92%; calc. for $C_{22}H_{30}ClCoN_4O_4$: C, 51.93; H, 5.94; N, 11.01%.

Crystal data

$[Co(C_{11}H_{15}N_2O)_2]·Cl$
M_r = 508.88
Monoclinic, $P2_1/n$
a = 9.802 (5) Å
b = 24.879 (13) Å
c = 10.425 (6) Å
β = 115.849 (7)°
V = 2288 (2) Å^3
Z = 4
D_x = 1.477 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2737 reflections
θ = 2.3–22.8°
μ = 0.90 mm^{-1}
T = 298 (2) K
Prism, dark red
0.29 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.780, T_{max} = 0.876
12017 measured reflections
4049 independent reflections
2768 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 25.0°
$h = -8 \rightarrow 11$
$k = -29 \rightarrow 25$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.113
S = 0.97
4049 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···Cl1^{i}	0.91	2.26	3.157 (3)	168
N4—H4···Cl1^{i}	0.91	2.55	3.458 (3)	172
O2—H2*A*···Cl1^{i}	0.82	2.34	3.154 (3)	170
O4—H4*B*···Cl1^{i}	0.82	2.75	3.500 (4)	154

Symmetry codes: (i) $1-x, -y, 1-z$.

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H and C—H distances of 0.90 and 0.96 Å, respectively, and $U_{iso}(H) = 1.2U_{eq}(C)$, $U_{iso}(H) = 1.2U_{eq}(N)$ and $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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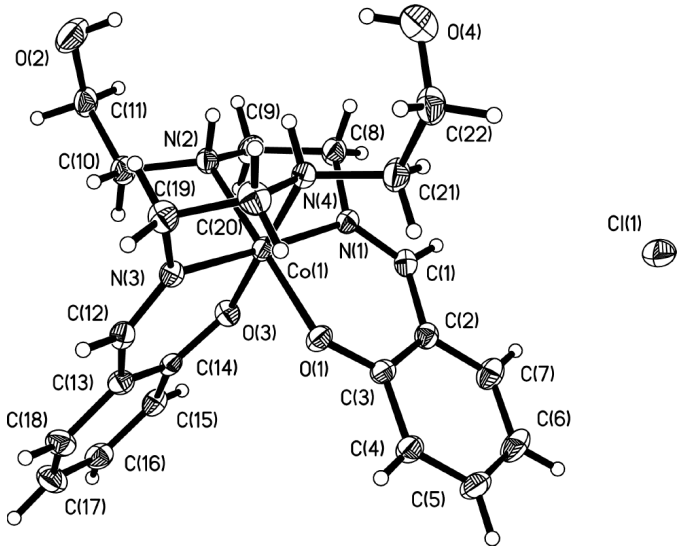

Figure 1
The structure of the title compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

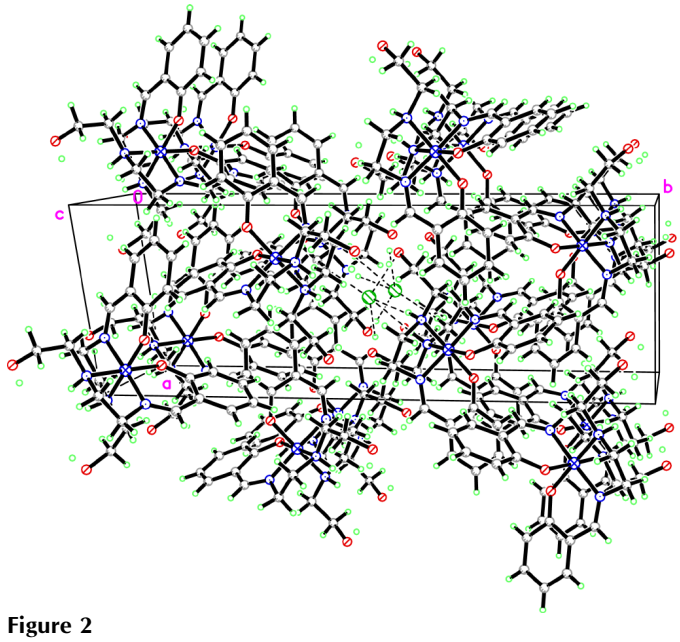

Figure 2
Crystal packing of (I), showing the hydrogen-bonded interactions as dashed lines.

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