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Bis{*N*-[2-(2-hydroxyethylamino)ethyl]-salicylideneimine}chromium(III) chloride

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.056
wR factor = 0.159
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.

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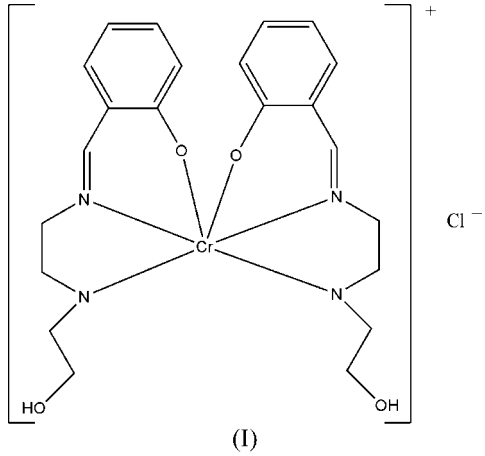
The title compound, $[Cr(C_{11}H_{15}N_2O_2)_2]Cl$, is a mononuclear chromium(III) complex with a distorted octahedral geometry defined by an N_4O_2 donor set.

Comment

Schiff bases obtained by condensation of *N*-2-hydroxyethylaminoethylamine and salicylaldehyde or analogues (*L*) have strong coordination abilities to transition metal ions. Recently, many such metal complexes have been structurally characterised: zinc(II) (Usman *et al.*, 2003; You *et al.*, 2004), cobalt(III) (Zhu *et al.*, 2003), silver(I) (Zhu *et al.*, 2000; Zou *et al.*, 2004), copper(II) (Qu *et al.*, 2004), nickel(II) (Ma *et al.*, 2005) and cadmium(II) (Yang *et al.*, 2004). However, no reports on related chromium(III) complexes have appeared. Here, the crystal structure of the title complex, (I), is described.



(I)

The mononuclear chromium(III) complex (Fig. 1) has a structure similar to that found for the cobalt(III) analogue (Zhu *et al.*, 2003), and comprises a complex cation and Cl^- anion. In the cation, the central atom is six-coordinated by four N and two O atoms derived from the two Schiff base ligands, forming a slightly distorted octahedron. In the crystal structure, there is a close association between the complex cation and Cl^- anion (Table 1). The Cl^- anion is stabilized by hydrogen bonding in a hydrophilic pocket located to one side of the cation and defined by two amine NH and two hydroxyl groups.

Experimental

Using a similar procedure to that in the literature (Zhu *et al.*, 2003), complex (I) was prepared as follows. Equimolar salicylaldehyde and

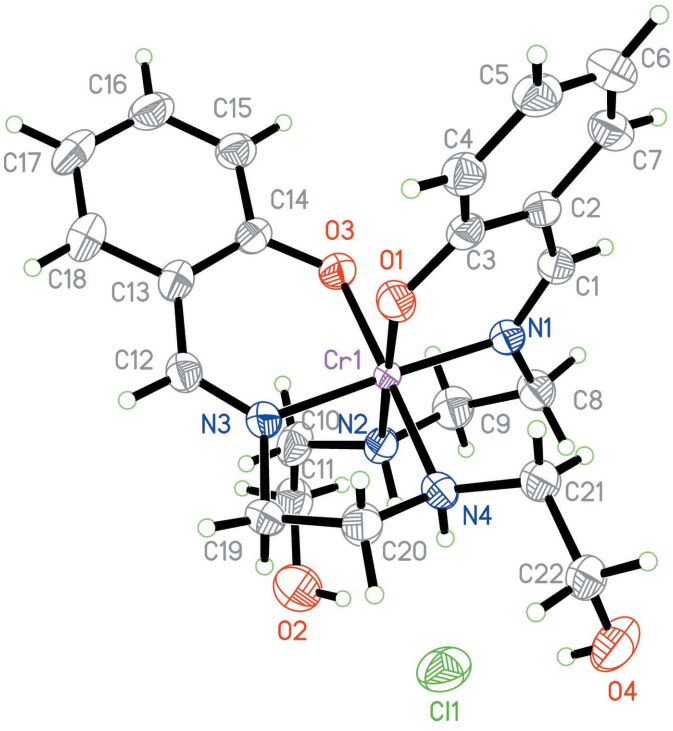


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

2-hydroxylaminoethylamine were dissolved in anhydrous ethanol. The mixture was stirred to give a clear colorless solution of *N*-[2-(2-hydroxyethylamino)ethyl]salicylideneimine. To this solution was added equimolar $CrCl_3·6H_2O$ in anhydrous ethanol. After standing, dark-blue crystals of (I) were formed. They were isolated, washed with ethanol three times and dried in a vacuum desiccator using silica gel (yield 48%; m.p. 584 K).

Crystal data

$[Cr(C_{11}H_{15}N_2O_2)_2]Cl$
M_r = 501.95
Monoclinic, $P2_1/n$
a = 9.818 (7) Å
b = 24.895 (18) Å
c = 10.431 (7) Å
β = 115.724 (11)°
V = 2297 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 298 (2) K
0.37 × 0.25 × 0.13 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.795, T_{max} = 0.920
12142 measured reflections
4052 independent reflections
2404 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.159
S = 0.93
4052 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···Cl1	0.91	2.55	3.457 (5)	172
N4—H4···Cl1	0.91	2.26	3.152 (4)	168
O2—H2*A*···Cl1	0.82	2.74	3.498 (5)	154
O4—H4*A*···Cl1	0.82	2.35	3.157 (5)	170

C-bound H atoms were included in the riding-model approximation with C—H = 0.93–0.97Å, and with U_{iso}(H) = 1.2U_{eq}(C). The H atoms attached to N and O 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}(N) and U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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