

Bis[4-chloro-2-[2-(isopropylamino)ethylimino-methyl]phenolato]cobalt(III) perchlorate

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Key indicators

Single-crystal X-ray study
 $T = 298$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.010$ Å
 Disorder in solvent or counterion
 R factor = 0.082
 wR factor = 0.238
 Data-to-parameter ratio = 18.5

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

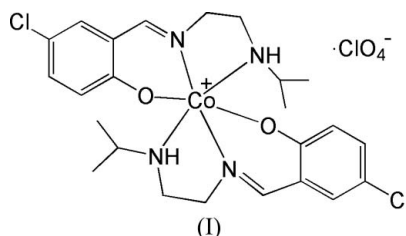
The title compound, $[\text{Co}(\text{C}_{12}\text{H}_{16}\text{ClN}_2\text{O})_2]\text{ClO}_4$, possesses two independent complex cations and two perchlorate anions in the asymmetric unit. Both Co^{III} atoms are six-coordinated by four N and two O atoms from two Schiff bases in slightly distorted octahedral coordination environments.

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Comment

Schiff base complexes are very important in coordination chemistry because of their easy preparation, interesting structures and excellent properties (Chang *et al.*, 1998; Chaturvedi, 1977; Archer & Wang, 1990; Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). Recently, the author has reported a few Schiff base compounds containing perchlorate anions (Yuan, 2005*a,b*). As a continuation of this work, a new cobalt(III) complex, (I), is reported here.



Compound (I) is a perchlorate salt of discrete mononuclear cobalt(III) complex cations (Fig. 1). The structure is similar to that recently reported for a cobalt(III) complex containing the 2,4-dichloro-6-[3-(cyclohexylamino)propyliminomethyl]phenolate ligand (Yuan, 2005*a*). There are two independent complex cations in the asymmetric unit along with two perchlorate anions. Both Co^{III} atoms are in a slightly distorted octahedral geometry formed by two O and four N atoms from two Schiff bases. The corresponding bond lengths and angles involving the Co atoms in the two cations are comparable to each other (Table 1) and to those of the above-mentioned related complex.

In the crystal structure, the cations are linked to the perchlorate anions *via* intermolecular N—H...O hydrogen bonds (Table 2), forming chains running along the *b* axis (Fig. 2). In addition, C—H...O and C—H...Cl interactions are observed.

Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.6 mg), *N*-isopropylethane-1,2-diamine (0.1 mmol, 10.2 mg), and $\text{Co}(\text{ClO}_4)_3 \cdot 7\text{H}_2\text{O}$ (0.1 mmol, 48.3 mg) were dissolved in MeOH (20 ml). The mixture was stirred at room temperature for 20 min to give a dark-brown solution. The

solution was left to stand in air for 12 d. Red plate-shaped crystals formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

[Co(C₁₂H₁₆ClN₂O)₂]ClO₄
M_r = 637.82
 Monoclinic, *P*2₁/*c*
a = 11.362 (1) Å
b = 16.951 (2) Å
c = 29.566 (3) Å
 β = 91.812 (2)°
V = 5691.5 (10) Å³

Z = 8
D_x = 1.489 Mg m⁻³
 Mo *K*α radiation
 μ = 0.93 mm⁻¹
T = 298 (2) K
 Plate, red
 0.30 × 0.18 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.768, *T_{max}* = 0.929

48467 measured reflections
 12990 independent reflections
 6337 reflections with *I* > 2σ(*I*)
R_{int} = 0.090
 θ_{max} = 27.5°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.082
wR (*F*²) = 0.238
S = 1.03
 12990 reflections
 703 parameters
 H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.101*P*)² + 3.5387*P*]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.91 e Å⁻³
 Δρ_{min} = -0.72 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—O1	1.891 (4)	Co2—O3	1.887 (4)
Co1—O2	1.884 (4)	Co2—O4	1.886 (4)
Co1—N1	1.903 (5)	Co2—N5	1.905 (5)
Co1—N2	2.041 (5)	Co2—N6	2.016 (5)
Co1—N3	1.907 (5)	Co2—N7	1.933 (6)
Co1—N4	2.012 (5)	Co2—N8	1.988 (6)
O2—Co1—O1	91.53 (18)	O4—Co2—O3	90.54 (19)
O2—Co1—N1	83.61 (19)	O4—Co2—N5	83.9 (2)
O1—Co1—N1	93.19 (18)	O3—Co2—N5	94.23 (18)
O2—Co1—N3	93.4 (2)	O4—Co2—N7	92.5 (2)
O1—Co1—N3	85.11 (19)	O3—Co2—N7	86.55 (19)
N1—Co1—N3	176.5 (2)	N5—Co2—N7	176.3 (2)
O2—Co1—N4	175.9 (2)	O4—Co2—N8	173.7 (2)
O1—Co1—N4	84.67 (19)	O3—Co2—N8	84.9 (2)
N1—Co1—N4	98.0 (2)	N5—Co2—N8	100.8 (2)
N3—Co1—N4	84.9 (2)	N7—Co2—N8	82.9 (3)
O2—Co1—N2	88.23 (19)	O4—Co2—N6	91.6 (2)
O1—Co1—N2	178.57 (18)	O3—Co2—N6	177.0 (2)
N1—Co1—N2	85.38 (19)	N5—Co2—N6	83.9 (2)
N3—Co1—N2	96.3 (2)	N7—Co2—N6	95.5 (2)
N4—Co1—N2	95.6 (2)	N8—Co2—N6	93.1 (2)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
N2—H2A⋯O11 ⁱ	0.91	2.27	3.130 (9)	157
N4—H4A⋯O9 ⁱⁱⁱ	0.91	2.57	3.464 (16)	168
N6—H6A⋯O7 ⁱⁱⁱ	0.91	2.43	3.253 (8)	151
C8—H8A⋯O9 ⁱ	0.97	2.53	3.359 (14)	143
C21—H21A⋯Cl3 ^{iv}	0.97	2.83	3.768 (7)	163

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (iii) $x, y, z - 1$; (iv) $x - 1, -y + \frac{3}{2}, z + \frac{1}{2}$

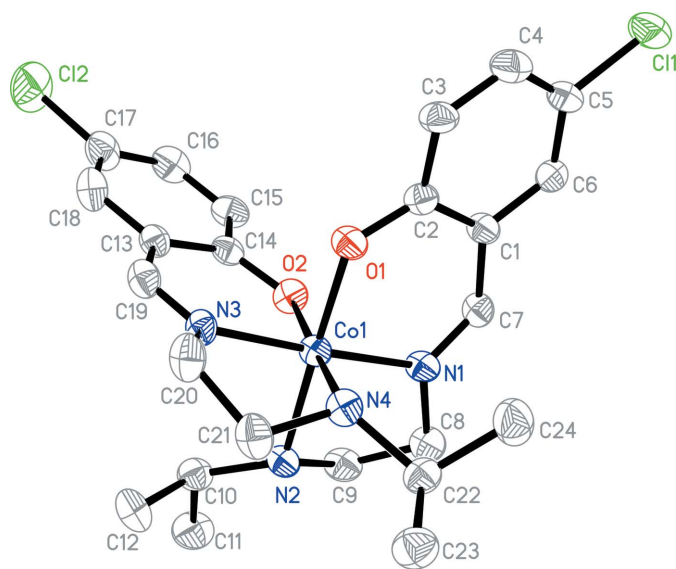


Figure 1

The structure of one of the independent cations of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are not shown. The second cation has essentially the same appearance.

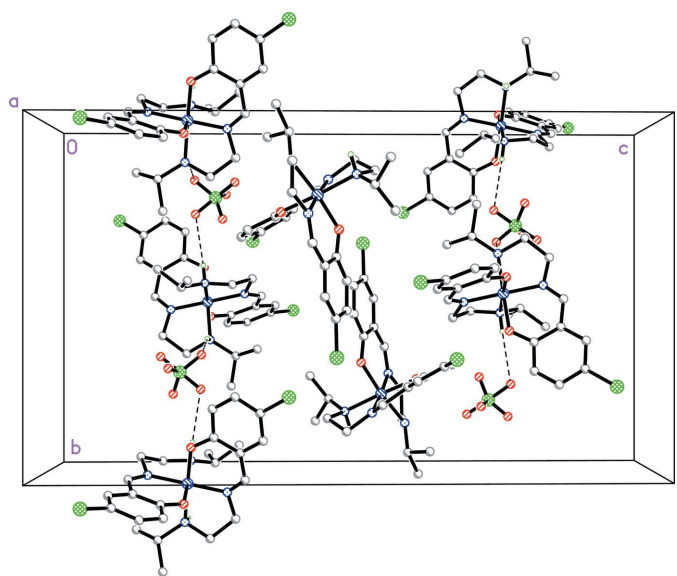


Figure 2

The crystal packing of (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds. Both disorder components are shown.

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98, N—H = 0.91 Å and *U*_{iso}(H) = 1.2 or 1.5*U*_{eq}(C,N). Atom O9 of one perchlorate anion is disordered over two distinct sites with occupancies of 0.585 (16) and 0.415 (16). The Cl—O and O⋯O distances in the disordered components were restrained to be equal. The *U*^{*ij*} components of atoms O6, O7, O9, O11, O12 and O9' were restrained to approximately isotropic behaviour.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

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