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trans-Bis{2-[3-(cyclohexylamino)propylimino-methyl]naphtholato}cobalt(III) perchlorate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
Disorder in solvent or counterion
R factor = 0.075
wR factor = 0.213
Data-to-parameter ratio = 15.4

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

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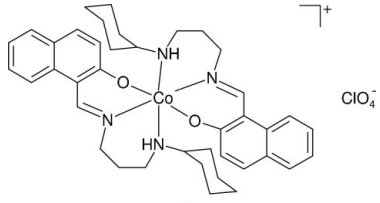
The title complex, $[Co(C_{20}H_{25}N_2O)_2]ClO_4$, is very similar to the mononuclear complex $[Co(C_{16}H_{23}N_2O)_2]ClO_4$, which we reported recently [You, Qu, Liu, Tan & Zhu (2003). *Acta Cryst.* E**59**, m1038–m1040]. The central Co^{III} atom, lying on an inversion center, is coordinated by four N atoms and two O atoms from two Schiff bases, giving an approximately octahedral coordination environment.

Comment

Recently, we have reported a few Schiff base complexes (You, Lin *et al.*, 2003, You *et al.* 2004). As an extension of our work on the structural characterization of Schiff base complexes, a mononuclear cobalt(III) complex is reported here. It is very similar to $[Co(C_{16}H_{23}N_2O)_2]ClO_4$, which we reported recently (You, Qu *et al.*, 2003).



(I)

The title complex, (I), is the perchlorate salt of a discrete centrosymmetric mononuclear cobalt(III) complex cation (Fig. 1). The structure is very similar to the complex cited above, with the ligand 2-[(3-cyclohexylaminopropylimino)-methyl]phenolate replaced by 3-[(3-cyclohexylaminopropyl-

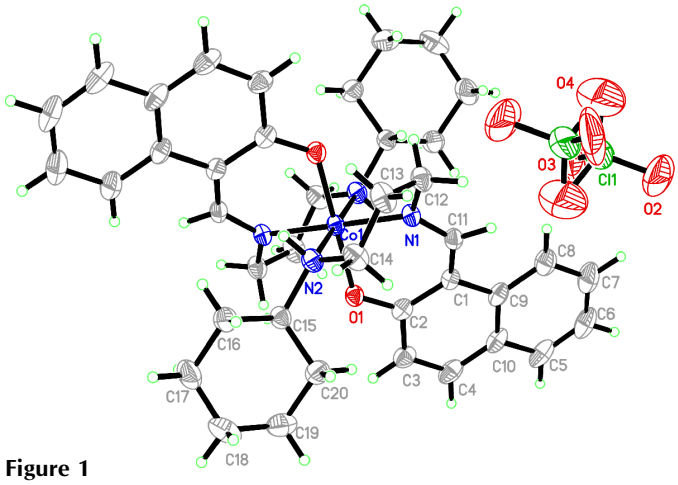


Figure 1
The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The unlabeled atoms are related by the symmetry code $(-x, -y, -z)$. The perchlorate anion is disordered about an inversion center and both components are shown.

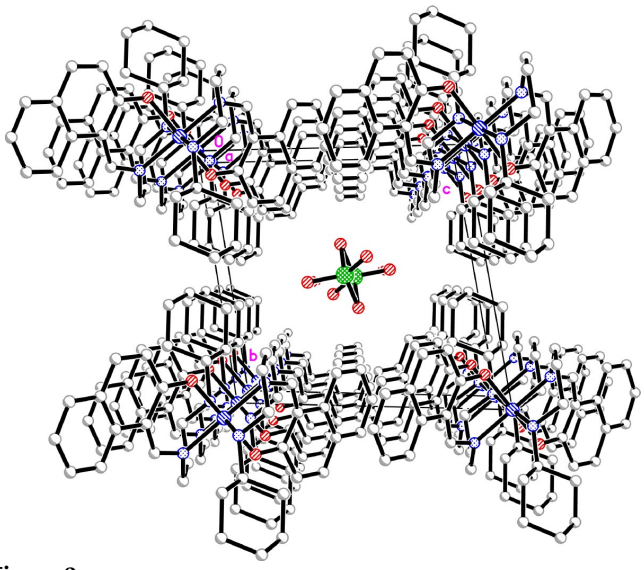


Figure 2
The crystal packing of (I), viewed along the *a* axis, including the disordered components of the anions. H atoms have been omitted for clarity.

imino)methyl]naphthalen-2-olate. All the bond lengths and angles are comparable to those of the previous complex (Table 1). In the title complex, the Co^{III} atom, lying on an inversion center, is also in a slightly distorted octahedral environment. The bond distances are similar, with values of 1.876 (3) (Co1—O1), 1.915 (4) (Co1—N1) and 1.999 (4) Å (Co1—N2). The three *trans* angles are all exactly 180°, as a result of centrosymmetry, and all other angles around Co1 are close to 90°, ranging from 89.34 (15) to 90.66 (15)°. The torsion angles N2—C14—C13—C12 and N1—C12—C13—C14 are −68.1 (6) and 15.8 (7)°, respectively. The dihedral angle between the two coordination planes defined by N1—Co1—N2 and N1—Co1—O1 is 90.1 (2)°. Atom Co1 deviates from the naphthalene ring plane by 0.6247 (2) Å. The conformation of the six-membered ring containing the Co, azomethine N (N1), amine N (N2) and three C atoms (C12, C13 and C14) is a twisted boat.

The crystal structure consists of $[Co(C_{20}H_{25}N_2O)_2]^+$ cations and ClO_4^- anions. As expected, the cyclohexyl groups in the complex adopt chair conformations to minimize steric effects as observed in the related complex. The perchlorate anion in the complex is disordered about an inversion center.

Experimental

N-Cyclohexyl-1,3-diaminopropane and salicylaldehyde were obtained commercially and were used without further purification. *N*-Cyclohexyl-1,3-diaminopropane (2.0 mmol, 312 mg) and 2-hydroxy-1-naphthaldehyde (2.0 mmol, 344 mg) were dissolved in methanol (20 ml). The mixture was stirred for 1 h to give a brown solution of *L* (2.0 mmol), where *L* is 3-[(3-cyclohexylaminopropylimino)methyl]-naphthalen-2-ol. To the solution of *L* was added a methanol solution (10 ml) of $Co(ClO_4)_3\cdot 7H_2O$ (1.0 mmol, 483 mg), with stirring. After keeping the resulting solution in air for 12 d, brown block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using P_4O_{10} (yield 70.3%). Analysis found: C 61.77, H 6.54, N 7.15%; calculated for $C_{40}H_{50}ClCoN_4O_6$: C 61.81, H 6.48, N 7.21%. Main IR data: 3440 (*m*), 3235 (*m*), 2925 (*s*), 2848 (*m*), 1614 (*s*), 1541 (*m*), 1450 (*s*), 1341 (*m*), 1312 (*s*), 1099 (*s*) cm^{-1}.

Crystal data

$[Co(C_{20}H_{25}N_2O)_2]ClO_4$
M_r = 777.22
Triclinic, $P\overline{1}$
a = 9.061 (2) Å
b = 10.378 (2) Å
c = 11.464 (2) Å
α = 78.01 (3)°
β = 67.79 (3)°
γ = 81.41 (3)°
V = 973.3 (3) $Å^3$
Z = 1
D_x = 1.326 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2138 reflections
θ = 2.7–25.6°
μ = 0.56 mm^{-1}
T = 293 (2) K
Block, brown
0.27 × 0.22 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.863, T_{max} = 0.946
4553 measured reflections
3849 independent reflections
2551 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.5°
$h = -11 \rightarrow 10$
$k = -13 \rightarrow 11$
$l = -14 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.213
S = 1.04
3849 reflections
250 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1068P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.79 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.30 e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.876 (3)	Co1—N2	1.999 (4)
Co1—N1	1.915 (4)		
O1—Co1—O1^{i}	180	N1—Co1—N2^{i}	90.66 (15)
O1—Co1—N1	90.34 (15)	O1—Co1—N2	89.87 (15)
O1—Co1—N1^{i}	89.66 (15)	N1—Co1—N2	89.34 (15)
N1—Co1—N1^{i}	180	N2^{i}—Co1—N2	180
O1—Co1—N2^{i}	90.13 (15)		

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

The perchlorate anion is disordered about the inversion center, and no constraints or restraints were used. 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 with U_{iso}(H) values fixed at 0.08 $Å^2$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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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