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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.046
 wR factor = 0.130
Data-to-parameter ratio = 16.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

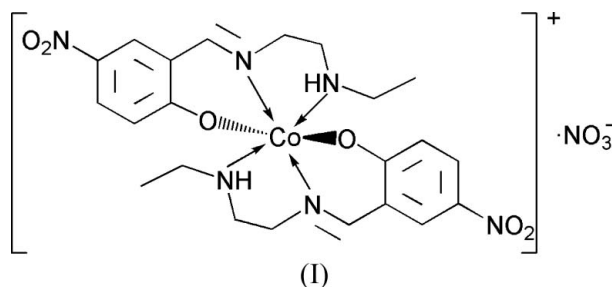
Bis{2-[2-(ethylamino)ethyliminomethyl]-4-nitrophenolato}cobalt(III) nitrate

In the title mononuclear cobalt(III) complex, $[\text{Co}(\text{C}_{11}\text{H}_{14}\text{N}_3\text{O}_3)_2]\text{NO}_3$, the octahedral Co^{III} atom is coordinated by two phenolate O atoms, two imine N atoms, and two amine N atoms from two Schiff base ligands. The Co^{III} complex and the nitrate anion possess crystallographic twofold rotation axis symmetry. The nitrate anions are linked to the cobalt(III) complexes through intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

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Comment

The design of multidentate ligands and their metallosupramolecular chemistry are of current interest (Henkel & Krebs, 2004; Tshuva & Lippard, 2004; Weston, 2005). The condensation reaction of an aromatic carbaldehyde with a primary amine has been shown to offer an easy and inexpensive way of preparing a variety of polydentate Schiff base ligands able to form a diverse array of metal complexes (Arici *et al.*, 2005; Salmon *et al.*, 2005; Hebbachi & Benali-Cherif, 2005; Sari *et al.*, 2006). We report here the crystal structure of the title mononuclear cobalt(III) complex, (I).



Complex (I) is a nitrate salt of bis{2-[2-(ethylamino)ethyliminomethyl]-4-nitrophenolato}cobalt(III). The octahedral Co^{III} atom in the complex is coordinated by two phenolate O atoms, two imine N atoms, and two amine N atoms from two Schiff base ligands (Fig. 1). The ions are each disposed about a crystallographic twofold rotation symmetry axis. All the bond values (Table 1) subtended at the metal centre are typical and comparable with the values observed in other similar cobalt(III) complexes (Meghdadi & Mahmoudkhani, 2006; Sun *et al.*, 2005; Wang *et al.*, 2004). In the crystal structure, the nitrate anions are linked to the cobalt(III) complexes through intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2 and Fig. 2).

Experimental

5-Nitrosalicylaldehyde (1.0 mmol, 168.2 mg), *N*-ethylethane-1,2-diamine (1.0 mmol, 88.2 mg) and $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.5 mmol, 145.5 mg) were dissolved in MeOH (100 ml). The mixture was stirred

at room temperature for about 1 h, giving a red solution. After allowing the solution to stand in air for about a week, red block-shaped crystals were formed.

Crystal data

| | |
|---|---|
| $[\text{Co}(\text{C}_{11}\text{H}_{14}\text{N}_3\text{O}_3)_2] \cdot \text{NO}_3$ | $Z = 4$ |
| $M_r = 593.44$ | $D_x = 1.514 \text{ Mg m}^{-3}$ |
| Orthorhombic, <i>Pbcn</i> | Mo $K\alpha$ radiation |
| $a = 12.041 (1) \text{ \AA}$ | $\mu = 0.72 \text{ mm}^{-1}$ |
| $b = 11.436 (1) \text{ \AA}$ | $T = 298 (2) \text{ K}$ |
| $c = 18.908 (2) \text{ \AA}$ | Block, red |
| $V = 2603.7 (4) \text{ \AA}^3$ | $0.32 \times 0.27 \times 0.23 \text{ mm}$ |

Data collection

| | |
|--|--|
| Bruker SMART APEX CCD area-detector diffractometer | 21071 measured reflections |
| ω scans | 3001 independent reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | 2148 reflections with $I > 2\sigma(I)$ |
| $T_{\min} = 0.802$, $T_{\max} = 0.851$ | $R_{\text{int}} = 0.047$ |
| | $\theta_{\max} = 27.5^\circ$ |

Refinement

| | |
|--|---|
| Refinement on F^2 | $w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.9222P]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.130$ | $(\Delta/\sigma)_{\max} < 0.001$ |
| $S = 1.03$ | $\Delta\rho_{\max} = 0.38 \text{ e \AA}^{-3}$ |
| 3001 reflections | $\Delta\rho_{\min} = -0.24 \text{ e \AA}^{-3}$ |
| 182 parameters | |
| H atoms treated by a mixture of independent and constrained refinement | |

Table 1

Selected geometric parameters (\AA , $^\circ$).

| | | | |
|-------------------------|-------------|-------------------------|------------|
| Co1—O1 | 1.899 (2) | Co1—N2 | 1.996 (2) |
| Co1—N1 | 1.911 (2) | | |
| O1—Co1—O1 ⁱ | 87.56 (11) | N1—Co1—N2 ⁱ | 93.69 (9) |
| O1—Co1—N1 ⁱ | 87.82 (8) | O1—Co1—N2 | 176.84 (8) |
| O1—Co1—N1 | 94.04 (8) | N1—Co1—N2 | 84.54 (9) |
| N1 ⁱ —Co1—N1 | 177.43 (13) | N2 ⁱ —Co1—N2 | 93.33 (13) |
| O1—Co1—N2 ⁱ | 89.57 (9) | | |

Symmetry code: (i) $-x, y, -z + \frac{1}{2}$.

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---|------------|--------------|--------------|----------------|
| $\text{N2}-\text{H2} \cdots \text{O4}^{\text{ii}}$ | 0.902 (10) | 2.288 (17) | 3.142 (4) | 158 (3) |
| $\text{N2}-\text{H2} \cdots \text{O4}^{\text{iii}}$ | 0.902 (10) | 2.337 (19) | 3.152 (4) | 150 (3) |

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

Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) \AA . The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 \AA and $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

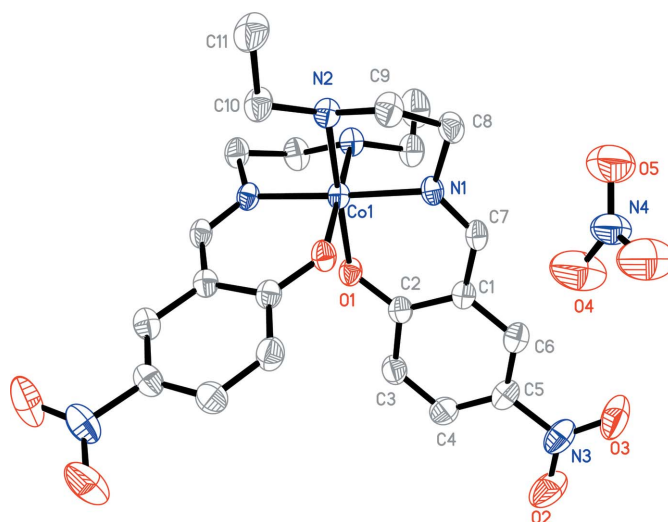


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are at the symmetry position $(-x, y, \frac{1}{2} - z)$ in the cation and $(1 - x, y, \frac{1}{2} - z)$ in the anion. H atoms have been omitted for clarity.

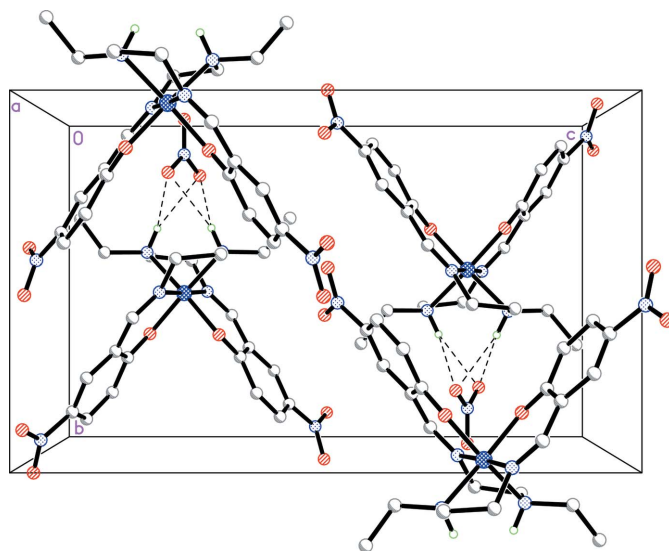


Figure 2

The crystal packing of (I). Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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