Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[4-bromo-2-(pyridin-2-ylmethyliminomethyl)-phenolato-κ^3N,N',O]cobalt(III) nitrate

Yu-Xi Sun

Department of Chemistry, Qufu Normal University, Qufu 273165, People's Republic of China

Correspondence e-mail: yuxisun@163.com

Received 4 January 2005
Accepted 12 January 2005
Online 22 January 2005

Key indicators

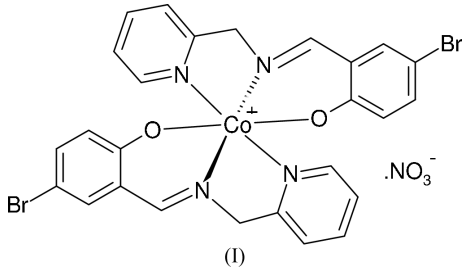
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.039
wR factor = 0.105
Data-to-parameter ratio = 17.4

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

The title compound, $[Co(C_{13}H_{10}BrN_2O)_2]NO_3$, is a mononuclear cobalt(III) complex. The Co^{III} atom is coordinated by four N atoms and two O atoms of two Schiff base ligands, forming a slightly distorted octahedral coordination configuration.

Comment

Cobalt compounds are present in the active sites of several important classes of metalloproteins. The study of cobalt compounds is of great interest in various aspects of chemistry (Downing & Urbach, 1969; Ganeshpure *et al.*, 1996; Bosnich, 1968; Costes *et al.*, 1995). The catalytic potential of Schiff base cobalt compounds has been widely studied (Boca *et al.*, 1998). As an extension of our work on the structural characterization of Schiff base complexes (Sun, 2005), the structure of the title mononuclear Schiff base cobalt(III) complex, (I), is reported here.



(I)

As illustrated in Fig. 1, compound (I) is the nitrate salt of a mononuclear cobalt(III) complex cation. Selected bond distances and angles are given in Table 1.

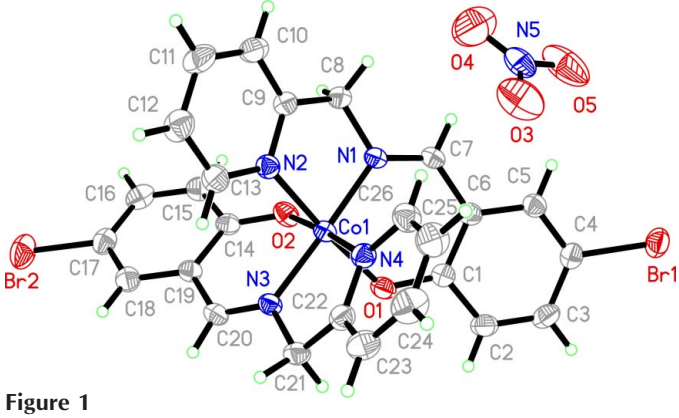


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

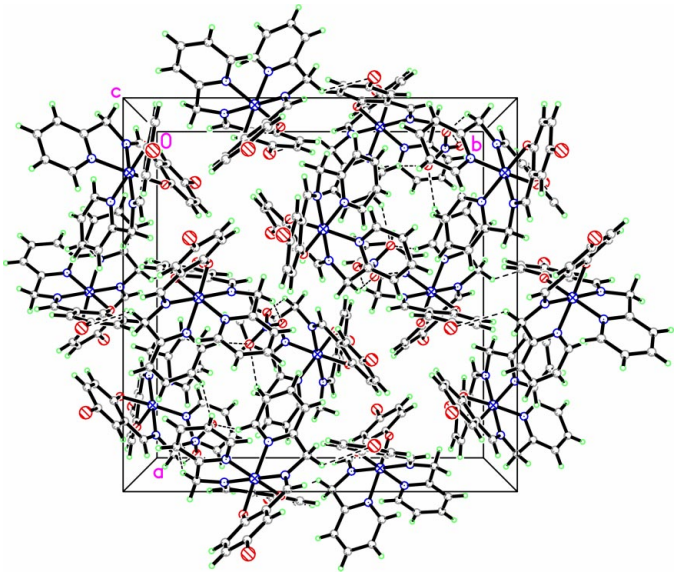


Figure 2
The crystal packing of (I), viewed along the *c* axis. C—H···O hydrogen bonds are shown as dashed lines.

The Co^{III} atom has an octahedral geometry and is coordinated by two Schiff base ligands. The Schiff base acts as a tridentate ligand through the phenolate O atom and two N atoms. The three *trans* angles at the Co^{III} atom are close to 180° (Table 1). All the other angles subtended at the Co^{III} atom are close to 90°, indicating a slightly distorted octahedral coordination configuration. The average Co—O bond length of 1.892 (2) Å is essentially the same as the value observed in a similar Schiff base cobalt(III) complex [1.891 (3) Å; Li *et al.*, 2004]. The average Co—N(imine) bond length of 1.894 (2) Å is a little shorter than the value observed in the same complex [1.933 (4) Å]. All the other bond lengths are in normal ranges (Allen *et al.*, 1987).

The crystal structure of (I) consists of $[Co(C_{13}H_{10}BrN_2O)_2]^+$ cations and NO_3^- anions (Fig. 2), linked by C—H···O hydrogen bonds (Table 2).

Experimental

5-Bromosalicylaldehyde (0.2 mmol, 40.2 mg) and 2-aminomethylpyridine (0.2 mmol, 21.6 mg) were dissolved in ethanol (15 ml). The mixture was stirred for 15 min to give a clear yellow solution. To this solution was added an aqueous solution (5 ml) of $Co(NO_3)_2{\cdot}4H_2O$ (0.1 mmol, 25.5 mg), with stirring. The mixture was stirred at room temperature for about 30 min and then filtered. After allowing the brown filtrate to stand in air for 15 d, brown block-shaped crystals of (I) were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$[Co(C_{13}H_{10}BrN_2O)_2]NO_3$
M_r = 701.22
Tetragonal, $P4_2/n$
a = 17.610 (1) Å
c = 17.206 (1) Å
V = 5336.0 (5) Å^3
Z = 8
D_x = 1.746 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6091 reflections
θ = 2.3–24.0°
μ = 3.69 mm^{-1}
T = 295 (2) K
Block, brown
0.28 × 0.19 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.393, T_{max} = 0.515
60 680 measured reflections
6123 independent reflections
4296 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 27.5°
$h = -22 \rightarrow 22$
$k = -22 \rightarrow 22$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 1.03
6123 reflections
352 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 4.6927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2	1.882 (2)	Co1—O1	1.902 (2)
Co1—N3	1.893 (2)	Co1—N4	1.953 (3)
Co1—N1	1.894 (2)	Co1—N2	1.954 (3)
O2—Co1—N3	92.38 (10)	N1—Co1—N4	98.45 (11)
O2—Co1—N1	85.79 (10)	O1—Co1—N4	88.71 (10)
N3—Co1—N1	177.71 (11)	O2—Co1—N2	90.62 (10)
O2—Co1—O1	91.65 (10)	N3—Co1—N2	95.61 (11)
N3—Co1—O1	87.92 (10)	N1—Co1—N2	83.04 (11)
N1—Co1—O1	93.51 (10)	O1—Co1—N2	175.73 (10)
O2—Co1—N4	175.72 (10)	N4—Co1—N2	89.30 (11)
N3—Co1—N4	83.37 (11)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8*B*···O3	0.97	2.47	3.313 (6)	146
C21—H21*B*···O5^{i}	0.97	2.43	3.197 (6)	136
C25—H25···O4^{ii}	0.93	2.47	3.332 (5)	153
C26—H26···O4	0.93	2.44	3.213 (5)	141

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

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2002); software used to prepare material for publication: *SHELXTL*.

The author thanks Qufu Normal University for funding this study.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–19.
Bruker (2002). *SMART* (Version 5.628), *SAINT* (Version 6.02) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Bosnich, B. (1968). *J. Am. Chem. Soc.* **90**, 627–632.
Boca, R., Elias, H., Haase, W., Hüber, M., Klement, M., Müller, L., Paulus, H., Svoboda, I. & Valko, M. (1998). *Inorg. Chim. Acta,* **278**, 127–135.

Costes, J. P., Dominiguez-Vera, J. M. & Laurent, J. P. (1995). *Polyhedron,* **14**, 2179–2187.
Downing, R. S. & Urbach, F. L. (1969). *J. Am. Chem. Soc.* **91**, 5977–5983.
Ganeshpure, P. A., Tembe, G. L. & Satish, S. (1996). *J. Mol. Catal. A,* **113**, L423–L425.
Li, S.-Y., You, Z.-L., Chen, B., Lin, Y.-S., Xiong, Z.-D. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, m999–m1001.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sun, Y.-X. (2005). *Acta Cryst.* E**61**, m39–m40.