[4-Bromo-2-(pyridin-2-ylmethyliminomethyl)-phenolato-κ^3O,N,N']methoxocobalt(III) perchlorate

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The title Schiff base compound, [Co(C$_{13}$H$_{10}$BrN$_2$O)-(CH$_3$O)]ClO$_4$, is a mononuclear cobalt(III) compound. The Co^{III} ion is coordinated by two N atoms and one O atom from a Schiff base ligand, and by another O atom from a coordinated methanolate ligand, giving an approximately square-planar geometry.

Comment

Cobalt complexes have been of great interest in coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Billson *et al.*, 2000; Kotera *et al.*, 2003; Fritsky *et al.*, 2003). As an extension of work on the structural characterization of cobalt complexes, the title mononuclear cobalt(II) compound, (I), is reported.

(I)
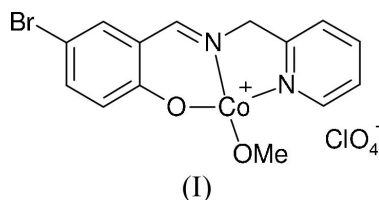
Compound (I) is a perchlorate salt of a mononuclear cobalt(III) complex (Fig. 1). The Co^{III} ion in the complex is four-coordinated by two N atoms and one O atom from the Schiff base ligand, and by another O atom from the methanol molecule, giving a square-planar geometry. The four coordinating atoms around the Co centre are approximately coplanar, giving a square-planar geometry with an average deviation of 0.039 (6) Å; the Co atom lies 0.021 (2) Å above this plane.

The C7═N1 bond length [1.274 (5) Å; Table 1] conforms to the value for a double bond, while the C8—N1 bond length [1.461 (5) Å] conforms to the value for a single bond. The Co1—O1 bond length [1.898 (3) Å] is a little longer than the corresponding value of 1.876 (3) Å observed in another Schiff base cobalt(III) complex (You *et al.*, 2003). The Co1—N1 bond length [1.940 (3) Å] is comparable with the value of 1.936 (4) Å observed in the same complex. Both *trans* angles in the CoN$_2$O$_2$ square plane are close to 180°, *viz.* 176.48 (14) and 175.10 (13)°, indicating a slightly distorted square-planar geometry. The smallest bond angles for the N1—Co1—N2 [82.96 (15)°] correlate with the strained ligand bite angle for the five-membered chelate ring.

In the crystal structure, the molecules are stacked along the *a* axis (Fig. 2). An O1⋯O6(1 − *x*,−*y*, 1 − *z*) short contact [2.665 (6) Å] is observed in the crystal structure.

Experimental

2–Aminomethylpyridine (0.1 mmol, 10.8 mg) and salicylaldehyde (0.1 mmol, 12.2 mg) were dissolved in methanol (10 ml). The mixture was stirred for 1 h to obtain a clear yellow solution. To this solution was added a methanol solution (10 ml) of $Co(ClO_4)_2 \cdot 6H_2O$ (0.1 mmol, 36.8 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.

Crystal data

$[Co(C_{13}H_{10}BrN_2O)(CH_3O)]ClO_4$
$M_r = 479.55$
Monoclinic, $P2_1/n$
$a = 7.194\ (2)$ Å
$b = 19.119\ (2)$ Å
$c = 12.694\ (2)$ Å
$\beta = 95.846\ (2)°$
$V = 1736.9\ (6)$ Å^3
$Z = 4$

$D_x = 1.834$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4575 reflections
$\theta = 2.4–24.7°$
$\mu = 3.48$ mm^{-1}
$T = 298\ (2)$ K
Block, brown
$0.23 \times 0.10 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.497$, $T_{max} = 0.761$
20 032 measured reflections

4190 independent reflections
2962 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 28.3°$
$h = -9 \rightarrow 9$
$k = -25 \rightarrow 25$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.134$
$S = 1.04$
4190 reflections
263 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 1.7215P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -1.00$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.898 (3)	Co1—N2	1.987 (3)
Co1—N1	1.940 (3)	Co1—O6	1.996 (3)
O1—Co1—N1	93.70 (13)	O1—Co1—O6	89.75 (12)
O1—Co1—N2	176.48 (14)	N1—Co1—O6	175.10 (13)
N1—Co1—N2	82.96 (15)	N2—Co1—O6	93.65 (13)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$. The O atoms of the perchlorate anion are disordered over two distinct sites with occupancies of 0.516 (19) and 0.484 (19). The Cl—O and O···O distances in both disordered components were restrained to be equal. The unassigned maximum residual density is 0.48 Å from atom Co1 and the minimum residual density is 0.77 Å from atom Br1.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.
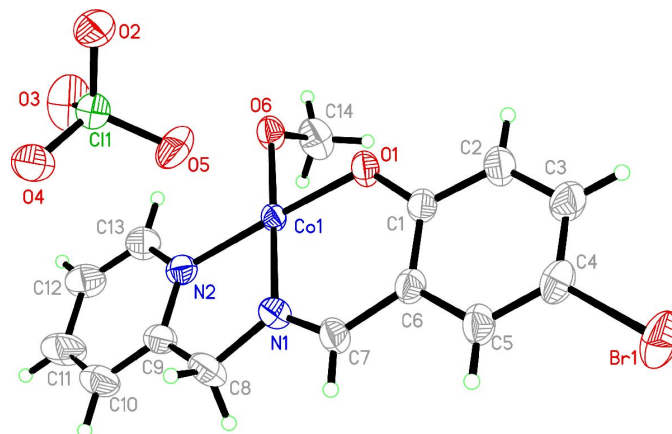

Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Only the major components of the disordered perchlorate anion are shown.
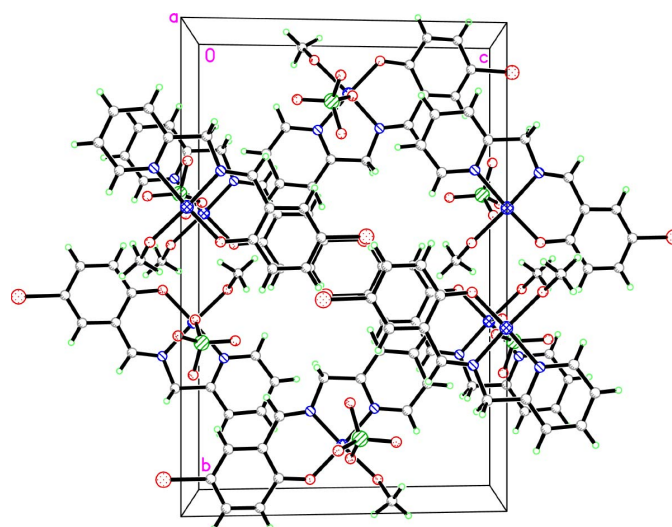

Figure 2
The crystal packing of (I), viewed along the a axis.

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