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Di-μ-oxo-bis[(2,2′-bipyridine)cobalt(III)] bis(perchlorate)

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Key indicators

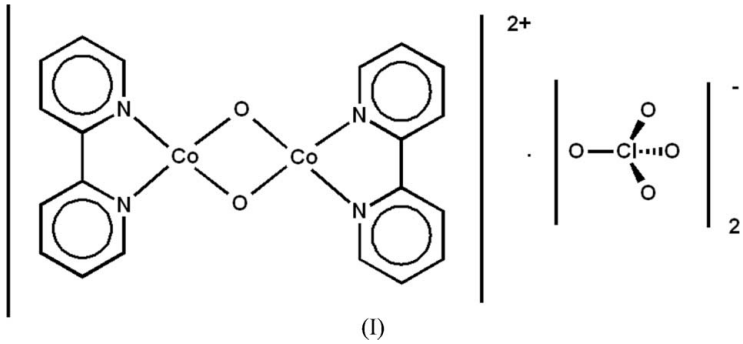
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.072
wR factor = 0.162
Data-to-parameter ratio = 16.8

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

In the title compound, $[Co_2O_2(C_{10}H_8N_2)_2](ClO_4)_2$, the binuclear complex cation has 2/m symmetry, and the perchlorate ion has mirror symmetry. The Co^{III} atoms are coordinated by two N atoms of the 2,2′-bipyridine ligand and two bridging O atoms in a square-planar geometry. The Co···Co distance in the complex is 2.8784 (19) Å.

Comment

Structures of Co^{III} complexes containing 2,2′-bipyridine (bpy) have been investigated (Sato & Saito, 1978; Ohba *et al.*, 1979; Chen *et al.*, 1998). In order to research the magnetic properties of complexes prepared from cobalt perchlorate and bipyridine, the structure of the compound (I) was determined.



(I)

In (I), the binuclear complex cation has an inversion centre, a twofold axis passing through the Co atoms and a mirror plane through the bridging O atoms (Fig. 1). Atoms Cl1/O2/O4 of the perchlorate ion lie on a mirror plane. The Co atom is coordinated by two N atoms of the bpy ligand and two bridging O atoms in a square-planar geometry (Table 1).

Experimental

Compound (I) was crystallized by slow evaporation of an aqueous solution of a mixture of $Co(ClO_4)_2{\cdot}6H_2O$ (2 mmol) and 2,2′-bipyridine (2 mmol) with $HClO_4$ (20 ml, 1N). Blue block-shaped crystals were obtained after several weeks (yield *ca* 90%).

Crystal data

$[Co_2O_2(C_{10}H_8N_2)_2](ClO_4)_2$
M_r = 661.13
Monoclinic, $C2/m$
a = 13.646 (5) Å
b = 15.289 (6) Å
c = 6.309 (2) Å
β = 113.798 (6)°
V = 1204.4 (8) Å^3
Z = 2
D_x = 1.823 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8119 reflections
θ = 2.1–28.4°
μ = 1.66 mm^{-1}
T = 298 K
Block, blue
0.24 × 0.16 × 0.08 mm

Data collection

Bruker Apex CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.691, T_{max} = 0.878
8119 measured reflections
1567 independent reflections

1301 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 28.4°
$h = -18 \rightarrow 18$
$k = -20 \rightarrow 20$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.162
S = 1.24
1567 reflections
93 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 2.5649P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.931 (3)	Co1···Co1^{i}	2.8784 (19)
Co1—N2	1.994 (4)		
O1—Co1—O1^{i}	83.6 (2)	N2—Co1—N2^{ii}	81.5 (2)
O1—Co1—N2	177.3 (2)	Co1—O1—Co1^{i}	96.4 (2)
O1^{i}—Co1—N2	97.50 (16)		

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, y, -z+2$.

H atoms were constrained to an ideal geometry with C—H distances of 0.93 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *SHELXTL*.

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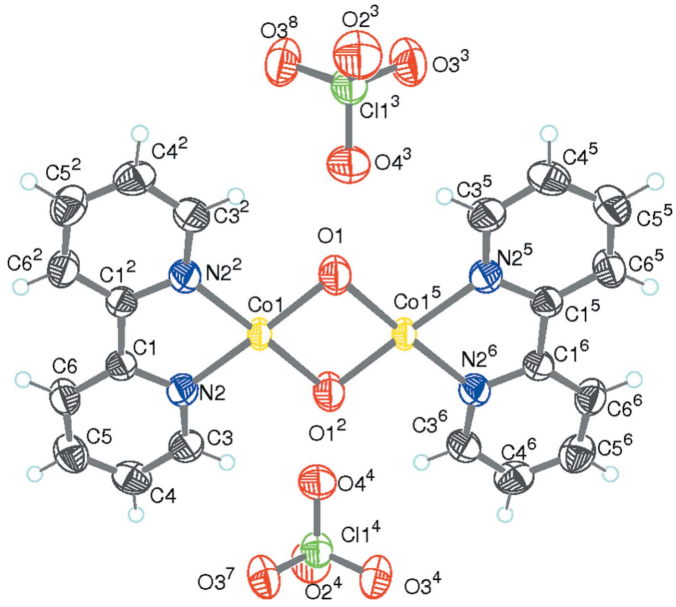

Figure 1
The cation and anion of (I). Displacement ellipsoids are shown at the 50% probability level. [Symmetry codes: (1) x, y, z; (2) $-x, y, -z$; (3) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (4) $-x+\frac{1}{2}, y+\frac{1}{2}, -z$; (5) $-x, -y, -z$; (6) $x, -y, z$; (7) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (8) $x+\frac{1}{2}, -y+\frac{1}{2}, z$.].

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