Hexakis(4-nitropyridine *N*-oxide-κN^1)cobalt(II) bis(perchlorate)

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Key indicators

Single-crystal X-ray study
$T = 298$ K
Mean σ(C–C) = 0.006 Å
Disorder in solvent or counterion
R factor = 0.067
wR factor = 0.181
Data-to-parameter ratio = 13.9

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

In the title complex, $[Co(C_5H_4N_2O_3)_6](ClO_4)_2$, six 4-nitropyridine *N*-oxide (npo) ligands coordinate to the Co^{II} atom *via* their *N*-oxide O atoms, resulting in an octahedral CoO$_6$ grouping. The Co^{II} ion occupies an inversion centre. A short contact of 2.841 (12) Å is observed between a pyridine N atom and a perchlorate O atom.
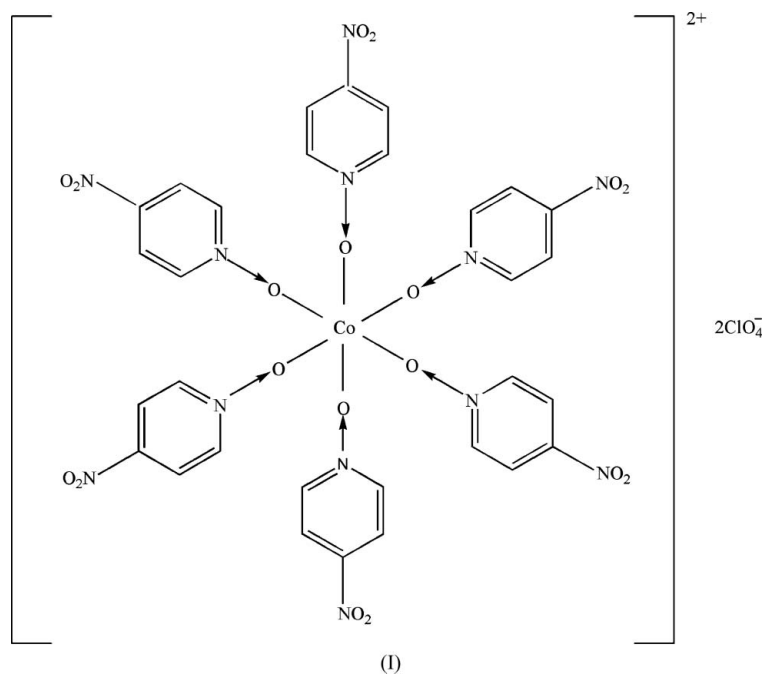
Comment

Pyridine *N*-oxide and its derivatives can act as bridging ligands in polynuclear metal complexes (Watson, 1969) or as monodentate ligands in mononulear complexes (Shi *et al.*, 2005). We report here the synthesis and structure of the title Co^{II} complex, (I), incorporating the 4-nitropyridine *N*-oxide (npo) ligand.

The molecular structure of (I) is shown in Fig. 1. The Co^{II} ion assumes a slightly distorted (Table 1) CoO$_6$ octahedral coordination geometry from the *N*-oxide O atoms of six monodentate npo ligands. Atom Co1 occupies an inversion centre.

In the crystal structure of (I), a short N4···O11^i [symmetry code: (i) = $\frac{3}{2} - x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$] contact of 2.841 (12) Å is observed between an *N*-oxide N atom and a perchlorate O atom (sum of van der Waals radii = 3.07 Å). A Coulombic attraction between the formal positive charge of N4 and the partial negative charge of O11 may be responsible for this.

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Experimental

An aqueous solution (10 ml) of 4-nitropyridine N-oxide (0.3375 g, 2.41 mmol) was added to an aqueous solution (15 ml) of Co(ClO$_4$)$_2$·6H$_2$O (0.2932 g, 0.801 mmol) and the mixture was stirred for a few minutes. Red single crystals of (I) were obtained after the solution was allowed to stand at room temperature for two weeks.

Crystal data

[Co(C$_5$H$_4$N$_2$O$_3$)$_6$](ClO$_4$)$_2$	$D_x = 1.732$ Mg m^{-3}
$M_r = 1098.44$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 5735
$a = 8.4969$ (12) Å	reflections
$b = 13.6406$ (19) Å	$\theta = 2.6–28.0°$
$c = 18.179$ (3) Å	$\mu = 0.65$ mm^{-1}
$\beta = 91.005$ (2)°	$T = 298$ (2) K
$V = 2106.7$ (5) Å^3	Prism, red
$Z = 2$	0.48 × 0.23 × 0.21 mm

Data collection

Bruker SMART CCD diffractometer	4487 independent reflections
	4006 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.041$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{max} = 27.0°$
	$h = -10 \rightarrow 10$
$T_{min} = 0.747$, $T_{max} = 0.876$	$k = -17 \rightarrow 10$
12139 measured reflections	$l = -23 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0878P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.067$	$+ 2.72P]$
$wR(F^2) = 0.181$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} < 0.001$
4487 reflections	$\Delta\rho_{max} = 0.96$ e Å^{-3}
323 parameters	$\Delta\rho_{min} = -0.64$ e Å^{-3}
H-atom parameters constrained	Extinction correction: SHELXL97
	Extinction coefficient: 0.0063 (12)

Table 1
Selected geometric parameters (Å, °).

Co1—O6	2.036 (2)	Co1—O7	2.109 (3)
Co1—O3	2.105 (2)		
Co1—O6—N4	128.39 (19)	Co1—O3—N5	132.5 (2)
Co1—O7—N6	115.01 (19)		

Three of the perchlorate O atoms are disordered over two sites in a 0.601 (13):0.393 (13) ratio (sum constrained to unity). The disordered O atoms were refined isotropically. All H atoms were included in
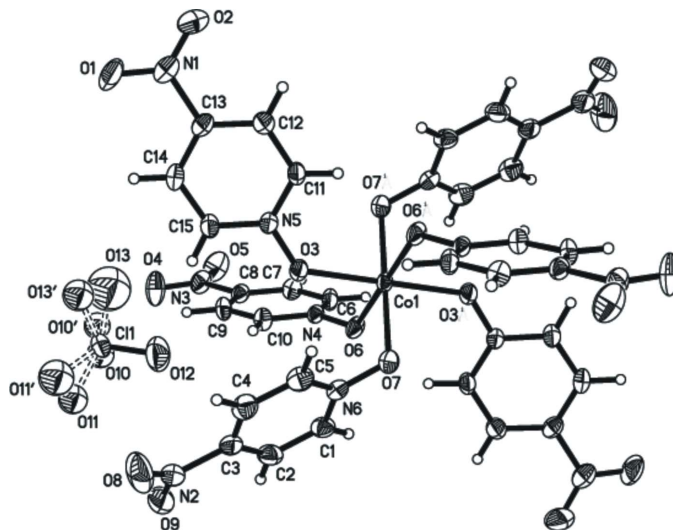

Figure 1
View of (I), showing 30% displacement ellipsoids for the non-H atoms. The Cl—O bonds of the disordered perchlorate O atoms are shown as dashed lines. Primed and unlabelled atoms are generated by the symmetry operation $(1 - x, 1 - y, 1 - z)$.

calculated positions and were included in the final cycles of refinement using a riding model [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C)].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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