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Key indicators

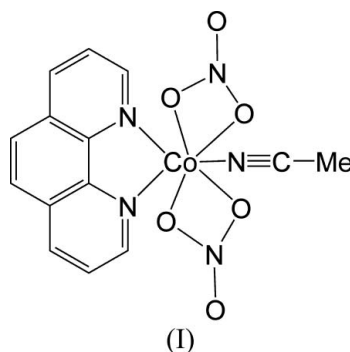
Single-crystal X-ray study
 $T = 150\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.036
 wR factor = 0.069
Data-to-parameter ratio = 15.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Acetonitrilebis(nitrato- $\kappa^2\text{O},\text{O}'$)(1,10-phenanthroline)cobalt(II)

In the title compound, $[\text{Co}(\text{NO}_3)_2(\text{C}_2\text{H}_3\text{N})(\text{C}_{12}\text{H}_8\text{N}_2)]$, the cobalt(II) centre adopts a seven-coordinate distorted pentagonal-bipyramidal geometry, being coordinated by a bidentate 1,10-phenanthroline, two bidentate nitrate anions and an acetonitrile ligand. The two axial sites are occupied by the acetonitrile ligand and one N-atom donor from the phenanthroline. The major distortions from ideal geometry occur within the equatorial plane, and are due to the narrow bite angle of the bidentate nitrate anions.

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Comment

The field of coordination frameworks and their potential applications have been increasingly growing over the last few decades (Braga *et al.*, 2005; Champness *et al.*, 2006). Our studies have led us to investigate a variety of transition metal(II) nitrate salts in combination with soft N-donor ligands (Barnett *et al.*, 2001; Barnett *et al.*, 2003*a,b*; Blake *et al.*, 2000; Khlobystov *et al.*, 2003). During our investigations, we have encountered the title compound, (I), as a by-product from an attempt to prepare a coordination polymer with the ligand 4,4'-(1,4-phenylene)bis(3,6-dipyridin-2-ylpyridazine). Thus, a new crystal structure containing the widely studied 1,10-phenanthroline ligand has been obtained and characterized.



The cobalt(II) centre adopts a seven-coordinate distorted pentagonal-bipyramidal geometry, the donor atoms being two N atoms supplied by a bidentate 1,10-phenanthroline, four O atoms from two bidentate nitrate anions and an N atom from an acetonitrile ligand. The two axial sites are occupied by the acetonitrile ligand and one N-atom donor from the phenanthroline; as the other phenanthroline N-atom donor occupies an equatorial site, this ligand bridges axial and equatorial sites. The major distortions from ideal geometry occur within the equatorial plane, and are due to the narrow bite angle (ca. 57°) of the nitrate anions.

A dihedral angle of $4.05 (14)^\circ$ is observed between the least-squares planes through the two nitrate anions which occupy four of the five equatorial positions of the cobalt(II) coordination environment. Dihedral angles of $105.1 (12)$ and $108.7 (12)^\circ$ are observed between the plane through the 1,10-phenanthroline group and those of the nitrates.

Experimental

The title compound was prepared by slow reaction of $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (10 mg, 0.034 mmol) and 1,10-phenanthroline (6 mg, 0.033 mmol) in acetonitrile (10 ml) in the presence of 4,4'-(1,4-phenylene)bis(3,6-dipyridin-2-ylpyridazine). Crystals were left to grow over a period of six months before being taken from the mother liquor for single-crystal X-ray diffraction studies.

Crystal data

$[\text{Co}(\text{NO}_3)_2(\text{C}_2\text{H}_3\text{N})(\text{C}_{12}\text{H}_8\text{N}_2)]$	$Z = 4$
$M_r = 404.2$	$D_x = 1.692 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 7.1414 (9) \text{ \AA}$	$\mu = 1.13 \text{ mm}^{-1}$
$b = 14.3837 (17) \text{ \AA}$	$T = 150 (2) \text{ K}$
$c = 15.4670 (19) \text{ \AA}$	Block, orange
$\beta = 92.906 (2)^\circ$	$0.14 \times 0.12 \times 0.10 \text{ mm}$
$V = 1586.7 (3) \text{ \AA}^3$	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	9772 measured reflections
ω scans	3637 independent reflections
Absorption correction: multi-scan (SHELXTL; Bruker, 2001)	2323 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.575$, $T_{\max} = 0.614$ (expected range = 0.840–0.896)	$R_{\text{int}} = 0.042$
	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0239P)^2]$
$wR(F^2) = 0.069$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.88$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3637 reflections	$\Delta\rho_{\text{max}} = 0.37 \text{ e \AA}^{-3}$
236 parameters	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$

Table 1

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

Co—N1	2.1087 (19)	Co—O3	2.2583 (18)
Co—N2	2.1180 (19)	Co—O4	2.3289 (19)
Co—N5	2.079 (2)	Co—O5	2.1224 (17)
Co—O1	2.2375 (17)		
N1—Co—N2	78.48 (7)	N5—Co—O1	87.02 (7)
N1—Co—N5	95.89 (7)	N5—Co—O3	93.68 (7)
N1—Co—O3	137.22 (7)	N5—Co—O4	85.53 (7)
N1—Co—O4	86.07 (7)	N5—Co—O5	94.82 (7)
N1—Co—O5	141.12 (7)	O1—Co—O3	56.74 (6)
N1—Co—O1	82.23 (7)	O1—Co—O4	165.41 (6)
N2—Co—N5	172.54 (8)	O1—Co—O5	135.63 (6)
N2—Co—O1	87.36 (7)	O3—Co—O4	136.29 (6)
N2—Co—O3	87.34 (7)	O3—Co—O5	78.93 (6)
N2—Co—O4	98.85 (7)	O4—Co—O5	57.68 (6)
N2—Co—O5	92.63 (7)		

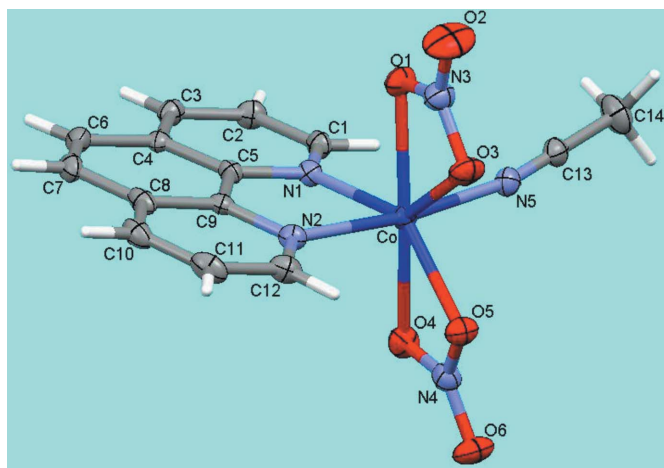


Figure 1

A view of the structure of the title compound, showing the atom-numbering scheme adopted. Displacement ellipsoids are drawn at the 50% probability level.

The methyl H atoms on the acetonitrile molecule were located in ΔF syntheses and refined as part of a rigid rotating group, with $\text{C—H} = 0.98 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. Aryl H atoms were positioned geometrically and refined using a riding model, with $\text{C—H} = 0.95 \text{ \AA}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* and *SHELXTL* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *MERCURY* (Macrae *et al.*, 2006); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2003) and *pubCIF* (Westrip, 2006).

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