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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
 R factor = 0.051
 wR factor = 0.169
 Data-to-parameter ratio = 17.9

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

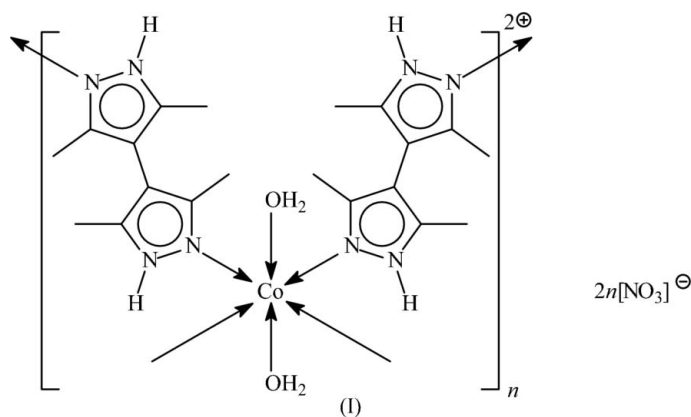
Poly[[diaquabis(μ -3,3',5,5'-tetramethyl-4,4'-bipyrazole- $\kappa^2\text{N:N}'$)cobalt(II)] dinitrate]

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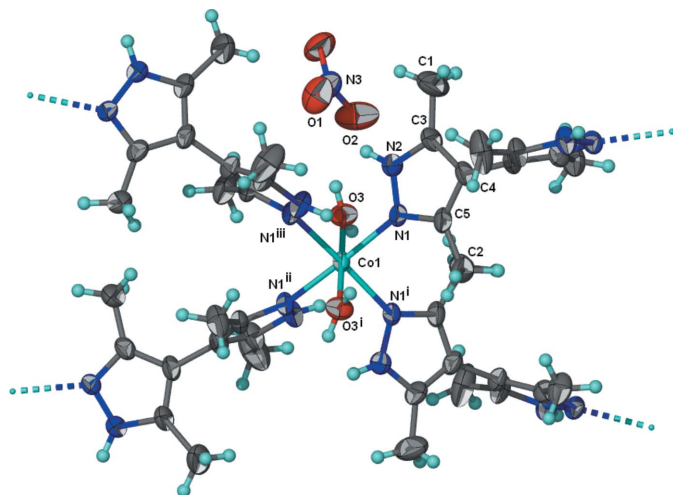
The Co atom in the title compound, $[\text{Co}(\text{C}_{10}\text{H}_{14}\text{N}_4)_2(\text{H}_2\text{O})_2](\text{NO}_3)_2$, is six-coordinate in a *trans*- N_4O_2 octahedral geometry as a consequence of bridging by the bipyrazole ligand; the bridging leads to the formation of a polycationic layer. The layers interact with the anions through hydrogen bonds, generating a three-dimensional hydrogen-bonded network. The structure is porous as 33.4% of its unit-cell volume is empty space. The Co atom lies on a special position of site symmetry 222, the bipyrazole ligand lies on a special position of site symmetry 2, the water molecule on another special position of site symmetry 2, and the nitrate anion on a special position of site symmetry *m*.

Comment

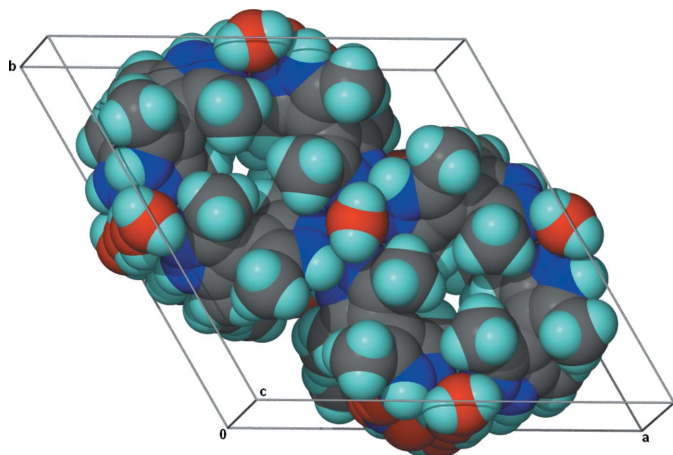
3,3',5,5'-Tetramethyl-4,4'-bipyrazole (Boldog, Rusanov *et al.*, 2003; Boldog, Sieler & Domasevitch, 2003) is an example of an *N*-heterocycle that has been used for the synthesis of coordination compounds for a long time (Usón *et al.*, 1982). The crystal structures of these compounds were determined only recently. They include the cadmium (Boldog *et al.*, 2001b; Boldog, Rusanov *et al.*, 2003; Boldog, Sieler & Domasevitch, 2003), cobalt (Boldog *et al.*, 2001a; Ponomarova *et al.*, 2002), copper (Boldog *et al.*, 2001b; He *et al.*, 2006; Komarchuk *et al.*, 2004; Kruger *et al.*, 2000), nickel (Kruger *et al.*, 1992; Ponomarova *et al.*, 2002), palladium (Yu *et al.*, 2005; Zhang *et al.*, 2004), silver (Boldog *et al.*, 2001b; Domasevitch *et al.*, 2005) and tungsten (Tang *et al.*, 2004) complexes. The 1:2 cobalt(II) dithionate adduct is a porous compound with 29% of its unit-cell volume as voids; the Co atom is covalently bonded to the dithionate units in an octahedral geometry. The zinc and cadmium analogs are isostructural (Rusanov *et al.*, 2003).



The title compound, (I), a 1:2 cobalt(II) dinitrate adduct, crystallizes with two coordinated water molecules; the anions


Figure 1

A portion of the layer structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radii. Symmetry codes are as given in Table 1.


Figure 2

A space-filling plot of the cationic layer structure, viewed along the *c* axis. The anions are not shown.

are not involved in coordination (Fig. 1). The metal atom is coordinated by the N atoms of four 3,3',5,5'-tetramethyl-4,4'-bipyrazole ligands, forming a square. The octahedron has the water molecules occupying *trans* positions. The Co atom lies on a special position of site symmetry 222, the bipyrazole ligand lies on a special position of site symmetry 2, the water molecule on another special position of site symmetry 2, and the nitrate anion on a special position of site symmetry *m*. The bridging nature of the ligand leads to the formation of a layer (Fig. 2); the anions are located between the layers and they interact through hydrogen bonds (Table 2). The structure is porous as 33.4% of it, as calculated by *PLATON* (Spek, 2003), is void space.

Experimental

3,3',5,5'-Tetramethyl-4,4'-bipyrazole (0.38 g, 2 mmol) and cobalt dinitrate hexahydrate (0.29 g, 1 mmol) were reacted in acetone (15 ml) to yield a deep-purple precipitate that was collected by

filtration. The compound was purified by recrystallization from acetonitrile, yielding block-shaped crystals.

Crystal data

[Co(C₁₀H₁₄N₄)₂(H₂O)₂](NO₃)₂
M_r = 599.49
 Hexagonal, *P6/mcc*
a = 19.922 (3) Å
c = 16.226 (2) Å
V = 5577.1 (9) Å³
Z = 6

D_x = 1.071 Mg m⁻³
 Mo *K*α radiation
 μ = 0.51 mm⁻¹
T = 295 (2) K
 Block, purple
 0.32 × 0.25 × 0.22 mm

Data collection

Bruker APEX2 area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.855, *T_{max}* = 0.897

26157 measured reflections
 1716 independent reflections
 996 reflections with *I* > 2σ(*I*)
R_{int} = 0.110
 θ_{max} = 25.0°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.051
wR(*F*²) = 0.169
S = 1.03
 1716 reflections
 96 parameters

H-atom parameters constrained
w = 1/[σ²(*F_o*²) + (0.101*P*)²]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 1.01 e Å⁻³
 Δρ_{min} = -0.60 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—O3	2.099 (4)	Co1—N1	2.151 (2)
O3—Co1—O3 ⁱ	180	O3—Co1—N1 ⁱⁱⁱ	92.3 (1)
O3—Co1—N1	87.7 (1)	N1—Co1—N1 ⁱⁱ	175.4 (1)
O3—Co1—N1 ⁱⁱ	87.7 (1)	N1—Co1—N1 ⁱ	96.0 (1)
O3—Co1—N1 ⁱ	92.3 (1)	N1—Co1—N1 ⁱⁱⁱ	84.2 (1)

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O3—H3 <i>o</i> ...O2	0.82	2.10	2.727 (4)	134
N2—H2 <i>n</i> ...O1	0.86	2.15	2.970 (4)	160

H atoms were positioned geometrically and included in the refinement in the riding-model approximation, with C—H = 0.96 Å, N—H = 0.86 Å and O—H = 0.82 Å, and with *U*_{iso}(H) values set at 1.2 or 1.5 (water O) times *U*_{eq}(C,N,O). The methyl groups were rotated to fit the electron density. The final difference Fourier map had a large peak that is not close to any atom. Attempts to refine this peak as a water O atom led to very high displacement parameters. A search for solvent-accessible voids in the crystal structure using *PLATON* (Spek, 2003) showed a potential solvent volume of 1228 Å³ showed only one relevant void around (0, 0, -0.02) with a solvent-accessible volume of 1209 Å³, with eight electrons in the void.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2006).

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