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## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.044  
 $wR$  factor = 0.119  
Data-to-parameter ratio = 14.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Aqua(2,9-dimethyl-1,10-phenanthroline- $\kappa^2N,N'$ )-dinitratocobalt(II)

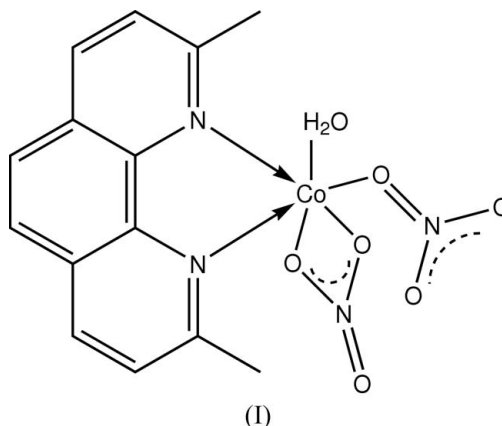
In the title compound,  $[\text{Co}(\text{NO}_3)_2(\text{C}_{14}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})]$ , the  $\text{Co}^{\text{II}}$  atom is coordinated by a bidentate 2,9-dimethyl-1,10-phenanthroline ligand, two nitrate ligands and one water molecule in a distorted octahedral environment. One of the nitrate ligands chelates in a bidentate manner and the other is monodentate. The molecule is stabilized by  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds involving water molecules and by  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds to form a two-dimensional network. The packing is further stabilized by  $\pi-\pi$  interactions.

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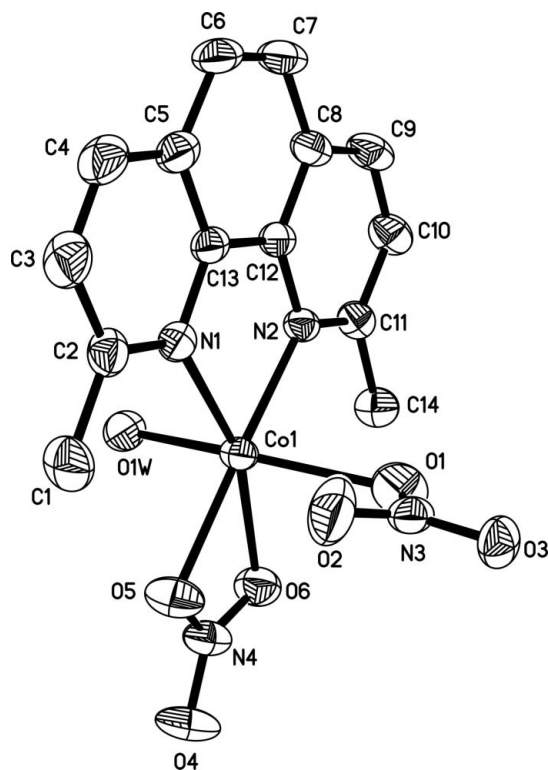
## Comment

Metal-phenanthroline complexes are good indicators for hybridization detection in DNA electrochemical biosensors (Wang *et al.*, 1996). In our search for new indicators (Zhang *et al.*, 2005), the title complex, (I), was synthesized.

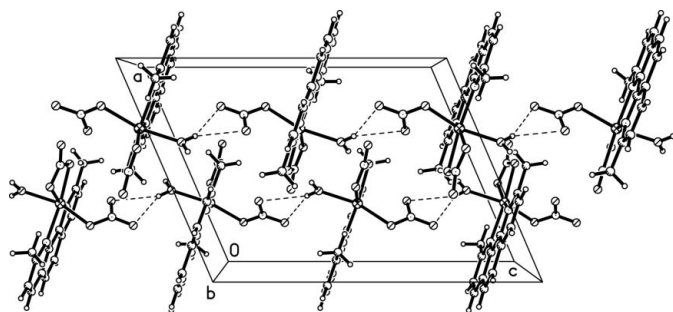


The structure of (I) consists of a  $\text{Co}^{\text{II}}$  atom coordinated by a bidentate  $N,N'$ -9,10-dimethyl-1,10-phenanthroline ligand, one bidentate and one monodentate nitrate anion and one water molecule in a distorted octahedral environment (Fig. 1). The water and  $\text{N}3/\text{O}1/\text{O}2/\text{O}3$  ligands occupy the axial positions, with an  $\text{O}1\text{W}-\text{Co}1-\text{O}1$  bond angle of  $151.2(1)^\circ$ . All the bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

There are two intramolecular  $\text{C}1-\text{H}1\text{A}\cdots\text{O}5$  and  $\text{C}14-\text{H}14\text{A}\cdots\text{O}6$  hydrogen bonds, forming two six-membered rings. In the crystal structure of (I), the water molecules act as donors to form  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2). These hydrogen bonds involving the nitrate anions link the molecules into chains along the  $c$  axis (Fig. 2). These chains are connected into a three-dimensional framework by other  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2). The short  $\text{Cg}5\cdots\text{Cg}5^i$  distance of  $3.564\text{ \AA}$  [ $\text{Cg}5$  is the centroid of the  $\text{C}5-$



**Figure 1**  
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted.



**Figure 2**  
A view of the crystal structure of (I), down the *b* axis, showing the chains. Intermolecular hydrogen bonds are denoted by dashed lines.

C8/C12/C13 ring; symmetry code: (i)  $-x, -y, 1 - z$ ] indicates  $\pi$ - $\pi$  stacking interactions between the phenanthroline ring systems.

## Experimental

To a solution of 2,9-dimethyl-1,10-phenanthroline (0.21 g, 1 mmol) in ethanol (10 ml) was added a solution of  $\text{Co}(\text{NO}_3)_2$  (0.12 g, 1 mmol) in distilled water (10 ml). The mixture was stirred and then refluxed for 9 h. The hot solution was then filtered into another flask containing ethanol-water (1:2 v/v). Brown crystals of (I) appeared over a period of one week by slow evaporation at room temperature (0.30 g, yield 75%).

## Crystal data

$[\text{Co}(\text{NO}_3)_2(\text{C}_{14}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})]$   
 $M_r = 409.22$   
 Monoclinic,  $P2_1/c$   
 $a = 11.1392$  (10) Å  
 $b = 10.8081$  (10) Å  
 $c = 15.0542$  (10) Å  
 $\beta = 113.287$  (5)°  
 $V = 1664.8$  (2) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.633$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 1.08$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Plate, brown  
 $0.28 \times 0.20 \times 0.08$  mm

## Data collection

Siemens SMART 1000 CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.752$ ,  $T_{\max} = 0.918$

9118 measured reflections  
 3287 independent reflections  
 2650 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$   
 $\theta_{\max} = 26.0^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.119$   
 $S = 1.03$   
 3287 reflections  
 235 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.3288P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.40$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.30$  e Å<sup>-3</sup>

**Table 1**  
Selected bond lengths (Å).

Co1—O1W	2.067 (2)	Co1—O5	2.130 (2)
Co1—N1	2.112 (2)	Co1—O1	2.211 (3)
Co1—N2	2.124 (2)	Co1—O6	2.309 (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>
O1W—H1W1...O2 <sup>i</sup>	0.82	2.49	3.096 (5)	132
O1W—H1W1...O3 <sup>l</sup>	0.82	2.06	2.825 (3)	155
O1W—H2W1...O4 <sup>ii</sup>	0.82	2.09	2.777 (4)	140
C1—H1A...O5	0.96	2.12	3.071 (4)	173
C7—H7A...O4 <sup>iii</sup>	0.93	2.54	3.418 (5)	158
C14—H14A...O6	0.96	2.38	3.333 (4)	172

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

Carbon-bound H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$  where  $x = 1.5$  for methyl H or 1.2 for aromatic H atoms. The water H atoms were located in a difference map and refined as riding, with O—H = 0.82 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ .

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); 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, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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