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shangao67@yahoo.com**Key indicators**Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$   
 $R$  factor = 0.031  
 $wR$  factor = 0.083  
Data-to-parameter ratio = 14.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**Diaqua(nitrato- $\kappa^2\text{O},\text{O}'$ )bis(4-pyridone- $\kappa\text{O}$ )-cobalt(II) nitrate**

In the title complex,  $[\text{Co}(\text{NO}_3)(\text{C}_5\text{H}_5\text{NO})_2(\text{H}_2\text{O})_2](\text{NO}_3)$ , the Co atom exists in an octahedral environment, defined by four O atoms of two 4-pyridone ligands and a chelating nitrate ion, as well as two water molecules. The Co atom and two nitrate ions lie on special positions with twofold rotation symmetry. A three-dimensional network structure is formed by intermolecular hydrogen bonds and  $\pi$ - $\pi$  interactions.

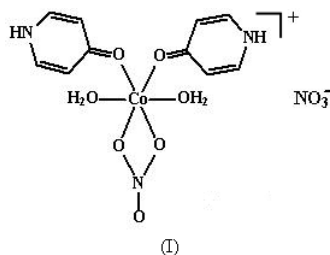
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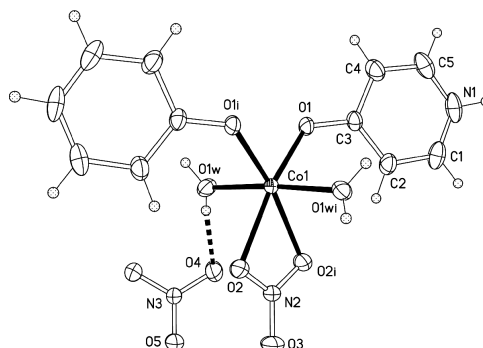
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**Comment**

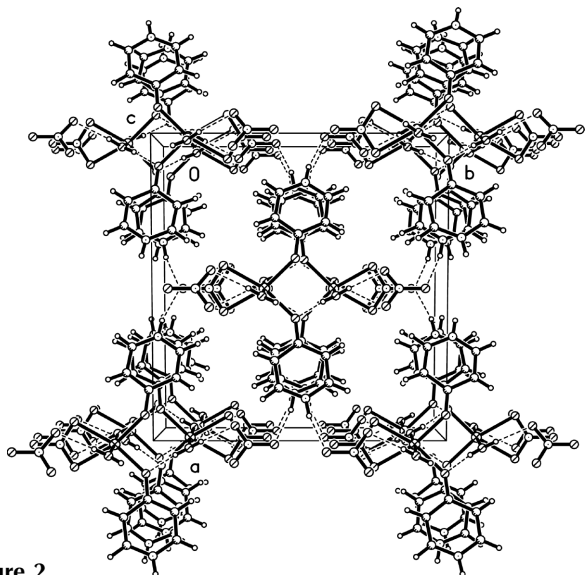
4-Hydroxypyridine has been widely used in pharmaceutical synthesis. However, the reported crystal structures of metal complexes with 4-hydroxypyridine or its tautomer, 4-pyridone, are rare (LaliaKantouri, 1996; Masse & Le Fur, 1998). Recently, we reported the structure of a complex,  $[\text{CoCl}_2(\text{C}_5\text{H}_5\text{ON})_2]$ , in which the Co atom shows a tetrahedral geometry (Gao *et al.*, 2004). In order to explore the effects of the counter-ions on the coordination geometry of the metal center, we used  $\text{Co}(\text{NO}_3)_2$  hexahydrate instead of  $\text{CoCl}_2$  hexahydrate in the reaction and synthesized a novel cobalt complex,  $[\text{Co}(\text{NO}_3)(\text{C}_5\text{H}_5\text{NO})_2(\text{H}_2\text{O})_2](\text{NO}_3)$ , (I), the crystal structure of which is reported here.



As shown in Fig. 1, the crystal structure of (I) consists of a  $[\text{Co}(\text{NO}_3)(\text{C}_5\text{H}_5\text{NO})_2(\text{H}_2\text{O})_2]^+$  cation and an  $\text{NO}_3^-$  anion. The uncoordinated  $\text{NO}_3^-$  anion forms an intermolecular hydrogen



**Figure 1**  
*ORTEP* (Johnson, 1976) plot of (I), shown with 50% probability ellipsoids. [Symmetry code as in Table 1.]



**Figure 2**  
Packing diagram of (I).

bond with a water molecule, with an O···O distance and O—H···O angle of 2.806 (2) Å and 166 (2)°, respectively. The Co atom and two nitrate ions lie on crystallographic twofold rotation axes. The Co atom has a slightly distorted octahedral geometry. Its equatorial plane is defined by two nitrate O atoms [Co—O = 2.193 (1) Å] and two carbonyl O atoms of 4-pyridone ligands [Co—O = 2.035 (1) Å], while the axial sites are occupied by two water molecules [Co—O = 2.060 (1) Å and O—Co—O = 175.97 (8)°]. The C1—C2, C4—C5 and C3—O1 bond lengths are 1.369 (3), 1.361 (3) and 1.287 (2) Å, respectively (Table 1). The dihedral angle between the planes of the coordinated nitrate ion and the pyridone ring is 28.26 (8)°. Individual molecules are stacked in an offset manner along the *c* direction through  $\pi$ – $\pi$  interactions of adjacent pyridone ligands, with a plane-to-plane separation of 3.866 (3) Å. Furthermore, O(water)—H···O(pyridone) and N(pyridone)—H···O(nitrate) intermolecular hydrogen bonds lead to a three-dimensional network (Table 2 and Fig. 2).

## Experimental

The title complex, (I), was synthesized by the addition of Co(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (1 mmol) to an ethanol solution of 4-hydroxypyridine (3 mmol). The mixed solution was allowed to evaporate at room temperature and pink prismatic crystals of (I) were isolated from the solution after about 7 d. Analysis calculated for C<sub>10</sub>H<sub>14</sub>CoN<sub>4</sub>O<sub>10</sub>: C 29.35, H 3.45, N 13.69%; found: C 29.53, H 3.38, N 13.55%.

### Crystal data

[Co(NO <sub>3</sub> )(C <sub>5</sub> H <sub>5</sub> NO) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ](NO <sub>3</sub> )	$D_x = 1.684 \text{ Mg m}^{-3}$
$M_r = 409.18$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 2419 reflections
$a = 14.842$ (3) Å	$\theta = 4.4$ – $27.5^\circ$
$b = 14.166$ (3) Å	$\mu = 1.13 \text{ mm}^{-1}$
$c = 7.721$ (2) Å	$T = 293$ (2) K
$\beta = 96.23$ (3)°	Prism, pink
$V = 1613.8$ (6) Å <sup>3</sup>	$0.38 \times 0.25 \times 0.18 \text{ mm}$
$Z = 4$	

### Data collection

Rigaku R-Axis RAPID diffractometer	1838 independent reflections
$\omega$ scans	1710 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{\text{int}} = 0.027$
$T_{\text{min}} = 0.674$ , $T_{\text{max}} = 0.823$	$\theta_{\text{max}} = 27.5^\circ$
7588 measured reflections	$h = -19 \rightarrow 19$
	$k = -18 \rightarrow 14$
	$l = -9 \rightarrow 10$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 1.1983P]$
$R[F^2 > 2\sigma(F^2)] = 0.031$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.083$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.61 \text{ e \AA}^{-3}$
1838 reflections	$\Delta\rho_{\text{min}} = -0.43 \text{ e \AA}^{-3}$
125 parameters	
H atoms treated by a mixture of independent and constrained refinement	

### Table 1

Selected geometric parameters (Å, °).

Co1—O1	2.035 (1)	O1—C3	1.287 (2)
Co1—O1W	2.060 (1)	C1—C2	1.369 (3)
Co1—O2	2.193 (1)	C4—C5	1.361 (3)
O1W—Co1—O1W <sup>i</sup>	175.97 (8)	O1—Co1—O1W <sup>i</sup>	91.58 (6)
O1W—Co1—O2	84.97 (6)	O1—Co1—O2 <sup>i</sup>	106.08 (5)
O1—Co1—O1 <sup>i</sup>	89.40 (8)	O1—Co1—O2	164.14 (6)
O1—Co1—O1W	91.28 (6)		

Symmetry code: (i)  $1 - x, y, \frac{1}{2} - z$ .

### Table 2

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W2···O1 <sup>ii</sup>	0.85 (2)	1.88 (3)	2.722 (2)	175 (3)
O1W—H1W1···O4	0.84 (2)	1.98 (3)	2.806 (2)	166 (2)
N1—H6···O5 <sup>iii</sup>	0.90 (3)	2.10 (3)	2.974 (2)	166 (3)

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

C-bound H atoms were placed in calculated positions [C—H = 0.93 Å (aromatic) and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ ] in the riding-model approximation. H atoms on nitrogen and of water were located in difference Fourier synthesis maps and refined with N—H, O—H and H···H distance restraints of 0.90 (1), 0.85 (1) and 1.39 (1) Å, respectively, and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N}, \text{O})$ .

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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