

## Hong-Yin He and Long-Guan Zhu\*

Department of Chemistry, Zhejiang University,  
Hangzhou 310027, People's Republic of China

Correspondence e-mail: chezlg@zju.edu.cn

## Key indicators

Single-crystal X-ray study

T = 293 K

Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ 

R factor = 0.041

wR factor = 0.078

Data-to-parameter ratio = 11.6

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.***trans*-Bis(3-aminopyridine)diaquabis-(4-cyanobenzoato)cobalt(II) dihydrate**

The reaction of cobalt(II) acetate with 4-cyanobenzoic acid and 3-aminopyridine gave the title centrosymmetric complex,  $[\text{Co}(\text{C}_8\text{H}_4\text{NO}_2)_2(\text{C}_5\text{H}_6\text{N}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$ . The coordination geometry around the  $\text{Co}^{\text{II}}$  ion is distorted octahedral, and the 4-cyanobenzoate and 3-aminopyridine ligands act in a monodentate fashion. The hydrogen bonds among the water molecules and cyano and amino groups ensure a two-dimensional hydrogen-bonding architecture.

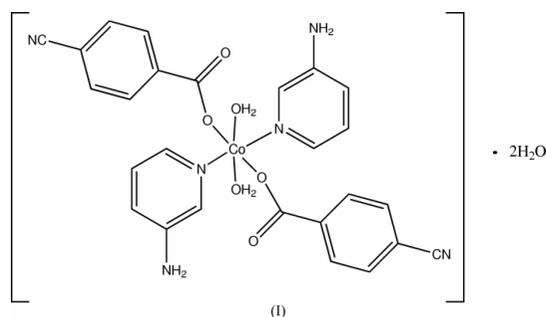
Received 14 November 2003

Accepted 20 November 2003

Online 29 November 2003

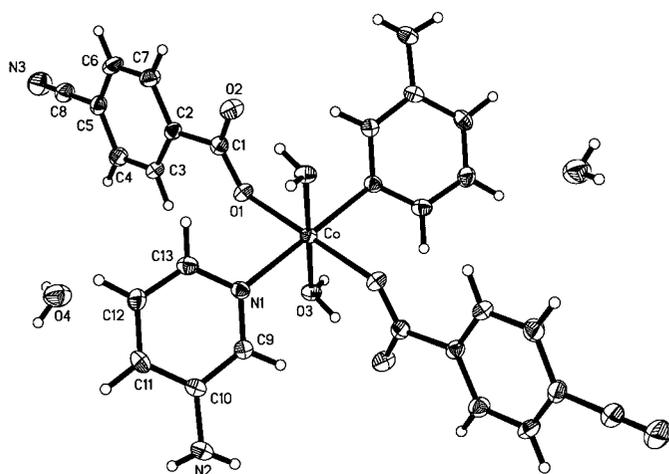
## Comment

The amino group of 3-aminopyridine (apy), in general, is difficult to coordinate to metal atoms (Akyuz, 1998; Kamaluddin, 2000); nevertheless, the amine group could provide a donor site for the formation of hydrogen bonds. In the present paper, we report the crystal structure of the title compound, (I), which contains apy and 4-cyanobenzoate (cba) ligands, both of which are building blocks for hydrogen bonds.

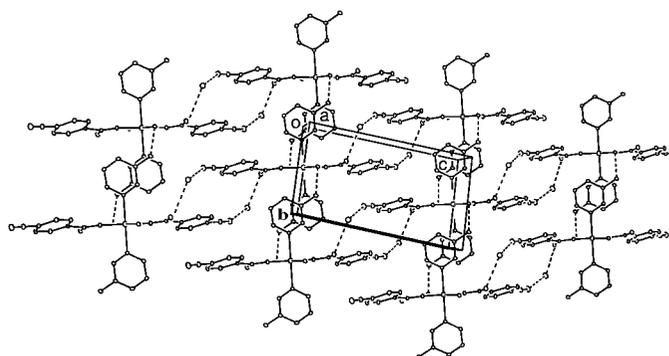


Complex (I) is monomeric and has a center of symmetry (Fig. 1). The geometry of the cobalt ion is distorted octahedral (Table 1). The carboxy group of the cba ligand coordinates in a monodentate mode, similar to those in  $[\text{Cu}(4,4'\text{-bipy})(\text{cba})_2]_n$  (He & Zhu, 2003),  $[\text{Co}(4,4'\text{-bipy})(\text{cba})_2(\text{H}_2\text{O})_2]_n$  (He *et al.*, 2003) and  $[\text{Cu}(\text{phen})(\text{H}_2\text{O})\text{Cl}(\text{cba})] \cdot \text{H}_2\text{O}$  (Zhou *et al.*, 2003). The  $\text{Co}-\text{O1}(\text{cba})$  distance [2.0777 (14)  $\text{\AA}$ ] is similar to that reported for  $[\text{Co}(4,4'\text{-bipy})(\text{cba})_2(\text{H}_2\text{O})_2]_2$  [2.0792 (12)  $\text{\AA}$ ].

The cyano group of the cba ligand forms a hydrogen bond with atom O4 (Table 2). Furthermore, there is a hydrogen bond between atoms O4 and O2 (the uncoordinated O atom of the carboxy group). Thus the  $\{[\text{Co}(\text{cba})_2](\text{H}_2\text{O})_2\}$  units form a one-dimensional chain *via* hydrogen bonds, in which a hydrogen-bonding  $[(\text{cba})_2(\text{H}_2\text{O})_2]$  loop is formed (Fig. 2). The amine group forms a hydrogen bond with atom O3 (of the coordinated water molecule). The combination of  $[\text{Co}(\text{apy})_2(\text{H}_2\text{O})_2]^{2+}$  and  $\{[\text{Co}(\text{cba})_2](\text{H}_2\text{O})_2\}$  units creates a two-dimensional hydrogen-bonded architecture (Fig. 2).



**Figure 1**  
ORTEP-3 diagram (Farrugia, 1997) of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. The labeled part of the molecule is related to the unlabeled part by the symmetry operation  $(-x, 1 - y, 2 - z)$ .



**Figure 2**  
View of the two-dimensional hydrogen-bonding network. H atoms have been omitted for clarity.

## Experimental

A methanol solution (20 ml) of  $\text{Co}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$  (0.0624 g, 0.25 mmol) was added to an aqueous solution (10 ml) of 4-cyanobenzoic acid (0.0757 g, 0.5 mmol) and 3-aminopyridine (0.0481 g, 0.5 mmol). After the mixture had been allowed to stand for three weeks at room temperature, purple crystals of (I) were obtained and dried at room temperature. Analysis calculated for  $\text{C}_{26}\text{H}_{28}\text{CoN}_6\text{O}_8$ : C 51.07, H 4.62, N 13.74%; found: C 51.13, H 4.67, N 13.82%.

### Crystal data

$[\text{Co}(\text{C}_8\text{H}_4\text{NO}_2)_2(\text{C}_5\text{H}_6\text{N}_2)_2 \cdot (\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$   
 $M_r = 611.47$   
 Triclinic,  $P\bar{1}$   
 $a = 7.2359$  (11) Å  
 $b = 7.7367$  (11) Å  
 $c = 13.2036$  (19) Å  
 $\alpha = 82.309$  (3)°  
 $\beta = 76.268$  (3)°  
 $\gamma = 72.365$  (2)°  
 $V = 682.76$  (17) Å<sup>3</sup>

$Z = 1$   
 $D_x = 1.487$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 1267 reflections  
 $\theta = 5.5\text{--}52.1^\circ$   
 $\mu = 0.69$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Plate, purple  
 $0.30 \times 0.15 \times 0.07$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1997)  
 $T_{\min} = 0.805$ ,  $T_{\max} = 0.960$   
 3999 measured reflections

2824 independent reflections  
 2360 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$   
 $\theta_{\max} = 26.8^\circ$   
 $h = -9 \rightarrow 9$   
 $k = -9 \rightarrow 9$   
 $l = -16 \rightarrow 8$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.078$   
 $S = 0.94$   
 2824 reflections  
 243 parameters

All H-atom parameters refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0241P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.46$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.28$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Co—O1	2.0777 (14)	Co—N1	2.1646 (17)
Co—O3	2.1202 (16)		
O1—Co—O3	89.44 (7)	O3—Co—N1	89.01 (7)
O1—Co—N1	87.02 (6)		

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D\text{—}H \cdots A$	$D\text{—}H$	$H \cdots A$	$D \cdots A$	$D\text{—}H \cdots A$
O3—H11 <sup>i</sup> ···O2 <sup>i</sup>	0.88 (3)	1.81 (3)	2.672 (2)	165 (3)
O3—H12 <sup>ii</sup> ···N2 <sup>ii</sup>	0.81 (3)	2.07 (3)	2.871 (3)	169 (2)
O4—H13 <sup>iii</sup> ···N3 <sup>iii</sup>	0.81 (3)	2.22 (4)	3.021 (4)	172 (3)
O4—H14 <sup>iv</sup> ···O2 <sup>iv</sup>	0.79 (4)	2.15 (4)	2.931 (3)	168 (4)

Symmetry codes: (i)  $-x, 1 - y, 2 - z$ ; (ii)  $x, 1 + y, z$ ; (iii)  $2 - x, 1 - y, 1 - z$ ; (iv)  $1 + x, y - 1, z$ .

All H atoms were located from difference Fourier maps and refined isotropically. The C—H, N—H and O—H bond lengths are 0.91 (2)–0.97 (2), 0.85 (2)–0.86 (3) and 0.79 (4)–0.88 (3) Å, respectively.

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SAINT and SHELXTL (Bruker, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

The project was supported by the National Natural Science Foundation of China (grant No. 50073019).

## References

- Akyuz, S. (1998). *J. Mol. Struct.* **449**, 23–27.  
 Bruker (1997). SMART (Version 5.044), SAINT (Version 5.01) and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.  
 He, H.-Y., Ma, A.-Q. & Zhu, L.-G. (2003). *Acta Cryst. E59*, m333–m335.  
 He, H.-Y. & Zhu, L.-G. (2003). *Acta Cryst. E59*, o174–o176.  
 Kamaluddin, A. T. (2000). *Colloids Surf. A*, **162**, 89–97.  
 Sheldrick, G. M. (1997). SADABS, SHELXL97 and SHELXS97. University of Göttingen, Germany.  
 Zhou, Y.-L., He, H.-Y., Zhang, Y. & Zhu, L.-G. (2003). *Acta Cryst. E59*, m605–m607.