Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Diaqua(4,4′-bipyridine)bis(4-cyanobenzoato)cobalt(II)

**Hong-Yin He, Ai-Qing Ma 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 $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.035
$wR$ factor = 0.087
Data-to-parameter ratio = 13.5

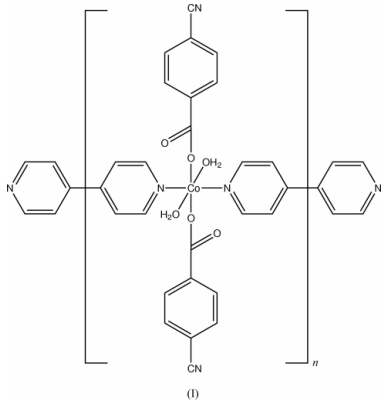
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 10 April 2003
Accepted 12 May 2003
Online 16 May 2003

In the title polymeric complex, $[Co(C_8H_4NO_2)_2(C_{10}H_8N_2)(H_2O)_2]_n$, the $Co^{II}$ atom, located on an inversion center, is surrounded by two N-donor molecules, two water molecules, and two 4-cyanobenzoate ligands, which impose an octahedral environment on the metal. 4-Cyanobenzoate, acting as a bridging linker, coordinates to the metal center in a monodentate fashion, in a skew mode. Both bridging spacers, *viz*. the 4,4′-bipyridine and 4-cyanobenzoate ligands, link adjacent metal atoms into a two-dimensional network.

## Comment

In the field of crystal engineering, 4,4′-bipyridine has been extensively used to construct novel one-, two-, and three-dimensional coordination polymers with potential applications as functional materials (Kitagawa & Kondo, 1998; Moulton & Zaworotko, 2001). The combination of 4,4′-bipyridine and carboxylic acid is largely directed toward interesting topologies (Tao *et al.*, 2002). 4–Cyanobenzoic acid (Hcba) has been used to develop new blue fluorescent materials; two crystal structures involving this ligand were recently reported (He & Zhu, 2003; Yuan *et al.*, 2001) and there are no reports of the cyano groups coordinating to a metal center or forming hydrogen bonds. Here we present the crystal structure of the $Co^{II}$ one-dimensional network of the title compound, (I), which provides an interesting example of the cyano group of Hcba as a hydrogen-bond acceptor.




(I)

The building block of the structure of (I) consists of one $Co^{II}$ atom, one 4,4′-bipyridine, two water molecules, and two cba ligands (Fig. 1). The $Co^{II}$ atom, located on an inversion center, displays an octahedral geometry. Two 4-cyanobenzoate groups and two pyridine rings of the 4,4′-bipyridine ligands are located on opposite sides to minimize repulsion between the

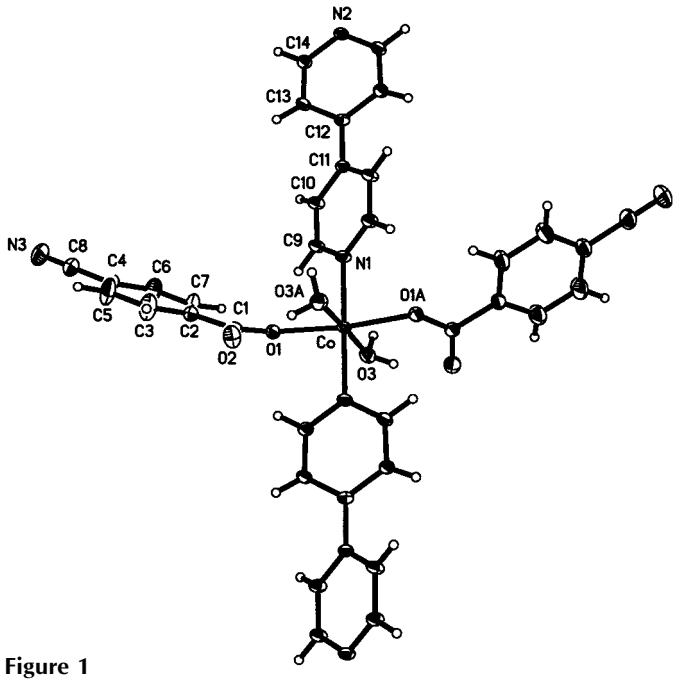



**Figure 1**
*ORTEP* diagram of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

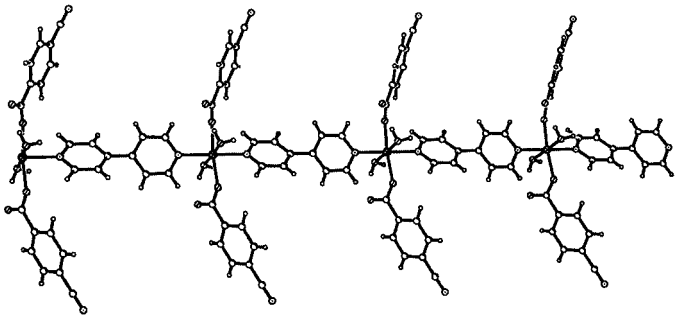


**Figure 2**
View of the one-dimensional network formed by the [$Co^{II}$(4,4′-bipyridine)] building block.

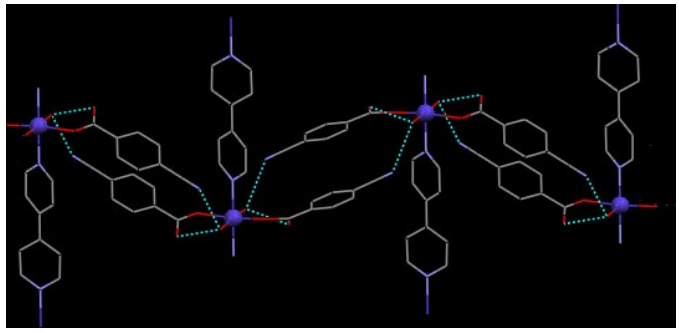


**Figure 3**
View of the one-dimensional hydrogen-bond network formed by the $[Co_2(cba)_2(H_2O)_2]$ building unit.

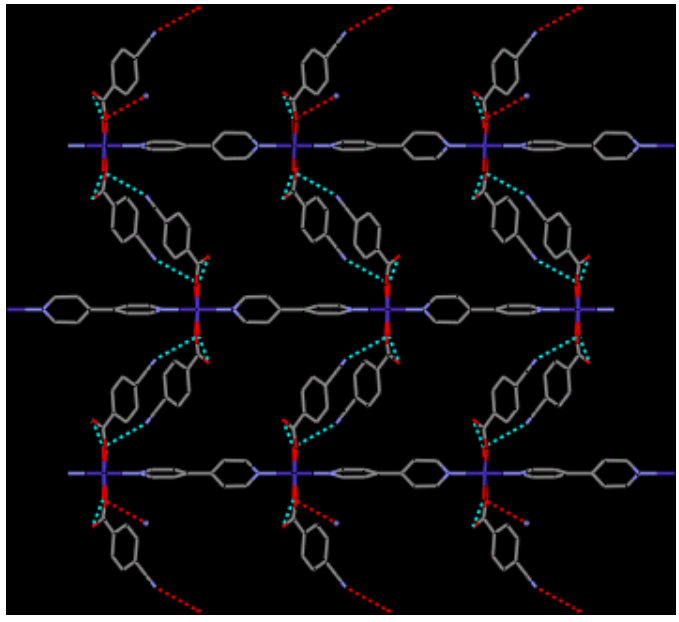


**Figure 4**
View of the two-dimensional network constructed by bridging linkers of 4,4′-bipyridine and 4-cyanobenzoate ligands.

ligands. The dihedral angle between the two rings of 4,4′-bipyridine is 30.44 (13)°, indicating a large torsion. The cobalt metal centers are linked by two bidentate 4,4′-bipyridine linear spacers, which leads to a one-dimensional chain along the *a* axis (Fig. 2). The Co—O1 bond length [2.0792 (12) Å] is shorter than that of Co—O3 [2.1548 (15) Å], indicating some distortion of the coordination geometry. The Co—N bond lengths are similar to those of other $Co^{II}$ complexes with a 4,4′-bipyridine bridging linker (Hu *et al.*, 2002). The 4-cyanobenzoate ligand is coordinated, in a monodentate fashion, in a skew mode [Co—O1—C1—C2 = 156.36 (11)°] to the cobalt center. The O—H···N hydrogen bonds between cyano groups and water molecules result in dimeric building units, *viz.* $[Co_2(cba)_2(H_2O)_2]$. Thus, the one-dimensional hydrogen-bonding network is extended by cba as a hydrogen-bonding bridging linker (Fig. 3). As expected, both cba and 4,4′-bipyridine acting as linkages create a two-dimensional framework, with a Co···Co distance for the cba linkage of 11.983 (2) Å and a Co···Co separation for the 4,4′-bipyridine linkage of 11.379 (2) Å (Fig. 4).

## Experimental

Crystals were grown by the layer method, using two solutions in a narrow tube with a diameter of 0.8 cm. The upper solution was 10 ml methanol containing 0.05 mol $l^{-1}$ 4-cyanbenzoic acid and 0.025 mol $l^{-1}$ 4,4′-bipyridine. The lower solution was 5 ml 0.05 mol $l^{-1}$ $Co(CH_3COO)_2{\cdot}4H_2O$ in water. After standing for two weeks, purple needle crystals of (I) were obtained and filtered off.

*Crystal data*

$[Co(C_8H_4NO_2)_2(C_{10}H_8N_2)(H_2O)_2]$
$M_r$ = 543.39
Monoclinic, *C*2/*c*
*a* = 10.8329 (9) Å
*b* = 11.3792 (9) Å
*c* = 19.7327 (16) Å
β = 97.662 (2)°
*V* = 2410.7 (3) Å$^3$
*Z* = 4
$D_x$ = 1.497 Mg m$^{-3}$
Mo *Kα* radiation
Cell parameters from 2702 reflections
θ = 5.2–55.6°
μ = 0.76 mm$^{-1}$
*T* = 293 (2) K
Block, purple
0.32 × 0.30 × 0.27 mm

*Data collection*

Bruker CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.605, $T_{max}$ = 0.815
7278 measured reflections
2830 independent reflections
2266 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029
$\theta_{max}$ = 28.2°
$h = -14 \rightarrow 14$
$k = -14 \rightarrow 14$
$l = -25 \rightarrow 18$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.087
$S$ = 1.00
2830 reflections
210 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0450P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å).

| | | | |
|---|---|---|---|
| Co—O1 | 2.0792 (12) | Co—N2$^{i}$ | 2.1517 (18) |
| Co—N1 | 2.1440 (18) | Co—O3 | 2.1548 (15) |

Symmetry code: (i) $x, 1 + y, z$.

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H10···O2$^{ii}$ | 0.82 (2) | 1.83 (3) | 2.620 (2) | 161 (2) |
| O3—H9···N3$^{iii}$ | 0.80 (3) | 2.15 (3) | 2.938 (2) | 167 (3) |

Symmetry codes: (ii) $-x, y, \frac{1}{2} - z$; (iii) $x - \frac{1}{2}, \frac{3}{2} - y, z - \frac{1}{2}$.

All H atoms were found in a difference Fourier map and refined isotropically.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We thank the National Natural Science Foundation of China for supporting this work (No. 50073019).

## References

Bruker (1997). *SMART* (Version 5.044), *SAINT* (Version 5.01) and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
He, H. Y. & Zhu, L. G. (2003). *Acta Cryst.* E**59**, o174–o176.
Hu, C. W., Wang, Y. H., Feng, L. Y., Li, Y. G., Wang, E. B., Hu, N. H. & Jia, H. G. (2002). *Inorg. Chem.* **41**, 6351–6357.
Kitagawa, S. & Kondo, M. (1998). *Bull. Chem. Soc. Jpn*, **71**, 1739–1753.
Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen,Germany.
Sheldrick, G. M. (1997). *SHELXL*97, *SHELXS*97 and *SHELXP*97. University of Göttingen, Germany.
Tao, J., Yin, X., Huang, R. B. & Zheng, L. S. (2002). *Inorg. Chem. Commun.* **5**, 1000–1002.
Yuan, R. X., Xiong, R. G., Chen, Z. F., You, X. Z., Peng, S. M. & Lee, G. H. (2001). *Inorg. Chem. Commun.* **4**, 430–433.