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μ-4,4′-Bipyridine-κ^2N:N'-bis[triaqua(pyridine-2,4-dicarboxylato-κ^2N,O)cobalt(II)] dihydrate

Xian-Ming Zhang

School of Chemistry and Material Science,
Shanxi Normal University, Linfen 041004,
People's Republic of China

Correspondence e-mail:
zhangxm@dns.sxtu.edu.cn

The title centrosymmetric dinuclear complex, $[Co_2(C_7H_3NO_4)_2(C_{10}H_8N_2)(H_2O)_6]\cdot 2H_2O$, has been synthesized hydrothermally. The cobalt(II) ion is coordinated in a slightly distorted octahedral environment by one N atom and one carboxylate O atom in *N*,*O*-chelating mode from one 2,4-pyridinedicarboxylate ligand, by one N atom from 4,4′-bipyridine, and by three water molecules. O—H···O hydrogen bonds link molecules into a three-dimensional framework.

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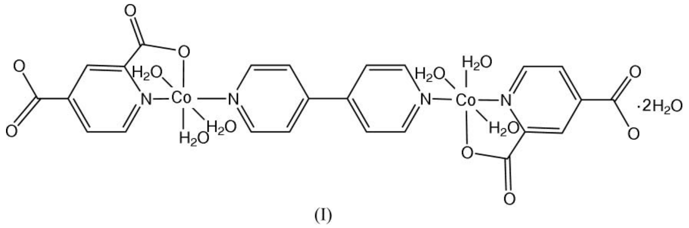
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.052
wR factor = 0.145
Data-to-parameter ratio = 12.8

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

Comment

Recently, the author and other groups have been exploiting the chelate and bridging pyridine-2,4-dicarboxylate ligand for coordination polymers and organic–inorganic hybrid compounds because of its flexible and varied coordination modes (Zhang & Chen, 2003; Zhang, 2005; Noro *et al.*, 2002; Liang *et al.*, 2002; Gerrard & Wood, 2000). The hydrothermal reaction of a copper salt, pyridine-2,4-dicarboxylate and 4,4′-bipyridine generated the porous mixed-valence copper(I,II) coordination polymer *catena*-[bis[(μ_2-4,4′-bipyridyl)(μ_2-pyridine-2,4-dicarboxylato-*N*,*O*,*O*′)]tricopper(I,II) tetrahydrate], which contains 'metal complex ligands' and is a three-dimensional framework constructed from fivefold parallel intertwining of two-dimensional (6,3)-nets (Zhang & Chen, 2003). Substitution of a cobalt salt for the copper salt resulted in the neutral dinuclear title complex, (I).



(I)

Compound (I) (Fig. 1) crystallizes in triclinic space group $P\overline{1}$ about an inversion center, and the asymmetric unit consists of one crystallographically independent cobalt(II) ion, one 2,4-pyridinedicarboxylate molecule, one-half of a 4,4′-bipyridyl (bipy) group, three coordinated water molecules and one solvent water molecule. All atoms reside on general positions and the inversion center is located at the mid-point of the bipy ligand. The Co^{II} ion is coordinated, in a slightly distorted octahedral environment (see Table 1), by one N atom and one carboyxlate O atom in *N*,*O*-chelate mode from one 2,4-pyridinedicarboxylate ligand, one N atom from bipy, and three water molecules. The μ_2-4,4′-bipyridine ligand bridges two [Co(2,4-pyridinedicarboxylate)(H_2O)$_3$] units to form the dinuclear molecule.

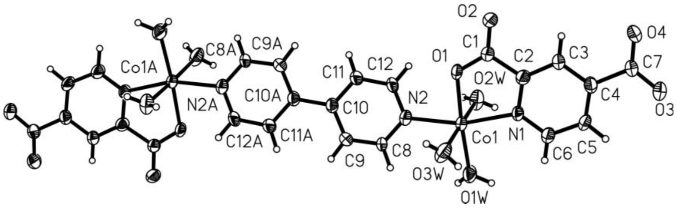


Figure 1
ORTEPII (Johnson, 1976) plot of the title compound. Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (*A*) $-x, -y, -z + 1$.]

In the crystal structure, O—H···O hydrogen bonds link the complexes and water molecules into a three-dimensional network (see Table 2 for hydrogen-bond geometries).

Experimental

A mixture of cobalt acetate tetrahydrate (0.125 g), 2,4-pyridinedicarboxylic acid (0.083 g), 4,4′-bipyridine (0.078 g) and water (7 ml) in a 1:1:1:780 molar ratio was stirred for 20 min in air, then transferred and sealed in a 15 ml Teflon-lined stainless steel container, which was heated to 433 K for 3 d. After cooling to room temperature, red needles of (I) were recovered as a single product in 65% yield. Analysis found: C 38.46, H 3.96, N 7.43%; calculated for $C_{24}H_{30}Co_2N_4O_{16}$: C 38.52, H 4.04, N 7.49%.

Crystal data

$[Co_2(C_7H_3NO_4)_2(C_{10}H_8N_2)(H_2O)_6]\cdot 2H_2O$
$M_r = 748.38$
Triclinic, $P\overline{1}$
$a = 6.413$ (1) Å
$b = 9.763$ (2) Å
$c = 12.113$ (2) Å
$\alpha = 79.54$ (3)°
$\beta = 79.26$ (3)°
$\gamma = 80.61$ (3)°
$V = 726.1$ (2) Å^3
$Z = 1$
$D_x = 1.711$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 126 reflections
$\theta = 2.6$–25°
$\mu = 1.23$ mm^{-1}
$T = 293$ (2) K
Needle, red
0.33 × 0.12 × 0.09 mm

Data collection

Bruker SMART APEX area-dector diffractometer
φ and ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.688$, $T_{max} = 0.898$
4961 measured reflections
3074 independent reflections
2285 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.2°$
$h = -8 \rightarrow 7$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.145$
$S = 1.12$
3074 reflections
241 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 0.6587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.29$ e Å^{-3}
$\Delta\rho_{min} = -0.61$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O3*W*	2.067 (3)	Co1—O2*W*	2.116 (3)
Co1—O1	2.075 (3)	Co1—N2	2.151 (3)
Co1—O1*W*	2.078 (3)	Co1—N1	2.157 (3)
O3*W*—Co1—O1	94.61 (14)	O1*W*—Co1—N2	97.01 (14)
O3*W*—Co1—O1*W*	85.80 (16)	O2*W*—Co1—N2	88.88 (14)
O1—Co1—O1*W*	175.66 (12)	O3*W*—Co1—N1	97.16 (14)
O3*W*—Co1—O2*W*	174.55 (15)	O1—Co1—N1	77.55 (11)
O1—Co1—O2*W*	90.22 (13)	O1*W*—Co1—N1	98.11 (14)
O1*W*—Co1—O2*W*	89.57 (15)	O2*W*—Co1—N1	86.34 (14)
O3*W*—Co1—N2	88.82 (14)	N2—Co1—N1	164.10 (12)
O1—Co1—N2	87.33 (12)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WB*···O4^{i}	0.74 (5)	2.07 (6)	2.791 (5)	167 (5)
O3*W*—H3*WA*···O1^{ii}	0.81 (6)	1.97 (6)	2.763 (5)	168 (6)
O3*W*—H3*WB*···O2^{iii}	0.86 (5)	1.93 (6)	2.761 (5)	163 (5)
O2*W*—H2*WA*···O3^{iv}	0.78 (6)	2.06 (6)	2.786 (5)	155 (6)
O4*W*—H4*WA*···O3^{v}	0.84 (8)	1.93 (8)	2.771 (5)	177 (8)
O2*W*—H2*WB*···O3^{vi}	0.88 (7)	1.94 (7)	2.808 (5)	172 (6)
O1*W*—H1*WA*···O4*W*^{vii}	0.89 (7)	1.81 (7)	2.695 (5)	176 (6)
O4*W*—H4*WB*···O4^{viii}	0.93 (11)	1.87 (11)	2.786 (6)	168 (9)

Symmetry codes: (i) $x+1, y-1, z$; (ii) $-x, -y, -z+1$; (iii) $x+1, y, z$; (iv) $-x, -y+1, -z$; (v) $x, y, z+1$; (vi) $x, y-1, z$; (vii) $-x+1, -y+1, -z+1$; (viii) $x+1, y, z+1$.

H atoms bonded to C atoms were placed in calculated positions (C—H = 0.93 Å) and refined in a riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms bonded to O atoms were located in Fourier maps and refined independently with isotropic displacement parameters. The highest peak in the final difference Fourier map was located 1.25 Å from Co1.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Winsonsin.
Gerrard, L. A. & Wood, P. T. (2000). *Chem. Commun.* pp. 2107–2108.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Liang, Y., Cao, C., Hong, M., Sun, D., Zhao, Y., Weng, J. & Wang, R. (2002). *Inorg. Chem. Commun.* **5**, 366–368.
Noro, S., Kitagawa, S., Yamashita, M. & Wada, T. (2002). *Chem. Commun.* pp. 222–223.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, X.-M. (2005). *Inorg. Chim. Acta*, **358**, 1865–1872.
Zhang, X.-M. & Chen, X.-M. (2003). *Eur. J. Inorg. Chem.* 413–417.