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catena-Poly[[[aqua(2,2′-bipyridine)cobalt(II)]-μ-5-nitrobenzene-1,3-dicarboxylato-κ^3O:O',O''] 0.25-hydrate]

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Key indicators

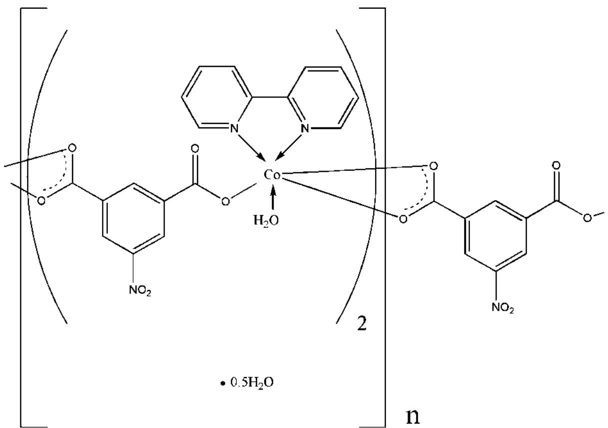
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
Disorder in solvent or counterion
R factor = 0.038
wR factor = 0.112
Data-to-parameter ratio = 12.9

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

In the title compound, $\{[Co(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]\cdot 0.25H_2O\}_n$, the coordination polyhedron of the Co^{II} ion is an octahedron. Each pair of adjacent Co^{II} ions is bridged by a dianion of 5-nitro-1,3-benzenedicarboxylic acid (H_2nmbdc) to form a chain running along the *a* axis. These chains are linked by π–π stacking interactions and O(water)—H$\cdots$O hydrogen bonds into a supramolecular structure.

Comment

The dianion of 5-nitro-1,3-benzenedicarboxylic acid (H_2nmbdc) can act as a bridging ligand in a bis-monodentate coordination mode (Xiao *et al.*, 2005) or a bis-bridging coordination mode (He *et al.*, 2004). In this paper, two carboxylate groups of the nmbdc ligand coordinate in a different mode than previously reported (Xie *et al.*, 2005).



(I)

In the title compound, (I), there are two Co^{II} atoms, two 2,2′-bipyridine molecules, two nmbdc ligands, two coordinated water molecules and a solvent water half-molecule in the asymmetric unit (Fig. 1). Each pair of adjacent Co^{II} atoms is bridged by an nmbdc ligand to form a chain running along the *a* axis. The mode of coordination of the two carboxylate groups on each nmbc ligand differs: one coordinates in a bidentate fashion and the other coordinates in a monodentate fashion. Each pair of adjacent chains is linked by π–π stacking interactions between the benzene rings and also O(water)—H$\cdots$O hydrogen bonds into double chains (Fig. 2 and Tables 2 and 3). The solvent water molecules are linked to the chains by O(water)—H$\cdots$O hydrogen bonds. In the crystal structure, there are many π–π stacking interactions involving the 2,2′-bipyridine ligands (Fig. 3). Geometric parameters for the π–π stacking interactions are listed in Table 3. The double chains are linked by these π–π stacking interactions into a supramolecular structure (Fig. 4).

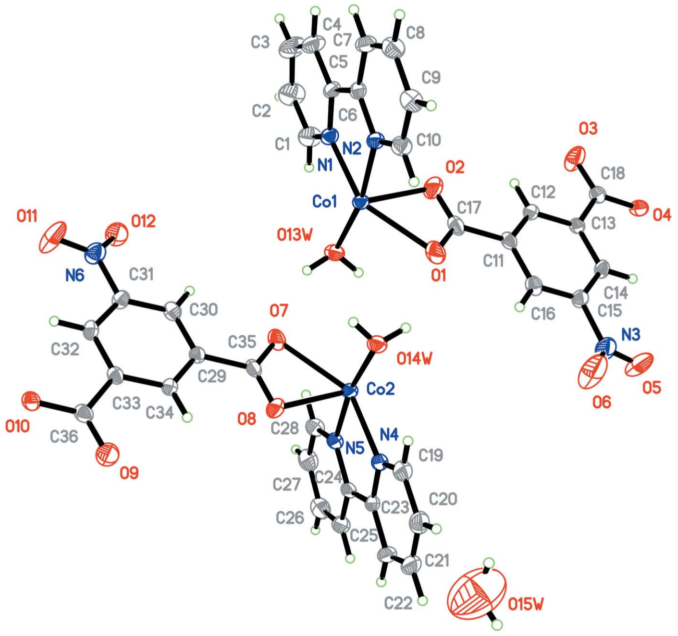


Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii.

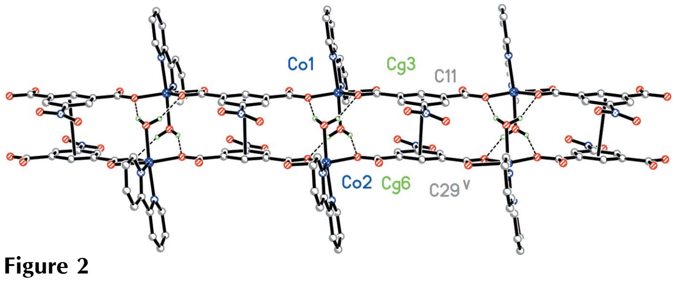


Figure 2
The double chains linked by π–π stacking interactions and hydrogen bonds along the *c* axis. For the sake of clarity, H atoms not involved in hydrogen bonding and solvent water molecules have been omitted [symmetry code: (v) $1 + x, y, z$].

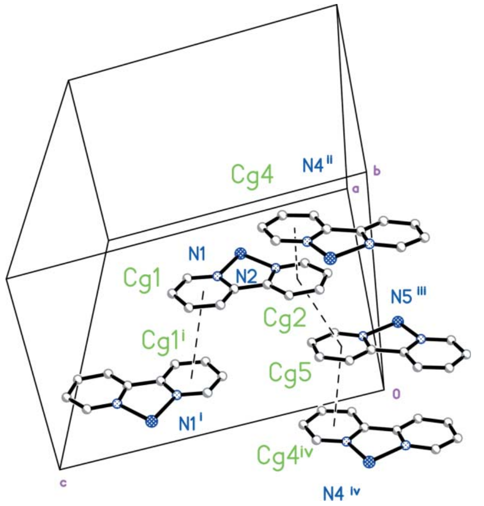


Figure 3
Part of the crystal structure of (I), showing π–π stacking interactions. For the sake of clarity, nmbdc ligands, water molecules and H atoms have been omitted [symmetry code: (i) $1 - x, -y, 1 - z$; (ii) $-\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z$; (iii) $\frac{3}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$; (iv) $\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$]

Experimental

A mixture of cobalt nitrate hexahydrate (0.073 g, 0.25 mmol), 5-nitroisophthalic acid (0.053 g, 0.25 mmol), 2,2′-bipyridine (0.039 g, 0.25 mmol), sodium hydroxide (0.02 g, 0.5 mmol) and water (10 ml) was stirred in air for 5 min, then transferred to and sealed in a 23 ml Teflon-lined stainless steel Parr bomb, which was heated at 433 K for 120 h and then cooled to room temperature. Red block-shaped crystals were obtained after washing with deionized water (yield 31%, based on Co).

Crystal data

$[Co(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]\cdot 0.25H_2O$
$M_r = 446.75$
Monoclinic, $P2_1/n$
$a = 10.0561\ (2)$ Å
$b = 23.3986\ (5)$ Å
$c = 15.3811\ (3)$ Å
$\beta = 96.317\ (1)°$
$V = 3597.18\ (13)$ Å^3
$Z = 8$
$D_x = 1.650$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3310 reflections
$\theta = 2.5$–$23.3°$
$\mu = 1.00$ mm^{-1}
$T = 293\ (2)$ K
Block, red
$0.26 \times 0.14 \times 0.12$ mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.780$, $T_{max} = 0.889$
28059 measured reflections
7054 independent reflections
4747 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 26.0°$
$h = -12 \rightarrow 12$
$k = -25 \rightarrow 28$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.112$
$S = 0.95$
7054 reflections
548 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -0.61$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.069 (2)	Co2—N4	2.077 (2)
Co1—N2	2.108 (2)	Co2—N5	2.114 (2)
Co1—O1	2.276 (2)	Co2—O7	2.307 (2)
Co1—O2	2.199 (2)	Co2—O8	2.176 (2)
Co1—O4^i	2.048 (2)	Co2—O10^{ii}	2.040 (2)
Co1—O13*W*	2.135 (2)	Co2—O14*W*	2.115 (2)
N1—Co1—N2	77.82 (9)	N4—Co2—N5	77.77 (9)
N1—Co1—O1	146.07 (9)	N4—Co2—O8	88.41 (9)
N1—Co1—O2	88.38 (9)	N4—Co2—O14*W*	95.01 (9)
N1—Co1—O13*W*	93.44 (8)	N4—Co2—O7	145.72 (9)
N2—Co1—O1	99.16 (9)	N5—Co2—O7	97.17 (9)
N2—Co1—O2	95.02 (9)	N5—Co2—O8	94.80 (9)
N2—Co1—O13*W*	169.57 (9)	N5—Co2—O14*W*	170.88 (9)
O2—Co1—O1	57.98 (8)	O8—Co2—O7	57.94 (8)
O4^i—Co1—N1	126.38 (9)	O10^{ii}—Co2—N4	125.63 (9)
O4^i—Co1—N2	91.83 (8)	O10^{ii}—Co2—N5	91.14 (9)
O4^i—Co1—O1	87.27 (8)	O10^{ii}—Co2—O7	88.01 (8)
O4^i—Co1—O2	145.22 (9)	O10^{ii}—Co2—O8	145.90 (8)
O4^i—Co1—O13*W*	88.80 (8)	O10^{ii}—Co2—O14*W*	88.58 (8)
O13*W*—Co1—O1	91.28 (9)	O14*W*—Co2—O7	91.93 (8)
O13*W*—Co1—O2	90.36 (9)	O14*W*—Co2—O8	90.52 (9)

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

m398 Xie *et al.* • $[Co(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]\cdot 0.25H_2O$ *Acta Cryst.* (2006). E**62**, m397–m399

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D$$\cdots$$A$	D—H$\cdots$$A$
O13W—H13$A$$\cdots$O7	0.853 (10)	1.99 (2)	2.741 (3)	147 (3)
O13W—H13$B$$\cdots$O10^{ii}	0.850 (10)	1.98 (2)	2.753 (3)	151 (3)
O14W—H14$B$$\cdots$O1	0.842 (10)	2.06 (2)	2.769 (3)	142 (3)
O14W—H14$C$$\cdots$O4^{i}	0.849 (10)	1.923 (18)	2.715 (3)	155 (3)
O15W—H15$A$$\cdots$O2^{iii}	0.86	2.28	2.833 (12)	123

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

Table 3
Geometric parameters of the π–π stacking interactions (Å, °).

$Cg1$ is the centroid of the ring containing N1, $Cg1^{i}$ is the centroid of the ring containing N1^{i}, $Cg2$ is the centroid of the ring containing N2, $Cg3$ is the centroid of the ring containing C11, $Cg4$ is the centroid of the ring containing N4^{ii}, $Cg4^{iv}$ is the centroid of the ring containing N4^{iv}, $Cg5$ is the centroid of the ring containing N5^{iii} and $Cg6$ is the centroid of the ring containing C29^{v}.

Rings	Distance	Dihedral angle
$Cg1\cdots Cg1^{i}$	3.977 (2)	0
$Cg2\cdots Cg4$	3.583 (2)	3.57 (5)
$Cg2\cdots Cg5$	3.889 (2)	6.65 (5)
$Cg3\cdots Cg6$	3.662 (2)	4.9 (1)
$Cg5\cdots Cg4^{iv}$	3.609 (2)	3.08 (5)

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

H atoms on C atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The coordinated water H atoms were located in difference Fourier maps, and were refined with distance restraints of O—H = 0.85 (2) Å and H$\cdots$H = 1.39 (2) Å. The uncoordinated water H atoms were located in difference Fourier maps and constrained to O—H = 0.86 Å, with U_{iso}(H) = 1.2U_{eq}(O). The 0.5 occupancy factor results from satisfactory elemental analyses.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

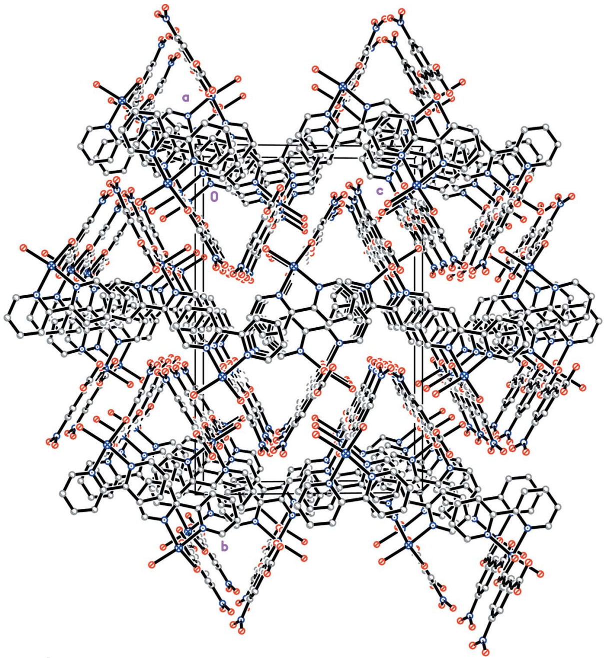


Figure 4
A packing diagram of (I). H atoms and solvent water molecules have been omitted.

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