

Poly[[[tetraaquacobalt(II)]- μ -bipyridine] terephthalate]

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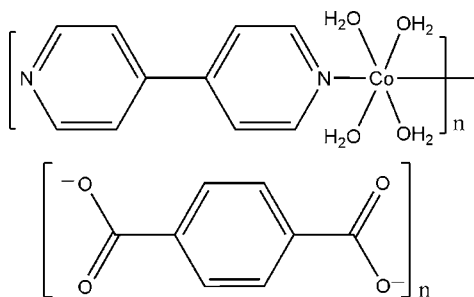
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.035; wR factor = 0.086; data-to-parameter ratio = 12.6.

The Co^{II} atom in the title complex, $\{[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_4](\text{C}_8\text{H}_4\text{O}_4)_n\}$, is coordinated by two N atoms of two bipyridine ligands and four O atoms of four water molecules in an octahedral geometry. The one-dimensional $[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_4]^{2+}$ cation chain is further extended into a supramolecular network *via* O–H \cdots O hydrogen-bond interactions. The Co atom lies on a twofold rotation axis; another twofold rotation axis passes through the carboxylate carbon atoms and the attached ring C atoms.

Related literature

For related literature, see: Banglin *et al.* (2001); Ferey (2001); Hill (1998); Manna *et al.* (2005); Pan *et al.* (2006); Wang *et al.* (2003); Wu *et al.* (2002); Halder & Kepert (2005).



Experimental

Crystal data

$[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_4](\text{C}_8\text{H}_4\text{O}_4)_n$
 $M_r = 451.29$
 Monoclinic, $P2_1/c$
 $a = 6.9516$ (16) Å
 $b = 11.309$ (3) Å

$c = 12.047$ (3) Å
 $\beta = 113.439$ (11)°
 $V = 868.9$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 1.04$ mm⁻¹
 $T = 298$ (2) K

0.23 × 0.20 × 0.18 mm

Data collection

Bruker APEX CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.796$, $T_{\text{max}} = 0.835$

4541 measured reflections
 1709 independent reflections
 1467 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.086$
 $S = 1.00$
 1709 reflections

136 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.38$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

D—H \cdots A	D—H	H \cdots A	D \cdots A	D—H \cdots A
O2—H2A \cdots O3 ⁱ	0.82	1.92	2.737 (2)	178
O1—H1A \cdots O4 ⁱⁱ	0.82	1.88	2.705 (2)	178
O2—H2B \cdots O4 ⁱⁱⁱ	0.82	2.15	2.927 (2)	158
O1—H1B \cdots O3 ^{iv}	0.82	1.91	2.728 (2)	173

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2081).

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supplementary materials

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Poly[[[tetraaquacobalt(II)]- μ -bipyridine] terephthalate]

H. Xu

Comment

Recently, research on organic-inorganic hybrid materials has attracted much attention owing to the wideness of potential applications in catalysis, materials chemistry and biochemistry (Hill, 1998; Banglin *et al.*, 2001; Ferey, 2001). These compounds and many frameworks may be obtained by the assembly of lower dimensional coordination polymers *via* noncovalent intermolecular forces such as hydrogen-bonding interactions. However in the formation of supramolecular assembly, an important target is to establish the possible connections between units. Here, we report the crystal structure of the title compound (I). Compound (I) consists of an infinite one-dimensional cationic chain $[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_4]$ and uncoordinated terephthalate anions (Fig. 1). The Co atom is hexacoordinated by two N atoms of the centrosymmetric bipyridine ligands and four O atoms of water molecules, forming an infinite one-dimensional cationic chain along the *b* axis. These chains are interconnected by the uncoordinated terephthalate anions through O—H \cdots O hydrogen-bonding interactions (Table 1), thus forming a fishing-net layer structure (Fig. 2). A three-dimensional supramolecular network is obtained through O—H \cdots O hydrogen-bonding interactions of the layers.

Experimental

The title compound was obtained by a diffusion method. In one arm of U-tube was placed $\text{Na}_2(\text{BDC})$ (42 mg, 0.2 mmol) in water/methanol (1:1; 10 ml) and in the other $\text{H}_{12}\text{Cl}_2\text{O}_{14}\text{Cu}$ (74 mg, 0.2 mmol) and bipy (31 mg, 0.2 mmol) in water/methanol (1:1; 10 ml). The purple platelike crystals were collected by filtration, washed with distilled water followed by methanol and dried under reduced pressure for 2 h.

Analysis found: C 48.09, H 4.41, N 6.06%; $\text{C}_{18}\text{H}_{20}\text{N}_2\text{O}_8\text{Co}$ requires: C 47.91, H 4.47, N 6.21%.

Refinement

The H-atoms were included in the riding-model approximation with C—H = 0.93 Å and O—H = 0.82 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C-aromatic})$.

Figures

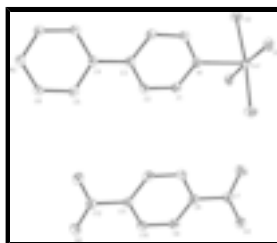


Fig. 1. The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted for clarity.



Fig. 2. three-dimensional superamolecular structure of (I). Hydrogen bond interactions was shown.

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Crystal data

$[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_4](\text{C}_8\text{H}_4\text{O}_4)$

$M_r = 451.29$

Monoclinic, $P2/c$

Hall symbol: $-P\ 2yc$

$a = 6.9516(16)\ \text{\AA}$

$b = 11.309(3)\ \text{\AA}$

$c = 12.047(3)\ \text{\AA}$

$\beta = 113.439(11)^\circ$

$V = 868.9(4)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 466$

$D_x = 1.725\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1738 reflections

$\theta = 3.2\text{--}26.4^\circ$

$\mu = 1.04\ \text{mm}^{-1}$

$T = 298(2)\ \text{K}$

Platelike, purple

$0.23 \times 0.20 \times 0.18\ \text{mm}$

Data collection

Bruker APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2)\ \text{K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.796$, $T_{\max} = 0.835$

4541 measured reflections

1709 independent reflections

1467 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 1.8^\circ$

$h = -8 \rightarrow 8$

$k = -13 \rightarrow 6$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.086$

$S = 1.00$

1709 reflections

136 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.34\ \text{e \AA}^{-3}$

$\Delta\rho_{\min} = -0.38\ \text{e \AA}^{-3}$

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	1.0000	0.10367 (3)	0.7500	0.02552 (16)
O1	0.8160 (2)	0.09545 (12)	0.84965 (13)	0.0328 (4)
H1A	0.7383	0.1504	0.8486	0.049*
H1B	0.7478	0.0347	0.8427	0.049*
O2	1.2845 (2)	0.11337 (13)	0.90757 (14)	0.0375 (4)
H2A	1.3146	0.1108	0.9806	0.056*
H2B	1.3833	0.1421	0.8961	0.056*
O3	0.3954 (3)	0.10827 (13)	0.15243 (14)	0.0408 (4)
O4	0.4395 (3)	0.72447 (14)	0.14960 (13)	0.0388 (4)
N1	1.0000	0.2930 (2)	0.7500	0.0276 (6)
N2	1.0000	0.9178 (2)	0.7500	0.0280 (6)
C1	0.9666 (3)	0.3547 (2)	0.64971 (18)	0.0290 (5)
H1	0.9431	0.3135	0.5787	0.035*
C2	0.9650 (3)	0.47594 (19)	0.64631 (18)	0.0279 (5)
H2	0.9404	0.5149	0.5739	0.033*
C3	1.0000	0.5404 (3)	0.7500	0.0240 (6)
C4	1.0000	0.6709 (2)	0.7500	0.0236 (6)
C5	0.9079 (3)	0.73486 (19)	0.64383 (18)	0.0297 (5)
H5	0.8440	0.6959	0.5702	0.036*
C6	0.9115 (4)	0.8560 (2)	0.64790 (18)	0.0312 (5)
H6	0.8488	0.8973	0.5756	0.037*
C7	0.5000	0.1599 (3)	0.2500	0.0296 (7)
C8	0.5000	0.2937 (3)	0.2500	0.0266 (7)
C9	0.4552 (3)	0.3556 (2)	0.14378 (18)	0.0298 (5)
H9	0.4237	0.3149	0.0716	0.036*
C10	0.4569 (3)	0.4778 (2)	0.14440 (18)	0.0289 (5)
H10	0.4286	0.5186	0.0725	0.035*
C11	0.5000	0.5404 (3)	0.2500	0.0262 (6)
C12	0.5000	0.6732 (3)	0.2500	0.0292 (7)

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0308 (3)	0.0183 (2)	0.0248 (2)	0.000	0.00822 (18)	0.000
O1	0.0393 (9)	0.0230 (8)	0.0393 (9)	0.0006 (6)	0.0191 (7)	0.0003 (6)
O2	0.0336 (9)	0.0429 (10)	0.0294 (8)	-0.0055 (7)	0.0058 (7)	0.0006 (7)
O3	0.0531 (11)	0.0316 (10)	0.0323 (9)	-0.0097 (7)	0.0111 (8)	-0.0022 (7)
O4	0.0501 (10)	0.0294 (9)	0.0326 (9)	0.0042 (8)	0.0118 (7)	0.0049 (7)
N1	0.0295 (13)	0.0213 (13)	0.0284 (13)	0.000	0.0076 (11)	0.000
N2	0.0326 (14)	0.0216 (13)	0.0281 (14)	0.000	0.0103 (11)	0.000
C1	0.0336 (12)	0.0245 (11)	0.0269 (11)	-0.0004 (9)	0.0099 (9)	-0.0036 (9)
C2	0.0342 (12)	0.0244 (11)	0.0240 (11)	0.0008 (9)	0.0106 (9)	0.0035 (9)
C3	0.0176 (13)	0.0228 (16)	0.0296 (15)	0.000	0.0072 (12)	0.000
C4	0.0240 (15)	0.0201 (15)	0.0269 (15)	0.000	0.0105 (12)	0.000
C5	0.0353 (12)	0.0228 (11)	0.0266 (11)	-0.0024 (9)	0.0076 (9)	-0.0032 (9)
C6	0.0412 (13)	0.0244 (11)	0.0235 (11)	0.0001 (10)	0.0081 (9)	0.0029 (9)
C7	0.0341 (17)	0.0271 (17)	0.0300 (17)	0.000	0.0155 (14)	0.000
C8	0.0204 (14)	0.0268 (16)	0.0294 (16)	0.000	0.0066 (12)	0.000
C9	0.0314 (12)	0.0286 (12)	0.0254 (11)	0.0016 (10)	0.0070 (9)	-0.0036 (9)
C10	0.0290 (11)	0.0313 (12)	0.0242 (11)	0.0015 (9)	0.0083 (9)	0.0042 (9)
C11	0.0191 (14)	0.0279 (17)	0.0286 (15)	0.000	0.0064 (12)	0.000
C12	0.0240 (15)	0.0274 (17)	0.0328 (17)	0.000	0.0078 (13)	0.000

Geometric parameters (\AA , $^\circ$)

Co1—O1	2.0754 (15)	C2—H2	0.9300
Co1—O2	2.1308 (16)	C3—C4	1.475 (4)
Co1—N1	2.142 (3)	C4—C5	1.385 (2)
O1—H1A	0.8199	C5—C6	1.370 (3)
O1—H1B	0.8200	C5—H5	0.9300
O2—H2A	0.8199	C6—H6	0.9300
O2—H2B	0.8199	C7—C8	1.514 (4)
O3—C7	1.253 (2)	C8—C9	1.381 (3)
O4—C12	1.253 (2)	C9—C10	1.382 (3)
N1—C1	1.333 (2)	C9—H9	0.9300
N2—C6	1.334 (2)	C10—C11	1.381 (3)
C1—C2	1.372 (3)	C10—H10	0.9300
C1—H1	0.9300	C11—C12	1.501 (4)
C2—C3	1.382 (2)		
O1 ⁱ —Co1—O1	174.86 (8)	C3—C2—H2	119.9
O1—Co1—N2 ⁱⁱ	87.43 (4)	C2—C3—C2 ⁱ	116.3 (3)
O1 ⁱ —Co1—O2	87.16 (6)	C2—C3—C4	121.86 (13)
O1—Co1—O2	93.11 (6)	C5 ⁱ —C4—C5	117.0 (3)
N2 ⁱⁱ —Co1—O2	92.95 (4)	C5—C4—C3	121.50 (13)
O1—Co1—O2 ⁱ	87.16 (6)	C6—C5—C4	119.6 (2)
O2—Co1—O2 ⁱ	174.10 (8)	C6—C5—H5	120.2

O1—Co1—N1	92.57 (4)	C4—C5—H5	120.2
N2 ⁱⁱ —Co1—N1	180.000 (1)	N2—C6—C5	123.5 (2)
O2—Co1—N1	87.05 (4)	N2—C6—H6	118.2
Co1—O1—H1A	120.7	C5—C6—H6	118.2
Co1—O1—H1B	116.3	O3—C7—O3 ^{iv}	124.5 (3)
H1A—O1—H1B	106.4	O3—C7—C8	117.76 (15)
Co1—O2—H2A	134.8	C9 ^{iv} —C8—C9	119.1 (3)
Co1—O2—H2B	114.4	C9—C8—C7	120.44 (14)
H2A—O2—H2B	108.8	C8—C9—C10	120.2 (2)
C1 ⁱ —N1—C1	116.9 (3)	C8—C9—H9	119.9
C1—N1—Co1	121.54 (13)	C10—C9—H9	119.9
C6—N2—C6 ⁱ	116.8 (3)	C11—C10—C9	121.1 (2)
C6—N2—Co1 ⁱⁱⁱ	121.62 (13)	C11—C10—H10	119.5
N1—C1—C2	123.12 (19)	C9—C10—H10	119.5
N1—C1—H1	118.4	C10—C11—C10 ^{iv}	118.3 (3)
C2—C1—H1	118.4	C10—C11—C12	120.85 (14)
C1—C2—C3	120.27 (19)	O4 ^{iv} —C12—O4	124.9 (3)
C1—C2—H2	119.9	O4—C12—C11	117.55 (14)
O1—Co1—N1—C1	-134.70 (11)	C6 ⁱ —N2—C6—C5	0.02 (16)
O2—Co1—N1—C1	132.32 (11)	Co1 ⁱⁱⁱ —N2—C6—C5	-179.98 (16)
C1 ⁱ —N1—C1—C2	-0.13 (14)	C4—C5—C6—N2	0.0 (3)
Co1—N1—C1—C2	179.87 (14)	O3—C7—C8—C9	-23.07 (14)
N1—C1—C2—C3	0.3 (3)	C9 ^{iv} —C8—C9—C10	0.48 (13)
C1—C2—C3—C2 ⁱ	-0.12 (13)	C7—C8—C9—C10	-179.52 (13)
C1—C2—C3—C4	179.88 (13)	C8—C9—C10—C11	-1.0 (3)
C2—C3—C4—C5	18.88 (14)	C9—C10—C11—C10 ^{iv}	0.49 (14)
C5 ⁱ —C4—C5—C6	0.02 (15)	C9—C10—C11—C12	-179.51 (14)
C3—C4—C5—C6	-179.98 (15)	C10—C11—C12—O4	6.91 (12)

Symmetry codes: (i) $-x+2, y, -z+3/2$; (ii) $x, y-1, z$; (iii) $x, y+1, z$; (iv) $-x+1, y, -z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O2—H2A \cdots O3 ^v	0.82	1.92	2.737 (2)	178
O1—H1A \cdots O4 ^{vi}	0.82	1.88	2.705 (2)	178
O2—H2B \cdots O4 ^{vii}	0.82	2.15	2.927 (2)	158
O1—H1B \cdots O3 ^{viii}	0.82	1.91	2.728 (2)	173

Symmetry codes: (v) $x+1, y, z+1$; (vi) $-x+1, -y+1, -z+1$; (vii) $-x+2, -y+1, -z+1$; (viii) $-x+1, -y, -z+1$.

Fig. 1

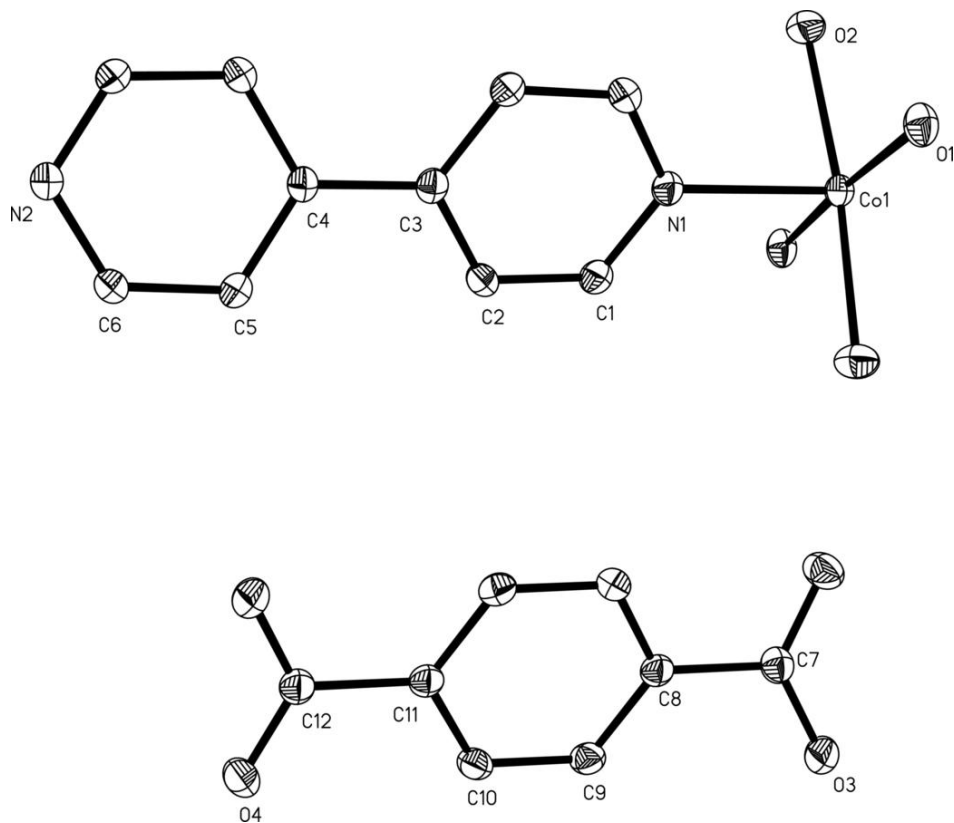


Fig. 2

