

catena-Poly[[bis(3,5-dicarboxybenzoato)cobalt(II)]- μ -4,4'-bipyridine]

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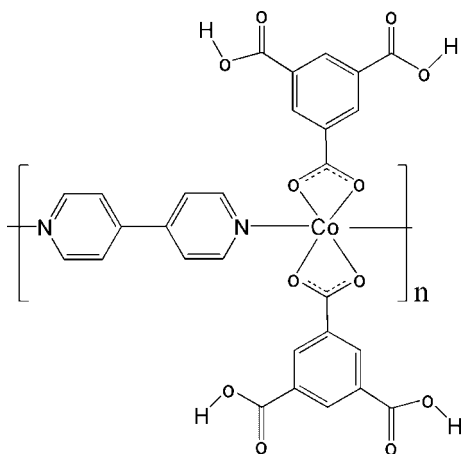
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.038; wR factor = 0.098; data-to-parameter ratio = 13.1.

In the title compound, $[\text{Co}(\text{C}_9\text{H}_5\text{O}_6)_2(\text{C}_{10}\text{H}_8\text{N}_2)]_n$, the asymmetric unit consists of one Co^{2+} ion with site symmetry 2, one mono-deprotonated 1,3,5-benzenetricarboxylic acid anion and one-half of a 4,4'-bipyridine (4,4'-bipy) molecule, in which two N and two C atoms have site symmetry 2. In the crystal structure, the Co^{2+} centre is coordinated by four O atoms from two bidentate carboxylate groups of two anions and two N atoms of two 4,4'-bipy molecules, resulting in infinite chains propagating in [010]. The cobalt coordination is distorted *trans*- CoO_4N_2 octahedral and interchain $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds complete the structure.

Related literature

For background, see: Feller *et al.* (2007); Brown *et al.* (2008).



Experimental

Crystal data

$[\text{Co}(\text{C}_9\text{H}_5\text{O}_6)_2(\text{C}_{10}\text{H}_8\text{N}_2)]$
 $M_r = 633.37$
 Monoclinic, $C2/c$
 $a = 10.6682$ (7) Å
 $b = 11.0490$ (7) Å
 $c = 22.6563$ (14) Å
 $\beta = 101.401$ (1)°

$V = 2617.9$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.73$ mm⁻¹
 $T = 293$ (2) K
 $0.18 \times 0.15 \times 0.13$ mm

Data collection

Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2001)
 $T_{\min} = 0.880$, $T_{\max} = 0.911$

7123 measured reflections
 2579 independent reflections
 2051 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.098$
 $S = 1.02$
 2579 reflections
 197 parameters

7 restraints
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.30$ e Å⁻³
 $\Delta\rho_{\min} = -0.73$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—N2 ⁱ	1.982 (2)	Co1—O1	2.0221 (14)
Co1—N1	1.992 (2)	Co1—O2	2.4354 (13)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 ⁱⁱ ···O2 ⁱⁱ	0.81	1.88	2.648 (2)	157
O5—H5 ⁱⁱⁱ ···O6 ⁱⁱⁱ	0.78	1.88	2.651 (2)	170

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2815).

References

- Brown, K. A., Martin, D. P. & LaDuca, R. L. (2008). *CrystEngComm*, **10**, 1305–1308.
- Bruker (2001). SMART and SAINT-Plus. Bruker AXS Inc., Madison, Wisconsin, USA.
- Feller, R. K., Forster, P. M., Wudl, F. & Cheetham, A. K. (2007). *Inorg. Chem.* **46**, 8717–8721.
- Sheldrick, G. M. (2001). SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2008). E64, m1400 [doi:10.1107/S1600536808032558]

***catena*-Poly[[bis(3,5-dicarboxybenzoato)cobalt(II)]- μ -4,4'-bipyridine]**

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Comment

Recently, many efforts in coordination chemistry and crystal engineering have been devoted to the construction of metal-organic coordination polymers (MOCs) employing both coordination bonds and/or hydrogen bonds, due to their appropriate strength and directionality (Feller *et al.* 2007). Dual-ligand or multidentate organic ligands are usually engaged in the construction of MOCs, among which carboxylates and *N,N*-bidentate ligands are all the simplest connectors potentially able to bridge metal ions (Brown *et al.* 2008). Herein, we report the title compound (I) containing organic dual-ligands (Fig. 1).

The structure of (I) presents a one-dimensional infinite chain (Fig.2), in which the Co^{2+} centre (site symmetry 2) is coordinated by four O atoms from two bidentate carboxylate groups of two 1,3,5-benzenetricarboxylic acid anions, two N atoms of two 4,4'-bipyridine molecules. The Co^{2+} cation resides in a distorted octahedral configuration. In the equatorial plane, it is chelated by four carboxylate oxygen atoms (O1, O2 and their symmetry equivalents) from two 1,3,5-benzenetricarboxylic acid anions (Table 1), in which the Co—O distances are very different.

In addition, these one-dimensional chains are linked together by O—H \cdots O hydrogen bonds between carboxylate groups generating a three-dimensional framework (Fig. 3 and Table 2).

Experimental

Solid $\text{Co}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$ (1 mmol, 0.245 g) was added to an aqueous solution (25 ml) of 1,3,5-benzenetricarboxylic acid (2 mmol, 0.420 g) and 4,4'-bipyridine (1 mmol, 0.156 g). The mixture was refluxed for two hours at 373 K. The solution was filtered, and the filtrate was kept at room temperature. After ten days, purple blocks of (I) were obtained.

Refinement

The O-bound H atoms were located in difference Fourier maps and refined as riding in their as-found relative positions with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The C-bound H atoms were geometrically placed (C—H = 0.93 Å) and refined as riding, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

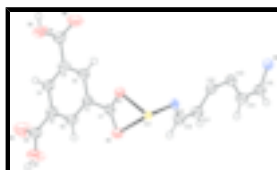


Fig. 1. Asymmetric unit of (I), showing displacement ellipsoids at the 50% probability level for the non-hydrogen atoms.

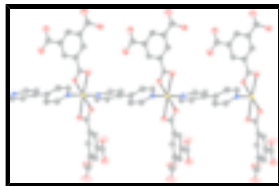


Fig. 2. One-dimensional chain structure of (I). H atoms are omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

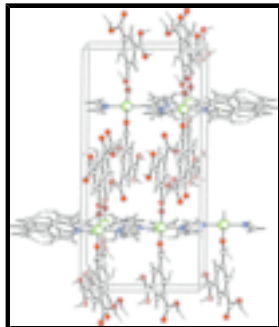


Fig. 3. Three-dimensional structure of (I) arising by means of hydrogen bonds. Displacement ellipsoids are drawn at the 50% probability level.

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Crystal data

[Co(C₉H₅O₆)₂(C₁₀H₈N₂)]

$M_r = 633.37$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 10.6682 (7) \text{ \AA}$

$b = 11.0490 (7) \text{ \AA}$

$c = 22.6563 (14) \text{ \AA}$

$\beta = 101.401 (1)^\circ$

$V = 2617.9 (3) \text{ \AA}^3$

$Z = 4$

$F_{000} = 1292$

$D_x = 1.607 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

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

Cell parameters from 1750 reflections

$\theta = 2.7\text{--}25.9^\circ$

$\mu = 0.73 \text{ mm}^{-1}$

$T = 293 (2) \text{ K}$

Block, purple

$0.18 \times 0.15 \times 0.13 \text{ mm}$

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2) \text{ K}$

ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2001)

$T_{\min} = 0.880$, $T_{\max} = 0.911$

7123 measured reflections

2579 independent reflections

2051 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

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

$\theta_{\text{min}} = 2.7^\circ$

$h = -13 \rightarrow 13$

$k = -13 \rightarrow 13$

$l = -27 \rightarrow 15$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.038$$

$$wR(F^2) = 0.098$$

$$S = 1.02$$

2579 reflections

197 parameters

7 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: difmap and geom

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 1.9201P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.73 \text{ e } \text{\AA}^{-3}$$

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	0.64801 (3)	0.2500	0.01788 (9)
O1	0.60733 (12)	0.64666 (13)	0.18575 (6)	0.0280 (3)
O2	0.40351 (13)	0.65638 (14)	0.14327 (6)	0.0347 (4)
O3	0.30786 (17)	0.7752 (2)	-0.06851 (8)	0.0661 (6)
H3	0.2523	0.7863	-0.0982	0.099*
O4	0.39825 (18)	0.6736 (2)	-0.13349 (8)	0.0692 (6)
O5	0.85792 (15)	0.55679 (17)	-0.04477 (7)	0.0509 (5)
H5	0.9287	0.5390	-0.0439	0.076*
O6	0.91135 (16)	0.5199 (2)	0.05406 (8)	0.0591 (6)
N1	0.5000	0.4678 (2)	0.2500	0.0232 (4)
N2	0.5000	-0.1726 (2)	0.2500	0.0274 (6)
C1	0.55508 (19)	0.64578 (18)	0.07857 (9)	0.0281 (5)
C2	0.67509 (19)	0.60572 (19)	0.07160 (9)	0.0298 (5)
H2	0.7360	0.5843	0.1053	0.036*
C3	0.70461 (19)	0.5975 (2)	0.01464 (10)	0.0306 (5)
C4	0.6137 (2)	0.6293 (2)	-0.03605 (10)	0.0338 (5)
H4	0.6326	0.6222	-0.0742	0.041*
C5	0.4946 (2)	0.6717 (2)	-0.02928 (10)	0.0329 (5)
C6	0.4664 (2)	0.6797 (2)	0.02785 (10)	0.0327 (5)
H6	0.3867	0.7084	0.0322	0.039*
C7	0.51892 (19)	0.65013 (18)	0.13895 (9)	0.0265 (5)
C8	0.8332 (2)	0.5551 (2)	0.00808 (10)	0.0362 (6)

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C9	0.3971 (2)	0.7059 (2)	-0.08302 (10)	0.0392 (6)
C10	0.4034 (2)	0.40519 (19)	0.21766 (10)	0.0321 (5)
H10	0.3356	0.4477	0.1947	0.039*
C11	0.3993 (2)	0.28136 (19)	0.21669 (10)	0.0330 (5)
H11	0.3295	0.2414	0.1938	0.040*
C12	0.5000	0.2156 (3)	0.2500	0.0284 (7)
C13	0.5000	0.0812 (3)	0.2500	0.0269 (7)
C14	0.38822 (19)	0.01470 (19)	0.23157 (10)	0.0333 (5)
H14	0.3108	0.0547	0.2192	0.040*
C15	0.3916 (2)	-0.1093 (2)	0.23148 (10)	0.0328 (5)
H15	0.3158	-0.1514	0.2181	0.039*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02150 (17)	0.01328 (16)	0.01973 (17)	0.000	0.00619 (13)	0.000
O1	0.0246 (6)	0.0345 (8)	0.0250 (7)	0.0022 (6)	0.0052 (5)	0.0008 (6)
O2	0.0252 (7)	0.0480 (9)	0.0314 (8)	0.0040 (7)	0.0071 (6)	0.0026 (7)
O3	0.0446 (10)	0.1163 (17)	0.0354 (10)	0.0378 (11)	0.0033 (8)	0.0035 (10)
O4	0.0557 (11)	0.1214 (18)	0.0293 (10)	0.0270 (12)	0.0052 (8)	-0.0022 (10)
O5	0.0367 (8)	0.0734 (12)	0.0478 (10)	0.0152 (8)	0.0210 (7)	0.0025 (9)
O6	0.0376 (9)	0.0938 (15)	0.0466 (10)	0.0261 (9)	0.0100 (8)	0.0094 (10)
N1	0.0263 (7)	0.0191 (7)	0.0246 (7)	0.000	0.0062 (6)	0.000
N2	0.0268 (12)	0.0246 (13)	0.0313 (13)	0.000	0.0072 (10)	0.000
C1	0.0268 (10)	0.0300 (10)	0.0276 (10)	0.0007 (9)	0.0057 (8)	-0.0005 (9)
C2	0.0250 (10)	0.0327 (11)	0.0308 (11)	0.0034 (9)	0.0030 (9)	0.0013 (9)
C3	0.0254 (10)	0.0333 (11)	0.0335 (11)	0.0015 (9)	0.0070 (9)	-0.0025 (9)
C4	0.0294 (10)	0.0441 (13)	0.0296 (11)	0.0011 (10)	0.0097 (9)	-0.0015 (10)
C5	0.0289 (11)	0.0410 (13)	0.0288 (11)	0.0011 (9)	0.0054 (9)	0.0003 (9)
C6	0.0256 (10)	0.0413 (12)	0.0320 (12)	0.0031 (9)	0.0071 (9)	-0.0010 (10)
C7	0.0259 (10)	0.0244 (10)	0.0291 (10)	0.0014 (8)	0.0050 (8)	0.0002 (9)
C8	0.0297 (11)	0.0435 (13)	0.0369 (13)	0.0022 (10)	0.0100 (10)	-0.0008 (10)
C9	0.0292 (11)	0.0614 (15)	0.0284 (12)	0.0044 (11)	0.0092 (9)	0.0027 (11)
C10	0.0317 (11)	0.0265 (11)	0.0370 (12)	0.0027 (9)	0.0042 (9)	0.0031 (9)
C11	0.0310 (11)	0.0271 (11)	0.0391 (12)	-0.0005 (9)	0.0030 (9)	-0.0002 (9)
C12	0.0267 (14)	0.0246 (15)	0.0354 (16)	0.000	0.0096 (12)	0.000
C13	0.0270 (14)	0.0238 (15)	0.0300 (16)	0.000	0.0057 (12)	0.000
C14	0.0246 (10)	0.0265 (11)	0.0464 (13)	0.0007 (9)	0.0015 (10)	0.0022 (10)
C15	0.0241 (10)	0.0276 (11)	0.0456 (13)	-0.0015 (9)	0.0044 (10)	0.0006 (10)

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

Co1—N2 ⁱ	1.982 (2)	C1—C7	1.494 (3)
Co1—N1	1.992 (2)	C2—C3	1.390 (3)
Co1—O1 ⁱⁱ	2.0221 (14)	C2—H2	0.9300
Co1—O1	2.0221 (14)	C3—C4	1.393 (3)
Co1—O2 ⁱⁱ	2.4354 (13)	C3—C8	1.485 (3)
Co1—O2	2.4354 (13)	C4—C5	1.391 (3)

O1—C7	1.273 (2)	C4—H4	0.9300
O2—C7	1.256 (2)	C5—C6	1.389 (3)
O3—C9	1.314 (3)	C5—C9	1.485 (3)
O3—H3	0.8127	C6—H6	0.9300
O4—C9	1.200 (3)	C10—C11	1.369 (3)
O5—C8	1.276 (3)	C10—H10	0.9300
O5—H5	0.7761	C11—C12	1.390 (3)
O6—C8	1.260 (3)	C11—H11	0.9300
N1—C10	1.333 (2)	C12—C11 ⁱⁱ	1.390 (3)
N1—C10 ⁱⁱ	1.333 (2)	C12—C13	1.485 (4)
N2—C15 ⁱⁱ	1.346 (2)	C13—C14	1.392 (2)
N2—C15	1.346 (2)	C13—C14 ⁱⁱ	1.392 (2)
N2—Co1 ⁱⁱⁱ	1.982 (2)	C14—C15	1.371 (3)
C1—C6	1.388 (3)	C14—H14	0.9300
C1—C2	1.393 (3)	C15—H15	0.9300
N2 ⁱ —Co1—N1	180.0	C1—C6—C5	121.1 (2)
N2 ⁱ —Co1—O1 ⁱⁱ	90.42 (4)	C1—C6—H6	119.5
N1—Co1—O1 ⁱⁱ	89.58 (4)	C5—C6—H6	119.5
N2 ⁱ —Co1—O1	90.42 (4)	O2—C7—O1	120.87 (19)
N1—Co1—O1	89.58 (4)	O2—C7—C1	120.51 (18)
O1 ⁱⁱ —Co1—O1	179.16 (8)	O1—C7—C1	118.62 (17)
C7—O1—Co1	99.65 (12)	O6—C8—O5	123.7 (2)
C9—O3—H3	109.1	O6—C8—C3	119.2 (2)
C8—O5—H5	110.6	O5—C8—C3	117.11 (19)
C10—N1—C10 ⁱⁱ	117.5 (2)	O4—C9—O3	123.8 (2)
C10—N1—Co1	121.23 (12)	O4—C9—C5	124.6 (2)
C10 ⁱⁱ —N1—Co1	121.23 (12)	O3—C9—C5	111.60 (19)
C15 ⁱⁱ —N2—C15	117.4 (2)	N1—C10—C11	123.1 (2)
C15 ⁱⁱ —N2—Co1 ⁱⁱⁱ	121.30 (12)	N1—C10—H10	118.5
C15—N2—Co1 ⁱⁱⁱ	121.30 (12)	C11—C10—H10	118.5
C6—C1—C2	118.9 (2)	C10—C11—C12	119.7 (2)
C6—C1—C7	119.49 (18)	C10—C11—H11	120.2
C2—C1—C7	121.58 (18)	C12—C11—H11	120.2
C3—C2—C1	120.52 (19)	C11 ⁱⁱ —C12—C11	116.9 (3)
C3—C2—H2	119.7	C11 ⁱⁱ —C12—C13	121.54 (13)
C1—C2—H2	119.7	C11—C12—C13	121.54 (13)
C2—C3—C4	120.00 (19)	C14—C13—C14 ⁱⁱ	116.3 (3)
C2—C3—C8	119.79 (18)	C14—C13—C12	121.83 (13)
C4—C3—C8	120.2 (2)	C14 ⁱⁱ —C13—C12	121.83 (13)
C5—C4—C3	119.7 (2)	C15—C14—C13	120.4 (2)
C5—C4—H4	120.1	C15—C14—H14	119.8
C3—C4—H4	120.1	C13—C14—H14	119.8
C6—C5—C4	119.72 (19)	N2—C15—C14	122.7 (2)
C6—C5—C9	120.1 (2)	N2—C15—H15	118.7
C4—C5—C9	120.2 (2)	C14—C15—H15	118.7

supplementary materials

N2 ⁱ —Co1—O1—C7	-88.18 (11)	C6—C1—C7—O1	-163.76 (19)
N1—Co1—O1—C7	91.82 (11)	C2—C1—C7—O1	17.7 (3)
O1 ⁱⁱ —Co1—O1—C7	91.82 (12)	C2—C3—C8—O6	4.3 (3)
N2 ⁱ —Co1—N1—C10	-141 (22)	C4—C3—C8—O6	-175.8 (2)
O1 ⁱⁱ —Co1—N1—C10	83.93 (12)	C2—C3—C8—O5	-175.6 (2)
O1—Co1—N1—C10	-96.07 (12)	C4—C3—C8—O5	4.3 (3)
N2 ⁱ —Co1—N1—C10 ⁱⁱ	39 (23)	C6—C5—C9—O4	-159.5 (3)
O1 ⁱⁱ —Co1—N1—C10 ⁱⁱ	-96.07 (12)	C4—C5—C9—O4	19.2 (4)
O1—Co1—N1—C10 ⁱⁱ	83.93 (12)	C6—C5—C9—O3	19.8 (3)
C6—C1—C2—C3	-1.3 (3)	C4—C5—C9—O3	-161.5 (2)
C7—C1—C2—C3	177.20 (19)	C10 ⁱⁱ —N1—C10—C11	0.39 (16)
C1—C2—C3—C4	-0.1 (3)	Co1—N1—C10—C11	-179.61 (16)
C1—C2—C3—C8	179.8 (2)	N1—C10—C11—C12	-0.8 (3)
C2—C3—C4—C5	1.4 (3)	C10—C11—C12—C11 ⁱⁱ	0.37 (15)
C8—C3—C4—C5	-178.4 (2)	C10—C11—C12—C13	-179.63 (15)
C3—C4—C5—C6	-1.3 (3)	C11 ⁱⁱ —C12—C13—C14	161.59 (15)
C3—C4—C5—C9	180.0 (2)	C11—C12—C13—C14	-18.41 (15)
C2—C1—C6—C5	1.5 (3)	C11 ⁱⁱ —C12—C13—C14 ⁱⁱ	-18.41 (15)
C7—C1—C6—C5	-177.08 (19)	C11—C12—C13—C14 ⁱⁱ	161.59 (15)
C4—C5—C6—C1	-0.2 (3)	C14 ⁱⁱ —C13—C14—C15	-0.70 (16)
C9—C5—C6—C1	178.6 (2)	C12—C13—C14—C15	179.30 (16)
Co1—O1—C7—O2	1.9 (2)	C15 ⁱⁱ —N2—C15—C14	-0.74 (16)
Co1—O1—C7—C1	-177.68 (15)	Co1 ⁱⁱⁱ —N2—C15—C14	179.26 (16)
C6—C1—C7—O2	16.6 (3)	C13—C14—C15—N2	1.5 (3)
C2—C1—C7—O2	-161.9 (2)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 ^{iv} —O2 ^{iv}	0.81	1.88	2.648 (2)	157
O5—H5 ^v —O6 ^v	0.78	1.88	2.651 (2)	170

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

Fig. 1

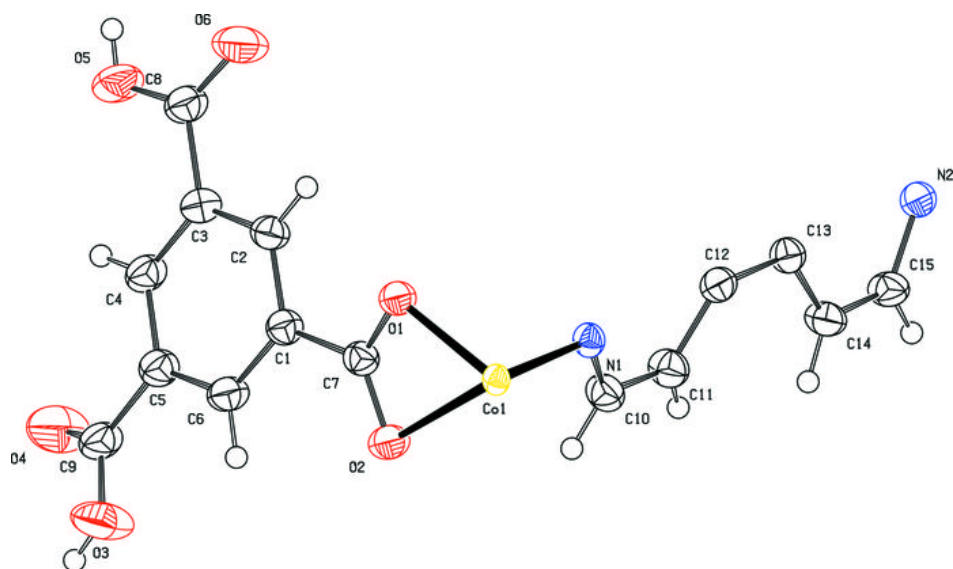


Fig. 2

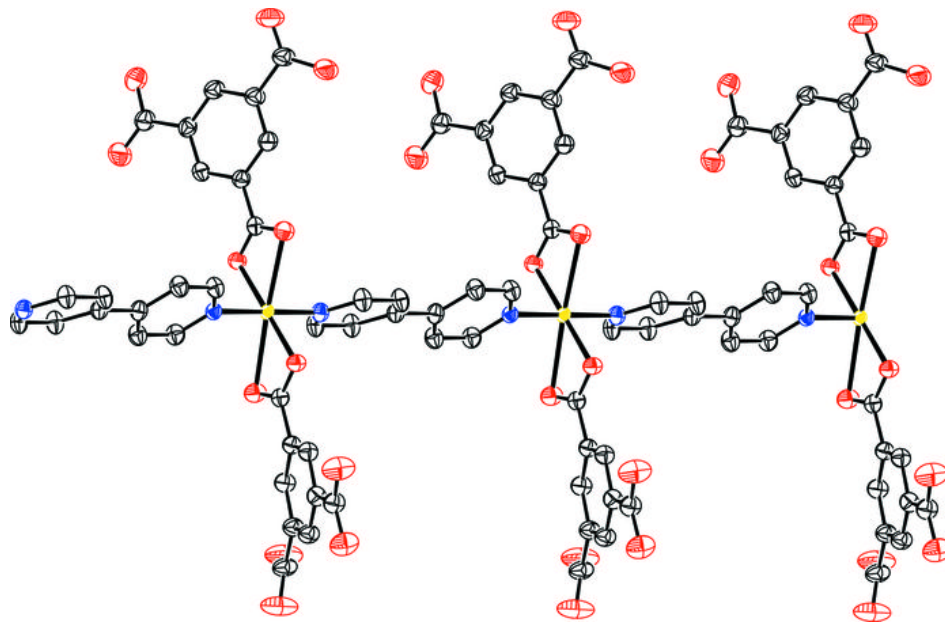


Fig. 3

