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Poly[[aqua(2,2-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)cobalt(II)] monohydrate]

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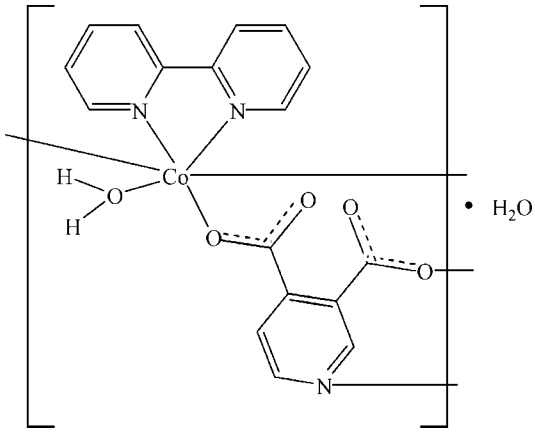
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.163; data-to-parameter ratio = 12.7.

The asymmetric unit of the title compound, $\{[Co(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)]\cdot H_2O\}_n$, contains one Co^{II} cation chelated by one 2,2′-bipyridine ligand and further coordinated by two monodentate carboxylate groups and one N atom belonging to three symmetry-related pyridine-3,4-dicarboxylate ligands (acting in a μ_3-*N*:*O*:*O*′ mode), and one water molecule. The result is a CoO_3N_3 polyhedron which exhibits an octahedral geometry. Each two neighboring Co^{II} cations are bridged by two independent pyridine-3,4-dicarboxylate ligands, which are further coordinated to a third and fourth Co^{II} cation though the pyridine N atom to form corrugated layers parallel to the (110) plane. There are two medium–strong intramolecular hydrogen bonds involving the coordinated water molecule and two intermolecular hydrogen bonds involving the solvent water molecule, linking layers into a three-dimensional packing network.

Related literature

For related literature, see: Li *et al.* (1993); Go *et al.* (2004); An *et al.* (2000); Baroni *et al.* (1996); Hundal *et al.* (2002).



Experimental

Crystal data

$[Co(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)]\cdot H_2O$
M_r = 416.25
Orthorhombic, *Pbca*
a = 15.7498 (5) Å
b = 12.3488 (10) Å
c = 17.0168 (5) Å
V = 3309.6 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 293 (2) K
0.43 × 0.36 × 0.23 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.654, T_{max} = 0.789
26510 measured reflections
3249 independent reflections
2562 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.163
S = 1.00
3249 reflections
256 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −1.07 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*W*···O6	0.82 (4)	2.03 (4)	2.830 (4)	165 (5)
O1—H2*W*···O2	0.82 (3)	1.839 (15)	2.646 (3)	166 (5)
O6—H3*W*···O2^{i}	0.83 (4)	2.04 (4)	2.841 (3)	166 (5)
O6—H4*W*···O4^{ii}	0.81 (4)	1.98 (4)	2.788 (3)	174 (5)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: BG2090).

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supplementary materials

Acta Cryst. (2007). E**63**, m2373 [**doi:10.1107/S1600536807040275**]

Poly[[aqua(2,2-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)cobalt(II)] monohydrate]

Z.-F. Li, S.-W. Wang, Q. Zhang and X.-J. Yu

Comment

Complexes containing carboxyl acids have been the interest of chemists these years due to their potential applications, such as catalysis, optics, information storage, medicine, molecular electrochemistry, biochemistry and biological pharmaceutics (Li *et al.*, 1993; Gao *et al.*, 2004; Go *et al.*, 2004). Thus far, N-containing aromatic carboxyl acid has been widely used in dye intermediates, organic synthesis, sensitization materials, functional pigments, *etc*. (An *et al.*, 2000). Pyridinecarboxylic acid is also a good ligand in coordination chemistry due to its strong coordination ability and versatile coordination modes for what it has received much attention it in recent decades (Baroni *et al.*, 1996; Hundal *et al.*, 2002)).

Herein, we report a new complex containing both ligands, namely poly[[aqua(2,2-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)cobalt(II)] monohydrate], (I).

The structure of (I) contains one cobalt cation chelated by one 2,2'-bipyridine ligand and further coordinated by two monodentate carboxylate groups and one N atom belonging to three-symmetry related pyridine-3,4-dicarboxylate ligands (acting in a μ_3-N:*O*:*O*' mode) and one water molecule. There is also a crystallization weater molecule. The result is a CoO_3N_3 polyhedron which exhibits an octahedral geometry (Fig. 1).

The Co^{II} atom is hexa-coordinated by three N and three O atoms exhibiting an octahedral geometry. Each two neighboring Co^{II} cations are bridged by two independent pyridine-3,4-dicarboxylate ligands, which are further coordinated to the third and the fourth Co^{II} cations though pyridine N atom to form corrugated layers parallel to the [110] plane (Fig. 2). There exist two medium–strong intramolecular hydrogen bonds involving the coordinated water molecule (Table 3, first and second entries) and two intermolecular hydrogen bonds (Table 3, third and fourth entries) wher the crystallization water takes part, linking layers into a three-dimensional packing network (Fig. 3).

Experimental

A mixture of cobalt chloride (1 mmol), pyridine-3,4-dicarboxylic acid (1 mmol) and 2,2-bipyridine (2 mmol) in a 1:1 solvent mixture of H_2O and ethanol was kept at 473 K for 10 d in a 25 ml Teflon-lined stainless steel autoclave. Red crystals were obtained after cooling to room temperature (yield 22%). Analysis calculated for $C_{17}H_{15}CoN_3O_6$: C 49.04, H 3.61, N 10.12%; found: C 48.89, H 3.41, N 10.06%.

Refinement

The H atoms of the water molecule were located from difference density maps and were refined with distance restraints of H···H = 1.38 (2)Å and O—H = 0.88 (2) Å, and with a fixed U_{iso}(H) value of 0.80 Å^2. All other H atoms were placed in calculated positions, with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq} of the respective carrier atom.

Figures

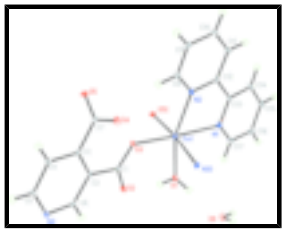

Fig. 1. The coordination of the Co atom in the title structure, drawn with 30% probability displacement ellipsoids. Atoms labeled with i at the symmetry positions ($x - 1/2$,$-y + 1/2$,$-z$).

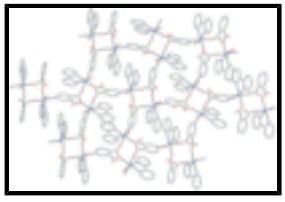

Fig. 2. A view of corrugated layers parallel to the [110] plane.

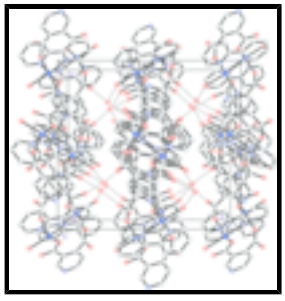

Fig. 3. Packing diagram formed *via* intermolecular hydrogen bonds.

Poly[[aqua(2,2-bipyridine)(μ$_3$-pyridine-3,4-dicarboxylato)cobalt(II)] monohydrate]

Crystal data

$[Co(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)]\cdot H_2O$	F_{000} = 1704
M_r = 416.25	D_x = 1.671 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3249 reflections
a = 15.7498 (5) Å	θ = 2.4–26.2º
b = 12.3488 (10) Å	μ = 1.08 mm^{-1}
c = 17.0168 (5) Å	*T* = 293 (2) K
V = 3309.6 (3) Å^3	Block, red
Z = 8	0.43 × 0.36 × 0.23 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	3249 independent reflections
Radiation source: fine-focus sealed tube	2562 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
T = 293(2) K	θ_{max} = 26.2º
φ and ω scans	θ_{min} = 2.4º

Absorption correction: multi-scan (SADABS; Bruker, 2001)
T_{min} = 0.654, T_{max} = 0.789
26510 measured reflections
h = −19→19
k = −15→15
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.163
S = 1.00
3249 reflections
256 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.119P)^2 + 0.8076P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −1.07 e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.1666 (2)	0.5122 (2)	0.05468 (19)	0.0207 (7)
C2	0.20645 (19)	0.6010 (2)	0.00657 (18)	0.0193 (6)
C3	0.1814 (2)	0.6283 (3)	−0.07012 (18)	0.0209 (7)
C4	0.2242 (2)	0.7129 (3)	−0.1059 (2)	0.0280 (8)
H4	0.2089	0.7350	−0.1562	0.034*
C5	0.2905 (2)	0.7654 (3)	−0.0662 (2)	0.0292 (8)
H5	0.3177	0.8225	−0.0914	0.035*
C6	0.2742 (2)	0.6578 (3)	0.04070 (19)	0.0222 (7)
H6	0.2906	0.6382	0.0913	0.027*
C7	0.1153 (2)	0.5687 (3)	−0.11957 (18)	0.0228 (7)
C8	−0.0243 (2)	0.2994 (3)	−0.1028 (2)	0.0300 (8)
H8	0.0076	0.3616	−0.1116	0.036*

C9	−0.0764 (3)	0.2621 (3)	−0.1624 (2)	0.0384 (9)
H9	−0.0793	0.2986	−0.2101	0.046*
C10	−0.1235 (3)	0.1708 (3)	−0.1501 (2)	0.0393 (9)
H10	−0.1583	0.1435	−0.1896	0.047*
C11	−0.1186 (2)	0.1197 (3)	−0.0777 (2)	0.0310 (8)
H11	−0.1514	0.0585	−0.0679	0.037*
C12	−0.06399 (19)	0.1603 (3)	−0.0191 (2)	0.0220 (7)
C13	−0.0539 (2)	0.1084 (3)	0.0589 (2)	0.0228 (7)
C14	−0.1060 (3)	0.0249 (3)	0.0844 (2)	0.0395 (10)
H14	−0.1502	0.0008	0.0527	0.047*
C15	−0.0923 (3)	−0.0224 (3)	0.1569 (2)	0.0419 (10)
H15	−0.1268	−0.0789	0.1738	0.050*
C16	−0.0271 (2)	0.0148 (3)	0.2043 (2)	0.0330 (8)
H16	−0.0160	−0.0162	0.2531	0.040*
C17	0.0208 (2)	0.0998 (3)	0.1760 (2)	0.0302 (8)
H17	0.0643	0.1262	0.2076	0.036*
Co1	0.06154 (3)	0.31049 (4)	0.06880 (3)	0.0275 (2)
H1W	0.171 (2)	0.264 (3)	0.190 (4)	0.080*
H2W	0.162 (3)	0.367 (2)	0.166 (3)	0.080*
H3W	0.262 (3)	0.107 (3)	0.204 (2)	0.080*
H4W	0.211 (3)	0.098 (3)	0.269 (2)	0.080*
N1	0.00877 (17)	0.1467 (2)	0.10612 (17)	0.0235 (6)
N2	−0.01773 (16)	0.2498 (2)	−0.03249 (17)	0.0225 (6)
N3	0.31687 (17)	0.7377 (2)	0.00600 (17)	0.0256 (6)
O1	0.13691 (16)	0.31271 (19)	0.18065 (16)	0.0300 (6)
O2	0.19348 (18)	0.4987 (2)	0.12382 (14)	0.0342 (6)
O3	0.11008 (14)	0.45667 (17)	0.02123 (14)	0.0261 (5)
O4	0.14178 (17)	0.4916 (2)	−0.15898 (15)	0.0367 (6)
O5	0.04092 (15)	0.6062 (2)	−0.12210 (15)	0.0331 (6)
O6	0.23530 (18)	0.13852 (19)	0.23886 (15)	0.0344 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0205 (15)	0.0129 (15)	0.0286 (18)	0.0010 (12)	0.0011 (13)	−0.0004 (12)
C2	0.0196 (15)	0.0138 (14)	0.0245 (16)	−0.0005 (11)	0.0047 (12)	−0.0019 (12)
C3	0.0175 (15)	0.0186 (16)	0.0266 (17)	0.0033 (12)	0.0029 (12)	−0.0012 (12)
C4	0.0306 (18)	0.0268 (17)	0.0265 (18)	0.0000 (14)	−0.0033 (15)	0.0069 (14)
C5	0.0284 (18)	0.0232 (18)	0.036 (2)	−0.0078 (14)	0.0013 (14)	0.0074 (14)
C6	0.0258 (16)	0.0204 (15)	0.0204 (16)	0.0005 (13)	0.0005 (13)	0.0010 (13)
C7	0.0262 (17)	0.0248 (17)	0.0174 (16)	0.0004 (13)	0.0025 (13)	0.0039 (13)
C8	0.0288 (18)	0.0287 (19)	0.032 (2)	−0.0021 (14)	0.0022 (16)	0.0076 (14)
C9	0.040 (2)	0.044 (2)	0.032 (2)	0.0019 (18)	−0.0035 (17)	0.0126 (17)
C10	0.036 (2)	0.044 (2)	0.039 (2)	−0.0031 (17)	−0.0118 (18)	0.0000 (18)
C11	0.0318 (19)	0.0277 (18)	0.033 (2)	−0.0084 (15)	−0.0068 (15)	−0.0010 (14)
C12	0.0192 (16)	0.0209 (16)	0.0259 (17)	0.0003 (12)	−0.0003 (13)	−0.0024 (13)
C13	0.0230 (16)	0.0170 (16)	0.0283 (18)	−0.0017 (12)	0.0013 (13)	−0.0034 (13)
C14	0.042 (2)	0.040 (2)	0.036 (2)	−0.0248 (18)	−0.0082 (18)	0.0037 (17)

C15	0.051 (2)	0.036 (2)	0.038 (2)	−0.0213 (19)	0.0000 (19)	0.0064 (17)
C16	0.041 (2)	0.0277 (19)	0.030 (2)	−0.0039 (15)	0.0008 (16)	0.0067 (15)
C17	0.0304 (18)	0.0310 (19)	0.0291 (19)	−0.0062 (15)	−0.0038 (15)	0.0003 (15)
Co1	0.0275 (3)	0.0217 (3)	0.0335 (3)	−0.00239 (18)	−0.00134 (19)	−0.00001 (18)
N1	0.0212 (14)	0.0225 (14)	0.0267 (15)	−0.0033 (11)	−0.0012 (11)	0.0028 (11)
N2	0.0211 (13)	0.0201 (14)	0.0263 (15)	−0.0007 (11)	0.0010 (11)	−0.0001 (11)
N3	0.0230 (14)	0.0219 (14)	0.0319 (16)	−0.0042 (11)	−0.0008 (12)	0.0006 (12)
O1	0.0341 (14)	0.0238 (13)	0.0320 (14)	−0.0035 (10)	−0.0030 (11)	0.0005 (10)
O2	0.0483 (15)	0.0269 (13)	0.0275 (14)	−0.0137 (11)	−0.0074 (11)	0.0062 (10)
O3	0.0278 (12)	0.0188 (11)	0.0317 (13)	−0.0065 (10)	−0.0014 (10)	0.0036 (9)
O4	0.0418 (15)	0.0306 (14)	0.0377 (15)	0.0108 (11)	−0.0022 (12)	−0.0153 (11)
O5	0.0226 (12)	0.0382 (15)	0.0386 (15)	0.0090 (11)	−0.0040 (11)	−0.0099 (12)
O6	0.0443 (16)	0.0290 (13)	0.0299 (14)	−0.0006 (12)	0.0059 (12)	−0.0001 (11)

Geometric parameters (Å, °)

C1—O3	1.259 (4)	C12—N2	1.343 (4)
C1—O2	1.262 (4)	C12—C13	1.483 (5)
C1—C2	1.506 (4)	C13—N1	1.358 (4)
C2—C6	1.403 (4)	C13—C14	1.387 (5)
C2—C3	1.404 (5)	C14—C15	1.382 (6)
C3—C4	1.384 (5)	C14—H14	0.9300
C3—C7	1.527 (4)	C15—C16	1.384 (6)
C4—C5	1.402 (5)	C15—H15	0.9300
C4—H4	0.9300	C16—C17	1.380 (5)
C5—N3	1.342 (5)	C16—H16	0.9300
C5—H5	0.9300	C17—N1	1.336 (5)
C6—N3	1.332 (4)	C17—H17	0.9300
C6—H6	0.9300	Co1—O5^{i}	2.118 (2)
C7—O4	1.237 (4)	Co1—O3	2.121 (2)
C7—O5	1.261 (4)	Co1—O1	2.243 (3)
C8—N2	1.348 (5)	Co1—N2	2.256 (3)
C8—C9	1.383 (6)	Co1—N1	2.276 (3)
C8—H8	0.9300	Co1—N3^{ii}	2.370 (3)
C9—C10	1.365 (6)	N3—Co1^{iii}	2.370 (3)
C9—H9	0.9300	O1—H1W	0.82 (4)
C10—C11	1.386 (5)	O1—H2W	0.82 (3)
C10—H10	0.9300	O5—Co1^{i}	2.118 (2)
C11—C12	1.410 (5)	O6—H3W	0.83 (4)
C11—H11	0.9300	O6—H4W	0.81 (4)
O3—C1—O2	125.9 (3)	C13—C14—H14	119.9
O3—C1—C2	116.5 (3)	C14—C15—C16	119.7 (3)
O2—C1—C2	117.6 (3)	C14—C15—H15	120.1
C6—C2—C3	118.6 (3)	C16—C15—H15	120.1
C6—C2—C1	117.1 (3)	C17—C16—C15	117.0 (3)
C3—C2—C1	124.2 (3)	C17—C16—H16	121.5
C4—C3—C2	116.9 (3)	C15—C16—H16	121.5
C4—C3—C7	116.9 (3)	N1—C17—C16	124.3 (3)

C2—C3—C7	126.0 (3)	N1—C17—H17	117.9
C3—C4—C5	120.0 (3)	C16—C17—H17	117.9
C3—C4—H4	120.0	$O5^{i}$—Co1—O3	91.41 (10)
C5—C4—H4	120.0	$O5^{i}$—Co1—O1	91.94 (10)
N3—C5—C4	123.6 (3)	O3—Co1—O1	97.05 (9)
N3—C5—H5	118.2	$O5^{i}$—Co1—N2	93.83 (9)
C4—C5—H5	118.2	O3—Co1—N2	100.98 (9)
N3—C6—C2	124.8 (3)	O1—Co1—N2	160.91 (9)
N3—C6—H6	117.6	$O5^{i}$—Co1—N1	91.94 (10)
C2—C6—H6	117.6	O3—Co1—N1	173.73 (10)
O4—C7—O5	125.3 (3)	O1—Co1—N1	88.13 (9)
O4—C7—C3	116.1 (3)	N2—Co1—N1	73.52 (10)
O5—C7—C3	118.4 (3)	$O5^{i}$—Co1—$N3^{ii}$	173.23 (10)
N2—C8—C9	123.0 (3)	O3—Co1—$N3^{ii}$	81.93 (9)
N2—C8—H8	118.5	O1—Co1—$N3^{ii}$	87.68 (10)
C9—C8—H8	118.5	N2—Co1—$N3^{ii}$	88.67 (10)
C10—C9—C8	119.0 (4)	N1—Co1—$N3^{ii}$	94.80 (10)
C10—C9—H9	120.5	C17—N1—C13	118.6 (3)
C8—C9—H9	120.5	C17—N1—Co1	125.6 (2)
C9—C10—C11	118.8 (4)	C13—N1—Co1	114.2 (2)
C9—C10—H10	120.6	C12—N2—C8	118.9 (3)
C11—C10—H10	120.6	C12—N2—Co1	116.3 (2)
C10—C11—C12	120.0 (3)	C8—N2—Co1	124.7 (2)
C10—C11—H11	120.0	C6—N3—C5	116.0 (3)
C12—C11—H11	120.0	C6—N3—$Co1^{iii}$	119.3 (2)
N2—C12—C11	120.3 (3)	C5—N3—$Co1^{iii}$	124.5 (2)
N2—C12—C13	116.7 (3)	Co1—O1—H1W	120 (4)
C11—C12—C13	123.0 (3)	Co1—O1—H2W	90 (4)
N1—C13—C14	120.3 (3)	H1W—O1—H2W	110 (3)
N1—C13—C12	117.2 (3)	C1—O3—Co1	123.1 (2)
C14—C13—C12	122.6 (3)	C7—O5—$Co1^{i}$	150.7 (2)
C15—C14—C13	120.1 (3)	H3W—O6—H4W	113 (3)
C15—C14—H14	119.9		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1W···O6	0.82 (4)	2.03 (4)	2.830 (4)	165 (5)
O1—H2W···O2	0.82 (3)	1.839 (15)	2.646 (3)	166 (5)
O6—H3W···$O2^{ii}$	0.83 (4)	2.04 (4)	2.841 (3)	166 (5)
O6—H4W···$O4^{iv}$	0.81 (4)	1.98 (4)	2.788 (3)	174 (5)

Symmetry codes: (ii) −*x*+1/2, *y*−1/2, *z*; (iv) *x*, −*y*+1/2, *z*+1/2.

Fig. 1

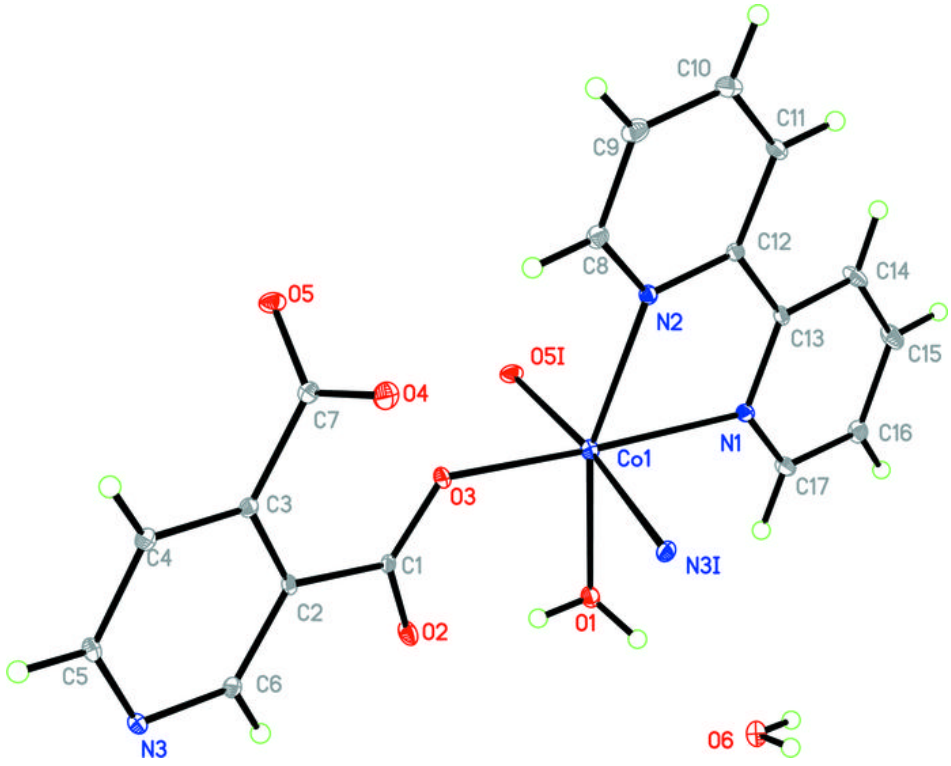
C10
C11
C9
C12
C8
C14
N2
C13
C15
O5I
O5
O4
C7
N1
C16
Co1
O3
C17
C3
N3I
C4
C1
C2
O1
O2
C5
C6
N3
O6

Fig. 2

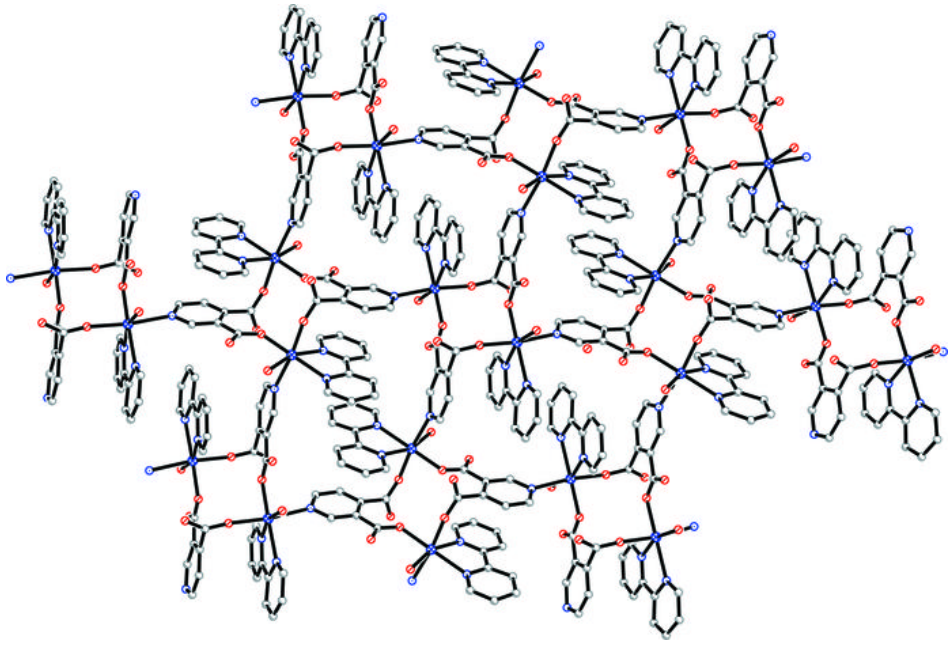

Fig. 3