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Poly[[(2,2-bipyridine-κ^2N,N')cobalt(II)]-μ_3-pyridine-3,4-dicarboxylato-$\kappa^4N{:}O^2{:}O^4,O^{4'}$]

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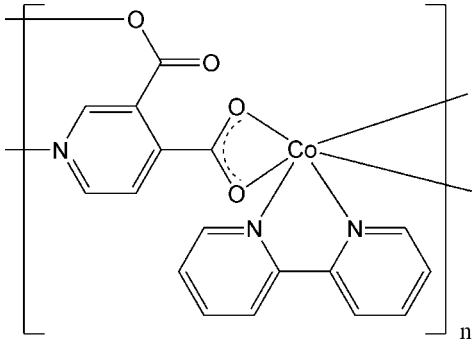
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.006 Å; R factor = 0.036; wR factor = 0.076; data-to-parameter ratio = 11.1.

In the title compound, $[Co(C_7H_3NO_4)(C_{10}H_8N_2)]_n$, the Co^{II} atom has a distorted octahedral coordination geometry, being coordinated by three N atoms and three carboxylate O atoms from chelating 2,2′-bipyridine and pyridine-3,4-dicarboxylate ligands. The compound exhibits a two-dimensional layer structure. This supramolecular network is consolidated by π–π stacking interactions [3.979 (3) Å].

Related literature

For related literature, see: Qin *et al.* (2005); Wang *et al.* (2005).



Experimental

Crystal data

$[Co(C_7H_3NO_4)(C_{10}H_8N_2)]$
M_r = 380.22
Monoclinic, Pc
a = 7.6088 (15) Å
b = 9.3094 (19) Å
c = 12.270 (4) Å
β = 122.38 (2)°
V = 734.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.20 mm^{-1}
T = 113 (2) K
0.10 × 0.08 × 0.04 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan *CrystalClear* (Rigaku/MSC, 2005)
T_{min} = 0.872, T_{max} = 0.954
5529 measured reflections
2503 independent reflections
2213 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.076
S = 1.00
2503 reflections
226 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Absolute structure: Flack (1983), with 744 Friedel pairs
Flack parameter: 0.011 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O4^{i}	0.95	2.20	3.118 (4)	163
C4—H4···O2^{ii}	0.95	2.43	2.990 (5)	117
C4—H4···O4^{ii}	0.95	2.38	2.940 (4)	117
C5—H5···O1^{iii}	0.95	2.42	3.337 (4)	161
C10—H10···O1^{iv}	0.95	2.59	3.224 (5)	124
C14—H14···O4^{v}	0.95	2.55	3.445 (4)	156
C17—H17···O4^{i}	0.95	2.51	3.394 (4)	155

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: ZL2031).

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supplementary materials

Acta Cryst. (2007). E**63**, m1789 [**doi:10.1107/S160053680702541X**]

Poly[[(2,2-bipyridine-κ^2N,N')cobalt(II)]-μ_3-pyridine-3,4-dicarboxylato-$\kappa^4N:O^2:O^4,O^{4'}$]

H.-H. Song and Y.-J. Li

Comment

The rational design and construction of metal-organic polymers is of current interest in the fields of supramolecular chemistry and crystal engineering. The pyridine-3,4-dicarboxylate anion (PDB) has recently been found by us and others to act as an excellent building block in the construction of coordination polymers. Some two-dimensional layered structures of metal-organic polymers containing PDB have been reported previously (Qin *et al.*, 2005; Wang *et al.*, 2005). We present here the crystal structure of the title compound, (I), which is another example of a coordination polymer compound with a layered structure.

As shown in Fig. 1, the asymmetric unit of (I) contains one Co ^{II} atom, one PDB and one 2,2'-bipyridine (bpy) ligand. The Co^{II} center exhibits a distorted octahedral geometry and its coordination environment is made up of three O atoms from two different PDB ligands and three N atoms from one chelating bpy and one PDB ligand. The Co—O bond distances range from 2.005 (2) to 2.206 (2) Å, while the Co—N bond distances range from 2.081 (3) to 2.145 (3) Å.

Each PDB ligand is connecting three different Co^{II} atoms, with the Co^{II} ions linked by the PDB ligands in such a way as to form a two-dimensionally layered structure as shown in Figure 2. The bpy groups bristle out in opposite directions and nearly perpendicular to the two-dimensional layer (Figure 3). Via π-π stacking interactions the bpy extend the layered structure into a three-dimensional supramolecular network, the closets face-to-face distance between neighbouring parallel planes is 3.979 (3)Å (Ring 1: N2, C8 to C12, Ring 2: N3, C13 to C17, symmetry code for Ring 2: x, $1 - y$, $1/2 + z$).

Experimental

A mixture of $CoCl_2 \cdot 6H_2O$ (0.3 mmol), pyridine-3,4-dicarboxylic acid (0.3 mmol), 2,2'-bipyridine (0.3 mmol), NaF (0.3 mmol) and water (8 mL) was placed in a 15 mL Teflon reactor, which was then heated to 443 K for 5 d. The reactor was cooled to room temperature at a rate of 10 K h^{-1}. CHN analysis for (I) (found/calculated): C 53.45 (53.70), H 2.87 (2.92), N 10.98% (11.05%).

Refinement

The H atoms were placed in calculated positions, with C—H = 0.95 Å, and treated as riding atoms in the final cycles of refinement, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

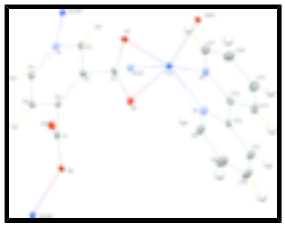


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme and with 30% probability displacement ellipsoids. [Symmetry codes: (#1) $x + 1, y, z$; (#2) $x + 1/2, -y, z + 1/2$; (#3) $x - 1, y, z$; (#4) $x - 1/2, -y, z - 1/2$.]

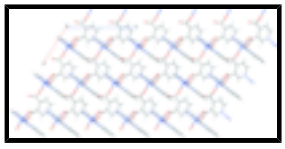


Fig. 2. A packing model of (I), view perpendicular to the two-dimensional layer. H atoms have been ommited for clarity.

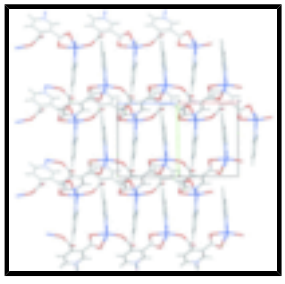


Fig. 3. A packing model of (I) showing the π-π interactions of the bipyridine units connecting the two-dimensional layers to a three-dimensional supramolecular structure. H atoms have been ommited for clarity.

Poly[[(2,2-bipyridine-κ^2*N*,*N*')cobalt(II)]-μ$_3$– pyridine-3,4-dicarboxylato-κ^4*N*:*O*^{4},*O*$^{4'}$:*O*^{2}]

Crystal data

$[Co(C_7H_3NO_4)(C_{10}H_8N_2)]$	$F_{000} = 386$
$M_r = 380.22$	$D_x = 1.720$ Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation λ = 0.71073 Å
a = 7.6088 (15) Å	Cell parameters from 2320 reflections
b = 9.3094 (19) Å	θ = 2.3–22.5º
c = 12.270 (4) Å	μ = 1.20 mm^{-1}
β = 122.38 (2)º	*T* = 113 (2) K
V = 734.0 (3) Å^3	Block, red
Z = 2	0.10 × 0.08 × 0.04 mm

Data collection

Rigaku Saturn diffractometer	2503 independent reflections
Radiation source: fine-focus sealed tube	2213 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.048$
Detector resolution: 7.31 pixels mm^{-1}	$\theta_{max} = 27.9$º
T = 113(2) K	$\theta_{min} = 2.2$º
ω scans	*h* = −10→9
Absorption correction: multi-scan	*k* = −12→12

CrystalClear (Rigaku/MSC, 2005)
T_{min} = 0.872, T_{max} = 0.954
5529 measured reflections

l = −10→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.076
S = 1.00
2503 reflections
226 parameters
2 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Extinction correction: none
Absolute structure: Flack (1983), with 744 Friedel pairs
Flack parameter: 0.011 (17)

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}
Co1	0.50834 (8)	0.24293 (4)	0.20068 (6)	0.00871 (11)
O1	0.4769 (4)	0.0409 (2)	0.2777 (3)	0.0112 (5)
O2	0.2656 (4)	0.2200 (3)	0.2460 (3)	0.0113 (6)
O3	−0.2251 (4)	0.2032 (3)	0.2097 (3)	0.0129 (6)
O4	−0.1534 (4)	0.0769 (3)	0.0818 (2)	0.0127 (5)
N1	0.2994 (5)	−0.1568 (3)	0.5116 (3)	0.0099 (6)
N2	0.4530 (5)	0.4600 (3)	0.1544 (3)	0.0128 (6)
N3	0.6816 (5)	0.3421 (3)	0.3838 (3)	0.0120 (7)
C1	0.3287 (5)	0.0950 (3)	0.2830 (4)	0.0101 (7)
C2	0.2350 (6)	0.0062 (4)	0.3423 (4)	0.0100 (7)
C3	0.3636 (5)	−0.0813 (3)	0.4451 (4)	0.0107 (7)
H3	0.5052	−0.0892	0.4708	0.013*

C4	0.0944 (5)	−0.1461 (3)	0.4696 (4)	0.0110 (7)
H4	0.0435	−0.2012	0.5122	0.013*
C5	−0.0422 (5)	−0.0603 (3)	0.3693 (4)	0.0113 (7)
H5	−0.1833	−0.0549	0.3451	0.014*
C6	0.0253 (5)	0.0196 (3)	0.3022 (3)	0.0092 (7)
C7	−0.1292 (5)	0.1065 (3)	0.1871 (3)	0.0099 (7)
C8	0.3328 (7)	0.5112 (4)	0.0342 (4)	0.0154 (8)
H8	0.2786	0.4457	−0.0360	0.018*
C9	0.2839 (7)	0.6566 (4)	0.0078 (4)	0.0233 (9)
H9	0.1985	0.6901	−0.0784	0.028*
C10	0.3635 (7)	0.7499 (4)	0.1107 (4)	0.0209 (9)
H10	0.3322	0.8495	0.0960	0.025*
C11	0.4897 (6)	0.6986 (4)	0.2361 (4)	0.0166 (8)
H11	0.5466	0.7620	0.3077	0.020*
C12	0.5303 (6)	0.5526 (4)	0.2537 (4)	0.0114 (7)
C13	0.6628 (6)	0.4874 (4)	0.3840 (4)	0.0128 (8)
C14	0.7617 (6)	0.5654 (4)	0.4969 (4)	0.0173 (8)
H14	0.7477	0.6669	0.4952	0.021*
C15	0.8815 (7)	0.4939 (4)	0.6129 (4)	0.0217 (9)
H15	0.9502	0.5458	0.6918	0.026*
C16	0.9007 (7)	0.3454 (4)	0.6133 (4)	0.0215 (9)
H16	0.9821	0.2941	0.6920	0.026*
C17	0.7985 (6)	0.2745 (4)	0.4967 (4)	0.0164 (8)
H17	0.8117	0.1731	0.4964	0.020*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.00969 (18)	0.00813 (19)	0.0088 (2)	−0.0001 (2)	0.00528 (17)	−0.0001 (2)
O1	0.0093 (12)	0.0120 (12)	0.0105 (14)	0.0022 (9)	0.0040 (12)	0.0012 (10)
O2	0.0130 (14)	0.0106 (12)	0.0115 (15)	−0.0013 (10)	0.0073 (13)	−0.0005 (11)
O3	0.0083 (13)	0.0113 (11)	0.0177 (16)	0.0008 (10)	0.0061 (13)	0.0022 (11)
O4	0.0110 (13)	0.0182 (13)	0.0061 (14)	−0.0008 (11)	0.0028 (12)	−0.0007 (10)
N1	0.0131 (16)	0.0094 (13)	0.0104 (18)	0.0003 (12)	0.0084 (16)	0.0001 (12)
N2	0.0193 (18)	0.0105 (14)	0.0128 (16)	−0.0007 (12)	0.0114 (16)	0.0002 (12)
N3	0.0130 (16)	0.0113 (14)	0.0116 (18)	−0.0008 (12)	0.0066 (16)	0.0031 (13)
C1	0.0066 (16)	0.0113 (16)	0.0083 (19)	−0.0012 (13)	0.0012 (16)	−0.0010 (14)
C2	0.0095 (17)	0.0102 (16)	0.0095 (19)	0.0015 (14)	0.0046 (17)	0.0016 (14)
C3	0.0109 (17)	0.0110 (16)	0.010 (2)	−0.0048 (13)	0.0057 (17)	−0.0065 (14)
C4	0.0116 (17)	0.0122 (16)	0.0103 (19)	−0.0027 (14)	0.0067 (17)	−0.0021 (14)
C5	0.0095 (17)	0.0123 (16)	0.0120 (19)	−0.0006 (13)	0.0056 (17)	−0.0016 (14)
C6	0.0093 (17)	0.0075 (15)	0.0088 (19)	−0.0017 (13)	0.0037 (16)	−0.0034 (13)
C7	0.0098 (17)	0.0104 (15)	0.0092 (19)	−0.0017 (13)	0.0048 (17)	0.0011 (13)
C8	0.023 (2)	0.0125 (18)	0.011 (2)	−0.0022 (16)	0.0093 (19)	0.0011 (15)
C9	0.033 (2)	0.0196 (19)	0.014 (2)	0.0044 (18)	0.010 (2)	0.0055 (17)
C10	0.034 (2)	0.0096 (17)	0.022 (2)	0.0023 (17)	0.016 (2)	0.0039 (16)
C11	0.022 (2)	0.0116 (16)	0.017 (2)	−0.0013 (15)	0.010 (2)	−0.0012 (15)
C12	0.0102 (16)	0.0113 (16)	0.014 (2)	−0.0036 (14)	0.0070 (18)	−0.0030 (14)

C13	0.0105 (17)	0.0149 (18)	0.016 (2)	−0.0003 (15)	0.0087 (18)	−0.0014 (16)
C14	0.021 (2)	0.0140 (17)	0.016 (2)	−0.0063 (15)	0.009 (2)	−0.0079 (16)
C15	0.026 (2)	0.020 (2)	0.013 (2)	−0.0017 (17)	0.006 (2)	−0.0076 (17)
C16	0.026 (2)	0.021 (2)	0.015 (2)	0.0049 (17)	0.009 (2)	0.0022 (17)
C17	0.0186 (19)	0.0164 (17)	0.015 (2)	0.0002 (15)	0.0094 (19)	0.0011 (15)

Geometric parameters (Å, °)

Co1—O3^{i}	2.005 (2)	C4—C5	1.365 (5)
Co1—N2	2.081 (3)	C4—H4	0.9500
Co1—N3	2.113 (3)	C5—C6	1.395 (4)
Co1—N1^{ii}	2.145 (3)	C5—H5	0.9500
Co1—O1	2.175 (2)	C6—C7	1.501 (5)
Co1—O2	2.206 (2)	C8—C9	1.395 (5)
Co1—C1	2.503 (3)	C8—H8	0.9500
O1—C1	1.267 (4)	C9—C10	1.377 (6)
O2—C1	1.249 (4)	C9—H9	0.9500
O3—C7	1.279 (4)	C10—C11	1.391 (6)
O3—Co1^{iii}	2.005 (2)	C10—H10	0.9500
O4—C7	1.235 (4)	C11—C12	1.384 (5)
N1—C3	1.350 (4)	C11—H11	0.9500
N1—C4	1.359 (4)	C12—C13	1.488 (6)
N1—Co1^{iv}	2.145 (3)	C13—C14	1.377 (5)
N2—C8	1.339 (5)	C14—C15	1.382 (6)
N2—C12	1.344 (5)	C14—H14	0.9500
N3—C17	1.336 (5)	C15—C16	1.390 (5)
N3—C13	1.361 (4)	C15—H15	0.9500
C1—C2	1.509 (4)	C16—C17	1.377 (6)
C2—C3	1.375 (5)	C16—H16	0.9500
C2—C6	1.401 (4)	C17—H17	0.9500
C3—H3	0.9500		
O3^{i}—Co1—N2	104.20 (11)	C2—C3—H3	118.2
O3^{i}—Co1—N3	89.16 (12)	N1—C4—C5	123.4 (3)
N2—Co1—N3	77.63 (12)	N1—C4—H4	118.3
O3^{i}—Co1—N1^{ii}	97.62 (11)	C5—C4—H4	118.3
N2—Co1—N1^{ii}	98.26 (12)	C4—C5—C6	120.1 (3)
N3—Co1—N1^{ii}	172.80 (12)	C4—C5—H5	120.0
O3^{i}—Co1—O1	99.20 (10)	C6—C5—H5	120.0
N2—Co1—O1	154.86 (9)	C5—C6—C2	117.1 (3)
N3—Co1—O1	93.81 (11)	C5—C6—C7	119.5 (3)
N1^{ii}—Co1—O1	87.51 (10)	C2—C6—C7	123.3 (3)
O3^{i}—Co1—O2	157.94 (10)	O4—C7—O3	127.0 (3)
N2—Co1—O2	95.05 (10)	O4—C7—C6	117.8 (3)
N3—Co1—O2	84.49 (11)	O3—C7—C6	115.2 (3)
N1^{ii}—Co1—O2	90.04 (10)	N2—C8—C9	122.7 (4)
O1—Co1—O2	60.33 (9)	N2—C8—H8	118.6

O3^{i}—Co1—C1	129.11 (11)	C9—C8—H8	118.6
N2—Co1—C1	124.77 (11)	C10—C9—C8	117.8 (4)
N3—Co1—C1	88.61 (11)	C10—C9—H9	121.1
N1^{ii}—Co1—C1	88.97 (11)	C8—C9—H9	121.1
O1—Co1—C1	30.42 (9)	C9—C10—C11	120.1 (3)
O2—Co1—C1	29.91 (10)	C9—C10—H10	119.9
C1—O1—Co1	89.25 (19)	C11—C10—H10	119.9
C1—O2—Co1	88.32 (18)	C12—C11—C10	118.3 (4)
C7—O3—Co1^{iii}	142.7 (2)	C12—C11—H11	120.8
C3—N1—C4	116.4 (3)	C10—C11—H11	120.8
C3—N1—Co1^{iv}	123.3 (2)	N2—C12—C11	122.3 (4)
C4—N1—Co1^{iv}	118.2 (2)	N2—C12—C13	115.3 (3)
C8—N2—C12	118.7 (3)	C11—C12—C13	122.3 (3)
C8—N2—Co1	124.4 (2)	N3—C13—C14	121.6 (4)
C12—N2—Co1	116.7 (2)	N3—C13—C12	114.5 (3)
C17—N3—C13	118.6 (4)	C14—C13—C12	123.8 (3)
C17—N3—Co1	125.9 (2)	C13—C14—C15	119.1 (3)
C13—N3—Co1	115.4 (3)	C13—C14—H14	120.5
O2—C1—O1	122.1 (3)	C15—C14—H14	120.5
O2—C1—C2	119.8 (3)	C14—C15—C16	119.6 (4)
O1—C1—C2	118.0 (3)	C14—C15—H15	120.2
O2—C1—Co1	61.77 (16)	C16—C15—H15	120.2
O1—C1—Co1	60.33 (16)	C17—C16—C15	118.2 (4)
C2—C1—Co1	175.8 (3)	C17—C16—H16	120.9
C3—C2—C6	119.5 (3)	C15—C16—H16	120.9
C3—C2—C1	118.6 (3)	N3—C17—C16	123.0 (3)
C6—C2—C1	121.7 (3)	N3—C17—H17	118.5
N1—C3—C2	123.6 (3)	C16—C17—H17	118.5
N1—C3—H3	118.2		
O3^{i}—Co1—O1—C1	170.5 (2)	O2—C1—C2—C6	33.5 (5)
N2—Co1—O1—C1	12.0 (4)	O1—C1—C2—C6	−149.5 (3)
N3—Co1—O1—C1	80.7 (2)	C4—N1—C3—C2	1.9 (5)
N1^{ii}—Co1—O1—C1	−92.2 (2)	Co1^{iv}—N1—C3—C2	−161.7 (3)
O2—Co1—O1—C1	−0.7 (2)	C6—C2—C3—N1	−0.1 (5)
O3^{i}—Co1—O2—C1	−22.9 (4)	C1—C2—C3—N1	174.8 (3)
N2—Co1—O2—C1	−173.9 (2)	C3—N1—C4—C5	−2.6 (5)
N3—Co1—O2—C1	−96.8 (2)	Co1^{iv}—N1—C4—C5	161.8 (3)
N1^{ii}—Co1—O2—C1	87.9 (2)	N1—C4—C5—C6	1.6 (5)
O1—Co1—O2—C1	0.7 (2)	C4—C5—C6—C2	0.3 (5)
O3^{i}—Co1—N2—C8	94.4 (3)	C4—C5—C6—C7	176.3 (3)
N3—Co1—N2—C8	−179.7 (3)	C3—C2—C6—C5	−1.0 (5)
N1^{ii}—Co1—N2—C8	−5.7 (3)	C1—C2—C6—C5	−175.8 (3)
O1—Co1—N2—C8	−107.5 (3)	C3—C2—C6—C7	−176.8 (3)
O2—Co1—N2—C8	−96.4 (3)	C1—C2—C6—C7	8.4 (5)
C1—Co1—N2—C8	−100.2 (3)	Co1^{iii}—O3—C7—O4	81.2 (5)
O3^{i}—Co1—N2—C12	−91.3 (2)	Co1^{iii}—O3—C7—C6	−97.6 (4)

N3—Co1—N2—C12	−5.3 (2)	C5—C6—C7—O4	−119.0 (3)
N1^{ii}—Co1—N2—C12	168.7 (2)	C2—C6—C7—O4	56.7 (5)
O1—Co1—N2—C12	66.8 (4)	C5—C6—C7—O3	59.9 (4)
O2—Co1—N2—C12	77.9 (2)	C2—C6—C7—O3	−124.4 (3)
C1—Co1—N2—C12	74.2 (3)	C12—N2—C8—C9	−0.2 (5)
O3^{i}—Co1—N3—C17	−73.7 (3)	Co1—N2—C8—C9	174.0 (3)
N2—Co1—N3—C17	−178.4 (3)	N2—C8—C9—C10	−0.1 (6)
O1—Co1—N3—C17	25.5 (3)	C8—C9—C10—C11	0.5 (6)
O2—Co1—N3—C17	85.2 (3)	C9—C10—C11—C12	−0.6 (5)
C1—Co1—N3—C17	55.5 (3)	C8—N2—C12—C11	0.2 (5)
O3^{i}—Co1—N3—C13	109.0 (2)	Co1—N2—C12—C11	−174.5 (2)
N2—Co1—N3—C13	4.2 (2)	C8—N2—C12—C13	−179.8 (3)
O1—Co1—N3—C13	−151.9 (2)	Co1—N2—C12—C13	5.6 (4)
O2—Co1—N3—C13	−92.2 (2)	C10—C11—C12—N2	0.2 (5)
C1—Co1—N3—C13	−121.9 (2)	C10—C11—C12—C13	−179.8 (3)
Co1—O2—C1—O1	−1.3 (4)	C17—N3—C13—C14	0.3 (5)
Co1—O2—C1—C2	175.5 (3)	Co1—N3—C13—C14	177.9 (3)
Co1—O1—C1—O2	1.3 (4)	C17—N3—C13—C12	179.8 (3)
Co1—O1—C1—C2	−175.5 (3)	Co1—N3—C13—C12	−2.7 (3)
O3^{i}—Co1—C1—O2	169.13 (19)	N2—C12—C13—N3	−1.8 (4)
N2—Co1—C1—O2	7.5 (3)	C11—C12—C13—N3	178.2 (3)
N3—Co1—C1—O2	81.3 (2)	N2—C12—C13—C14	177.6 (3)
N1^{ii}—Co1—C1—O2	−91.9 (2)	C11—C12—C13—C14	−2.3 (5)
O1—Co1—C1—O2	−178.7 (4)	N3—C13—C14—C15	−0.5 (5)
O3^{i}—Co1—C1—O1	−12.2 (3)	C12—C13—C14—C15	−179.9 (3)
N2—Co1—C1—O1	−173.8 (2)	C13—C14—C15—C16	0.3 (5)
N3—Co1—C1—O1	−99.9 (2)	C14—C15—C16—C17	0.1 (6)
N1^{ii}—Co1—C1—O1	86.8 (2)	C13—N3—C17—C16	0.1 (5)
O2—Co1—C1—O1	178.7 (4)	Co1—N3—C17—C16	−177.2 (3)
O2—C1—C2—C3	−141.3 (4)	C15—C16—C17—N3	−0.3 (6)
O1—C1—C2—C3	35.7 (5)		

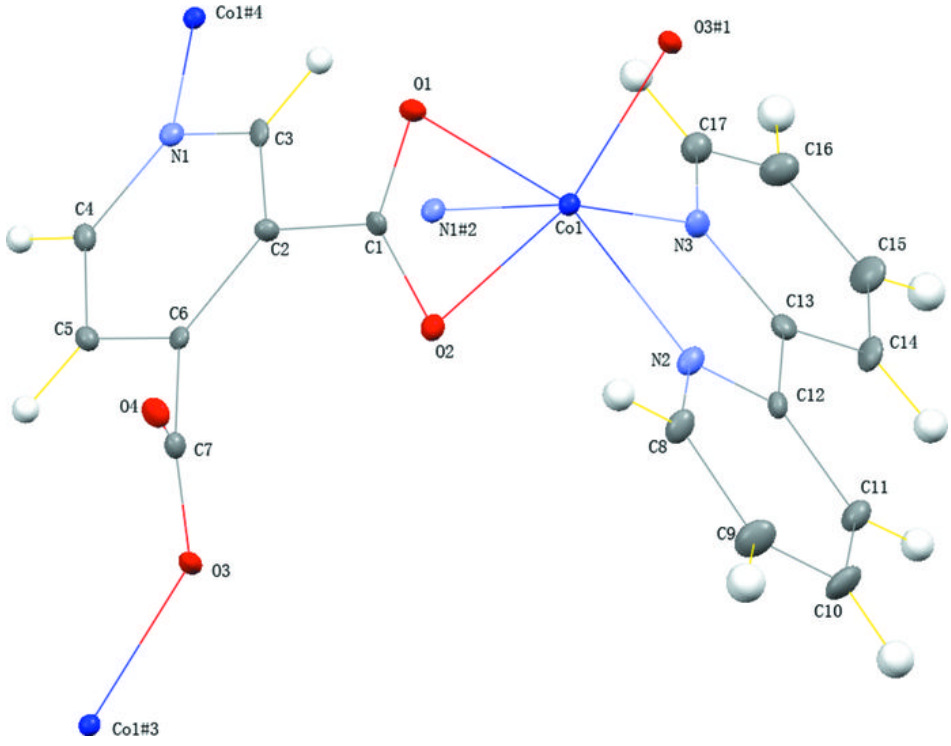
Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*, −*y*, *z*−1/2; (iii) *x*−1, *y*, *z*; (iv) *x*, −*y*, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O4^{v}	0.95	2.20	3.118 (4)	163
C4—H4···O2^{iv}	0.95	2.43	2.990 (5)	117
C4—H4···O4^{iv}	0.95	2.38	2.940 (4)	117
C5—H5···O1^{iii}	0.95	2.42	3.337 (4)	161
C10—H10···O1^{vi}	0.95	2.59	3.224 (5)	124
C14—H14···O4^{vii}	0.95	2.55	3.445 (4)	156
C17—H17···O4^{v}	0.95	2.51	3.394 (4)	155

Symmetry codes: (v) *x*+1, −*y*, *z*+1/2; (iv) *x*, −*y*, *z*+1/2; (iii) *x*−1, *y*, *z*; (vi) *x*, *y*+1, *z*; (vii) *x*+1, −*y*+1, *z*+1/2.

Fig. 1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C17
C16
N1
C3
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N1#2
Co1
N3
C15
C2
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C13
C5
C6
O2
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O4
C12
C8
C7
C11
C9
O3
C10
Co1#3

Fig. 2

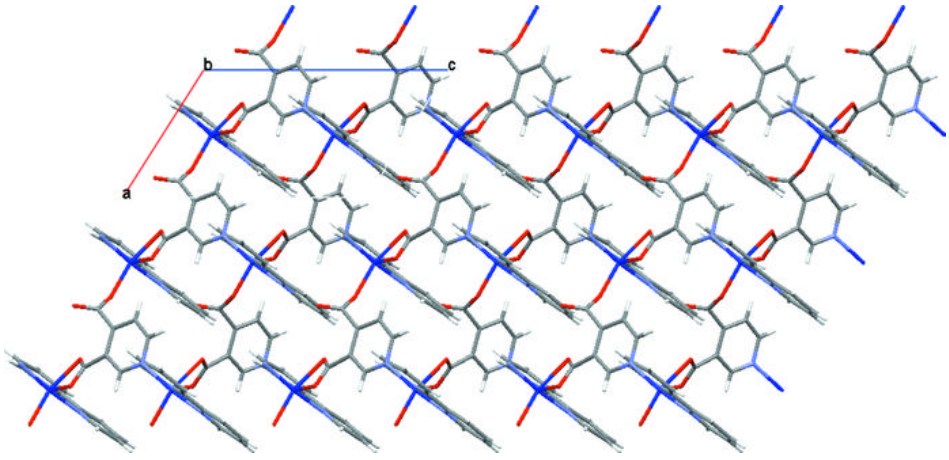

Fig. 3