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Poly[propane-1,3-diammonium [diaqua-(μ_4-4-benzene-1,2,4,5-tetracarboxylato)-cobaltate(II)] hemihydrate]

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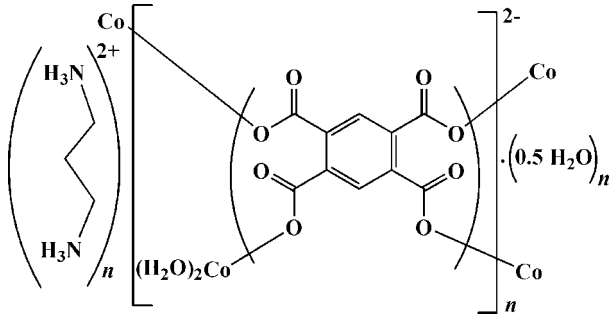
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; disorder in solvent or counterion; R factor = 0.022; wR factor = 0.066; data-to-parameter ratio = 18.9.

The title polymeric compound, $\{(C_3H_{12}N_2)[Co(C_{10}H_2O_8)(H_2O)_2]\cdot 0.5H_2O\}_n$, was obtained by the reaction of cobalt(II) nitrate hexahydrate with the proton-transfer compound $(pnH_2)_2(btc)\cdot 2H_2O$ (pn = propane-1,3-diamine and $btcH_4$ = benzene-1,2,4,5-tetracarboxylic acid) in aqueous solution. Each Co^{2+} ion is situated on a crystallographic twofold rotation axis and is coordinated in a distorted octahedral geometry by six O atoms [Co—O = 2.0650 (9)–2.1107 (8) Å] from two coordinated water molecules and four $(btc)^{4-}$ ligands which also act as bridging ligands between Co^{2+} ions. In the crystal structure, a wide range of non-covalent interactions consisting of O—H···O, N—H···O and C—H···O hydrogen bonds, as well as ion pairing, van der Waals forces and C—H···π stacking between the propane-1,3-diammonium ions and the aromatic rings of benzene-1,2,4,5-tetracarboxylate ligands, connect the various fragments, forming a three-dimensional supramolecular structure. The crystal studied was an inversion twin.

Related literature

For related literature, see: Aghabozorg, Attar Gharamaleki *et al.* (2007); Aghabozorg, Bahrami *et al.* (2007); Aghabozorg, Ghadermazi & Attar Gharamaleki (2006); Aghabozorg, Ghadermazi *et al.* (2007); Aghabozorg, Ghasemikhah, Ghadermazi *et al.* (2006); Aghabozorg, Ghasemikhah, Soleimannejad *et al.* (2006); Aghabozorg, Manteghi & Ghadermazi (2007); Aghabozorg, Zabihi *et al.* (2006); Sharif *et al.* (2007).



Experimental

Crystal data

$(C_3H_{12}N_2)[Co(C_{10}H_2O_8)(H_2O)_2]\cdot 0.5H_2O$
M_r = 430.23
Orthorhombic, *Ima*2
a = 16.4011 (3) Å
b = 7.1786 (1) Å
c = 14.2586 (2) Å
V = 1678.76 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.09 mm^{-1}
T = 100 (2) K
0.22 × 0.18 × 0.13 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.796, T_{max} = 0.872
19141 measured reflections
2526 independent reflections
2479 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.066
S = 1.00
2526 reflections
134 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack (1983), with 1214 Friedel pairs
Flack parameter: 0.375 (11)

Table 1
Selected geometric parameters (Å, °).

Co1—O1^{i}	2.0650 (9)	Co1—O5	2.1107 (8)
Co1—O4	2.0910 (9)		
O1^{i}—Co1—O4	174.14 (4)	O5^{ii}—Co1—O5	177.26 (6)

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

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

Cg is the centroid of the aromatic ring

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5*B*···O3	0.89	1.85	2.680 (1)	153
O5—H5*A*···O2^{iii}	0.89	1.91	2.737 (1)	154
N1—H1*B*···O2^{iii}	0.91	1.93	2.831 (1)	168
N1—H1*C*···O4^{iv}	0.91	1.95	2.843 (2)	166
N1—H1*D*···O3^{i}	0.91	2.11	2.988 (2)	161
C7—H7*B*···*Cg*^{v}	0.99	2.98	3.767 (2)	137
C8—H8*B*···*Cg*^{vi}	0.99	2.61	3.439 (2)	141

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

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Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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, 2005); software used to prepare material for publication: *SHELXTL* Bruker, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2167).

References

Aghabozorg, H., Attar Gharamaleki, J., Ghasemikhah, P., Ghadermazi, M. & Soleimannejad, J. (2007). *Acta Cryst.*, ***E63***, m1710-m1711.

Aghabozorg, H., Bahrami, Z., Tabatabaie, M., Ghadermazi, M. & Attar Gharamaleki, J. (2007). *Acta Cryst.*, ***E63***, m2022-m2023.

Aghabozorg, H., Ghadermazi, M., Sheshmani, S. & Attar Gharamaleki, J. (2007). *Acta Cryst.*, ***E63***, o2985-o2986.

Aghabozorg, H., Ghadermazi, M. & Attar Gharamaleki, J. (2006). *Acta Cryst.*, ***E62***, o3174-o3176.

Aghabozorg, H., Ghasemikhah, P., Ghadermazi, M., Attar Gharamaleki, J. & Sheshmani, S. (2006). *Acta Cryst.*, ***E62***, m2022-m2023.

Aghabozorg, H., Ghasemikhah, P., Soleimannejad, J., Ghadermazi, M. & Attar Gharamaleki, J. (2006). *Acta Cryst.*, ***E62***, m2266-m2268.

Aghabozorg, H., Manteghi, F. & Ghadermazi, M. (2007). *Acta Cryst.*, ***E6***3, Submitted.

Aghabozorg, H., Zabihi, F., Ghadermazi, M., Attar Gharamaleki, J. & Sheshmani, S. (2006). *Acta Cryst.*, ***E62***, m2269-m2271.

Bruker (2005). *APEXII* (Version 2.0-1), *SAINT* (Version 7.23A), *SADABS* (Version 2004/1), *XPREP* (Version 2005/2) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Sharif, M. A., Aghabozorg, H., Motyeian, E., Ghadermazi, M. & Attar Gharamaleki, J. (2007). *Acta Cryst.*, ***E63***, m2235-m2236.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*, University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, m2793-m2794 [**doi:10.1107/S1600536807050659**]

Poly[propane-1,3-diammonium [diaqua(μ_4-4-benzene-1,2,4,5-tetracarboxylato)cobaltate(II)] hemihydrate]

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Comment

We have reported cases in which proton transfer from benzene-1,2,4,5-tetracarboxylic acid ($btcH_4$) to propane-1,3-diamine (pn), piperazine (pipz) and 1,10-phenanthroline (phen), resulted in the formation of novel self assembled $(pnH_2)_2(btc)\cdot 2H_2O$ (Aghabozorg, Ghadermazi *et al*., 2007), $(pipzH_2)_2(btc)\cdot 6.2H_2O$ (Aghabozorg, Manteghi, Ghadermazi 2007) and $(phenH)_4(btcH_3)_2(btcH_2)$ (Aghabozorg, Ghadermazi & Attar Gharamaleki, 2006) systems, respectively. The resulting compounds, with some remaining sites as electron donors, can coordinate to metal ions (Aghabozorg, Ghasemikhah, Ghadermazi *et al.*, 2006; Aghabozorg, Ghasemikhah, Soleimannejad *et al.*, 2006). For the crystal structures of related complexes, see: Aghabozorg, Bahrami, *et al.*, (2007); Aghabozorg, Zabihi *et al.*, 2006; Aghabozorg, Attar Gharamaleki *et al.*, 2007).

Here, we report a new polymeric compound obtained from reaction of $(pnH_2)_2(btc)\cdot 2H_2O$ with cobalt(II) nitrate. The crystal structure of the title polymeric compound is shown in Fig. 1. The negative charge of the anionic complex is neutralized by dicationic propane-1,3-diammonium ions. The Co^{2+} atom is situated on a crystallographic twofold rotation axis.

Co^{2+} is six-coordinated by four $(btc)^{4-}$ groups and two coordinated water molecules, *i.e.* each $(btc)^{4-}$ fragments coordinates through one O atom of the $(COO)^-$ fragments, which also act as bridging ligands between other Co^{2+} ions. O5 and O5a atoms of two coordinated water molecules occupy the axial positions, while four O atoms of $(btc)^{4-}$ fragments form the equatorial plane. The axial bond is slightly longer than the equatorial bond lengths. The $O5^{iii}$—Co1—O5 bond angle is slightly deviated from linearity. The coordination around Co^{2+} is distorted octahedral.

A considerable feature of the compound (Sharif *et al.*, 2007) is the presence of C—H···π stacking interactions between C—H groups of $(pnH_2)^{2+}$ cations and aromatic rings of $(btc)^{4-}$ fragments (Fig. 2). The most important feature of the crystal structure is the presence of a large number of O—H···O, N—H···O and C—H···O hydrogen bonds between $(pnH_2)^{2+}$ and $[Co(H_2O)_2(btc)]^{2-}$ fragments and uncoordinated water molecules with D···A distances ranging from 2.679 (1) Å to 3.251 (2) Å. Hydrogen bonding, ion pairing, C—H···π stacking and van der Waals forces are effective in the stabilization of the crystal structure, resulting in the formation of an interesting supramolecular structure (Fig. 3).

Experimental

The proton-transfer compound was prepared by a reaction between propane-1,3-diamine and benzene-1,2,4,5-tetracarboxylic acid [Aghabozorg, Ghadermazi *et al.*, 2007]. Starting with a 1:1 molar ratio of the reactants in THF, a puffy white precipitate was obtained. By recrystallization in an aqueous solution, pale-yellow crystals were obtained. A solution of $Co(NO_3)_2\cdot 6H_2O$ (196 mg, 0.5 mmol) in water (15 ml) was added to an aqueous solution of $(pnH_2)_2(btc)\cdot 2H_2O$ (253 mg,

1.0 mmol) in water (15 ml) in a 1:2 molar ratio. Colorless crystals suitable for X-ray characterization were obtained after a few days at room temperature.

Refinement

The hydrogen atoms of the NH~3~ group and water molecules were found in the difference Fourier map. The H(C) atom positions were calculated. All hydrogen atoms were refined in isotropic approximation in riding model with with the *U*iso~(H) parameters equal to 1.2 *U*~eq~(Ci), 1.2 *U*~eq~(Oi) and 1.2 *U*~eq~(Ni) where U(Ci), U(Oi) and U(Ni) are respectively the equivalent thermal parameters of the carbon, oxygen and nitrigen atoms to which corresponding H atoms are bonded. Water molecule H(6 A)—O(6)—H(6B) has a total ocuppancy equal to 1/2 and is disordered by two positions, H(6B) atom is common for two positions. There is pseudo-symmetry in the crystal (space group Imma). However, the cation and water molecule are strongly disordered in the suggested Imma setting. One of the carbonyl O atoms is also disordered in Imma by two positions. Our attempt to solve the disordered structure in Imma group did not lead to acceptable R1 and wR2 values. The space group Ima2 is non-centrosymmetric so the Flack parameter can be calculated. The crystal is a racemic twin, so we used the TWIN instruction to refine the structure. In this case the Flack parameter is equal to the twin parameter of TWIN refinement (BASF). A total of 1206 Friedel pairs was measured.

Figures

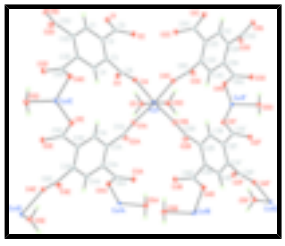


Fig. 1. Full environment of Co1 center for compound (I). Atoms Co1C and Co1F belong to a twofold axis. Co Atoms labeled with A—G are obtained by the following symmetry operations: A: x, 1.5 − y, −1/2 + z B: 1 − x, 1/2 + y, −1/2 + z C: 1 − x, 1 − y, z D: 1.5 − x, y, z E: 1.5 − x, 1.5 − y, −1/2 + z F: −1/2 + x, −1/2 + y, −1/2 + z G: −1/2 + x, 1 − y, z.

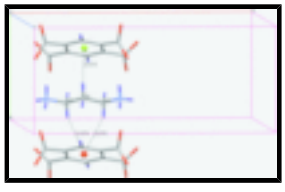


Fig. 2. The C—H···π distances (measured to the centre of phenyl ring) are 2.61 Å (1/2 + x, 1/2 + y, 1/2 + z) and 2.98 Å (1/2 + x,-1/2 + y, 1/2 + z) and the C–H···π angles are 141° and 137°, respectively.

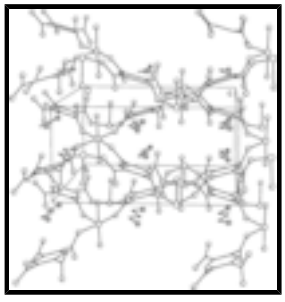


Fig. 3. Crystal packing of the title compound viewed along a crystal axis. Hydrogen atoms are omitted for clarity.

Poly[propane-1,3-diammonium [diaqua(μ$_4$-4-benzene-1,2,4,5-tetracarboxylato)cobaltate(II)] hemihydrate]

Crystal data

$(C_3H_{12}N_2)[Co(C_{10}H_2O_8)(H_2O_1)_2]\cdot 0.5H_2O$ $F_{000} = 888$

M_r = 430.23	D_x = 1.702 Mg m^{-3}
Orthorhombic, *Ima*2	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: I 2 -2a	Cell parameters from 6735 reflections
a = 16.4011 (3) Å	θ = 2.5–46.7º
b = 7.17860 (10) Å	μ = 1.09 mm^{-1}
c = 14.2586 (2) Å	T = 100 (2) K
V = 1678.76 (5) Å^3	Prism, colourless
Z = 4	0.22 × 0.18 × 0.13 mm

Data collection

Bruker APEXII CCD diffractometer	2526 independent reflections
Radiation source: fine-focus sealed tube	2479 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 100(2) K	θ_{max} = 30.0º
ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (SADABS; Bruker, 2005)	h = −23→23
T_{min} = 0.796, T_{max} = 0.872	k = −10→10
19141 measured reflections	l = −20→20

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.022	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.066	$(\Delta/\sigma)_{max}$ = 0.004
S = 1.00	$\Delta\rho_{max}$ = 0.81 e Å^{-3}
2526 reflections	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
134 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983)
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.375 (11)
Secondary atom site location: difference Fourier map	

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}	Occ. (<1)
Co1	0.5000	0.5000	0.82749 (2)	0.00585 (4)	
O1	0.59187 (6)	0.93889 (14)	1.23336 (6)	0.01174 (18)	
O2	0.54019 (5)	0.69011 (13)	1.15830 (6)	0.01297 (17)	
O3	0.56026 (5)	0.86184 (13)	0.96344 (7)	0.01294 (16)	
O4	0.58410 (6)	0.55896 (14)	0.93363 (6)	0.01095 (17)	
C1	0.7500	0.8092 (3)	1.17061 (12)	0.0095 (3)	
H1A	0.7500	0.8483	1.2343	0.011*	
C2	0.67589 (7)	0.78092 (16)	1.12452 (9)	0.0090 (2)	
C3	0.67626 (7)	0.72442 (17)	1.03074 (8)	0.0083 (2)	
C4	0.7500	0.6944 (2)	0.98435 (12)	0.0095 (3)	
H4A	0.7500	0.6535	0.9210	0.011*	
C5	0.59580 (7)	0.80529 (17)	1.17606 (8)	0.0093 (2)	
C6	0.59980 (7)	0.71361 (17)	0.97228 (8)	0.0090 (2)	
O5	0.45721 (5)	0.77721 (11)	0.82396 (8)	0.01252 (15)	
H5B	0.4770	0.8192	0.8781	0.015*	
H5A	0.4806	0.8255	0.7732	0.015*	
N1	0.40163 (6)	0.73402 (16)	0.54638 (8)	0.0136 (2)	
H1B	0.4460	0.7422	0.5844	0.020*	
H1C	0.4044	0.8241	0.5016	0.020*	
H1D	0.4006	0.6200	0.5185	0.020*	
C7	0.32604 (8)	0.75991 (19)	0.60320 (9)	0.0136 (2)	
H7A	0.3248	0.8881	0.6288	0.016*	
H7B	0.3264	0.6718	0.6566	0.016*	
C8	0.2500	0.7265 (3)	0.54340 (14)	0.0133 (3)	
H8A	0.2500	0.5971	0.5195	0.016*	
H8B	0.2500	0.8123	0.4890	0.016*	
O6	0.2991 (5)	0.9781 (12)	0.8219 (7)	0.071 (2)	0.25
H6A	0.3333	0.8845	0.8105	0.085*	0.25
H6B	0.2500	0.9320	0.8101	0.085*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.00543 (8)	0.00700 (8)	0.00512 (8)	−0.00108 (6)	0.000	0.000
O1	0.0107 (4)	0.0125 (4)	0.0120 (4)	−0.0006 (4)	0.0035 (3)	−0.0034 (3)
O2	0.0105 (4)	0.0155 (4)	0.0129 (4)	−0.0035 (3)	0.0009 (3)	−0.0023 (3)
O3	0.0122 (3)	0.0118 (4)	0.0149 (4)	0.0024 (3)	−0.0036 (3)	−0.0017 (3)
O4	0.0107 (4)	0.0114 (4)	0.0107 (4)	−0.0002 (3)	−0.0025 (3)	−0.0008 (3)
C1	0.0094 (7)	0.0114 (6)	0.0077 (7)	0.000	0.000	−0.0018 (6)
C2	0.0103 (5)	0.0077 (5)	0.0091 (5)	0.0004 (4)	0.0010 (4)	−0.0016 (4)
C3	0.0061 (4)	0.0094 (5)	0.0095 (5)	0.0000 (4)	0.0000 (4)	−0.0007 (4)
C4	0.0095 (7)	0.0090 (6)	0.0099 (8)	0.000	0.000	−0.0009 (6)

C5	0.0084 (5)	0.0106 (5)	0.0089 (5)	0.0006 (4)	0.0000 (4)	0.0009 (4)
C6	0.0080 (4)	0.0114 (5)	0.0078 (5)	−0.0011 (4)	0.0011 (4)	0.0003 (4)
O5	0.0144 (3)	0.0129 (3)	0.0103 (3)	0.0005 (3)	−0.0004 (4)	0.0000 (3)
N1	0.0095 (4)	0.0143 (5)	0.0170 (5)	0.0001 (4)	0.0009 (4)	0.0029 (4)
C7	0.0121 (5)	0.0122 (5)	0.0166 (6)	0.0004 (4)	0.0004 (4)	0.0010 (5)
C8	0.0099 (6)	0.0132 (7)	0.0169 (7)	0.000	0.000	0.0012 (6)
O6	0.056 (3)	0.120 (6)	0.036 (3)	0.056 (4)	0.014 (4)	0.001 (4)

Geometric parameters (Å, °)

Co1—O1^{i}	2.0650 (9)	C4—H4A	0.9500
Co1—O4	2.0910 (9)	O5—H5B	0.8899
Co1—O5	2.1107 (8)	O5—H5A	0.8901
O1—C5	1.2615 (16)	N1—C7	1.4926 (16)
O1—Co1^{ii}	2.0650 (9)	N1—H1B	0.9100
O2—C5	1.2569 (15)	N1—H1C	0.9100
O3—C6	1.2525 (15)	N1—H1D	0.9100
O4—C6	1.2659 (16)	C7—C8	1.5297 (17)
C1—C2	1.3967 (15)	C7—H7A	0.9900
C1—C2^{iii}	1.3967 (15)	C7—H7B	0.9900
C1—H1A	0.9500	C8—C7^{iv}	1.5297 (17)
C2—C3	1.3973 (14)	C8—H8A	0.9900
C2—C5	1.5153 (17)	C8—H8B	0.9900
C3—C4	1.3952 (14)	O6—O6^{iv}	1.612 (15)
C3—C6	1.5077 (17)	O6—H6A	0.8900
C4—C3^{iii}	1.3952 (14)	O6—H6B	0.8873
O1^{i}—Co1—O1^{v}	98.92 (5)	O1—C5—C2	116.50 (11)
O1^{i}—Co1—O4	174.14 (4)	O3—C6—O4	126.57 (11)
O1^{v}—Co1—O4	86.91 (3)	O3—C6—C3	116.27 (11)
O4—Co1—O4^{vi}	87.26 (5)	O4—C6—C3	117.07 (11)
O1^{i}—Co1—O5^{vi}	91.54 (4)	Co1—O5—H5B	100.2
O1^{v}—Co1—O5^{vi}	86.68 (4)	Co1—O5—H5A	104.1
O4—Co1—O5^{vi}	89.36 (4)	H5B—O5—H5A	114.6
O4^{vi}—Co1—O5^{vi}	92.62 (4)	C7—N1—H1B	109.5
O1^{v}—Co1—O5	91.54 (4)	C7—N1—H1C	109.5
O4—Co1—O5	92.62 (4)	H1B—N1—H1C	109.5
O4^{vi}—Co1—O5	89.36 (4)	C7—N1—H1D	109.5
O5^{vi}—Co1—O5	177.26 (6)	H1B—N1—H1D	109.5
C5—O1—Co1^{ii}	128.29 (8)	H1C—N1—H1D	109.5
C6—O4—Co1	128.82 (8)	N1—C7—C8	110.80 (11)
C2—C1—C2^{iii}	120.99 (16)	N1—C7—H7A	109.5
C2—C1—H1A	119.5	C8—C7—H7A	109.5
C2^{iii}—C1—H1A	119.5	N1—C7—H7B	109.5
C1—C2—C3	119.25 (13)	C8—C7—H7B	109.5
C1—C2—C5	120.62 (11)	H7A—C7—H7B	108.1

C3—C2—C5	120.10 (12)	C7—C8—C7^{iv}	109.24 (15)
C4—C3—C2	120.15 (13)	C7—C8—H8A	109.8
C4—C3—C6	116.80 (11)	C7^{iv}—C8—H8A	109.8
C2—C3—C6	122.71 (12)	C7—C8—H8B	109.8
C3—C4—C3^{iii}	120.18 (15)	C7^{iv}—C8—H8B	109.8
C3—C4—H4A	119.9	H8A—C8—H8B	108.3
C3^{iii}—C4—H4A	119.9	O6^{iv}—O6—H6A	129.1
O2—C5—O1	126.41 (11)	H6A—O6—H6B	104.9
O2—C5—C2	117.09 (11)		
O1^{v}—Co1—O4—C6	88.68 (11)	Co1^{ii}—O1—C5—C2	−172.14 (8)
O4^{vi}—Co1—O4—C6	−91.95 (11)	C1—C2—C5—O2	−140.38 (14)
O5^{vi}—Co1—O4—C6	175.39 (11)	C3—C2—C5—O2	37.76 (15)
O5—Co1—O4—C6	−2.72 (11)	C1—C2—C5—O1	39.04 (18)
C2^{iii}—C1—C2—C3	−0.4 (2)	C3—C2—C5—O1	−142.82 (11)
C2^{iii}—C1—C2—C5	177.80 (11)	Co1—O4—C6—O3	10.12 (19)
C1—C2—C3—C4	0.84 (16)	Co1—O4—C6—C3	−166.26 (8)
C5—C2—C3—C4	−177.32 (13)	C4—C3—C6—O3	−114.56 (14)
C1—C2—C3—C6	−172.23 (14)	C2—C3—C6—O3	58.73 (15)
C5—C2—C3—C6	9.60 (15)	C4—C3—C6—O4	62.21 (17)
C2—C3—C4—C3^{iii}	−1.3 (2)	C2—C3—C6—O4	−124.50 (12)
C6—C3—C4—C3^{iii}	172.13 (10)	N1—C7—C8—C7^{iv}	−178.35 (9)
Co1^{ii}—O1—C5—O2	7.22 (19)		

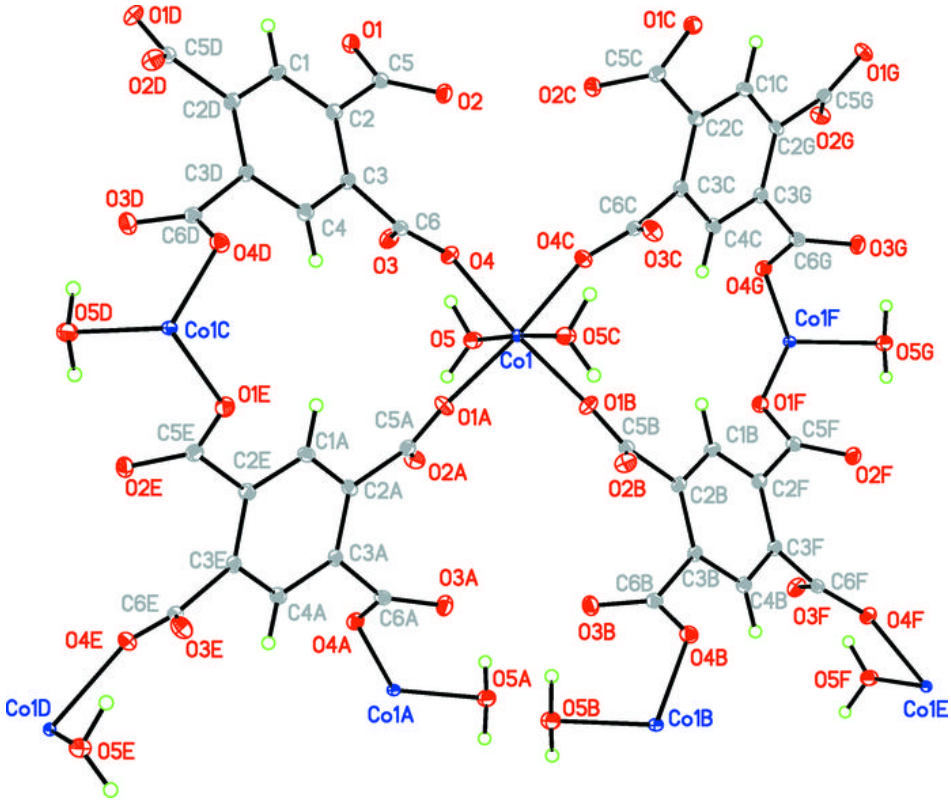
Symmetry codes: (i) −*x*+1, *y*−1/2, *z*−1/2; (ii) *x*, −*y*+3/2, *z*+1/2; (iii) −*x*+3/2, *y*, *z*; (iv) −*x*+1/2, *y*, *z*; (v) *x*, −*y*+3/2, *z*−1/2; (vi) −*x*+1, −*y*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5B···O3	0.89	1.85	2.680 (1)	153
O5—H5A···O2^{v}	0.89	1.91	2.737 (1)	154
N1—H1B···O2^{v}	0.91	1.93	2.831 (1)	168
N1—H1C···O4^{vii}	0.91	1.95	2.843 (2)	166
N1—H1D···O3^{i}	0.91	2.11	2.988 (2)	161
C7—H7B···Cg^{viii}	0.99	2.98	3.767 (2)	137
C8—H8B···Cg^{ix}	0.99	2.61	3.439 (2)	141

Symmetry codes: (v) *x*, −*y*+3/2, *z*−1/2; (vii) −*x*+1, *y*+1/2, *z*−1/2; (i) −*x*+1, *y*−1/2, *z*−1/2; (viii) *x*+1/2, *y*−1/2, *z*+1/2; (ix) *x*+1/2, *y*+1/2, *z*+1/2.

Fig. 1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C2
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C6B
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Co1E

Fig. 2

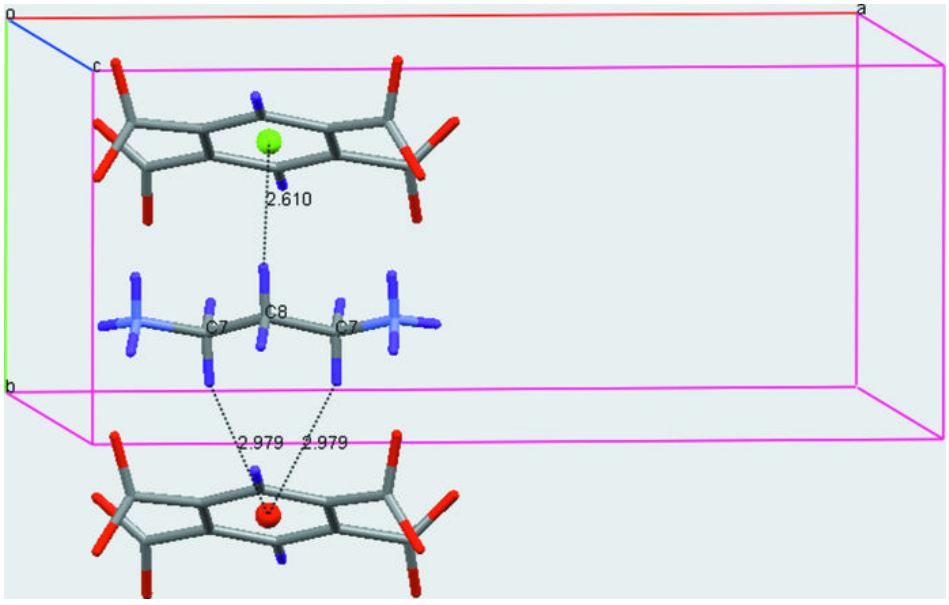

Fig. 3