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catena-Poly[[diaquabis(methanol)-cobalt(II)]-μ-phthalato]

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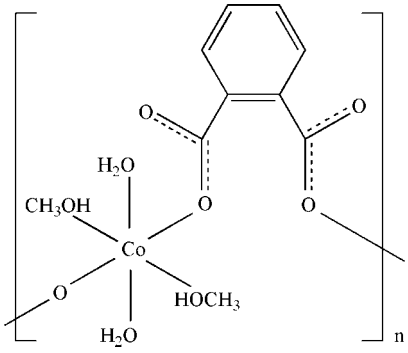
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.076; wR factor = 0.133; data-to-parameter ratio = 12.2.

In the crystal structure of the polymeric title compound, $[Co(\mu\text{-}C_8H_4O_4)(CH_3OH)_2(H_2O)_2]_n$, two independent Co^{II} atoms both occupy special positions with $\bar{1}$ site symmetry. Each Co^{II} atom assumes a distorted octahedral coordination geometry. The phthalate anion acts as a bridging ligand and leads to the formation of a zigzag chain running along the c axis. O—H···O and C—H···O hydrogen bonds connect the chains and result in the formation of a three-dimensional structure.

Related literature

For related crystal structures, see: Baca *et al.* (2003, 2006).



Experimental

Crystal data

$[Co(C_8H_4O_4)(CH_4O)_2(H_2O)_2]$
M_r = 323.16
Monoclinic, $P2_1/c$
a = 10.0810 (9) Å
b = 9.9429 (9) Å
c = 13.2735 (12) Å
β = 90.300 (2)°
V = 1330.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.778, T_{max} = 0.826
5378 measured reflections
2351 independent reflections
2172 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.133
S = 1.26
2351 reflections
193 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	2.080 (3)	Co2—O3	2.077 (4)
Co1—O5	2.148 (4)	Co2—O7	2.098 (4)
Co1—O6	2.037 (4)	Co2—O8	2.083 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H2···O2^{i}	0.82 (5)	1.75 (6)	2.557 (5)	167 (7)
O7—H1···O5^{ii}	0.82 (5)	2.00 (5)	2.817 (6)	175 (8)
O6—H6*C*···O4^{i}	0.85 (5)	1.93 (5)	2.764 (5)	165 (6)
O6—H6*D*···O3^{iii}	0.85 (4)	1.85 (4)	2.699 (5)	176 (6)
O8—H8*A*···O1^{ii}	0.84 (3)	1.88 (3)	2.716 (5)	170 (6)
O8—H8*B*···O4^{iv}	0.85 (4)	1.94 (5)	2.770 (5)	166 (5)
C5—H5*A*···O2^{v}	0.93	2.49	3.331 (7)	150

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 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: IS2201).

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supplementary materials

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catena-Poly[[diaquabis(methanol)cobalt(II)]-μ-phthalato]

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Comment

Phthalate anion is a versatile ligand and a large number of multi-nuclear complexes with it as a bridging ligand have been reported (Baca *et al.*, 2003, 2006). Here we report the crystal structure of a novel coordination polymer dealing with phthalate anion, (I).

Fig. 1 shows the asymmetric unit and the symmetry-related fragment of (I). Atoms Co1 and Co2 lie in an inversion centre and are in a distorted octahedral CoO_6 coordination geometry (Table 1). Each phthalate anion as a μ_2-bridging ligand joins two adjacent Co^{II} atoms with separation of 6.6367 (6) Å and it results in the formation of a zigzag one-dimensional chain along the *c* axis. The overall crystal structure of (I) is a super-molecular three-dimensional network, which attributes to the connection between chains by the O—H···O and C—H···O hydrogen bonds (Table 2 and Fig. 2).

Experimental

A methanol solution (50 ml) containing phthalic acid (3.32 g, 0.02 mol) and cobalt acetate (1.77 g, 0.01 mol) was refluxed for 50 min and the reaction solid was separated and dried. The dried solid (0.2 g) was dissolved in H_2O (20 ml) and pink single crystals were obtained after the solution had been allowed to stand at room temperature for about a month.

Refinement

H atoms of water molecules and hydroxyl groups were located in a difference Fourier map and were refined with distance restraints of O—H = 0.85 (2) Å for water molecules and 0.82 (2) Å for hydroxyl groups, and with U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were placed in calculated positions (C—H = 0.93 or 0.96 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

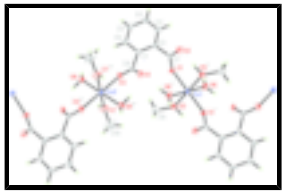

Fig. 1. The coordination structure of (I), with the atom numbering scheme and thermal ellipsoids drawn at the 30% probability level [symmetry codes: (i) −*x* + 1, −*y*, −*z* + 2; (ii) −*x* + 1, −*y*, −*z* + 1].

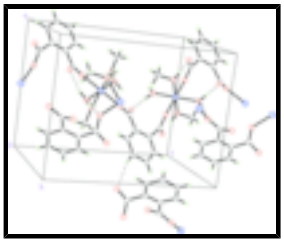

Fig. 2. A packing diagram of (I), showing hydrogen bonds (dashed lines).

catena-Poly[[diaquabis(methanol)cobalt(II)]-μ-phthalato]

Crystal data

$[Co(C_8H_4O_4)(CH_4O)_2(H_2O)_2]$	$F_{000} = 668$
$M_r = 323.16$	$D_x = 1.613$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2648 reflections
$a = 10.0810$ (9) Å	$\theta = 2.6$–$27.6°$
$b = 9.9429$ (9) Å	$\mu = 1.32$ mm^{-1}
$c = 13.2735$ (12) Å	$T = 293$ (2) K
$\beta = 90.300$ (2)°	Prism, pink
$V = 1330.4$ (2) Å^3	0.20 × 0.20 × 0.15 mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD diffractometer	2351 independent reflections
Radiation source: fine-focus sealed tube	2172 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 293(2)$ K	$\theta_{max} = 25.1°$
φ and ω scans	$\theta_{min} = 2.0°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -6 \rightarrow 12$
$T_{min} = 0.778$, $T_{max} = 0.826$	$k = -11 \rightarrow 11$
5378 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.077$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.133$	$w = 1/[\sigma^2(F_o^2) + (0.0199P)^2 + 5.7387P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.27$	$(\Delta/\sigma)_{max} < 0.001$
2351 reflections	$\Delta\rho_{max} = 0.49$ e Å^{-3}

193 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}
8 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.5000	0.0000	1.0000	0.0270 (3)
Co2	0.5000	0.0000	0.5000	0.0291 (3)
O1	0.3636 (3)	0.1108 (3)	0.9162 (3)	0.0247 (8)
O2	0.1792 (4)	−0.0057 (4)	0.9467 (3)	0.0421 (10)
O3	0.4035 (4)	0.1133 (4)	0.6087 (3)	0.0316 (9)
O4	0.3505 (4)	−0.0417 (3)	0.7224 (3)	0.0304 (9)
O5	0.6557 (4)	0.1154 (4)	0.9317 (3)	0.0352 (9)
H2	0.717 (5)	0.087 (7)	0.966 (4)	0.053*
O6	0.5027 (5)	0.1347 (4)	1.1156 (3)	0.0374 (10)
H6C	0.553 (5)	0.120 (6)	1.166 (3)	0.056*
H6D	0.471 (6)	0.214 (3)	1.117 (4)	0.056*
O7	0.6667 (4)	0.1246 (4)	0.5157 (4)	0.0459 (11)
H1	0.661 (8)	0.198 (4)	0.488 (5)	0.069*
O8	0.4320 (4)	0.1280 (4)	0.3867 (3)	0.0343 (10)
H8A	0.412 (6)	0.210 (3)	0.388 (5)	0.051*
H8B	0.499 (4)	0.115 (5)	0.349 (4)	0.051*
C1	0.2433 (5)	0.0782 (5)	0.8981 (4)	0.0250 (12)
C2	0.1755 (5)	0.1554 (5)	0.8149 (4)	0.0273 (12)
C3	0.0660 (6)	0.2309 (6)	0.8391 (5)	0.0417 (15)
H3A	0.0314	0.2250	0.9037	0.050*
C4	0.0059 (6)	0.3155 (7)	0.7695 (5)	0.0482 (18)
H4A	−0.0682	0.3658	0.7871	0.058*
C5	0.0578 (6)	0.3241 (6)	0.6739 (5)	0.0460 (17)
H5A	0.0200	0.3822	0.6270	0.055*
C6	0.1661 (6)	0.2462 (6)	0.6475 (5)	0.0400 (14)
H6B	0.1996	0.2512	0.5825	0.048*
C7	0.2251 (5)	0.1606 (5)	0.7175 (4)	0.0267 (12)
C8	0.3358 (5)	0.0702 (5)	0.6825 (4)	0.0236 (12)
C9	0.6831 (7)	0.1107 (7)	0.8252 (5)	0.0537 (18)

H9A	0.7566	0.1687	0.8104	0.080*
H9B	0.6064	0.1400	0.7882	0.080*
H9C	0.7047	0.0202	0.8062	0.080*
C10	0.7954 (9)	0.0949 (10)	0.5518 (8)	0.098 (4)
H10A	0.8493	0.1743	0.5489	0.147*
H10B	0.8341	0.0259	0.5108	0.147*
H10C	0.7902	0.0642	0.6202	0.147*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0288 (6)	0.0185 (5)	0.0336 (6)	−0.0006 (5)	−0.0035 (4)	0.0013 (5)
Co2	0.0353 (6)	0.0198 (5)	0.0321 (6)	0.0021 (5)	0.0001 (5)	−0.0005 (5)
O1	0.0189 (19)	0.0197 (18)	0.035 (2)	−0.0017 (15)	−0.0050 (15)	0.0037 (16)
O2	0.037 (2)	0.043 (2)	0.045 (2)	−0.012 (2)	−0.0051 (19)	0.015 (2)
O3	0.044 (2)	0.0190 (19)	0.032 (2)	0.0042 (18)	0.0052 (18)	−0.0024 (16)
O4	0.051 (3)	0.0164 (19)	0.0236 (19)	0.0067 (17)	0.0021 (18)	0.0000 (15)
O5	0.032 (2)	0.034 (2)	0.040 (2)	−0.0033 (19)	−0.0020 (18)	0.0073 (19)
O6	0.055 (3)	0.022 (2)	0.035 (2)	0.011 (2)	−0.011 (2)	−0.0040 (18)
O7	0.039 (3)	0.022 (2)	0.076 (3)	−0.002 (2)	−0.011 (2)	0.005 (2)
O8	0.041 (3)	0.023 (2)	0.038 (2)	0.0115 (19)	0.0017 (19)	0.0029 (18)
C1	0.029 (3)	0.021 (3)	0.025 (3)	0.002 (2)	−0.002 (2)	−0.004 (2)
C2	0.023 (3)	0.024 (3)	0.035 (3)	0.000 (2)	−0.003 (2)	−0.003 (2)
C3	0.032 (3)	0.046 (4)	0.046 (4)	0.013 (3)	0.003 (3)	−0.002 (3)
C4	0.032 (3)	0.050 (4)	0.063 (5)	0.021 (3)	−0.002 (3)	−0.005 (3)
C5	0.043 (4)	0.038 (4)	0.057 (4)	0.011 (3)	−0.012 (3)	0.010 (3)
C6	0.042 (4)	0.034 (3)	0.043 (3)	0.002 (3)	−0.005 (3)	0.009 (3)
C7	0.026 (3)	0.017 (3)	0.037 (3)	−0.001 (2)	−0.002 (2)	−0.002 (2)
C8	0.037 (3)	0.019 (3)	0.014 (2)	−0.001 (2)	−0.007 (2)	0.004 (2)
C9	0.057 (5)	0.037 (4)	0.067 (5)	−0.002 (3)	0.008 (4)	0.009 (4)
C10	0.074 (6)	0.102 (8)	0.118 (8)	−0.039 (6)	−0.034 (6)	0.048 (7)

Geometric parameters (Å, °)

Co1—O1^{i}	2.080 (3)	O7—H1	0.82 (5)
Co1—O1	2.080 (3)	O8—H8A	0.84 (3)
Co1—O5^{i}	2.148 (4)	O8—H8B	0.85 (4)
Co1—O5	2.148 (4)	C1—C2	1.506 (7)
Co1—O6	2.037 (4)	C2—C3	1.374 (8)
Co1—O6^{i}	2.037 (4)	C2—C7	1.389 (8)
Co2—O3	2.077 (4)	C3—C4	1.386 (9)
Co2—O3^{ii}	2.077 (4)	C3—H3A	0.9300
Co2—O7	2.098 (4)	C4—C5	1.377 (9)
Co2—O7^{ii}	2.098 (4)	C4—H4A	0.9300
Co2—O8^{ii}	2.083 (4)	C5—C6	1.385 (9)
Co2—O8	2.083 (4)	C5—H5A	0.9300
O1—C1	1.277 (6)	C6—C7	1.392 (8)

O2—C1	1.239 (6)	C6—H6B	0.9300
O3—C8	1.271 (6)	C7—C8	1.508 (7)
O4—C8	1.240 (6)	C9—H9A	0.9600
O5—C9	1.443 (8)	C9—H9B	0.9600
O5—H2	0.82 (5)	C9—H9C	0.9600
O6—H6C	0.85 (4)	C10—H10A	0.9600
O6—H6D	0.85 (5)	C10—H10B	0.9600
O7—C10	1.411 (9)	C10—H10C	0.9600
O6—Co1—O6^{i}	180.000 (1)	Co2—O7—H1	115 (5)
O6—Co1—O1^{i}	86.52 (15)	Co2—O8—H8A	131 (4)
O6^{i}—Co1—O1^{i}	93.48 (15)	Co2—O8—H8B	94 (4)
O6—Co1—O1	93.48 (15)	H8A—O8—H8B	110 (3)
O6^{i}—Co1—O1	86.52 (15)	O2—C1—O1	124.8 (5)
O1^{i}—Co1—O1	180.000 (1)	O2—C1—C2	119.3 (5)
O6—Co1—O5^{i}	92.29 (17)	O1—C1—C2	115.8 (5)
O6^{i}—Co1—O5^{i}	87.71 (17)	C3—C2—C7	119.4 (5)
O1^{i}—Co1—O5^{i}	88.50 (14)	C3—C2—C1	118.0 (5)
O1—Co1—O5^{i}	91.50 (14)	C7—C2—C1	122.4 (5)
O6—Co1—O5	87.71 (17)	C2—C3—C4	121.6 (6)
O6^{i}—Co1—O5	92.29 (17)	C2—C3—H3A	119.2
O1^{i}—Co1—O5	91.50 (14)	C4—C3—H3A	119.2
O1—Co1—O5	88.50 (14)	C5—C4—C3	119.0 (6)
O5^{i}—Co1—O5	180.0	C5—C4—H4A	120.5
O3—Co2—O3^{ii}	180.00 (14)	C3—C4—H4A	120.5
O3—Co2—O8^{ii}	89.05 (15)	C4—C5—C6	120.2 (6)
O3^{ii}—Co2—O8^{ii}	90.95 (15)	C4—C5—H5A	119.9
O3—Co2—O8	90.95 (15)	C6—C5—H5A	119.9
O3^{ii}—Co2—O8	89.05 (15)	C5—C6—C7	120.5 (6)
O8^{ii}—Co2—O8	180.00 (15)	C5—C6—H6B	119.8
O3—Co2—O7	89.33 (17)	C7—C6—H6B	119.8
O3^{ii}—Co2—O7	90.67 (17)	C2—C7—C6	119.3 (5)
O8^{ii}—Co2—O7	91.63 (17)	C2—C7—C8	122.4 (5)
O8—Co2—O7	88.37 (17)	C6—C7—C8	118.2 (5)
O3—Co2—O7^{ii}	90.67 (17)	O4—C8—O3	124.6 (5)
O3^{ii}—Co2—O7^{ii}	89.33 (17)	O4—C8—C7	119.3 (5)
O8^{ii}—Co2—O7^{ii}	88.37 (17)	O3—C8—C7	115.9 (4)
O8—Co2—O7^{ii}	91.63 (17)	O5—C9—H9A	109.5
O7—Co2—O7^{ii}	180.00 (18)	O5—C9—H9B	109.5
C1—O1—Co1	126.2 (3)	H9A—C9—H9B	109.5
C8—O3—Co2	127.4 (3)	O5—C9—H9C	109.5
C9—O5—Co1	122.7 (4)	H9A—C9—H9C	109.5
C9—O5—H2	113 (5)	H9B—C9—H9C	109.5
Co1—O5—H2	98 (5)	O7—C10—H10A	109.5
Co1—O6—H6C	119 (4)	O7—C10—H10B	109.5

Co1—O6—H6D	128 (4)	H10A—C10—H10B	109.5
H6C—O6—H6D	112 (3)	O7—C10—H10C	109.5
C10—O7—Co2	130.1 (5)	H10A—C10—H10C	109.5
C10—O7—H1	114 (6)	H10B—C10—H10C	109.5
O6—Co1—O1—C1	−110.5 (4)	O2—C1—C2—C7	−126.5 (6)
O6^{i}—Co1—O1—C1	69.5 (4)	O1—C1—C2—C7	56.9 (7)
O5^{i}—Co1—O1—C1	−18.1 (4)	C7—C2—C3—C4	−2.0 (9)
O5—Co1—O1—C1	161.9 (4)	C1—C2—C3—C4	173.3 (6)
O8^{ii}—Co2—O3—C8	−43.5 (4)	C2—C3—C4—C5	−0.1 (10)
O8—Co2—O3—C8	136.5 (4)	C3—C4—C5—C6	1.7 (10)
O7—Co2—O3—C8	−135.1 (4)	C4—C5—C6—C7	−1.2 (10)
O7^{ii}—Co2—O3—C8	44.9 (4)	C3—C2—C7—C6	2.6 (8)
O6—Co1—O5—C9	−158.0 (4)	C1—C2—C7—C6	−172.6 (5)
O6^{i}—Co1—O5—C9	22.0 (4)	C3—C2—C7—C8	−173.6 (5)
O1^{i}—Co1—O5—C9	115.6 (4)	C1—C2—C7—C8	11.3 (8)
O1—Co1—O5—C9	−64.4 (4)	C5—C6—C7—C2	−1.0 (9)
O3—Co2—O7—C10	114.6 (7)	C5—C6—C7—C8	175.3 (5)
O3^{ii}—Co2—O7—C10	−65.4 (7)	Co2—O3—C8—O4	25.4 (7)
O8^{ii}—Co2—O7—C10	25.6 (7)	Co2—O3—C8—C7	−150.5 (4)
O8—Co2—O7—C10	−154.4 (7)	C2—C7—C8—O4	28.2 (8)
Co1—O1—C1—O2	18.8 (8)	C6—C7—C8—O4	−148.0 (5)
Co1—O1—C1—C2	−164.9 (3)	C2—C7—C8—O3	−155.7 (5)
O2—C1—C2—C3	58.3 (7)	C6—C7—C8—O3	28.1 (7)
O1—C1—C2—C3	−118.3 (6)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H2···O2^{i}	0.82 (5)	1.75 (6)	2.557 (5)	167 (7)
O7—H1···O5^{iii}	0.82 (5)	2.00 (5)	2.817 (6)	175 (8)
O6—H6C···O4^{i}	0.85 (5)	1.93 (5)	2.764 (5)	165 (6)
O6—H6D···O3^{iv}	0.85 (4)	1.85 (4)	2.699 (5)	176 (6)
O8—H8A···O1^{iii}	0.84 (3)	1.88 (3)	2.716 (5)	170 (6)
O8—H8B···O4^{ii}	0.85 (4)	1.94 (5)	2.770 (5)	166 (5)
C5—H5A···O2^{v}	0.93	2.49	3.331 (7)	150

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

Fig. 1

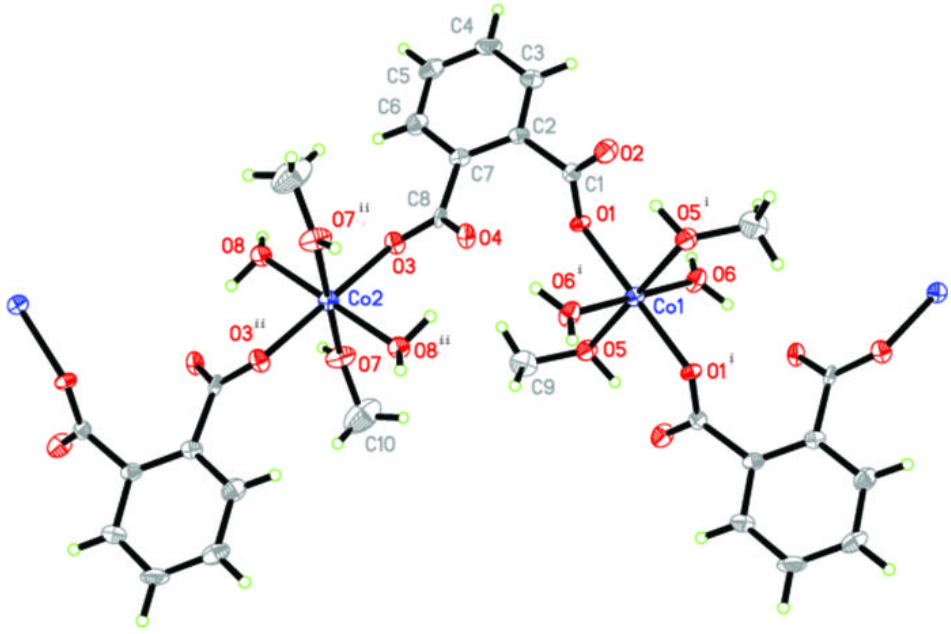
C4
C3
C5
C6
C2
C7
C8
C1
O2
O1
O4
O3
O8
O7 ii
Co2
O3 ii
O7
O8 ii
C10
O5 i
O6
O6 i
Co1
O5
C9
O1 i

Fig. 2