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catena-Poly[bis[(1,10-phenanthroline)-cobalt(II)]- μ_4 -3,6-dicarboxycyclohexane-1,2,4,5-tetracarboxylato]

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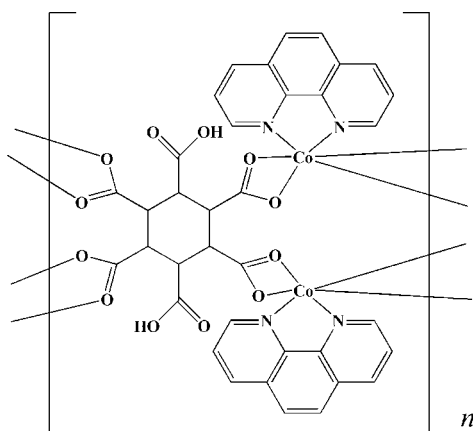
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.031; wR factor = 0.083; data-to-parameter ratio = 15.1.

In the title compound, $[\text{Co}_2(\text{C}_{12}\text{H}_8\text{O}_{12})(\text{C}_{12}\text{H}_8\text{N}_2)_2]_n$, each 3,6-dicarboxycyclohexane-1,2,4,5-tetracarboxylate ($\text{H}_2\text{chhc}^{4-}$) anion has crystallographically imposed C_2 symmetry and bridges four six-coordinate Co atoms, generating polymeric chains running along [010]. These chains are further extended into a three-dimensional network *via* $\text{O}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions and interchain $\pi-\pi$ stacking interactions [centroid-centroid distance = 3.662 (2) Å].

Related literature

For the design and synthesis of coordination polymer complexes and their potential applications, see: Biradha *et al.* (2006); Bauer *et al.* (2007); Zacher *et al.* (2011). For the 1,2,3,4,5,6-cyclohexanehexacarboxylate ligand, see: Li *et al.* (2006); Wang *et al.* (2008); Thuéry & Masci (2010). For related structures, see: Konar *et al.* (2004); Li *et al.* (2006).



Experimental

Crystal data

$[\text{Co}_2(\text{C}_{12}\text{H}_8\text{O}_{12})(\text{C}_{12}\text{H}_8\text{N}_2)_2]$
 $M_r = 822.46$
 Monoclinic, $C2/c$
 $a = 22.180$ (4) Å
 $b = 8.9520$ (18) Å
 $c = 16.426$ (3) Å
 $\beta = 93.33$ (3)°

$V = 3256.0$ (11) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.10$ mm⁻¹
 $T = 295$ K
 $0.31 \times 0.23 \times 0.15$ mm

Data collection

Siemens P4 diffractometer
 Absorption correction: ψ scan
 (XSCANS; Siemens, 1996)
 $T_{\min} = 0.702$, $T_{\max} = 0.784$
 4566 measured reflections
 3753 independent reflections

3312 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 3 standard reflections every 97 reflections
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.083$
 $S = 1.03$
 3753 reflections
 248 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.38$ e Å⁻³
 $\Delta\rho_{\min} = -0.33$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—O1	2.2002 (13)	Co1—O6 ⁱ	2.1519 (13)
Co1—O2	2.0890 (13)	Co1—N1	2.1012 (15)
Co1—O5 ⁱ	2.1211 (13)	Co1—N2	2.1016 (15)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O4}-\text{H4A}\cdots\text{O2}^{\text{ii}}$	0.79 (3)	1.89 (3)	2.627 (2)	156 (2)

Symmetry code: (ii) $-x, -y + 2, -z$.

Data collection: XSCANS (Siemens, 1996); cell refinement: XSCANS; data reduction: XSCANS; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5153).

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supporting information

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catena-Poly[bis[(1,10-phenanthroline)cobalt(II)]- μ_4 -3,6-dicarboxycyclohexane-1,2,4,5-tetracarboxylato]

Wei Xu

S1. Comment

The rational design and construction of metal-organic coordination polymers with flexible multidentate ligands have received more and more attention due to their intriguing structural topologies and novel properties for potential applications (Biradha, *et al.*, 2006; Bauer, *et al.*, 2007; Zacher, *et al.*, 2011). As a typical flexible cycloalkane polycarboxylic acid ligand, we have focused on the 1,2,3,4,5,6-cyclohexanehexacarboxylic acid (H_6chhc) whose coordination chemistry remains practically unexplored. We were particularly aware that the greater flexibility of this ligand would make the prediction and control of the final coordination networks that it generates more difficult. (Wang, *et al.*, 2008; Thuéry & Masci, 2010). Herein, we report a new cobalt coordination polymer, $[Co_2(phen)_2(H_2chhc)]_n$, resulting from reaction of Co^{2+} cations, phen and H_6chhc under hydrothermal conditions. It is isostructural with the previously reported $[Ni_2(phen)_2(H_2chhc)]_n$ complex (Li, *et al.*, 2006).

The asymmetric unit of the title compound consists of one Co^{2+} cation, one phen ligand and one-half of a H_2chhc^+ anion lying across a twofold rotation axis. The Co atoms are each in an octahedral environment defined by two N atoms of one phen ligand and four O atoms of two carboxylate groups from different H_2chhc^+ anions. The Co-O bond lengths fall in the range 2.089 (1)-2.200 (1) Å and the two Co-N distances are 2.101 (2) and 2.102 (2) Å (Table 1), thus falling in the expected region (Konar, *et al.*, 2004). The octahedral coordination around the Co atoms are strongly distorted since the diametrical and non-diametrical bond angles indicate significant deviations from 180° and 90°, respectively. The H_2chhc^+ ligands assume an *e,e,e,e,e,e*-conformation with the central ring adopting a chair-shaped configuration, the carboxylate and carboxyl groups being located at the equatorial sites. Each carboxylate group of the H_2chhc^+ anion chelates one Co atom. As a result, the H_2chhc^+ anions are each coordinated to four $[Co(phen)]^{2+}$ units, leading to polymeric chains $[Co_2(phen)_2(H_2chhc)]_n$ running along the [010] direction with the phen ligands *exo*-orientated (Fig. 1). The phen ligands of two adjacent supramolecular chains are stacked *via* the quinoline fragments (centroid-centroid distance = 3.662 (2) Å). Obviously, such π - π stacking interactions are responsible for the supramolecular assembly of the one-dimensional chains into two-dimensional layers parallel to (001) (Fig. 2). The layers are further connected to form a three-dimensional framework *via* interlayer O-H \cdots O hydrogen bonds ($d(O4\cdots O2^{\#1}) = 2.627$ (2) Å, $\angle O4-H4A\cdots O2^{\#1} = 156$ (2)°, #1 = -x, 2-y, -z).

S2. Experimental

$CoCl_2 \cdot 6H_2O$ (0.238 g, 1.0 mmol), H_6chhc (0.173 g, 0.5 mmol), phen (0.200 g, 1.0 mmol) and NaOH 1.5 mL (1 M) were stirred in 20 mL H_2O . The resulting mixture was placed in a 23 mL Teflon-lined autoclave and heated at 170 °C for 3 days. The reaction system was cooled to room temperature at a rate of 20 °C/h, and small amount of pink crystals of the title complex was obtained.

S3. Refinement

All H atoms bound to C were position geometrically and refined as riding, with $C-H = 0.93 \text{ \AA}$ and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms attached to O were located in difference Fourier maps and refined freely with $U_{iso}(H) = 1.5U_{eq}(O)$.

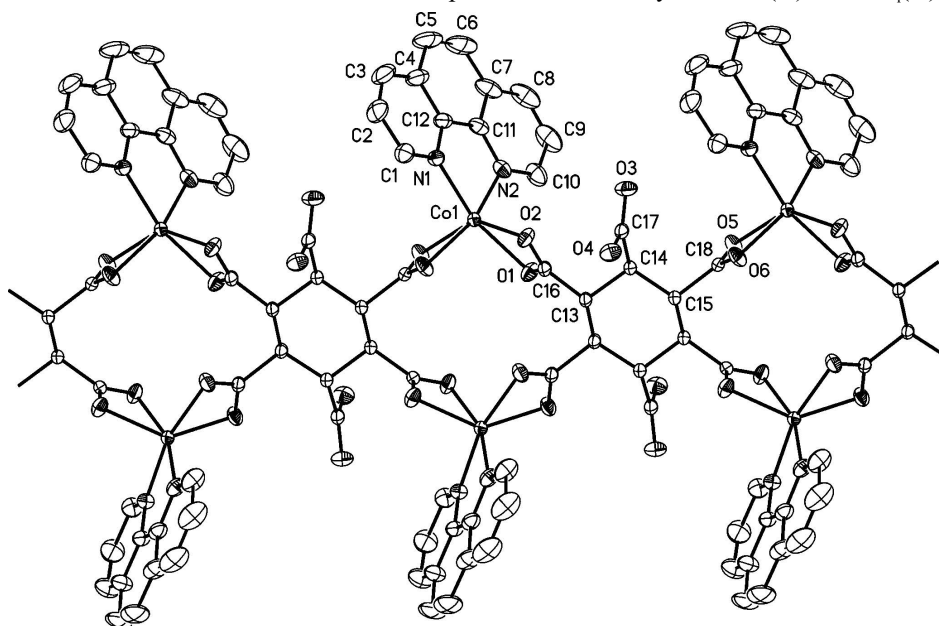


Figure 1

ORTEP view of the polymer chain $[Co_2(phen)_2(H_2chhc)]_n$ of the title complex. The displacement ellipsoids are drawn at 40% probability level, hydrogen atoms are omitted for clarity.

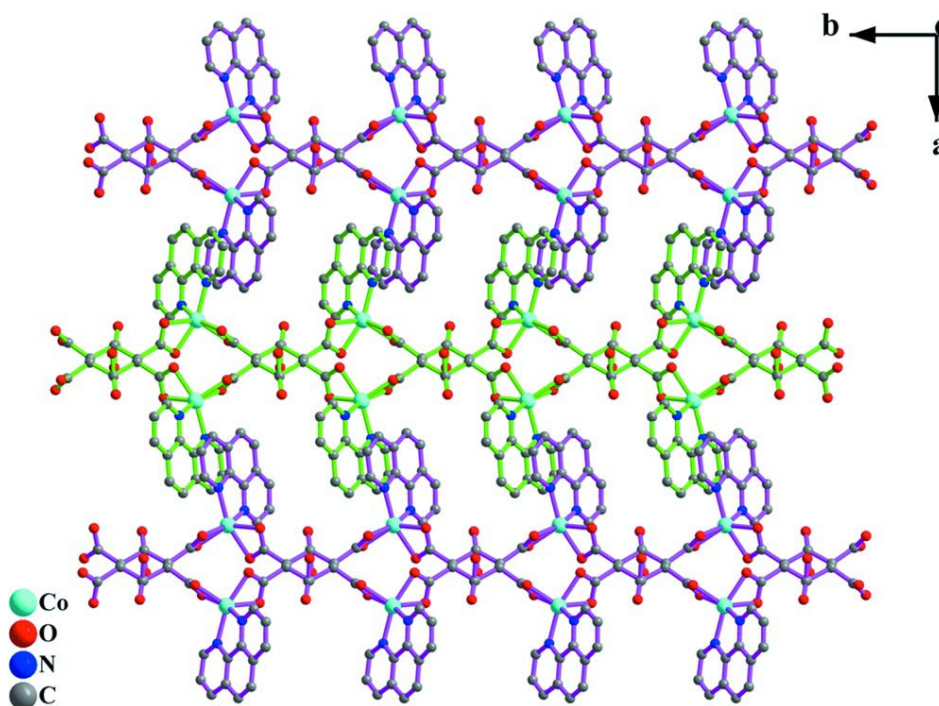


Figure 2

A view of a single layer of the title complex.

catena-Poly[bis[(1,10-phenanthroline)cobalt(II)]- μ_4 -3,6- dicarboxycyclohexane-1,2,4,5-tetracarboxylato]*Crystal data*

[Co₂(C₁₂H₈O₁₂)(C₁₂H₈N₂)₂]

$M_r = 822.46$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 22.180\ (4)\ \text{\AA}$

$b = 8.9520\ (18)\ \text{\AA}$

$c = 16.426\ (3)\ \text{\AA}$

$\beta = 93.33\ (3)^\circ$

$V = 3256.0\ (11)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1672$

$D_x = 1.678\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 25 reflections

$\theta = 5.0\text{--}12.5^\circ$

$\mu = 1.10\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Block, pink

$0.31 \times 0.23 \times 0.15\ \text{mm}$

Data collection

Siemens P4

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\theta/2\theta$ scans

Absorption correction: ψ scan

(*XSCANS*; Siemens, 1996)

$T_{\min} = 0.702$, $T_{\max} = 0.784$

4566 measured reflections

3753 independent reflections

3312 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.5^\circ$

$h = -28 \rightarrow 1$

$k = -1 \rightarrow 11$

$l = -21 \rightarrow 21$

3 standard reflections every 97 reflections

intensity decay: none

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.083$

$S = 1.03$

3753 reflections

248 parameters

0 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

$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 2.2781P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.38\ \text{e \AA}^{-3}$

$\Delta\rho_{\min} = -0.33\ \text{e \AA}^{-3}$

Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00077 (19)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.098444 (9)	0.64743 (2)	0.140367 (13)	0.02138 (9)
O1	0.07208 (6)	0.79951 (15)	0.23735 (7)	0.0330 (3)
O2	0.04781 (7)	0.83776 (14)	0.10892 (7)	0.0327 (3)
O3	0.08305 (7)	1.16900 (18)	0.04746 (9)	0.0433 (4)
O4	-0.01738 (6)	1.14637 (17)	0.04776 (8)	0.0363 (3)
H4A	-0.0159 (12)	1.148 (3)	-0.0004 (19)	0.054*
O5	0.09100 (5)	1.45307 (15)	0.21296 (8)	0.0314 (3)
O6	0.01745 (5)	1.51543 (15)	0.12579 (8)	0.0329 (3)
N1	0.13438 (6)	0.55177 (17)	0.03690 (9)	0.0277 (3)
N2	0.18993 (7)	0.70526 (19)	0.16045 (9)	0.0322 (3)
C1	0.10617 (9)	0.4793 (2)	-0.02411 (11)	0.0378 (4)
H1A	0.0642	0.4771	-0.0272	0.045*
C2	0.13708 (13)	0.4053 (3)	-0.08457 (14)	0.0544 (6)
H2A	0.1159	0.3563	-0.1272	0.065*
C3	0.19861 (13)	0.4065 (3)	-0.07970 (15)	0.0591 (7)
H3A	0.2196	0.3561	-0.1186	0.071*
C4	0.23052 (10)	0.4833 (3)	-0.01624 (14)	0.0472 (5)
C5	0.29531 (12)	0.4955 (4)	-0.00706 (19)	0.0673 (8)
H5A	0.3186	0.4468	-0.0441	0.081*
C6	0.32300 (10)	0.5748 (4)	0.05321 (19)	0.0686 (9)
H6A	0.3649	0.5806	0.0569	0.082*
C7	0.28897 (9)	0.6512 (3)	0.11216 (16)	0.0517 (6)
C8	0.31442 (11)	0.7393 (4)	0.17623 (18)	0.0660 (8)
H8A	0.3561	0.7516	0.1821	0.079*
C9	0.27855 (12)	0.8067 (4)	0.22961 (17)	0.0658 (8)
H9A	0.2954	0.8650	0.2719	0.079*
C10	0.21599 (11)	0.7875 (3)	0.22011 (14)	0.0487 (5)
H10A	0.1917	0.8338	0.2568	0.058*
C11	0.22540 (8)	0.6391 (2)	0.10648 (12)	0.0339 (4)
C12	0.19595 (8)	0.5557 (2)	0.04106 (11)	0.0318 (4)
C13	0.00497 (7)	1.00717 (17)	0.20407 (9)	0.0213 (3)
H13A	-0.0344	0.9985	0.1741	0.026*
C14	0.03623 (7)	1.15052 (16)	0.17600 (9)	0.0205 (3)
H14A	0.0778	1.1519	0.1998	0.025*
C15	0.00349 (7)	1.29201 (17)	0.20377 (9)	0.0194 (3)
H15A	-0.0367	1.2958	0.1758	0.023*
C16	0.04335 (8)	0.87293 (17)	0.18323 (10)	0.0234 (3)
C17	0.03790 (8)	1.15477 (18)	0.08330 (10)	0.0256 (3)
C18	0.03920 (7)	1.42928 (17)	0.17948 (9)	0.0209 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02179 (13)	0.01718 (13)	0.02545 (13)	-0.00066 (8)	0.00385 (8)	-0.00008 (8)
O1	0.0451 (7)	0.0284 (6)	0.0258 (6)	0.0125 (6)	0.0031 (5)	0.0002 (5)

O2	0.0497 (8)	0.0259 (6)	0.0228 (6)	0.0115 (6)	0.0048 (5)	-0.0013 (5)
O3	0.0426 (8)	0.0505 (9)	0.0389 (7)	0.0011 (7)	0.0212 (6)	0.0015 (6)
O4	0.0402 (7)	0.0477 (9)	0.0209 (6)	0.0031 (6)	0.0014 (5)	-0.0005 (6)
O5	0.0286 (6)	0.0283 (6)	0.0368 (6)	-0.0066 (5)	-0.0040 (5)	0.0084 (5)
O6	0.0274 (6)	0.0276 (6)	0.0431 (7)	-0.0037 (5)	-0.0031 (5)	0.0141 (6)
N1	0.0265 (7)	0.0298 (7)	0.0272 (7)	0.0006 (6)	0.0044 (5)	-0.0008 (6)
N2	0.0299 (7)	0.0335 (8)	0.0328 (7)	-0.0094 (6)	-0.0004 (6)	0.0029 (7)
C1	0.0407 (10)	0.0412 (11)	0.0313 (9)	-0.0015 (8)	0.0005 (7)	-0.0037 (8)
C2	0.0764 (17)	0.0522 (14)	0.0353 (11)	-0.0025 (13)	0.0089 (10)	-0.0145 (10)
C3	0.0742 (17)	0.0589 (15)	0.0469 (13)	0.0132 (14)	0.0256 (12)	-0.0108 (12)
C4	0.0444 (11)	0.0513 (13)	0.0479 (12)	0.0140 (10)	0.0206 (9)	0.0045 (10)
C5	0.0411 (13)	0.086 (2)	0.0782 (18)	0.0230 (14)	0.0307 (13)	0.0099 (17)
C6	0.0245 (10)	0.096 (2)	0.087 (2)	0.0121 (13)	0.0166 (11)	0.0225 (18)
C7	0.0236 (9)	0.0692 (17)	0.0620 (14)	-0.0055 (9)	0.0005 (9)	0.0216 (12)
C8	0.0310 (11)	0.092 (2)	0.0729 (17)	-0.0238 (13)	-0.0132 (11)	0.0211 (16)
C9	0.0571 (15)	0.081 (2)	0.0564 (15)	-0.0368 (15)	-0.0180 (12)	0.0040 (14)
C10	0.0505 (13)	0.0511 (13)	0.0438 (11)	-0.0208 (11)	-0.0043 (9)	-0.0023 (10)
C11	0.0229 (8)	0.0386 (10)	0.0404 (10)	-0.0019 (7)	0.0025 (7)	0.0106 (8)
C12	0.0278 (8)	0.0337 (9)	0.0348 (9)	0.0038 (7)	0.0091 (7)	0.0062 (8)
C13	0.0275 (7)	0.0155 (7)	0.0213 (7)	-0.0008 (6)	0.0037 (6)	-0.0001 (6)
C14	0.0228 (7)	0.0161 (7)	0.0227 (7)	-0.0001 (6)	0.0036 (5)	0.0001 (6)
C15	0.0209 (7)	0.0157 (7)	0.0217 (7)	0.0000 (5)	0.0020 (5)	0.0003 (6)
C16	0.0302 (8)	0.0168 (7)	0.0238 (7)	-0.0003 (6)	0.0051 (6)	0.0008 (6)
C17	0.0342 (8)	0.0179 (7)	0.0252 (8)	0.0015 (6)	0.0077 (6)	0.0009 (6)
C18	0.0238 (7)	0.0167 (7)	0.0228 (7)	0.0008 (6)	0.0058 (6)	-0.0014 (6)

Geometric parameters (Å, °)

Co1—O1	2.2002 (13)	C3—H3A	0.9300
Co1—O2	2.0890 (13)	C4—C12	1.406 (3)
Co1—O5 ⁱ	2.1211 (13)	C4—C5	1.440 (3)
Co1—O6 ⁱ	2.1519 (13)	C5—C6	1.338 (5)
Co1—N1	2.1012 (15)	C5—H5A	0.9300
Co1—N2	2.1016 (15)	C6—C7	1.435 (4)
Co1—C18 ⁱ	2.4599 (16)	C6—H6A	0.9300
Co1—C16	2.4827 (16)	C7—C8	1.407 (4)
O1—C16	1.250 (2)	C7—C11	1.412 (3)
O2—C16	1.270 (2)	C8—C9	1.359 (4)
O3—C17	1.198 (2)	C8—H8A	0.9300
O4—C17	1.329 (2)	C9—C10	1.398 (3)
O4—H4A	0.79 (3)	C9—H9A	0.9300
O5—C18	1.263 (2)	C10—H10A	0.9300
O5—Co1 ⁱⁱ	2.1211 (13)	C11—C12	1.435 (3)
O6—C18	1.247 (2)	C13—C16	1.523 (2)
O6—Co1 ⁱⁱⁱ	2.1519 (13)	C13—C13 ⁱⁱⁱ	1.538 (3)
N1—C1	1.321 (2)	C13—C14	1.542 (2)
N1—C12	1.364 (2)	C13—H13A	0.9800
N2—C10	1.330 (3)	C14—C17	1.526 (2)

N2—C11	1.355 (3)	C14—C15	1.542 (2)
C1—C2	1.405 (3)	C14—H14A	0.9800
C1—H1A	0.9300	C15—C18	1.528 (2)
C2—C3	1.363 (4)	C15—C15 ⁱⁱⁱ	1.535 (3)
C2—H2A	0.9300	C15—H15A	0.9800
C3—C4	1.405 (4)	C18—Co1 ⁱⁱ	2.4599 (16)
O2—Co1—N1	110.87 (6)	C5—C6—C7	121.0 (2)
O2—Co1—N2	109.77 (6)	C5—C6—H6A	119.5
N1—Co1—N2	79.58 (6)	C7—C6—H6A	119.5
O2—Co1—O5 ⁱ	138.57 (6)	C8—C7—C11	116.6 (2)
N1—Co1—O5 ⁱ	99.55 (6)	C8—C7—C6	124.6 (2)
N2—Co1—O5 ⁱ	102.70 (6)	C11—C7—C6	118.8 (2)
O2—Co1—O6 ⁱ	89.26 (5)	C9—C8—C7	120.5 (2)
N1—Co1—O6 ⁱ	92.27 (6)	C9—C8—H8A	119.8
N2—Co1—O6 ⁱ	160.89 (6)	C7—C8—H8A	119.8
O5 ⁱ —Co1—O6 ⁱ	61.34 (5)	C8—C9—C10	119.2 (2)
O2—Co1—O1	60.84 (5)	C8—C9—H9A	120.4
N1—Co1—O1	165.26 (6)	C10—C9—H9A	120.4
N2—Co1—O1	91.64 (6)	N2—C10—C9	122.4 (2)
O5 ⁱ —Co1—O1	93.89 (5)	N2—C10—H10A	118.8
O6 ⁱ —Co1—O1	99.50 (6)	C9—C10—H10A	118.8
O2—Co1—C18 ⁱ	115.12 (6)	N2—C11—C7	122.6 (2)
N1—Co1—C18 ⁱ	96.96 (6)	N2—C11—C12	117.47 (15)
N2—Co1—C18 ⁱ	132.85 (6)	C7—C11—C12	119.9 (2)
O5 ⁱ —Co1—C18 ⁱ	30.88 (5)	N1—C12—C4	122.56 (19)
O6 ⁱ —Co1—C18 ⁱ	30.46 (5)	N1—C12—C11	117.50 (16)
O1—Co1—C18 ⁱ	97.68 (5)	C4—C12—C11	119.94 (18)
O2—Co1—C16	30.74 (5)	C16—C13—C13 ⁱⁱⁱ	109.53 (11)
N1—Co1—C16	140.98 (6)	C16—C13—C14	108.82 (12)
N2—Co1—C16	104.00 (6)	C13 ⁱⁱⁱ —C13—C14	112.70 (10)
O5 ⁱ —Co1—C16	116.86 (6)	C16—C13—H13A	108.6
O6 ⁱ —Co1—C16	93.24 (6)	C13 ⁱⁱⁱ —C13—H13A	108.6
O1—Co1—C16	30.20 (5)	C14—C13—H13A	108.6
C18 ⁱ —Co1—C16	106.99 (5)	C17—C14—C13	110.89 (13)
C16—O1—Co1	87.50 (10)	C17—C14—C15	108.29 (12)
C16—O2—Co1	92.02 (10)	C13—C14—C15	111.56 (12)
C17—O4—H4A	110 (2)	C17—C14—H14A	108.7
C18—O5—Co1 ⁱⁱ	89.55 (10)	C13—C14—H14A	108.7
C18—O6—Co1 ⁱⁱ	88.55 (10)	C15—C14—H14A	108.7
C1—N1—C12	118.65 (16)	C18—C15—C15 ⁱⁱⁱ	109.99 (10)
C1—N1—Co1	128.96 (13)	C18—C15—C14	108.86 (12)
C12—N1—Co1	112.02 (12)	C15 ⁱⁱⁱ —C15—C14	111.64 (10)
C10—N2—C11	118.66 (18)	C18—C15—H15A	108.8
C10—N2—Co1	128.76 (15)	C15 ⁱⁱⁱ —C15—H15A	108.8
C11—N2—Co1	112.44 (12)	C14—C15—H15A	108.8
N1—C1—C2	122.6 (2)	O1—C16—O2	119.22 (15)
N1—C1—H1A	118.7	O1—C16—C13	121.57 (14)

C2—C1—H1A	118.7	O2—C16—C13	119.17 (14)
C3—C2—C1	118.9 (2)	O1—C16—Co1	62.30 (9)
C3—C2—H2A	120.6	O2—C16—Co1	57.23 (8)
C1—C2—H2A	120.6	C13—C16—Co1	174.86 (12)
C2—C3—C4	120.5 (2)	O3—C17—O4	124.52 (17)
C2—C3—H3A	119.8	O3—C17—C14	124.24 (17)
C4—C3—H3A	119.8	O4—C17—C14	111.20 (14)
C3—C4—C12	116.8 (2)	O6—C18—O5	120.56 (15)
C3—C4—C5	124.8 (2)	O6—C18—C15	119.79 (14)
C12—C4—C5	118.3 (2)	O5—C18—C15	119.64 (14)
C6—C5—C4	122.0 (2)	O6—C18—Co1 ⁱⁱ	60.99 (9)
C6—C5—H5A	119.0	O5—C18—Co1 ⁱⁱ	59.57 (8)
C4—C5—H5A	119.0	C15—C18—Co1 ⁱⁱ	178.92 (11)

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

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4A ^{iv} ⋯O2 ^{iv}	0.79 (3)	1.89 (3)	2.627 (2)	156 (2)

Symmetry code: (iv) $-x, -y+2, -z$.