



Crystal structure of poly[[μ -1,1'-(butane-1,4-diyl)bis(1*H*-benzimidazole)- κ^2 N³:N^{3'}]-{ μ -4,4'-[1,4-phenylenebis(oxy)]dibenzoato- κ^4 O,O':O'',O'''}cobalt(II)]

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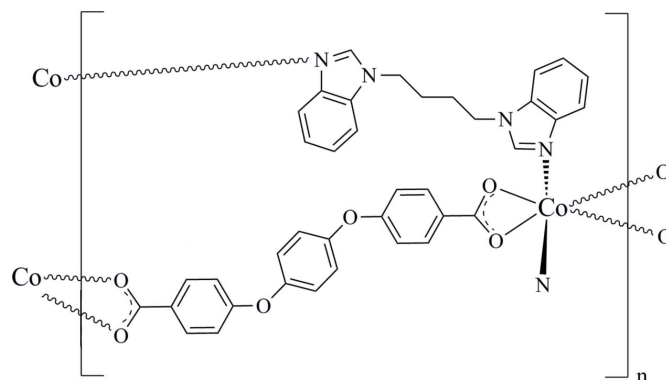
In the title compound, $[\text{Co}(\text{C}_{20}\text{H}_{12}\text{O}_6)(\text{C}_{18}\text{H}_{18}\text{N}_4)]_n$, the Co^{II} atom, located on a twofold rotation axis, is hexacoordinated to four O from two bis-bidentate 4,4'-[phenylenebis(oxy)]-dibenzoate (*L*) ligands and two N atoms from two 1,1'-(butane-1,4-diyl)bis(1*H*-benzimidazole) (bbbm) ligands, forming a distorted octahedral *cis*-N₂O₄ coordination environment. Polymeric zigzag chains along [102] are built up by the bridging *L* ligands. These chains are additionally connected by the bbbm ligands to produce a two-dimensional coordination polymer parallel too (010).

Keywords: crystal structure; metal–organic frameworks; bis-benzimidazole; dicarboxylate.

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1. Related literature

As a result of their intriguing variety of architectures and topologies, metal–organic frameworks (MOFs) with transition metal Co have received extensive interest. Bis-benzimidazole ligands bearing with butyl spacers are a good choice for the assembly of versatile entangled structures, see: Liu *et al.* (2008). Complexes with dicarboxylate ligands represent the most reliable and typical building blocks which can be jointly applied to synthesize a wide range of compounds with coordination networks, see: Du *et al.* (2013). For the potential properties of metal–organic complexes involving polycarboxylate ligands or bis-benzimidazole, see: Li *et al.* (2011); Wang *et al.* (2004); Sun *et al.* (2009); Wang *et al.* (2005); Łyszczek & Mazur (2012); Meng *et al.* (2003).



2. Experimental

2.1. Crystal data

$[\text{Co}(\text{C}_{20}\text{H}_{12}\text{O}_6)(\text{C}_{18}\text{H}_{18}\text{N}_4)]$
 $M_r = 697.59$
 Monoclinic, $C2/c$
 $a = 16.961$ (4) Å
 $b = 16.446$ (3) Å
 $c = 12.987$ (3) Å
 $\beta = 117.022$ (3)°

$V = 3227.1$ (12) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.59$ mm⁻¹
 $T = 296$ K
 $0.27 \times 0.24 \times 0.19$ mm

2.2. Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
 $T_{\text{min}} = 0.858$, $T_{\text{max}} = 0.897$

7207 measured reflections
 2836 independent reflections
 2385 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.140$
 $S = 1.02$
 2836 reflections

222 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.61$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.65$ e Å⁻³

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: IM2463).

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supporting information

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Crystal structure of poly[[μ -1,1'-(butane-1,4-diyl)bis(1*H*-benzimidazole)- κ^2 N³:N^{3'}]{ μ -4,4'-[1,4-phenylenebis(oxy)]dibenzoato- κ^4 O,O':O'',O'''}cobalt(II)]

Chen Xie and ChangGe Zheng

S1. Comment

Because of the intriguing varieties of architectures and topologies, metal-organic frameworks (MOFs) with transition-metal Co have received extensive interests. The bis-benzimidazole ligands bearing with butyl spacers are a good choice for the assembly of versatile entangled structures. (Ying-Ying Liu *et al.*, 2008) Complexes with the dicarboxylate ligands represent the most reliable and typical building blocks which can be jointly applied to synthesize a wide range of desired coordination networks (Du *et al.*, 2013).

Single-crystal X-ray diffraction analyses reveal that Co(II) is six-coordinate. The asymmetric unit contains one Co(II) atom, a dicarboxylate ligand and a bbbm ligand. Two carboxylate groups adopt a chelating bidentate mode to connect one Co(II) atoms. The Co—O bond length is 2.3705 (24)Å (O1) and 2.0422 (21)Å (O2), the Co—N bond length is 2.0797 (26)Å.

S2. Synthesis and crystallization

A mixture of 1,4-bis(4-carboxylphenoxy)benzene (0.035 g, 0.1 mmol), 1,1'-(1,4-butyl) bis-benzimidazole (0.029 g, 0.1 mmol), Co(NO₃)₂·H₂O (0.029 g, 0.1 mmol), and deionized water (9 mL) was stirred for 10 min at ambient temperature. Then the mixture was sealed in a Teflon-lined stainless vessel(25 mL) and heated at 160 °C for 3 days. The vessel was cooled to 50 °C by 9 °C decrease per hour, then cooled to ambient temperature directly. Amaranth transparent block-like crystal were obtained by filtration and washed with deionized water. Yield: 34.2 mg(49 %, based on Co) Elemental analysis (%) calcd. for CoC₃₈H₃₀N₄O₆: C 65.33, H 4.3, N 8.02. Found: C 65.38, H 4.39, N 8.11.

S3. Refinement

The H atoms bonded to C atoms were introduced at calculated positions and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) and C—H distances of 0.93–0.97 Å.

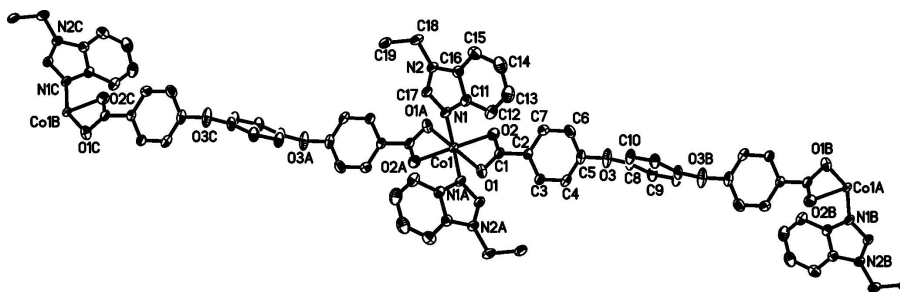


Figure 1

The molecular structure of $[\text{Co}(\text{C}_{20}\text{H}_{12}\text{O}_6)(\text{C}_{18}\text{H}_{18}\text{N}_4)]_n$, with the non-H atom-numbering scheme and 30% probability displacement ellipsoids.

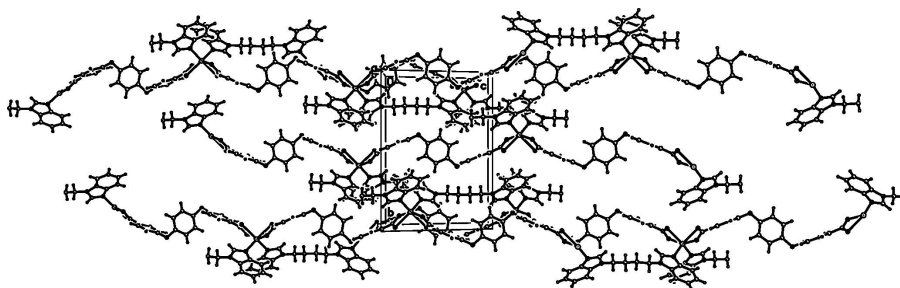


Figure 2

Three-dimensional network structure of $[\text{Co}(\text{C}_{20}\text{H}_{12}\text{O}_6)(\text{C}_{18}\text{H}_{18}\text{N}_4)]_n$ formed by C—H—O interaction.

Poly[[μ -1,1'-(butane-1,4-diyl)bis(1*H*-benzimidazole)- $\kappa^2\text{N}^3:\text{N}^3'$][μ -4,4'-[1,4-phenylenebis(oxy)]dibenzoato- $\kappa^4\text{O},\text{O}':\text{O}'',\text{O}'''$]cobalt(II)]

Crystal data

$[\text{Co}(\text{C}_{20}\text{H}_{12}\text{O}_6)(\text{C}_{18}\text{H}_{18}\text{N}_4)]$

$M_r = 697.59$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 16.961(4)\ \text{\AA}$

$b = 16.446(3)\ \text{\AA}$

$c = 12.987(3)\ \text{\AA}$

$\beta = 117.022(3)^\circ$

$V = 3227.1(12)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1444$

$D_x = 1.436\ \text{Mg m}^{-3}$

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

Cell parameters from 2720 reflections

$\theta = 2.7\text{--}26.5^\circ$

$\mu = 0.59\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Block, purple

$0.27 \times 0.24 \times 0.19\ \text{mm}$

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ϕ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2007)

$T_{\min} = 0.858$, $T_{\max} = 0.897$

7207 measured reflections

2836 independent reflections

2385 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 1.8^\circ$

$h = -15 \rightarrow 20$

$k = -17 \rightarrow 19$

$l = -14 \rightarrow 15$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.140$
 $S = 1.02$
 2836 reflections
 222 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-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0857P)^2 + 2.0556P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.61 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.65 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	0.10089 (3)	0.7500	0.0377 (2)
N1	0.46215 (15)	0.17924 (14)	0.84527 (17)	0.0426 (5)
O2	0.37200 (15)	0.07207 (16)	0.63915 (18)	0.0635 (6)
O1	0.46556 (13)	0.00024 (14)	0.60520 (19)	0.0591 (6)
N2	0.42235 (15)	0.21416 (15)	0.98059 (18)	0.0437 (5)
C16	0.36476 (17)	0.25422 (16)	0.8810 (2)	0.0424 (6)
C1	0.38817 (18)	0.02076 (17)	0.5798 (2)	0.0432 (6)
C2	0.31148 (17)	-0.01457 (15)	0.4757 (2)	0.0378 (6)
C3	0.32303 (18)	-0.03657 (17)	0.3804 (2)	0.0422 (6)
H3	0.3786	-0.0317	0.3830	0.051*
C17	0.47733 (18)	0.17001 (18)	0.9539 (2)	0.0438 (6)
H17	0.5214	0.1365	1.0064	0.053*
O3	0.10093 (17)	-0.10366 (14)	0.1800 (2)	0.0759 (8)
C11	0.39104 (18)	0.23265 (16)	0.7975 (2)	0.0417 (6)
C4	0.2531 (2)	-0.06546 (17)	0.2819 (2)	0.0477 (7)
H4	0.2610	-0.0801	0.2181	0.057*
C19	0.5047 (2)	0.2089 (2)	1.1943 (2)	0.0537 (7)
H19A	0.5404	0.2550	1.1945	0.064*
H19B	0.5351	0.1598	1.1908	0.064*
C7	0.22884 (19)	-0.0219 (2)	0.4712 (2)	0.0512 (7)
H7	0.2205	-0.0064	0.5344	0.061*
C13	0.2759 (2)	0.3149 (2)	0.6626 (3)	0.0696 (10)
H13	0.2448	0.3361	0.5885	0.084*
C8	0.05289 (18)	-0.04860 (18)	0.0917 (2)	0.0508 (7)
C10	0.0458 (2)	0.0333 (2)	0.1086 (2)	0.0576 (8)

H10	0.0771	0.0557	0.1819	0.069*
C5	0.1718 (2)	-0.07240 (18)	0.2787 (2)	0.0510 (7)
C12	0.3458 (2)	0.26448 (19)	0.6859 (3)	0.0572 (8)
H12	0.3628	0.2517	0.6291	0.069*
C18	0.4176 (2)	0.2131 (2)	1.0912 (2)	0.0584 (8)
H18A	0.3825	0.1667	1.0916	0.070*
H18B	0.3873	0.2618	1.0961	0.070*
C15	0.2935 (2)	0.30607 (19)	0.8577 (3)	0.0579 (8)
H15	0.2766	0.3200	0.9142	0.069*
C9	0.0075 (2)	-0.08197 (19)	-0.0168 (3)	0.0540 (8)
H9	0.0127	-0.1371	-0.0282	0.065*
C14	0.2497 (2)	0.3356 (2)	0.7465 (3)	0.0712 (10)
H14	0.2015	0.3700	0.7270	0.085*
C6	0.15846 (19)	-0.0521 (2)	0.3733 (3)	0.0591 (8)
H6	0.1032	-0.0586	0.3708	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0393 (3)	0.0508 (4)	0.0221 (3)	0.000	0.0133 (2)	0.000
N1	0.0524 (13)	0.0490 (13)	0.0281 (11)	0.0031 (10)	0.0198 (10)	-0.0016 (9)
O2	0.0606 (13)	0.0822 (16)	0.0457 (12)	-0.0111 (12)	0.0223 (10)	-0.0246 (11)
O1	0.0415 (11)	0.0632 (14)	0.0567 (13)	-0.0011 (10)	0.0083 (10)	-0.0031 (10)
N2	0.0495 (12)	0.0512 (14)	0.0342 (11)	-0.0018 (10)	0.0224 (10)	-0.0083 (10)
C16	0.0454 (14)	0.0390 (15)	0.0415 (14)	-0.0052 (12)	0.0185 (12)	-0.0062 (11)
C1	0.0465 (15)	0.0505 (16)	0.0281 (13)	0.0015 (12)	0.0130 (12)	0.0040 (11)
C2	0.0410 (13)	0.0369 (14)	0.0307 (13)	0.0026 (11)	0.0122 (11)	0.0039 (10)
C3	0.0439 (14)	0.0455 (15)	0.0342 (13)	0.0032 (12)	0.0152 (12)	0.0033 (11)
C17	0.0487 (15)	0.0527 (17)	0.0289 (13)	0.0023 (12)	0.0167 (11)	-0.0044 (11)
O3	0.0741 (16)	0.0512 (13)	0.0501 (13)	-0.0189 (11)	-0.0175 (12)	0.0059 (10)
C11	0.0491 (14)	0.0376 (14)	0.0340 (13)	-0.0043 (11)	0.0150 (12)	-0.0022 (10)
C4	0.0630 (18)	0.0448 (16)	0.0292 (13)	-0.0035 (14)	0.0155 (13)	0.0015 (11)
C19	0.0625 (18)	0.069 (2)	0.0373 (15)	-0.0063 (15)	0.0293 (14)	0.0003 (14)
C7	0.0501 (16)	0.065 (2)	0.0415 (15)	-0.0023 (14)	0.0236 (13)	-0.0036 (13)
C13	0.074 (2)	0.056 (2)	0.059 (2)	0.0119 (18)	0.0134 (18)	0.0121 (16)
C8	0.0381 (14)	0.0515 (18)	0.0407 (15)	-0.0122 (12)	-0.0016 (12)	0.0025 (12)
C10	0.0562 (17)	0.0547 (18)	0.0371 (15)	-0.0159 (15)	-0.0004 (13)	-0.0108 (13)
C5	0.0519 (16)	0.0420 (15)	0.0364 (15)	-0.0090 (13)	0.0001 (12)	0.0038 (12)
C12	0.0714 (19)	0.0513 (18)	0.0424 (16)	0.0000 (15)	0.0203 (15)	0.0041 (13)
C18	0.0693 (19)	0.076 (2)	0.0417 (16)	-0.0016 (17)	0.0352 (15)	-0.0120 (15)
C15	0.0546 (17)	0.0518 (18)	0.069 (2)	-0.0027 (14)	0.0294 (16)	-0.0109 (15)
C9	0.0506 (16)	0.0442 (16)	0.0478 (17)	-0.0096 (13)	0.0055 (14)	-0.0062 (13)
C14	0.0576 (19)	0.055 (2)	0.084 (3)	0.0104 (16)	0.0178 (19)	0.0052 (18)
C6	0.0381 (14)	0.068 (2)	0.064 (2)	-0.0069 (14)	0.0170 (14)	0.0044 (16)

Geometric parameters (Å, °)

Co1—O2	2.042 (2)	C4—H4	0.9300
Co1—O2 ⁱ	2.042 (2)	C19—C18	1.477 (4)
Co1—N1	2.080 (2)	C19—C19 ⁱⁱ	1.526 (5)
Co1—N1 ⁱ	2.080 (2)	C19—H19A	0.9700
Co1—O1	2.371 (2)	C19—H19B	0.9700
Co1—O1 ⁱ	2.371 (2)	C7—C6	1.382 (4)
N1—C17	1.322 (3)	C7—H7	0.9300
N1—C11	1.390 (3)	C13—C12	1.363 (5)
O2—C1	1.255 (4)	C13—C14	1.392 (5)
O1—C1	1.246 (3)	C13—H13	0.9300
N2—C17	1.346 (3)	C8—C9	1.377 (4)
N2—C16	1.383 (4)	C8—C10	1.378 (5)
N2—C18	1.474 (3)	C10—C9 ⁱⁱⁱ	1.378 (4)
C16—C15	1.395 (4)	C10—H10	0.9300
C16—C11	1.393 (4)	C5—C6	1.387 (4)
C1—C2	1.503 (4)	C12—H12	0.9300
C2—C7	1.381 (4)	C18—H18A	0.9700
C2—C3	1.387 (4)	C18—H18B	0.9700
C3—C4	1.375 (4)	C15—C14	1.378 (5)
C3—H3	0.9300	C15—H15	0.9300
C17—H17	0.9300	C9—C10 ⁱⁱⁱ	1.378 (4)
O3—C8	1.396 (4)	C9—H9	0.9300
O3—C5	1.397 (3)	C14—H14	0.9300
C11—C12	1.398 (4)	C6—H6	0.9300
C4—C5	1.365 (4)		
O2—Co1—O2 ⁱ	153.16 (15)	C3—C4—H4	120.3
O2—Co1—N1	92.67 (9)	C18—C19—C19 ⁱⁱ	111.6 (3)
O2 ⁱ —Co1—N1	103.95 (9)	C18—C19—H19A	109.3
O2—Co1—N1 ⁱ	103.95 (9)	C19 ⁱⁱ —C19—H19A	109.3
O2 ⁱ —Co1—N1 ⁱ	92.67 (9)	C18—C19—H19B	109.3
N1—Co1—N1 ⁱ	103.44 (13)	C19 ⁱⁱ —C19—H19B	109.3
O2—Co1—O1	58.59 (8)	H19A—C19—H19B	108.0
O2 ⁱ —Co1—O1	101.36 (9)	C2—C7—C6	120.4 (3)
N1—Co1—O1	150.83 (8)	C2—C7—H7	119.8
N1 ⁱ —Co1—O1	89.54 (8)	C6—C7—H7	119.8
O2—Co1—O1 ⁱ	101.36 (9)	C12—C13—C14	122.0 (3)
O2 ⁱ —Co1—O1 ⁱ	58.59 (8)	C12—C13—H13	119.0
N1—Co1—O1 ⁱ	89.54 (8)	C14—C13—H13	119.0
N1 ⁱ —Co1—O1 ⁱ	150.83 (8)	C9—C8—C10	120.3 (3)
O1—Co1—O1 ⁱ	91.42 (11)	C9—C8—O3	115.4 (3)
C17—N1—C11	104.9 (2)	C10—C8—O3	124.3 (3)
C17—N1—Co1	126.90 (19)	C9 ⁱⁱⁱ —C10—C8	120.0 (3)
C11—N1—Co1	124.46 (17)	C9 ⁱⁱⁱ —C10—H10	120.0
C1—O2—Co1	97.48 (18)	C8—C10—H10	120.0
C1—O1—Co1	82.61 (17)	C4—C5—C6	121.4 (3)

C17—N2—C16	107.1 (2)	C4—C5—O3	119.6 (3)
C17—N2—C18	126.5 (2)	C6—C5—O3	118.9 (3)
C16—N2—C18	126.1 (2)	C13—C12—C11	118.0 (3)
N2—C16—C15	131.9 (3)	C13—C12—H12	121.0
N2—C16—C11	105.5 (2)	C11—C12—H12	121.0
C15—C16—C11	122.6 (3)	N2—C18—C19	114.2 (2)
O1—C1—O2	121.2 (3)	N2—C18—H18A	108.7
O1—C1—C2	120.7 (2)	C19—C18—H18A	108.7
O2—C1—C2	118.1 (2)	N2—C18—H18B	108.7
C7—C2—C3	119.4 (2)	C19—C18—H18B	108.7
C7—C2—C1	121.3 (2)	H18A—C18—H18B	107.6
C3—C2—C1	119.2 (2)	C14—C15—C16	116.4 (3)
C4—C3—C2	120.5 (3)	C14—C15—H15	121.8
C4—C3—H3	119.7	C16—C15—H15	121.8
C2—C3—H3	119.7	C10 ⁱⁱⁱ —C9—C8	119.7 (3)
N1—C17—N2	113.0 (2)	C10 ⁱⁱⁱ —C9—H9	120.1
N1—C17—H17	123.5	C8—C9—H9	120.1
N2—C17—H17	123.5	C15—C14—C13	121.4 (3)
C8—O3—C5	116.9 (2)	C15—C14—H14	119.3
N1—C11—C16	109.5 (2)	C13—C14—H14	119.3
N1—C11—C12	131.0 (3)	C7—C6—C5	118.8 (3)
C16—C11—C12	119.5 (3)	C7—C6—H6	120.6
C5—C4—C3	119.4 (3)	C5—C6—H6	120.6
C5—C4—H4	120.3		
O2—Co1—N1—C17	114.1 (2)	C16—N2—C17—N1	1.6 (3)
O2 ⁱ —Co1—N1—C17	-44.6 (3)	C18—N2—C17—N1	175.4 (3)
N1 ⁱ —Co1—N1—C17	-140.8 (3)	C17—N1—C11—C16	-0.2 (3)
O1—Co1—N1—C17	104.9 (3)	Co1—N1—C11—C16	159.27 (18)
O1 ⁱ —Co1—N1—C17	12.8 (2)	C17—N1—C11—C12	-179.7 (3)
O2—Co1—N1—C11	-40.8 (2)	Co1—N1—C11—C12	-20.2 (4)
O2 ⁱ —Co1—N1—C11	160.4 (2)	N2—C16—C11—N1	1.1 (3)
N1 ⁱ —Co1—N1—C11	64.21 (19)	C15—C16—C11—N1	-178.7 (3)
O1—Co1—N1—C11	-50.1 (3)	N2—C16—C11—C12	-179.3 (2)
O1 ⁱ —Co1—N1—C11	-142.2 (2)	C15—C16—C11—C12	0.9 (4)
O2 ⁱ —Co1—O2—C1	-48.23 (18)	C2—C3—C4—C5	0.0 (4)
N1—Co1—O2—C1	-177.02 (19)	C3—C2—C7—C6	1.0 (4)
N1 ⁱ —Co1—O2—C1	78.4 (2)	C1—C2—C7—C6	177.9 (3)
O1—Co1—O2—C1	-2.29 (17)	C5—O3—C8—C9	156.8 (3)
O1 ⁱ —Co1—O2—C1	-86.95 (19)	C5—O3—C8—C10	-26.4 (5)
O2—Co1—O1—C1	2.31 (17)	C9—C8—C10—C9 ⁱⁱⁱ	0.6 (6)
O2 ⁱ —Co1—O1—C1	162.98 (16)	O3—C8—C10—C9 ⁱⁱⁱ	-176.1 (3)
N1—Co1—O1—C1	13.2 (3)	C3—C4—C5—C6	-1.0 (4)
N1 ⁱ —Co1—O1—C1	-104.39 (17)	C3—C4—C5—O3	-178.4 (2)
O1 ⁱ —Co1—O1—C1	104.77 (18)	C8—O3—C5—C4	-86.4 (4)
C17—N2—C16—C15	178.2 (3)	C8—O3—C5—C6	96.1 (4)
C18—N2—C16—C15	4.4 (5)	C14—C13—C12—C11	0.6 (5)
C17—N2—C16—C11	-1.6 (3)	N1—C11—C12—C13	178.3 (3)

C18—N2—C16—C11	-175.4 (3)	C16—C11—C12—C13	-1.1 (4)
Co1—O1—C1—O2	-3.8 (3)	C17—N2—C18—C19	40.2 (4)
Co1—O1—C1—C2	175.3 (2)	C16—N2—C18—C19	-147.2 (3)
Co1—O2—C1—O1	4.4 (3)	C19 ⁱⁱ —C19—C18—N2	179.41 (19)
Co1—O2—C1—C2	-174.77 (19)	N2—C16—C15—C14	-179.9 (3)
O1—C1—C2—C7	152.1 (3)	C11—C16—C15—C14	-0.1 (4)
O2—C1—C2—C7	-28.8 (4)	C10—C8—C9—C10 ⁱⁱⁱ	-0.6 (6)
O1—C1—C2—C3	-31.1 (4)	O3—C8—C9—C10 ⁱⁱⁱ	176.4 (3)
O2—C1—C2—C3	148.1 (3)	C16—C15—C14—C13	-0.4 (5)
C7—C2—C3—C4	0.0 (4)	C12—C13—C14—C15	0.2 (5)
C1—C2—C3—C4	-176.9 (2)	C2—C7—C6—C5	-2.0 (5)
C11—N1—C17—N2	-0.8 (3)	C4—C5—C6—C7	2.0 (5)
Co1—N1—C17—N2	-159.67 (18)	O3—C5—C6—C7	179.4 (3)

Symmetry codes: (i) $-x+1, y, -z+3/2$; (ii) $-x+1, y, -z+5/2$; (iii) $-x, -y, -z$.