metal-organic compounds

catena-Poly[[[2-(2-pyridyl)-1*H*-benzimidazole]cobalt(II)]-*μ*-benzene-1,4-dicarboxylato]

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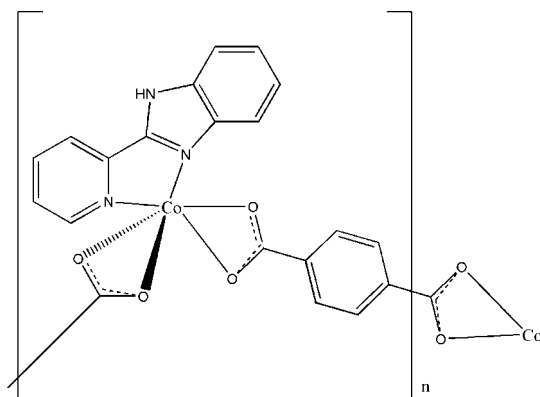Correspondence e-mail: jsuxie@163.com

In the title coordination polymer, $[Co(C_8H_4O_4)(C_{12}H_9N_3)]_n$, the Co^{II} atom exists in an octahedral coordination environment formed by four carboxylate O atoms from two benzene-1,4-dicarboxylate ligands, and two N atoms from the 2-(2-pyridyl)benzimidazole ligand. Bridging by the benzene-1,4-dicarboxylate ligand leads to a zigzag chain structure, and intermolecular N—H···O hydrogen bonds as well as π–π interactions between the pyridyl ring and the benzene ring of the 2-(2-pyridyl)benzimidazole ligand (centroid–centroid distances = 3.678 and 3.697 Å) link the chains into a three-dimensional framework.

Related literature

For related literature, see: Sun *et al.* (2001); Zhang *et al.* (2003); Cano *et al.* (1997); Alcade *et al.* (1992).

Experimental

Crystal data

$[Co(C_8H_4O_4)(C_{12}H_9N_3)]$
$M_r = 418.26$
Monoclinic, $P2_1/c$
$a = 7.2518 (7)$ Å
$b = 20.6995 (19)$ Å
$c = 11.3088 (11)$ Å
$\beta = 95.914 (5)°$
$V = 1688.5 (3)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.05$ mm^{-1}
$T = 293 (2)$ K
$0.20 \times 0.15 \times 0.08$ mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
$T_{min} = 0.828$, $T_{max} = 0.923$
12922 measured reflections
3866 independent reflections
3170 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.100$
$S = 1.10$
3866 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O2^i	0.86	2.27	2.913 (3)	132
N3—H3B···O4^{ii}	0.86	2.36	2.963 (3)	127

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

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2531).

References

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Cano, J., Munno, G. D., Sanz, J. L., Ruiz, R., Faus, J., Lloret, F., Julve, M. & Caneschi, A. (1997). *J. Chem. Soc. Dalton Trans.* pp. 1915–1923.
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Sun, D. F., Cao, R., Liang, Y. C., Shi, Q., Su, W. P. & Hong, M. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 2335–2340.
Zhang, L. J., Zhao, X. L., Cheng, P., Xu, J. Q., Tang, X., Cui, X. B., Xu, W. & Wang, T. G. (2003). *Bull. Chem. Soc. Jpn*, **76**, 1179–1184.

supplementary materials

catena-Poly[[[2-(2-pyridyl)-1*H*-benzimidazole]cobalt(II)]-$^\mu$-benzene-1,4-dicarboxylato]

C.-K. Xia, W. Wu, Q.-Y. Chen and J.-M. Xie

Comment

benzene-1,4-dicarboxylatic acid is often used to bridge metal atoms with 2,2'-bipyridine or 1,10-phenanthroline as auxiliary ligands (Sun *et al.*, 2001; Zhang *et al.*, 2003; Cano *et al.*, 1997). Those compounds demonstrate various network topologies. In the title compound the Co^{II} atom is six coordinated (Fig. 1), bonded to two nitrogen atoms of the chelating 2-(2-pyridyl)benzimidazole ligand, and bridged by the benzene-1,4-dicarboxylate into a zigzag chain (Fig. 2). The chains are further connected into a three-dimensional framework *via* intermolecular N—H⋯O hydrogen bonds as well as π-π interactions (perpendicular distance: 3.54 Å, centroid⋯centroid distances: 3.678Å and 3.697 Å) (Fig. 3).

Experimental

2-(2-pyridyl)benzimidazole was synthesized according to the literature method of Alcade *et al.* (1992). A solution of Co(CH$_3$COO)$_2$·4H$_2$O (0.128 g, 0.51 mmol), 2-(2-pyridyl)benzimidazole (0.10 g, 0.51 mmol), benzene-1,4-dicarboxylatic acid (0.085 g, 0.51 mmol) and H$_2$O (15 ml) stirred under ambient conditions, then sealed in a Teflon-lined steel vessel, heated at 160 °C for 5 days, and cooled to room temperature. The resulting product was recovered by filtration, washed with distilled water and dried in air (80% yield).

Refinement

After checking their presence in the difference map, all H atoms were positioned geometrically and allowed to ride on their attached atoms with C—H and N—H bond lengths of 0.93–0.97Å and 0.86 Å, respectively, and U_{iso}(H) = 1.2U_{eq}(C,*N*).
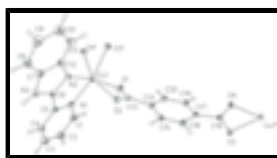
Figures

Fig. 1. The structure of the title compound with the atomic labels and 30% probability displacement ellipsoids for non-H atoms. Symmetry codes: (i)*x* − 1, 1/2 − *y*, *z* − 1/2; (ii) 1 + *x*, 1/2 − *y*, 1/2 + *z*.
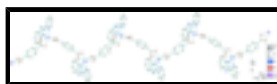

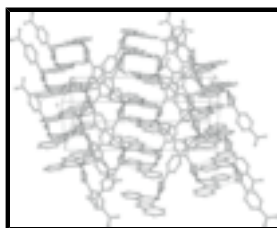Fig. 2. A view of the zigzag chain of the title compound.

Fig. 3. Packing diagram.

catena-Poly[[2-(2-pyridyl)-1H-benzimidazole]cobalt(II)]-µ-\ benzene-1,4-dicarboxylato]

Crystal data

$[Co(C_8H_4O_4)(C_{12}H_9N_3)]$	$F_{000} = 852$
$M_r = 418.26$	$D_x = 1.645$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -p 2ybc	Cell parameters from 3393 reflections
$a = 7.2518$ (7) Å	$\theta = 3.2–27.5º$
$b = 20.6995$ (19) Å	$\mu = 1.05$ mm^{-1}
$c = 11.3088$ (11) Å	$T = 293$ (2) K
$\beta = 95.914$ (5)º	Prism, red
$V = 1688.5$ (3) Å^3	$0.20 \times 0.15 \times 0.08$ mm
$Z = 4$	

Data collection

Rigaku CCD diffractometer	3866 independent reflections
Radiation source: fine-focus sealed tube	3170 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.042$
Detector resolution: 14.6306 pixels mm^{-1}	$\theta_{max} = 27.5º$
$T = 293(2)$ K	$\theta_{min} = 3.3º$
ω scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2002)	$k = -24 \rightarrow 26$
$T_{min} = 0.828$, $T_{max} = 0.923$	$l = -14 \rightarrow 14$
12922 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 1.1421P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
3866 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
253 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.21952 (5)	0.389651 (17)	0.65376 (3)	0.02542 (12)
C1	0.1887 (4)	0.51415 (16)	0.8068 (3)	0.0420 (7)
H1A	0.1646	0.4867	0.8685	0.050*
C2	0.2052 (5)	0.57978 (18)	0.8292 (3)	0.0541 (9)
H2A	0.1906	0.5961	0.9042	0.065*
C3	0.2433 (5)	0.62015 (16)	0.7392 (3)	0.0547 (10)
H3A	0.2567	0.6643	0.7525	0.066*
C4	0.2617 (4)	0.59479 (14)	0.6290 (3)	0.0421 (8)
H4A	0.2882	0.6215	0.5668	0.051*
C5	0.2403 (4)	0.52938 (13)	0.6114 (2)	0.0291 (6)
C6	0.2538 (3)	0.49664 (12)	0.4984 (2)	0.0259 (5)
C7	0.2778 (4)	0.47506 (14)	0.3107 (2)	0.0320 (6)
C8	0.2962 (5)	0.47506 (16)	0.1891 (3)	0.0429 (8)
H8A	0.3118	0.5131	0.1475	0.051*
C9	0.2899 (5)	0.41577 (18)	0.1343 (3)	0.0498 (8)
H9A	0.3018	0.4137	0.0533	0.060*
C10	0.2664 (5)	0.35865 (16)	0.1960 (3)	0.0440 (8)
H10A	0.2617	0.3197	0.1549	0.053*
C11	0.2500 (4)	0.35825 (15)	0.3156 (3)	0.0375 (7)
H11A	0.2354	0.3199	0.3565	0.045*
C12	0.2559 (4)	0.41753 (13)	0.3730 (2)	0.0276 (6)
C13	0.4583 (4)	0.35217 (12)	0.8096 (2)	0.0251 (5)
C14	0.6013 (4)	0.31788 (12)	0.8909 (2)	0.0248 (5)
C15	0.7883 (4)	0.32392 (13)	0.8738 (2)	0.0280 (6)
H15A	0.8250	0.3527	0.8175	0.034*
C16	0.9190 (4)	0.28677 (13)	0.9411 (2)	0.0297 (6)
H16A	1.0440	0.2915	0.9314	0.036*
C17	0.8643 (3)	0.24263 (12)	1.0228 (2)	0.0238 (5)
C18	1.0033 (4)	0.19638 (13)	1.0811 (2)	0.0259 (6)
C19	0.6783 (4)	0.23799 (13)	1.0420 (2)	0.0272 (6)
H19A	0.6417	0.2093	1.0984	0.033*
C20	0.5484 (4)	0.27602 (13)	0.9769 (2)	0.0276 (6)
H20A	0.4244	0.2736	0.9910	0.033*

O1	0.2913 (3)	0.35225 (10)	0.83061 (17)	0.0363 (5)
O2	0.5059 (2)	0.37898 (9)	0.71660 (16)	0.0305 (4)
O3	1.1733 (2)	0.20703 (9)	1.08103 (17)	0.0317 (4)
O4	0.9473 (2)	0.14397 (9)	1.12442 (16)	0.0289 (4)
N1	0.2062 (3)	0.48882 (11)	0.7003 (2)	0.0309 (5)
N2	0.2420 (3)	0.43282 (10)	0.49134 (18)	0.0263 (5)
N3	0.2760 (3)	0.52381 (11)	0.3928 (2)	0.0324 (5)
H3B	0.2871	0.5644	0.3792	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0241 (2)	0.02434 (19)	0.02722 (19)	−0.00096 (15)	−0.00035 (14)	0.00107 (15)
C1	0.0434 (18)	0.0478 (19)	0.0339 (15)	0.0057 (15)	−0.0011 (14)	−0.0110 (14)
C2	0.057 (2)	0.057 (2)	0.0458 (19)	0.0125 (18)	−0.0064 (16)	−0.0267 (18)
C3	0.065 (2)	0.0334 (18)	0.061 (2)	0.0101 (16)	−0.0160 (18)	−0.0165 (16)
C4	0.0448 (19)	0.0275 (16)	0.0506 (18)	0.0008 (13)	−0.0115 (15)	−0.0029 (13)
C5	0.0232 (14)	0.0252 (14)	0.0369 (14)	0.0032 (11)	−0.0058 (11)	−0.0025 (11)
C6	0.0214 (13)	0.0234 (13)	0.0317 (13)	0.0003 (10)	−0.0026 (11)	0.0021 (11)
C7	0.0300 (15)	0.0320 (15)	0.0336 (14)	0.0001 (12)	0.0017 (12)	0.0031 (12)
C8	0.0472 (19)	0.0464 (19)	0.0355 (16)	−0.0029 (15)	0.0065 (14)	0.0095 (14)
C9	0.058 (2)	0.061 (2)	0.0325 (16)	0.0019 (18)	0.0107 (15)	−0.0008 (16)
C10	0.049 (2)	0.0437 (19)	0.0397 (16)	0.0035 (15)	0.0077 (15)	−0.0099 (15)
C11	0.0410 (18)	0.0315 (16)	0.0412 (16)	−0.0003 (13)	0.0101 (14)	−0.0042 (13)
C12	0.0241 (14)	0.0292 (14)	0.0299 (13)	0.0010 (11)	0.0047 (11)	0.0004 (11)
C13	0.0254 (13)	0.0239 (13)	0.0257 (12)	−0.0022 (11)	0.0006 (10)	−0.0011 (10)
C14	0.0242 (13)	0.0255 (13)	0.0244 (12)	0.0020 (11)	0.0012 (10)	−0.0006 (10)
C15	0.0260 (14)	0.0291 (14)	0.0295 (13)	−0.0017 (11)	0.0059 (11)	0.0064 (11)
C16	0.0214 (13)	0.0343 (15)	0.0339 (14)	0.0008 (11)	0.0048 (11)	0.0035 (12)
C17	0.0222 (13)	0.0241 (13)	0.0250 (12)	0.0015 (10)	0.0018 (10)	−0.0021 (10)
C18	0.0275 (14)	0.0264 (14)	0.0240 (12)	0.0029 (11)	0.0042 (11)	−0.0037 (10)
C19	0.0272 (14)	0.0275 (14)	0.0276 (13)	0.0000 (11)	0.0064 (11)	0.0041 (11)
C20	0.0230 (13)	0.0316 (15)	0.0290 (13)	0.0004 (11)	0.0066 (11)	0.0001 (11)
O1	0.0231 (10)	0.0493 (13)	0.0364 (11)	0.0021 (9)	0.0030 (8)	0.0105 (9)
O2	0.0252 (10)	0.0363 (11)	0.0297 (9)	0.0023 (8)	0.0016 (8)	0.0089 (8)
O3	0.0228 (10)	0.0272 (10)	0.0443 (11)	0.0010 (8)	−0.0004 (8)	0.0019 (8)
O4	0.0259 (10)	0.0276 (10)	0.0334 (10)	0.0014 (8)	0.0040 (8)	0.0054 (8)
N1	0.0286 (12)	0.0315 (13)	0.0315 (11)	0.0010 (10)	−0.0015 (10)	−0.0046 (10)
N2	0.0261 (12)	0.0239 (11)	0.0284 (11)	−0.0001 (9)	0.0006 (9)	0.0004 (9)
N3	0.0375 (14)	0.0215 (12)	0.0375 (12)	−0.0010 (10)	0.0000 (11)	0.0064 (10)

Geometric parameters (Å, °)

Co1—N2	2.064 (2)	C9—H9A	0.9300
Co1—O4ⁱ	2.0872 (18)	C10—C11	1.371 (4)
Co1—N1	2.124 (2)	C10—H10A	0.9300
Co1—O2	2.1362 (18)	C11—C12	1.387 (4)
Co1—O1	2.1577 (19)	C11—H11A	0.9300

Co1—O3ⁱ	2.1765 (18)	C12—N2	1.389 (3)
C1—N1	1.332 (4)	C13—O1	1.257 (3)
C1—C2	1.385 (5)	C13—O2	1.268 (3)
C1—H1A	0.9300	C13—C14	1.493 (3)
C2—C3	1.367 (5)	C14—C20	1.386 (4)
C2—H2A	0.9300	C14—C15	1.395 (3)
C3—C4	1.371 (5)	C15—C16	1.386 (4)
C3—H3A	0.9300	C15—H15A	0.9300
C4—C5	1.375 (4)	C16—C17	1.386 (4)
C4—H4A	0.9300	C16—H16A	0.9300
C5—N1	1.352 (4)	C17—C19	1.392 (4)
C5—C6	1.459 (4)	C17—C18	1.493 (4)
C6—N2	1.326 (3)	C18—O3	1.253 (3)
C6—N3	1.344 (3)	C18—O4	1.274 (3)
C7—N3	1.372 (4)	C19—C20	1.381 (4)
C7—C8	1.395 (4)	C19—H19A	0.9300
C7—C12	1.401 (4)	C20—H20A	0.9300
C8—C9	1.373 (5)	N3—O2ⁱⁱ	2.913 (3)
C8—H8A	0.9300	N3—O4ⁱⁱⁱ	2.963 (3)
C9—C10	1.392 (5)	N3—H3B	0.8600
N2—Co1—O4ⁱ	99.39 (8)	C11—C10—H10A	119.1
N2—Co1—N1	79.16 (9)	C9—C10—H10A	119.1
O4ⁱ—Co1—N1	107.17 (8)	C10—C11—C12	117.1 (3)
N2—Co1—O2	100.22 (8)	C10—C11—H11A	121.5
O4ⁱ—Co1—O2	152.82 (7)	C12—C11—H11A	121.5
N1—Co1—O2	94.88 (8)	C11—C12—N2	130.6 (3)
N2—Co1—O1	161.16 (8)	C11—C12—C7	121.1 (3)
O4ⁱ—Co1—O1	99.31 (7)	N2—C12—C7	108.3 (2)
N1—Co1—O1	97.47 (9)	O1—C13—O2	120.4 (2)
O2—Co1—O1	61.38 (7)	O1—C13—C14	120.4 (2)
N2—Co1—O3ⁱ	94.88 (8)	O2—C13—C14	119.2 (2)
O4ⁱ—Co1—O3ⁱ	61.77 (7)	O1—C13—Co1	61.04 (13)
N1—Co1—O3ⁱ	166.70 (8)	O2—C13—Co1	60.05 (13)
O2—Co1—O3ⁱ	97.89 (7)	C14—C13—Co1	169.17 (18)
O1—Co1—O3ⁱ	91.91 (8)	C20—C14—C15	119.8 (2)
N2—Co1—C18ⁱ	97.03 (8)	C20—C14—C13	120.3 (2)
O4ⁱ—Co1—C18ⁱ	31.22 (8)	C15—C14—C13	119.7 (2)
N1—Co1—C18ⁱ	137.68 (9)	C16—C15—C14	119.6 (2)
O2—Co1—C18ⁱ	126.96 (8)	C16—C15—H15A	120.2
O1—Co1—C18ⁱ	97.74 (8)	C14—C15—H15A	120.2
O3ⁱ—Co1—C18ⁱ	30.60 (7)	C17—C16—C15	120.4 (2)
N2—Co1—C13	131.17 (9)	C17—C16—H16A	119.8
O4ⁱ—Co1—C13	126.29 (8)	C15—C16—H16A	119.8
N1—Co1—C13	100.00 (8)	C16—C17—C19	119.9 (2)
O2—Co1—C13	30.95 (7)	C16—C17—C18	119.4 (2)

O1—Co1—C13	30.65 (7)	C19—C17—C18	120.5 (2)
O3^i—Co1—C13	92.88 (8)	O3—C18—O4	120.2 (2)
C18^i—Co1—C13	112.83 (8)	O3—C18—C17	120.4 (2)
N1—C1—C2	122.5 (3)	O4—C18—C17	119.2 (2)
N1—C1—H1A	118.8	O3—C18—Co1^{iv}	62.20 (14)
C2—C1—H1A	118.8	O4—C18—Co1^{iv}	58.13 (13)
C3—C2—C1	118.9 (3)	C17—C18—Co1^{iv}	172.09 (18)
C3—C2—H2A	120.5	C20—C19—C17	119.8 (2)
C1—C2—H2A	120.5	C20—C19—H19A	120.1
C2—C3—C4	119.3 (3)	C17—C19—H19A	120.1
C2—C3—H3A	120.4	C19—C20—C14	120.5 (2)
C4—C3—H3A	120.4	C19—C20—H20A	119.8
C3—C4—C5	119.2 (3)	C14—C20—H20A	119.8
C3—C4—H4A	120.4	C13—O1—Co1	88.31 (15)
C5—C4—H4A	120.4	C13—O2—Co1	89.00 (15)
N1—C5—C4	122.1 (3)	C18—O3—Co1^{iv}	87.20 (15)
N1—C5—C6	113.4 (2)	C18—O4—Co1^{iv}	90.65 (15)
C4—C5—C6	124.6 (3)	C1—N1—C5	118.0 (3)
N2—C6—N3	112.1 (2)	C1—N1—Co1	128.0 (2)
N2—C6—C5	120.4 (2)	C5—N1—Co1	113.55 (17)
N3—C6—C5	127.5 (2)	C6—N2—C12	105.9 (2)
N3—C7—C8	132.5 (3)	C6—N2—Co1	112.86 (17)
N3—C7—C12	106.0 (2)	C12—N2—Co1	141.17 (18)
C8—C7—C12	121.5 (3)	C6—N3—C7	107.7 (2)
C9—C8—C7	116.3 (3)	C6—N3—O2^{ii}	141.83 (18)
C9—C8—H8A	121.9	C7—N3—O2^{ii}	100.21 (17)
C7—C8—H8A	121.9	C6—N3—O4^{iii}	107.15 (17)
C8—C9—C10	122.2 (3)	C7—N3—O4^{iii}	128.03 (18)
C8—C9—H9A	118.9	O2^{ii}—N3—O4^{iii}	73.09 (7)
C10—C9—H9A	118.9	C6—N3—H3B	126.2
C11—C10—C9	121.8 (3)	C7—N3—H3B	126.2
N1—C1—C2—C3	−0.9 (5)	O1—C13—O2—Co1	−9.6 (2)
C1—C2—C3—C4	0.9 (5)	C14—C13—O2—Co1	167.6 (2)
C2—C3—C4—C5	0.3 (5)	N2—Co1—O2—C13	−178.84 (15)
C3—C4—C5—N1	−1.6 (5)	O4^i—Co1—O2—C13	−43.3 (2)
C3—C4—C5—C6	179.1 (3)	N1—Co1—O2—C13	101.32 (16)
N1—C5—C6—N2	−3.3 (4)	O1—Co1—O2—C13	5.47 (14)
C4—C5—C6—N2	176.0 (3)	O3^i—Co1—O2—C13	−82.40 (15)
N1—C5—C6—N3	175.9 (3)	C18^i—Co1—O2—C13	−71.90 (17)
C4—C5—C6—N3	−4.8 (4)	O4—C18—O3—Co1^{iv}	4.1 (2)
N3—C7—C8—C9	−179.5 (3)	C17—C18—O3—Co1^{iv}	−171.4 (2)
C12—C7—C8—C9	0.6 (5)	O3—C18—O4—Co1^{iv}	−4.3 (2)
C7—C8—C9—C10	0.0 (5)	C17—C18—O4—Co1^{iv}	171.3 (2)
C8—C9—C10—C11	−0.7 (5)	C2—C1—N1—C5	−0.3 (4)
C9—C10—C11—C12	0.6 (5)	C2—C1—N1—Co1	171.6 (2)

C10—C11—C12—N2	179.5 (3)	C4—C5—N1—C1	1.6 (4)
C10—C11—C12—C7	0.0 (4)	C6—C5—N1—C1	−179.1 (2)
N3—C7—C12—C11	179.4 (3)	C4—C5—N1—Co1	−171.4 (2)
C8—C7—C12—C11	−0.7 (4)	C6—C5—N1—Co1	7.9 (3)
N3—C7—C12—N2	−0.2 (3)	N2—Co1—N1—C1	−179.7 (3)
C8—C7—C12—N2	179.8 (3)	O4^{i}—Co1—N1—C1	83.7 (3)
N2—Co1—C13—O1	172.07 (15)	O2—Co1—N1—C1	−80.2 (3)
O4^{i}—Co1—C13—O1	−32.30 (19)	O1—Co1—N1—C1	−18.5 (3)
N1—Co1—C13—O1	87.79 (16)	O3^{i}—Co1—N1—C1	116.0 (4)
O2—Co1—C13—O1	170.6 (2)	C18^{i}—Co1—N1—C1	91.7 (3)
O3^{i}—Co1—C13—O1	−88.89 (16)	C13—Co1—N1—C1	−49.4 (3)
C18^{i}—Co1—C13—O1	−64.94 (17)	N2—Co1—N1—C5	−7.54 (18)
N2—Co1—C13—O2	1.5 (2)	O4^{i}—Co1—N1—C5	−104.12 (18)
O4^{i}—Co1—C13—O2	157.15 (13)	O2—Co1—N1—C5	91.96 (18)
N1—Co1—C13—O2	−82.77 (16)	O1—Co1—N1—C5	153.68 (18)
O1—Co1—C13—O2	−170.6 (2)	O3^{i}—Co1—N1—C5	−71.8 (4)
O3^{i}—Co1—C13—O2	100.56 (15)	C18^{i}—Co1—N1—C5	−96.1 (2)
C18^{i}—Co1—C13—O2	124.51 (15)	C13—Co1—N1—C5	122.76 (18)
N2—Co1—C13—C14	−87.5 (10)	N3—C6—N2—C12	−0.5 (3)
O4^{i}—Co1—C13—C14	68.2 (10)	C5—C6—N2—C12	178.8 (2)
N1—Co1—C13—C14	−171.8 (10)	N3—C6—N2—Co1	177.46 (17)
O2—Co1—C13—C14	−89.0 (10)	C5—C6—N2—Co1	−3.2 (3)
O1—Co1—C13—C14	100.5 (10)	C11—C12—N2—C6	−179.1 (3)
O3^{i}—Co1—C13—C14	11.6 (10)	C7—C12—N2—C6	0.4 (3)
C18^{i}—Co1—C13—C14	35.5 (10)	C11—C12—N2—Co1	3.9 (5)
O1—C13—C14—C20	12.1 (4)	C7—C12—N2—Co1	−176.6 (2)
O2—C13—C14—C20	−165.1 (2)	O4^{i}—Co1—N2—C6	111.45 (18)
Co1—C13—C14—C20	−82.2 (10)	N1—Co1—N2—C6	5.60 (18)
O1—C13—C14—C15	−173.2 (2)	O2—Co1—N2—C6	−87.46 (18)
O2—C13—C14—C15	9.7 (4)	O1—Co1—N2—C6	−75.7 (3)
Co1—C13—C14—C15	92.5 (10)	O3^{i}—Co1—N2—C6	173.60 (18)
C20—C14—C15—C16	1.6 (4)	C18^{i}—Co1—N2—C6	142.90 (18)
C13—C14—C15—C16	−173.2 (2)	C13—Co1—N2—C6	−88.3 (2)
C14—C15—C16—C17	1.7 (4)	O4^{i}—Co1—N2—C12	−71.6 (3)
C15—C16—C17—C19	−3.5 (4)	N1—Co1—N2—C12	−177.5 (3)
C15—C16—C17—C18	171.0 (2)	O2—Co1—N2—C12	89.5 (3)
C16—C17—C18—O3	18.1 (4)	O1—Co1—N2—C12	101.2 (4)
C19—C17—C18—O3	−167.5 (2)	O3^{i}—Co1—N2—C12	−9.5 (3)
C16—C17—C18—O4	−157.5 (2)	C18^{i}—Co1—N2—C12	−40.2 (3)
C19—C17—C18—O4	16.9 (4)	C13—Co1—N2—C12	88.7 (3)
C16—C17—C19—C20	2.0 (4)	N2—C6—N3—C7	0.4 (3)
C18—C17—C19—C20	−172.4 (2)	C5—C6—N3—C7	−178.8 (3)
C17—C19—C20—C14	1.3 (4)	N2—C6—N3—O2^{ii}	−134.5 (2)
C15—C14—C20—C19	−3.1 (4)	C5—C6—N3—O2^{ii}	46.3 (4)

C13—C14—C20—C19	171.6 (2)	N2—C6—N3—O4^{iii}	141.23 (18)
O2—C13—O1—Co1	9.5 (2)	C5—C6—N3—O4^{iii}	−38.0 (3)
C14—C13—O1—Co1	−167.6 (2)	C8—C7—N3—C6	179.9 (3)
N2—Co1—O1—C13	−18.8 (3)	C12—C7—N3—C6	−0.1 (3)
O4^{i}—Co1—O1—C13	154.12 (15)	C8—C7—N3—O2^{ii}	−26.5 (4)
N1—Co1—O1—C13	−97.02 (16)	C12—C7—N3—O2^{ii}	153.47 (18)
O2—Co1—O1—C13	−5.52 (14)	C8—C7—N3—O4^{iii}	50.0 (4)
O3^{i}—Co1—O1—C13	92.43 (16)	C12—C7—N3—O4^{iii}	−130.1 (2)
C18^{i}—Co1—O1—C13	122.59 (16)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···O2^{ii}	0.86	2.27	2.913 (3)	132
N3—H3B···O4^{iii}	0.86	2.36	2.963 (3)	127

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

Fig. 1

Fig. 2

Fig. 3