

catena-Poly[[aqua(4,4'-bipyridine- κ^2N,N')cobalt(II)]- μ -3-(4-carboxylatophenoxy)propionato- $\kappa^3O:O',O''$]

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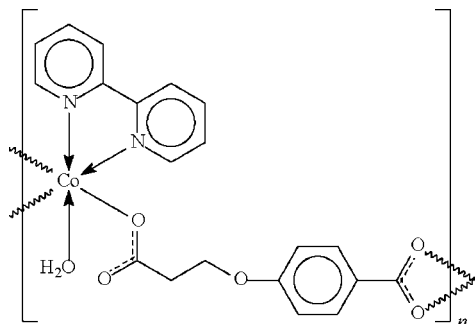
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.034; wR factor = 0.086; data-to-parameter ratio = 15.8.

In the crystal structure of the polymeric title compound, $[\text{Co}(\text{C}_{10}\text{H}_8\text{O}_5)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]_n$, the Co^{II} atom is O,O' -chelated by the aromatic carboxylate end of the 3-(4-carboxylatophenoxy)propionate dianion, and is covalently bonded (through one O atom) by the aliphatic carboxylate end of another dianion; it is also coordinated by a water molecule to give an octahedral coordination environment. The compound adopts a helical chain structure that propagates along the c axis of the orthorhombic unit cell. The coordinated water molecule engages in both intrachain and interchain hydrogen bonding; the interchain hydrogen bonds result in a honeycomb motif. The crystal structure is an inversion twin and the ratio of the two twin components refined to 0.47 (2):0.53 (2).

Related literature

For the isostructural manganese compound, see: Kong *et al.* (2007).



Experimental

Crystal data

$[\text{Co}(\text{C}_{10}\text{H}_8\text{O}_5)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$
 $M_r = 441.29$
 Orthorhombic, $P2_12_12_1$
 $a = 6.7193$ (2) Å
 $b = 16.1369$ (5) Å
 $c = 17.2762$ (7) Å
 $V = 1873.2$ (1) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.96$ mm⁻¹
 $T = 295$ (2) K
 $0.38 \times 0.25 \times 0.17$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.546$, $T_{\max} = 0.854$
 18344 measured reflections
 4282 independent reflections
 3233 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.087$
 $S = 1.00$
 4282 reflections
 271 parameters
 2 restraints
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.33$ e Å⁻³
 $\Delta\rho_{\min} = -0.35$ e Å⁻³
 Absolute structure: Flack (1983), with 1820 Friedel pairs
 Flack parameter: 0.47 (2)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1W}-\text{H1W2}\cdots\text{O2}$	0.86 (1)	1.80 (2)	2.644 (3)	166 (6)
$\text{O1W}-\text{H1W1}\cdots\text{O4}^i$	0.85 (1)	2.01 (2)	2.837 (3)	164 (5)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2489).

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supplementary materials

Acta Cryst. (2007). E63, m2852 [doi:10.1107/S1600536807052191]

***catena*-Poly[[aqua(4,4'-bipyridine- κ^2N,N')cobalt(II)]- μ -3-(4-carboxylatophenoxy)propionato- $\kappa^3O:O',O''$]**

L.-L. Kong, S. Gao, L.-H. Huo and S. W. Ng

Experimental

Cobalt dichloride hexahydrate (2 mmol), 3-(4-carboxylatophenoxy)propionic acid (2 mmol) and 2,2'-bipyridine (2 mmol) were dissolved in a 3:1 ethanol–water solution. Aqueous 0.1 *M* sodium hydroxide was added until the solution registered a pH of 7. The solution was set aside for the growth of crystals over several days. CH&N analysis. Calc. for $C_{20}H_{18}N_2O_6Co$: C 54.43, H 4.11, N 6.35%. Found: C 54.45, H 4.10, N 6.36%.

Refinement

The carbon-bound H atoms were placed in calculated positions [$C-H = 0.93-0.97$ Å and $U_{iso}(H) = 1.2-1.5U_{eq}(C)$], and were included in the refinement in the riding-model approximation. The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of $O-H = 0.85$ (1) Å; their $U_{iso}(H)$ values were freely refined.

Figures

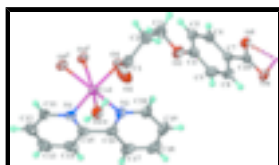


Fig. 1. Part of the polymeric structure of the title compound, showing 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii. Symmetry code: (i) $5/2 - x, 1 - y, z - 1/2$.

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Crystal data

$[Co(C_{10}H_8O_5)(C_{10}H_8N_2)(H_2O)]$

$M_r = 441.29$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 6.7193$ (2) Å

$b = 16.1369$ (5) Å

$c = 17.2762$ (7) Å

$V = 1873.2$ (1) Å³

$Z = 4$

$F_{000} = 908$

$D_x = 1.565$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 14469 reflections

$\theta = 3.0-27.5^\circ$

$\mu = 0.96$ mm⁻¹

$T = 295$ (2) K

Block, pink

$0.38 \times 0.25 \times 0.17$ mm

Data collection

Rigaku R-Axis RAPID diffractometer	4282 independent reflections
Radiation source: fine-focus sealed tube	3233 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.041$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{\text{max}} = 27.5^\circ$
$T = 295(2)$ K	$\theta_{\text{min}} = 3.3^\circ$
ω scans	$h = -8 \rightarrow 8$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -20 \rightarrow 20$
$T_{\text{min}} = 0.546$, $T_{\text{max}} = 0.854$	$l = -22 \rightarrow 22$
18344 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2]$
$wR(F^2) = 0.087$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\text{max}} = 0.001$
4282 reflections	$\Delta\rho_{\text{max}} = 0.33 \text{ e } \text{\AA}^{-3}$
271 parameters	$\Delta\rho_{\text{min}} = -0.35 \text{ e } \text{\AA}^{-3}$
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 1820 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.47 (2)

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	0.76489 (5)	0.398602 (19)	0.855061 (19)	0.03280 (11)
O1	0.8432 (3)	0.51878 (12)	0.86177 (15)	0.0497 (5)
O2	0.5641 (3)	0.58949 (13)	0.84844 (18)	0.0748 (8)
O3	0.9850 (3)	0.64927 (14)	0.98563 (12)	0.0493 (6)
O4	1.4181 (3)	0.62191 (12)	1.31063 (11)	0.0381 (5)
O5	1.6780 (3)	0.60698 (13)	1.23548 (11)	0.0392 (4)
O1W	0.4572 (3)	0.43293 (15)	0.86584 (15)	0.0471 (5)
H1W1	0.351 (5)	0.421 (3)	0.841 (3)	0.13 (2)*
H1W2	0.472 (10)	0.4855 (10)	0.858 (3)	0.15 (2)*
N1	0.7355 (3)	0.26736 (12)	0.86476 (13)	0.0380 (5)
N2	0.7761 (3)	0.37846 (13)	0.97567 (12)	0.0372 (5)
C1	0.7464 (5)	0.58424 (15)	0.85589 (15)	0.0405 (6)

C2	0.8697 (5)	0.66325 (17)	0.85777 (19)	0.0478 (7)
H2A	0.7878	0.7080	0.8774	0.057*
H2B	0.9084	0.6774	0.8053	0.057*
C3	1.0561 (5)	0.65662 (19)	0.90742 (18)	0.0468 (8)
H3A	1.1336	0.6083	0.8930	0.056*
H3B	1.1384	0.7056	0.9016	0.056*
C4	1.1199 (4)	0.63966 (18)	1.04414 (19)	0.0400 (8)
C5	1.3226 (4)	0.62954 (18)	1.03432 (18)	0.0382 (7)
H5	1.3781	0.6289	0.9850	0.046*
C6	1.4423 (4)	0.62027 (17)	1.09954 (18)	0.0358 (7)
H6	1.5785	0.6128	1.0932	0.043*
C7	1.3635 (4)	0.62183 (18)	1.17393 (17)	0.0325 (6)
C8	1.1589 (4)	0.6321 (2)	1.18138 (19)	0.0407 (8)
H8	1.1024	0.6334	1.2305	0.049*
C9	1.0378 (5)	0.6405 (2)	1.11728 (19)	0.0464 (8)
H9	0.9011	0.6466	1.1234	0.056*
C10	1.4924 (4)	0.61640 (16)	1.24370 (16)	0.0315 (6)
C11	0.7263 (5)	0.21451 (17)	0.80494 (18)	0.0465 (7)
H11	0.7152	0.2359	0.7551	0.056*
C12	0.7325 (6)	0.12974 (18)	0.8145 (2)	0.0577 (9)
H12	0.7225	0.0946	0.7720	0.069*
C13	0.7535 (5)	0.09824 (18)	0.8873 (2)	0.0597 (8)
H13	0.7629	0.0413	0.8949	0.072*
C14	0.7608 (5)	0.15235 (17)	0.9502 (2)	0.0512 (8)
H14	0.7712	0.1320	1.0004	0.061*
C15	0.7525 (4)	0.23639 (15)	0.93690 (16)	0.0372 (6)
C16	0.7603 (4)	0.29919 (16)	0.99980 (15)	0.0362 (6)
C17	0.7481 (5)	0.2795 (2)	1.07764 (16)	0.0496 (7)
H17	0.7364	0.2246	1.0935	0.059*
C18	0.7535 (5)	0.3428 (2)	1.13136 (17)	0.0583 (8)
H18	0.7468	0.3308	1.1839	0.070*
C19	0.7688 (5)	0.4237 (2)	1.10691 (18)	0.0569 (8)
H19	0.7711	0.4669	1.1426	0.068*
C20	0.7804 (5)	0.43962 (19)	1.02912 (17)	0.0471 (7)
H20	0.7917	0.4943	1.0126	0.056*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03360 (18)	0.03556 (17)	0.02925 (18)	−0.00088 (17)	0.00086 (18)	0.00136 (15)
O1	0.0485 (12)	0.0362 (10)	0.0644 (15)	−0.0022 (9)	0.0008 (12)	−0.0018 (11)
O2	0.0542 (14)	0.0514 (14)	0.119 (3)	0.0054 (11)	−0.0266 (16)	−0.0056 (16)
O3	0.0396 (12)	0.0774 (15)	0.0309 (12)	−0.0002 (10)	−0.0106 (9)	−0.0001 (10)
O4	0.0337 (10)	0.0499 (11)	0.0308 (11)	0.0015 (9)	0.0002 (8)	−0.0032 (9)
O5	0.0267 (9)	0.0581 (11)	0.0328 (10)	0.0010 (9)	−0.0034 (7)	−0.0006 (10)
O1W	0.0331 (11)	0.0588 (13)	0.0495 (14)	0.0017 (10)	−0.0034 (11)	−0.0037 (11)
N1	0.0351 (12)	0.0369 (10)	0.0420 (13)	−0.0033 (11)	0.0067 (14)	0.0017 (9)
N2	0.0335 (13)	0.0472 (12)	0.0310 (12)	0.0040 (12)	−0.0005 (11)	0.0013 (9)

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C1	0.0499 (16)	0.0399 (13)	0.0317 (13)	0.0009 (14)	−0.0089 (19)	−0.0005 (11)
C2	0.063 (2)	0.0423 (15)	0.0385 (17)	−0.0063 (14)	−0.0131 (18)	0.0071 (15)
C3	0.0505 (18)	0.0504 (17)	0.0396 (18)	−0.0072 (15)	−0.0044 (15)	0.0055 (14)
C4	0.0359 (16)	0.0460 (18)	0.0380 (19)	−0.0072 (13)	−0.0068 (14)	0.0012 (14)
C5	0.0383 (16)	0.0469 (17)	0.0295 (16)	0.0001 (12)	0.0008 (12)	−0.0038 (13)
C6	0.0270 (14)	0.0418 (16)	0.0385 (17)	0.0002 (12)	0.0006 (12)	−0.0029 (13)
C7	0.0291 (13)	0.0356 (15)	0.0328 (16)	−0.0032 (11)	−0.0033 (12)	−0.0006 (12)
C8	0.0317 (15)	0.060 (2)	0.0301 (17)	−0.0012 (13)	0.0019 (12)	0.0024 (14)
C9	0.0300 (15)	0.070 (2)	0.0388 (19)	−0.0044 (14)	0.0002 (14)	0.0043 (15)
C10	0.0296 (14)	0.0310 (13)	0.0338 (15)	−0.0004 (11)	−0.0019 (11)	−0.0017 (11)
C11	0.0461 (18)	0.0483 (15)	0.0451 (17)	−0.0067 (15)	0.0103 (17)	−0.0053 (13)
C12	0.052 (2)	0.0440 (15)	0.077 (2)	−0.0061 (17)	0.009 (2)	−0.0126 (16)
C13	0.0485 (17)	0.0352 (14)	0.095 (3)	−0.002 (2)	0.005 (2)	−0.0002 (16)
C14	0.0350 (16)	0.0498 (16)	0.069 (2)	−0.0011 (17)	−0.004 (2)	0.0180 (14)
C15	0.0249 (12)	0.0419 (13)	0.0448 (15)	0.0003 (14)	0.0014 (16)	0.0085 (11)
C16	0.0224 (12)	0.0503 (14)	0.0358 (14)	0.0015 (14)	0.0008 (14)	0.0079 (11)
C17	0.0361 (15)	0.0694 (17)	0.0432 (17)	0.0053 (18)	0.0027 (18)	0.0180 (14)
C18	0.0426 (17)	0.102 (3)	0.0300 (16)	0.007 (2)	0.0007 (19)	0.0098 (15)
C19	0.0479 (19)	0.085 (2)	0.0381 (17)	0.0034 (19)	0.0011 (18)	−0.0131 (16)
C20	0.0482 (19)	0.0572 (16)	0.0358 (16)	0.0035 (16)	−0.0003 (15)	−0.0056 (13)

Geometric parameters (Å, °)

Co1—O1	2.013 (2)	C5—C6	1.392 (4)
Co1—O5 ⁱ	2.103 (2)	C5—H5	0.93
Co1—N2	2.110 (2)	C6—C7	1.390 (4)
Co1—N1	2.134 (2)	C6—H6	0.93
Co1—O1W	2.148 (2)	C7—C8	1.391 (4)
Co1—O4 ⁱ	2.289 (2)	C7—C10	1.487 (4)
O1—C1	1.245 (3)	C8—C9	1.380 (4)
O2—C1	1.234 (4)	C8—H8	0.93
O3—C4	1.367 (4)	C9—H9	0.93
O3—C3	1.438 (4)	C11—C12	1.379 (4)
O4—C10	1.263 (3)	C11—H11	0.93
O5—C10	1.265 (3)	C12—C13	1.364 (5)
O1W—H1W1	0.85 (1)	C12—H12	0.93
O1W—H1W2	0.86 (1)	C13—C14	1.395 (5)
N1—C11	1.341 (3)	C13—H13	0.93
N1—C15	1.348 (3)	C14—C15	1.377 (4)
N2—C16	1.350 (3)	C14—H14	0.93
N2—C20	1.352 (4)	C15—C16	1.487 (4)
C1—C2	1.521 (4)	C16—C17	1.384 (4)
C2—C3	1.522 (4)	C17—C18	1.381 (5)
C2—H2A	0.97	C17—H17	0.93
C2—H2B	0.97	C18—C19	1.377 (5)
C3—H3A	0.97	C18—H18	0.93
C3—H3B	0.97	C19—C20	1.370 (4)
C4—C5	1.382 (4)	C19—H19	0.93
C4—C9	1.379 (4)	C20—H20	0.93

O1—Co1—O5 ⁱ	92.87 (9)	C4—C5—H5	120.6
O1—Co1—N2	94.72 (9)	C6—C5—H5	120.6
O5 ⁱ —Co1—N2	163.10 (8)	C5—C6—C7	121.8 (3)
O1—Co1—N1	167.43 (10)	C5—C6—H6	119.1
O5 ⁱ —Co1—N1	92.95 (8)	C7—C6—H6	119.1
N2—Co1—N1	76.87 (9)	C6—C7—C8	117.7 (3)
O1—Co1—O1W	89.89 (9)	C6—C7—C10	121.8 (2)
O5 ⁱ —Co1—O1W	105.76 (8)	C8—C7—C10	120.5 (3)
N2—Co1—O1W	89.35 (9)	C9—C8—C7	121.3 (3)
N1—Co1—O1W	99.22 (9)	C9—C8—H8	119.3
O1—Co1—O4 ⁱ	85.14 (8)	C7—C8—H8	119.3
O5 ⁱ —Co1—O4 ⁱ	59.64 (7)	C8—C9—C4	119.9 (3)
N2—Co1—O4 ⁱ	106.00 (8)	C8—C9—H9	120.0
N1—Co1—O4 ⁱ	88.21 (8)	C4—C9—H9	120.0
O1W—Co1—O4 ⁱ	164.19 (8)	O4—C10—O5	120.1 (3)
C1—O1—Co1	132.6 (2)	O4—C10—C7	120.5 (2)
C4—O3—C3	118.9 (2)	O5—C10—C7	119.4 (2)
C10—O4—Co1 ⁱⁱ	85.92 (15)	N1—C11—C12	122.5 (3)
C10—O5—Co1 ⁱⁱ	94.29 (17)	N1—C11—H11	118.8
Co1—O1W—H1W1	134 (4)	C12—C11—H11	118.8
Co1—O1W—H1W2	98 (5)	C13—C12—C11	118.9 (3)
H1W1—O1W—H1W2	104 (5)	C13—C12—H12	120.5
C11—N1—C15	118.7 (2)	C11—C12—H12	120.5
C11—N1—Co1	125.10 (19)	C12—C13—C14	119.2 (3)
C15—N1—Co1	115.65 (17)	C12—C13—H13	120.4
C16—N2—C20	118.9 (2)	C14—C13—H13	120.4
C16—N2—Co1	116.62 (17)	C15—C14—C13	119.0 (3)
C20—N2—Co1	124.24 (19)	C15—C14—H14	120.5
O2—C1—O1	125.8 (3)	C13—C14—H14	120.5
O2—C1—C2	119.0 (2)	N1—C15—C14	121.5 (3)
O1—C1—C2	115.1 (3)	N1—C15—C16	115.2 (2)
C1—C2—C3	113.7 (2)	C14—C15—C16	123.2 (3)
C1—C2—H2A	108.8	N2—C16—C17	121.5 (3)
C3—C2—H2A	108.8	N2—C16—C15	115.0 (2)
C1—C2—H2B	108.8	C17—C16—C15	123.5 (2)
C3—C2—H2B	108.8	C18—C17—C16	118.8 (3)
H2A—C2—H2B	107.7	C18—C17—H17	120.6
O3—C3—C2	105.2 (3)	C16—C17—H17	120.6
O3—C3—H3A	110.7	C19—C18—C17	119.9 (3)
C2—C3—H3A	110.7	C19—C18—H18	120.1
O3—C3—H3B	110.7	C17—C18—H18	120.1
C2—C3—H3B	110.7	C20—C19—C18	118.8 (3)
H3A—C3—H3B	108.8	C20—C19—H19	120.6
O3—C4—C5	125.2 (3)	C18—C19—H19	120.6
O3—C4—C9	114.3 (3)	N2—C20—C19	122.2 (3)
C5—C4—C9	120.5 (3)	N2—C20—H20	118.9

supplementary materials

C4—C5—C6	118.8 (3)	C19—C20—H20	118.9
O5 ⁱ —Co1—O1—C1	91.4 (3)	C10—C7—C8—C9	177.5 (3)
N2—Co1—O1—C1	−103.7 (3)	C7—C8—C9—C4	−0.8 (5)
N1—Co1—O1—C1	−151.1 (4)	O3—C4—C9—C8	−179.4 (3)
O1W—Co1—O1—C1	−14.4 (3)	C5—C4—C9—C8	0.8 (5)
O4 ⁱ —Co1—O1—C1	150.6 (3)	Co1 ⁱⁱ —O4—C10—O5	−2.4 (2)
O1—Co1—N1—C11	−127.3 (4)	Co1 ⁱⁱ —O4—C10—C7	178.3 (2)
O5 ⁱ —Co1—N1—C11	−9.8 (3)	Co1 ⁱⁱ —O5—C10—O4	2.6 (3)
N2—Co1—N1—C11	−176.2 (3)	Co1 ⁱⁱ —O5—C10—C7	−178.0 (2)
O1W—Co1—N1—C11	96.7 (3)	C6—C7—C10—O4	176.6 (3)
O4 ⁱ —Co1—N1—C11	−69.3 (3)	C8—C7—C10—O4	−0.7 (4)
O1—Co1—N1—C15	44.2 (6)	C6—C7—C10—O5	−2.7 (4)
O5 ⁱ —Co1—N1—C15	161.7 (2)	C8—C7—C10—O5	179.9 (3)
N2—Co1—N1—C15	−4.6 (2)	C15—N1—C11—C12	0.3 (5)
O1W—Co1—N1—C15	−91.8 (2)	Co1—N1—C11—C12	171.6 (3)
O4 ⁱ —Co1—N1—C15	102.2 (2)	N1—C11—C12—C13	−1.6 (6)
O1—Co1—N2—C16	−170.7 (2)	C11—C12—C13—C14	2.3 (6)
O5 ⁱ —Co1—N2—C16	−54.3 (4)	C12—C13—C14—C15	−1.9 (5)
N1—Co1—N2—C16	−0.2 (2)	C11—N1—C15—C14	0.1 (5)
O1W—Co1—N2—C16	99.5 (2)	Co1—N1—C15—C14	−172.0 (2)
O4 ⁱ —Co1—N2—C16	−84.4 (2)	C11—N1—C15—C16	−179.6 (3)
O1—Co1—N2—C20	15.3 (3)	Co1—N1—C15—C16	8.3 (3)
O5 ⁱ —Co1—N2—C20	131.7 (3)	C13—C14—C15—N1	0.7 (5)
N1—Co1—N2—C20	−174.2 (3)	C13—C14—C15—C16	−179.7 (3)
O1W—Co1—N2—C20	−74.5 (3)	C20—N2—C16—C17	0.1 (5)
O4 ⁱ —Co1—N2—C20	101.6 (3)	Co1—N2—C16—C17	−174.2 (2)
Co1—O1—C1—O2	4.8 (5)	C20—N2—C16—C15	178.8 (3)
Co1—O1—C1—C2	−174.7 (2)	Co1—N2—C16—C15	4.5 (3)
O2—C1—C2—C3	148.8 (3)	N1—C15—C16—N2	−8.5 (4)
O1—C1—C2—C3	−31.6 (4)	C14—C15—C16—N2	171.9 (3)
C4—O3—C3—C2	178.1 (2)	N1—C15—C16—C17	170.1 (3)
C1—C2—C3—O3	−67.7 (3)	C14—C15—C16—C17	−9.5 (5)
C3—O3—C4—C5	−5.5 (4)	N2—C16—C17—C18	−0.4 (5)
C3—O3—C4—C9	174.6 (3)	C15—C16—C17—C18	−178.9 (3)
O3—C4—C5—C6	−179.9 (3)	C16—C17—C18—C19	0.7 (5)
C9—C4—C5—C6	−0.1 (5)	C17—C18—C19—C20	−0.7 (6)
C4—C5—C6—C7	−0.7 (4)	C16—N2—C20—C19	−0.2 (5)
C5—C6—C7—C8	0.7 (4)	Co1—N2—C20—C19	173.7 (2)
C5—C6—C7—C10	−176.7 (3)	C18—C19—C20—N2	0.4 (5)
C6—C7—C8—C9	0.0 (5)		

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

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W2 \cdots O2	0.86 (1)	1.80 (2)	2.644 (3)	166 (6)

O1W—H1W1...O4ⁱⁱⁱ 0.85 (1) 2.01 (2) 2.837 (3) 164 (5)
 Symmetry codes: (iii) $-x+3/2, -y+1, z-1/2$.

Fig. 1

