Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[diaquabis(1*H*-indole-3-acetato-κ*O*)cobalt(II)]-μ-4,4′-bipyridine-κ^2*N*:*N*′] tetrahydrate]

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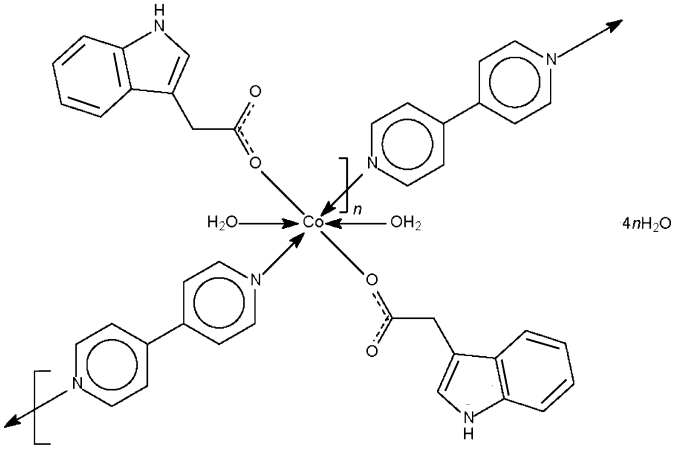
Received 9 April 2008; accepted 18 April 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.040; wR factor = 0.103; data-to-parameter ratio = 11.4.

The 4,4′-bipyridine spacer in the title compound, $[Co(C_{10}H_8NO_2)_2(C_{10}H_8N_2)(H_2O)_2]\cdot 4H_2O$, links the diaquacobalt(II) dicarboxylate units into a linear chain; the metal atom lies on a center of inversion in an octahedral environment. The coordinated and uncoordinated water molecules interact through O—H···O hydrogen bonds to form a three-dimensional network.

Related literature

For examples of diaqua transition-metal dicarboxylates that are linked by 4,4′-bipyridine, see: Deng *et al.* (2005); Gao *et al.* (2006); He *et al.* (2003); Hou *et al.* (2007); Li *et al.* (2006); Pedireddi & Varughese (2004); Yan *et al.* (2005); Zhang *et al.* (1999); Zheng, Su & Feng (2006); Zheng, Tong & Chen (2006).



Experimental

Crystal data

$[Co(C_{10}H_8NO_2)_2(C_{10}H_8N_2)(H_2O)_2]\cdot 4H_2O$
M_r = 671.56
Monoclinic, $P2_1/c$
a = 11.5011 (3) Å
b = 16.0953 (4) Å
c = 8.8302 (2) Å
β = 111.784 (1)°
V = 1517.86 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 295 (2) K
0.35 × 0.20 × 0.08 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.810, T_{max} = 0.951
11131 measured reflections
2584 independent reflections
1771 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.102
S = 1.03
2584 reflections
226 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.182 (2)	Co1—N2	2.184 (2)
Co1—O1*W*	2.042 (2)		
O1—Co1—O1*W*	89.74 (7)	O1—Co1—N2^{i}	88.42 (7)
O1—Co1—O1*W*^{i}	90.26 (7)	O1*W*—Co1—N2	91.63 (8)
O1—Co1—N2	91.58 (7)	O1*W*—Co1—N2^{i}	88.37 (8)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2	0.85 (3)	1.76 (3)	2.585 (2)	165 (3)
O1*W*—H1*W*2···O2*W*	0.85 (3)	1.89 (3)	2.724 (3)	171 (3)
O2*W*—H2*W*1···O3*W*^{ii}	0.85 (3)	1.89 (3)	2.735 (3)	173 (3)
O2*W*—H2*W*2···O2^{iii}	0.84 (3)	1.94 (3)	2.752 (3)	162 (3)
O3*W*—H3*W*1···O1	0.85 (3)	2.00 (3)	2.854 (3)	179 (3)
O3*W*—H3*W*2···O2*W*^{i}	0.85 (3)	2.03 (3)	2.872 (3)	168 (3)

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

We thank Daqing Petroleum Institute and the University of Malaya for generously supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2234).

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supporting information

Acta Cryst. (2008). E**64**, m706–m707 [doi:10.1107/S1600536808010842]

catena-Poly[[[diaquabis(1*H*-indole-3-acetato-κO)cobalt(II)]-μ-4,4′-bipyridine-κ^2N:N'] tetrahydrate]

Ji-Wei Liu and Seik Weng Ng

S1. Comment

There are many crystallographic examples of transition metal di(carboxylates) that are linked by the 4,4′-bipyridine spacer ligand. Among these are examples that have coordinated water; the water entities engage in hydrogen bonding that consolidates the structure.

The title diaquadi(indole-3-carboxylato)cobalt–4,4′-bipyridine tetrahydrate (Scheme I) exists as a chain. The metal atom is coordinated by two unidentate carboxylate groups, two water molecules and two 4,4′-bipyridine ligands in an octahedral geometry (Fig. 1). The spacer ligand links the mononuclear units into a linear chain. The chains are further linked by hydrogen bonds into a three-dimensional network (Table 2).

S2. Experimental

Cobalt(II) sulfate septahydrate (0.28 g, 1 mmol) and 4,4′-bipyridine (0.16 g, 1 mmol) were added to a hot aqueous solution of indole-3-acetic acid (0.12 g, 1 mmol); the pH was adjusted to 6 with 0.1*M* sodium hydroxide. The solution was allowed to evaporate at room temperature. Single crystals are separated from the filtered solution after several days.

S3. Refinement

Hydrogen atoms were treated as riding, with C–H = 0.93 to 0.97 Å and were included in the refinement with U(H) set to 1.2 times U_{eq}(C). The water and amino H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H = N–H = 0.85±0.01 Å and H···H 1.39±0.01 Å. Their temperature factors were tied to those of the parent atoms by a factor of 1.5

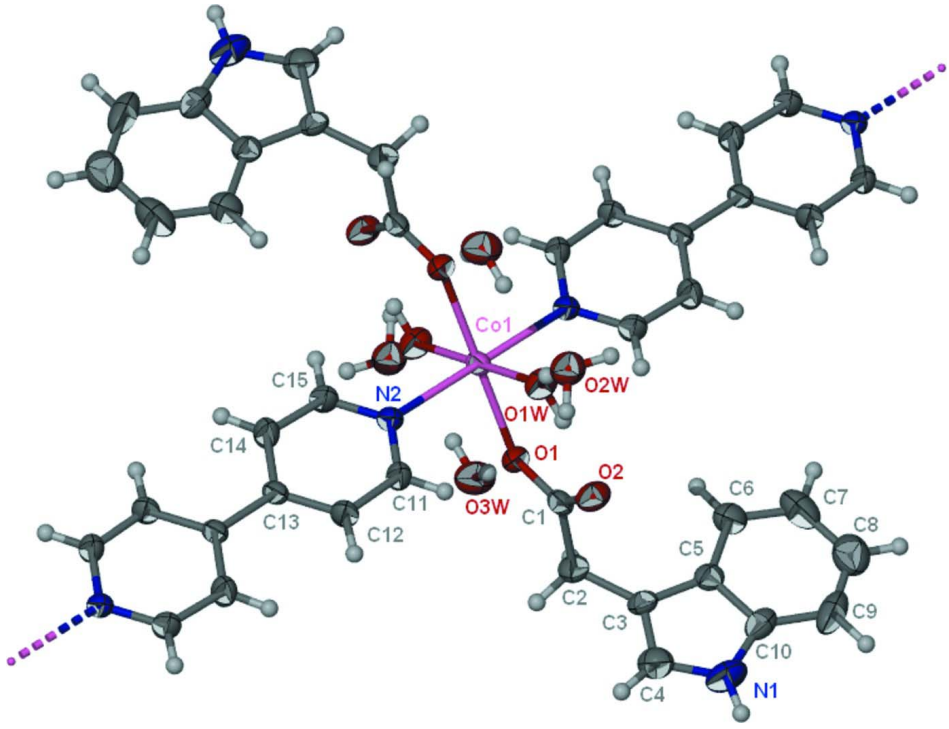

Figure 1

Thermal displacement ellipsoid plot (Barbour, 2001) illustrating the coordination geometry of cobalt in $Co(C_{10}H_8N_2)(C_{10}H_8NO_2)_2(H_2O)_2{\cdot}4H_2O$. Displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radii.

catena-Poly[[[diaquabis(1_H_-indole-3-acetato- κO)cobalt(II)]-μ-4,4′-bipyridine-κ^2N:N'] tetrahydrate]

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Monoclinic, $P2_1/c$
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$b = 16.0953$ (4) Å
$c = 8.8302$ (2) Å
$\beta = 111.784$ (1)°
$V = 1517.86$ (6) Å^3
$Z = 2$
$F(000) = 702$
$D_x = 1.469$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2534 reflections
$\theta = 2.3$–$21.7°$
$\mu = 0.63$ mm^{-1}
$T = 295$ K
Block, pink
0.35 × 0.20 × 0.08 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.810$, $T_{max} = 0.951$
11131 measured reflections
2584 independent reflections
1771 reflections with $I > 2^{-}I$)
$R_{int} = 0.037$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -13\rightarrow13$
$k = -17\rightarrow19$
$l = -10\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.102$
$S = 1.03$
2584 reflections
226 parameters
10 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
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.1356P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.5000	0.02917 (19)
O1	0.57914 (16)	0.50222 (11)	0.7661 (2)	0.0353 (5)
O2	0.60753 (17)	0.63848 (12)	0.8108 (2)	0.0454 (5)
O1W	0.50557 (18)	0.62679 (12)	0.4969 (2)	0.0423 (5)
H1W1	0.539 (2)	0.6396 (16)	0.5967 (13)	0.063*
H1W2	0.472 (2)	0.6689 (12)	0.441 (3)	0.063*
O2W	0.4133 (2)	0.77242 (13)	0.3416 (3)	0.0535 (6)
H2W1	0.387 (2)	0.7955 (17)	0.409 (3)	0.080*
H2W2	0.4825 (18)	0.7928 (19)	0.348 (4)	0.080*
O3W	0.6525 (2)	0.34501 (14)	0.9218 (3)	0.0617 (6)
H3W1	0.631 (3)	0.3921 (10)	0.877 (3)	0.093*
H3W2	0.644 (3)	0.3081 (13)	0.850 (3)	0.093*
N1	0.8052 (3)	0.72774 (16)	1.3063 (3)	0.0603 (8)
H1N	0.806 (3)	0.7654 (15)	1.373 (3)	0.090*
N2	0.30936 (19)	0.50106 (13)	0.4973 (3)	0.0335 (6)
C1	0.6121 (2)	0.56454 (19)	0.8587 (3)	0.0339 (7)
C2	0.6562 (3)	0.55025 (19)	1.0415 (3)	0.0443 (8)
H2A	0.5834	0.5440	1.0709	0.053*
H2B	0.7028	0.4985	1.0676	0.053*
C3	0.7364 (3)	0.61775 (17)	1.1427 (3)	0.0374 (7)
C4	0.7058 (3)	0.6757 (2)	1.2330 (4)	0.0530 (9)
H4	0.6285	0.6796	1.2436	0.064*
C5	0.8624 (3)	0.63474 (17)	1.1623 (3)	0.0369 (7)
C6	0.9462 (3)	0.5963 (2)	1.1030 (4)	0.0522 (8)
H6	0.9216	0.5504	1.0344	0.063*
C7	1.0646 (3)	0.6275 (3)	1.1475 (5)	0.0712 (11)
H7	1.1208	0.6022	1.1088	0.085*
C8	1.1028 (3)	0.6955 (3)	1.2485 (5)	0.0776 (12)
H8	1.1842	0.7149	1.2761	0.093*
C9	1.0246 (3)	0.7352 (2)	1.3093 (4)	0.0656 (10)
H9	1.0510	0.7812	1.3771	0.079*
C10	0.9034 (3)	0.70374 (18)	1.2654 (3)	0.0460 (8)
C11	0.2700 (2)	0.55901 (17)	0.5739 (4)	0.0393 (7)

H11	0.3255	0.6011	0.6273	0.047*
C12	0.1515 (2)	0.56060 (17)	0.5789 (3)	0.0401 (7)
H12	0.1300	0.6025	0.6362	0.048*
C13	0.0644 (2)	0.50028 (16)	0.4993 (3)	0.0309 (6)
C14	0.1058 (2)	0.44017 (18)	0.4190 (4)	0.0439 (8)
H14	0.0521	0.3977	0.3633	0.053*
C15	0.2258 (3)	0.44290 (18)	0.4212 (4)	0.0439 (8)
H15	0.2503	0.4014	0.3659	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0262 (3)	0.0343 (3)	0.0289 (3)	0.0001 (2)	0.0124 (2)	0.0008 (3)
O1	0.0385 (11)	0.0364 (11)	0.0311 (11)	−0.0045 (9)	0.0129 (9)	−0.0043 (10)
O2	0.0620 (14)	0.0377 (13)	0.0338 (12)	−0.0019 (11)	0.0146 (10)	0.0007 (11)
O1W	0.0498 (12)	0.0364 (12)	0.0347 (11)	0.0023 (10)	0.0088 (10)	0.0033 (10)
O2W	0.0640 (15)	0.0449 (14)	0.0537 (15)	−0.0024 (12)	0.0243 (12)	−0.0021 (11)
O3W	0.0847 (17)	0.0520 (14)	0.0557 (15)	0.0017 (15)	0.0343 (14)	0.0021 (12)
N1	0.081 (2)	0.0483 (19)	0.0477 (19)	0.0026 (17)	0.0200 (17)	−0.0148 (15)
N2	0.0311 (12)	0.0415 (14)	0.0303 (13)	−0.0024 (12)	0.0142 (10)	−0.0054 (12)
C1	0.0275 (14)	0.045 (2)	0.0317 (17)	−0.0034 (14)	0.0144 (12)	−0.0003 (17)
C2	0.0499 (18)	0.053 (2)	0.0284 (17)	−0.0093 (16)	0.0130 (14)	−0.0004 (16)
C3	0.0463 (17)	0.0416 (18)	0.0240 (16)	−0.0032 (15)	0.0125 (13)	−0.0028 (14)
C4	0.051 (2)	0.063 (2)	0.046 (2)	0.0047 (18)	0.0186 (16)	−0.0020 (18)
C5	0.0443 (17)	0.0373 (18)	0.0297 (16)	−0.0010 (15)	0.0145 (13)	0.0031 (15)
C6	0.056 (2)	0.054 (2)	0.052 (2)	−0.0043 (17)	0.0275 (17)	−0.0029 (17)
C7	0.059 (2)	0.087 (3)	0.078 (3)	−0.001 (2)	0.037 (2)	0.010 (2)
C8	0.053 (2)	0.102 (3)	0.071 (3)	−0.022 (2)	0.015 (2)	0.019 (3)
C9	0.073 (3)	0.058 (2)	0.049 (2)	−0.026 (2)	0.0027 (19)	0.0010 (19)
C10	0.059 (2)	0.0398 (19)	0.0331 (19)	−0.0060 (17)	0.0094 (16)	−0.0011 (16)
C11	0.0318 (16)	0.0437 (18)	0.0445 (19)	−0.0071 (14)	0.0166 (13)	−0.0130 (16)
C12	0.0348 (16)	0.0449 (19)	0.0467 (19)	−0.0023 (14)	0.0221 (14)	−0.0130 (15)
C13	0.0266 (14)	0.0405 (17)	0.0276 (15)	0.0003 (14)	0.0125 (11)	−0.0003 (14)
C14	0.0317 (16)	0.049 (2)	0.054 (2)	−0.0066 (14)	0.0191 (14)	−0.0151 (16)
C15	0.0361 (17)	0.052 (2)	0.049 (2)	−0.0035 (16)	0.0225 (15)	−0.0193 (17)

Geometric parameters (Å, º)

Co1—O1	2.182 (2)	C3—C4	1.355 (4)
Co1—O1^{i}	2.182 (2)	C3—C5	1.421 (3)
Co1—O1W^{i}	2.042 (2)	C4—H4	0.9300
Co1—O1W	2.042 (2)	C5—C6	1.400 (4)
Co1—N2	2.184 (2)	C5—C10	1.402 (4)
Co1—N2^{i}	2.184 (2)	C6—C7	1.365 (4)
O1—C1	1.260 (3)	C6—H6	0.9300
O2—C1	1.258 (3)	C7—C8	1.376 (5)
O1W—H1W1	0.85 (3)	C7—H7	0.9300
O1W—H1W2	0.85 (3)	C8—C9	1.365 (5)

O2W—H2W1	0.85 (3)	C8—H8	0.9300
O2W—H2W2	0.84 (3)	C9—C10	1.396 (4)
O3W—H3W1	0.85 (3)	C9—H9	0.9300
O3W—H3W2	0.85 (3)	C11—C12	1.380 (3)
N1—C10	1.364 (4)	C11—H11	0.9300
N1—C4	1.371 (4)	C12—C13	1.385 (3)
N1—H1N	0.84 (1)	C12—H12	0.9300
N2—C11	1.327 (3)	C13—C14	1.384 (3)
N2—C15	1.331 (3)	C13—C13^{ii}	1.487 (5)
C1—C2	1.519 (4)	C14—C15	1.374 (3)
C2—C3	1.489 (4)	C14—H14	0.9300
C2—H2A	0.9700	C15—H15	0.9300
C2—H2B	0.9700		

O1—Co1—O1^{i}	180.0	N1—C4—H4	124.9
O1—Co1—O1W	89.74 (7)	C6—C5—C10	118.7 (3)
O1—Co1—O1W^{i}	90.26 (7)	C6—C5—C3	133.0 (3)
O1—Co1—N2	91.58 (7)	C10—C5—C3	108.3 (2)
O1—Co1—N2^{i}	88.42 (7)	C7—C6—C5	118.8 (3)
O1W—Co1—O1W^{i}	180.0	C7—C6—H6	120.6
O1W—Co1—N2	91.63 (8)	C5—C6—H6	120.6
O1W—Co1—N2^{i}	88.37 (8)	C6—C7—C8	121.6 (3)
N2—Co1—N2^{i}	180.0	C6—C7—H7	119.2
C1—O1—Co1	128.05 (17)	C8—C7—H7	119.2
Co1—O1W—H1W1	104 (2)	C9—C8—C7	121.9 (3)
Co1—O1W—H1W2	143 (2)	C9—C8—H8	119.1
H1W1—O1W—H1W2	111 (2)	C7—C8—H8	119.1
H2W1—O2W—H2W2	111 (2)	C8—C9—C10	117.2 (3)
H3W1—O3W—H3W2	110 (2)	C8—C9—H9	121.4
C10—N1—C4	109.2 (3)	C10—C9—H9	121.4
C10—N1—H1N	127 (3)	N1—C10—C9	131.6 (3)
C4—N1—H1N	124 (3)	N1—C10—C5	106.5 (3)
C11—N2—C15	115.6 (2)	C9—C10—C5	121.9 (3)
C11—N2—Co1	122.10 (17)	N2—C11—C12	123.9 (2)
C15—N2—Co1	122.25 (17)	N2—C11—H11	118.1
O2—C1—O1	124.7 (3)	C12—C11—H11	118.1
O2—C1—C2	117.2 (3)	C11—C12—C13	120.5 (2)
O1—C1—C2	118.1 (2)	C11—C12—H12	119.7
C3—C2—C1	114.6 (2)	C13—C12—H12	119.7
C3—C2—H2A	108.6	C14—C13—C12	115.4 (2)
C1—C2—H2A	108.6	C14—C13—C13^{ii}	122.2 (3)
C3—C2—H2B	108.6	C12—C13—C13^{ii}	122.4 (3)
C1—C2—H2B	108.6	C15—C14—C13	120.3 (3)
H2A—C2—H2B	107.6	C15—C14—H14	119.8
C4—C3—C5	105.8 (3)	C13—C14—H14	119.8
C4—C3—C2	128.1 (3)	N2—C15—C14	124.2 (3)
C5—C3—C2	126.1 (2)	N2—C15—H15	117.9
C3—C4—N1	110.2 (3)	C14—C15—H15	117.9

C3—C4—H4	124.9		
O1W^{i}—Co1—O1—C1	178.5 (2)	C2—C3—C5—C10	179.3 (3)
O1W—Co1—O1—C1	−1.5 (2)	C10—C5—C6—C7	−0.1 (4)
N2—Co1—O1—C1	−93.1 (2)	C3—C5—C6—C7	−178.7 (3)
N2^{i}—Co1—O1—C1	86.9 (2)	C5—C6—C7—C8	−0.2 (5)
O1W^{i}—Co1—N2—C11	144.9 (2)	C6—C7—C8—C9	0.1 (6)
O1W—Co1—N2—C11	−35.1 (2)	C7—C8—C9—C10	0.2 (5)
O1—Co1—N2—C11	54.6 (2)	C4—N1—C10—C9	−179.1 (3)
O1^{i}—Co1—N2—C11	−125.4 (2)	C4—N1—C10—C5	0.4 (3)
O1W^{i}—Co1—N2—C15	−34.0 (2)	C8—C9—C10—N1	178.9 (3)
O1W—Co1—N2—C15	146.0 (2)	C8—C9—C10—C5	−0.5 (5)
O1—Co1—N2—C15	−124.2 (2)	C6—C5—C10—N1	−179.2 (3)
O1^{i}—Co1—N2—C15	55.8 (2)	C3—C5—C10—N1	−0.2 (3)
Co1—O1—C1—O2	−2.0 (4)	C6—C5—C10—C9	0.4 (4)
Co1—O1—C1—C2	175.64 (15)	C3—C5—C10—C9	179.4 (3)
O2—C1—C2—C3	−24.1 (3)	C15—N2—C11—C12	0.7 (4)
O1—C1—C2—C3	158.1 (2)	Co1—N2—C11—C12	−178.1 (2)
C1—C2—C3—C4	106.8 (3)	N2—C11—C12—C13	−1.0 (4)
C1—C2—C3—C5	−72.4 (4)	C11—C12—C13—C14	0.6 (4)
C5—C3—C4—N1	0.4 (3)	C11—C12—C13—C13^{ii}	−179.7 (3)
C2—C3—C4—N1	−179.0 (3)	C12—C13—C14—C15	−0.2 (4)
C10—N1—C4—C3	−0.5 (4)	C13^{ii}—C13—C14—C15	−179.8 (3)
C4—C3—C5—C6	178.7 (3)	C11—N2—C15—C14	−0.2 (4)
C2—C3—C5—C6	−2.0 (5)	Co1—N2—C15—C14	178.7 (2)
C4—C3—C5—C10	−0.1 (3)	C13—C14—C15—N2	−0.1 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2	0.85 (3)	1.76 (3)	2.585 (2)	165 (3)
O1*W*—H1*W*2···O2*W*	0.85 (3)	1.89 (3)	2.724 (3)	171 (3)
O2*W*—H2*W*1···O3*W*^{iii}	0.85 (3)	1.89 (3)	2.735 (3)	173 (3)
O2*W*—H2*W*2···O2^{iv}	0.84 (3)	1.94 (3)	2.752 (3)	162 (3)
O3*W*—H3*W*1···O1	0.85 (3)	2.00 (3)	2.854 (3)	179 (3)
O3*W*—H3*W*2···O2*W*^{i}	0.85 (3)	2.03 (3)	2.872 (3)	168 (3)
N1—H1*N*···O2^{v}	0.84 (1)	2.64 (3)	3.142 (3)	120 (3)

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