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Aqua(iminodiacetato-κ^3O,N,O')(1,10-phenanthroline-κ^2N,N')cobalt(II) monohydrate

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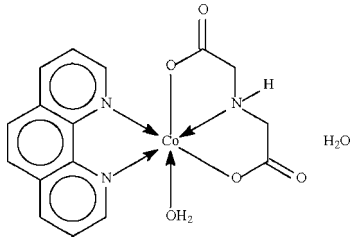
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.009 Å; R factor = 0.048; wR factor = 0.126; data-to-parameter ratio = 14.7.

The iminodiacetate dianion in the title compound, $[Co(C_4H_5NO_4)(C_{12}H_8N_2)(H_2O)]\cdot H_2O$, chelates to the cobalt(II) atom, its N and two O atoms occupying the *fac* sites of the distorted octahedron around the metal atom. The metal atom is also chelated by the *N*-heterocycle. The dianion, and coordinated and uncoordinated water molecules interact through hydrogen bonds, generating a layer motif. The crystal studied was a racemic twin with a 0.62 (2):0.38 (2) domain ratio.

Related literature

For structural examples of the *N*-heterocycle adducts of cobalt iminodiacetate, see: Su & Xu (2004); Xu *et al.* (1989).



Experimental

Crystal data

$[Co(C_4H_5NO_4)(C_{12}H_8N_2)(H_2O)]\cdot H_2O$
M_r = 406.26
Monoclinic, *Pn*
a = 6.7884 (3) Å
b = 12.0903 (5) Å
c = 10.4945 (4) Å
β = 108.357 (3)°
V = 817.49 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.09 mm^{-1}
T = 100 (2) K
0.35 × 0.02 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.701, T_{max} = 0.979
6417 measured reflections
3639 independent reflections
2997 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.126
S = 1.00
3639 reflections
248 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Absolute structure: Flack (1983), 1746 Friedel pairs
Flack parameter: 0.38 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O2^{i}	0.84 (5)	1.82 (4)	2.656 (5)	174 (6)
O1w—H12···O4^{ii}	0.84 (6)	1.87 (4)	2.682 (5)	162 (6)
O2w—H21···O1^{i}	0.84 (5)	1.98 (4)	2.815 (5)	174 (7)
O2w—H22···O4	0.84 (6)	2.05 (5)	2.871 (5)	165 (6)

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

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2563).

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supporting information

Acta Cryst. (2009). E**65**, m41 [doi:10.1107/S1600536808041226]

Aqua(iminodiacetato-κ^3O,N,O')(1,10-phenanthroline-κ^2N,N')cobalt(II) monohydrate

Hwa Loong Ng, Chew Hee Ng and Seik Weng Ng

S1. Experimental

An aqueous solution of cobalt(II) chloride (0.24 g, 1 mmol) was mixed with an aqueous solutin of disodium iminodiacetate monohydrate (0.20 g, 1 mmol); this was added to a water-methanol solution of 1,10-phenanthroline (0.20 g, 1 mmol). The solution was set aside for the growth of orange crystals.

S2. Refinement

Carbon-bound hydrogen atoms were placed at calculated positions (C–H 0.95–0.99 Å) and were treated as riding on their parent atoms, with U(H) set to 1.2 times U_{eq}(C). The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H 0.84±0.01 Å; their temperature factors were freely refined. The amino H-atom could not be located, and was treated as riding.

The structure is a racemic twin. The explicit refinement of the Flack parameter gave the twin component as 0.38 (2).

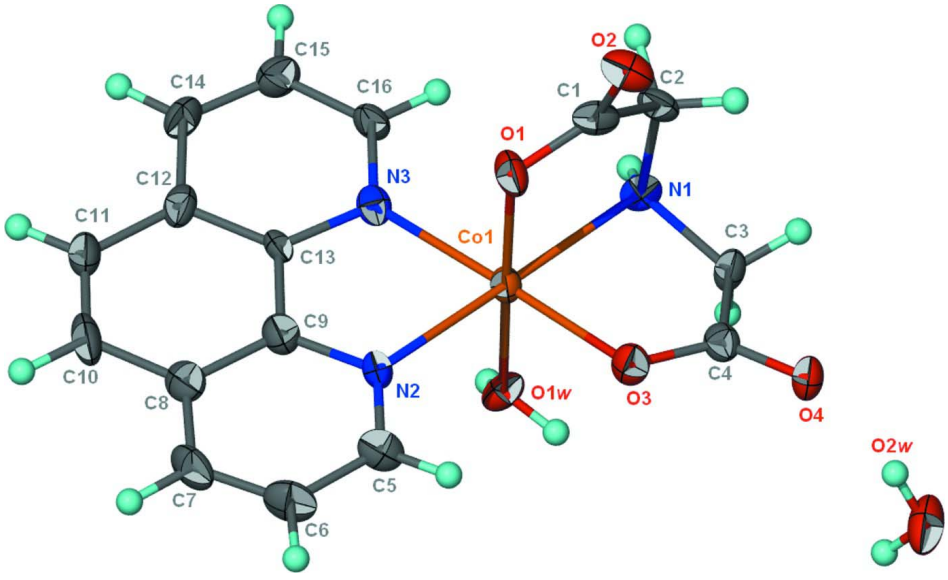

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $Co(C_{12}H_8N_2)(C_4H_5NO_4)(H_2O)\cdot H_2O$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Aqua(iminodiacetato-κ^3O,N,O')(1,10- phenanthroline-κ^2N,N')cobalt(II) monohydrate

Crystal data

$[Co(C_4H_5NO_4)(C_{12}H_8N_2)(H_2O)]\cdot H_2O$
$M_r = 406.26$
Monoclinic, *Pn*
Hall symbol: P 2yac
$a = 6.7884$ (3) Å
$b = 12.0903$ (5) Å
$c = 10.4945$ (4) Å
$\beta = 108.357$ (3)°
$V = 817.49$ (6) Å^3
$Z = 2$
$F(000) = 418$
$D_x = 1.650$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1265 reflections
$\theta = 2.6$–$24.5°$
$\mu = 1.09$ mm^{-1}
$T = 100$ K
Prism, orange
0.35 × 0.02 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.701$, $T_{max} = 0.979$
6417 measured reflections
3639 independent reflections
2997 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.7°$
$h = -8\rightarrow8$
$k = -15\rightarrow15$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.126$
$S = 1.00$
3639 reflections
248 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}
Absolute structure: Flack (1983), 1746 Friedel pairs
Absolute structure parameter: 0.38 (2)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.49999 (10)	0.85733 (5)	0.50000 (8)	0.01527 (16)
O1	0.4183 (7)	0.8730 (3)	0.6730 (4)	0.0222 (9)
O2	0.3360 (6)	1.0019 (3)	0.7965 (4)	0.0254 (8)
O3	0.7258 (6)	0.9787 (3)	0.5790 (3)	0.0196 (9)
O4	0.7806 (5)	1.1607 (3)	0.5786 (3)	0.0190 (7)
O1W	0.5702 (6)	0.8446 (3)	0.3211 (4)	0.0194 (9)
H11	0.652 (7)	0.896 (3)	0.317 (5)	0.029*
H12	0.493 (7)	0.830 (4)	0.243 (2)	0.029*
O2W	0.9365 (7)	1.2706 (3)	0.3875 (4)	0.0307 (9)
H21	0.939 (10)	1.225 (4)	0.327 (4)	0.046*
H22	0.870 (9)	1.243 (4)	0.435 (5)	0.046*
N1	0.3129 (7)	1.0058 (4)	0.4480 (4)	0.0162 (10)

H1	0.2104	0.9968	0.3727	0.019*
N2	0.6902 (8)	0.7165 (4)	0.5733 (5)	0.0171 (10)
N3	0.2824 (7)	0.7278 (4)	0.4343 (4)	0.0168 (11)
C1	0.3389 (7)	0.9654 (4)	0.6867 (5)	0.0193 (10)
C2	0.2335 (7)	1.0313 (4)	0.5604 (5)	0.0202 (10)
H2A	0.0826	1.0160	0.5320	0.024*
H2B	0.2533	1.1112	0.5814	0.024*
C3	0.4607 (8)	1.0907 (4)	0.4324 (5)	0.0183 (10)
H3A	0.4062	1.1653	0.4414	0.022*
H3B	0.4760	1.0849	0.3419	0.022*
C4	0.6704 (8)	1.0754 (4)	0.5382 (5)	0.0177 (10)
C5	0.8890 (9)	0.7128 (5)	0.6410 (5)	0.0217 (13)
H5	0.9625	0.7806	0.6638	0.026*
C6	0.9974 (10)	0.6143 (5)	0.6811 (6)	0.0256 (13)
H6	1.1410	0.6154	0.7310	0.031*
C7	0.8948 (9)	0.5164 (5)	0.6478 (5)	0.0246 (13)
H7	0.9666	0.4485	0.6736	0.030*
C8	0.6812 (10)	0.5167 (5)	0.5748 (5)	0.0221 (13)
C9	0.5835 (10)	0.6199 (5)	0.5401 (7)	0.0210 (14)
C10	0.5597 (10)	0.4182 (5)	0.5380 (6)	0.0269 (14)
H10	0.6247	0.3481	0.5601	0.032*
C11	0.3534 (10)	0.4234 (4)	0.4720 (6)	0.0230 (12)
H11A	0.2754	0.3570	0.4500	0.028*
C12	0.2518 (10)	0.5267 (5)	0.4351 (5)	0.0205 (13)
C13	0.3668 (10)	0.6250 (4)	0.4676 (6)	0.0128 (12)
C14	0.0390 (9)	0.5374 (4)	0.3682 (5)	0.0220 (12)
H14	−0.0462	0.4734	0.3459	0.026*
C15	−0.0462 (10)	0.6399 (4)	0.3350 (6)	0.0238 (14)
H15	−0.1902	0.6475	0.2884	0.029*
C16	0.0795 (8)	0.7328 (5)	0.3699 (6)	0.0182 (11)
H16	0.0175	0.8035	0.3467	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0158 (3)	0.0120 (3)	0.0173 (3)	0.0003 (3)	0.0041 (2)	−0.0001 (3)
O1	0.033 (3)	0.0132 (18)	0.024 (2)	0.0052 (16)	0.0135 (19)	0.0029 (14)
O2	0.0220 (19)	0.032 (2)	0.0207 (17)	0.0070 (16)	0.0052 (14)	−0.0024 (16)
O3	0.017 (2)	0.0178 (19)	0.021 (2)	0.0012 (15)	0.0013 (16)	0.0033 (15)
O4	0.0219 (18)	0.0127 (17)	0.0210 (17)	−0.0021 (14)	0.0048 (14)	0.0012 (13)
O1W	0.014 (2)	0.023 (2)	0.0183 (19)	−0.0049 (15)	0.0022 (16)	0.0039 (15)
O2W	0.049 (3)	0.0175 (19)	0.029 (2)	−0.0081 (18)	0.0165 (19)	−0.0030 (15)
N1	0.010 (2)	0.022 (3)	0.012 (2)	−0.0009 (18)	−0.0025 (17)	0.0020 (19)
N2	0.019 (2)	0.011 (2)	0.022 (2)	0.0010 (19)	0.0077 (19)	−0.0011 (19)
N3	0.021 (2)	0.015 (2)	0.014 (2)	0.0008 (19)	0.0053 (19)	−0.0012 (18)
C1	0.012 (2)	0.027 (3)	0.017 (2)	0.001 (2)	0.0017 (19)	−0.001 (2)
C2	0.015 (2)	0.021 (2)	0.025 (3)	0.0072 (19)	0.008 (2)	0.003 (2)
C3	0.017 (3)	0.013 (2)	0.022 (2)	−0.002 (2)	0.002 (2)	0.0032 (19)

C4	0.020 (3)	0.016 (3)	0.017 (2)	0.001 (2)	0.007 (2)	0.001 (2)
C5	0.019 (3)	0.026 (3)	0.018 (3)	0.002 (2)	0.003 (2)	−0.004 (2)
C6	0.017 (3)	0.034 (3)	0.022 (3)	0.008 (3)	0.002 (2)	0.004 (2)
C7	0.027 (3)	0.021 (3)	0.026 (3)	0.012 (2)	0.008 (2)	0.008 (2)
C8	0.027 (3)	0.020 (3)	0.023 (3)	0.004 (2)	0.013 (2)	0.007 (2)
C9	0.023 (3)	0.018 (3)	0.024 (3)	0.001 (2)	0.009 (2)	0.000 (2)
C10	0.041 (4)	0.011 (2)	0.033 (3)	0.004 (2)	0.017 (3)	0.002 (2)
C11	0.029 (3)	0.013 (2)	0.030 (3)	−0.001 (2)	0.014 (2)	0.001 (2)
C12	0.029 (3)	0.015 (3)	0.022 (3)	−0.004 (2)	0.013 (3)	0.000 (2)
C13	0.016 (3)	0.010 (3)	0.013 (2)	0.003 (2)	0.006 (2)	0.0001 (19)
C14	0.019 (3)	0.019 (3)	0.027 (3)	−0.007 (2)	0.006 (2)	−0.002 (2)
C15	0.019 (3)	0.025 (3)	0.027 (3)	−0.005 (2)	0.006 (2)	−0.003 (2)
C16	0.012 (2)	0.016 (3)	0.023 (3)	0.003 (2)	0.001 (2)	−0.003 (2)

Geometric parameters (Å, º)

Co1—O1	2.067 (4)	C3—C4	1.516 (7)
Co1—O1W	2.083 (4)	C3—H3A	0.9900
Co1—O3	2.095 (4)	C3—H3B	0.9900
Co1—N3	2.113 (5)	C5—C6	1.394 (8)
Co1—N2	2.129 (5)	C5—H5	0.9500
Co1—N1	2.167 (5)	C6—C7	1.362 (8)
O1—C1	1.269 (6)	C6—H6	0.9500
O2—C1	1.240 (6)	C7—C8	1.411 (8)
O3—C4	1.260 (6)	C7—H7	0.9500
O4—C4	1.267 (6)	C8—C9	1.406 (9)
O1W—H11	0.84 (5)	C8—C10	1.430 (8)
O1W—H12	0.84 (6)	C9—C13	1.429 (8)
O2W—H21	0.84 (5)	C10—C11	1.355 (9)
O2W—H22	0.84 (6)	C10—H10	0.9500
N1—C2	1.476 (6)	C11—C12	1.420 (8)
N1—C3	1.480 (6)	C11—H11A	0.9500
N1—H1	0.8800	C12—C14	1.399 (9)
N2—C5	1.313 (8)	C12—C13	1.403 (8)
N2—C9	1.360 (8)	C14—C15	1.365 (8)
N3—C16	1.331 (7)	C14—H14	0.9500
N3—C13	1.368 (7)	C15—C16	1.389 (8)
C1—C2	1.518 (6)	C15—H15	0.9500
C2—H2A	0.9900	C16—H16	0.9500
C2—H2B	0.9900		
O1—Co1—O1W	177.6 (2)	C4—C3—H3A	109.6
O1—Co1—O3	87.34 (16)	N1—C3—H3B	109.6
O1W—Co1—O3	93.54 (15)	C4—C3—H3B	109.6
O1—Co1—N3	90.07 (17)	H3A—C3—H3B	108.1
O1W—Co1—N3	89.20 (16)	O3—C4—O4	124.0 (5)
O3—Co1—N3	175.53 (17)	O3—C4—C3	118.3 (5)
O1—Co1—N2	93.20 (16)	O4—C4—C3	117.7 (4)

O1W—Co1—N2	88.95 (17)	N2—C5—C6	123.2 (6)
O3—Co1—N2	97.62 (17)	N2—C5—H5	118.4
N3—Co1—N2	78.88 (15)	C6—C5—H5	118.4
O1—Co1—N1	81.23 (15)	C7—C6—C5	119.1 (6)
O1W—Co1—N1	96.68 (15)	C7—C6—H6	120.4
O3—Co1—N1	79.47 (17)	C5—C6—H6	120.4
N3—Co1—N1	103.74 (19)	C6—C7—C8	119.5 (5)
N2—Co1—N1	173.79 (18)	C6—C7—H7	120.2
C1—O1—Co1	114.9 (3)	C8—C7—H7	120.2
C4—O3—Co1	114.3 (3)	C9—C8—C7	117.5 (5)
Co1—O1W—H11	109 (3)	C9—C8—C10	119.0 (5)
Co1—O1W—H12	130 (3)	C7—C8—C10	123.5 (5)
H11—O1W—H12	109 (5)	N2—C9—C8	121.7 (6)
H21—O2W—H22	109 (5)	N2—C9—C13	118.4 (6)
C2—N1—C3	111.9 (4)	C8—C9—C13	119.9 (6)
C2—N1—Co1	107.7 (3)	C11—C10—C8	121.0 (5)
C3—N1—Co1	103.8 (3)	C11—C10—H10	119.5
C2—N1—H1	111.0	C8—C10—H10	119.5
C3—N1—H1	111.0	C10—C11—C12	121.0 (6)
Co1—N1—H1	111.0	C10—C11—H11A	119.5
C5—N2—C9	118.9 (5)	C12—C11—H11A	119.5
C5—N2—Co1	128.7 (4)	C14—C12—C13	116.9 (5)
C9—N2—Co1	112.4 (4)	C14—C12—C11	123.6 (5)
C16—N3—C13	117.0 (5)	C13—C12—C11	119.5 (6)
C16—N3—Co1	129.6 (4)	N3—C13—C12	123.5 (6)
C13—N3—Co1	113.4 (4)	N3—C13—C9	116.9 (6)
O2—C1—O1	123.4 (5)	C12—C13—C9	119.6 (6)
O2—C1—C2	118.9 (4)	C15—C14—C12	119.9 (5)
O1—C1—C2	117.6 (4)	C15—C14—H14	120.0
N1—C2—C1	113.4 (4)	C12—C14—H14	120.0
N1—C2—H2A	108.9	C14—C15—C16	119.5 (6)
C1—C2—H2A	108.9	C14—C15—H15	120.3
N1—C2—H2B	108.9	C16—C15—H15	120.3
C1—C2—H2B	108.9	N3—C16—C15	123.3 (5)
H2A—C2—H2B	107.7	N3—C16—H16	118.4
N1—C3—C4	110.3 (4)	C15—C16—H16	118.4
N1—C3—H3A	109.6		

O3—Co1—O1—C1	66.7 (4)	Co1—O3—C4—C3	−4.4 (6)
N3—Co1—O1—C1	−116.9 (4)	N1—C3—C4—O3	31.4 (6)
N2—Co1—O1—C1	164.2 (4)	N1—C3—C4—O4	−149.6 (4)
N1—Co1—O1—C1	−13.1 (4)	C9—N2—C5—C6	−0.1 (8)
O1—Co1—O3—C4	−96.3 (4)	Co1—N2—C5—C6	−178.6 (4)
O1W—Co1—O3—C4	81.5 (4)	N2—C5—C6—C7	0.8 (9)
N2—Co1—O3—C4	170.9 (3)	C5—C6—C7—C8	−0.6 (8)
N1—Co1—O3—C4	−14.7 (4)	C6—C7—C8—C9	−0.3 (8)
O1—Co1—N1—C2	−1.0 (3)	C6—C7—C8—C10	−178.6 (5)
O1W—Co1—N1—C2	177.7 (3)	C5—N2—C9—C8	−0.9 (8)

O3—Co1—N1—C2	−89.9 (3)	Co1—N2—C9—C8	177.9 (4)
N3—Co1—N1—C2	86.9 (3)	C5—N2—C9—C13	179.4 (5)
O1—Co1—N1—C3	117.8 (3)	Co1—N2—C9—C13	−1.9 (6)
O1W—Co1—N1—C3	−63.4 (3)	C7—C8—C9—N2	1.0 (8)
O3—Co1—N1—C3	28.9 (3)	C10—C8—C9—N2	179.4 (5)
N3—Co1—N1—C3	−154.3 (3)	C7—C8—C9—C13	−179.2 (5)
O1—Co1—N2—C5	−90.5 (5)	C10—C8—C9—C13	−0.8 (7)
O1W—Co1—N2—C5	90.7 (5)	C9—C8—C10—C11	−0.7 (8)
O3—Co1—N2—C5	−2.8 (5)	C7—C8—C10—C11	177.6 (5)
N3—Co1—N2—C5	−180.0 (5)	C8—C10—C11—C12	1.1 (8)
O1—Co1—N2—C9	90.9 (4)	C10—C11—C12—C14	−179.3 (5)
O1W—Co1—N2—C9	−88.0 (4)	C10—C11—C12—C13	0.0 (8)
O3—Co1—N2—C9	178.6 (4)	C16—N3—C13—C12	1.3 (8)
N3—Co1—N2—C9	1.4 (4)	Co1—N3—C13—C12	179.6 (4)
O1—Co1—N3—C16	84.0 (5)	C16—N3—C13—C9	−178.2 (5)
O1W—Co1—N3—C16	−93.7 (5)	Co1—N3—C13—C9	0.1 (6)
N2—Co1—N3—C16	177.2 (5)	C14—C12—C13—N3	−1.7 (8)
N1—Co1—N3—C16	3.0 (5)	C11—C12—C13—N3	179.0 (5)
O1—Co1—N3—C13	−94.1 (4)	C14—C12—C13—C9	177.8 (5)
O1W—Co1—N3—C13	88.3 (4)	C11—C12—C13—C9	−1.5 (7)
N2—Co1—N3—C13	−0.8 (4)	N2—C9—C13—N3	1.2 (7)
N1—Co1—N3—C13	−175.0 (3)	C8—C9—C13—N3	−178.5 (5)
Co1—O1—C1—O2	−158.4 (4)	N2—C9—C13—C12	−178.3 (5)
Co1—O1—C1—C2	24.6 (6)	C8—C9—C13—C12	1.9 (7)
C3—N1—C2—C1	−101.0 (5)	C13—C12—C14—C15	1.4 (8)
Co1—N1—C2—C1	12.5 (5)	C11—C12—C14—C15	−179.2 (5)
O2—C1—C2—N1	157.4 (4)	C12—C14—C15—C16	−0.9 (9)
O1—C1—C2—N1	−25.4 (6)	C13—N3—C16—C15	−0.7 (8)
C2—N1—C3—C4	77.1 (5)	Co1—N3—C16—C15	−178.7 (4)
Co1—N1—C3—C4	−38.8 (4)	C14—C15—C16—N3	0.5 (9)
Co1—O3—C4—O4	176.7 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H11···O2^{i}	0.84 (5)	1.82 (4)	2.656 (5)	174 (6)
O1*w*—H12···O4^{ii}	0.84 (6)	1.87 (4)	2.682 (5)	162 (6)
O2*w*—H21···O1^{i}	0.84 (5)	1.98 (4)	2.815 (5)	174 (7)
O2*w*—H22···O4	0.84 (6)	2.05 (5)	2.871 (5)	165 (6)
N1—H1···O2^{ii}	0.88	2.41	3.126 (6)	139

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