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Tetraaquabis{3-carboxy-5-[(4-carboxyphenyl)diazenyl]benzoato-κO^1}cobalt(II) dihydrate

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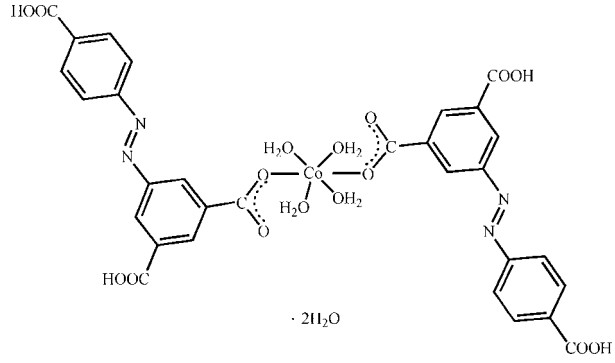
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.105; data-to-parameter ratio = 15.0.

In the title complex, $[Co(C_{15}H_9N_2O_6)_2(H_2O)_4]\cdot 2H_2O$, the Co^{II} ion is located on an inversion center and is coordinated by two monodentate 3-carboxy-5-[(4-carboxyphenyl)diazenyl]benzoate ligands and four water molecules in a distorted octahedral geometry. In the crystal, intermolecular O—H···O hydrogen bonds link the molecules into a three-dimensional supramolecular network.

Related literature

For background to coordination polymers, see: Kitagawa *et al.* (2004); Moulton & Zaworotko (2001).



Experimental

Crystal data

$[Co(C_{15}H_9N_2O_6)_2(H_2O)_4]\cdot 2H_2O$ M_r = 793.51
Monoclinic, $P2_1/c$
a = 19.347 (10) Å
b = 7.105 (3) Å
c = 12.379 (6) Å
β = 103.020 (9)°
V = 1657.9 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 296 K
0.26 × 0.21 × 0.18 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.858, T_{max} = 0.896
16990 measured reflections
3795 independent reflections
3435 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.105
S = 1.02
3795 reflections
253 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O5^{i}	0.82	1.82	2.605 (2)	160
O6—H6A···O1^{ii}	0.82	1.78	2.574 (2)	164
O7—H7A···O3^{iii}	0.83 (1)	1.92 (1)	2.746 (2)	170 (3)
O7—H7B···O1W^{iv}	0.82	2.05	2.791 (2)	151
O8—H8A···O1	0.82	1.98	2.697 (2)	145
O8—H8B···O1W	0.87 (1)	1.94 (1)	2.797 (2)	169 (2)
O1W—H1WA···O8^{v}	0.85 (1)	2.12 (1)	2.957 (2)	169 (3)
O1W—H1WB···O3^{vi}	0.85 (1)	2.15 (2)	2.937 (2)	155 (3)

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{5}{2}$; (iii) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (v) $-x, y+\frac{1}{2}, -z+\frac{5}{2}$; (vi) $x, y, z+1$.

Data collection: *SMART* (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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2481).

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supporting information

Acta Cryst. (2011). E**67**, m1689 [https://doi.org/10.1107/S1600536811045557]

Tetraaquabis{3-carboxy-5-[(4-carboxyphenyl)diazenyl]benzoato-κO^1}cobalt(II) dihydrate

Liang Bai and Jun Zhao

S1. Comment

The formation of coordination polymers is an active area of research as these compounds have potential uses in gas storage, molecular sieves, magnetism and so on (Kitagawa *et al.*, 2004; Moulton & Zaworotko, 2001). During the synthesis of polymeric complexes using 5-[(4-carboxyphenyl)diazenyl]isophthalate (*L*) as bridging ligand, to our surprise, the title monomeric Co(II) complex was obtained.

The title complex is a centrosymmetric mononuclear complex. The Co^{II} ion, which is located on an inversion center, is six-coordinated by two carboxylate O atoms from two *L* ligands and four water O atoms, resulting in a distorted octahedral geometry (Fig. 1). In the *L* ligand, two benzene rings is almost coplanar and the dihedral angle is 4.62 (4)°. A three-dimensional supramolecular network structure is formed through the extended hydrogen bonding interactions between water molecules and carboxylate O atoms (Table 1, Fig. 2).

S2. Experimental

A mixture of 5-[(4-carboxyphenyl)diazenyl]isophthalic acid (0.031 g, 0.1 mmol), $Co(CH_3CO_2)_2.4H_2O$ (0.025 g, 0.1 mmol) and water (10 ml) was stired vigorously for 30 min and then sealed in a Teflon-lined stainless-steel autoclave. The autoclave was heated and maintained at 393 K for 3 days and then cooled to room temperature at 5 K h^{-1}. Red prism crystals suitable for X-ray analysis were obtained.

S3. Refinement

H atoms of water molecules were identified from a difference Fourier map and refined with a restraint of O—H = 0.85 (1) Å and with U_{iso}(H) = 1.5U_{eq}(O). The other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93, O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

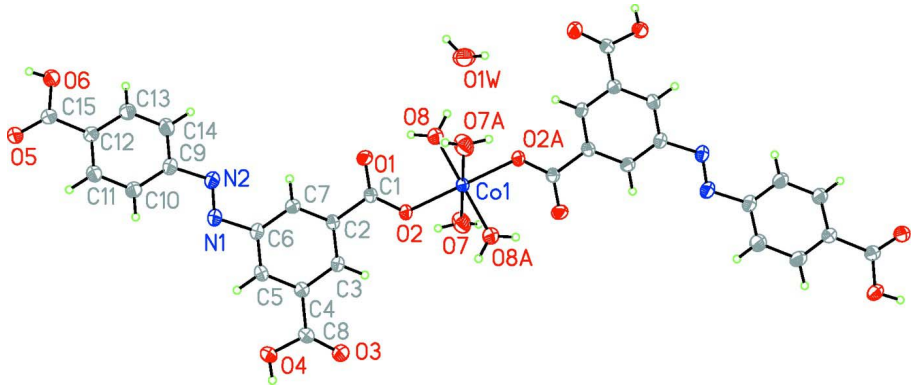

Figure 1

The molecular structure of the title compound, showing the 50% probability displacement ellipsoids. [Symmetry code: (A) -*x*, -*y*+1, -*z*+2.]

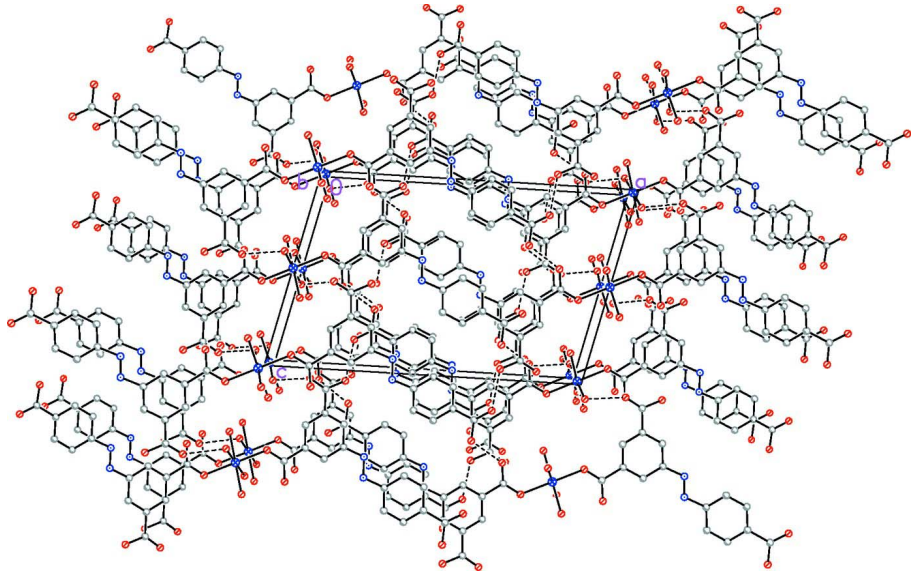

Figure 2

The crystal packing of the title compound, showing the three-dimensional network structure formed by hydrogen bonding interactions (dashed lines). H atoms are omitted for clarity.

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$c = 12.379\ (6)$ Å
$\beta = 103.020\ (9)°$
$V = 1657.9\ (14)$ Å^3
$Z = 2$
$F(000) = 818$
$D_x = 1.590$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4430 reflections
$\theta = 3.1–27.5°$
$\mu = 0.61$ mm^{-1}
$T = 296$ K
Prism, red
0.26 × 0.21 × 0.18 mm

Data collection

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.858, T_{max} = 0.896
16990 measured reflections
3795 independent reflections
3435 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −25→25
k = −9→9
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.105
S = 1.02
3795 reflections
253 parameters
9 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
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.5749P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.0000	0.5000	1.0000	0.02445 (11)
O5	0.74586 (6)	0.0750 (2)	1.15653 (10)	0.0380 (3)
O6	0.71026 (7)	0.0661 (2)	1.31469 (10)	0.0449 (4)
H6A	0.7499	0.0212	1.3377	0.067*
O1	0.17152 (6)	0.4276 (2)	1.07663 (10)	0.0379 (3)
N1	0.39438 (7)	0.3211 (2)	0.92114 (12)	0.0314 (3)
N2	0.41162 (7)	0.2937 (2)	1.02335 (12)	0.0345 (3)
O8	0.05213 (6)	0.35528 (19)	1.14721 (10)	0.0334 (3)
H8A	0.0949	0.3524	1.1506	0.050*
C7	0.27274 (8)	0.3904 (2)	0.94775 (13)	0.0263 (3)
H7C	0.2866	0.3648	1.0232	0.032*
O3	0.15235 (7)	0.5636 (3)	0.55330 (11)	0.0453 (4)
C2	0.20334 (8)	0.4436 (2)	0.90172 (13)	0.0250 (3)
O7	−0.03319 (7)	0.2493 (2)	0.91850 (12)	0.0435 (3)
H7B	0.0013	0.1921	0.9072	0.065*
C12	0.62389 (8)	0.1432 (2)	1.15653 (13)	0.0278 (3)
O2	0.08675 (7)	0.48577 (19)	0.92636 (10)	0.0340 (3)
C5	0.30177 (8)	0.4156 (3)	0.76885 (13)	0.0283 (3)
H5A	0.3347	0.4056	0.7247	0.034*
C1	0.15001 (8)	0.4543 (2)	0.97381 (13)	0.0258 (3)
C6	0.32179 (8)	0.3752 (2)	0.88120 (13)	0.0268 (3)
O4	0.26546 (7)	0.5081 (2)	0.55360 (11)	0.0396 (3)
H4A	0.2520	0.5338	0.4876	0.059*
C9	0.48438 (9)	0.2430 (3)	1.06321 (14)	0.0311 (4)

C15	0.69910 (9)	0.0914 (3)	1.20755 (13)	0.0289 (3)
C10	0.53469 (9)	0.2432 (3)	0.99908 (14)	0.0338 (4)
H10A	0.5216	0.2765	0.9246	0.041*
C3	0.18298 (9)	0.4847 (2)	0.78833 (14)	0.0265 (3)
H3A	0.1366	0.5210	0.7572	0.032*
C11	0.60397 (9)	0.1942 (3)	1.04523 (14)	0.0339 (4)
H11A	0.6375	0.1953	1.0019	0.041*
C14	0.50395 (10)	0.1931 (4)	1.17404 (16)	0.0461 (5)
H14A	0.4705	0.1940	1.2175	0.055*
C4	0.23232 (9)	0.4712 (2)	0.72194 (14)	0.0263 (3)
C13	0.57344 (10)	0.1416 (3)	1.22021 (15)	0.0429 (5)
H13A	0.5863	0.1057	1.2943	0.051*
C8	0.21179 (9)	0.5190 (2)	0.60178 (14)	0.0287 (4)
O1W	0.04442 (9)	0.5355 (2)	1.34499 (12)	0.0469 (4)
H8B	0.0450 (9)	0.420 (4)	1.2030 (16)	0.070*
H7A	−0.0701 (6)	0.190 (3)	0.919 (2)	0.070*
H1WB	0.0831 (8)	0.557 (4)	1.3910 (19)	0.070*
H1WA	0.0176 (11)	0.631 (3)	1.339 (2)	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01671 (17)	0.0366 (2)	0.02086 (17)	−0.00116 (11)	0.00589 (12)	−0.00045 (11)
O5	0.0253 (6)	0.0628 (9)	0.0262 (6)	0.0058 (6)	0.0061 (5)	−0.0019 (6)
O6	0.0285 (7)	0.0810 (10)	0.0242 (6)	0.0165 (7)	0.0040 (5)	0.0094 (6)
O1	0.0218 (6)	0.0720 (9)	0.0200 (6)	−0.0032 (6)	0.0049 (4)	0.0026 (6)
N1	0.0205 (7)	0.0448 (8)	0.0285 (7)	0.0055 (6)	0.0048 (5)	0.0014 (6)
N2	0.0219 (7)	0.0525 (9)	0.0280 (7)	0.0057 (7)	0.0033 (5)	0.0038 (6)
O8	0.0256 (6)	0.0478 (7)	0.0274 (6)	0.0015 (5)	0.0070 (5)	0.0016 (5)
C7	0.0215 (7)	0.0362 (8)	0.0205 (7)	−0.0001 (6)	0.0035 (6)	0.0003 (6)
O3	0.0310 (7)	0.0787 (10)	0.0258 (6)	0.0186 (7)	0.0057 (5)	0.0077 (7)
C2	0.0188 (7)	0.0340 (8)	0.0229 (7)	−0.0008 (6)	0.0064 (6)	−0.0016 (6)
O7	0.0344 (7)	0.0473 (8)	0.0529 (8)	−0.0135 (6)	0.0184 (6)	−0.0153 (6)
C12	0.0240 (8)	0.0352 (8)	0.0232 (8)	0.0031 (7)	0.0031 (6)	−0.0002 (6)
O2	0.0168 (6)	0.0630 (9)	0.0231 (6)	0.0034 (5)	0.0067 (5)	0.0014 (5)
C5	0.0210 (7)	0.0403 (9)	0.0256 (8)	0.0020 (7)	0.0092 (6)	−0.0011 (7)
C1	0.0173 (7)	0.0379 (8)	0.0229 (8)	−0.0027 (6)	0.0058 (6)	−0.0022 (6)
C6	0.0185 (7)	0.0347 (8)	0.0264 (8)	0.0021 (6)	0.0034 (6)	−0.0006 (6)
O4	0.0295 (7)	0.0689 (10)	0.0226 (6)	0.0052 (6)	0.0104 (5)	0.0056 (5)
C9	0.0214 (8)	0.0427 (10)	0.0284 (8)	0.0040 (7)	0.0036 (6)	0.0012 (7)
C15	0.0252 (8)	0.0374 (9)	0.0231 (7)	0.0013 (7)	0.0036 (6)	−0.0014 (6)
C10	0.0267 (8)	0.0503 (11)	0.0237 (8)	0.0057 (8)	0.0044 (6)	0.0070 (7)
C3	0.0173 (7)	0.0385 (9)	0.0234 (8)	0.0016 (6)	0.0038 (6)	−0.0005 (6)
C11	0.0252 (8)	0.0515 (11)	0.0257 (8)	0.0059 (8)	0.0074 (6)	0.0044 (7)
C14	0.0279 (9)	0.0834 (16)	0.0284 (9)	0.0098 (10)	0.0096 (7)	0.0080 (9)
C4	0.0216 (8)	0.0355 (8)	0.0219 (8)	0.0008 (6)	0.0054 (6)	−0.0003 (6)
C13	0.0289 (9)	0.0767 (15)	0.0226 (8)	0.0104 (9)	0.0050 (7)	0.0091 (9)
C8	0.0253 (8)	0.0393 (9)	0.0226 (8)	0.0028 (7)	0.0074 (6)	−0.0013 (6)

O1W	0.0532 (10)	0.0503 (8)	0.0350 (8)	0.0024 (7)	0.0051 (7)	−0.0050 (6)

Geometric parameters (Å, º)

Co1—O7^{i}	2.0766 (15)	C12—C13	1.386 (2)
Co1—O7	2.0766 (15)	C12—C11	1.392 (2)
Co1—O2	2.0850 (15)	C12—C15	1.496 (2)
Co1—O2^{i}	2.0850 (15)	O2—C1	1.253 (2)
Co1—O8^{i}	2.1371 (14)	C5—C6	1.387 (2)
Co1—O8	2.1371 (14)	C5—C4	1.396 (2)
O5—C15	1.220 (2)	C5—H5A	0.9300
O6—C15	1.307 (2)	O4—C8	1.311 (2)
O6—H6A	0.8200	O4—H4A	0.8200
O1—C1	1.261 (2)	C9—C10	1.388 (2)
N1—N2	1.249 (2)	C9—C14	1.385 (3)
N1—C6	1.432 (2)	C10—C11	1.378 (2)
N2—C9	1.429 (2)	C10—H10A	0.9300
O8—H8A	0.8200	C3—C4	1.396 (2)
O8—H8B	0.867 (9)	C3—H3A	0.9300
C7—C2	1.388 (2)	C11—H11A	0.9300
C7—C6	1.394 (2)	C14—C13	1.386 (3)
C7—H7C	0.9300	C14—H14A	0.9300
O3—C8	1.213 (2)	C4—C8	1.490 (2)
C2—C3	1.401 (2)	C13—H13A	0.9300
C2—C1	1.511 (2)	O1W—H1WB	0.845 (10)
O7—H7B	0.8200	O1W—H1WA	0.847 (10)
O7—H7A	0.831 (9)		
O7^{i}—Co1—O7	180.0	C4—C5—H5A	120.0
O7^{i}—Co1—O2	93.60 (6)	O2—C1—O1	124.44 (15)
O7—Co1—O2	86.40 (6)	O2—C1—C2	117.21 (15)
O7^{i}—Co1—O2^{i}	86.40 (6)	O1—C1—C2	118.33 (14)
O7—Co1—O2^{i}	93.60 (6)	C5—C6—C7	120.21 (15)
O2—Co1—O2^{i}	180.0	C5—C6—N1	115.60 (14)
O7^{i}—Co1—O8^{i}	92.09 (6)	C7—C6—N1	124.19 (15)
O7—Co1—O8^{i}	87.91 (6)	C8—O4—H4A	109.5
O2—Co1—O8^{i}	85.55 (6)	C10—C9—C14	119.78 (16)
O2^{i}—Co1—O8^{i}	94.45 (6)	C10—C9—N2	124.45 (15)
O7^{i}—Co1—O8	87.91 (6)	C14—C9—N2	115.77 (15)
O7—Co1—O8	92.09 (6)	O5—C15—O6	122.68 (16)
O2—Co1—O8	94.45 (6)	O5—C15—C12	124.70 (15)
O2^{i}—Co1—O8	85.55 (6)	O6—C15—C12	112.62 (14)
O8^{i}—Co1—O8	180.00 (4)	C11—C10—C9	120.31 (16)
C15—O6—H6A	109.5	C11—C10—H10A	119.8
N2—N1—C6	114.14 (13)	C9—C10—H10A	119.8
N1—N2—C9	113.99 (14)	C4—C3—C2	120.03 (15)
Co1—O8—H8A	109.5	C4—C3—H3A	120.0
Co1—O8—H8B	107.1 (19)	C2—C3—H3A	120.0

H8A—O8—H8B	108.1	C10—C11—C12	120.16 (16)
C2—C7—C6	120.20 (15)	C10—C11—H11A	119.9
C2—C7—H7C	119.9	C12—C11—H11A	119.9
C6—C7—H7C	119.9	C9—C14—C13	119.95 (17)
C7—C2—C3	119.73 (14)	C9—C14—H14A	120.0
C7—C2—C1	119.85 (14)	C13—C14—H14A	120.0
C3—C2—C1	120.41 (14)	C5—C4—C3	119.77 (15)
Co1—O7—H7B	109.5	C5—C4—C8	119.68 (15)
Co1—O7—H7A	127.2 (15)	C3—C4—C8	120.55 (15)
H7B—O7—H7A	118.8	C12—C13—C14	120.34 (17)
C13—C12—C11	119.45 (15)	C12—C13—H13A	119.8
C13—C12—C15	120.04 (15)	C14—C13—H13A	119.8
C11—C12—C15	120.52 (15)	O3—C8—O4	123.37 (16)
C1—O2—Co1	126.97 (12)	O3—C8—C4	124.27 (16)
C6—C5—C4	120.06 (15)	O4—C8—C4	112.36 (15)
C6—C5—H5A	120.0	H1WB—O1W—H1WA	110.4 (16)

C6—N1—N2—C9	−178.97 (15)	C13—C12—C15—O6	−6.3 (3)
C6—C7—C2—C3	−0.9 (3)	C11—C12—C15—O6	173.41 (17)
C6—C7—C2—C1	178.26 (16)	C14—C9—C10—C11	−0.1 (3)
O7^{i}—Co1—O2—C1	69.81 (16)	N2—C9—C10—C11	179.18 (19)
O7—Co1—O2—C1	−110.19 (16)	C7—C2—C3—C4	0.3 (3)
O8^{i}—Co1—O2—C1	161.62 (16)	C1—C2—C3—C4	−178.89 (15)
O8—Co1—O2—C1	−18.38 (16)	C9—C10—C11—C12	0.4 (3)
Co1—O2—C1—O1	−0.7 (3)	C13—C12—C11—C10	0.2 (3)
Co1—O2—C1—C2	177.75 (11)	C15—C12—C11—C10	−179.49 (18)
C7—C2—C1—O2	−173.46 (16)	C10—C9—C14—C13	−0.7 (3)
C3—C2—C1—O2	5.7 (2)	N2—C9—C14—C13	180.0 (2)
C7—C2—C1—O1	5.1 (3)	C6—C5—C4—C3	−0.5 (3)
C3—C2—C1—O1	−175.70 (17)	C6—C5—C4—C8	178.47 (16)
C4—C5—C6—C7	−0.2 (3)	C2—C3—C4—C5	0.4 (3)
C4—C5—C6—N1	−179.43 (16)	C2—C3—C4—C8	−178.52 (15)
C2—C7—C6—C5	0.9 (3)	C11—C12—C13—C14	−1.0 (3)
C2—C7—C6—N1	−179.93 (16)	C15—C12—C13—C14	178.7 (2)
N2—N1—C6—C5	176.98 (16)	C9—C14—C13—C12	1.2 (4)
N2—N1—C6—C7	−2.3 (3)	C5—C4—C8—O3	177.86 (18)
N1—N2—C9—C10	6.9 (3)	C3—C4—C8—O3	−3.2 (3)
N1—N2—C9—C14	−173.76 (19)	C5—C4—C8—O4	−2.3 (2)
C13—C12—C15—O5	174.2 (2)	C3—C4—C8—O4	176.63 (16)
C11—C12—C15—O5	−6.1 (3)		

Symmetry code: (i) −*x*, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O5^{ii}	0.82	1.82	2.605 (2)	160
O6—H6*A*···O1^{iii}	0.82	1.78	2.574 (2)	164

O7—H7*A*···O3^{iv}	0.83 (1)	1.92 (1)	2.746 (2)	170 (3)
O7—H7*B*···O1*W*^{v}	0.82	2.05	2.791 (2)	151
O8—H8*A*···O1	0.82	1.98	2.697 (2)	145
O8—H8*B*···O1*W*	0.87 (1)	1.94 (1)	2.797 (2)	169 (2)
O1*W*—H1*WA*···O8^{vi}	0.85 (1)	2.12 (1)	2.957 (2)	169 (3)
O1*W*—H1*WB*···O3^{vii}	0.85 (1)	2.15 (2)	2.937 (2)	155 (3)

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