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catena-Poly[[[diaqua(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-4-hydroxy-3-sulfonatobenzoato-$\kappa^2O^3:O^1$] sesquihydrate]

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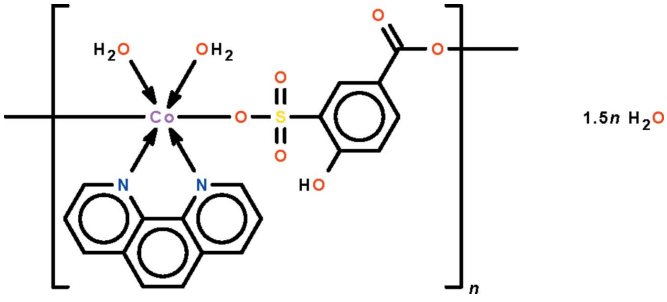
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; some non-H atoms missing; R factor = 0.035; wR factor = 0.096; data-to-parameter ratio = 14.5.

The 1,10-phenanthroline-chelated Co^{II} atom in the polymeric title compound, $\{[Co(C_7H_4O_6S)(C_{12}H_8N_2)(H_2O)_2]\cdot 1.5H_2O\}_n$, is connected to the sulfonate O atom of one 4-hydroxy-3-sulfonatobenzoate dianion and to the carboxylate O atom of another dianion. It is also coordinated by two water molecules in a *trans*-CoN_2O_4 octahedral environment. The dianion links adjacent metal atoms into a chain running along [110]. The chains are linked by O—H···O hydrogen bonds into a three-dimensional network.

Related literature

For the isotypic Mn^{II} derivative, see: Fang *et al.* (2011).



Experimental

Crystal data

$[Co(C_7H_4O_6S)(C_{12}H_8N_2)(H_2O)_2]\cdot 1.5H_2O$
M_r = 518.35
Monoclinic, $C2/c$
a = 8.3369 (4) Å
b = 17.3630 (6) Å
c = 28.6382 (10) Å
β = 93.189 (1)°
V = 4139.1 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 293 K
0.21 × 0.18 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.819, T_{max} = 0.874
20042 measured reflections
4727 independent reflections
4053 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
S = 1.04
4727 reflections
326 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O4W	0.83 (1)	1.79 (1)	2.617 (2)	171 (3)
O1w—H11···O6^{i}	0.85 (1)	1.69 (1)	2.526 (2)	169 (3)
O1w—H12···O3W	0.84 (1)	1.99 (1)	2.790 (1)	161 (2)
O2w—H21···O2^{ii}	0.83 (1)	1.93 (1)	2.752 (2)	168 (3)
O2w—H22···O1W^{iii}	0.83 (1)	1.93 (1)	2.756 (2)	171 (3)
O3w—H31···O2	0.85 (1)	1.92 (1)	2.754 (2)	167 (3)
O4w—H41···O4^{iv}	0.83 (1)	2.29 (2)	2.952 (2)	137 (3)
O4w—H42···O5^{v}	0.84 (1)	1.96 (1)	2.795 (2)	176 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); 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, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5892).

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supporting information

Acta Cryst. (2012). E**68**, m721 [doi:10.1107/S1600536812018752]

catena-Poly[[[diaqua(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-4-hydroxy-3-sulfonatobenzoato-κ^2O^3:O^1] sesquihydrate]

Xiang-Qian Fang, Shan Gao and Seik Weng Ng

S1. Comment

The title cobalt(II) compound (Scheme I, Fig. 1) is isostructural with the manganese(II) derivative, which we reported recently (Fang *et al.*, 2011). The 1,10-phenanthroline chelated Co^{II} atom is connected to the sulfonate O atom of one ($C_7H_4O_6S$) dianion and to the carboxylate O atom of another dianion. It is also coordinated by two water molecules in an octahedral environment. The dianion links adjacent metal atoms into a chain along [1 1 0]. The chains are linked by O–H···O hydrogen bonds into a three-dimensional network (Table 1).

S2. Experimental

A methanol solution (5 ml) of 1,10-phenanthroline (1 mmol) was added to an aqueous solution (10 ml) of cobalt(II) dichloride (1 mmol), 2-hydroxy-5-carboxybenzenesulfonic acid (2 mmol) and lithium hydroxide (4 mmol). Pink crystals were isolated from the solution after several days.

S3. Refinement

All H atoms were located in a difference map. Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C). H-atoms bonded to O were isotropically refined with a distance restraint of O–H 0.84±0.01 Å.

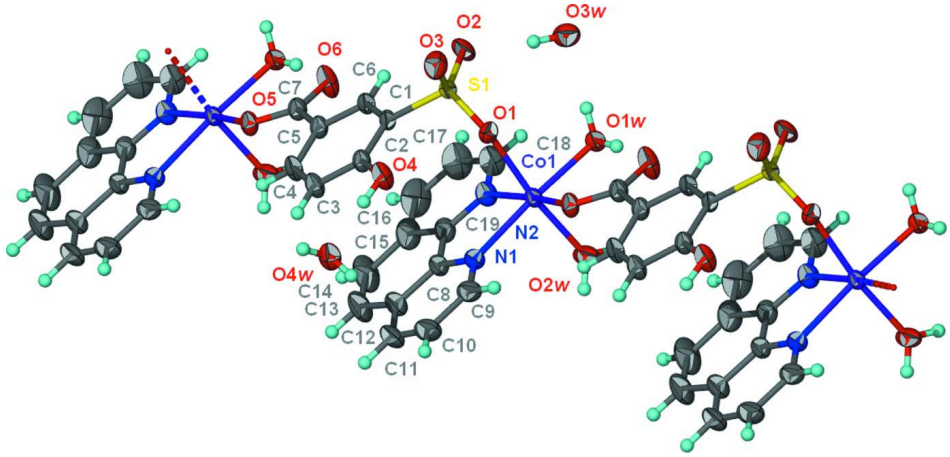

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of a portion of the structure of polymeric $[Co(H_2O)_2(C_{12}H_8N_2)(C_7H_4O_6S)]_n\cdot 1.5nH_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

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$c = 28.6382$ (10) Å
$\beta = 93.189$ (1)°
$V = 4139.1$ (3) Å^3
$Z = 8$
$F(000) = 2128$
$D_x = 1.664$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 16110 reflections
$\theta = 3.0$–27.5°
$\mu = 0.99$ mm^{-1}
$T = 293$ K
Prism, pink
0.21 × 0.18 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.819$, $T_{max} = 0.874$
20042 measured reflections
4727 independent reflections
4053 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -10\rightarrow10$
$k = -22\rightarrow22$
$l = -36\rightarrow37$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.096$
$S = 1.04$
4727 reflections
326 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
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 2.0124P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Co1	0.61702 (3)	0.233252 (12)	0.341796 (8)	0.02663 (9)
S1	1.01602 (5)	0.26449 (2)	0.376637 (16)	0.02890 (11)
O1	0.85592 (16)	0.23081 (7)	0.37033 (5)	0.0356 (3)
O2	1.09098 (19)	0.27300 (8)	0.33199 (6)	0.0465 (4)
O3	1.1137 (2)	0.22279 (8)	0.41122 (6)	0.0512 (4)
O4	0.8735 (2)	0.31178 (7)	0.46465 (5)	0.0430 (3)
O5	1.08477 (16)	0.62905 (7)	0.37595 (4)	0.0335 (3)
O6	1.1048 (2)	0.54895 (8)	0.31558 (5)	0.0536 (4)
O1W	0.69134 (16)	0.17451 (7)	0.28018 (4)	0.0316 (3)
O2W	0.39077 (18)	0.22382 (11)	0.30945 (5)	0.0524 (4)
O3W	1.0000	0.19799 (15)	0.2500	0.0502 (5)

O4W	0.7312 (2)	0.35058 (9)	0.54035 (5)	0.0429 (3)
N1	0.52131 (18)	0.30093 (9)	0.39551 (5)	0.0340 (3)
N2	0.6524 (2)	0.34674 (9)	0.31625 (6)	0.0376 (3)
C1	0.9907 (2)	0.35987 (9)	0.39700 (6)	0.0282 (3)
C2	0.9196 (2)	0.37256 (10)	0.43952 (6)	0.0308 (4)
C3	0.8980 (3)	0.44848 (11)	0.45451 (6)	0.0379 (4)
H3	0.8491	0.4578	0.4824	0.045*
C4	0.9488 (3)	0.50940 (10)	0.42819 (6)	0.0379 (4)
H4A	0.9343	0.5595	0.4386	0.045*
C5	1.0217 (2)	0.49711 (10)	0.38621 (6)	0.0314 (4)
C6	1.0407 (2)	0.42151 (10)	0.37083 (6)	0.0308 (4)
H6	1.0875	0.4125	0.3426	0.037*
C7	1.0749 (2)	0.56273 (10)	0.35690 (6)	0.0337 (4)
C8	0.5290 (2)	0.37789 (11)	0.38715 (7)	0.0386 (4)
C9	0.4570 (3)	0.27742 (14)	0.43451 (7)	0.0437 (5)
H9	0.4500	0.2248	0.4402	0.052*
C10	0.3995 (3)	0.32857 (18)	0.46737 (8)	0.0594 (7)
H10	0.3574	0.3102	0.4946	0.071*
C11	0.4060 (3)	0.40557 (18)	0.45891 (9)	0.0651 (7)
H11A	0.3665	0.4400	0.4803	0.078*
C12	0.4721 (3)	0.43345 (14)	0.41810 (9)	0.0544 (6)
C13	0.4873 (4)	0.51322 (16)	0.40639 (13)	0.0776 (10)
H13	0.4504	0.5503	0.4266	0.093*
C14	0.5536 (4)	0.53590 (14)	0.36690 (13)	0.0798 (9)
H14	0.5605	0.5882	0.3604	0.096*
C15	0.6139 (3)	0.48139 (13)	0.33467 (10)	0.0597 (7)
C16	0.6870 (4)	0.50107 (15)	0.29369 (11)	0.0742 (9)
H16	0.6988	0.5527	0.2859	0.089*
C17	0.7411 (4)	0.44549 (15)	0.26510 (10)	0.0711 (8)
H17	0.7908	0.4584	0.2379	0.085*
C18	0.7202 (3)	0.36828 (13)	0.27749 (8)	0.0521 (6)
H18	0.7556	0.3303	0.2576	0.063*
C19	0.5997 (2)	0.40207 (11)	0.34500 (7)	0.0407 (4)
H4	0.829 (3)	0.3290 (15)	0.4878 (6)	0.062 (8)*
H11	0.665 (4)	0.1300 (9)	0.2888 (9)	0.072 (9)*
H12	0.7900 (12)	0.1745 (13)	0.2762 (7)	0.037 (6)*
H21	0.3019 (19)	0.2343 (14)	0.3198 (9)	0.054 (7)*
H22	0.371 (3)	0.2041 (13)	0.2833 (5)	0.049 (7)*
H31	1.022 (4)	0.2272 (13)	0.2731 (7)	0.064 (9)*
H41	0.663 (3)	0.3175 (13)	0.5465 (10)	0.066 (9)*
H42	0.789 (3)	0.3586 (17)	0.5647 (6)	0.070 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03140 (14)	0.02203 (14)	0.02687 (14)	−0.00093 (8)	0.00532 (9)	−0.00072 (8)
S1	0.0284 (2)	0.0234 (2)	0.0354 (2)	−0.00200 (14)	0.00557 (17)	−0.00556 (16)
O1	0.0321 (6)	0.0297 (6)	0.0449 (7)	−0.0070 (5)	0.0020 (6)	−0.0050 (5)

O2	0.0537 (9)	0.0385 (8)	0.0502 (8)	−0.0041 (6)	0.0275 (7)	−0.0121 (6)
O3	0.0526 (9)	0.0364 (7)	0.0626 (10)	0.0058 (6)	−0.0151 (8)	−0.0030 (7)
O4	0.0706 (10)	0.0267 (6)	0.0337 (7)	−0.0100 (6)	0.0203 (7)	−0.0009 (6)
O5	0.0480 (7)	0.0227 (6)	0.0303 (6)	−0.0087 (5)	0.0069 (5)	−0.0014 (5)
O6	0.0967 (13)	0.0307 (7)	0.0358 (7)	−0.0174 (8)	0.0263 (8)	−0.0050 (6)
O1W	0.0364 (7)	0.0294 (6)	0.0298 (6)	−0.0029 (5)	0.0083 (5)	0.0005 (5)
O2W	0.0314 (7)	0.0876 (13)	0.0381 (8)	0.0092 (7)	−0.0003 (6)	−0.0220 (8)
O3W	0.0420 (12)	0.0638 (15)	0.0454 (12)	0.000	0.0063 (9)	0.000
O4W	0.0595 (9)	0.0395 (8)	0.0305 (7)	−0.0083 (7)	0.0088 (6)	0.0000 (6)
N1	0.0318 (8)	0.0364 (8)	0.0338 (7)	0.0031 (6)	0.0014 (6)	−0.0048 (7)
N2	0.0484 (9)	0.0272 (7)	0.0373 (8)	0.0003 (7)	0.0036 (7)	0.0030 (6)
C1	0.0325 (8)	0.0232 (7)	0.0290 (8)	−0.0046 (6)	0.0038 (6)	−0.0054 (6)
C2	0.0404 (9)	0.0252 (8)	0.0273 (8)	−0.0067 (7)	0.0061 (7)	−0.0014 (7)
C3	0.0566 (12)	0.0295 (9)	0.0291 (8)	−0.0072 (8)	0.0153 (8)	−0.0053 (7)
C4	0.0556 (12)	0.0248 (8)	0.0342 (9)	−0.0069 (8)	0.0113 (8)	−0.0068 (7)
C5	0.0411 (10)	0.0243 (8)	0.0292 (8)	−0.0085 (7)	0.0063 (7)	−0.0012 (7)
C6	0.0375 (9)	0.0270 (8)	0.0286 (8)	−0.0066 (7)	0.0086 (7)	−0.0039 (7)
C7	0.0417 (10)	0.0270 (8)	0.0331 (9)	−0.0079 (7)	0.0077 (7)	−0.0020 (7)
C8	0.0350 (9)	0.0353 (9)	0.0448 (10)	0.0081 (8)	−0.0038 (8)	−0.0124 (8)
C9	0.0369 (10)	0.0572 (12)	0.0374 (10)	0.0007 (9)	0.0064 (8)	−0.0043 (9)
C10	0.0449 (12)	0.090 (2)	0.0444 (12)	0.0010 (12)	0.0119 (9)	−0.0207 (12)
C11	0.0502 (13)	0.0847 (19)	0.0608 (14)	0.0121 (13)	0.0062 (11)	−0.0426 (14)
C12	0.0466 (12)	0.0519 (13)	0.0640 (14)	0.0140 (10)	−0.0033 (10)	−0.0260 (11)
C13	0.080 (2)	0.0485 (14)	0.103 (2)	0.0220 (14)	−0.0041 (18)	−0.0385 (16)
C14	0.107 (2)	0.0255 (11)	0.105 (2)	0.0165 (13)	−0.009 (2)	−0.0125 (14)
C15	0.0707 (17)	0.0281 (10)	0.0788 (17)	0.0043 (10)	−0.0089 (14)	0.0001 (11)
C16	0.105 (2)	0.0338 (12)	0.0823 (19)	−0.0094 (13)	−0.0047 (17)	0.0228 (13)
C17	0.106 (2)	0.0467 (14)	0.0613 (15)	−0.0139 (14)	0.0112 (15)	0.0195 (13)
C18	0.0737 (16)	0.0395 (11)	0.0439 (11)	−0.0062 (10)	0.0110 (11)	0.0070 (9)
C19	0.0442 (11)	0.0270 (9)	0.0500 (11)	0.0046 (7)	−0.0051 (9)	−0.0025 (8)

Geometric parameters (Å, º)

Co1—O2W	2.0613 (15)	C2—C3	1.401 (2)
Co1—O5^{i}	2.0813 (12)	C3—C4	1.379 (3)
Co1—O1	2.1107 (14)	C3—H3	0.9300
Co1—N1	2.1262 (15)	C4—C5	1.393 (2)
Co1—N2	2.1281 (15)	C4—H4A	0.9300
Co1—O1W	2.1586 (12)	C5—C6	1.396 (2)
S1—O3	1.4418 (16)	C5—C7	1.497 (2)
S1—O1	1.4592 (13)	C6—H6	0.9300
S1—O2	1.4616 (14)	C8—C12	1.410 (3)
S1—C1	1.7724 (16)	C8—C19	1.435 (3)
O4—C2	1.345 (2)	C9—C10	1.398 (3)
O4—H4	0.832 (10)	C9—H9	0.9300
O5—C7	1.275 (2)	C10—C11	1.360 (4)
O5—Co1^{ii}	2.0813 (12)	C10—H10	0.9300
O6—C7	1.246 (2)	C11—C12	1.405 (4)

O1W—H11	0.845 (10)	C11—H11A	0.9300
O1W—H12	0.837 (10)	C12—C13	1.432 (4)
O2W—H21	0.833 (10)	C13—C14	1.345 (5)
O2W—H22	0.832 (10)	C13—H13	0.9300
O3W—H31	0.846 (10)	C14—C15	1.432 (4)
O4W—H41	0.832 (10)	C14—H14	0.9300
O4W—H42	0.837 (10)	C15—C16	1.395 (4)
N1—C9	1.330 (3)	C15—C19	1.415 (3)
N1—C8	1.360 (3)	C16—C17	1.359 (4)
N2—C18	1.327 (3)	C16—H16	0.9300
N2—C19	1.354 (3)	C17—C18	1.400 (3)
C1—C6	1.384 (2)	C17—H17	0.9300
C1—C2	1.401 (2)	C18—H18	0.9300

O2W—Co1—O5^{i}	90.19 (7)	C3—C4—H4A	119.5
O2W—Co1—O1	173.02 (6)	C5—C4—H4A	119.5
O5^{i}—Co1—O1	86.81 (5)	C4—C5—C6	118.59 (16)
O2W—Co1—N1	89.90 (6)	C4—C5—C7	121.63 (16)
O5^{i}—Co1—N1	94.41 (5)	C6—C5—C7	119.76 (15)
O1—Co1—N1	96.61 (6)	C1—C6—C5	120.89 (15)
O2W—Co1—N2	93.43 (7)	C1—C6—H6	119.6
O5^{i}—Co1—N2	172.07 (5)	C5—C6—H6	119.6
O1—Co1—N2	90.34 (6)	O6—C7—O5	124.64 (16)
N1—Co1—N2	78.56 (6)	O6—C7—C5	117.87 (16)
O2W—Co1—O1W	83.81 (6)	O5—C7—C5	117.48 (15)
O5^{i}—Co1—O1W	91.37 (5)	N1—C8—C12	122.7 (2)
O1—Co1—O1W	89.96 (5)	N1—C8—C19	117.46 (16)
N1—Co1—O1W	171.47 (6)	C12—C8—C19	119.8 (2)
N2—Co1—O1W	96.03 (6)	N1—C9—C10	122.7 (2)
O3—S1—O1	111.20 (9)	N1—C9—H9	118.7
O3—S1—O2	113.52 (10)	C10—C9—H9	118.7
O1—S1—O2	111.40 (9)	C11—C10—C9	119.1 (2)
O3—S1—C1	108.44 (9)	C11—C10—H10	120.5
O1—S1—C1	106.87 (8)	C9—C10—H10	120.5
O2—S1—C1	104.95 (8)	C10—C11—C12	120.5 (2)
S1—O1—Co1	151.26 (9)	C10—C11—H11A	119.7
C2—O4—H4	107 (2)	C12—C11—H11A	119.7
C7—O5—Co1^{ii}	126.22 (11)	C11—C12—C8	116.6 (2)
Co1—O1W—H11	96 (2)	C11—C12—C13	124.9 (2)
Co1—O1W—H12	116.1 (15)	C8—C12—C13	118.5 (3)
H11—O1W—H12	109 (3)	C14—C13—C12	121.7 (2)
Co1—O2W—H21	129.3 (19)	C14—C13—H13	119.1
Co1—O2W—H22	124.7 (18)	C12—C13—H13	119.1
H21—O2W—H22	106 (3)	C13—C14—C15	121.6 (2)
H41—O4W—H42	108 (3)	C13—C14—H14	119.2
C9—N1—C8	118.34 (17)	C15—C14—H14	119.2
C9—N1—Co1	128.54 (14)	C16—C15—C19	117.4 (2)
C8—N1—Co1	113.11 (12)	C16—C15—C14	124.4 (3)

C18—N2—C19	118.44 (18)	C19—C15—C14	118.2 (3)
C18—N2—Co1	128.46 (14)	C17—C16—C15	120.6 (2)
C19—N2—Co1	113.09 (13)	C17—C16—H16	119.7
C6—C1—C2	120.24 (15)	C15—C16—H16	119.7
C6—C1—S1	119.96 (13)	C16—C17—C18	118.5 (3)
C2—C1—S1	119.80 (13)	C16—C17—H17	120.7
O4—C2—C1	119.26 (15)	C18—C17—H17	120.7
O4—C2—C3	121.90 (15)	N2—C18—C17	123.1 (2)
C1—C2—C3	118.84 (15)	N2—C18—H18	118.4
C4—C3—C2	120.35 (16)	C17—C18—H18	118.4
C4—C3—H3	119.8	N2—C19—C15	122.0 (2)
C2—C3—H3	119.8	N2—C19—C8	117.78 (17)
C3—C4—C5	121.08 (16)	C15—C19—C8	120.2 (2)

O3—S1—O1—Co1	171.77 (16)	Co1^{ii}—O5—C7—O6	10.2 (3)
O2—S1—O1—Co1	−60.5 (2)	Co1^{ii}—O5—C7—C5	−168.98 (12)
C1—S1—O1—Co1	53.6 (2)	C4—C5—C7—O6	−164.0 (2)
O2W—Co1—O1—S1	115.4 (5)	C6—C5—C7—O6	14.1 (3)
O5^{i}—Co1—O1—S1	−179.94 (18)	C4—C5—C7—O5	15.2 (3)
N1—Co1—O1—S1	−85.86 (18)	C6—C5—C7—O5	−166.62 (18)
N2—Co1—O1—S1	−7.34 (18)	C9—N1—C8—C12	0.2 (3)
O1W—Co1—O1—S1	88.68 (18)	Co1—N1—C8—C12	179.86 (16)
O2W—Co1—N1—C9	86.52 (17)	C9—N1—C8—C19	179.64 (17)
O5^{i}—Co1—N1—C9	−3.66 (17)	Co1—N1—C8—C19	−0.6 (2)
O1—Co1—N1—C9	−90.95 (17)	C8—N1—C9—C10	−1.0 (3)
N2—Co1—N1—C9	−179.96 (18)	Co1—N1—C9—C10	179.36 (16)
O2W—Co1—N1—C8	−93.15 (14)	N1—C9—C10—C11	1.5 (4)
O5^{i}—Co1—N1—C8	176.67 (13)	C9—C10—C11—C12	−1.1 (4)
O1—Co1—N1—C8	89.38 (13)	C10—C11—C12—C8	0.3 (4)
N2—Co1—N1—C8	0.37 (13)	C10—C11—C12—C13	−178.7 (3)
O2W—Co1—N2—C18	−92.3 (2)	N1—C8—C12—C11	0.2 (3)
O1—Co1—N2—C18	81.8 (2)	C19—C8—C12—C11	−179.3 (2)
N1—Co1—N2—C18	178.5 (2)	N1—C8—C12—C13	179.3 (2)
O1W—Co1—N2—C18	−8.2 (2)	C19—C8—C12—C13	−0.2 (3)
O2W—Co1—N2—C19	89.16 (14)	C11—C12—C13—C14	179.2 (3)
O1—Co1—N2—C19	−96.71 (14)	C8—C12—C13—C14	0.2 (4)
N1—Co1—N2—C19	−0.04 (14)	C12—C13—C14—C15	−0.6 (5)
O1W—Co1—N2—C19	173.29 (14)	C13—C14—C15—C16	−178.6 (3)
O3—S1—C1—C6	121.28 (16)	C13—C14—C15—C19	1.0 (5)
O1—S1—C1—C6	−118.75 (15)	C19—C15—C16—C17	0.3 (4)
O2—S1—C1—C6	−0.35 (18)	C14—C15—C16—C17	179.9 (3)
O3—S1—C1—C2	−58.89 (17)	C15—C16—C17—C18	0.7 (5)
O1—S1—C1—C2	61.08 (16)	C19—N2—C18—C17	0.5 (4)
O2—S1—C1—C2	179.48 (15)	Co1—N2—C18—C17	−178.0 (2)
C6—C1—C2—O4	−179.27 (17)	C16—C17—C18—N2	−1.1 (5)
S1—C1—C2—O4	0.9 (2)	C18—N2—C19—C15	0.5 (3)
C6—C1—C2—C3	1.0 (3)	Co1—N2—C19—C15	179.22 (17)
S1—C1—C2—C3	−178.80 (15)	C18—N2—C19—C8	−179.00 (19)

O4—C2—C3—C4	179.05 (19)	Co1—N2—C19—C8	−0.3 (2)
C1—C2—C3—C4	−1.3 (3)	C16—C15—C19—N2	−0.9 (4)
C2—C3—C4—C5	0.4 (3)	C14—C15—C19—N2	179.5 (2)
C3—C4—C5—C6	0.8 (3)	C16—C15—C19—C8	178.6 (2)
C3—C4—C5—C7	178.95 (19)	C14—C15—C19—C8	−1.0 (4)
C2—C1—C6—C5	0.1 (3)	N1—C8—C19—N2	0.6 (3)
S1—C1—C6—C5	179.94 (14)	C12—C8—C19—N2	−179.85 (19)
C4—C5—C6—C1	−1.0 (3)	N1—C8—C19—C15	−178.87 (19)
C7—C5—C6—C1	−179.22 (17)	C12—C8—C19—C15	0.6 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O4*W*	0.83 (1)	1.79 (1)	2.617 (2)	171 (3)
O1w—H11···O6^{i}	0.85 (1)	1.69 (1)	2.526 (2)	169 (3)
O1w—H12···O3*W*	0.84 (1)	1.99 (1)	2.790 (1)	161 (2)
O2w—H21···O2^{iii}	0.83 (1)	1.93 (1)	2.752 (2)	168 (3)
O2w—H22···O1*W*^{iv}	0.83 (1)	1.93 (1)	2.756 (2)	171 (3)
O3w—H31···O2	0.85 (1)	1.92 (1)	2.754 (2)	167 (3)
O4w—H41···O4^{v}	0.83 (1)	2.29 (2)	2.952 (2)	137 (3)
O4w—H42···O5^{vi}	0.84 (1)	1.96 (1)	2.795 (2)	176 (3)

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