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

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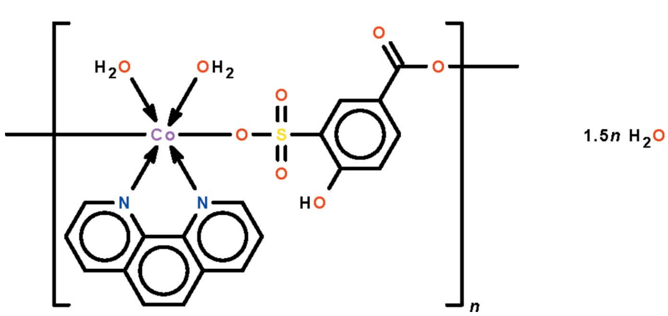
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; some non-H atoms missing; $R$ factor = 0.035; $wR$ factor = 0.096; data-to-parameter ratio = 14.5.

The 1,10-phenanthroline-chelated $Co^{II}$ atom in the polymeric title compound, $\{[Co(C_7H_4O_6S)(C_{12}H_8N_2)(H_2O)_2]\cdot1.5H_2O\}_n$, 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*

$[Co(C_7H_4O_6S)(C_{12}H_8N_2)(H_2O)_2]\cdot1.5H_2O$
$M_r$ = 518.35
Monoclinic, $C2/c$
$a$ = 8.3369 (4) Å
$b$ = 17.3630 (6) Å
$c$ = 28.6382 (10) Å
$\beta$ = 93.189 (1)°
$V$ = 4139.1 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 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···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$^{ii}$ | 0.83 (1) | 1.93 (1) | 2.752 (2) | 168 (3) |
| O2w—H22···O1$W^{iii}$ | 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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# supplementary materials

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

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

**Xiang-Qian Fang, Shan Gao and Seik Weng Ng**

### 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).

### 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.

### 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.

### Computing details

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO* (Rigaku, 1998); 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).

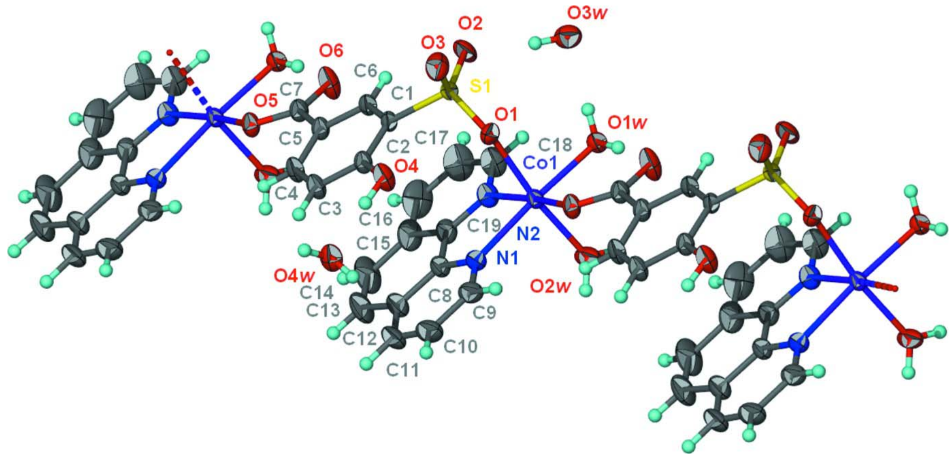


**Figure 1**

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.

## *catena*-Poly[[[diaqua(1,10-phenanthroline- κ²*N*,*N*′)cobalt(II)]-μ-4-hydroxy-3-sulfonatobenzoato- κ²*O*³:*O*¹] sesquihydrate]

### *Crystal data*

$[Co(C_7H_4O_6S)(C_{12}H_8N_2)(H_2O)_2]\cdot 1.5H_2O$
$M_r = 518.35$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 8.3369$ (4) Å
$b = 17.3630$ (6) Å
$c = 28.6382$ (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
$\omega$ 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 $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -10 \rightarrow 10$
$k = -22 \rightarrow 22$
$l = -36 \rightarrow 37$

### *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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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 |

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| 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) |

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| 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) $-x+2, -y+1, -z+1$.