

catena-Poly[[[diaquacobalt(II)]- μ -(*E*)-1,2-bis(4-pyridyl)ethylene- κ^2 N:N'] bis(4-aminobenzenesulfonate) hexahydrate]

 Zhong-Xiang Du^a and Jun-Xia Li^{a,b*}

^aCollege of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, People's Republic of China, and ^bCollege of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin, Guangxi 541004, People's Republic of China

Correspondence e-mail: ljx6281@126.com

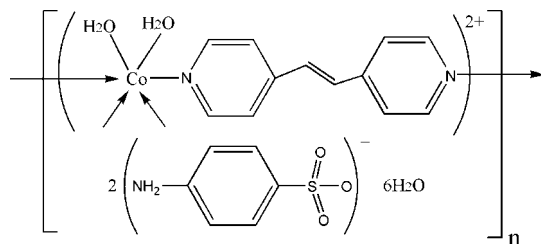
Received 4 November 2007; accepted 13 November 2007

Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.051; wR factor = 0.155; data-to-parameter ratio = 14.8.

In the title compound, $\{[\text{Co}(\text{C}_{12}\text{H}_{10}\text{N}_2)(\text{H}_2\text{O})_2](\text{C}_6\text{H}_4\text{NO}_3\text{S})_2 \cdot 6\text{H}_2\text{O}\}_n$, a cobalt coordination polymer, the repeat unit comprises a cobalt complex cation, two 4-aminobenzene-sulfonate anions and six uncoordinated water molecules. In the doubly charged cobalt cation, each Co atom lies on a center of symmetry and is six-coordinated in a distorted octahedral geometry formed by four O atoms of four coordinated water molecules, and two N atoms from two (*E*)-1,2-bis(4-pyridyl)ethylene (bpe) ligands. The bpe ligands bridge the Co atoms, forming a one-dimensional linear chain. Intermolecular O—H...O, O—H...N and N—H...O hydrogen-bonding interactions stabilize this chain structure.

Related literature

For related literature, see: Du & Li (2007); Gunderman *et al.* (1996); Huang *et al.* (2004); Starynowicz (1992).



Experimental

Crystal data

$[\text{Co}(\text{C}_{12}\text{H}_{10}\text{N}_2)(\text{H}_2\text{O})_2] \cdot (\text{C}_6\text{H}_4\text{NO}_3\text{S})_2 \cdot 6\text{H}_2\text{O}$
 $M_r = 729.63$
 Monoclinic, $P2_1/c$

$a = 13.4351$ (15) Å
 $b = 7.9688$ (9) Å
 $c = 15.7183$ (18) Å
 $\beta = 104.1330$ (10)°

$V = 1631.9$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 0.72$ mm⁻¹
 $T = 291$ (2) K
 $0.30 \times 0.20 \times 0.09$ mm

Data collection

Bruker APEX II CCD area-detector diffractometer
 Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
 $T_{\text{min}} = 0.814$, $T_{\text{max}} = 0.941$

12048 measured reflections
 3035 independent reflections
 2395 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.155$
 $S = 1.05$
 3035 reflections
 205 parameters

144 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.83$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—O1	1.985 (3)	Co1—O3 ⁱⁱ	2.458 (3)
Co1—N2 ⁱ	2.009 (3)		
O1 ⁱ —Co1—O1	180	O3 ⁱⁱ —Co1—O3 ⁱⁱ	180
O1—Co1—N2 ⁱ	90.67 (11)	O3 ⁱⁱ —Co1—N2 ⁱ	88.75 (11)
O1—Co1—N2	89.33 (11)	O3—Co1—N2 ⁱ	172.76 (9)
N2 ⁱ —Co1—N2	180		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1W...O6 ⁱⁱⁱ	0.83	1.86	2.674 (4)	164
O1—H2W...O5 ^{iv}	0.83	1.99	2.806 (5)	173
O2—H3W...O4 ^v	0.85	1.92	2.771 (7)	179
O2—H4W...N1 ^{vi}	1.03	2.20	2.841 (8)	118
O3—H5W...O7 ^{vi}	0.83	1.92	2.743 (4)	168
O3—H6W...O4	0.84	2.08	2.800 (5)	143
O4—H7W...O5	0.87	2.08	2.714 (6)	129
O4—H8W...O3 ^{vii}	0.83	2.21	2.886 (5)	139
N1—H1A...O7 ^v	0.86	2.21	2.997 (5)	152
N1—H1B...O2 ^{viii}	0.86	1.98	2.841 (8)	175

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation of China (No. 20471026) and the Natural Science Foundation of Henan province (No. 0311021200).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2470).

References

- Bruker (2004). *APEX2*, *SAINTE* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Du, Z.-X. & Li, J.-X. (2007). *Acta Cryst.* **E63**, m2133–m2134.
- Gunderman, B. J., Squattrito, P. J. & Dubey, S. N. (1996). *Acta Cryst.* **C52**, 1131–1134.
- Huang, M.-H., Bi, L.-H. & Dong, S.-J. (2004). *Acta Cryst.* **C60**, m30–m32.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Starynowicz, P. (1992). *Acta Cryst.* **C48**, 1414–1416.

supplementary materials

Acta Cryst. (2007). E63, m3080-m3081 [doi:10.1107/S1600536807058461]

***catena*-Poly[[[diaquacobalt(II)]- μ -(*E*)-1,2-bis(4-pyridyl)ethylene- κ^2 N:N'] bis(4-aminobenzenesulfonate) hexahydrate]**

Z.-X. Du and J.-X. Li

Comment

In the previous literatures, the complexes containing 4-aminobenzenesulfonate as monodentate ligand (Du & Li, 2007., Gunderman *et al.*, 1996; Huang *et al.*, 2004; Starynowicz, 1992) have been reported. In our paper, we describe another new compound (I) in which 4-aminobenzenesulfonate does not participate in coordination, (Fig. 1).

Compound (I) is a Co coordination polymer and the structural unit is comprised of a cobalt complex cation, two 4-aminobenzenesulfonate anions and six uncoordinated water molecules.

In the doubly charged cobalt cation, each Co symmetrical center has distorted octahedral geometry, formed by four O atoms of four coordinated water molecules, two N atoms from two (*E*)-1,2-bis(4-pyridyl)ethylene (bpe) ligands (Table 1). The bpe ligand plays as a bridging ligand linking neighbouring Co^{II} atoms into a one-dimensional linear chain with the Co1...Co1(-x + 1, y, z) separation distance of 13.435 (2) Å.

4-Aminobenzenesulfonate anions here does not take part in coordination but involve in intermolecular hydrogen bonds with coordinated and uncoordinated water molecules (Table 2). The chain structure is stabilized *via* these hydrogen bonding interactions and as well as electrostatic force (Fig. 2).

Experimental

A 10 ml water solution of Co(Cl)₂·6H₂O (0.238 g, 1 mmol) was dropped into 10 ml methanol solution of (*E*)-1,2-bis(4-pyridyl)ethylene (0.182 g, 1 mmol) and 4-aminobenzenesulfonic acid (0.346 g, 2 mmol) and then the mixture was stirred for 5 h at 343 K. The filtrate was stayed in air for about two weeks to obtain red block-shaped crystals. Analysis, found (%): C 39.42, H 5.15, N 7.71, S 8.82. C₂₄H₃₈CoN₄O₁₄S₂ requires(%): C 39.47, H 5.21, N 7.67, S 8.77. [CCDC: 656072].

Refinement

H atoms bonded to C and N were positioned geometrically with C—H distance of 0.93 Å and N—H of 0.86 Å, respectively, and treated as riding atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C or N})$. The O—H hydrogen atoms were located in a difference Fourier map and refined isotropically, with O—H distance in the range of 0.8250–1.0288 Å.

Figures

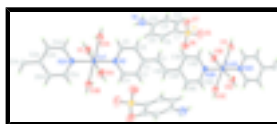


Fig. 1. The segment of the polymeric structure of (I) with atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The uncoordinated water molecules have been omitted. [Symmetry codes: (A) $-x + 2, -y + 1, -z$; (B) $-x + 1, -y + 1, -z$; (C) $-1 + x, y, z$.]

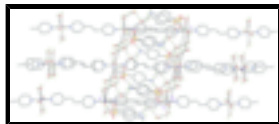


Fig. 2. Packing diagram of (I), showing the hydrogen bonds as dashed lines. H atoms on C atoms have been omitted for clarity.

catena-Poly[[[diaquacobalt(II)]- μ -(*E*)-1,2-bis(4-pyridyl)ethylene- κ^2 N:N'] bis(4-aminobenzenesulfonate) hexahydrate]

Crystal data

[Co(C₁₂H₁₀N₂)(H₂O)₂](C₆H₆NO₃S)₂·6H₂O

$M_r = 729.63$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 13.4351$ (15) Å

$b = 7.9688$ (9) Å

$c = 15.7183$ (18) Å

$\beta = 104.1330$ (10)°

$V = 1631.9$ (3) Å³

$Z = 2$

$F_{000} = 762$

$D_x = 1.485$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2927 reflections

$\theta = 2.7$ – 24.2 °

$\mu = 0.72$ mm⁻¹

$T = 291$ (2) K

Block, red

$0.30 \times 0.20 \times 0.09$ mm

Data collection

Bruker APEX II CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 291$ (2) K

φ and ω scans

Absorption correction: multi-scan

SADABS (Sheldrick, 1996)

$T_{\min} = 0.814$, $T_{\max} = 0.941$

12048 measured reflections

3035 independent reflections

2395 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 25.5$ °

$\theta_{\min} = 2.7$ °

$h = -16 \rightarrow 16$

$k = -9 \rightarrow 9$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.155$

$S = 1.05$

3035 reflections

205 parameters

144 restraints

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0893P)^2 + 1.4053P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.83$ e Å⁻³

$\Delta\rho_{\min} = -0.49$ e Å⁻³

Extinction correction: none

Primary atom site location: structure-invariant direct methods

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and

goodness of fit S are based on F^2 , conventional R -factors R are based

on F , with F set to zero for negative F^2 . The threshold expression of

$F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is

not relevant to the choice of reflections for refinement. R -factors based

on F^2 are statistically about twice as large as those based on F , and R -

factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	1.0000	0.5000	0.0000	0.0305 (2)
S1	0.20531 (8)	-0.04540 (13)	0.13300 (7)	0.0519 (3)
O1	1.00684 (18)	0.2545 (4)	0.0220 (2)	0.0587 (8)
H1W	0.9589	0.1931	-0.0039	0.088*
H2W	1.0497	0.2017	0.0588	0.088*
O2	0.7714 (5)	0.9228 (9)	0.0977 (4)	0.160 (2)
H3W	0.8184	0.8814	0.1386	0.240*
H4W	0.6946	0.9382	0.0949	0.240*
O3	0.0514 (2)	0.5633 (4)	0.1577 (2)	0.0614 (8)
H5W	0.1010	0.6284	0.1636	0.092*
H6W	0.0534	0.5159	0.2058	0.092*
O4	0.0764 (3)	0.2844 (5)	0.2693 (3)	0.1046 (13)
H7W	0.1093	0.1920	0.2643	0.157*
H8W	0.0185	0.2582	0.2756	0.157*
O5	0.1560 (3)	0.1016 (5)	0.1560 (3)	0.0924 (12)
O6	0.1664 (3)	-0.0819 (6)	0.0398 (2)	0.0910 (12)
O7	0.1974 (2)	-0.1889 (4)	0.1860 (2)	0.0788 (10)
N1	0.6514 (3)	0.0765 (6)	0.2018 (3)	0.0829 (13)

supplementary materials

H1A	0.6824	0.1329	0.2472	0.099*
H1B	0.6858	0.0332	0.1678	0.099*
N2	0.8530 (2)	0.4986 (3)	0.0078 (2)	0.0392 (7)
C1	0.5415 (3)	0.4745 (5)	0.0290 (3)	0.0447 (9)
H1D	0.5320	0.4262	0.0803	0.054*
C2	0.6476 (3)	0.4871 (4)	0.0201 (3)	0.0412 (8)
C3	0.6745 (3)	0.5588 (5)	-0.0527 (3)	0.0457 (9)
H3	0.6241	0.6045	-0.0981	0.055*
C4	0.7758 (3)	0.5612 (5)	-0.0566 (3)	0.0436 (8)
H4	0.7920	0.6080	-0.1057	0.052*
C5	0.8270 (3)	0.4325 (5)	0.0778 (2)	0.0435 (8)
H5	0.8787	0.3896	0.1232	0.052*
C6	0.7273 (3)	0.4256 (5)	0.0855 (3)	0.0445 (8)
H6	0.7133	0.3787	0.1355	0.053*
C7	0.3369 (3)	0.0009 (4)	0.1491 (3)	0.0453 (9)
C8	0.3922 (3)	-0.0651 (5)	0.0940 (3)	0.0513 (10)
H8	0.3588	-0.1266	0.0451	0.062*
C9	0.4968 (3)	-0.0405 (6)	0.1107 (3)	0.0560 (10)
H9	0.5338	-0.0872	0.0737	0.067*
C10	0.5476 (3)	0.0555 (6)	0.1838 (3)	0.0554 (10)
C11	0.4897 (3)	0.1229 (5)	0.2368 (3)	0.0590 (11)
H11	0.5221	0.1879	0.2847	0.071*
C12	0.3864 (3)	0.0969 (5)	0.2209 (3)	0.0544 (10)
H12	0.3493	0.1431	0.2580	0.065*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0108 (3)	0.0324 (4)	0.0491 (4)	-0.0001 (2)	0.0086 (2)	0.0038 (3)
S1	0.0409 (6)	0.0450 (6)	0.0632 (7)	-0.0035 (4)	0.0003 (5)	0.0099 (4)
O1	0.0310 (14)	0.0484 (16)	0.088 (2)	-0.0015 (11)	-0.0011 (13)	0.0101 (14)
O2	0.145 (5)	0.218 (6)	0.127 (4)	0.059 (4)	0.053 (4)	0.037 (4)
O3	0.0460 (16)	0.0704 (18)	0.0687 (19)	-0.0153 (14)	0.0159 (14)	0.0019 (15)
O4	0.130 (3)	0.093 (3)	0.105 (3)	-0.007 (3)	0.056 (3)	0.009 (2)
O5	0.066 (2)	0.071 (2)	0.142 (3)	0.0020 (18)	0.030 (2)	-0.008 (2)
O6	0.059 (2)	0.131 (3)	0.068 (2)	-0.034 (2)	-0.0116 (17)	0.011 (2)
O7	0.0564 (19)	0.064 (2)	0.103 (2)	-0.0148 (15)	-0.0042 (17)	0.0334 (18)
N1	0.056 (2)	0.101 (3)	0.086 (3)	-0.032 (2)	0.006 (2)	-0.008 (3)
N2	0.0248 (14)	0.0424 (16)	0.0510 (17)	-0.0017 (11)	0.0105 (12)	0.0015 (13)
C1	0.0292 (18)	0.054 (2)	0.053 (2)	-0.0032 (15)	0.0133 (15)	0.0029 (17)
C2	0.0265 (17)	0.0450 (19)	0.054 (2)	-0.0030 (14)	0.0146 (15)	-0.0021 (15)
C3	0.0240 (17)	0.058 (2)	0.054 (2)	0.0029 (15)	0.0083 (15)	0.0109 (18)
C4	0.0272 (17)	0.053 (2)	0.051 (2)	0.0019 (15)	0.0106 (15)	0.0101 (17)
C5	0.0260 (17)	0.053 (2)	0.052 (2)	0.0009 (15)	0.0094 (15)	0.0081 (17)
C6	0.0273 (17)	0.056 (2)	0.050 (2)	-0.0014 (16)	0.0099 (15)	0.0059 (17)
C7	0.044 (2)	0.0371 (19)	0.048 (2)	-0.0065 (15)	-0.0004 (16)	0.0065 (15)
C8	0.052 (2)	0.050 (2)	0.047 (2)	-0.0099 (18)	0.0013 (17)	-0.0044 (17)
C9	0.055 (2)	0.064 (2)	0.047 (2)	-0.011 (2)	0.0091 (18)	0.0040 (18)

C10	0.047 (2)	0.055 (2)	0.057 (2)	-0.0178 (19)	0.0005 (19)	0.0111 (19)
C11	0.058 (2)	0.053 (2)	0.056 (2)	-0.0100 (19)	-0.004 (2)	-0.0114 (19)
C12	0.052 (2)	0.051 (2)	0.055 (2)	-0.0014 (18)	0.0025 (18)	-0.0072 (18)

Geometric parameters (Å, °)

Co1—O1 ⁱ	1.985 (3)	N2—C4	1.354 (5)
Co1—O1	1.985 (3)	C1—C1 ⁱⁱ	1.321 (8)
Co1—N2 ⁱ	2.009 (3)	C1—C2	1.469 (5)
Co1—N2 ⁱ	2.009 (3)	C1—H1D	0.9300
Co1—O3 ⁱⁱ	2.458 (3)	C2—C6	1.380 (5)
Co1—O3 ⁱⁱ	2.458 (3)	C2—C3	1.403 (5)
S1—O7	1.434 (3)	C3—C4	1.378 (5)
S1—O5	1.435 (4)	C3—H3	0.9300
S1—O6	1.460 (4)	C4—H4	0.9300
S1—C7	1.763 (4)	C5—C6	1.375 (5)
O1—H1W	0.8319	C5—H5	0.9300
O1—H2W	0.8250	C6—H6	0.9300
O2—H3W	0.8496	C7—C8	1.376 (6)
O2—H4W	1.0288	C7—C12	1.391 (5)
O3—H5W	0.8322	C8—C9	1.379 (6)
O3—H6W	0.8390	C8—H8	0.9300
O4—H7W	0.8721	C9—C10	1.411 (6)
O4—H8W	0.8349	C9—H9	0.9300
N1—C10	1.364 (6)	C10—C11	1.378 (7)
N1—H1A	0.8600	C11—C12	1.365 (6)
N1—H1B	0.8600	C11—H11	0.9300
N2—C5	1.341 (5)	C12—H12	0.9300
O1 ⁱ —Co1—O1	179.998 (1)	C6—C2—C1	120.0 (3)
O1 ⁱ —Co1—N2 ⁱ	89.33 (11)	C3—C2—C1	123.6 (3)
O1—Co1—N2 ⁱ	90.67 (11)	C4—C3—C2	119.7 (3)
O1 ⁱ —Co1—N2	90.67 (11)	C4—C3—H3	120.2
O1—Co1—N2	89.33 (11)	C2—C3—H3	120.2
N2 ⁱ —Co1—N2	180.0	N2—C4—C3	123.1 (3)
O1—Co1—N2	89.33 (11)	N2—C4—H4	118.4
N2 ⁱ —Co1—N2	180.0	C3—C4—H4	118.4
O3 ⁱⁱ —Co1—O3 ⁱⁱ	180.0	N2—C5—C6	122.8 (3)
O3 ⁱⁱ —Co1—N2 ⁱ	88.75 (11)	N2—C5—H5	118.6
O3—Co1—N2 ⁱ	172.76 (9)	C6—C5—H5	118.6
O7—S1—O5	113.6 (3)	C5—C6—C2	121.1 (4)
O7—S1—O6	111.4 (2)	C5—C6—H6	119.5
O5—S1—O6	110.0 (3)	C2—C6—H6	119.5
O7—S1—C7	107.27 (18)	C8—C7—C12	119.8 (4)
O5—S1—C7	107.6 (2)	C8—C7—S1	120.4 (3)
O6—S1—C7	106.7 (2)	C12—C7—S1	119.7 (3)
Co1—O1—H1W	119.9	C7—C8—C9	120.5 (4)

supplementary materials

Co1—O1—H2W	128.3	C7—C8—H8	119.8
H1W—O1—H2W	111.5	C9—C8—H8	119.8
H3W—O2—H4W	129.1	C8—C9—C10	120.0 (4)
H5W—O3—H6W	109.4	C8—C9—H9	120.0
H7W—O4—H8W	107.9	C10—C9—H9	120.0
C10—N1—H1A	120.0	N1—C10—C11	121.7 (4)
C10—N1—H1B	120.0	N1—C10—C9	120.1 (5)
H1A—N1—H1B	120.0	C11—C10—C9	118.2 (4)
C5—N2—C4	116.9 (3)	C12—C11—C10	121.9 (4)
C5—N2—Co1	120.6 (2)	C12—C11—H11	119.0
C4—N2—Co1	122.5 (2)	C10—C11—H11	119.0
C1 ⁱⁱ —C1—C2	126.1 (5)	C11—C12—C7	119.6 (4)
C1 ⁱⁱ —C1—H1D	116.9	C11—C12—H12	120.2
C2—C1—H1D	116.9	C7—C12—H12	120.2
C6—C2—C3	116.4 (3)		
O1 ⁱ —Co1—N2—C5	-126.6 (3)	C1—C2—C6—C5	178.6 (4)
O1—Co1—N2—C5	53.4 (3)	O7—S1—C7—C8	92.7 (4)
N2 ⁱ —Co1—N2—C5	13 (10)	O5—S1—C7—C8	-144.7 (4)
O1 ⁱ —Co1—N2—C4	54.1 (3)	O6—S1—C7—C8	-26.8 (4)
O1—Co1—N2—C4	-125.9 (3)	O7—S1—C7—C12	-83.6 (4)
N2 ⁱ —Co1—N2—C4	-166 (10)	O5—S1—C7—C12	38.9 (4)
C1 ⁱⁱ —C1—C2—C6	-178.8 (5)	O6—S1—C7—C12	156.8 (3)
C1 ⁱⁱ —C1—C2—C3	0.9 (8)	C12—C7—C8—C9	1.8 (6)
C6—C2—C3—C4	1.4 (6)	S1—C7—C8—C9	-174.6 (3)
C1—C2—C3—C4	-178.3 (4)	C7—C8—C9—C10	-1.2 (6)
C5—N2—C4—C3	-0.2 (6)	C8—C9—C10—N1	178.3 (4)
Co1—N2—C4—C3	179.0 (3)	C8—C9—C10—C11	-0.2 (6)
C2—C3—C4—N2	-0.8 (6)	N1—C10—C11—C12	-177.4 (4)
C4—N2—C5—C6	0.6 (6)	C9—C10—C11—C12	1.0 (7)
Co1—N2—C5—C6	-178.7 (3)	C10—C11—C12—C7	-0.5 (7)
N2—C5—C6—C2	0.1 (6)	C8—C7—C12—C11	-0.9 (6)
C3—C2—C6—C5	-1.1 (6)	S1—C7—C12—C11	175.5 (3)

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

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1W \cdots O6 ⁱⁱⁱ	0.83	1.86	2.674 (4)	164
O1—H2W \cdots O5 ^{iv}	0.83	1.99	2.806 (5)	173
O2—H3W \cdots O4 ^v	0.85	1.92	2.771 (7)	179
O2—H4W \cdots N1 ^{vi}	1.03	2.20	2.841 (8)	118
O3—H5W \cdots O7 ^{vi}	0.83	1.92	2.743 (4)	168
O3—H6W \cdots O4	0.84	2.08	2.800 (5)	143
O4—H7W \cdots O5	0.87	2.08	2.714 (6)	129
O4—H8W \cdots O3 ^{vii}	0.83	2.21	2.886 (5)	139
N1—H1A \cdots O7 ^v	0.86	2.21	2.997 (5)	152

N1—H1B \cdots O2^{viii}

0.86

1.98

2.841 (8)

175

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

Fig. 1

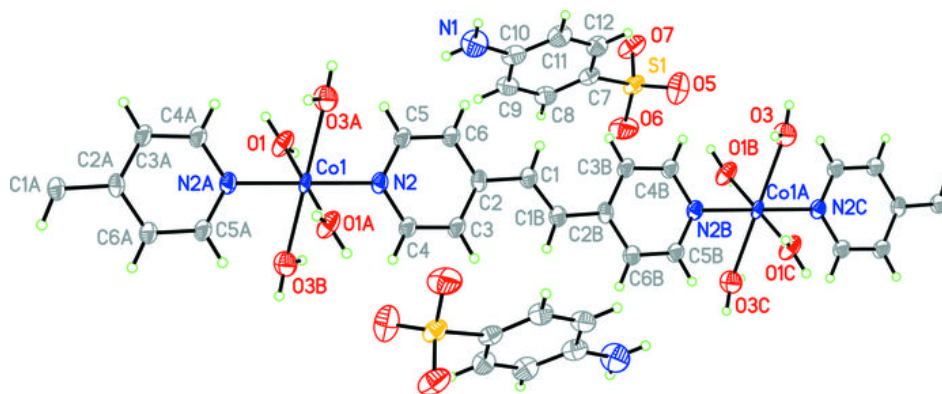


Fig. 2

