Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquacobalt(II) 4-hydroxybenzenesulfonate dihydrate

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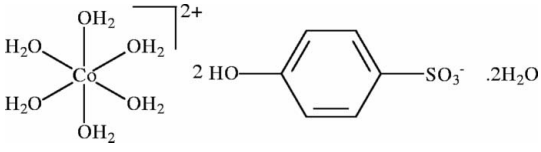
Received 8 August 2007; accepted 18 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.001 Å; disorder in main residue; R factor = 0.034; wR factor = 0.090; data-to-parameter ratio = 12.2.

In the title compound, $[Co(H_2O)_6](C_6H_6O_4S)_2{\cdot}2H_2O$, the Co^{II} ion lies on an inversion center and is octahedrally coordinated by six water molecules. Two independent water molecules in the $[Co(H_2O)_6]^{2+}$ cation are disordered over two sites, with half occupancy for each site. The 4-hydroxybenzenesulfonate (L^-) anion does not coordinate to the cobalt ion but rather acts as a counter-ion. The asymmetric unit is completed by an uncoordinated water molecule. The crystal structure is composed of alternating layers of $[Co(H_2O)_6]^{2+}$ cations and L^- anions, with the lattice water molecules located in channels along the a direction. The $[Co(H_2O)_6]^{2+}$ cations, L^- anions and solvent water molecules are connected through a complex pattern of hydrogen-bonding interactions.

Related literature

For related literature, see: Ma *et al.* (2003); Sharma *et al.* (2006).



Experimental

Crystal data

$[Co(H_2O)_6](C_6H_6O_4S)_2{\cdot}2H_2O$
M_r = 549.38
Monoclinic, $P2_1/c$
a = 5.843 (2) Å
b = 7.224 (3) Å
c = 25.459 (9) Å
β = 94.837 (1)°
V = 1070.8 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.07 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
T_{min} = 0.673, T_{max} = 0.814
7850 measured reflections
2427 independent reflections
2051 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.090
S = 1.02
2427 reflections
199 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O1	0.845 (4)	1.928 (4)	2.7667 (11)	171.4 (4)
O1W—H1WB···O4^{i}	0.846 (4)	1.927 (4)	2.7609 (9)	168.0 (5)
O2WA—H2WA···O3^{ii}	0.846 (4)	2.127 (6)	2.8625 (12)	145.2 (8)
O2WA—H2WB···O4W	0.844 (4)	1.757 (4)	2.5967 (12)	172.7 (8)
O3WA—H3WB···O4W^{iii}	0.843 (4)	1.806 (4)	2.6398 (14)	169.6 (5)
O3WB—H3WC···O2	0.847 (4)	1.886 (5)	2.7193 (13)	167.9 (5)
O4—H4···O3^{iv}	0.840 (8)	1.916 (7)	2.7543 (10)	175.6 (8)
O4W—H4WA···O2WB^{v}	0.840 (4)	1.785 (4)	2.6227 (13)	175.6 (4)
O4W—H4WA···O2WA^{v}	0.840 (4)	2.040 (5)	2.8436 (12)	160.1 (6)
O4W—H4WB···O2^{vi}	0.844 (4)	1.986 (5)	2.8244 (10)	171.9 (6)
O2WB—H2WD···O3^{ii}	0.844 (4)	1.941 (4)	2.7833 (13)	175.1 (6)
O3WB—H3WD···O3WB^{vii}	0.845 (4)	1.945 (8)	2.6474 (19)	139.8 (11)

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

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors gratefully acknowledge financial support by the NSF of Fujian Province (grant No. E0510031).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2133).

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supplementary materials

Acta Cryst. (2007). E**63**, m2597 [**doi:10.1107/S1600536807045904**]

Hexaaquacobalt(II) 4-hydroxybenzenesulfonate dihydrate

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Comment

The crystal structures of $[Co(H_2O)_6]^{2+}$ with 3-carboxy-4-hydroxybenzenesulfonate as counter-ion (Ma *et al.*, 2003) and $[Co(NH_3)_6]^{3+}$ with 4-hydroxybenzenesulfonate (Sharma *et al.*, 2006) have been reported. We have now characterized the title compound, $[Co(H_2O)_6]^{2+}$ 4-hydroxybenzenesulfonate as a dihydrate, for which we report the synthesis and the crystal structure (Scheme, I).

As shown in Fig. 1, the asymmetric unit of (I) consists of one L^- anion, one-half hexaaquacobalt(II) cation as well as one lattice water molecule. The Co^{II} ion is located on an inversion center, and all other atoms are in general positions. The Co1 atom displays a slightly distorted octahedral environment, coordinated by six water molecules with the Co—O bond lengths ranging from 2.0574 (11) to 2.1032 (10) Å, similar to those found in the above cited hexaaquacobalt compound (Ma *et al.*, 2003). The 4-hydroxybenzenesulfonate anion acts as a counter-ion, with normal bond lengths (Sharma *et al.*, 2006).

The crystal structure of (I) can be regarded as a H-bonding 3-D framework, composed of alternating layers of $[Co(H_2O)_6]^{2+}$ cations and L^- sulfonate anions, with the lattice water molecules located in the channels along the [100] direction (Fig. 2). Within the sulfonate layers, the L^- anions are connected to form a zigzag chain along the [010] direction through the inter-molecular O3···O4 H-bonds, with O3···O4 separation of 2.7543 (10) Å. The chains are bridged by hexaaquacobalt(II) cations through the O1W···O4 and O2W···O3 H-bonds [O1W···O4 = 2.7609 (9); O2WA···O3 = 2.8625 (12) Å] to form the 3-D framework. The O4W lattice water molecules H-bond to the O2W and O3W coordinated water molecules, and O1 and O2 atoms of L^- anions, to further stabilize the crystal structure.

Experimental

A mixture of H*L* (549 mg, 1 mmol) and $CoCO_3$ (60 mg, 0.5 mmol) was added into 15 ml water and stirred at room temperature for 1 h. Red crystals of (I) suitable for single-crystal X-ray diffraction analysis were obtained after leaving the solution to stand at room temperature for several days (56% yield based on $CoCO_3$).

Refinement

Water molecules O2W and O3W were found to be disordered over two positions, and refined with site occupancies 1/2 for O2WA, O2WB, O3WA and O3WB. Water H atoms and hydroxyl H4 atom were located in a difference Fourier map and refined with a regularized geometry, the O—H and H···H distances being restrained to 0.85 (1) and 1.34 (2) Å, respectively, and with U_{iso}(H) = 1.5U_{eq}(carrier O). The C-bonded H atoms were placed in idealized positions and allowed to ride on their respective parent atoms, with C—H distances constrained to 0.93 Å, and U_{iso}(H) = 1.2U_{eq}(carrier C).

Figures

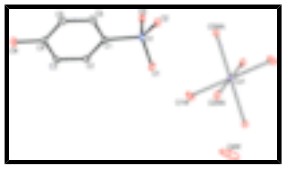

Fig. 1. *ORTEP* drawing with 30% probability thermal ellipsoids. Hydrogen atoms are omitted for clarity, as disordered 'B' sites for O2W and O3W.

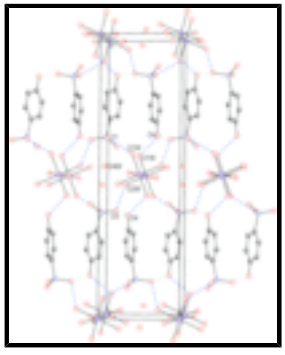

Fig. 2. 3-D packing diagram viewed along the [100] direction with the dashed lines representing the O···O contacts for H-bonds. The H-bonds around the O4W atoms are omitted for clarity. All H atoms and disordered O atoms have been omitted.

Hexaaquacobalt(II) 4-hydroxybenzenesulfonate dihydrate

Crystal data

$[Co(H_2O)_6](C_6H_6O_4S)_2{\cdot}2H_2O$	F_{000} = 570
M_r = 549.38	D_x = 1.704 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5365 reflections
a = 5.843 (2) Å	θ = 2.3–27.5º
b = 7.224 (3) Å	μ = 1.07 mm^{-1}
c = 25.459 (9) Å	T = 293 (2) K
β = 94.8370 (10)º	Prism, red
V = 1070.8 (7) Å^3	0.40 × 0.30 × 0.20 mm
Z = 2	

Data collection

Rigaku Mercury CCD diffractometer	2427 independent reflections
Radiation source: rotating anode generator	2051 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.9º
Absorption correction: multi-scan (CrystalClear; Rigaku, 2002)	h = −7→7
T_{min} = 0.673, T_{max} = 0.814	k = −7→9
7850 measured reflections	l = −32→32

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.090$	$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 0.0596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.009$
2427 reflections	$\Delta\rho_{max} = 0.75$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.57$ e Å^{-3}
18 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.0000	1.0000	1.0000	0.01164 (3)	
O1W	−0.14944 (9)	0.91860 (7)	0.926835 (19)	0.03708 (16)	
H1WA	−0.1214 (11)	0.8278 (5)	0.90746 (18)	0.056*	
H1WB	−0.2298 (8)	0.9937 (5)	0.9076 (2)	0.056*	
O2WA	0.03598 (15)	1.26230 (12)	0.96743 (3)	0.0185 (2)	0.50
H2WA	0.0732 (10)	1.2458 (13)	0.93638 (13)	0.028*	0.50
H2WB	−0.0793 (6)	1.3331 (7)	0.9643 (4)	0.028*	0.50
O2WB	0.16007 (14)	1.23240 (13)	0.97331 (3)	0.0186 (2)	0.50
H2WC	0.2844 (6)	1.2132 (14)	0.99136 (19)	0.028*	0.50
H2WD	0.1907 (13)	1.2767 (10)	0.94403 (13)	0.028*	0.50
O3WA	0.29704 (14)	0.84098 (11)	0.99253 (3)	0.0149 (2)	0.50
H3WA	0.4229 (6)	0.8969 (7)	0.9974 (4)	0.022*	0.50
H3WB	0.3033 (15)	0.7408 (5)	1.0096 (2)	0.022*	0.50
O3WB	0.31335 (15)	0.92872 (14)	0.97466 (4)	0.0284 (3)	0.50
H3WC	0.3241 (16)	0.8382 (5)	0.95388 (19)	0.043*	0.50
H3WD	0.4383 (6)	0.9879 (7)	0.9752 (5)	0.043*	0.50
S1	0.19699 (3)	0.55915 (2)	0.865589 (6)	0.01538 (4)	
O1	−0.04225 (7)	0.60173 (6)	0.873004 (17)	0.01916 (12)	
O2	0.36032 (8)	0.67549 (6)	0.897272 (17)	0.02085 (12)	
O3	0.24658 (8)	0.36089 (6)	0.873832 (16)	0.02103 (12)	
O4	0.35295 (8)	0.67622 (7)	0.642301 (17)	0.02172 (12)	
H4	0.4713 (12)	0.7379 (11)	0.6375 (3)	0.033*	
C1	0.23829 (10)	0.60609 (8)	0.79905 (2)	0.01407 (15)	
C2	0.07181 (11)	0.55567 (9)	0.75978 (2)	0.01730 (16)	
H2A	−0.0662	0.5051	0.7686	0.021*	
C3	0.11117 (11)	0.58080 (9)	0.70694 (2)	0.01842 (17)	
H3A	−0.0005	0.5486	0.6803	0.022*	
C4	0.32027 (11)	0.65489 (8)	0.69470 (2)	0.01541 (15)	

C5	0.48649 (11)	0.70370 (9)	0.73403 (2)	0.01702 (16)
H5A	0.6251	0.7532	0.7252	0.020*
C6	0.44820 (11)	0.67946 (8)	0.78660 (2)	0.01726 (16)
H6A	0.5604	0.7115	0.8131	0.021*
O4W	−0.30549 (11)	1.49300 (7)	0.96527 (3)	0.0577 (2)
H4WA	−0.2574 (11)	1.5769 (6)	0.98621 (17)	0.087*
H4WB	−0.4113 (7)	1.5371 (9)	0.94433 (18)	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01328 (5)	0.01141 (5)	0.01034 (5)	0.00068 (4)	0.00169 (4)	0.00001 (4)
O1W	0.0524 (3)	0.0345 (3)	0.0210 (2)	0.0267 (2)	−0.0169 (2)	−0.0160 (2)
O2WA	0.0286 (4)	0.0132 (4)	0.0146 (4)	0.0043 (4)	0.0066 (3)	0.0016 (3)
O2WB	0.0186 (4)	0.0219 (4)	0.0154 (4)	−0.0024 (4)	0.0016 (3)	0.0043 (4)
O3WA	0.0150 (4)	0.0159 (4)	0.0139 (4)	0.0008 (3)	0.0016 (3)	−0.0006 (3)
O3WB	0.0135 (4)	0.0342 (5)	0.0379 (5)	−0.0018 (4)	0.0050 (4)	−0.0190 (5)
S1	0.02079 (7)	0.01546 (7)	0.01016 (6)	0.00447 (6)	0.00284 (6)	−0.00033 (6)
O1	0.0213 (2)	0.0205 (2)	0.01664 (19)	0.00334 (19)	0.00750 (17)	−0.00017 (18)
O2	0.0234 (2)	0.0258 (2)	0.01320 (19)	0.0017 (2)	0.00036 (18)	−0.00523 (18)
O3	0.0315 (2)	0.0187 (2)	0.01380 (19)	0.0059 (2)	0.00675 (18)	0.00249 (18)
O4	0.0250 (2)	0.0289 (2)	0.01156 (19)	−0.0076 (2)	0.00335 (18)	0.00095 (18)
C1	0.0184 (3)	0.0134 (3)	0.0106 (2)	0.0033 (2)	0.0022 (2)	−0.0001 (2)
C2	0.0147 (3)	0.0210 (3)	0.0165 (3)	0.0015 (3)	0.0033 (2)	0.0027 (2)
C3	0.0163 (3)	0.0252 (3)	0.0133 (3)	−0.0005 (3)	−0.0015 (2)	0.0009 (3)
C4	0.0209 (3)	0.0144 (3)	0.0114 (2)	0.0020 (3)	0.0041 (2)	0.0006 (2)
C5	0.0171 (3)	0.0155 (3)	0.0186 (3)	−0.0037 (3)	0.0025 (2)	0.0023 (2)
C6	0.0213 (3)	0.0135 (3)	0.0164 (3)	−0.0029 (3)	−0.0022 (3)	−0.0006 (2)
O4W	0.0375 (3)	0.0214 (3)	0.1061 (5)	−0.0087 (2)	−0.0417 (3)	0.0174 (3)

Geometric parameters (Å, °)

Co1—O3WB	2.0574 (11)	O3WB—H3WD	0.845 (4)
Co1—O3WB^{i}	2.0574 (11)	S1—O1	1.4591 (7)
Co1—O2WB	2.0645 (11)	S1—O2	1.4621 (6)
Co1—O2WB^{i}	2.0645 (11)	S1—O3	1.4728 (8)
Co1—O1W	2.0745 (8)	S1—C1	1.7640 (8)
Co1—O1W^{i}	2.0745 (8)	O4—C4	1.3721 (9)
Co1—O2WA	2.0861 (11)	O4—H4	0.840 (8)
Co1—O2WA^{i}	2.0861 (11)	C1—C2	1.3836 (9)
Co1—O3WA	2.1032 (10)	C1—C6	1.3969 (10)
Co1—O3WA^{i}	2.1032 (10)	C2—C3	1.3956 (10)
O1W—H1WA	0.845 (4)	C2—H2A	0.9300
O1W—H1WB	0.846 (4)	C3—C4	1.3931 (10)
O2WA—H2WA	0.846 (4)	C3—H3A	0.9300
O2WA—H2WB	0.844 (4)	C4—C5	1.3806 (9)
O2WB—H2WC	0.838 (4)	C5—C6	1.3868 (10)
O2WB—H2WD	0.844 (4)	C5—H5A	0.9300

O3WA—H3WA	0.839 (4)	C6—H6A	0.9300
O3WA—H3WB	0.843 (4)	O4W—H4WA	0.840 (4)
O3WB—H3WC	0.847 (4)	O4W—H4WB	0.844 (4)
O3WB—Co1—O3WB^{i}	180.000 (1)	O2WA^{i}—Co1—O3WA^{i}	110.40 (4)
O3WB—Co1—O2WB	70.15 (4)	O3WA—Co1—O3WA^{i}	180.00 (4)
O3WB^{i}—Co1—O2WB	109.85 (4)	Co1—O1W—H1WA	131.0 (4)
O3WB—Co1—O2WB^{i}	109.85 (4)	Co1—O1W—H1WB	120.6 (3)
O3WB^{i}—Co1—O2WB^{i}	70.15 (4)	H1WA—O1W—H1WB	106.6 (5)
O2WB—Co1—O2WB^{i}	180.0	Co1—O2WA—H2WA	106.6 (6)
O3WB—Co1—O1W	88.04 (4)	Co1—O2WA—H2WB	118.8 (4)
O3WB^{i}—Co1—O1W	91.96 (4)	H2WA—O2WA—H2WB	105.2 (7)
O2WB—Co1—O1W	95.91 (3)	Co1—O2WB—H2WC	94.6 (6)
O2WB^{i}—Co1—O1W	84.09 (3)	Co1—O2WB—H2WD	137.3 (5)
O3WB—Co1—O1W^{i}	91.96 (4)	H2WC—O2WB—H2WD	108.0 (7)
O3WB^{i}—Co1—O1W^{i}	88.04 (4)	Co1—O3WA—H3WA	116.3 (4)
O2WB—Co1—O1W^{i}	84.09 (3)	Co1—O3WA—H3WB	115.0 (6)
O2WB^{i}—Co1—O1W^{i}	95.91 (3)	H3WA—O3WA—H3WB	109.7 (8)
O1W—Co1—O1W^{i}	180.0	Co1—O3WB—H3WC	120.3 (7)
O3WB—Co1—O2WA	88.88 (4)	Co1—O3WB—H3WD	131.2 (5)
O3WB^{i}—Co1—O2WA	91.12 (4)	H3WC—O3WB—H3WD	107.0 (9)
O2WB—Co1—O2WA	21.07 (3)	O1—S1—O2	113.29 (3)
O2WB^{i}—Co1—O2WA	158.93 (3)	O1—S1—O3	111.45 (3)
O1W—Co1—O2WA	87.10 (3)	O2—S1—O3	111.65 (3)
O1W^{i}—Co1—O2WA	92.90 (3)	O1—S1—C1	107.09 (3)
O3WB—Co1—O2WA^{i}	91.12 (4)	O2—S1—C1	106.47 (3)
O3WB^{i}—Co1—O2WA^{i}	88.88 (4)	O3—S1—C1	106.41 (3)
O2WB—Co1—O2WA^{i}	158.93 (3)	C4—O4—H4	112.6 (5)
O2WB^{i}—Co1—O2WA^{i}	21.07 (3)	C2—C1—C6	120.88 (6)
O1W—Co1—O2WA^{i}	92.90 (3)	C2—C1—S1	119.90 (5)
O1W^{i}—Co1—O2WA^{i}	87.10 (3)	C6—C1—S1	118.99 (4)
O2WA—Co1—O2WA^{i}	180.000 (1)	C1—C2—C3	119.96 (6)
O3WB—Co1—O3WA	21.88 (4)	C1—C2—H2A	120.0
O3WB^{i}—Co1—O3WA	158.12 (4)	C3—C2—H2A	120.0
O2WB—Co1—O3WA	90.81 (4)	C4—C3—C2	118.98 (6)
O2WB^{i}—Co1—O3WA	89.19 (4)	C4—C3—H3A	120.5
O1W—Co1—O3WA	92.99 (3)	C2—C3—H3A	120.5
O1W^{i}—Co1—O3WA	87.01 (3)	O4—C4—C5	121.96 (6)
O2WA—Co1—O3WA	110.40 (4)	O4—C4—C3	117.21 (5)
O2WA^{i}—Co1—O3WA	69.60 (4)	C5—C4—C3	120.83 (6)
O3WB—Co1—O3WA^{i}	158.12 (4)	C4—C5—C6	120.46 (6)
O3WB^{i}—Co1—O3WA^{i}	21.88 (4)	C4—C5—H5A	119.8
O2WB—Co1—O3WA^{i}	89.19 (4)	C6—C5—H5A	119.8

O2WB^{i}—Co1—O3WA^{i}	90.81 (4)	C5—C6—C1	118.89 (5)
O1W—Co1—O3WA^{i}	87.01 (3)	C5—C6—H6A	120.6
O1W^{i}—Co1—O3WA^{i}	92.99 (3)	C1—C6—H6A	120.6
O2WA—Co1—O3WA^{i}	69.60 (4)	H4WA—O4W—H4WB	108.5 (6)
O1—S1—C1—C2	−41.52 (6)	C1—C2—C3—C4	0.72 (10)
O2—S1—C1—C2	−163.00 (5)	C2—C3—C4—O4	179.56 (6)
O3—S1—C1—C2	77.78 (6)	C2—C3—C4—C5	−0.24 (10)
O1—S1—C1—C6	143.96 (5)	O4—C4—C5—C6	−179.69 (6)
O2—S1—C1—C6	22.48 (6)	C3—C4—C5—C6	0.10 (10)
O3—S1—C1—C6	−96.74 (6)	C4—C5—C6—C1	−0.42 (9)
C6—C1—C2—C3	−1.07 (10)	C2—C1—C6—C5	0.91 (9)
S1—C1—C2—C3	−175.48 (5)	S1—C1—C6—C5	175.37 (5)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O1	0.845 (4)	1.928 (4)	2.7667 (11)	171.4 (4)
O1W—H1WB···O4^{ii}	0.846 (4)	1.927 (4)	2.7609 (9)	168.0 (5)
O2WA—H2WA···O3^{iii}	0.846 (4)	2.127 (6)	2.8625 (12)	145.2 (8)
O2WA—H2WB···O4W	0.844 (4)	1.757 (4)	2.5967 (12)	172.7 (8)
O3WA—H3WB···O4W^{i}	0.843 (4)	1.806 (4)	2.6398 (14)	169.6 (5)
O3WB—H3WC···O2	0.847 (4)	1.886 (5)	2.7193 (13)	167.9 (5)
O4—H4···O3^{iv}	0.840 (8)	1.916 (7)	2.7543 (10)	175.6 (8)
O4W—H4WA···O2WB^{v}	0.840 (4)	1.785 (4)	2.6227 (13)	175.6 (4)
O4W—H4WA···O2WA^{v}	0.840 (4)	2.040 (5)	2.8436 (12)	160.1 (6)
O4W—H4WB···O2^{vi}	0.844 (4)	1.986 (5)	2.8244 (10)	171.9 (6)
O2WB—H2WD···O3^{iii}	0.844 (4)	1.941 (4)	2.7833 (13)	175.1 (6)
O3WB—H3WD···O3WB^{vii}	0.845 (4)	1.945 (8)	2.6474 (19)	139.8 (11)

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

Fig. 1

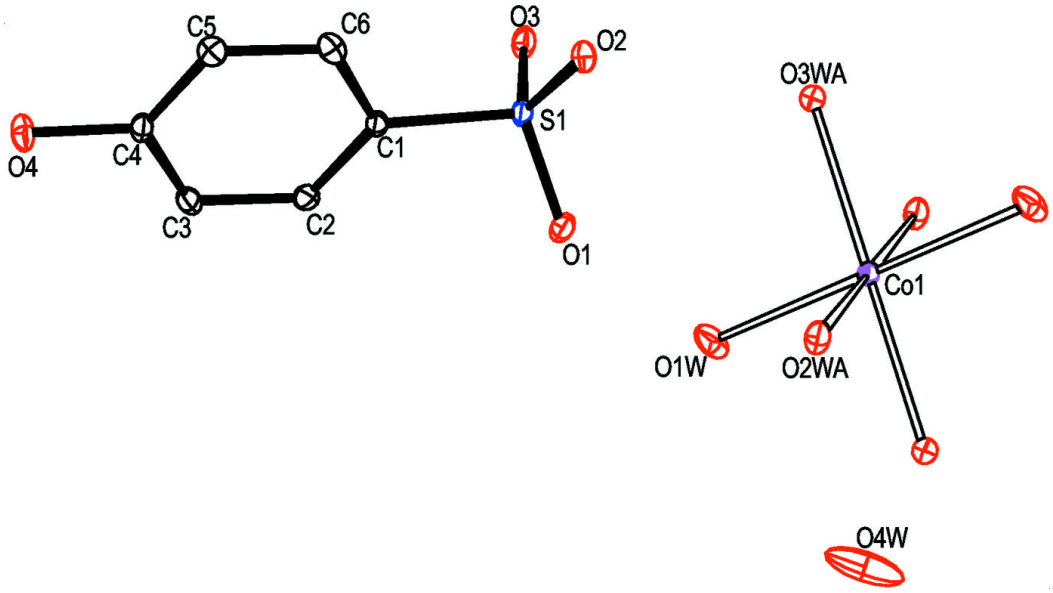

Fig. 2