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Hexaaquacobalt(II) bis(5-benzoyl-2-methoxy-4-oxidobenzenesulfonato-κ^2O,O')bis(pyridine-κN)cobaltate(II) tetrahydrate

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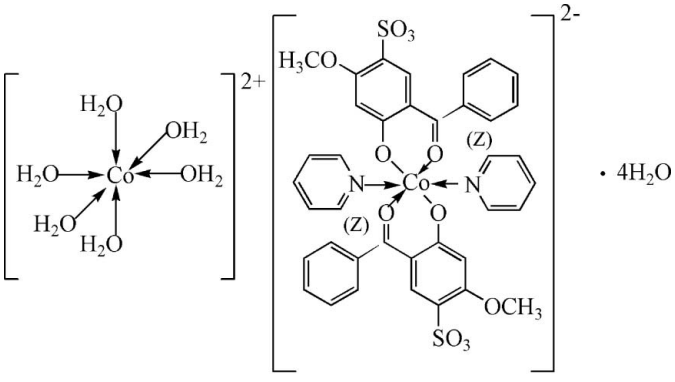
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.103; data-to-parameter ratio = 12.6.

The ionic title compound, $[Co(H_2O)_6][Co(C_{14}H_{10}O_6S)_2(C_5H_5N)_2]\cdot 4H_2O$, consists of octahedrally coordinated $[Co(H_2O)_6]^{2+}$ and $[Co(C_{14}H_{10}O_6S)_2(C_5H_5N)_2]^{2-}$ ions along with four solvent water molecules. Both ions lie on inversion sites. In the anion, two 5-benzoyl-2-methoxy-4-oxidobenzenesulfonate ligands chelate the Co atom; the pyridine ligands occupy *trans* positions. A three-dimensional network structure results from hydrogen bonding involving the aqua ligands, sulfonate groups and solvent water molecules.

Related literature

For related literature, see: Russell & Ward (1996); Shiu *et al.* (2004).



(I)

Experimental

Crystal data

$[Co(H_2O)_6][Co(C_{14}H_{10}O_6S)_2(C_5H_5N)_2]\cdot 4H_2O$
M_r = 1068.78
Monoclinic, $P2_1/c$
a = 20.373 (3) Å
b = 7.1181 (9) Å
c = 17.497 (3) Å
β = 111.514 (4)°
V = 2360.5 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 193 (2) K
0.32 × 0.21 × 0.06 mm

Data collection

Rigaku Mercury diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.768, T_{max} = 0.950
22147 measured reflections
4319 independent reflections
3462 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.103
S = 1.14
4319 reflections
343 parameters
13 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.005 (2)	Co2—O8	2.037 (3)
Co1—O2	2.080 (2)	Co2—O9	2.075 (3)
Co1—N1	2.173 (3)	C7—O2	1.254 (4)
Co2—O7	2.113 (2)		
O1^i—Co1—O1	180	N1^i—Co1—N1	180
O1—Co1—O2	86.87 (9)	O7—Co2—O8	87.83 (10)
O1—Co1—N1^i	90.28 (9)	O7—Co2—O9	87.25 (10)
O1—Co1—N1	89.72 (9)	O8—Co2—O9	90.10 (12)
O2—Co1—N1	93.47 (9)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O6^{ii}	0.82 (3)	2.059 (16)	2.855 (3)	164 (4)
O7—H7B···O5^{iii}	0.82 (3)	1.98 (3)	2.788 (3)	172 (4)
O8—H8A···O11	0.829 (10)	1.827 (13)	2.651 (4)	173 (5)
O8—H8B···O4^{iv}	0.82 (3)	1.99 (3)	2.821 (3)	178 (4)
O9—H9A···O10	0.83 (3)	1.93 (4)	2.753 (4)	170 (5)
O9—H9B···O4^{v}	0.83 (4)	1.95 (5)	2.763 (3)	169 (5)
O10—H10A···O5	0.82 (3)	2.04 (2)	2.813 (3)	158 (4)
O10—H10B···O6^{ii}	0.82 (3)	2.019 (16)	2.822 (3)	166 (5)
O11—H11A···O10^{vi}	0.82 (3)	2.03 (3)	2.853 (5)	177 (5)
O11—H11B···O6	0.82 (5)	2.09 (5)	2.899 (4)	166 (4)

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

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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2003223) and the program of NCET (NCET-04–0836) of the Chinese Ministry of Education.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2246).

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supplementary materials

Acta Cryst. (2007). E**63**, m1397-m1398 [**doi:10.1107/S1600536807017746**]

Hexaaquacobalt(II) bis(5-benzoyl-2-methoxy-4-oxidobenzenesulfonato-κ^2O,O')bis(pyridine-κN)cobaltate(II) tetrahydrate

Y.-C. Liu, T. Yuan, Z.-F. Chen, H. Liang and Y. Zhang

Comment

Although the crystal structure of guanidinium 5-benzoyl-4- hydroxybenznesulfonate (sulisobenzone) methanol solvate $[C(NH_2)_3^+\cdot(C_{14}H_{11}O_3)SO_3^-.\ CH_3OH]$ (II) was first reported by Russell and Ward in 1996), there is no study on a metal derivative of the aion.

The title compound (I) consists of $[Co(H_2O)_6]^{2+}$, $[Co(C_5H_5N)_2(C_{14}H_{10}O_6S)_2Co]^{2-}$ and four lattice water molecules; the composition is related to $[Co(H_2O)_6][Co(C_7H_3NO_4)_2]\cdot 2H_2O$ (III) (Shiu *et al.*, 2004). The cation and anion lie on inversion sites. In (I), two cobalt atoms are octahedrally coordinated, with Co1 surrounded by two N atoms of two pyridine ligands, and four O atoms of two sulisobenzone ligands; the Co2 is ligated by six O atoms of water molecules (Fig. 1). The Co1—O bond lengths are shorter than those of (III). The geometric parameters of 5-benzoyl-4-hydroxy-2-methoxybenzenesulfonate are comparable with those of (II) (Russell & Ward, 1996). The methoxyl group is oriented away from the sulfonate group so that the sulfonate group is sterically accessible for hydrogen bonding with cation and the lattice water donors.

The packing is governed by hydrogen bonds involving the aqua ligands, sulfonate groups and lattice water molecules (Fig.2 and Table 2) to give rise to a three-dimensional network motif.

Experimental

Cobalt nitrate hydrate (0.2 mmol), 5-benzoyl-4-hydroxy-2-mehtoxybenzenesulfonic acid (0.2 mmol), ethanol (2 ml), H_2O (2 ml) and pyridine (0.2 ml), were placed in a Pyrex tube (*ca* 20 cm). The tube was frozen with liquid N_2, evacuated under vacuum, sealed with a torch and heated at 353 K for two days to give orange-red plate crystals (I), with a yield of 85%.

Refinement

H atoms on C atoms were positioned geometrically and were treated as riding and refined isotropically, with C—H distances of 0.95 Å and $U_{iso}(H) = 1.2_{eq}(C)$. H atoms bound to water O were located in a difference map and refined isotropically with restraint of O—H = 0.82 Å.

Figures

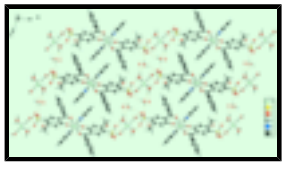

Fig. 1. The structure of compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.

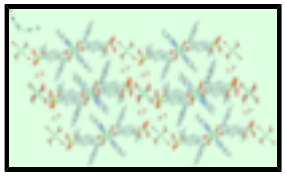

Fig. 2. The packing diagram for compound (I) (dashed lines indicate hydrogen bonds).

Hexaaquacobalt(II) bis(5-benzoyl-2-methoxy-4-oxidobenzenesulfonato- κ^2O,O')bis(pyridine-κN)cobaltate(II) tetrahydrate

Crystal data

$[Co(H_2O)_6][Co(C_{14}H_{10}O_6S)_2(C_5H_5N)_2]\cdot 4H_2O$	$F_{000} = 1108$
$M_r = 1068.78$	$D_x = 1.504$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
Hall symbol: -p 2ybc	Cell parameters from 6940 reflections
$a = 20.373$ (3) Å	$\theta = 3.0$–$25.3°$
$b = 7.1181$ (9) Å	$\mu = 0.87$ mm^{-1}
$c = 17.497$ (3) Å	$T = 193$ (2) K
$\beta = 111.514$ (4)°	Platelet, orange
$V = 2360.5$ (6) Å^3	0.32 × 0.21 × 0.06 mm
$Z = 2$	

Data collection

Rigaku Mercury diffractometer	4319 independent reflections
Radiation source: fine-focus sealed tube	3462 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.058$
Detector resolution: 7.31 pixels mm^{-1}	$\theta_{max} = 25.3°$
$T = 193(2)$ K	$\theta_{min} = 3.1°$
ω scans	$h = -23\rightarrow24$
Absorption correction: multi-scan (Jacobson, 1998)	$k = -8\rightarrow8$
$T_{min} = 0.768$, $T_{max} = 0.950$	$l = -20\rightarrow21$
22147 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.103$	$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 2.5747P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{max} < 0.001$

4319 reflections	$\Delta\rho_{max} = 0.68$ e Å^{-3}
343 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
13 restraints	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.5000	0.02003 (16)
Co2	0.0000	0.5000	0.0000	0.02028 (16)
S1	0.12304 (4)	0.49322 (11)	0.41394 (4)	0.01826 (18)
O1	0.42104 (11)	0.6814 (3)	0.48558 (13)	0.0250 (5)
O2	0.42779 (11)	0.3420 (3)	0.40685 (13)	0.0244 (5)
O3	0.19800 (11)	0.8273 (3)	0.49728 (14)	0.0281 (5)
O4	0.11333 (11)	0.4893 (3)	0.49252 (12)	0.0241 (5)
O5	0.11111 (11)	0.3096 (3)	0.37406 (13)	0.0248 (5)
O6	0.08083 (11)	0.6411 (3)	0.36010 (13)	0.0259 (5)
O7	−0.04346 (13)	0.4972 (4)	0.09263 (15)	0.0278 (5)
H7A	−0.062 (2)	0.402 (4)	0.102 (3)	0.056 (14)*
H7B	−0.0636 (18)	0.593 (3)	0.098 (2)	0.038 (12)*
O8	0.06503 (16)	0.7105 (4)	0.06326 (16)	0.0422 (7)
H8A	0.078 (2)	0.726 (7)	0.1136 (8)	0.071 (16)*
H8B	0.080 (2)	0.796 (4)	0.042 (2)	0.053 (14)*
O9	0.07215 (14)	0.3021 (4)	0.06926 (16)	0.0334 (6)
H9A	0.071 (3)	0.273 (7)	0.1146 (16)	0.084 (18)*
H9B	0.080 (3)	0.207 (4)	0.047 (3)	0.088 (19)*
O10	0.06752 (15)	0.1624 (4)	0.21393 (16)	0.0382 (6)
H10A	0.081 (2)	0.232 (5)	0.2539 (17)	0.059 (15)*
H10B	0.0248 (7)	0.146 (7)	0.200 (3)	0.077 (18)*
O11	0.1141 (2)	0.7821 (6)	0.22309 (19)	0.0633 (9)
H11A	0.101 (4)	0.892 (3)	0.2191 (18)	0.25 (5)*
H11B	0.104 (4)	0.724 (5)	0.258 (2)	0.14 (3)*
N1	0.53214 (13)	0.6648 (4)	0.41518 (16)	0.0246 (6)
C1	0.35542 (16)	0.6346 (4)	0.46664 (18)	0.0205 (7)
C2	0.31166 (16)	0.7572 (5)	0.49088 (19)	0.0216 (7)

H2	0.3311	0.8703	0.5189	0.026*
C3	0.24190 (16)	0.7166 (4)	0.47481 (19)	0.0217 (7)
C4	0.21184 (16)	0.5472 (4)	0.43321 (19)	0.0198 (7)
C5	0.25249 (16)	0.4312 (4)	0.40683 (18)	0.0199 (7)
H5	0.2317	0.3202	0.3779	0.024*
C6	0.32401 (15)	0.4683 (4)	0.42047 (18)	0.0198 (7)
C7	0.36210 (16)	0.3416 (4)	0.38757 (18)	0.0195 (7)
C8	0.32306 (15)	0.1984 (5)	0.32385 (18)	0.0201 (7)
C9	0.34515 (17)	0.0129 (5)	0.3360 (2)	0.0265 (7)
H9C	0.3817	−0.0236	0.3857	0.032*
C10	0.3137 (2)	−0.1189 (5)	0.2755 (2)	0.0370 (9)
H10	0.3278	−0.2467	0.2847	0.044*
C11	0.2619 (2)	−0.0669 (6)	0.2019 (2)	0.0398 (10)
H11	0.2415	−0.1575	0.1600	0.048*
C12	0.24051 (19)	0.1172 (6)	0.1902 (2)	0.0348 (9)
H12	0.2050	0.1535	0.1397	0.042*
C13	0.26956 (17)	0.2501 (5)	0.25025 (19)	0.0276 (8)
H13	0.2533	0.3763	0.2417	0.033*
C14	0.22528 (18)	0.9989 (5)	0.5402 (2)	0.0344 (9)
H14A	0.2663	0.9712	0.5899	0.052*
H14B	0.1888	1.0599	0.5555	0.052*
H14C	0.2394	1.0828	0.5046	0.052*
C15	0.52623 (18)	0.8529 (5)	0.4150 (2)	0.0308 (8)
H15	0.5084	0.9089	0.4527	0.037*
C16	0.5445 (2)	0.9684 (5)	0.3632 (2)	0.0377 (9)
H16	0.5387	1.1006	0.3645	0.045*
C17	0.5716 (2)	0.8887 (6)	0.3094 (2)	0.0422 (10)
H17	0.5847	0.9649	0.2728	0.051*
C18	0.5793 (2)	0.6978 (6)	0.3096 (2)	0.0397 (9)
H18	0.5987	0.6395	0.2738	0.048*
C19	0.55858 (18)	0.5911 (5)	0.3625 (2)	0.0312 (8)
H19	0.5633	0.4585	0.3614	0.037*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0128 (3)	0.0263 (3)	0.0220 (3)	−0.0002 (3)	0.0076 (2)	−0.0032 (3)
Co2	0.0220 (3)	0.0177 (3)	0.0250 (3)	−0.0001 (3)	0.0131 (3)	0.0001 (3)
S1	0.0163 (4)	0.0187 (4)	0.0218 (4)	−0.0006 (3)	0.0093 (3)	−0.0008 (3)
O1	0.0154 (11)	0.0268 (13)	0.0335 (13)	−0.0009 (10)	0.0100 (10)	−0.0030 (10)
O2	0.0169 (12)	0.0304 (13)	0.0272 (12)	0.0007 (10)	0.0096 (10)	−0.0061 (10)
O3	0.0200 (12)	0.0248 (13)	0.0423 (14)	0.0001 (10)	0.0147 (11)	−0.0123 (11)
O4	0.0276 (12)	0.0257 (12)	0.0252 (11)	−0.0012 (10)	0.0168 (10)	0.0003 (10)
O5	0.0243 (12)	0.0232 (12)	0.0299 (12)	−0.0051 (10)	0.0134 (10)	−0.0072 (10)
O6	0.0212 (12)	0.0258 (13)	0.0294 (12)	0.0039 (10)	0.0077 (10)	0.0027 (10)
O7	0.0351 (14)	0.0200 (13)	0.0384 (13)	0.0014 (13)	0.0253 (12)	0.0017 (12)
O8	0.0600 (19)	0.0413 (17)	0.0288 (15)	−0.0267 (15)	0.0203 (14)	−0.0054 (13)
O9	0.0402 (15)	0.0336 (15)	0.0313 (14)	0.0141 (13)	0.0190 (13)	0.0047 (13)

O10	0.0318 (16)	0.0519 (19)	0.0294 (15)	−0.0063 (14)	0.0094 (13)	−0.0052 (13)
O11	0.091 (3)	0.064 (2)	0.0414 (18)	−0.018 (2)	0.0311 (18)	0.0007 (16)
N1	0.0212 (14)	0.0286 (16)	0.0254 (14)	0.0004 (12)	0.0101 (12)	−0.0028 (13)
C1	0.0177 (16)	0.0216 (17)	0.0234 (16)	−0.0011 (13)	0.0092 (14)	0.0019 (14)
C2	0.0188 (16)	0.0198 (17)	0.0267 (17)	−0.0010 (13)	0.0087 (14)	−0.0043 (14)
C3	0.0201 (16)	0.0210 (18)	0.0274 (17)	0.0035 (14)	0.0128 (14)	0.0000 (14)
C4	0.0159 (15)	0.0196 (17)	0.0254 (16)	−0.0012 (13)	0.0093 (14)	0.0008 (13)
C5	0.0181 (16)	0.0193 (16)	0.0215 (16)	0.0008 (13)	0.0066 (14)	−0.0008 (13)
C6	0.0150 (15)	0.0236 (18)	0.0204 (15)	0.0007 (13)	0.0061 (13)	0.0000 (13)
C7	0.0186 (16)	0.0210 (17)	0.0202 (16)	0.0026 (13)	0.0088 (13)	0.0038 (13)
C8	0.0171 (16)	0.0263 (18)	0.0208 (16)	−0.0003 (14)	0.0113 (14)	−0.0009 (14)
C9	0.0245 (17)	0.0262 (19)	0.0278 (17)	0.0015 (15)	0.0086 (15)	0.0022 (15)
C10	0.045 (2)	0.024 (2)	0.045 (2)	−0.0031 (17)	0.020 (2)	−0.0050 (17)
C11	0.041 (2)	0.039 (2)	0.039 (2)	−0.0124 (19)	0.014 (2)	−0.0161 (19)
C12	0.0287 (19)	0.045 (2)	0.0264 (19)	−0.0027 (18)	0.0049 (16)	−0.0053 (17)
C13	0.0230 (18)	0.0299 (19)	0.0282 (18)	0.0039 (15)	0.0075 (15)	−0.0001 (15)
C14	0.0285 (19)	0.0266 (19)	0.050 (2)	0.0001 (17)	0.0167 (17)	−0.0184 (18)
C15	0.0291 (19)	0.030 (2)	0.0333 (19)	0.0034 (16)	0.0118 (16)	−0.0031 (16)
C16	0.038 (2)	0.029 (2)	0.042 (2)	−0.0036 (17)	0.0113 (19)	0.0038 (18)
C17	0.039 (2)	0.050 (3)	0.042 (2)	−0.007 (2)	0.0193 (19)	0.012 (2)
C18	0.040 (2)	0.049 (3)	0.040 (2)	−0.0003 (19)	0.0261 (19)	0.0011 (19)
C19	0.034 (2)	0.031 (2)	0.0322 (19)	0.0018 (17)	0.0172 (17)	−0.0017 (16)

Geometric parameters (Å, °)

Co1—O1^{i}	2.005 (2)	C1—C6	1.443 (4)
Co1—O1	2.005 (2)	C2—C3	1.375 (4)
Co1—O2^{i}	2.080 (2)	C2—H2	0.9500
Co1—O2	2.080 (2)	C3—C4	1.426 (4)
Co1—N1^{i}	2.173 (3)	C4—C5	1.364 (4)
Co1—N1	2.173 (3)	C5—C6	1.412 (4)
Co2—O7	2.113 (2)	C5—H5	0.9500
Co2—O8	2.037 (3)	C6—C7	1.440 (4)
Co2—O8^{ii}	2.037 (3)	C7—C8	1.505 (4)
Co2—O9	2.075 (3)	C8—C9	1.386 (5)
Co2—O9^{ii}	2.075 (3)	C8—C13	1.397 (4)
Co2—O7^{ii}	2.113 (2)	C9—C10	1.383 (5)
S1—O5	1.459 (2)	C9—H9C	0.9500
S1—O4	1.459 (2)	C10—C11	1.382 (5)
S1—O6	1.463 (2)	C10—H10	0.9500
S1—C4	1.757 (3)	C11—C12	1.373 (5)
O1—C1	1.297 (4)	C11—H11	0.9500
C7—O2	1.254 (4)	C12—C13	1.376 (5)
O3—C3	1.354 (4)	C12—H12	0.9500
O3—C14	1.435 (4)	C13—H13	0.9500
O7—H7A	0.82 (3)	C14—H14A	0.9800
O7—H7B	0.82 (3)	C14—H14B	0.9800
O8—H8A	0.829 (10)	C14—H14C	0.9800

O8—H8B	0.83 (3)	C15—C16	1.372 (5)
O9—H9A	0.83 (3)	C15—H15	0.9500
O9—H9B	0.83 (4)	C16—C17	1.376 (5)
O10—H10A	0.82 (3)	C16—H16	0.9500
O10—H10B	0.82 (3)	C17—C18	1.368 (6)
O11—H11A	0.82 (3)	C17—H17	0.9500
O11—H11B	0.82 (5)	C18—C19	1.378 (5)
N1—C19	1.333 (4)	C18—H18	0.9500
N1—C15	1.344 (4)	C19—H19	0.9500
C1—C2	1.419 (4)		
O1^{i}—Co1—O1	180.00 (13)	C3—C2—H2	119.2
O1^{i}—Co1—O2^{i}	86.87 (9)	C1—C2—H2	119.2
O1—Co1—O2^{i}	93.13 (9)	O3—C3—C2	124.2 (3)
O1^{i}—Co1—O2	93.13 (9)	O3—C3—C4	115.8 (3)
O1—Co1—O2	86.87 (9)	C2—C3—C4	120.1 (3)
O2^{i}—Co1—O2	180.0	C5—C4—C3	119.0 (3)
O1^{i}—Co1—N1^{i}	89.72 (9)	C5—C4—S1	120.9 (2)
O1—Co1—N1^{i}	90.28 (9)	C3—C4—S1	120.1 (2)
O2^{i}—Co1—N1^{i}	93.47 (9)	C4—C5—C6	123.1 (3)
O2—Co1—N1^{i}	86.53 (9)	C4—C5—H5	118.4
O1^{i}—Co1—N1	90.28 (9)	C6—C5—H5	118.4
O1—Co1—N1	89.72 (9)	C5—C6—C7	119.3 (3)
O2^{i}—Co1—N1	86.53 (9)	C5—C6—C1	117.8 (3)
O2—Co1—N1	93.47 (9)	C7—C6—C1	122.9 (3)
N1^{i}—Co1—N1	180.0	O2—C7—C6	124.7 (3)
O7—Co2—O8	87.83 (10)	O2—C7—C8	115.0 (3)
O7—Co2—O9	87.25 (10)	C6—C7—C8	120.3 (3)
O8—Co2—O8^{ii}	180.0 (3)	C9—C8—C13	119.5 (3)
O8—Co2—O9	90.10 (12)	C9—C8—C7	118.5 (3)
O8^{ii}—Co2—O9	89.90 (12)	C13—C8—C7	121.7 (3)
O8—Co2—O9^{ii}	89.90 (12)	C10—C9—C8	119.7 (3)
O8^{ii}—Co2—O9^{ii}	90.10 (12)	C10—C9—H9C	120.2
O9—Co2—O9^{ii}	180.0 (2)	C8—C9—H9C	120.2
O8—Co2—O7^{ii}	92.17 (10)	C11—C10—C9	120.9 (4)
O8^{ii}—Co2—O7^{ii}	87.83 (10)	C11—C10—H10	119.6
O9—Co2—O7^{ii}	92.75 (10)	C9—C10—H10	119.6
O9^{ii}—Co2—O7^{ii}	87.25 (10)	C12—C11—C10	119.1 (3)
O8^{ii}—Co2—O7	92.17 (10)	C12—C11—H11	120.4
O9^{ii}—Co2—O7	92.75 (10)	C10—C11—H11	120.4
O7^{ii}—Co2—O7	180.00 (9)	C11—C12—C13	121.2 (3)
O5—S1—O4	112.16 (13)	C11—C12—H12	119.4
O5—S1—O6	112.40 (13)	C13—C12—H12	119.4
O4—S1—O6	111.69 (13)	C12—C13—C8	119.6 (3)
O5—S1—C4	105.46 (14)	C12—C13—H13	120.2

O4—S1—C4	108.01 (14)	C8—C13—H13	120.2
O6—S1—C4	106.67 (14)	O3—C14—H14A	109.5
C1—O1—Co1	124.8 (2)	O3—C14—H14B	109.5
C7—O2—Co1	126.2 (2)	H14A—C14—H14B	109.5
C3—O3—C14	118.5 (2)	O3—C14—H14C	109.5
Co2—O7—H7A	121 (3)	H14A—C14—H14C	109.5
Co2—O7—H7B	117 (3)	H14B—C14—H14C	109.5
H7A—O7—H7B	112 (4)	N1—C15—C16	123.6 (3)
Co2—O8—H8A	124 (3)	N1—C15—H15	118.2
Co2—O8—H8B	125 (3)	C16—C15—H15	118.2
H8A—O8—H8B	111 (4)	C15—C16—C17	118.6 (4)
Co2—O9—H9A	118 (4)	C15—C16—H16	120.7
Co2—O9—H9B	119 (4)	C17—C16—H16	120.7
H9A—O9—H9B	109 (5)	C18—C17—C16	118.8 (4)
H10A—O10—H10B	109 (5)	C18—C17—H17	120.6
H11A—O11—H11B	112 (6)	C16—C17—H17	120.6
C19—N1—C15	116.6 (3)	C17—C18—C19	119.1 (4)
C19—N1—Co1	124.0 (2)	C17—C18—H18	120.5
C15—N1—Co1	119.4 (2)	C19—C18—H18	120.5
O1—C1—C2	117.8 (3)	N1—C19—C18	123.3 (4)
O1—C1—C6	123.9 (3)	N1—C19—H19	118.4
C2—C1—C6	118.3 (3)	C18—C19—H19	118.4
C3—C2—C1	121.7 (3)		
$O2^{i}$—Co1—O1—C1	−145.3 (2)	C3—C4—C5—C6	1.6 (5)
O2—Co1—O1—C1	34.7 (2)	S1—C4—C5—C6	179.8 (2)
$N1^{i}$—Co1—O1—C1	−51.8 (2)	C4—C5—C6—C7	−177.6 (3)
N1—Co1—O1—C1	128.2 (2)	C4—C5—C6—C1	1.8 (5)
$O1^{i}$—Co1—O2—C7	154.5 (3)	O1—C1—C6—C5	177.8 (3)
O1—Co1—O2—C7	−25.5 (3)	C2—C1—C6—C5	−4.1 (4)
$N1^{i}$—Co1—O2—C7	65.0 (3)	O1—C1—C6—C7	−2.8 (5)
N1—Co1—O2—C7	−115.0 (3)	C2—C1—C6—C7	175.3 (3)
$O1^{i}$—Co1—N1—C19	35.2 (3)	Co1—O2—C7—C6	7.8 (4)
O1—Co1—N1—C19	−144.8 (3)	Co1—O2—C7—C8	−173.65 (19)
$O2^{i}$—Co1—N1—C19	122.0 (3)	C5—C6—C7—O2	−167.5 (3)
O2—Co1—N1—C19	−58.0 (3)	C1—C6—C7—O2	13.1 (5)
$O1^{i}$—Co1—N1—C15	−144.2 (2)	C5—C6—C7—C8	14.0 (4)
O1—Co1—N1—C15	35.8 (2)	C1—C6—C7—C8	−165.4 (3)
$O2^{i}$—Co1—N1—C15	−57.3 (2)	O2—C7—C8—C9	51.5 (4)
O2—Co1—N1—C15	122.7 (2)	C6—C7—C8—C9	−129.8 (3)
Co1—O1—C1—C2	154.4 (2)	O2—C7—C8—C13	−123.0 (3)
Co1—O1—C1—C6	−27.5 (4)	C6—C7—C8—C13	55.6 (4)
O1—C1—C2—C3	−178.7 (3)	C13—C8—C9—C10	−0.4 (5)
C6—C1—C2—C3	3.1 (5)	C7—C8—C9—C10	−175.1 (3)
C14—O3—C3—C2	0.4 (5)	C8—C9—C10—C11	2.0 (5)
C14—O3—C3—C4	179.3 (3)	C9—C10—C11—C12	−1.8 (6)
C1—C2—C3—O3	179.2 (3)	C10—C11—C12—C13	0.0 (6)
C1—C2—C3—C4	0.4 (5)	C11—C12—C13—C8	1.6 (5)

O3—C3—C4—C5	178.3 (3)	C9—C8—C13—C12	−1.3 (5)
C2—C3—C4—C5	−2.8 (5)	C7—C8—C13—C12	173.1 (3)
O3—C3—C4—S1	0.1 (4)	C19—N1—C15—C16	1.2 (5)
C2—C3—C4—S1	179.1 (2)	Co1—N1—C15—C16	−179.4 (3)
O5—S1—C4—C5	4.0 (3)	N1—C15—C16—C17	−1.2 (6)
O4—S1—C4—C5	124.1 (3)	C15—C16—C17—C18	−0.1 (6)
O6—S1—C4—C5	−115.7 (3)	C16—C17—C18—C19	1.2 (6)
O5—S1—C4—C3	−177.8 (2)	C15—N1—C19—C18	0.0 (5)
O4—S1—C4—C3	−57.8 (3)	Co1—N1—C19—C18	−179.4 (3)
O6—S1—C4—C3	62.4 (3)	C17—C18—C19—N1	−1.2 (6)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7A···O6^{iii}	0.82 (3)	2.059 (16)	2.855 (3)	164 (4)
O7—H7B···O5^{iv}	0.82 (3)	1.98 (3)	2.788 (3)	172 (4)
O8—H8A···O11	0.829 (10)	1.827 (13)	2.651 (4)	173 (5)
O8—H8B···O4^{v}	0.82 (3)	1.99 (3)	2.821 (3)	178 (4)
O9—H9A···O10	0.83 (3)	1.93 (4)	2.753 (4)	170 (5)
O9—H9B···O4^{vi}	0.83 (4)	1.95 (5)	2.763 (3)	169 (5)
O10—H10A···O5	0.82 (3)	2.04 (2)	2.813 (3)	158 (4)
O10—H10B···O6^{iii}	0.82 (3)	2.019 (16)	2.822 (3)	166 (5)
O11—H11A···O10^{vii}	0.82 (3)	2.03 (3)	2.853 (5)	177 (5)
O11—H11B···O6	0.82 (5)	2.09 (5)	2.899 (4)	166 (4)

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

Fig. 1

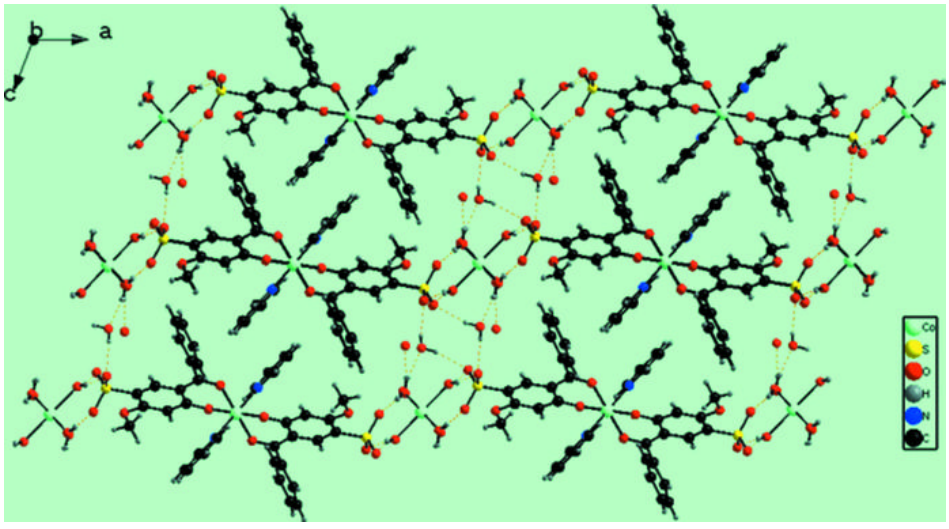

Fig. 2