

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Hexaaquacobalt(II) bis(4-amino-3-methylbenzenesulfonate)

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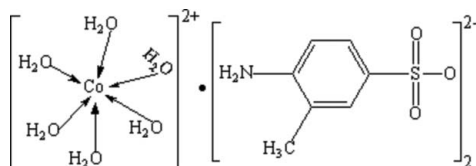
Received 26 October 2009; accepted 4 November 2009

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.025; wR factor = 0.073; data-to-parameter ratio = 13.4.

In the title molecular salt, $[\text{Co}(\text{H}_2\text{O})_6](\text{C}_7\text{H}_8\text{NO}_3\text{S})_2$, the Co^{2+} cation lies on an inversion centre. In the crystal, the components are linked by $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, thereby generating sheets parallel to (001).

Related literature

For background to hydrogen-bonded networks, see: Tai *et al.* (2007).



Experimental

Crystal data

 $[\text{Co}(\text{H}_2\text{O})_6](\text{C}_7\text{H}_8\text{NO}_3\text{S})_2$ $M_r = 539.43$ Monoclinic, $P2_1/n$ $a = 6.309$ (1) Å $b = 7.0513$ (11) Å $c = 24.262$ (4) Å $\beta = 94.080$ (2)° $V = 1076.6$ (3) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 1.06$ mm⁻¹ $T = 293$ K

0.21 × 0.16 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2000)

 $T_{\min} = 0.809$, $T_{\max} = 0.884$

5530 measured reflections

1921 independent reflections

1690 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.019$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.025$ $wR(F^2) = 0.073$ $S = 1.10$

1921 reflections

143 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.42$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.33$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—O6	2.0515 (14)	Co1—O5	2.0868 (13)
Co1—O4	2.0866 (13)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A ⁱ ···O2 ⁱ	0.86	2.47	3.214 (2)	145
N1—H1B ⁱ ···O4	0.86	2.56	3.129 (2)	125
O4—H7 ⁱ ···O2 ⁱ	0.85	2.00	2.8300 (19)	167
O4—H8 ⁱ ···O3 ⁱⁱ	0.85	1.92	2.7675 (19)	176
O5—H9 ⁱ ···O1 ⁱⁱⁱ	0.85	1.94	2.7828 (19)	170
O5—H10 ⁱ ···O3 ^{iv}	0.85	1.95	2.7963 (19)	174
O6—H11 ⁱ ···O1 ^{iv}	0.85	1.93	2.7711 (19)	169
O6—H12 ⁱ ···O2 ⁱⁱ	0.85	1.90	2.7419 (19)	173

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

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

The authors would like to thank the Program for New Century Excellent Talents in Universities for a research grant.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5188).

References

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supporting information

Acta Cryst. (2009). E65, m1548 [doi:10.1107/S1600536809046583]

Hexaaquacobalt(II) bis(4-amino-3-methylbenzenesulfonate)

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S1. Experimental

A solution of 1.0 mmol 4-amino-3-methyl-benzenesulfonic acid and 1.0 mmol NaOH in 10 ml ethanol was added to a solution of 0.5 mmol $\text{Co}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$ in 5 ml ethanol at room temperature. The mixture was refluxed for 4 h with stirring, then the resulting precipitate was filtered, washed, and dried *in vacuo* over P_4O_{10} for 48 h. Pink blocks of (I) were obtained by slowly evaporating from methanol at room temperature.

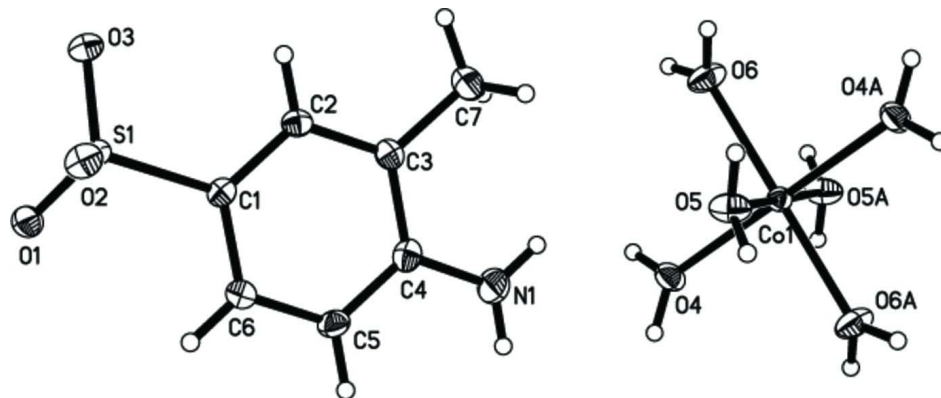


Figure 1

The molecular structure of (I) showing 30% displacement ellipsoids. Atoms with suffix A are generated by the symmetry operation $(1-x, 1-y, -z)$.

Hexaaquacobalt(II) bis(4-amino-3-methylbenzenesulfonate)

Crystal data

$[\text{Co}(\text{H}_2\text{O})_6](\text{C}_7\text{H}_8\text{NO}_3\text{S})_2$

$M_r = 539.43$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 6.309$ (1) Å

$b = 7.0513$ (11) Å

$c = 24.262$ (4) Å

$\beta = 94.080$ (2)°

$V = 1076.6$ (3) Å³

$Z = 2$

$F(000) = 562$

$D_x = 1.664$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3103 reflections

$\theta = 3.3\text{--}28.3^\circ$

$\mu = 1.06$ mm⁻¹

$T = 293$ K

Block, pink

$0.21 \times 0.16 \times 0.12$ mm

Data collection

Bruker SMART CCD diffractometer	5530 measured reflections
Radiation source: fine-focus sealed tube	1921 independent reflections
Graphite monochromator	1690 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.019$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$\theta_{\text{max}} = 25.1^\circ$, $\theta_{\text{min}} = 1.7^\circ$
$T_{\text{min}} = 0.809$, $T_{\text{max}} = 0.884$	$h = -7 \rightarrow 7$
	$k = -8 \rightarrow 6$
	$l = -25 \rightarrow 28$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.025$	$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 0.4723P]$
$wR(F^2) = 0.073$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1921 reflections	$\Delta\rho_{\text{max}} = 0.42 \text{ e } \text{\AA}^{-3}$
143 parameters	$\Delta\rho_{\text{min}} = -0.33 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001x \text{Fc}^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0268 (16)
Secondary atom site location: difference Fourier map	

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	0.5000	0.5000	0.0000	0.02153 (14)
S1	0.59383 (7)	0.51047 (6)	0.403529 (19)	0.02233 (15)
O1	0.5037 (2)	0.66812 (19)	0.43304 (5)	0.0324 (3)
O2	0.5014 (2)	0.32921 (19)	0.41856 (5)	0.0315 (3)
O3	0.8256 (2)	0.50668 (17)	0.41067 (6)	0.0311 (3)
O4	0.3989 (2)	0.73519 (19)	0.04326 (6)	0.0363 (3)
H7	0.2775	0.7762	0.0506	0.054*
H8	0.4888	0.8156	0.0567	0.054*
O5	0.4048 (2)	0.3100 (2)	0.05939 (6)	0.0365 (4)
H9	0.2842	0.2560	0.0589	0.055*
H10	0.4924	0.2201	0.0664	0.055*
O6	0.7970 (2)	0.50949 (18)	0.04025 (7)	0.0418 (4)
H12	0.8684	0.6054	0.0519	0.063*
H11	0.8706	0.4134	0.0507	0.063*
N1	0.3463 (3)	0.6380 (3)	0.16739 (7)	0.0474 (5)

H1A	0.2229	0.6845	0.1580	0.057*
H1B	0.4320	0.6115	0.1425	0.057*
C1	0.5244 (3)	0.5467 (2)	0.33285 (7)	0.0232 (4)
C2	0.6647 (3)	0.5036 (2)	0.29306 (8)	0.0247 (4)
H2	0.7980	0.4545	0.3039	0.030*
C3	0.6088 (3)	0.5326 (2)	0.23743 (8)	0.0260 (4)
C4	0.4060 (3)	0.6062 (3)	0.22179 (8)	0.0289 (4)
C5	0.2676 (3)	0.6489 (3)	0.26221 (8)	0.0307 (4)
H5	0.1341	0.6985	0.2518	0.037*
C6	0.3248 (3)	0.6188 (3)	0.31715 (8)	0.0289 (4)
H6	0.2301	0.6467	0.3437	0.035*
C7	0.7578 (4)	0.4865 (3)	0.19380 (9)	0.0360 (5)
H7A	0.8888	0.4387	0.2110	0.054*
H7B	0.7854	0.5991	0.1733	0.054*
H7C	0.6945	0.3923	0.1693	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0198 (2)	0.0217 (2)	0.0232 (2)	-0.00091 (13)	0.00196 (14)	-0.00005 (12)
S1	0.0203 (3)	0.0220 (3)	0.0245 (3)	-0.00008 (16)	-0.00023 (18)	0.00040 (16)
O1	0.0316 (7)	0.0326 (7)	0.0328 (7)	0.0041 (6)	0.0005 (6)	-0.0082 (6)
O2	0.0299 (7)	0.0284 (7)	0.0359 (8)	-0.0036 (6)	0.0002 (6)	0.0071 (6)
O3	0.0220 (7)	0.0343 (8)	0.0362 (8)	0.0004 (5)	-0.0024 (6)	0.0012 (5)
O4	0.0278 (7)	0.0340 (8)	0.0476 (9)	-0.0019 (6)	0.0072 (6)	-0.0164 (6)
O5	0.0270 (7)	0.0361 (8)	0.0474 (9)	0.0027 (6)	0.0088 (6)	0.0160 (7)
O6	0.0311 (8)	0.0281 (8)	0.0633 (11)	-0.0004 (6)	-0.0171 (7)	-0.0025 (6)
N1	0.0528 (12)	0.0596 (13)	0.0288 (9)	0.0205 (10)	-0.0043 (8)	0.0047 (9)
C1	0.0247 (9)	0.0198 (8)	0.0248 (9)	-0.0011 (7)	-0.0006 (7)	0.0021 (7)
C2	0.0236 (9)	0.0197 (9)	0.0307 (10)	0.0007 (7)	0.0009 (8)	0.0008 (7)
C3	0.0304 (10)	0.0196 (9)	0.0283 (10)	-0.0003 (7)	0.0041 (8)	-0.0009 (7)
C4	0.0375 (11)	0.0222 (9)	0.0263 (10)	0.0008 (8)	-0.0019 (8)	0.0025 (7)
C5	0.0268 (10)	0.0306 (10)	0.0338 (11)	0.0077 (8)	-0.0042 (8)	0.0003 (8)
C6	0.0261 (10)	0.0307 (10)	0.0299 (10)	0.0031 (8)	0.0031 (8)	-0.0011 (8)
C7	0.0418 (12)	0.0335 (11)	0.0334 (11)	0.0050 (9)	0.0085 (10)	0.0004 (8)

Geometric parameters (Å, °)

Co1—O6 ⁱ	2.0515 (14)	N1—C4	1.365 (2)
Co1—O6	2.0515 (14)	N1—H1A	0.8600
Co1—O4 ⁱ	2.0866 (13)	N1—H1B	0.8600
Co1—O4	2.0866 (13)	C1—C6	1.386 (2)
Co1—O5	2.0868 (13)	C1—C2	1.389 (3)
Co1—O5 ⁱ	2.0868 (13)	C2—C3	1.386 (3)
S1—O1	1.4593 (13)	C2—H2	0.9300
S1—O3	1.4603 (14)	C3—C4	1.407 (3)
S1—O2	1.4617 (13)	C3—C7	1.500 (3)
S1—C1	1.7580 (18)	C4—C5	1.392 (3)

O4—H7	0.8498	C5—C6	1.372 (3)
O4—H8	0.8498	C5—H5	0.9300
O5—H9	0.8500	C6—H6	0.9300
O5—H10	0.8499	C7—H7A	0.9600
O6—H12	0.8499	C7—H7B	0.9600
O6—H11	0.8499	C7—H7C	0.9600
O6 ⁱ —Co1—O6	180.0	H12—O6—H11	105.7
O6 ⁱ —Co1—O4 ⁱ	92.07 (6)	C4—N1—H1A	120.0
O6—Co1—O4 ⁱ	87.93 (6)	C4—N1—H1B	120.0
O6 ⁱ —Co1—O4	87.93 (6)	H1A—N1—H1B	120.0
O6—Co1—O4	92.07 (6)	C6—C1—C2	120.05 (17)
O4 ⁱ —Co1—O4	180.0	C6—C1—S1	118.67 (14)
O6 ⁱ —Co1—O5	90.56 (6)	C2—C1—S1	121.28 (14)
O6—Co1—O5	89.44 (6)	C3—C2—C1	120.94 (17)
O4 ⁱ —Co1—O5	87.15 (6)	C3—C2—H2	119.5
O4—Co1—O5	92.85 (6)	C1—C2—H2	119.5
O6 ⁱ —Co1—O5 ⁱ	89.44 (6)	C2—C3—C4	118.72 (17)
O6—Co1—O5 ⁱ	90.56 (6)	C2—C3—C7	121.77 (18)
O4 ⁱ —Co1—O5 ⁱ	92.85 (6)	C4—C3—C7	119.51 (17)
O4—Co1—O5 ⁱ	87.15 (6)	N1—C4—C5	120.13 (17)
O5—Co1—O5 ⁱ	180.0	N1—C4—C3	120.29 (18)
O1—S1—O3	112.18 (8)	C5—C4—C3	119.58 (17)
O1—S1—O2	111.56 (9)	C6—C5—C4	121.08 (17)
O3—S1—O2	111.60 (7)	C6—C5—H5	119.5
O1—S1—C1	106.81 (8)	C4—C5—H5	119.5
O3—S1—C1	107.24 (8)	C5—C6—C1	119.63 (17)
O2—S1—C1	107.10 (8)	C5—C6—H6	120.2
Co1—O4—H7	133.5	C1—C6—H6	120.2
Co1—O4—H8	120.2	C3—C7—H7A	109.5
H7—O4—H8	106.2	C3—C7—H7B	109.5
Co1—O5—H9	125.3	H7A—C7—H7B	109.5
Co1—O5—H10	113.7	C3—C7—H7C	109.5
H9—O5—H10	103.7	H7A—C7—H7C	109.5
Co1—O6—H12	129.0	H7B—C7—H7C	109.5
Co1—O6—H11	125.2		
O1—S1—C1—C6	-38.02 (17)	C2—C3—C4—N1	179.47 (17)
O3—S1—C1—C6	-158.47 (14)	C7—C3—C4—N1	-0.9 (3)
O2—S1—C1—C6	81.62 (16)	C2—C3—C4—C5	0.3 (3)
O1—S1—C1—C2	142.30 (14)	C7—C3—C4—C5	179.96 (17)
O3—S1—C1—C2	21.85 (16)	N1—C4—C5—C6	-179.70 (19)
O2—S1—C1—C2	-98.06 (15)	C3—C4—C5—C6	-0.6 (3)
C6—C1—C2—C3	0.4 (3)	C4—C5—C6—C1	0.7 (3)
S1—C1—C2—C3	-179.97 (13)	C2—C1—C6—C5	-0.6 (3)

C1—C2—C3—C4	-0.2 (3)	S1—C1—C6—C5	179.75 (15)
C1—C2—C3—C7	-179.85 (17)		

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

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N1—H1A...O2 ⁱⁱ	0.86	2.47	3.214 (2)	145
N1—H1B...O4	0.86	2.56	3.129 (2)	125
O4—H7...O2 ⁱⁱ	0.85	2.00	2.8300 (19)	167
O4—H8...O3 ⁱⁱⁱ	0.85	1.92	2.7675 (19)	176
O5—H9...O1 ^{iv}	0.85	1.94	2.7828 (19)	170
O5—H10...O3 ^v	0.85	1.95	2.7963 (19)	174
O6—H11...O1 ^v	0.85	1.93	2.7711 (19)	169
O6—H12...O2 ⁱⁱⁱ	0.85	1.90	2.7419 (19)	173

Symmetry codes: (ii) $-x+1/2, y+1/2, -z+1/2$; (iii) $-x+3/2, y+1/2, -z+1/2$; (iv) $-x+1/2, y-1/2, -z+1/2$; (v) $-x+3/2, y-1/2, -z+1/2$.