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Hexaaquacobalt(II) 1,5-naphthalenedisulfonate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.024
wR factor = 0.069
Data-to-parameter ratio = 14.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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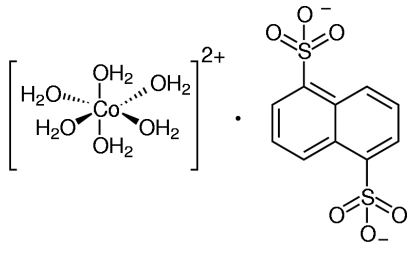
The title compound, $[Co(H_2O)_6][C_{10}H_6(SO_3)_2]$, is made up of $[Co(H_2O)_6]^{2+}$ cations and 1,5-naphthalenedisulfonate $[C_{10}H_6(SO_3)_2]^{2-}$ anions. The Co atom, which lies on a centre of symmetry, is coordinated by six water molecules to form a distorted octahedron. The anion also lies on a centre of symmetry. A three-dimensional supramolecular framework is formed *via* hydrogen bonds between the anions and cations.

Comment

Studies of molecular layered materials consisting of guanidinium cations and organosulfonate anions have shown that RSO_3^- groups are good hydrogen-bond acceptors for hydrogen-bonded frameworks (Russell & Ward, 1997). For the 1,5-naphthalenedisulfonate group, a one-dimensional Ag^I polymer has been obtained in which the group acts as a bridge between metal centres. It is also a hydrogen-bond acceptor, giving rise to chain and layer structures (Cai *et al.*, 2001). The NH_3-substituted 1,5-naphthalenedisulfonate anion has also been used in synthesizing other layered compounds (Gunderman *et al.*, 1995, 1997).



(I)

As shown in Fig. 1, the title compound, (I), consists of $[C_{10}H_6(SO_3)_2]^{2-}$ anions and $[Co(H_2O)_6]^{2+}$ cations. In the cation, the Co atom occupies an inversion site and is coordi-

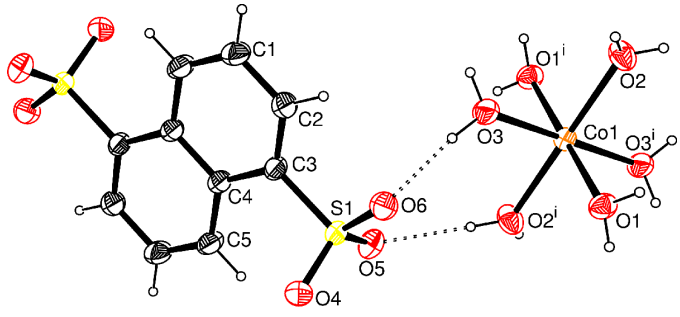


Figure 1
A view of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii [symmetry code: (i) $-x, -y, -z$].

nated by six water molecules in an octahedral geometry (Table 1). The cation interacts with the sulfonate groups *via* hydrogen bonds (Table 2). The 1,5-naphthalenedisulfonate group lies on another inversion site. The structure can be envisaged as one in which layers of anions alternate with layers of cations, the layers being linked *via* hydrogen bonds to give rise to a three-dimensional network (Table 2).

Experimental

To an aqueous solution (40 ml) of $Co(NO_3)_2\cdot 6H_2O$ (5.82 g, 20 mmol), an aqueous solution (40 ml) of sodium 1,5-naphthalenedisulfonate (6.65 g, 20 mmol) was slowly added. Pink single crystals of (I) were isolated over several days.

Crystal data

$[Co(H_2O)_6][C_{10}H_6O_6S_2]$
M_r = 453.29
Monoclinic, $P2_1/c$
a = 13.195 (3) Å
b = 6.668 (1) Å
c = 9.666 (2) Å
β = 92.14 (3)°
V = 849.9 (3) Å^3
Z = 2
D_x = 1.771 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6525 reflections
θ = 3.1–27.5°
μ = 1.32 mm^{-1}
T = 293 (2) K
Prism, pink
0.30 × 0.28 × 0.26 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.680, T_{max} = 0.712
8159 measured reflections
1952 independent reflections
1829 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 27.5°
$h = -17 \rightarrow 17$
$k = -8 \rightarrow 8$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.069
S = 1.07
1952 reflections
139 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.2109P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.108 (1)	S1—O4	1.453 (1)
Co1—O2	2.102 (1)	S1—O5	1.458 (1)
Co1—O3	2.042 (1)	S1—O6	1.463 (1)
O1—Co1—O2	91.35 (5)	O2^i—Co1—O1	88.65 (5)
O1—Co1—O3	87.74 (5)	O3^i—Co1—O1	92.26 (5)
O2—Co1—O3	87.78 (5)	O3^i—Co1—O2	92.22 (5)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O5^i	0.85 (1)	1.95 (1)	2.795 (2)	178 (2)
O1—H1B···O6^{ii}	0.85 (1)	1.93 (1)	2.760 (2)	169 (2)
O2—H2A···O1^{ii}	0.84 (1)	2.08 (1)	2.905 (2)	165 (2)
O2—H2B···O5^{iii}	0.85 (1)	2.01 (1)	2.856 (2)	178 (2)
O3—H3A···O4^{iv}	0.85 (1)	1.86 (1)	2.703 (2)	171 (2)
O3—H3B···O6	0.855 (9)	1.86 (1)	2.711 (2)	173 (2)

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

The H atoms of the water molecules were located in Fourier difference maps and refined isotropically, with O—H restrained to 0.85 (1) Å. The H atoms attached to the C atoms were included in calculated positions and treated as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Molecular Structure Corporation & Rigaku, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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