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Diammonium hexaaquacobalt(II) bis(sulfate)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(S–O) = 0.002 Å
R factor = 0.031
wR factor = 0.073
Data-to-parameter ratio = 10.5

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

In the title compound,$(NH_4)_2[Co(H_2O)_6](SO_4)_2$, six water molecules are coordinated to one Co^{2+} cation, which lies on an inversion centre. The geometry around the Co^{2+} cation is that of an octahedron. The coordinated water molecules, uncoordinated ammonium cations and sulfate anions are linked by hydrogen bonds into a network structure.

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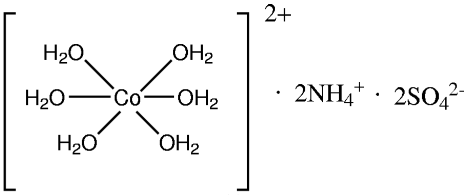
Comment

In the synthesis of crystal structures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Directional intermolecular interactions are the primary tools in achieving this goal and hydrogen bonding is currently the best among these (Zaworotko, 1997; Braga & Grepioni, 2000). Against this background, we report here the structure of the title compound, (I).



(I)

The asymmetric unit of (I) consists of one half of a $[Co(H_2O)_6]^{2+}$ cation, an NH_4^+ cation and a sulfate anion. The cobalt cation lies on an inversion centre, and the geometry around the Co^{2+} ion is that of an octahedron, with bonds to six water molecules (Fig. 1 and Table 1). The two ammonium cations lie beside the Co^{2+} ion to balance charges.

The coordinated water molecules, uncoordinated ammonia cations and sulfate anions interact through hydrogen bonds (Fig. 2 and Table 2), generating a three-dimensional network.

Experimental

Cobalt sulfate heptahydrate (0.06 g, 0.2 mmol) was dissolved in water (10 ml) and the solution was mixed with a dimethylformamide solu-

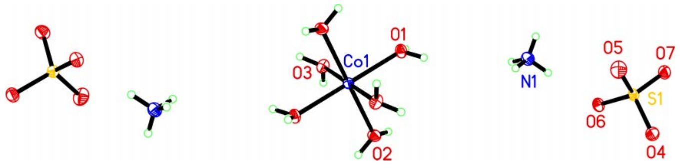


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Only the contents of the asymmetric unit are labelled.

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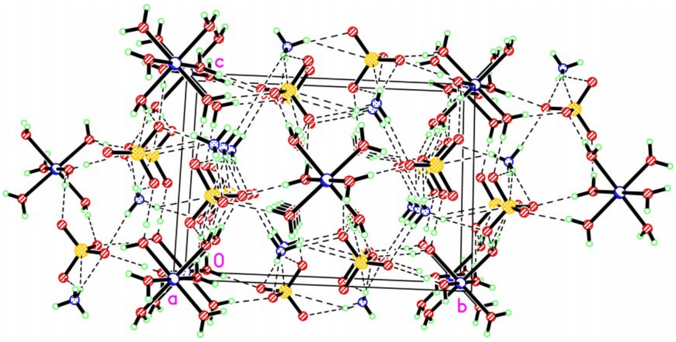

Figure 2
A view of the three-dimensional network formed by the hydrogen-bonding interactions in (I), which are shown as dashed lines.

tion (10 ml) of 5-sulfoisophthalic acid monosodium salt (0.11 g, 0.4 mmol) and ammonium pyrrolidine dithiocarbamate (0.07 g, 0.4 mmol). Ammonia (0.2 ml) was added dropwise. The reaction mixture was filtered and allowed to stand. Yellow prism-shaped crystals of (I) were separated from the solution after about three months. As shown by the present crystal structure analysis, the 5-sulfoisophthalic acid monosodium salt and ammonium pyrrolidine dithiocarbamate entities were not incorporated into the product.

Crystal data

$(NH_4)_2[Co(H_2O)_6](SO_4)_2$
$M_r = 395.23$
Monoclinic, $P2_1/c$
$a = 6.2362$ (13) Å
$b = 12.521$ (3) Å
$c = 9.2553$ (19) Å
$\beta = 107.038$ (4)°
$V = 691.0$ (2) Å^3
$Z = 2$

$D_x = 1.900$ Mg m$^{-3$}
Mo $K\alpha$ radiation
Cell parameters from 1237 reflections
$\theta = 2.3$–25.3°
$\mu = 1.62$ mm^{-1}
$T = 298$ (2) K
Prism, yellow
0.21 × 0.06 × 0.05 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.84$, $T_{max} = 0.91$
3595 measured reflections

1237 independent reflections
1126 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.2°$
$h = -7 \rightarrow 7$
$k = -15 \rightarrow 14$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.073$
$S = 1.05$
1237 reflections
118 parameters
Only coordinates of H atoms refined

$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 0.6682P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.064 (2)	Co1—O2	2.103 (2)
Co1—O3	2.101 (2)		
O1^i—Co1—O1	180	O3—Co1—O2	91.04 (8)
O1^i—Co1—O3	90.40 (8)	O1—Co1—O2^i	91.32 (8)
O1—Co1—O3	89.60 (8)	O3—Co1—O2^i	88.96 (8)
O3^i—Co1—O3	180	O2—Co1—O2^i	180
O1—Co1—O2	88.68 (8)		

Symmetry code: (i) $-x, 2-y, 2-z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O6^i	0.83 (1)	1.96 (1)	2.783 (3)	173 (3)
O2—H2B···O7^{ii}	0.83 (1)	2.01 (1)	2.833 (3)	176 (3)
O3—H3A···O7^{iii}	0.84 (1)	1.93 (1)	2.759 (3)	172 (3)
O3—H3B···O5^{iv}	0.84 (1)	1.88 (1)	2.710 (3)	177 (4)
O1—H1A···O4^v	0.84 (1)	1.87 (1)	2.705 (3)	173 (3)
O1—H1B···O6^{ii}	0.83 (1)	1.94 (1)	2.768 (3)	169 (3)
N1—H4D···O6	0.85 (4)	2.00 (4)	2.847 (4)	171 (3)
N1—H4A···O4^v	0.83 (4)	2.22 (4)	2.996 (4)	157 (3)
N1—H4A···O5^v	0.83 (4)	2.47 (4)	3.151 (4)	140 (3)
N1—H4B···O4^{ii}	0.82 (4)	2.17 (4)	2.973 (4)	166 (4)
N1—H4C···O7^{vi}	0.80 (4)	2.13 (4)	2.903 (4)	165 (4)

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

All H atoms were located in a difference Fourier map and their positional parameters were refined. U_{iso}(H) values were set equal to $1.5U_{eq}$(carrier atom). The water H atoms were refined with the O—H and H···H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively.

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

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