Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

1,4-Diazoniabicyclo[2.2.2]octane hexaaqua-cobalt(II) bis(sulfate)

Ya-Juan Zhao, Xin-Hua Li* and Shun Wang

School of Chemistry and Materials Science, Wenzhou Normal College, Zhejiang, Wenzhou 325027, People's Republic of China

Correspondence e-mail: lixinhua01@126.com

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.029
wR factor = 0.079
Data-to-parameter ratio = 11.4

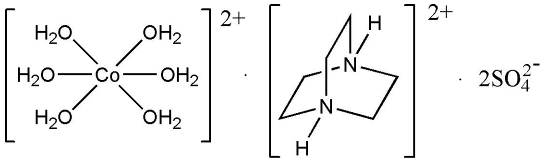
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 3 March 2005
Accepted 7 March 2005
Online 18 March 2005

The title compound, $(C_6H_{14}N_2)[Co(H_2O)_6](SO_4)_2$, consists of hexaaquacobalt(II) cations, 1,4-diazabicyclo[2,2,2]octane cations and sulfate anions, linked by O—H···O hydrogen bonds. The geometry around the Co^{2+} cation is octahedral.

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). In this paper, we report the structure of the title compound, (I).



(I)

The asymmetric unit of (I) consists of a 1,4-diazabicyclo[2,2,2]octane cation, a hexaaquacobalt(II) cation and two sulfate anions. The Co^{2+} cation lies in a general position and the geometry around it is octahedral, with bonds to six water molecules (Fig. 1 and Table 1). The coordinated water molecules, 1,4-diazabicyclo[2,2,2]octane cations and sulfate anions interact through hydrogen bonds (Table 2), generating a three-dimensional network (Fig. 2).

Experimental

Cobalt(II) sulfate heptahydrate (0.06 g, 0.2 mmol) was dissolved in water (10 ml) and the solution was mixed with a dimethylformamide solution (10 ml) of 5-sulfoisophthalic acid monosodium salt (0.11 g, 0.4 mmol) and 1,4-diazabicyclo[2,2,2]octane (0.05 g, 0.4 mmol). The reaction mixture was filtered and allowed to stand. Pink prism-shaped crystals of (I) separated from the solution after about three months. As shown by the present crystal structure analysis, no component of the 5-sulfoisophthalic acid monosodium salt was incorporated into the product.

Crystal data

$(C_6H_{14}N_2)[Co(H_2O)_6](SO_4)_2$
M_r = 473.34
Monoclinic, $P2_1/c$
a = 12.0488 (8) Å
b = 12.1842 (8) Å
c = 12.1390 (8) Å
β = 104.20 (1)°
V = 1727.8 (2) Å^3
Z = 4

D_x = 1.820 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3079 reflections
θ = 1.7–25.1°
μ = 1.31 mm^{-1}
T = 298 (2) K
Prism, pink
0.29 × 0.26 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\rm min} = 0.69$, $T_{\rm max} = 0.77$
8951 measured reflections
3079 independent reflections
2920 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\rm max} = 25.1°$
$h = -14 \rightarrow 12$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.079$
$S = 1.06$
3079 reflections
269 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 1.1451P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.29$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.44$ e Å^{-3}
Extinction correction: *SHELXTL* (Bruker, 2002)
Extinction coefficient: 0.0642 (18)

Table 1
Selected geometric parameters (Å, °).

Co1—O2	2.0705 (17)	Co1—O1	2.0816 (16)
Co1—O4	2.0728 (16)	Co1—O3	2.1053 (17)
Co1—O5	2.0798 (17)	Co1—O6	2.1466 (16)
O2—Co1—O4	86.86 (7)	O5—Co1—O3	88.36 (8)
O2—Co1—O5	175.82 (7)	O1—Co1—O3	89.01 (7)
O4—Co1—O5	93.86 (7)	O2—Co1—O6	89.04 (7)
O2—Co1—O1	91.75 (7)	O4—Co1—O6	92.45 (7)
O4—Co1—O1	178.43 (7)	O5—Co1—O6	86.82 (7)
O5—Co1—O1	87.57 (7)	O1—Co1—O6	88.27 (7)
O2—Co1—O3	95.75 (8)	O3—Co1—O6	174.56 (7)
O4—Co1—O3	90.39 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6*C*···O12$^{\rm i}$	0.83 (3)	1.95 (3)	2.780 (2)	177 (4)
O2—H2*C*···O9	0.82 (3)	1.94 (3)	2.752 (2)	171 (4)
O1—H1*C*···O8	0.81 (3)	1.98 (3)	2.776 (2)	168 (4)
O2—H2*D*···O13$^{\rm ii}$	0.79 (3)	1.98 (3)	2.753 (2)	164 (4)
O4—H4*D*···O13$^{\rm i}$	0.84 (3)	1.85 (3)	2.691 (2)	174 (4)
O1—H1*D*···O10$^{\rm iii}$	0.80 (3)	1.90 (3)	2.691 (2)	169 (4)
O5—H5*C*···O12$^{\rm iv}$	0.79 (3)	1.98 (3)	2.765 (2)	171 (4)
O6—H6*D*···O8$^{\rm v}$	0.83 (3)	2.16 (3)	2.985 (2)	173 (4)
O3—H3*C*···O9$^{\rm iii}$	0.82 (3)	1.98 (3)	2.802 (3)	179 (4)
O5—H5*D*···O10$^{\rm v}$	0.81 (2)	1.89 (3)	2.688 (2)	169 (4)
O4—H4*C*···O11$^{\rm iv}$	0.82 (3)	1.90 (3)	2.698 (2)	167 (4)
O3—H3*D*···O14$^{\rm vi}$	0.81 (2)	2.01 (3)	2.790 (2)	160 (4)
N2—H2*N*···O7$^{\rm iii}$	0.86 (2)	1.86 (3)	2.685 (3)	159 (3)
N1—H1*N*···O14$^{\rm vii}$	0.89 (2)	2.03 (3)	2.796 (3)	145 (3)
N1—H1*N*···O12$^{\rm vii}$	0.89 (2)	2.23 (3)	2.995 (3)	145 (3)

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

Water and amine H atoms were located in a difference Fourier map and refined isotropically, with O—H and N—H distance restraints of 0.82 (3) and 0.86 (3) Å, respectively. All other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.97 Å, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent atom).

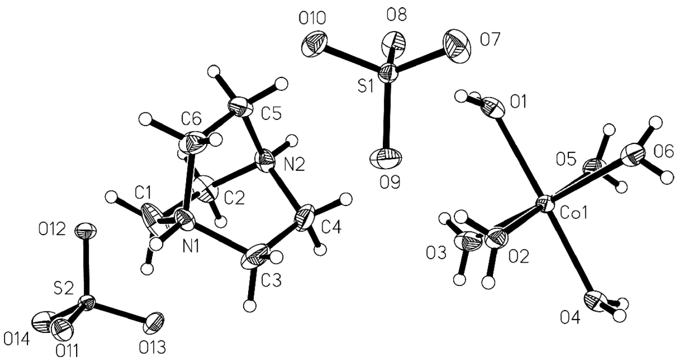


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme and with displacement ellipsoids at the 50% probability level.

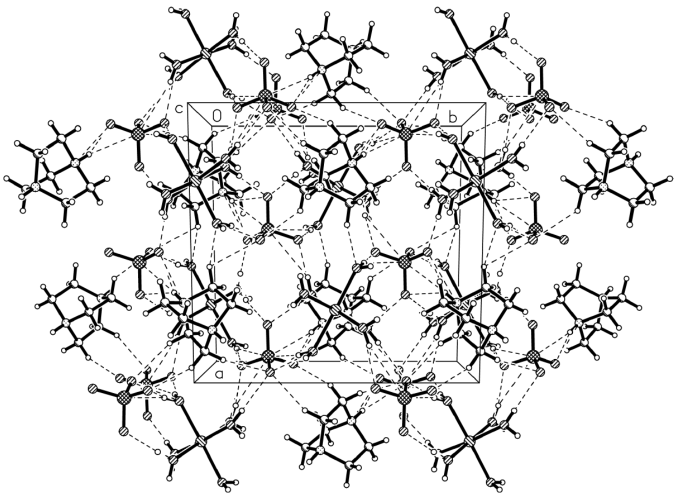


Figure 2
A perspective view of the three-dimensional network of (I), assembled *via* hydrogen bonds, which are shown as dashed lines.

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*.

The authors acknowledge financial support from the Zhejiang Provincial Natural Science Foundation of China (grant Nos. Y404294 and Y404118), the Natural Science Foundation of China (grant No. 20471043) and the '151' Distinguished Person Foundation of Zhejiang Province.

References

Braga, D. & Grepioni, F. (2000). *Acc. Chem. Res.* **33**, 601–608.
Braga, D., Grepioni, F. & Desiraju, G. R. (1998). *Chem. Rev.* **98**, 1375–1386.
Bruker (2002). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 2311–2315.
Desiraju, G. R. (1997). *J. Chem. Soc. Chem. Commun.* pp. 1475–1476.
Zaworotko, M. J. (1997). *Nature (London)*, **386**, 220–226.

m672 Zhao *et al.* • $(C_6H_{14}N_2)[Co(H_2O)_6](SO_4)_2$ *Acta Cryst.* (2005). E**61**, m671–m672