Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(benzylammonium) tetraaquadisulfatomanganate(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.103
Data-to-parameter ratio = 14.9

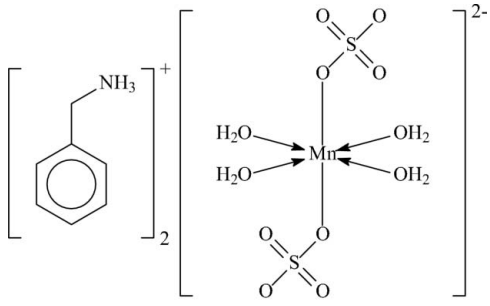
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 6 September 2005
Accepted 8 September 2005
Online 14 September 2005

The cation and anion of the title compound, $(C_7H_{10}N)_2[Mn(SO_4)_2(H_2O)_4]$, are linked by hydrogen bonds into a three-dimensional network structure. The Mn atom of the anion lies on a centre of inversion in an octahedral coordination geometry of water and sulfate ligands.

Comment

The Tutton salts $M^I_2[M^{II}(H_2O)_6](SO_4)_2$, where M^I is a monovalent metal or ammonium and M^{II} is a divalent transition metal, are a well studied class of salts (Mahadevan Pillai *et al.*, 1997) that typically afford large well defined crystals. Such salts have been reported to undergo multiple phase transitions, and some of the phases also exhibit ferroelectricity/ferroelasticity (Kirpichnikova *et al.*, 1990; Vlokh, Bublyk *et al.*, 1991; Vlokh, Karpustyanyuk *et al.*, 1991). Interest in the double alkylammonium–metal sulfates arises from the information that can be obtained from them on the structural features of the ammonium ion (Naumov *et al.*, 2002).



(I)

Bis(benzylammonium) tetraaquadisulfatomanganate, (I), is a member of the triad of double sulfates which has cadmium and copper salts as the other members. The formulation of the compound (Fig. 1) was established previously (Jordanovska *et al.*, 2000).

In the crystal structure, the Mn atom lies on a centre of inversion, and the octahedrally coordinated anion interacts with the cation through hydrogen bonds (Table 2) to give rise to a tightly held three-dimensional network structure.

Two other tetraaquadisulfatomanganate salts that have been crystallographically authenticated are the ethylenediammonium (Chaabouni *et al.*, 1996) and histaminium (Wojtczak & Jaskólski, 1989) salts.

Experimental

The compound could be synthesized on a large scale, as it forms as colourless crystalline blocks of centimetre dimensions by merely

evaporating, at ambient temperature, an aqueous solution of manganese(II) sulfate and two molar equivalents of benzylammonium sulfate in the presence of sulfuric acid (Jordanovska *et al.*, 2000). The crystal of (I) used for the present diffraction measurements was cut from a large specimen.

Crystal data

$(C_7H_{10}N)_2[Mn(SO_4)_2(H_2O)_4]$	$Z = 1$
$M_r = 535.44$	$D_x = 1.551$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 6.5934$ (4) Å	Cell parameters from 2764 reflections
$b = 8.0307$ (5) Å	$\theta = 2.6$–$28.3°$
$c = 11.2873$ (8) Å	$\mu = 0.82$ mm^{-1}
$\alpha = 80.620$ (1)°	$T = 295$ (2) K
$\beta = 82.639$ (1)°	Irregular block, colourless
$\gamma = 77.613$ (1)°	0.30 × 0.30 × 0.30 mm
$V = 573.24$ (6) Å^3	

Data collection

Bruker APEX area-detector diffractometer	2533 independent reflections
φ and ω scans	2371 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.017$
$T_{min} = 0.631$, $T_{max} = 0.791$	$\theta_{max} = 27.5°$
3583 measured reflections	$h = -8 \rightarrow 8$
	$k = -9 \rightarrow 10$
	$l = -8 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2 + 0.1241P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.033$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.103$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
$S = 1.10$	$\Delta\rho_{min} = -0.44$ e Å^{-3}
2533 reflections	
170 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.219 (1)	Mn1—O2*W*	2.188 (1)
Mn1—O1*W*	2.159 (1)		
O1—Mn1—O1*W*	93.24 (5)	O1—Mn1—O2*W*^{i}	92.45 (5)
O1—Mn1—O1*W*^{i}	86.76 (5)	O1*W*—Mn1—O2*W*	90.30 (5)
O1—Mn1—O2*W*	87.55 (5)	O1*W*—Mn1—O2*W*^{i}	89.70 (5)

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*
O1*W*—H1*W*1···O2^{ii}	0.84 (1)	1.91 (1)	2.754 (2)	178 (3)
O1*W*—H1*W*2···O4^{iii}	0.84 (1)	1.90 (1)	2.740 (2)	173 (3)
O2*W*—H2*W*1···O2	0.85 (1)	1.92 (1)	2.746 (2)	164 (3)
O2*W*—H2*W*2···O3^{ii}	0.84 (1)	1.89 (1)	2.726 (2)	175 (3)
N1—H1N1···O2	0.86 (1)	1.99 (1)	2.807 (2)	160 (2)
N1—H1N2···O1^{iv}	0.86 (1)	2.21 (2)	2.991 (2)	152 (2)
N1—H1N3···O3^{v}	0.86 (1)	1.95 (1)	2.813 (2)	176 (2)

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

C-bound H atoms were positioned geometrically [C—H_{phenyl} = 0.93 Å and C—$H_{methylene}$ = 0.97 Å; U_{iso}(H) = 1.2U_{eq}C] and were included in the refinement in the riding-model approximation. Ammonium and water H atoms were found in difference Fourier maps and refined with a distance restraint of N—H = O—H = 0.85 (1) Å.

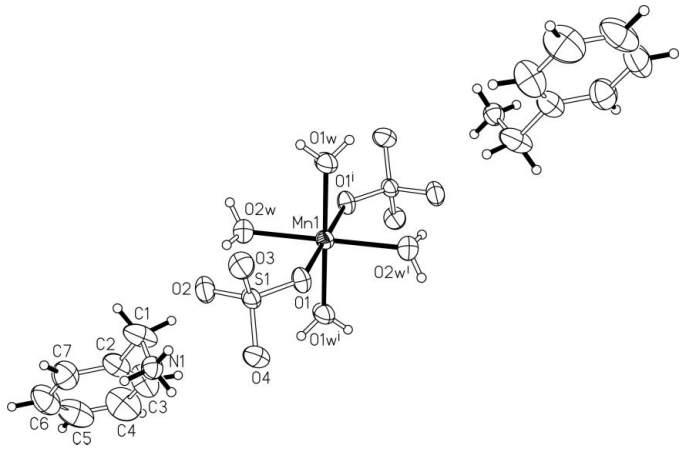


Figure 1
A plot of (I), showing displacement ellipsoids at the 50% probability level. H atoms are drawn as small spheres of arbitrary radii. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; method used to solve structure: difference Fourier, with Mn1 at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

We thank the Department of Chemistry, Central China Normal University, for collecting the diffraction data. We also thank Sv. Kiril i Metodij University and the University of Malaya for supporting this work.

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