Crystal structure of tetraaquamanganese(II) selenate monohydrate, $\text{Mn}(\text{H}_2\text{O})_4\text{SeO}_4 \cdot \text{H}_2\text{O}$

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oxygen atoms shared with the SeO_4 tetrahedra. As a consequence, chains of corner linked $\text{Mn1}(\text{OH}_2)_4\text{--SeO}_4\text{--Mn2}(\text{OH}_2)_4\text{--SeO}_4$ units are formed, running along [110]. The almost regular octahedra ($d(\text{Mn--O}) = 2.127 \text{ \AA} - 2.212 \text{ \AA}$) and slightly distorted tetrahedra ($d(\text{Se--O}) = 1.629 \text{ \AA} - 1.645 \text{ \AA}$) of adjacent chains are linked by the fifth, non-coordinating water molecule and a system of hydrogen bonds. Eight are of normal strength, $d(\text{O}\cdots\text{O}) = 2.730 \text{ \AA} - 2.883 \text{ \AA}$, and three bonds are weaker, $d(\text{O}\cdots\text{O}_2) = 3.114 \text{ \AA}$, $d(\text{O}_6\cdots\text{O}_2, \text{O}_7) = 2.924 \text{ \AA}, 3.113 \text{ \AA}$, respectively, showing that H3 is probably involved in a bifurcated bond.

Table 1. Data collection and handling.

Crystal:	colorless prisma, size $0.2 \times 0.2 \times 0.25 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation ($0.71069 \text{ \AA}$)
μ :	61.77 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC6R, ω
$2\theta_{\text{max}}$:	50.1°
$N(hkl)_{\text{measured}}, N(hkl)_{\text{unique}}$:	2860, 1430
Criterion for $I_{\text{obs}}, N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1349
$N(\text{param})_{\text{refined}}$:	144
Programs:	SHELXL-97 [4], DIAMOND [5]

Abstract

$\text{H}_{10}\text{MnO}_9\text{Se}$, triclinic, $P\bar{1}$ (No. 2), $a = 6.471(3) \text{ \AA}$, $b = 10.898(3) \text{ \AA}$, $c = 6.263(4) \text{ \AA}$, $\alpha = 81.45(2)^\circ$, $\beta = 109.43(2)^\circ$, $\gamma = 104.37(3)^\circ$, $V = 402.4 \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.017$, $wR_{\text{ref}}(F^2) = 0.043$, $T = 293 \text{ K}$.

Source of material

In the course of systematic structure investigations of Tutton salts [1,2], tetraaquamanganese(II) selenate monohydrate has been prepared as a starting material from a solution of $\text{MnCO}_3 \cdot 5\text{H}_2\text{O}$ in diluted selenic acid.

Experimental details

A small single crystal was fixed in a 0.3 mm diameter capillary using silica glass wool. In order to prevent dehydration of the sample, a drop of water was added prior to sealing the capillary.

Discussion

$\text{Mn}(\text{H}_2\text{O})_4\text{SeO}_4 \cdot \text{H}_2\text{O}$ is isotypic with $\text{MgSO}_4 \cdot 5\text{H}_2\text{O}$ and $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ [3]. The structure is composed of $\text{MnO}_2(\text{OH}_2)_4$ octahedra, whose equatorial corners are occupied by water molecule oxygens, whereas the remaining apical corners are occupied by

Table 2. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	2i	0.889(7)	0.127(4)	0.246(7)	0.06(1)
H(2)	2i	0.745(7)	0.021(4)	0.227(6)	0.06(1)
H(3)	2i	0.355(6)	0.194(3)	0.133(5)	0.05(1)
H(4)	2i	0.360(6)	0.123(3)	0.313(6)	0.05(1)
H(5)	2i	0.567(6)	0.398(3)	0.413(5)	0.034(9)
H(6)	2i	0.343(8)	0.381(4)	0.365(6)	0.07(1)
H(7)	2i	0.800(6)	0.399(3)	0.946(6)	0.03(1)
H(8)	2i	0.847(6)	0.386(3)	0.144(6)	0.05(1)
H(9)	2i	0.574(8)	0.130(4)	0.694(7)	0.07(1)
H(10)	2i	0.455(6)	0.187(4)	0.728(6)	0.05(1)

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Mn(1)	1 <i>a</i>	0	0	0	0.0257(3)	0.0193(2)	0.0205(2)	0.0049(2)	0.0074(2)	0.0000(2)
Mn(2)	1 <i>e</i>	1/2	1/2	0	0.0190(2)	0.0192(2)	0.0177(2)	0.0038(2)	0.0059(2)	−0.0005(2)
Se(1)	2 <i>i</i>	0.02649(3)	0.29021(2)	0.64961(3)	0.0175(1)	0.0179(1)	0.0152(1)	0.00338(8)	0.00452(8)	−0.00004(8)
O(1)	2 <i>i</i>	0.9163(3)	0.1436(2)	0.7193(3)	0.0285(8)	0.0240(8)	0.0295(8)	−0.0005(7)	0.0051(7)	0.0075(6)
O(2)	2 <i>i</i>	0.2792(3)	0.3292(2)	0.8305(3)	0.0220(8)	0.0262(8)	0.0298(9)	0.0024(6)	−0.0033(7)	−0.0043(7)
O(3)	2 <i>i</i>	0.8656(3)	0.3835(2)	0.6514(3)	0.0328(9)	0.0359(9)	0.0264(8)	0.0164(7)	0.0085(7)	−0.0032(7)
O(4)	2 <i>i</i>	0.0502(3)	0.2962(2)	0.3959(3)	0.0349(9)	0.0301(8)	0.0193(7)	0.0094(7)	0.0127(7)	−0.0003(6)
O(5)	2 <i>i</i>	0.8167(4)	0.0735(2)	0.1644(4)	0.045(1)	0.034(1)	0.044(1)	0.0000(9)	0.025(1)	−0.0126(9)
O(6)	2 <i>i</i>	0.3111(3)	0.1207(2)	0.1843(3)	0.038(1)	0.027(1)	0.031(1)	−0.0005(8)	0.0063(8)	−0.0022(8)
O(7)	2 <i>i</i>	0.4671(3)	0.4008(2)	0.3167(3)	0.0279(9)	0.047(1)	0.0210(9)	0.0055(8)	0.0080(8)	0.0079(8)
O(8)	2 <i>i</i>	0.7644(3)	0.4087(2)	0.0302(4)	0.032(1)	0.055(1)	0.0234(9)	0.0252(9)	0.0085(9)	−0.0002(8)
O(9)	2 <i>i</i>	0.4503(3)	0.1313(2)	0.6592(4)	0.026(1)	0.043(1)	0.043(1)	0.0061(8)	0.0087(8)	−0.0001(9)

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