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*Note added in proof*: Only late in the editorial process was it discovered that a structure for this same crystal had also been determined by Leclaire, Borel & Monier (1980) (preceding paper) and reported under the alternative name tachydrite. The structure of Leclaire *et al.* (refined to $R = 0{\cdot}021$) is in close agreement with ours. As shown in Table 1, the differences between the structure parameters are not greater than the sum of the reported standard errors, except for $z_{Mg}$ and $y_{H(2)}$ where they are $1{\cdot}7(\sum\sigma)$. The standard errors given by Leclaire *et al.*, are generally less than ours, and the hydrogen atoms are somewhat better resolved. We believe, however, that in the case of the unit-cell parameters, where the differences are more substantial, the results of Erd *et al.* (1979), obtained from a calibrated powder diffractometer pattern made with Cu $K\alpha$ radiation, are more reliable.

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# Manganese(II) Sulfite Trihydrate

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**Abstract.** $\alpha$-$MnSO_3.3H_2O$, monoclinic, $P2_1/n$, $a = 6{\cdot}659\,(2)$, $b = 8{\cdot}920\,(2)$, $c = 8{\cdot}806\,(2)$ Å, $\beta = 96{\cdot}10\,(2)°$, $Z = 4$, $D_x = 2{\cdot}41$ Mg m$^{-3}$, $\mu$(Mo $K\alpha$) = $2{\cdot}99$ mm$^{-1}$. Final $R = 0{\cdot}049$ for 1449 diffractometer data. The structure is isomorphous with $\alpha$-$FeSO_3.3H_2O$ [L.-G. Johansson & O. Lindqvist (1979). *Acta Cryst.* B**35**, 1017–1020].

**Introduction.** Georgii & Barrie (1976) have shown that $Mn^{2+}$ and $Fe^{2+}$ have high catalytic activity in the oxidation reaction $SO_2 + \frac{1}{2}O_2 + H_2O \rightarrow H_2SO_4$. In order to investigate the relations between the dimensions and the stability of the sulfite ion the structure of $\alpha$-$MnSO_3.3H_2O$ has been refined. Crystals of $\alpha$-$MnSO_3.3H_2O$ were prepared in the same way as for the isomorphous $\alpha$-$FeSO_3.3H_2O$ (Bugli & Pannetier, 1968). They have a pale rose colour and oxidize slowly in air like $\alpha$-$FeSO_3.3H_2O$.

A crystal $0{\cdot}1 \times 0{\cdot}2 \times 0{\cdot}2$ mm was mounted in a glass capillary on a Syntex $P2_1$ diffractometer. Graphite-monochromated Mo $K\alpha$ radiation and a variable scan rate and range were used. 1738 reflections with $h \geq 0$ and $k \geq 0$ were measured out to $2\theta = 60°$, and 1449 were considered significant having

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Table 1. *Atomic parameters for* α-$MnSO_3.3H_2O$

| | *x* | *y* | *z* | $B_{iso}$ (Å$^2$) |
|---|---|---|---|---|
| Mn | 0·43045 (6) | 0·24605 (5) | 0·14290 (5) | 1·08 (1) |
| S | 0·8255 (1) | 0·0701 (1) | 0·3263 (1) | 1·16 (1) |
| O(1) | 0·9557 (4) | 0·1983 (3) | 0·4045 (3) | 1·64 (4) |
| O(2) | 0·7231 (4) | 0·1415 (3) | 0·1806 (3) | 1·73 (5) |
| O(3) | 0·5206 (4) | 0·4632 (3) | 0·2325 (3) | 1·55 (4) |
| O(4) | 0·1106 (4) | 0·3472 (3) | 0·1444 (3) | 1·65 (4) |
| O(5) | 0·2630 (4) | 0·0443 (3) | 0·0734 (3) | 2·18 (5) |
| O(6) | 0·3631 (4) | 0·1665 (3) | 0·3746 (3) | 1·65 (4) |

$I > 3\sigma(I)$. The intensity of a standard reflection showed that the crystal was stable during data collection. Integrated intensities were obtained with the Lehmann & Larsen (1974) profile-analysis method (program *LELA*; Lindqvist & Ljungström, 1979). Lorentz and polarization corrections were performed with a local program (*SYN*). No absorption correction was made.

The cell parameters have been determined from a Guinier focused powder photograph* with $Pb(NO_3)_2$ as internal standard (program *POWDER*; Lindqvist & Wengelin, 1967).

The refinement was started from the positions of α-$FeSO_3.3H_2O$ (Johansson & Lindqvist, 1979), with the block-diagonal approximation (program *BLOCK*; Lindgren, 1977). The final refinement was carried out with anisotropic thermal parameters* and gave $R$ = 0·049. The positional parameters and isotropic temperature factors, the latter obtained in a previous refinement ($R$ = 0·065), are given in Table 1. Scattering factors (Doyle & Turner, 1968) were used for $Mn^0$, $S^0$ and $O^0$. The structure factors were weighted according to $w = [\sigma^2(F) + 0{\cdot}00025F^2]^{-1}$.

**Discussion.** Coordination distances and angles are listed in Table 2, and are given with the same notation as α-$FeSO_3.3H_2O$ (Johansson & Lindqvist, 1979). The S–O distances are not significantly different in the compounds, the average values being 1·536 Å for α-$FeSO_3.3H_2O$ and 1·535 Å for α-$MnSO_3.3H_2O$, but in both cases the S–O(1) bond is significantly longer than the other two S–O bonds. This is because O(1) is more strongly hydrogen bonded to the water molecules than O(2) and O(3) (Table 3).

All Mn–O bonds are longer than the corresponding Fe–O bonds, with average values 2·243 and 2·180 Å for $M$—$O_{aq}$, and 2·161 and 2·125 Å for the $M$–$O_{sulfite}$ bonds, respectively. This is in good agreement with the reported values of ionic radii for $Mn^{2+}$ and $Fe^{2+}$, 0·80 and 0·76 Å, respectively (Pauling, 1960). In α-$FeSO_3.3H_2O$ the Fe–O(3) distance is ~0·1 Å shorter than the other Fe–$O_{sulfite}$ distances. Such a difference is not present in α-$MnSO_3.3H_2O$. Baggio & Baggio (1976) reported the structure of an orthorhombic phase of $MnSO_3.3H_2O$. The average S–O distance is given as 1·525 Å while the average Mn–$O_{sulfite}$ and Mn–$O_{aq}$ distances are 2·164 and 2·210 Å respectively.

The positions of the H atoms have not been established in either of the two phases, but the O–O distances possible for hydrogen bonding are similar in α-$MnSO_3.3H_2O$ (Table 3) and in α-$FeSO_3.3H_2O$. Neutron diffraction data for α-$MnSO_3.3D_2O$ have been collected.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35313 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Coordination distances* (Å) *and angles* (°)

| | | | |
|---|---|---|---|
| Mn–O(1) | 2·180 (2) | S–O(1) | 1·550 (3) |
| Mn–O(2) | 2·152 (2) | S–O(2) | 1·526 (2) |
| Mn–O(3) | 2·150 (2) | S–O(3) | 1·529 (3) |
| Mn–O(4) | 2·312 (2) | | |
| Mn–O(5) | 2·169 (2) | | |
| Mn–O(6) | 2·249 (2) | | |

| | | O···O distance |
|---|---|---|
| O(1)–Mn–O(2) | 94·9 (1) | 3·193 (3) |
| O(1)–Mn–O(3) | 95·8 (1) | 3·214 (3) |
| O(1)–Mn–O(4) | 94·7 (1) | 3·305 (3) |
| O(1)–Mn–O(5) | 90·4 (1) | 3·086 (3) |
| O(1)–Mn–O(6) | 171·1 (1) | 4·416 (4) |
| O(2)–Mn–O(3) | 96·9 (1) | 3·220 (3) |
| O(2)–Mn–O(4) | 170·4 (1) | 4·449 (4) |
| O(2)–Mn–O(5) | 96·5 (1) | 3·225 (4) |
| O(2)–Mn–O(6) | 89·3 (1) | 3·094 (3) |
| O(3)–Mn–O(4) | 82·4 (1) | 2·943 (3) |
| O(3)–Mn–O(5) | 164·6 (1) | 4·280 (4) |
| O(3)–Mn–O(6) | 91·5 (1) | 3·151 (3) |
| O(4)–Mn–O(5) | 83·1 (1) | 2·973 (3) |
| O(4)–Mn–O(6) | 81·1 (1) | 2·966 (3) |
| O(5)–Mn–O(6) | 81·3 (1) | 2·878 (3) |
| O(1)–S–O(2) | 104·2 (1) | 2·427 (3) |
| O(1)–S–O(3) | 104·3 (1) | 2·431 (3) |
| O(2)–S–O(3) | 103·4 (1) | 2·396 (3) |

Table 3. *Possible hydrogen bonding*

| | O···O(*W*) | O(*W*)···O | O O(*W*)–O |
|---|---|---|---|
| O(2)···O(*W*5)···O(3) | 2·791 (3) Å | 2·773 (3) Å | 114·9 (1)° |
| Alternative I | | | |
| O(1)···O(*W*4)···O(*W*6) | 2·926 (3) | 2·746 (3) | 115·3 (1) |
| O(1)···O(*W*6)···O(*W*4) | 2·766 (3) | 2·857 (3) | 100·0 (1) |
| Alternative II | | | |
| O(1)···O(*W*4)···O(*W*6) | 2·926 (3) | 2·857 (3) | 121·7 (1) |
| O(1)···O(*W*6)···O(*W*4) | 2·766 (3) | 2·746 (3) | 115·2 (1) |

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*Note added in proof*: The structure of α-$MnSO_3.3H_2O$ has been determined independently by B. Engelen & C. Freiburg [*Z. Naturforsch. Teil B* (1979). **34**, 1495–1499]. They obtained an $R$ value of 0·021 including H atom positions, but there are no significant differences with respect to the Mn and S coordination.

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# Structure of Sodium Sulfate Tellurate

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**Abstract.** $Te(OH)_6.Na_2SO_4$, monoclinic, *Cc*, $a$ = 5·459 (5), $b$ = 10·306 (7), $c$ = 15·349 (10) Å, $\beta$ = 94·73 (5)°, $V$ = 861 (2) Å$^3$, $Z$ = 4, $D_x$ = 2·87 Mg m$^{-3}$. The structure has been determined using the Patterson method and refined to an $R$ value of 0·027 for 2431 independent reflections. The interest of this structure is the presence of two different anions in the same crystal.

**Introduction.** This study is part of a systematic investigation of alkali phosphate- and sulfate-tellurate salts. The chemical preparation and crystal data of the title compound have been reported elsewhere (Zilber, 1980).

A piezo-electric test on the crystal proved to be inconclusive so that doubt remained as to whether the correct space group is *C*2/*c* or *Cc*.

The crystal used was a small, almost cubic prism of approximate dimensions 0·12 × 0·12 × 0·12 mm. 2476 reflections were recorded on a Philips PW 1100 four-circle diffractometer equipped with a graphite monochromator. The radiation used was that of a silver anticathode [$\lambda$(Ag $K\alpha$) = 0·5608 Å]. The angular range was taken between 3 and 23° ($\theta$), the scan speed was 0·02° s$^{-1}$ and the scan width 1·30°. The background was measured for 10 s at each end of the scan range. An $\omega$ scan was used. Because of the small size of the crystal and the radiation used, no correction for absorption was made. Nevertheless, a Lorentz–polarization correction was applied to the data.

The structure was solved using the heavy-atom method. A Patterson function allowed the location of the Te atoms. A Fourier synthesis gave an $R$ factor of 0·53 and allowed the positioning of the O atoms, thus confirming the space group *Cc*. A few more refinements gave the positions of the S and Na atoms. Finally, the unweighted $R$ ($R = \sum||F_o| - |F_c||/\sum|F_o|$) came down to a value of 0·027 and the weighted $R$ $\{R_w = [\sum w(|F_o| - |F_c|)^2/\sum wF_o^2]^{1/2}\}$ to a value of 0·039 for 2431 independent reflections. The quantity minimized was $\sum w(|F_o| - |F_c|)^2$ with $w = \sigma^{-2}(F_o)$ determined by counting statistics. The reflections had $I > 3\sigma(I)$.

Table 1. *Positional parameters* (×10$^4$) *with their estimated standard deviations, and* $B_{eq}$ *for* $Te(OH)_6.Na_2SO_4$

| | $x$ | $y$ | $z$ | $B_{eq}$ (Å$^2$) |
|---|---|---|---|---|
| Te | 0 | 77 (2) | 0 | 0·63 |
| S | 3873 (3) | 2457 (1) | 7483·7 (9) | 0·85 |
| Na(1) | 3405 (5) | 2455 (3) | 1216 (2) | 1·42 |
| Na(2) | 4589 (6) | 747 (3) | 3104 (2) | 1·64 |
| O(1) | 2092 (9) | 3250 (5) | 6937 (3) | 1·45 |
| O(2) | 6353 (8) | 3005 (6) | 7460 (3) | 1·72 |
| O(3) | 3799 (10) | 1116 (5) | 7175 (3) | 1·69 |
| O(4) | 3063 (9) | 2509 (5) | 8392 (3) | 1·42 |
| O(1H) | 1764 (9) | 4877 (7) | 4422 (3) | 2·35 |
| O(2H) | 8235 (6) | 4861 (4) | 5613 (2) | 0·69 |
| O(3H) | 4942 (9) | 3072 (4) | 5194 (3) | 1·35 |
| O(4H) | 3631 (8) | 5318 (4) | 6088 (3) | 1·19 |
| O(5H) | 6386 (8) | 4736 (4) | 3927 (3) | 1·24 |
| O(6H) | 5383 (8) | 6770 (4) | 4890 (2) | 1·08 |

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