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**Manganese bromide tetrahydrate.** By E. D. CROZIER and N. ALBERDING, *Physics Department, Simon Fraser University, Burnaby, BC, Canada V5A 1S6*, and B. R. SUNDHEIM, *Chemistry Department, New York University, 4 Washington Place, New York, NY 10003, USA*

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### Abstract

An EXAFS investigation of  $\text{MnBr}_2 \cdot 4\text{H}_2\text{O}$  has indicated that while the unit-cell dimensions and positional parameters reported by Sudarsanan [*Acta Cryst.* (1975). B31, 2720–2721] are correct, the calculated bond lengths are in error.

The crystal structure of  $\text{MnBr}_2 \cdot 4\text{H}_2\text{O}$  as determined by X-ray diffraction has been reported by Sudarsanan (1975). Discrepancy exists between the Mn–Br bond lengths reported by Sudarsanan and the average bond lengths determined in an EXAFS analysis of polycrystalline  $\text{MnBr}_2 \cdot 4\text{H}_2\text{O}$  at 295K. The Mn and Br *K* edge EXAFS Mn–Br bond lengths are  $2.624 \pm 0.02$  and  $2.628 \pm 0.02$  Å. Details of the EXAFS experiment and analysis are provided as part of a larger study of molten salts containing  $\text{MnBr}_4^{2-}$  and  $\text{MnBr}_3^-$  ions (Crozier, Alberding & Sundheim, 1983). The X-ray diffraction results tabulated in Table 3 of Sudarsanan are repeated in column 2 of our Table 1. Column 3 lists the bond lengths that we have calculated from the unit-cell dimensions and positional parameters given in Tables 1 and 2 of Sudarsanan. Column 4 shows the estimates obtained by adding 0.14 Å, the difference between the ionic radii of Br and Cl (Pauling, 1960), to the Mn–Cl bond lengths determined for the isostructural  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$  (Zalkin, Forrester & Templeton, 1964). Column 4 also

includes the Mn–O bond lengths calculated for  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ . Thus, on the basis of the agreement of the EXAFS result and columns 3 and 4, it is concluded that Tables 1 and 2 of Sudarsanan correctly describe the crystal structure of  $\text{MnBr}_2 \cdot 4\text{H}_2\text{O}$  but that Table 3 and the conclusions based on it are in error.

Table 1. Bond lengths (Å) in  $\text{MnBr}_2 \cdot 4\text{H}_2\text{O}$

|          | Table 3<br>(Sudarsanan, 1975) | Recalculated | Estimated from<br>$\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ |
|----------|-------------------------------|--------------|---|
| Mn–Br(1) | 2.802                         | 2.652 (2)    | 2.640   |
| Mn–Br(2) | 2.913                         | 2.627 (2)    | 2.615   |
| Mn–O(1)  | 2.247                         | 2.218 (6)    | 2.224   |
| Mn–O(2)  | 2.221                         | 2.191 (6)    | 2.209   |
| Mn–O(3)  | 2.475                         | 2.176 (6)    | 2.184   |
| Mn–O(4)  | 2.369                         | 2.216 (6)    | 2.181   |

### References

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