

appreciably unequal, these sites would also be disordered in $P1$. Similarly, the occupancy of at least one of the two (M , Zr) sites would be disordered if there is any Zr present. (The possibility that one site is entirely M and the other entirely Zr is ruled out both by the values of the parameter P_2 and by the relatively unsatisfactory results obtained by GBG.) In any event, there is little prospect of detecting any slight deviations from the centrosymmetric $P\bar{1}$ structure, particularly since GBG followed the usual (and regrettable) procedure of deleting the weakest reflections from their data set (see Marsh, 1981).

Finally, we come to the title question: How much Zr is present in either compound? I believe that the answer is 'Only a small amount'. The small amount would presumably be accompanied by a corresponding deficiency in the occupancy of the Na^+ sites; according to Goodenough, Hong & Kafalas (1976), such a deficiency would be a prerequisite for Na^+ mobility. It also seems probable that the amount of Zr can vary from one preparation to another, along with the conductivity of the crystals. I see little chance that the site of the additional proton, H, is other than fully occupied, because of the very short $\text{O}\cdots\text{O}$ distance. Indeed, this strong $\text{O}\cdots\text{H}\cdots\text{O}$ bond increases the rigidity of the MHP_2O_7 framework (note the small size of

the U_{eq} values, Tables 1 and 2), which is another requirement for rapid ion transport (Goodenough *et al.*, 1976). Thus, the correct formula for the compounds is, presumably, $\text{Na}_{1-2x}\text{M}_{1-x}\text{Zr}_x\text{HP}_2\text{O}_7$, with x being 0.1 or less. Note, though, that the results reported here (Tables 1 and 2) were based on a model corresponding to $x = 0$ – that is, to NaMHP_2O_7 .

I greatly appreciate the advice and comments of Dr E. Fowles.

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