

atoms by difference Fourier techniques, H-atom positions refined, 3000 data points, 0.64–2.61 Å *d* space range, 848 contributing reflections, $R_{wp} = 0.0193$, neutron scattering lengths (Koester & Steyert, 1977), other refinement information in Table 1.*

Results and discussion

The final difference plot for the neutron TOF Rietveld refinement is shown in Fig. 1. The atom positions (both H and non-H) closely agree with those of $\text{NaMn}_2(\text{OH})(\text{H}_2\text{O})(\text{MoO}_4)_2$ (Clearfield, Moini & Rudolf, 1985). The Ni–O bond distances are very similar to each other [2.066 (3)–2.078 (5) Å], and the bond angles indicate the formation of a slightly distorted octahedron [81.1 (2)–98.9 (2)°]. On the other hand, the MoO_4 unit forms a regular tetrahedron consisting of three Mo–O bonds with very close distances [1.751 (7)–1.779 (5) Å] and one which is relatively longer [1.833 (10) Å]. The arrangement of the hydroxyl and water groups found for the $\text{NaMn}_2(\text{OH})(\text{H}_2\text{O})(\text{MoO}_4)_2$ structure is therefore confirmed. The O4–H1 distance of 1.009 (11) Å is about 0.14 Å longer than in the X-ray Mn phase. This lengthening is due to the neutron technique (Ceccarelli, Jeffrey & Taylor, 1981). The fully occupied H1 position is found to be hydrogen bonded, in the *c* direction, to O1 at a distance of 1.724 (11) Å. On the other hand, the half-occupied H2 does not enter into any hydrogen bonding with framework O atoms. The O4–H2 bonding vector is primarily in the *a* direction and is symmetry constrained. The lack of hydrogen bonding by this H atom results in the rather

long O4–H2 distance of 1.294 (26) Å, and compared with the other H atom (*cf.* e.s.d.'s) is much more free to move. The coordination of O atoms around the Na atom represents a distorted octahedral arrangement with two of the angles approximately 12° from the ideal arrangement. Final atom positions show the title compound to be isostructural with $\text{NaMn}_2(\text{OH})(\text{H}_2\text{O})(\text{MoO}_4)_2$.

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* Positional and thermal parameters and all important bond distances and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43149 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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