*American Mineralogist, Volume 85, pages 745–752, 2000*

# Two proton positions in the very strong hydrogen bond of serandite, $NaMn_2[Si_3O_8(OH)]$

**STEVEN D. JACOBSEN,[1,2,]* JOSEPH R. SMYTH,[1,2] R. JEFFREY SWOPE,[1] AND ROBERT I. SHELDON[3]**

[1]Department of Geological Sciences, University of Colorado, Boulder, Colorado 80309-0399, U.S.A.
[2]Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany
[3]Los Alamos National Laboratory, Los Alamos, New Mexico, 87545, U.S.A.

## ABSTRACT

The crystal structure and hydrogen positions of serandite, $NaMn_2[Si_3O_8(OH)]$, have been refined from single-crystal X-ray and time-of-flight neutron diffraction data at ambient conditions. The proton occupies an asymmetric, double-well position between O3 and O4, confirming one of the shortest asymmetric hydrogen bonds known in minerals with $d$(O3…O4) = 2.464(1) Å (X-ray) and 2.467(1) Å (neutron). The proton position closest to O3 has about 84% occupancy and an O-H distance of 1.078(3) Å, and the position closest to O4 has an occupancy of 16% and an O-H distance of 1.07(1) Å. The $d$(H…O) of these hydrogen bonds is 1.413(3) Å and 1.41(1) Å, respectively. Hydrogen bond angles are 164° for H1 and 168° for H2. The $Si^{IV}$-OH bond length [1.628(1) Å] is intermediate in length among the three other Si-O bonds in the dominantly (84%) hydrated Si1 tetrahedron. These new structure data for a very strong hydrogen bond may be useful for extending spectroscopy-structure correlation diagrams into the region of very low energy O-H stretching.