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A variable-temperature neutron diffraction study of serandite: A Mn-silicate framework with a very strong, two-proton site, hydrogen bond

Edward R. Williams[1] and Mark T. Weller[1,*]

[1]Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, U.K.

Abstract

A variable-temperature powder neutron diffraction study of serandite, $Na(Mn,Ca)_2Si_3O_8(OH)$, has been undertaken over the temperature range 4–800 K to investigate the behavior of the very strong hydrogen bond in this mineral. At 4 K the O(D)···O(A) distance in serandite has been determined to be extremely short at 2.413(10) Å. The distribution of hydrogen along the O3···O4 direction at low temperatures confirms that reported previously at room temperature with one site, bonded to O3, strongly, but not exclusively, favored; the origin of the occupation of this preferred site has been assigned to additional weak hydrogen bonding interactions. At higher temperatures the hydrogen distribution along the O3···O4 direction becomes increasingly random as the thermal energy and motion outweigh the weak hydrogen bonding. The data also show that calcium substitutes only on one manganese site, Mn2 in the mineral structure.

Keywords: Hydrogen bonding, serandite, neutron powder diffraction, variable-temperature