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Sursassite: Hydrogen bonding, cation order, and pumpellyite intergrowth

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Abstract

The crystal chemistry of sursassite, simplified formula $Mn_2^{2+}Al_3Si_3O_{11}(OH)_3$, from six different localities [(1) Falotta, Switzerland, (2) Woodstock, New Brunswick, Canada, (3) Kamisugai, Japan, (4) Kamogawa, Japan, (5) Molinello, Italy, and (6) Gambatesa, Italy] was studied using electron microprobe analysis (EMPA), Fourier transform infrared spectroscopy (FTIR), and single-crystal X-ray diffraction methods. The structure has two symmetry independent Mn sites. The Mn1 site is seven coordinated by O and hosts, in addition to Mn^{2+}, up to 20% Ca, whereas Mn2 has octahedral coordination and is strongly selective for Mn^{2+}. In the simplified formula, three smaller octahedral M sites are occupied by Al. However, M1 also accepts significant amounts of divalent cations, such as Cu, Mg, Fe, and Mn, whereas M2 is occupied exclusively by Al. The unit-cell parameters of sursassite are a = 8.698–8.728, b = 5.789–5.807, c = 9.778–9.812 Å, β = 108.879–109.060°, V = 465.7–470.0 Å^3, the space group is $P2_1/m$. Structure refinements converged to R_1 values of 2.15–6.62%. In agreement with bond-valence analyses, at least three OH groups, depending on the concentration of divalent cations at M1, are found at the O6, O7, and O11 positions. However, the bond-valence sum at O10 is always low, thus partial hydroxylation is assumed at O10 to maintain charge balance. Owing to the influence of divalent cations at M1 in sursassite the hydrogen-bond systems in sursassite and isostructural macfallite are different. The FTIR spectrum in the region of OH-stretching vibrations is characterized by three strong bands at 3511, 3262, and around 2950 cm^{-1}, the latter being broad. The band at 2950 cm^{-1} is assigned to strong hydrogen bonds between O6 and O10 (O6···O10 = 2.66 Å). Residual difference-Fourier peaks in the refinement of the Kamogawa and Molinello (specimen 1) crystals indicated less than 5% pumpellyite intergrowth.

Keywords: Sursassite, hydrogen bond, infrared spectroscopy, crystal structure, macfallite, pumpellyite