LOCATION OF HYDROGEN ATOMS IN PREHNITE

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The mineral prehnite, $Ca_2Al(AlSi_3O_{10})(OH)_2$, is an important metamorphic mineral, paired with pumpellyite as metamorphic grade indicator between the zeolite and greenschist facies, and is also present in the higher levels of subduction zones. The structure of prehnite can be described as a mixed layer silicate consisting of stacked sheets of SiO_4 and $(Si,Al)O_4$ tetrahedra linked by sheets of $AlO_4(OH)_2$ octahedra. Ca atoms occupy cages formed by the framework (Fig 1). Previous studies using high precision single crystal x-ray diffraction were performed on prehnite specimens from Austria, Norway, Mali; and South Africa to determine the space group symmetry and Al/Si arrangement (Detrie, 2006). The hydrogen atom was not able to be determined using x-ray diffraction because the hydrogen atom is not a strong scatterer of electrons; therefore x-rays are unsuitable for determining the location of hydrogen. In order to determine the location of hydrogen, a proposal for a neutron diffraction study was submitted to ISIS, a pulsed neutron source located near Oxford, UK. Two days of beamtime were granted on the time-of-flight diffractometer, POLARIS. A 2.7 g natural sample of prehnite from Mali was powdered and measured at room temperature and at 2 K in a cryostat. Data from two sets of detector banks is being refined using the Rietveld method to determine the location hydrogen atoms in the structure. These locations will illustrate how the hydrogen atom aids in linking the octahedral sheets, as well as resolve strength and directionality of the hydrogen bonding. This study compliments our previous Raman spectroscopic study, allowing for a more comprehensive interpretation of behavior, and provides a basis for upcoming high-pressure x-ray and spectroscopic studies of this important mineral.

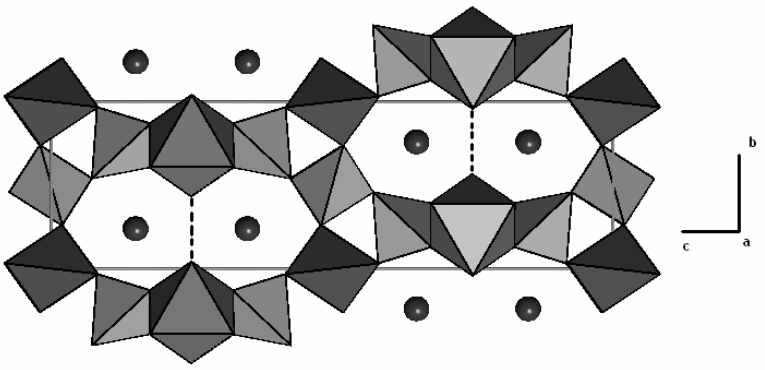

Figure 1: View of the prehnite unit cell down (100) showing AlO_4 tetrahedra (medium gray), SiO_4 tetrahedra (light gray) and AlO_6 octahedra (dark gray) with Ca atoms (black spheres). The dashed line represents the hydrogen environment currently under investigation.

References Cited:

Detrie, T.A., Ross, N.L., Zhou, J., and Angel, R.J. (2006) High pressure Raman spectroscopic study of prehnite $Ca_2Al(AlSi_3O_{10})(OH)_2$. (*in* Geological Society of America, 2006 Annual Meeting) Abstracts with Programs- Geological Society of America, 38 (7), 293.

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