



Neutron diffraction studies on hydrous layer silicates: Structure and dynamics of intercalates

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The crystal structures of most of the naturally occurring hydrous layer silicate minerals, e.g. magadiite and kenyaite, are still unknown because of severe disorder in the structure. In layer silicates an extensive part of the structure is made of surface-like, negatively charged silicate units which are accessible for interaction with solvent and cations. Because of its periodic order diffraction techniques can be used to study the structure and composition of the material, and, in particular, the interaction of the solvent and cations with the silicate surface. RUB-18 is a synthetic member of the family of hydrous sodium layer silicates which has been studied intensively owing to the excellent crystallinity of the material. This material serves as model system for investigations of the interaction of silicate surfaces with solvent (water) and cations.

RUB-18, $\text{Na}_8[\text{Si}_{32}\text{O}_{64}(\text{OH})_8] \cdot 32\text{H}_2\text{O}$, was studied as parent material and in modified and exchanged forms using powder Neutron diffraction data recorded at D2B, ILL Grenoble(F) and HRPT, PSI Villingen(CH).

In combination with NMR and QENS experiments the proton disorder and proton dynamics were studied in the parent material at temperatures between RT and 345 K. It has been shown that local disorder of protons at RT changes to proton conduction at temperatures above ca. 310 K.

The structure of the Ca- and H-exchanged forms, $\text{Ca}_8[\text{Si}_{32}\text{O}_{72}] \cdot 16\text{H}_2\text{O}$ and $\text{H}_{16}[\text{Si}_{32}\text{O}_{72}]$, were studied using a combination of Neutron and X-ray powder diffraction. The structure analyses showed that in the Ca-form 50% of the hydrate water with respect to the Na-salt is removed whereas the H-form is water free.

In order to study the molecular interaction of organic molecules with the silicate surface acetone and glycine were intercalated. Powder Neutron diffraction data were used to refine the crystal structures which show the intercalation of the organic molecules in stoichiometric relation between the silicate layers.