Structure Solution of the Highly Disordered Layer Silicate H-RUB-18
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H-RUB-18 is a layer silicate of the chemical formula Si$_3$O$_{56}$(OH)$_{16}$. At standard pressure two modifications of H-RUB-18 are known, a low temperature (α-) form stable at temperatures $T < \sim 343$ K and a high temperature (β-) form stable between $\sim 343$K and the decomposition temperature. One of H-RUB-18 remarkable properties is the intercalation of organic molecules$^1$.

H-RUB-18 is obtained from the layer silicate Na-RUB-18 ($\text{Na}_8\text{[Si}_3\text{O}_{64}(\text{OH})_8]\times 32\text{H}_2\text{O}$) by ion exchange with diluted acids. From chemical analysis it is known that all Na$^+$-ions are replaced by protons. Karl-Fischer titration and thermal analysis proved that in contrast to most layer silicates H-RUB-18 contains no free hydrate.

The powder diffraction pattern of H-RUB-18 is of low resolution. Because of the poor periodic register of neighboring layers only a few broad reflections with anisotropic linewidths arise from the background. Therefore it is not possible to solve the structure only from the XRD-data. NMR studies give hints that the layerlike silicate anions of H-RUB-18 and Na-RUB-18$^2$ have the same topology. Moreover the NMR spectra indicated that the silicate units are fairly ordered at short range (i.e. within the layerlike unit).

Based on all experimental evidence an approximate model of the crystal structure was developed. This model served as starting conformation for MD-calculations, which have been performed with the program package InsightII$^3$ using a forcefield specifically developed and tested for this type of problem. Depending on the simulation conditions two reasonable structures were obtained, which are in good agreement with the powder pattern of the α- or β- form of H-RUB-18. These structures are used as start values for the Rietfeld refinement by TOPAS$^4$. Since the simulation also showed different possible sites for the atoms, the resulting stacking faults become obvious and offer the possibility of a reasonable refinement using split positions for certain atoms.