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ABSTRACT BOOK

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NMR INVESTIGATION OF NATROLITE STRUCTURE

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The mineral natrolite ($\text{Na}_2\text{Al}_2\text{Si}_3\text{O}_{10}\text{H}_2\text{O}$) is the typical channel-type compound with porous structure (zeolite). The natrolite unit cell is orthorhombic with space group $Fdd2$. The natrolite aluminosilicate framework contains AlO_4 and SiO_4 tetrahedra, bonded via common oxygen atoms. The water molecules are situated at regular positions within the channels and form hydrogen bonds to oxygen's atoms of the aluminosilicate structure. The sodium ions are situated at regular positions within the channels also.

In this study we have undertaken a detailed investigation of natrolite structure by Nuclear Magnetic Resonance (NMR) of ^1H , ^{23}Na and ^{27}Al nuclei. From the temperature dependencies of the NMR spectra of ^1H nuclei it follows that there are two different kinds of the water molecular motion. The molecular motion of the first kind is the 180° flip motion and second one is the diffusion of the water molecules. From NMR data it follows that water molecules diffuse along the vacancies whose positions coincide with the regular positions of water molecules. From the temperature dependencies of the NMR spectra of ^{23}Na and ^{27}Al nuclei it follows that observed transformations of NMR spectra are concerned with the diffusion of the water molecules and with the dehydration of water molecules. The obtained results have been compared with results published early [1-13].

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