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ABSTRACTS

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DQ-10/13 **MODEL OF WATER DIFFUSION IN A NATROLITE**

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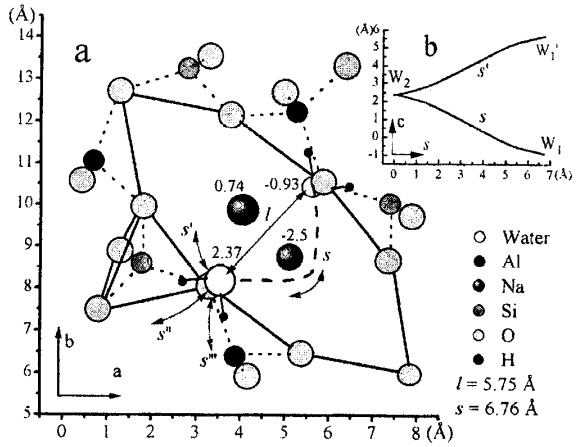

Fig.1. Projection of the trajectory water molecule in a natrolite channel. (a) - projection on (001) plane, (b) - vertical profile of trajectory. *s* - path of diffusion, *l* - short distance between water positions.

The water mobility at different path of diffusion in natrolite ($Na_{16}[Al_{16}Si_{24}O_{80}]\cdot 16H_2O$) was investigated using ^{1}H-NMR line-shape analysis. Earlier it has been known that molecular motion in natrolite of the first kind is the 180^0 flip motion and second one is the regular diffusion of water molecules [1,2]. From our investigation it was be obtained that for temperatures higher then 250 K the diffusion along the c-axis is begin with activation energy 39.7 kJ/mol (fig.1; s, s'). From the analysis of a natrolite structure and NMR date it follows, that the 180° flip motion take place simultaneously with diffusion along the c-axis. Besides in a natrolite there are two paths for diffusion in channels perpendicular c-axes (s", s"'). If temperatures is higher than 350 K water molecules diffuses in channels of a perpendicular c-axis. It is possible to assume that for one from paths of diffusion the barrier is 58.5 kJ/mol. For the other diffusion path the barrier is ~ 70 kJ/mol.

From ^{1}H line shape studies a distribution of correlation time for diffusing molecules was observed [3]. In the report it is discussed the possible reasons for distribution of correlation time such as heterogeneous distribution of vacancies in zeolite channel and the availability of nonequivalent paths for a diffusion. In the fig. 1 it is shown one from possible real trajectory (*s*) of water molecule diffusion. This trajectory fulfils the condition of minimum deformation of electronic orbit of ions. The results of evaluations of interaction forces of ions and water molecules for all possible paths for diffusion are represented.

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