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ABSTRACTS

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EQ – 11/8 NMR STUDY OF THE MOLECULAR MOBILITY AND DEHYDRATION IN NATROLITE, A FIBROUS ZEOLITE.

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The temperature dependencies of NMR spectra of ^1H nucleis in natrolite $Na_2Al_2Si_3O_{10}\cdot 2H_2O$ have been studied. The water and Na^+ occur in zig-zag chains along the zeolite channel. Together with the two oxygen atoms and of the two sodium ions they give a tetrahedral geometry about the water molecule. From NMR data it follows that water molecules diffuse along the vacancies whose positions coincide with the regular positions of water molecules [1]. At room temperature the intermolecular dipolar interactions between magnetic moments of the water protons lead to the broadening of the doublet lines and the observed NMR spectrum consists the non-resolved doublets. The heating of the crystal induces the motional average of the intra- and intermolecular dipolar H-H interactions and at the high temperature the single narrow doublet is observed [1]. Width and speed of a line narrowing depends on a thermal history of a crystal. The temperature dependence of a linewidth the doublet component is given in Fig. 1. It is possible to select two cases. The first case when a crystal the first time heats up above than room temperature. The second case, when a crystal previously heated up above 120°C. In second case we observed a linewidth narrowing has a place in two stages (curve 2). After exposure of a crystal during 2 day at the room temperature and normal humidity the initial dependence of spectrum was restored (curve 1). The presence of two steps a line narrowing is result of change in the mechanisms or paths of a molecular diffusion after heating of crystal. The reason it can be effect of partial dehydration of a crystal. Earlier thermal measurements of a natrolite were realising on powders [2,3]. For a comparison with NMR data the study of lose/regain water was done on monocrystal. After heating a crystal of natrolite up to 120°C a weight loss does not exceed the error of measuring. The study of dehydration of a natrolite has shown that in temperature range up to 180°C natrolite crystal loses about 0.4 % of water. In conditions of normal humidity and room temperature during 2-3 day the initial water content are restored. For example, the rehydration of a powder on air is happens during a few hours. The partial dehydration is creating a quantity of vacancies much greater, than quantity of equilibrium vacancies. After crystal is cooling up to room temperature this vacancies quantity are fixed. In the result it distorted chains Na···-···H_2O···-···Na···-... in a natrolite channels. And it rises the barrier of diffusion from 45 up to 63 kJ/mol. The other models of molecular mobility also are discussed.

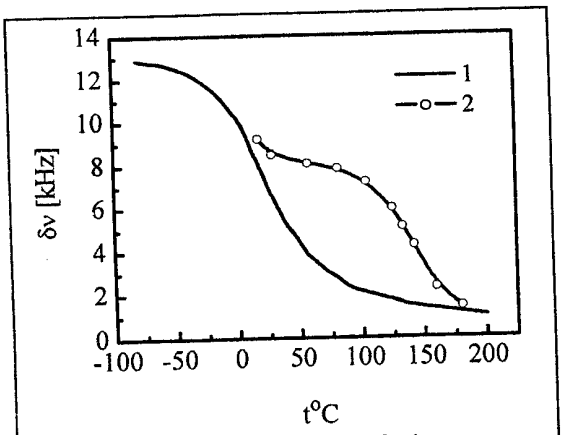

Fig. 1. Linewidth (δν) of the proton resonance vs. temperature in natrolite when the magnetic field $\mathbf{B}_0$ is parallel to *b* direction. 1- is the first cases; 2- is the second case (15 hours after heating).

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