MITT.ÖSTERR.MINER.GES. 149 (2004)

NMR STUDIES OF MOLECULAR DIFFUSION AND PROTON TRANSFER IN HYDRATED MINERALS

Moroz, N.K.

Institute of Inorganic Chemistry, Russian Academy of Sciences, Siberian Branch
Avenue Lavretiev 3, 630090 Novosibirsk, Russian Federation
e-mail: moroz@che.nsk.su

The physical-chemical properties of hydrated minerals in which the H_2O molecules are located in structural cavities, channels or between layers, essentially depend on the librational and translational motions of the water molecules (WINKLER, 1996; PAUKOV et al., 2002). Along with infrared-, dielectric-spectroscopy, and incoherent neutron scattering, the most often used technique to determine the low-frequency dynamics of molecular H_2O in minerals is ^{1}H-NMR spectroscopy (STEBBINS, 1988). Recently, we proposed a new wide-line ^{1}H NMR approach based on the consideration of the anisotropy of the fluctuations of the intramolecular proton-proton interaction, arising during the process of the H_2O molecular diffusion. With this approach, a number of intriguing results, such as the pressure-enhanced H_2O self-diffusion in natural zeolites (MOROZ et al., 2001), have been obtained. The ensuing development of the approach discussed enabled us to suggest a way to measure the rates of the proton-transfer reactions in water subsystems of hydrated microporous minerals (AFANASSYEV et al., 2000; AFANASSYEV & MOROZ, 2003). It has been shown that the intermolecular proton transfer is due to the interaction of water molecules with the protonic defects, presented by the acid (Brønsted) cites. As a rule, these reactions are exhibited at temperatures corresponding to the intense H_2O self-diffusion. These circumstances allow one to use water molecules as a NMR molecular probe for visualization of the active acid sites and consequently for characterization of the catalytic activity of minerals even if the site concentration is small enough that obstacle its detection with available spectroscopic techniques (MOROZ et al., 2003).

This work was supported by Russian Academy of Sciences (Program #26, Hydrogen Energetic).

References

AFANASSYEV, I.S. & MOROZ, N.K. (2003): Solid State Ionics, **160**: 125-129.

AFANASSYEV, I.S., MOROZ, N.K. & BELITSKY, I.A. (2000): J. Phys. Chem. B, **104**: 6804-6808.

MOROZ, N.K., AFANASSYEV, I.S., PAUKSHTIS, E.A. & VALUEVA, G.P. (2003): Phys. Chem. Minerals, **30**: 243-247.

MOROZ, N.K., KHOLOPOV, E.V., BELITSKY, I.A. & FURSENKO, B.A. (2001): Micropor. Mesopor. Mater., **42**: 113-119.

PAUKOV, I.E., MOROZ, N.K., KOVALEVSKAYA, Y.A. & BELITSKY, I.A. (2002): Phys. Chem. Minerals, **29**: 300-306.

STEBBINS, J.F. (1988): In: HAWTHORNE, F.C. (ed.) Spectroscopic Methods in Mineralogy and Geology. Rev. Mineral., 18, Miner. Soc. Amer., Washington D.C., 405-429.

WINKLER, B. (1996): Phys. Chem. Minerals, **23**: 310-318.