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Lithium Ion and Water Mobility in Hydrated Li-LSX Zeolite Studied by ^{1}H, ^{6}Li and ^{7}Li NMR Spectroscopy and Diffusometry

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Crystallites of zeolite LSX with a diameter of about 10 µm are shown to allow the simultaneous investigation of intracrystalline mass transfer phenomena of water molecules and lithium ions in hydrated zeolite Li-LSX by NMR diffusometry. By MAS NMR spectroscopy with the ^{1}H and ^{6}Li nuclei, the water molecules and lithium ions are found to yield two signals, a major and a minor one, which may be attributed to locations in the sodalite cages and the supercages, respectively. By ^{1}H and ^{6}Li exchange spectroscopy the mean residence times in the sodalite cages at 373 K are found to be about 150 ms for the water molecules and about 40 ms for the lithium cations [1].

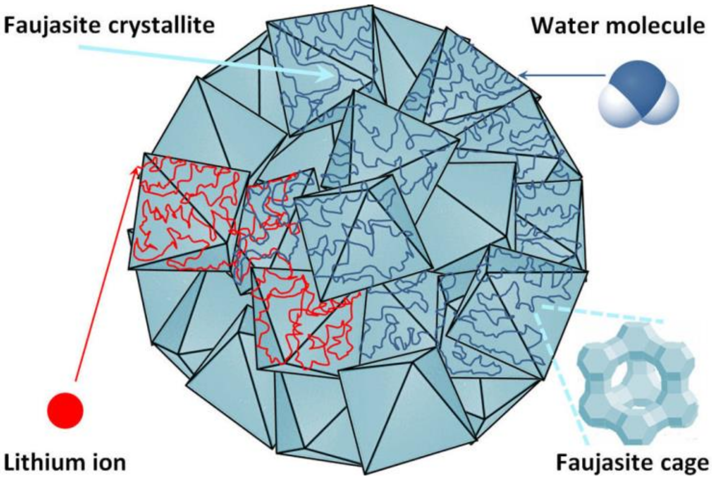

Fig. 1. Lithium and water diffusion in Li-LSX zeolite Li-LSX [2].

PFG NMR measurements of cation diffusion in zeolites were first published in Refs. [1] and [2]. Whilst, under the given experimental conditions, the water diffusivity at 373 K could be determined to be of the order of 2.5×10^{-10} m^{2}s^{-1} or even larger, the diffusivity of the lithium ions in the same sample and at the same temperature was found to be $(2.0 \pm 0.8) \times 10^{-11}$ m^{2}s^{-1}. This yields to a Haven factor of about 10 for the ion conductivity in the zeolite Li-LSX. The observed propagation patterns reveal, for both the water molecules and the cations, two types of transport resistances, acting in addition to the diffusion resistance of the genuine pore network. They are attributed to the interfaces at the boundary between the purely crystalline regions (crystallites) within the Li-LSX particles (intergrowths) under study and to the external surface of either the particles themselves or crystallite aggregates within these particles.

The new options provided by the high-intensity device for PFG NMR diffusion measurement applied in this study for the measurement of the intracrystalline diffusion of both the cations and the guest molecules in zeolite Li-LSX, in purposeful combination with the information accessible by PFG MAS NMR and two-dimensional MAS NMR spectroscopy, have all potentials for opening new routes for a deeper understanding of the dynamic processes in host-guest systems under the involvement of exchangeable cations.

References

[1] D. Freude, S. Beckert, F. Stallmach, R. Kurzhals, D. Täschner, H. Toufar, J. Kärger, J. Haase: Ion and water mobility in hydrated Li-LSX zeolite studied by ^{1}H, ^{6}Li and ^{7}Li NMR spectroscopy and diffusometry. *Microporous Mesoporous Mater.* **172** (2013) 174–181.

[2] S. Beckert, F. Stallmach, H. Toufar, D. Freude, J. Kärger, J. Haase: Tracing Water and Cation Diffusion in Hydrated Zeolites of Type Li-LSX by Pulsed Field Gradient NMR. *J. Phys. Chem. C* **117** (2013) 24866−24872.