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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].

As to our knowledge, PFG NMR measurements of cation diffusion in zeolites have never been performed. 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 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.

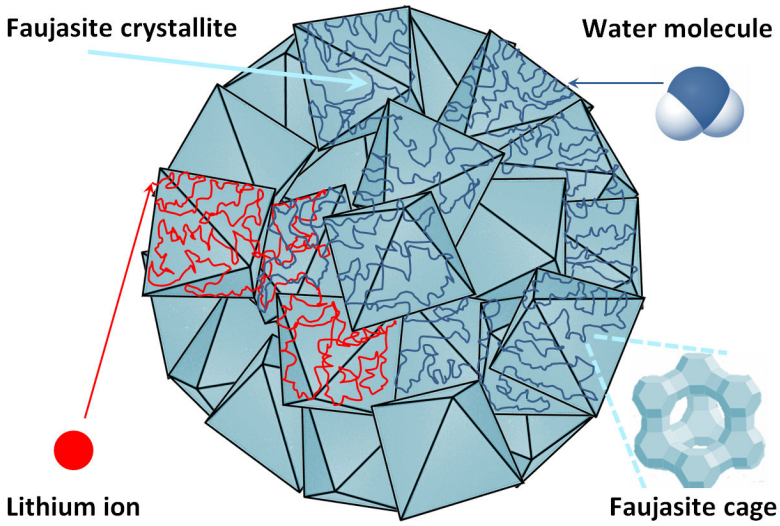

Figure 1: Water and ion diffusion in the package of zeolite crystallites.

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 Materials **172**, 174–181 (2013)