Diffusion of Water in Li-Montmorillonite Studied by Quasielastic Neutron Scattering

D. J. Cebula[1], R. K. Thomas and J. W. White

Physical Chemistry Laboratory, South Parks Road, Oxford, OX1 3QZ, United Kingdom
Institut Laue-Langevin, X156 Centre de Tri, Grenoble 38042 Cedex, France

[1] Present address: Institut Laue-Langevin, Grenoble, France.

Abstract: The diffusion of water in Li-montmorillonite was studied by incoherent quasielastic neutron scattering. Experiments were carried out on sedimented samples equilibrated at relative humidities of 32%, 58%, and 98%, corresponding approximately to 1, 2, and 3 molecular layers of water in the clay. At all three humidities, although the mobility of the water molecules is less than in bulk water, all water molecules in the system undergo translational diffusion, at least over short distances (>5 Å), with correlation times shorter than 5×10^{-11} sec.

Various models of molecular motion have been used to account for the exact shape of the scattering. The only completely successful model is one where a water molecule undergoes jump-translational diffusion and rotational diffusion. The mean square jump length is $10-15$ Å^2 with a residence time between jumps of $4-2 \times 10^{-11}$ sec. The translational diffusion coefficient increases with humidity, having values of 4, 7, and 10×10^{-10} m^2/sec for the three humidities. These values can be combined with values previously obtained by tracer measurements to give an estimate of $0.75-0.8$ for the tortuosity factor. Although the samples are anisotropic, there is no clear evidence that the diffusion of water over distances $5-20$ Å is anisotropic. An upper limit of 3 can be deduced for the rate of diffusion parallel to the direction perpendicular to the platelets.

Key Words: Diffusion • Montmorillonite • Neutron scattering • Water

Clays and Clay Minerals; August 1981 v. 29; no. 4; p. 241-248; DOI: 10.1346/CCMN.1981.0290401

Clay Minerals Society (www.clays.org)