Effects of Clay Fraction and Temperature on the H₂O Self-Diffusivity in Hectorite Gel: A Pulsed-Field-Gradient Spin-Echo Nuclear Magnetic Resonance Study

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Abstract: Self-diffusion coefficients of H_2O molecules in Na-rich hectorite gel were measured by ¹H nuclear magnetic resonance (NMR). Spin-echo pulse sequences with magnetic field gradient pulses for the translational diffusion measurement were applied to the hectorite gel at the Larmor frequency of 20 MHz. Effects of clay fraction (0– 51.2 wt. %) and temperature (20.0– 60.3° C) were studied. The results show: (1) Phenomenologically, the self-diffusion coefficient, *D*, of ¹H₂O in the clay gel is expressed by the normalized diffusivity, $D/D_0 = \exp(-0.0257w)$, where D_0 is the water self-diffusivity in bulk water at temperature and *w* is the weight fraction of the hectorite (wt. %). (2) The activation energy of H₂O diffusivity in the hectorite gel is nearly equal to that in bulk water. Hence, the normalized diffusivity, D/D_0 , obeys a temperature-independent curve. (3) The exponential dependence of D/D_0 on *w* for w <30 wt. % is explained by a random-walk model, in which free or unbound H₂O molecules migrate in the geometrically complex and tortuous pore structure of randomly scattered clay-mineral grains.

Key Words: Complexity of Pore Structure • Hectorite • H₂O • NMR • Self-Diffusion

Clays and Clay Minerals; December 2000 v. 48; no. 6; p. 603-609; DOI: <u>10.1346/CCMN.2000.0480602</u> © 2000, The Clay Minerals Society Clay Minerals Society (<u>www.clays.org</u>)