Monte Carlo Simulation of the Total Radial Distribution Function for Interlayer Water in Sodium and Potassium Montmorillonites

Garrison Sposito, Park Sung-Ho and Rebecca Sutton

Earth Sciences Division, Mail Stop 90-1116, Lawrence Berkeley National Laboratory, Berkeley, California 94720-3110

Abstract: Monte Carlo simulations based on tested water-water, cation-water, and water-clay potential functions were applied to calculate radial distribution functions for O-O, O-H and H-H spatial correlations in the interlayer region of the two-layer hydrates of Na- and K-montmorillonite. The simulated radial distribution functions then were used to compute the total radial distribution function for interlayer water, a physical quantity that can be determined experimentally by H/D isotopic-difference neutron diffraction. The simulated total radial distribution functions were compared with that for bulk liquid water, and with a total radial distribution function determined experimentally for the two-layer hydrate of Na-montmorillonite by Powell *et al.* (1997). This comparison suggested that water molecules in the two-layer hydrate of montmorillonite have nearest-neighbor configurations which differ significantly from the tetrahedral ordering of nearest neighbors that characterizes bulk liquid water.

Key Words: Adsorbed Water • Montmorillonite • Neutron Diffraction • Water

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