Monte Carlo Simulation of Interlayer Molecular Structure in Swelling Clay Minerals. 2. Monolayer Hydrates

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Abstract: Monte Carlo (MC) simulations of interlayer molecular structure in monolayer hydrates of Na-saturated Wyoming-type montmorillonites and vermiculite were performed. Detailed comparison of the stimulation results with experimental diffraction and thermodynamic data for these clay-water systems indicated good semiquantitative to quantitative agreement. The MC simulations revealed that, in the monolayer hydrate, interlayer water molecules tend to increase their occupation of the midplane as layer charge increases. As the percentage of tetrahedral layer charge increases, water molecules are induced to interact with the siloxane surface O atoms through hydrogen bonding and Na^+ counter-ions are induced to form inner-sphere surface complexes. These results suggest the need for careful diffraction experiments on a series of monolayer hydrates of montmorillonite whose layer charge and tetrahedral isomorphic substitution charge vary systematically.

Key Words: Clay water systems • Monte Carlo simulation • swelling clays

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