
Mixed Layering of Illite-Smectite: Results from High-Resolution Transmission Electron Microscopy and Lattice-Energy Calculations

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Abstract: Mixed layering of illite-smectite was studied both experimentally, by using high-resolution transmission electron microscopy (HRTEM) and analytical electron microscopy (AEM), and theoretically, by using lattice-energy calculations.

Samples from a hydrothermal origin show the transformation of smectite to illite with different ordering types in the illite-smectite layer sequences. Ordering ranges from complete disordered (Reichweite, $R = 0$ type) in the less transformed samples to increased local order, with IS and IIS sequences ($R = 1$ and $R = 2$, respectively; I = illite, S = smectite) in more illitized samples.

Lattice-energy calculations are used to determine the structure of the illite-smectite sequence, which corresponds to the minimum energy. The unit layers are: $O_{0.5}TI' TO_{0.5}$ (O, T, and I' , respectively, denote the octahedral and tetrahedral sheets, and the interlayer. The 0.5 signifies half of the octahedral cations.) For example, the arrangements of the perfectly ordered \cdots ISIS \cdots and \cdots IISIIS \cdots sequences are respectively $\cdots O_M(TI' T)_1 O_M(TI' T)_S \cdots$ and $\cdots O_M(TI' T)_1 O_1(TI' T)_1 O_M(TI' T)_S \cdots$ (the subscripts I, S, and M, respectively, refer to compositions of illite, smectite, and midway between at 0.5).

Such arrangements produce a polar model for TOT layers, which display a $T_1 O_M T_S$ structure in the case of IS adjacent layers.

Furthermore, the lattice energies of \cdots ISIS \cdots and \cdots IISIIS \cdots are found to be nearly equal to the corresponding sums of the lattice energies of illite and smectite. This result indicates that interstratified illite-smectite and the two-phase assemblage of illite + smectite have similar stabilities.

On the basis of the above model, the solid-state transformation of one smectite layer to one illite layer, which produces mixed-layer sequences, involves the transformation of an $O_{0.5}TI' TO_{0.5}$ unit of smectite into the same corresponding unit of illite.

Key Words: HRTEM-AEM • Illite-Smectite • Lattice-Energy Calculations • Mixed Layering • Polar 2:1 Layers

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