
Rotationally Disordered Illite/Smectite in Paleozoic K-Bentonites

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Abstract: The three-dimensional crystal structure of rotationally disordered illite/smectite (I/S) in K-bentonite samples from the Appalachian basin and neighboring areas is described using the parameters of 1) P_0 , the proportion of zero-degree layer stacking rotations, such as in the polytype series *IMd-IM*; 2) P_{cv} , the proportion of 2:1 layers with *cis*-vacant (*cv*) octahedral sites that are randomly interstratified with *trans*-vacant (*tv*) layers; and 3) P_{60} , the proportion of layers with $n \cdot 60^\circ$ rotations (as opposed to $n \cdot 120^\circ$) in the rotated layers. These parameters were determined by computer modeling of experimental randomly oriented powder X-ray diffraction patterns.

The proportion of *cv* interstratification in the I/S increases with Al and decreases with Mg and Fe content. The proportion of $n \cdot 60^\circ$ rotations in the rotated layers increases with Mg and Fe content. The *cv* 120° disordered structure correlates with tetrahedral Al for Si substitution and increasing tetrahedral charge. The *tv* $n \cdot 60^\circ$ disordered structures correlate with octahedral Mg for Al substitution. The data indicate that the type of unit cell and nature of rotational disorder in I/S is controlled by the octahedral Mg content. The three-dimensional structures do not show any systematic correlation with Reichweite and percent expandability as determined from diffraction patterns of oriented sample preparations.

Key Words: Bentonite • *Cis*-vacant octahedra • Crystal structure • Illite/Smectite • Polytype • Rotational disorder • X-ray diffraction

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