
Three-Dimensional Crystal Structures of Illite-Smectite Minerals in Paleozoic K-Bentonites from the Appalachian Basin

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Abstract: The three-dimensional crystal structures of illite-smectite (I-S) in K-bentonite samples from the Appalachian Basin are characterized by rotational disorder in the stacking sequence of 2:1 illite layers, different proportions of $n60^\circ$ rotations (as opposed to $n120^\circ$ in the rotated layers, and layers with centrosymmetric *trans*-vacant (*tv*) octahedral sites that are randomly interstratified with noncentric *cis*-vacant (*cv*) layers. The proportion of *cv* interstratification in the I-S increases with tetrahedral Al and decreases with octahedral Mg and Fe content. The I-S minerals in the northern Appalachian basin K-bentonites are characterized by high (79% average) proportions of *cv* (P_{cv}) layers. In contrast, I-S from equivalent K-bentonites from the southern Appalachian basin has low P_{cv} values (38% average). These values do not correlate with expandability or rotational disorder. The geographic distribution of these I-S structural parameters may have resulted from possibly short-term, hot, and advective fluid migrations that differed in Mg concentrations and/or other physical and chemical parameters.

Key Words: Bentonite • *Cis*-Vacant Octahedra • Crystal Structure • Illite-Smectite • Polytype • Rotational • Disorder • X-ray Diffraction

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