
The Nature of Cation-Substitution Sites in Phyllosilicates

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Abstract: A fundamental property of electrostatic potentials is their additivity. This study demonstrates that the electrostatic potential of a negatively charged, cation-substituted phyllosilicate layer can be represented as the sum of two potentials. Viewing cation substitution as a defect, one potential is derived from the atoms in a charge-neutral, unsubstituted layer such as pyrophyllite or talc. The “neutral-layer” potential rapidly decays to zero with distance from the layer and is determined primarily by the atoms in the first two atomic planes parallel to the (001) surface, i.e., the basal oxygens and tetrahedral cations. The second component, characterized as a “defect” potential, is a long-range potential derived from cation-substitution. The model used to compute the electrostatic potentials, a two-dimensional Ewald lattice sum, represents the atoms of a single phyllosilicate layer as point charges.

Key Words: Beidellite • Cation-substitution site • Electrostatic potential • Hectorite • Montmorillonite • Vermiculite

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