Electrostatic Potential at the Basal (001) Surface of Talc and Pyrophyllite as Related to Tetrahedral Sheet Distortions

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Abstract: Maps of the electrostatic potentials at the basal plane of talc and pyrophyllite, computed using a two-dimensional Ewald lattice-sum, reveal the effects caused by structural distortion of the phyllosilicate layer. Rotation and tilting of basal tetrahedra in phyllosilicates dramatically perturb the electrostatic potential near the (001) surface. A potential high exists at the center of each six-fold ring of the talc (001) surface. Concerted counter-rotations of basal tetrahedra by 10 °, as are typical in pyrophyllite, cause the potential lows above basal oxygens rotated into the ring to overlap, eliminating the ring-centered potential highs. Expansion of the vacant site in dioctahedral minerals tilts the basal tetrahedra by 4 ° and moves one-third of the basal oxygens about 0.2 Å toward the center of each phyllosilicate layer and away from the (001) surface, thereby producing corrugations of the basal surface. This shift dramatically reduces the contribution of these displaced basal oxygens to the (001) surface potential. Rotation and tilting of basal tetrahedra may influence the arrangement of interlayer water molecules on smectites and other swelling phyllosilicates by the effect that these distortions have on the (001) surface potential.

Key Words: Basal oxygen sheet • Electrostatic potential • Pyrophyllite • Talc • Tetrahedral sheet distortion

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