The Surface Coulomb Energy and Proton Coulomb Potentials of Pyrophyllite {010}, {110}, {100}, and {130} Edges

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Abstract: This paper describes structural models of four pyrophyllite edge faces: {010}, {110}, {100}, and {130}. Water molecules chemisorbed to Lewis acid sites stabilize edge faces both crystallochemically and electrostatically. The detailed assignment of protons to surface oxygens and the orientation of OH bond-vectors both influence the surface Coulomb energy.

The geometry chosen for the electrostatic calculations was infinite pyrophyllite ribbon the thickness of a single phyllosilicate layer and the width of 50 to 70 unit cells. Such a phyllosilicate ribbon has only two edges, a top and bottom, which were simulated using the edge-face models mentioned above. About 94% of the surface Coulomb energy is confined to the edge-face repeat unit. The surface Coulomb energies of the four edge faces are on the order of $2-3$ nJ/m, varying $\pm$ 1 nJ/m with proton assignment. The Coulomb potential, measured either within the layer or parallel to the layer, has a distinct negative trend near the edge face that can be traced to chemisorbed water molecules. Finally, the correlation between proton Coulomb potentials at the edge face and the coordination environment of the protons is poor, obscured by long-range interactions.

Key Words: Edge structure • Electrostatic potential • Lattice sum • Pyrophyllite

Clays and Clay Minerals; June 1993 v. 41; no. 3; p. 305-316; DOI: 10.1346/CCMN.1993.0410305