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# Model for Crystalline Swelling of 2:1 Phyllosilicates

David A. Laird

USDA, Agricultural Research Service, National Soil Tilth Laboratory, 2150 Pammel Drive, Ames, IA 50011

**Abstract:** A macroscopic energy balance model for crystalline swelling of 2:1 phyllosilicates is presented. Crystalline swelling for a static system is modeled by a balance among the potential energies of attraction, repulsion and resistance. The potential energy of attraction is due to both the electrostatic interaction between the interlayer cations and the negative surface charge sites and to van der Waals attraction between layers. The potential energy of repulsion is due to the net hydration energy for the interlayer cations, the net hydration energy for the negative surface charge sites and Born repulsion. The potential energy of resistance represents irreversible work needed to overcome the mechanical resistance of the clay water system to both expansion and collapse. The potential energy of resistance is responsible for both hysteresis and the stepwise nature of crystalline swelling.

A numerical solution of the crystalline swelling model is presented and shown to yield reasonable estimates of basal spacings for octahedrally charged clays. Measured and predicted basal spacings are directly compared and are in general agreement ( $r^2 = 0.39$ ). Most of the scatter for the measured vs. predicted basal spacing relationship is attributed to inaccuracies of the assumptions used for the numerical solution. The crystalline swelling model readily accounts for the effects of layer charge and nature of the interlayer cations upon crystalline swelling, but does not account for the effect of charge site location upon crystalline swelling.

**Key Words:** Crystalline Swelling • 2:1 Phyllosilicates

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