Hard and Soft Acid-Base Model Applied to Bivalent Cation Selectivity on a 2:1 Clay Mineral

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Abstract: We applied the hard and soft acid-base (HSAB) model (Xu and Harsh 1990a, 1990b) to bivalent cation exchange on a purified Ca-montmorillonite. As a result, a satisfactory model is proposed to describe the gradual selectivity of exchange with Ca for 4 of the 6 metals studied (Cd, Cu, Pb, Zn). The selectivity is predicted as a function of the differences of electronegativity and softness of the metals. The deviation of Ni and Co data from the predicting model is interpreted in terms of hydration (Ni and Co being the most strongly hydrated ions). The fitting parameters of the model, α and β, are related to the electronegativity and softness characteristics of the surface, respectively. Their ratio gives information on the nature of bonding. Results suggest that covalent bonding modifies electrostatic interactions, which in turn affect selectivity, with an increasing influence of covalent bondings in the order: Pb < Cd < Zn < Cu.

To balance the lack of representativity of the model for the small molar fraction (N_M), we propose to associate to the HSAB model an equation describing the variation of the Vanselow selectivity coefficient as a function of the molar fraction of metal on clay.

Key Words: Bivalent Cations • Covalent Bonding • Electronegativity • HSAB • Montmorillonite • Selectivity Coefficient • Softness

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