Alkali Cation Selectivity and Surface Charge of 2:1 Clay Minerals

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Abstract: A critical demand in environmental modeling and a desirable but elusive goal of research on the ion exchange properties of the charged solid surface has been to determine the selectivity coefficient from fundamental properties of the ions and surface. We developed a Hard and Soft Acid and Base (HSAB) Model to describe exchangeable cation selectivity on solid surfaces. Our previous work has shown that the model quantitatively describes alkali cation exchange on clay minerals in terms of the absolute electronegativity and softness of the exchangeable cations and two fitting parameters: α and β. This study was conducted to determine the relationship between α and β and surface charge characteristics of 2:1 clays. The layer charge and cation selectivity of seven smectites and one vermiculite were used. The regression of log K v o against four combinations of charge properties was performed and the appropriate relationship between α, β, and surface charge was selected based on both statistical criteria (R^2) and their consistency with the assumptions of the HSAB model. The selected model was then cross-validated using separate cation exchange data from the literature. It was found that α and β are linearly related to the amount of charge arising from mineral tetrahedral and octahedral sites, respectively. These results make it possible to predict the alkali cation selectivity of 2:1 clay minerals from their chemical composition data and the alkali cation properties.

Key Words: Hard/soft acid/base model • Ion exchange • Isomorphic substitution • Layer charge • Lewis acid • Lewis base • Smectite • Surface complexation • Vermiculite

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