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Monte Carlo simulations of ordering of Al, Fe, and Mg cations in the octahedral sheet of smectites and illites

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ABSTRACT

The ordering of Al^{3+}, Fe^{3+}, and Mg^{2+} cations along the octahedral sheet in dioctahedral 2:1 phyllosilicates was studied theoretically. The distribution of Fe^{3+}/Mg^{2+} was studied in the octahedral sheet and is compared with the Al^{3+}/Fe^{3+} and Al^{3+}/Mg^{2+} distributions. The cation exchange interaction parameters J_n, as first, second, third, and fourth nearest neighbors were calculated by means of empirical interatomic potentials. Several compositions with different interlayer cations, and tetrahedral charge close to ferric smectites, illites, and nontronites were studied. From these J_n values, a trend to form FeMg pairs was observed in the Fe/Mg system. Monte Carlo (MC) simulations based on the previously calculated cation exchange potentials J_n of these systems showed ordering phase transitions in the distribution of the octahedral cations, with different ordering patterns in each case. The two-species model was extended to a three-species ordering MC simulation model. A new procedure to study the ordering of three species is presented in this paper. We present for the first time a theoretical study of the ordering of three octahedral cations Al^{3+}, Fe^{3+}, and Mg^{2+} in clays, describing compositions more realistic for dioctahedral clay minerals, by means of Monte Carlo simulations based only on atomistic models. Short-range ordering of Fe was found in compositions of smectites and illites reproducing experimental cation distribution patterns.