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A computational investigation of the Al/Fe/Mg order-disorder behavior in the dioctahedral sheet of phyllosilicates

ERIKA J. PALIN,[1,*] MARTIN T. DOVE,[1] ALFONSO HERNÁNDEZ-LAGUNA,[2] AND C. IGNACIO SAINZ-DÍAZ[2]

[1]Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, U.K.
[2]Departamento de Ciencias de la Tierra y Química Ambiental, Estación Experimental del Zaidín (CSIC), C/ Profesor Albareda, 1, 18008-Granada, Spain

ABSTRACT

In previous papers, we investigated via Monte Carlo simulation the order-disorder behavior of an individual octahedral phyllosilicate sheet, with respect to two-species systems Al/Fe, Al/Mg, and Fe/Mg, and some three-species systems Al/Fe/Mg that were relevant to clay compositions found in nature. We have extended the work on Al/Fe/Mg systems to include a wide range of different octahedral compositions that can represent different natural and synthetic clay minerals, by means of Monte Carlo simulations based only on atomistic models. In many cases, phase transitions do not occur, in that long-range order is not attained, but most systems exhibit short-range order at low temperatures. The ordering of the octahedral cations is highly dependent on the cation composition.