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Investigation of Al/Si ordering in tetrahedral phyllosilicate sheets by Monte Carlo simulation

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ABSTRACT

We have investigated by Monte Carlo simulation the Al/Si ordering behavior of the tetrahedral phyllosilicate sheet, with a variety of compositions from Al_1Si_1 to Al_1Si_7, using atomic interaction parameters determined for the tetrahedral sheet in muscovite. Three different ordering schemes operate, depending on composition, with relatively Al-poor systems ordering in a muscovite-like (Al:Si = 1:3) pattern and relatively Al-rich compositions ordering in an "ABABAB" or margarite-like (Al:Si = 1:1) pattern, where ABABAB indicates the arrangement of atoms around a hexagonal ring of tetrahedral cation sites. The pattern corresponding to Al:Si = 1:2 occurs in intermediate compositions, but always in conjunction with another ordering pattern, except for one composition close to Al:Si = 1:2. Simulations of the same composition but with different ordering schemes can show different behavior, and this is evidence for metastability fields. The transition temperature for order-disorder T_c is strongly dependent on composition, and the dilution effect can be observed at low Al concentrations, with a critical concentration x_c between 0.12 and 0.15.