American Mineralogist, Volume 101, pages 1207–1216, 2016

Compressibility of $2M_1$ muscovite-paragonite series minerals: A computational study to 6 GPa

Noemí Hernández-Haro[1,3], Daniel Muñoz-Santiburcio[1,†], Carlos Pérez Del Valle[2], Joaquin Ortega-Castro[3], Claro I. Sainz-Díaz[1], Carlos J. Garrido[1], and Alfonso Hernández-Laguna[1,*]

[1]Instituto Andaluz de Ciencias de la Tierra (CSIC-UGR), Avenida de las Palmeras 4, 18100-Armilla, Granada, Spain
[2]Université Grenoble Alpes, DCM F-38000 Grenoble Cedex 9, France
[3]Departament de Química, Institut d'Investigació en Ciències de la Salut (IUNICS), Universitat de les Illes Balears, E-07122 Palma de Mallorca, Spain

Abstract

The muscovite–paragonite (Ms–Pg) series $[K_{1-x}Na_xAl_2(Si_{4-y}Al_y)O_{10}(OH)_2]$ is a group of micas with end-members of Ms ($x = 0$, $y \approx 1$) and Pg ($x = 1$, $y \approx 1$). This mineral series is found in the Earth's crust and upper mantle. The series shows a wide immiscibility gap between the end-members.

Density functional theory (DFT) is used to show the compression in five models of the $2M_1$ polytype Ms-Pg series to 6 GPa. Bulk moduli and cell-parameter moduli were obtained from a least-square fitting of pressures and volumes to a third-order Birch-Murnaghan equation of state. Bulk-modulus values of the end-members of the series agree with the range of experimental values. Bond lengths and atomic-group geometries were studied as a function of the pressure and composition of the series by determining the moduli. Compression mechanism has been determined.

The excess volumes, V^{ex}, were higher for the Na-rich members than for the K-rich members. V^{ex} follow a Redlich-Kister behavior. The excess free energy, G^{ex}, was calculated isobarically in a semiempirical way: the DFT excess volume data were calculated in one experimental model (A from Roux and Hovis 1996) in a Redlich-Kister function. The G^{ex} as a function of the composition of the Ms-Pg join of the A model show two minima with constant composition to 0.75 GPa, evolving to richer end-member compositions at greater pressures. Therefore, the solvus should increase the gap of immiscibility at high pressure.

Keywords: Muscovite-paragonite series, DFT calculations, pressure behavior of atomic groups and crystal geometry, bulk modulus, cell-parameter moduli, bonds and atomic-group moduli, compression mechanism, excess volume, excess free energy