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Computational study of the elastic behavior of the $2M_1$ muscovite-paragonite series

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Abstract

Elastic properties are an important issue in explaining the behavior of seisms and to ascertain the mineralogical composition of the Earth's shells through which seismic waves pass. Computational methods can yield an additional, detailed, free-of-heterogeneity model knowledge of the mineral series of interest. Therefore, a computational study on the influence of the interlayer cation in the muscovite-paragonite (Ms-Pg) series on the crystal cell, internal geometry, and the elastic properties was made to shed light on the mineralogical, geophysical, and geochemical properties of the series. These properties have been calculated by means of Density Functional Theory (SIESTA2.0.2 code). The crystal structure and internal geometry agreed with the range of experimental values in the literature. In general, elastic stiffness constants (EC) agreed with the known experimental values. ECs of different interlayer cation configurations for the middle concentration sample showed very similar values, except for C_{33}, The majority of ECs, with the exception of C_{33} and C_{66}, decreased as a function of Na' [Na/(Na+K)], many of which showed ideal crystalline solution behavior, and some showed mixing terms. The polycrystalline bulk modulus registered similar values for the end-members of the series and a minimum at Na' = 0.5, although an estimate of the value at room temperature made the Pg stiffer than Ms; while the shear modulus showed a decreasing trend as a function of the Na'. Velocities of the sound waves lowered as a function of Na'. Local deformabilities were also studied, where the highest deformability was found for the interlayer space. The results are discussed in the framework of the mineralogical, geochemical, and geophysical knowledge of the series.

Keywords: Muscovite-paragonite series, crystal structure, local geometries, elastic-stiffness constants, bulk and shear moduli, local deformabilities, DFT calculations