

High-pressure behavior of $2M_1$ muscovite

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ABSTRACT

The crystal structure and pressure influence (between 0–6 GPa) on $2M_1$ muscovite have been calculated by quantum-mechanical methods based on density functional theory (DFT) with optimized numerical LCAO basis sets and norm-conserving pseudopotentials. Tensions between 0.8 and 0 GPa have been also studied. Volumes as a function of pressure, computed from the generalized gradient approximation, are closer to the experimental data than volumes calculated from the local density approximation. The crystal structure, bond distances, and main geometrical features agree with previous experimental values. A third-order Birch-Murnaghan equation is fitted, giving a bulk modulus of 60.1 GPa, which reasonably agrees with the experimental data. Axis compressibilities are slightly smaller than those of the experimental data. The most compressible axis is the c axis. Bond strains, angles, the main geometrical features, and polyhedral strains are studied as a function of pressure, and these vary according to the experimental behavior. Tetrahedral $\langle\alpha\rangle$ and $\langle\rho_2\rangle$ angles and corrugation show an oscillating behavior in the range of pressures used. The most important compressibilities are those related to the interlayer space, as it corresponds to the weakest bonding in the structure. The highest compressibility in the T-O-T layer along the [001] direction is determined by the octahedral sheet thickness. The compressibilities along the a and b axes are determined by the tetrahedra, as the most compressible polyhedra, and the α angle. Therefore, with our results the utility of periodic DFT methods for studying crystal structure and the effect of hydrostatic pressure on $2M_1$ muscovite are once again validated, and they are suitable to describe the compression of the crystal structure in detail.

Keywords: Muscovite, crystal structure, pressure, DFT, equations of states, compressibility, bulk modulus