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RESEARCH ARTICLE

Influence of B-site cation in lattice dynamics of bilayered Ruddlesden–Popper Sr₃B₂O₇ (B = Zr, Mo, Sn, Hf) compounds

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Abstract

The Raman and infrared (IR) wavenumbers for the Ruddlesden–Popper Sr_{n+1}B_nO_{3n+1} (B = Zr, Mo, Sn, Hf) bilayered tetragonal compounds with n = 2 of symmetry and phase I4/mmm (Z = 2) have been analyzed with Wilson's GF matrix method. Theoretical assignments for the optical wavenumbers have been reported for the first time for the bilayered tetragonal Sr₃Zr₂O₇, Sr₃Mo₂O₇, Sr₃Sn₂O₇, and Sr₃Hf₂O₇ compounds in phase I4/mmm with the use of 10 short-range force constants. Using the available data of the isostructural compounds Sr₃Ti₂O₇, Sr₃Mn₂O₇, and Sr₃Fe₂O₇, we have tried to calculate the vibrational modes of the Sr₃B₂O₇ (B = Zr, Mo, Sn, Hf) compounds in phase I4/mmm by the comparative method. Also, we have compared all these Sr₃B₂O₇ (B = Zr, Mo, Sn, Hf) compounds together in terms of wavenumbers and force constants. The appropriate optical vibrational modes have been assigned to the bilayered tetragonal Sr₃B₂O₇ (B = Zr, Mo, Sn, Hf) compounds in phase I4/mmm. The impact of cation-B (B = Zr, Mo, Sn, Hf) exchange on the lattice dynamics of the tetragonal bilayered Sr₃B₂O₇ (B = Zr, Mo, Sn, Hf) isostructural compounds has been analyzed by comparison of the zone center vibrational modes, force constants, and bond lengths. To understand the structure more clearly, an attempt is also made to analyze the effect of B-cations on the affected apical bonds. It was observed that the B-site substitutions have the least influence on the Sr layer and the equatorial bonds of octahedra; meanwhile, the outer apical bonds of the octahedra have shown the maximum impact. For each normal mode of the bilayered tetragonal Sr₃B₂O₇ (B = Zr, Mo, Sn, Hf) Ruddlesden–Popper phase, the potential energy distribution (PED) has been analyzed for the noteworthy effects of short-range force constants on calculated wavenumbers.