DOI: https://doi.org/10.36094/sc.v89.2024.Lattice_Dynamical_Investigation_of_Raman_and.Das 235

Sci. and Cult. 90 (5–6) : 235-238 (2024)

LATTICE DYNAMICAL INVESTIGATION OF RAMAN AND IR WAVE NUMBERS AT THE ZONE CENTER OF ORTHORHOMBIC PEROVSKITE $LUFEO_3$

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Herein, we have investigated the Raman and infrared wave numbers of orthorhombic perovskite $LuFeO_3$ by using normal coordinate analysis in light of a short-range valence band force-field model. For the calculation of zone center phonons, we have employed 9 stretching and 7 bending force constants in the Wilson GF matrix method. Our calculated wave numbers agree well with the observed wave numbers. The Raman wave numbers have been assigned to their specific mode of vibrations. The infrared wave numbers have been calculated and assigned. The potential energy distribution has also been determined to signify the contribution of the force constants toward the Raman and infrared wave numbers.