ABSTRACT

The elastic properties are basic cohesive properties related to the anharmonicity of the crystal lattice. Elastic constants also provide insight into the nature of binding forces between the atoms as they are represented by the derivatives of the internal energy. A complete set of higher order elastic constants of these materials is essential to estimate the physical parameters such as thermal expansion, Debye temperature, compressibility and acoustic anisotropy. The fundamental significance to the elastic constants is implied by their appearance as the derivatives of elastic energy with respect to strain. There exist various theoretical as well as experimental methods for the determination of the higher order elastic constants of solids. The present objective is to study the vibrational anharmonicity of long wavelength acoustic modes of trigonal crystals; CaCO$_3$, Bi and LiNbO$_3$. Here we make an attempt to calculate the complete set of second and third-order elastic constants. Pressure derivatives of the second-order elastic constants and generalized Gruneisen parameters of elastic waves are also determined. Low temperature lattice thermal expansions of these trigonal crystals are evaluated. The results are compared with those obtained by other workers wherever such data are available.

Key Words
Elastic constants, Gruneisen parameters, Thermal expansion