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Pressure-Dependent Elastic, Mechanical, and Ultrasonic Analysis of CaAuBi Compound

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The Lennard–Jones potential model is used to investigate the effects of pressure on the elastic and ultrasonic properties of CaAuBi half-Heusler compound. Potential model technique approaches is used to evaluate second- and third-order elastic constants of CaAuBi compound at various pressures (0–15 GPa). The pressure dependence of elastic constants is studied and it has been observed that the elastic constants of the half-Heusler CaAuBi compound increase monotonically as pressure is increased. The hexagonal half-Heusler CaAuBi compound is mechanically stable at different pressures according to Born's elastic stability criteria. The Voigt–Reuss–Hill method was used to compute elastic parameters such as Young's modulus Y, shear modulus G, bulk modulus B, and Poisson's ratio ν under various pressures. For the provided pressure range, the second-order elastic constants were also utilized to determine ultrasonic velocities along with z-axis at various angles. The half-Heusler CaAuBi compound's hardness, ultrasonic attenuation, melting temperature, and anisotropy are also determined. The computation have been also satisfactory in estimating the thermal conductivity $k_{(\min)}$ and Debye average velocity under varied pressure.

Keywords: elastic properties, thermal conductivity, ultrasonic properties, thermo-physical properties.