

Optical Phonons and Chemical Bonding in TlSbS₂, TlSbSe₂, and Tl₃SbS₃ Crystals

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Abstract

The optical phonons at $k = 0$ of TlSbS₂, TlSbSe₂, and Tl₃SbS₃ have been investigated by infrared reflectivity measurements from 50 to 4000 cm⁻¹ at 300 K. The factor group analysis of vibrational modes of TlSbS₂ and Tl₃SbS₃ crystal lattices has been made. The dielectric constant dispersion for $E \parallel a$ and $E \parallel b$ has been determined by classical dispersion relations. The Szigeti effective charges, the Born dynamic effective charge, and the Tl, Sb, S (Se) relative ion charges were calculated in dependence on the polarization of the incident light.