

Infrared vibrational Modes in Tl_3SbS_3 , Tl_3AsS_3 , and Tl_3AsSe_3 crystals

Syrbu N. N., Krasovsky V. T., Grincheshen I. N.

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Abstract

Reflectivity spectra of Tl_3SbS_3 , Tl_3AsS_3 , and Tl_3AsSe_3 crystals have been investigated in the wave number range $50-600\text{ cm}^{-1}$ for the polarizations $E\parallel c$ and $E \perp c$. The fundamental phonon parameters, the limiting dielectric constants ϵ_∞ and ϵ_S and the reflectivity spectra contours have been calculated by using classical dispersion relations for both $E\parallel c$ and $E \perp c$ configurations. The Szigeti effective charges and the relative ion charges of As, Tl, Sb, Se, S anions and cations have been calculated in dependence on the incident light polarization.