



Double Davydov resonance in the vibrational spectra of Tl_3AsS_4 and Tl_3PS_4 crystals

N. N. Syrbu V. T. Krasovsky

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Abstract

Raman spectra of Tl_3AsS_4 and Tl_3PS_4 have been investigated at 300 and 77 K. The vibrational modes A_g , B_{1g} , B_{2g} and B_{3g} are determined. The vibrational mode splittings caused by Davydov resonances are determined. Infrared reflectivity spectra of Tl_3AsS_4 and Tl_3PS_4 crystals have been investigated for the polarizations $E\parallel a$, $E\parallel b$ and $E\parallel c$ in the range 50–4000 cm^{-1} . Reflectivity spectra contours are calculated and the main vibrational mode parameters are determined. The effective ionic charges of the anions and cations of the crystals are determined.