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Davydov multiplets in vibrational spectra of and crystals

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Abstract

In this paper the Raman vibrational spectra for all actually realized geometries of and crystals at 77 K, and infrared reflectivity spectra for both and polarizations in the range from 50 to at 300 K have been investigated. The contours of the reflectivity spectra are calculated by means of the classical dispersion relations of the multi-oscillator model, and the fundamental phonon parameters and the static and high-frequency dielectric constants are determined as well. Davydov multiplet vibrational modes have been revealed in both crystals.