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Far-infrared spectroscopy investigation and lattice dynamics simulations in CsCdBr3 and CsCdBr3: R3+ crystals

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Abstract

Polarized infrared reflectivity spectra of CsCdBr3 crystal were measured at temperatures 20 and 300 K in the wave number range of 10-650 cm-1. Frequencies and damping of the optically active lattice modes at the Brillouin zone center were determined. The lattice dynamics of CsCdBr3 crystal is studied in the framework of the rigid ion model, the phonon density of states, and the spectral representations of correlation functions of relative displacements of a Cd2+ ion and the nearest neighbor Br- ions in the perfect lattice are presented. The local dynamics of the lattice containing impurity rare-earth ions that form symmetrical pair centers substituted for three adjacent Cd2+ ions is analyzed with the formalism of lattice Green's functions. It is argued that resonance and localized vibrations whose frequencies lie near the boundary of the continuous phonon spectrum of a perfect lattice are induced in CsCdBr3: R3+ crystals. The corresponding vibronic satellites have been found in the optical spectra of symmetrical dimers in CsCdBr3: Yb3+, CsCdBr3: Tm3+, and CsCdBr3: Pr3+ single crystals.