SPECTROSCOPIC INVESTIGATION OF THE LATTICE DYNAMICS IN HYDROGEN-BONDED CRYSTAL NH_4IO_3

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The lattice dynamics of the ammonium iodate crystal NH_4IO_3 has been investigated by means of IR, Raman and NQR methods near the phase transition temperature 367 K (T_c). It is known, that NH_4IO_3 crystal grows from water solution and has orthorhombic syngony (C_{2v}^9, z = 4). In contrast with other hydrogen-bonded iodate crystals, which undergo the order-disorder phase transitions, the phase transition in NH_4IO_3 crystal has clear marks of the displacive type phase transition. First, ^{127}I NQR measurements allow to assign the low frequency bands observed in IR and Raman spectra of NH_4IO_3 crystal to the lattice vibrational associated with librational and translational vibrations of the NH_4^+ and IO_3^- ions ($\nu < 120$ cm^{-1}) and with internal vibrations of N−H and I−O ions ($\nu < 850$ cm^{-1}), whereas high frequency bands were associated with NH...O hydrogen bond. Second, the potential barriers for such vibrations were estimated from the spectroscopic data. Further, it was shown, that the temperature dependence of the asymmetry parameter of the ^{127}I in the pretransition temperature range ((T_c- 50) ÷ T_c) can not be described by a simple Arrheniuse's law. In the present paper we attempted to explain this deviation by the decreasing of potential barriers for reorientational vibrations of NH_4^+ and IO_3^- ions due to the temperature expansion of the crystal volume and the change in the hydrogen bonds network in the pretransition temperature range.