SPECTROSCOPIC INVESTIGATION OF THE CRYSTAL STRUCTURE OF THE BINARY SYSTEM $LiIO_3-HIO_3$

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The lattice dynamics of the pseudo-binary system $LiIO_3-HIO_3$ has been investigated by means of the IR and Raman spectroscopies and the NQR technique. The spectral changes, observed in the $2600-400$ cm^{-1} region, indicate the formation of variable "intermolecular" hydrogen bonds O-H$\cdots$O in the system between the quasi molecular halogenate groups IO_3^-, HIO_3 and $H(IO_3)_2^-$. By the analysis of low-frequency Raman spectra of the mixed crystals $Li_{1-x}H_xIO_3$ with varying the concentration x in the range from 0 to 1, the critical x values of HIO_3 content were evaluated at which the hydrogen bonds of different strength are formed and the different crystal structure of the binary system is observed. Thus for the concentration range $0-0.22$ the IR absorption spectra show wide and weak O-H stretching bands. That concentration range corresponds to α-modification $LiIO_3$ crystal doped by protons (C_6^6 space group). Within the intermediate concentration range $0.06 < x < 0.22$ two separate crystals α-$LiIO_3$ and $2LiIO_3{\cdot}HIO_3$ (with unknown crystal structure) exist as it follows from the NQR data. For concentrations $x > 0.35$ the vibrational spectra of the system correspond to Li-doped orthorhombic α-HIO_3 crystal. From the NQR and Raman data the amorphous ("glass") phase was detected in the concentration range $0.22-0.35$. Our results help to solve some contradictions concerning the binary system structure obtained by different experimental methods.