Intermolecular Interaction and Molecular Dynamics in Carboxylic Acid Crystals

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In this work we report about investigation of Davydov splitting value temperature changes for CH_2 rocking vibrations of pure crystalline carboxylic acids $CH_3(CH)_{n-2}COOH$ with odd (n=15,17,19) and even (n=10,14,16,22) number n of carbon atoms in the temperature region from 100K to the crystal melting temperature by FTIR spectra.

A statistic and dynamic model is proposed which provides adequate description of the observed effect. In the framework of this model the damping of vibrational excitons on orientational defects of different nature takes place. Genesis of such defects is connected with excitation of conformational, librational and rotational degrees of freedom of H-bonded molecular dimers at the different temperatures.

Theoretical analysis of the effect of resonance dynamical intermolecular interaction on the spectra of intramolecular vibrations of the crystals was performed in terms of stochastic equations with account of mentioned mechanisms. Computer simulation of such dependence was performed for crystalline normal chain carboxylic acids. Good agreement between the experimental and computer simulation results was obtained.

Keywords: intermolecular interactions, computer simulation, carboxylic acids