COMPUTER SIMULATION OF TEMPERATURE TRANSFORMATION OF ISOTROPIC RAMAN BAND CONTOURS OF INTRAMOLECULAR VIBRATIONS OF LIQUID CH_3I

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S u m m a r y

The computer simulation of the influence of a specific resonant dynamic intermolecular interaction, caused by the existence of a local ordering of molecules in liquid, on the formation of isotropic Raman intramolecular vibrational bands in liquid CH_3I is performed at various temperatures. It is determined that the temperature narrowing of spectral vibrational bands of liquid methyl iodide is related to a growing similarity for the frequencies of the resonant splitting components of vibration modes as the structural elements of appropriate spectral bands owing to temperature disordering of the local molecular surrounding in liquids. The satisfactory agreement between the results of computer analysis, appropriate experimental data, and theoretical estimations is obtained.