DEVIATION OF THE C—H BOND IN LIQUID AND GASEOUS CHLOROMETHANE AND IODOMETHANE

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S u m m a r y

The method of $3N$ matrices has been used to solve the inverse spectral problem of vibrational spectroscopy for molecules of chloromethane, $ClCH_3$, and iodomethane, ICH_3, belonging to the liquid or gaseous phases. The deviation angles of C—H bonds have been calculated irrespective of the models of the molecular force field and the environment. A comparison of the calculated values of the shape parameter of molecular vibration modes, the parameter of anharmonicity, and the deviation angle of chemical bonds, which are characteristic of molecules belonging to different states of aggregation, has been carried out. The frequencies of characteristic vibrations of molecules and the approximation of identical parameters of anharmonicity for all vibration modes have been chosen for calculations. The formalism of a "non-full" basis of the vibration shapes has been used.