INTERMOLECULAR INTERACTION IN LIQUID CHLOROFORM AND ITS SOLUTIONS. NON-EMPIRICAL CALCULATIONS AND RAMAN SPECTRA

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It was studied Raman spectra of C-H and C-D vibrations of chloroform and its solution with acetonitrile. It was found that in pure chloroform the band maxima frequency noncoincidance in parallel and perpendicular polarized components of Raman spectra line. Difference is 1.8 cm-1 for chloroform and 1.5 cm-1 for deuteried chloroform. At dilution in neutral solvent this frequence difference is decreased. The results was explained by molecular aggregation in pure liquid, when for monomers and aggregates correspond two near placed and overlapping bands with different values of depolarization ratio. The calculations on base of DFT method (B3LYP) show that the such aggregations formation in liquid is possible, at this in dimmer the hydrogen atom of C-H band of one molecule is oriented to one of three atoms chlorine of other molecule of chloroform. The frequency difference of monomer and dimer vibrations is 2 cm-1. In mixture with acetonitrile the bands C-H and C-D are experienced high frequency shift in comparison with place of band in pare liquid, at this the band with concentration change go through maximum that indicates about band complexity in mixture