MANIFESTATION OF INTERMOLECULAR INTERACTIONS IN RAMAN SPECTRA AND *AB INITIO* CALCULATIONS OF MOLECULAR AGGREGATION IN LIQUID ETHYLENE GLYCOL

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S u m m a r y

We present the results of a study of intermolecular interactions in ethylene glycol by Raman spectra. For a more reasonable assumptions about the possibility of the existence of aggregated intermolecular complexes and monomeric molecules of ethylene glycol in the liquid, as well as manifestations of these formations in spectra, we carried out *ab initio* calculations of the normal vibration frequencies, depolarization ratios of bands, formation energy, and other physical and optical characteristics for aggregated complexes of molecules. Calculations were carried out in the framework of a self-consistent field (RHF) using the basis 6-31G++(d, p) with full optimization of the geometry of molecules. Calculations showed a possibility of the formation of an intermolecular H-bond between the H atom of the O–H group of one molecule and the O atom of another molecule. For a dimeric aggregate, the intermolecular H-bond length is 1.986 Å. In molecules of the dimer, there is a slight change of bonds' lengths, but also there is a significant change of the charge distribution between atoms. The energy of dimer formation is 4.6 kcal/mole, the dipole moment of an aggregate is 6.35 D (in the monomeric molecule, the dipole moment is 2.73 D). In Raman spectra, there are some features of the manifestation of the H-bonding between molecules: asymmetry of bands and splitting of bands that are the features that accompany the H-bond formation.