AGGREGATION OF BENZENE MOLECULES WITH MOLECULES OF METHANOL AND FORMIC ACID

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S u m m a r y

Calculations and experimental studies of Raman scattering spectra show that there is a dimeric aggregation of benzene molecules with the molecule of methyl alcohol with the use of π-electrons of the benzene ring. In this process, the H-active hydrogen atom of O–H group is oriented to the edge of the benzene ring (a distance along the normal to the plane of the benzene ring is 2.850 Å). The unusual position of the H-active hydrogen atom is conditioned by the interaction of two hydrogen atoms of the alcohol's methyl group with π-electrons of the benzene ring. In Raman scattering spectra, the aggregation of molecules in the liquid state of the substance leads to a broadening of the band of full-symmetric vibrations with the maximum at 992 cm^{-1}, as well as to a shift of this band toward lower frequencies by ~ 1 cm^{-1}. The band at 992 cm^{-1} is narrowed more than twice at the strong dilution of the benzene–methyl alcohol mixture by a large amount of heptane. The aggregation of benzene molecules takes place also with the molecules of formic acid with the use of π-electrons of the benzene ring. As in the case of the benzene–methyl alcohol mixture, the H-active hydrogen atom of O–H group of the acid is shifted toward the edge of the benzene ring. The energy of the benzene–formic acid dimerization is 9.2 kJ/mole.