Solvent Effect on Assembling and Interactions in Solutions of Phenol: Infrared Spectroscopic and Density Functional Theory Study

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This work provides new insight into assembling of phenol in various solvents and competition between different kinds of interactions. To examine both weak and strong interactions, we selected a series of non-aromatic and aromatic solvents. Infrared spectra were measured at low (0.05 M) and high (2 M) phenol content. In addition, we performed density functional theory calculations of the structures and harmonic vibrational spectra of 1:1 complexes of phenol with the solvents and the associates of phenol from dimer to tetramer. Based on these results, we divided the solvents into three groups. The first group consists of non-aromatic solvents weakly interacting with phenol. Depending on the concentration, molecules of phenol in these solvents remain non-bonded or self-associated. In diluted solutions of phenol in chlorinated non-aromatic solvents do not appear free OH groups, since they are involved in a weak OH···Cl interaction. It is of note that in diluted solutions of phenol in tetramethyl ethylene both the non-bonded and bonded OH coexists due to solvent–solvent interactions. The second group consists of aromatic solvents with methyl or chlorine substituents. At low concentration, the molecules of phenol are involved in the phenol–solvent OH···π interaction and the strength of these interactions depends on the solvent properties. At a higher phenol content an equilibrium exists between phenol–solvent OH···π and phenol–phenol OH···OH interactions. Finally, the third group includes the aromatic and non-aromatic solvents with highly polar group (C≡N). In these solvents, regardless of the concentration all molecules of phenol are involved in the solute–solvent OH···NC interaction. Comparison of the experimental and theoretical band parameters reveals that molecules of phenol in non-aromatic solvents prefer the cyclic associates, while in the aromatic solvents they tend to form the linear associates.

Słowa kluczowe

Infrared spectroscopy, IR spectroscopy, density functional theory calculations, DFT, vibrational spectra, phenol, hydrogen bonding, OH–OH interaction, OH–π interaction, solvent effect, self-association

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