INVESTIGATION OF INTERMOLECULAR INTERACTIONS IN VARIOUS SOLUTIONS OF ANILINE USING RAMAN SPECTROSCOPY AND DFT CALCULATIONS

A. Jumabaev[a], H. Hushvaktov[a], I. Doroshenko[a,b], U. Holikulov[a], B. Khudaykulov[a]

[a]Sharof Rashidov Samarkand State University, 15 University Blvd., Samarkand, 140104 Uzbekistan

[b]Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Str.,Kyiv 01601, Ukraine

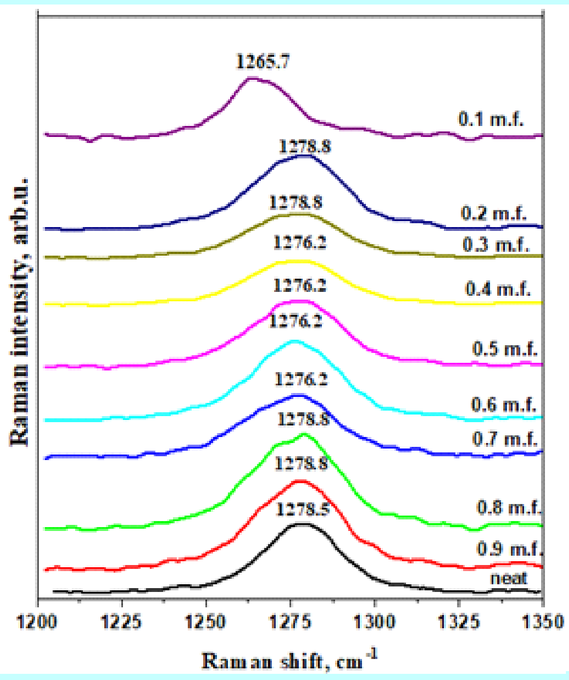
M O T I V A T I O N

There are a number of problems in studying the spectral manifestation of the nature of intermolecular interactions. That is why scientific research work on the structure, properties, intermolecular hydrogen bonds and molecular structure of liquids is being conducted intensively all over the world. Such studies are of great scientific and practical importance and occupy an important place in the activity of living organisms. Also, this research creates opportunities for effective use of compressed gases and liquids in practice. In recent years, hydrogen bonding as a special type of interaction, which plays an important role in the existence of biomolecules, is causing great interest in the world. Its manifestation in vibrational spectra has not been fully explained to date.

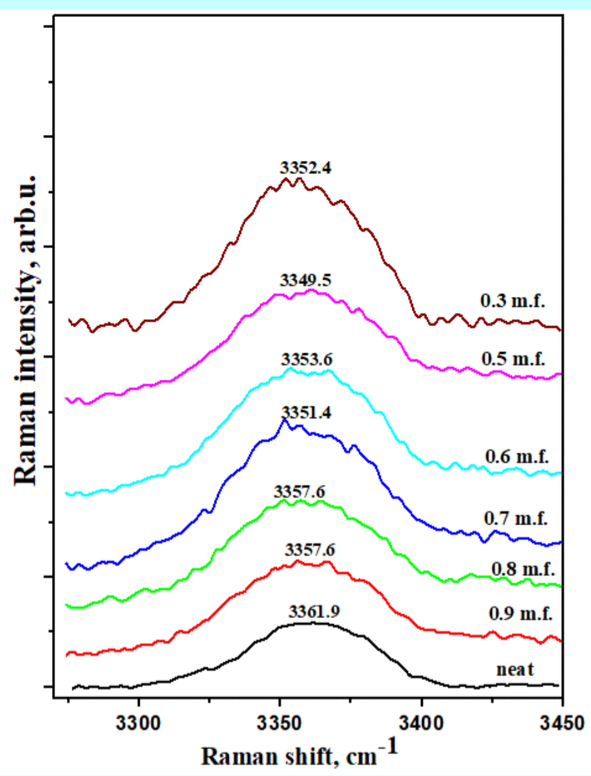
THE PURPOSE AND TASK OF THE WORK

The study of the nature of weak intermolecular interactions has been quite interesting in recent years because they play a significant role in determining the physicochemical properties of molecular structures in a condensed medium. Aniline is a simple amine representative of aromatic ring substances, and N-H vibration gives good results in the study of hydrogen bonding. This work utilized Raman spectroscopy to investigate the effect of water on aniline vibrational modes. The intermolecular interactions of aniline and water molecules were investigated using the DFT approach using the B3LYP/6-311++G(d,p) basis set. The effect of various solvent concentrations on the N-H, C-H stretching, and C-H breathing vibrations of aniline was investigated. *The Raman spectra of aniline-water complexes were simulated. NBO analysis was performed to examine the mechanism of intermolecular and intramolecular charge transfer. MEP, HUMO-LUMO gap energy, and other electronic properties are described. Interactions at important connection points were studied by applying topological (AIM, NCI, RDG, ELF, and LOL) analyses.*

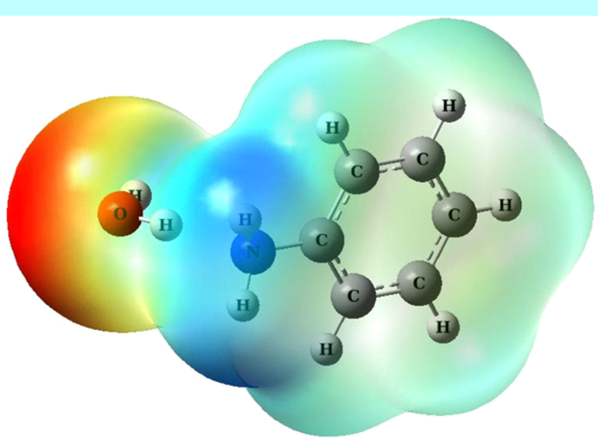
Raman scattering spectra of C-N stretching vibrational band of aniline in aqueos solution



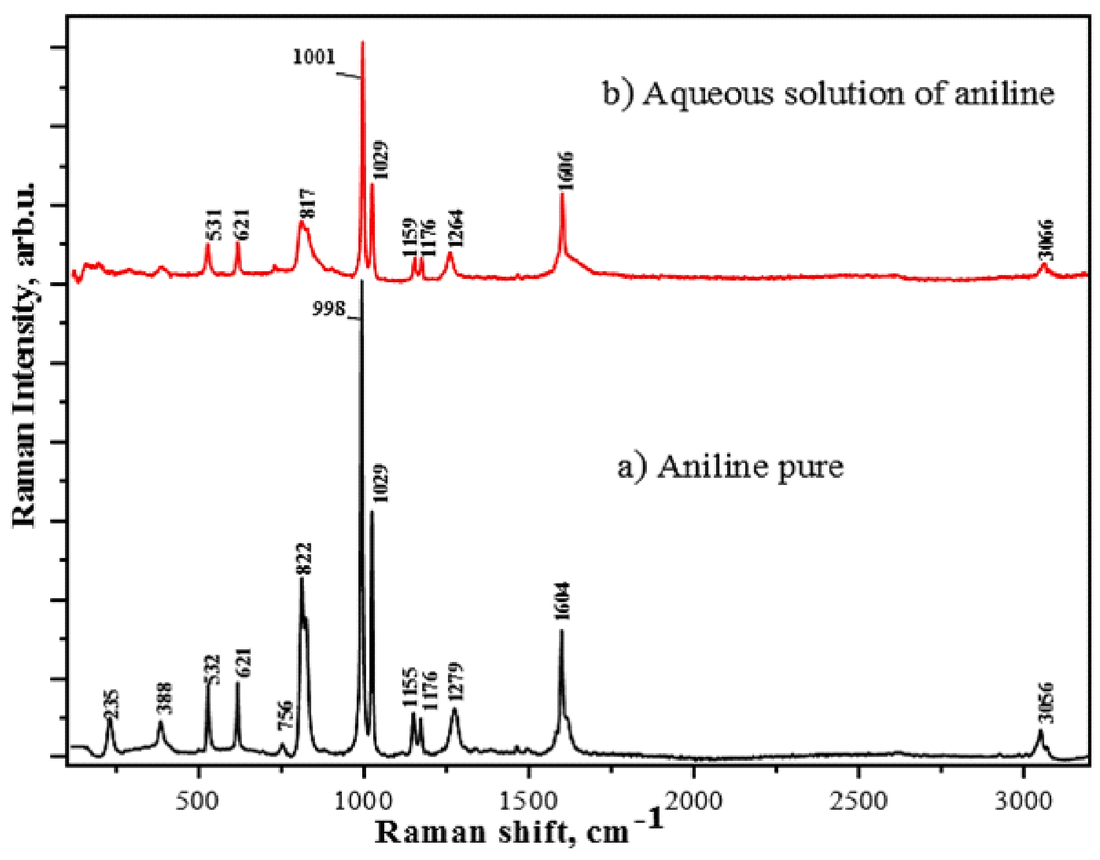
Raman scattering spectra of N-H stretching vibrational band of aniline in aqueos solution



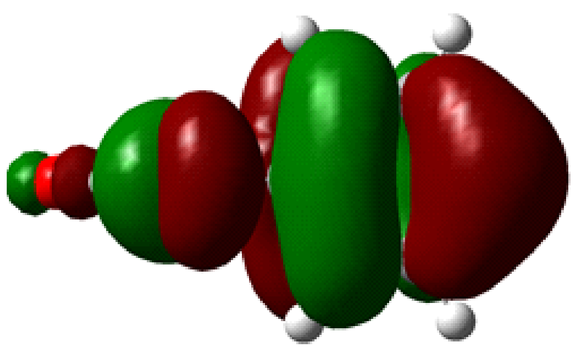
MEP Diagram for aniline-water



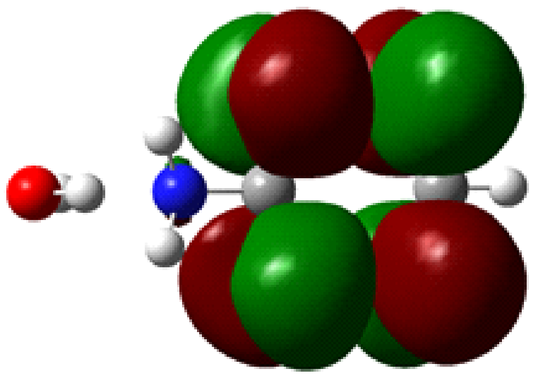
Raman spectra of aniline



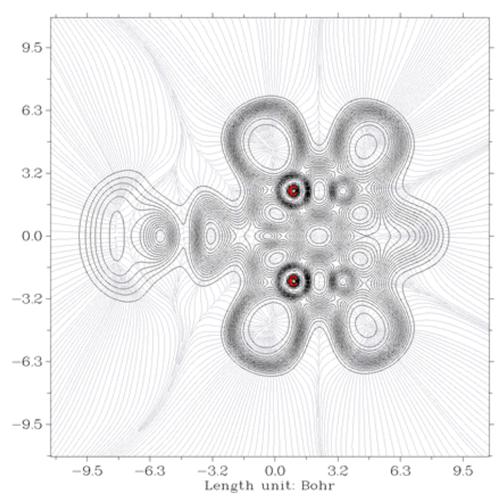
HOMO orbital of aniline-water complexes



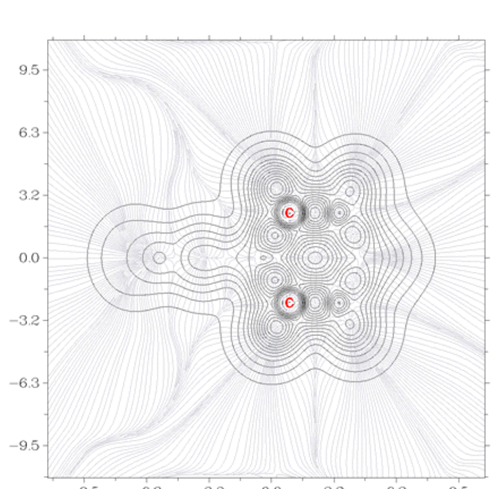
LUMO orbital of aniline-water complexes



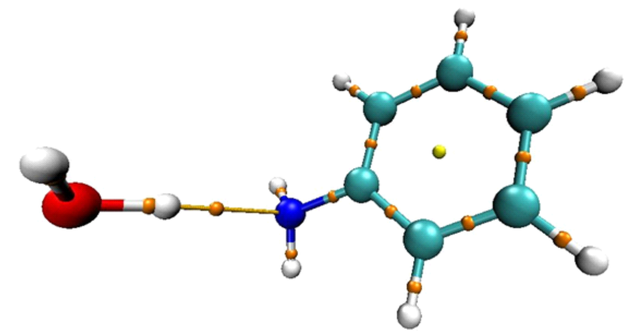
Electron localization function (ELF) analysis for aniline-water complexes



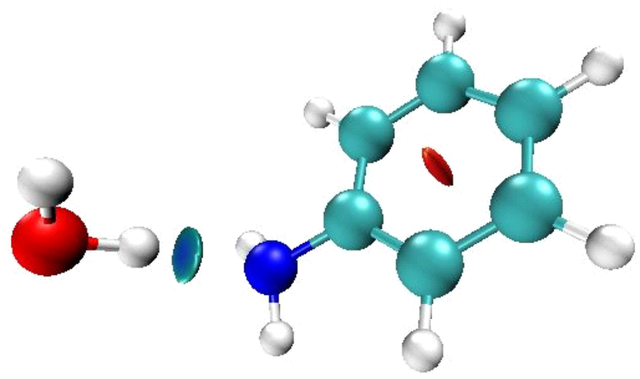
Localized orbital locator (LOL) analysis for aniline-water complexes



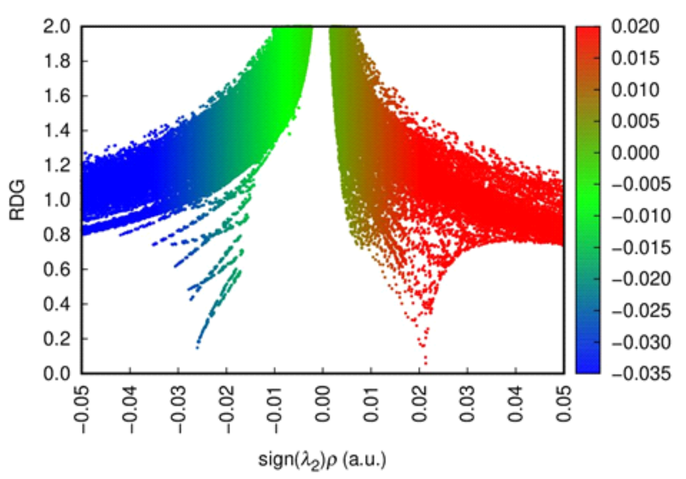
Atoms in molecules (AIM) analysis of title molecules of aniline-water solution



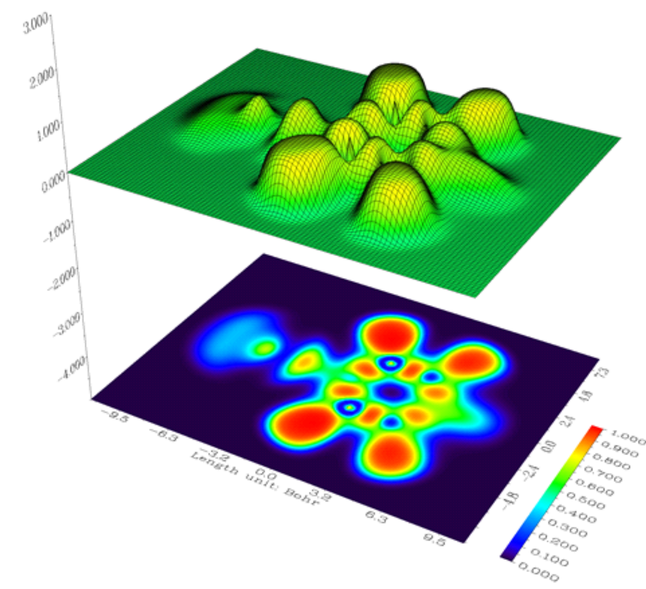
Noncovalent interaction (NCI) analysis of aniline-water complexes



Reduced density gradient (RDG) analysis of aniline-water complexes



Electron localization function (ELF) analysis for aniline-water complexes



Localized orbital locator (LOL) analysis for aniline-water complexes