Study of noncovalent interactions in various solutions of thiophene-2-carboxylic acid

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THE PURPOSE AND TASK

The purpose of this research is to investigate noncovalent interactions in various thiophene-2-carboxylic acid (TCA) solutions through experiments and simulations. Raman and infrared (IR) spectroscopy were utilized to investigate the vibrational characteristics of TCA in various solvent solutions. Experimental data analyzed using computing approaches include, highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) frontier molecular orbitals and molecular electrostatic potential (MEP) mapping. These analyses revealed vital information on TCA's electrical structure and proclivity for noncovalent interactions.

Noncovalent interactions, such as hydrogen bonding and van der Waals interactions were investigated further using the atom in molecule (AIM), noncovalent interaction index (NCI) and reduced density gradient (RDG) approaches, which identify the presence and type of weak interactions in molecular clusters. Electron localization function (ELF) and localized orbital occupier (LOL) analyses were utilized to study the electron localization and binding areas of TCA and its solvent complexes, providing more insight into binding behavior. The results reveal that solvent polarity has a major effect on noncovalent interactions, as seen by shifts in vibrational frequencies and changes in the molecule's electrical environment. A combined experimental and computational investigation yields a comprehensive understanding of how noncovalent interactions influence molecular behavior in solution. This study emphasizes the significance of these interactions in defining the chemical and physical properties of thiophene-2-carboxylic acid in a variety of environments, as well as providing useful insights for future chemistry and material science applications.

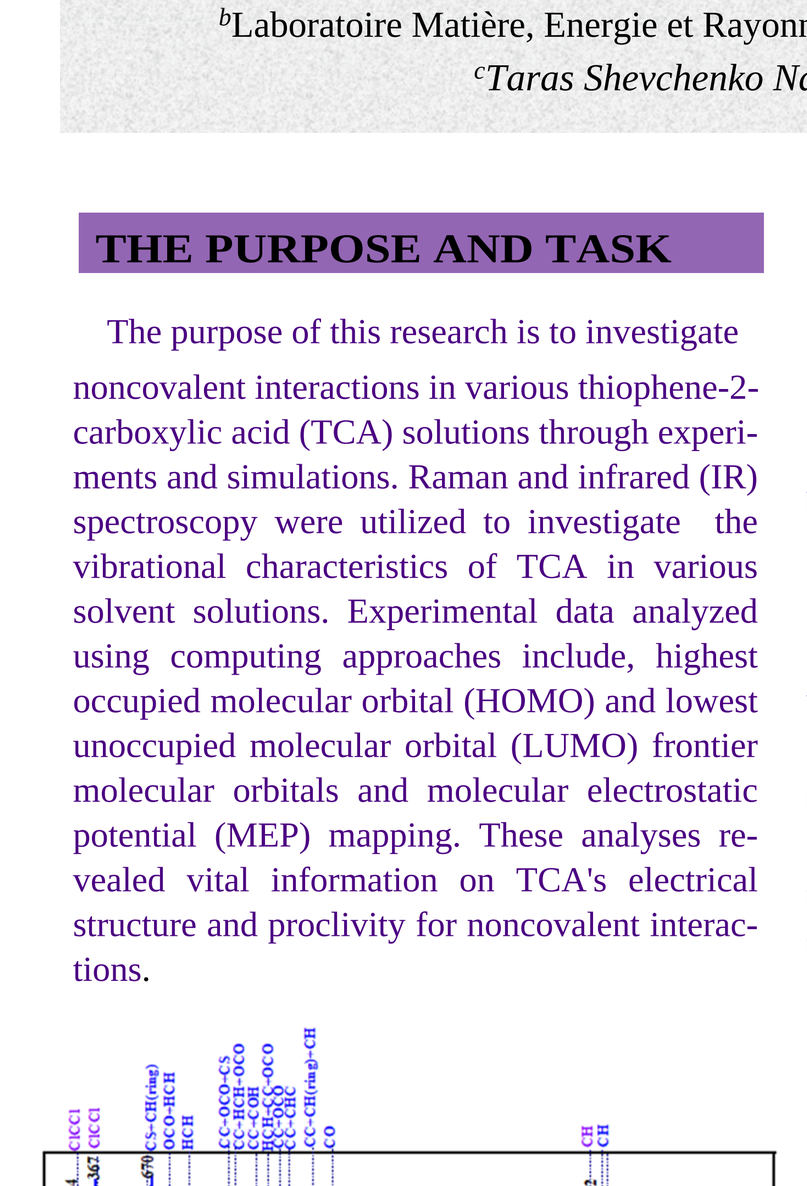


Figure 1. Raman spectra of TCA in chloroform solutions

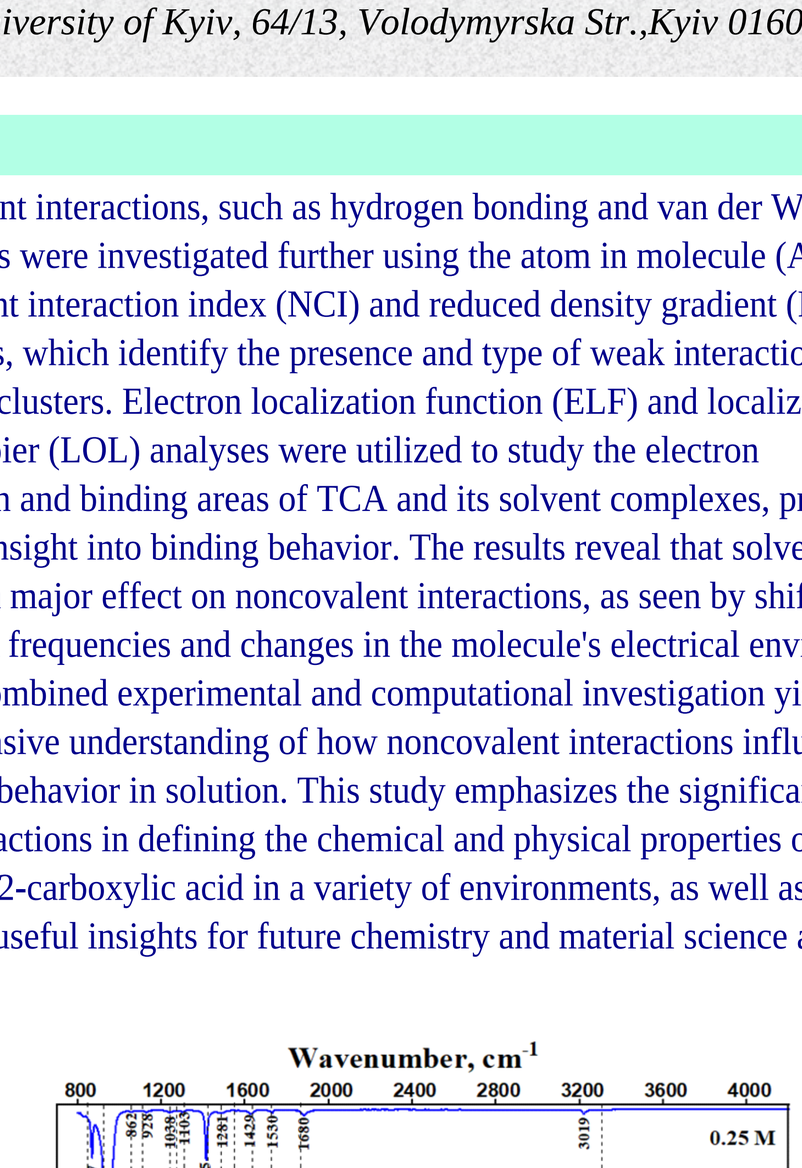


Figure 2. FTIR spectra of TCA in chloroform solutions

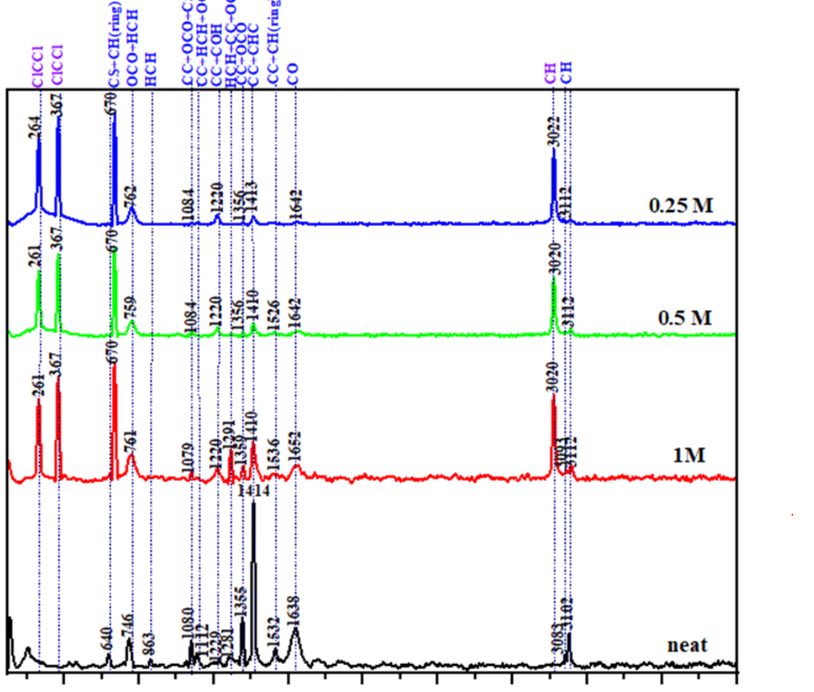


Figure 3. Raman spectra of TCA in ethanol solutions

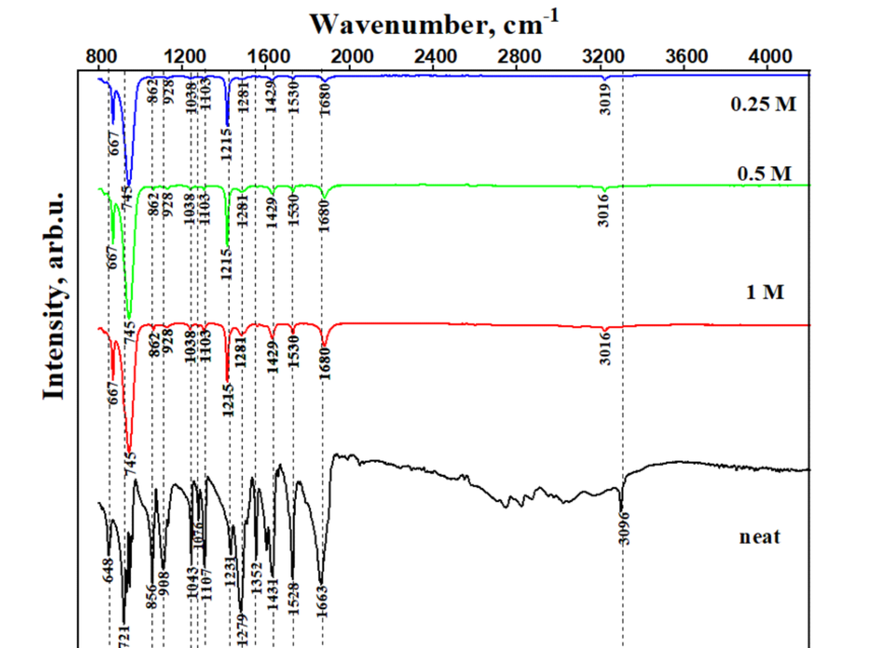
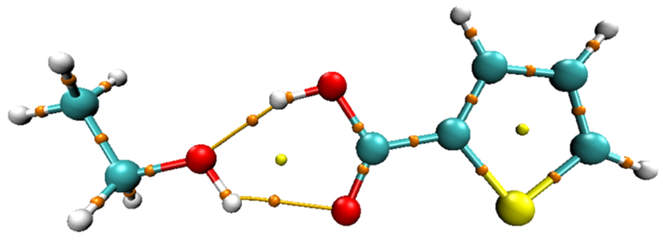
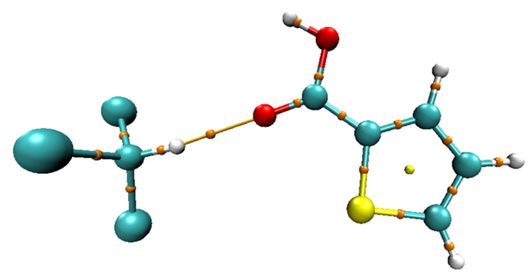


Figure 4. FTIR spectra of TCA in ethanol solutions

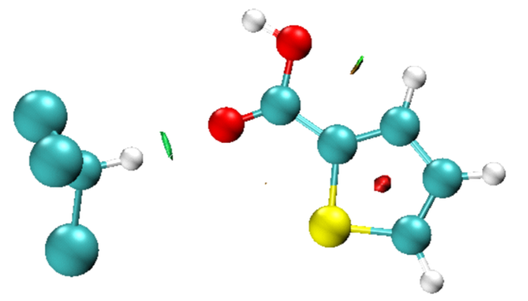


AIM analysis of TCA-ethanol

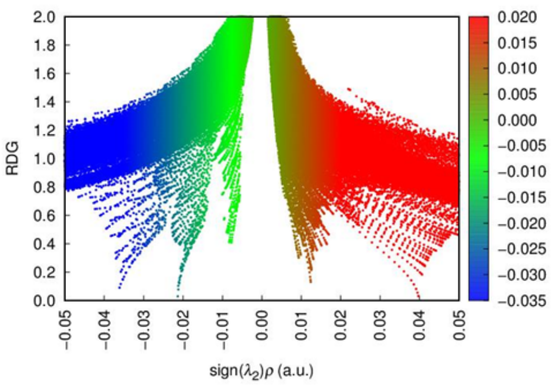


AIM analysis of TCA-chloform

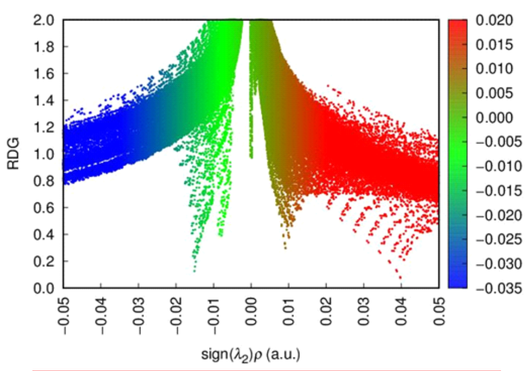
NCI analysis of TCA-ethanol



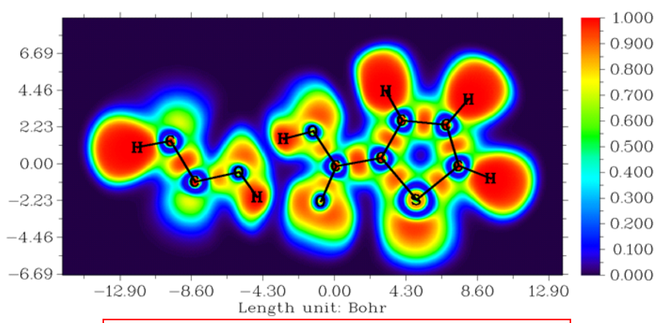
NCI analysis of TCA-chloroform



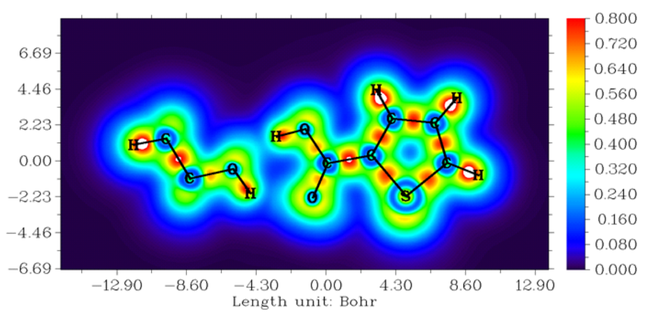
RDG analysis of TCA-ethanol



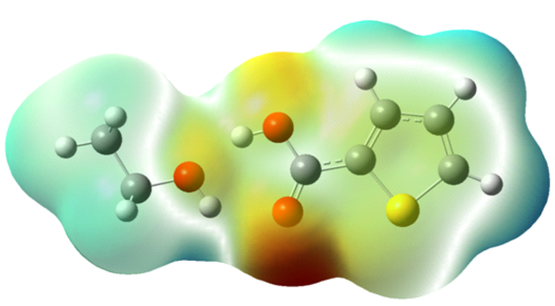
RDG analysis of TCA-chloform



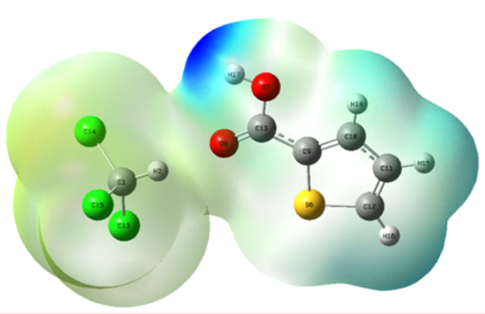
ELF analysis of TCA-ethanol



LOL analysis of TCA-ethanol



MEP Diagram for TCA-ethanol



MEP Diagram for TCA-chloform