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

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This research aims to investigate noncovalent interactions in various thiophene-2-carboxylic acid (TCA) solutions through experiments and simulations. Raman and infrared (IR) spectroscopy were utilized to analyse 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, molecular electrostatic potential (MEP) mapping, and Mulliken charge distribution assessments. These analyses revealed vital information on TCA's electrical structure and propensity for noncovalent interactions. Noncovalent interactions, such as hydrogen bonding, van der Waals interactions, and p-p stacking, were investigated further using the 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 behaviour. 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 behaviour 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.

Type of presence

Presence online

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