

PROBING HALOGEN BONDING INTERACTIONS BETWEEN HEPTAFLUORO-2-IODOPROPANE AND THREE AZABENZENES WITH RAMAN SPECTROSCOPY AND DENSITY FUNCTIONAL THEORY

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The potential formation of halogen bonded complexes between a donor, heptafluoro-2-iodopropane (HFP), and the three acceptor heterocyclic azines (azabenzene: pyridine, pyrimidine, and pyridazine) is investigated herein through normal mode analysis via Raman spectroscopy, density functional theory, and natural electron configuration analysis. Theoretical Raman spectra of the halogen bonded complexes are in good agreement with experimental data providing insight into the structure of these complexes. The exhibited shifts in vibrational frequency of as high as 8 cm⁻¹ for each complex demonstrate, in conjunction with NEDA analysis, significant evidence of charge transfer from the halogen bond acceptor to donor. Here, an interesting charge flow mechanism is proposed involving a conduit-like flow of electron density from each azabenzene's interacting nitrogen atom through the halogen bond and iodine atom to the highly electron-withdrawing fluorine atoms. This mechanism provides further insight into the formation and fundamental nature of halogen bonding and its effects on neighboring atoms. The present findings provide novel and deeper characterization of halogen bonding with applications in supramolecular and organometallic chemistry.