TAILOR MADE SYNTHESIS OF T-SHAPED AND π-STACKED DIMERS IN THE GAS PHASE: CONCEPT FOR EFFICIENT DRUG DESIGN AND MATERIAL SYNTHESIS

SUMIT KUMAR and ALOKE DAS, *Indian Institute of Science Education and Research (IISER), 900 NCL Innovation Park, Dr. Homi Bhabha Road, Pune-411008, Maharashtra, India..*

Non-covalent interactions play a key role in governing the specific functional structures of biomolecules as well as materials. Thus molecular level understanding of these intermolecular interactions can help in efficient drug design and material synthesis. It has been found from X-ray crystallography that pure hydrocarbon solids (i.e. benzene, hexaflurobenzene) have mostly slanted T-shaped (herringbone) packing arrangement whereas mixed solid hydrocarbon crystals (i.e. solid formed from mixtures of benzene and hexafluorobenzene) exhibit preferentially parallel displaced (PD) π-stacked arrangement. Gas phase spectroscopy of the dimeric complexes of the building blocks of solid pure benzene and mixed benzene-hexafluorobenzene adducts exhibit similar structural motifs observed in the corresponding crystal strcutures. In this talk, I will discuss about the jet-cooled dimeric complexes of indole with hexafluorobenzene and p-xylene in the gas phase using Resonant two photon ionzation and IR-UV double resonance spectroscopy combined with quantum chemistry calculations. In stead of studying benzene...p-xylene and benzene...hexafluorobenzene dimers, we have studied corresponding indole complexes because N-H group is much more sensitive IR probe compared to C-H group. We have observed that indole...hexafluorobenzene dimer has parallel displaced (PD) π-stacked structure whereas indole...p-xylene has slanted T-shaped structure. We have shown here selective switching of dimeric structure from T-shaped to π-stacked by changing the substituent from electron donating (-CH3) to electron withdrawing group (fluorine) in one of the complexing partners. Thus, our results demonstrate that efficient engineering of the non-covalent interactions can lead to efficient drug design and material synthesis.