n→π* NON-COVALENT INTERACTION IS WEAK BUT STRONG IN ACTION

SANTOSH KUMAR SINGH, ALOKE DAS, *Department of Chemistry, Indian Institute of Science Education and Research, Pune, Maharshtra, India*.

n→π* interaction is a newly discovered non-covalent interaction which involves delocalization of lone pair (n) electrons of an electronegative atom into π* orbital of a carbonyl group or an aromatic ring. It is widely observed in materials, biomolecules (protein, DNA, RNA), amino acids, neurotransmitter and drugs. However, due to its weak strength and counterintuitive nature its existence is debatable. Such weak interactions are often masked by solvent effects in condense phase or physiological conditions thereby, making it difficult to prove the presence of such weak interactions. Therefore, we have used isolated gas phase spectroscopy in combination with quantum chemical calculations to study n→π* interaction in several molecules where, our molecular systems are free from solvent effects or any external forces. Herein I will be discussing two of the molecular systems (phenyl formate and salicin) where, we have observed the significance of n→π* interaction in determining the conformational specificity of the molecules. We have proved the existence of n→π* interaction for the first time through IR spectroscopy by probing the carbonyl stretching frequency of phenyl formate. Our study is further pursued on a drug named salicin where, we have observed that its conformational preferences is ruled by n→π* interaction even though a strong hydrogen bonding interaction is present in the molecule. Our results show that n→π* interaction, in spite of its weak strength, should not be overlooked as it existence can play an important role in governing the structures of molecules like other strong non-covalent interactions do.