Invited Lecture
Inter-Disciplinary Explorations in Chemistry (I-DEC 2018)

Exploring n→π* interaction in the monomeric building block of Collagen

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Abstract:
n→π* interaction is quite weak (~ 1-2 kcal/mol) but a very important non-covalent interaction widely present in biomolecules and materials.[1-3] In spite of the immense significance of the n→π* interaction in the structure and function of variety of molecular systems, this interaction was not explored by the scientific community until last 15 years due to its weak and counterintuitive nature. This non-covalent interaction is analogous to the well-known and relatively much stronger hydrogen-bonding interaction (n→σ* interaction) in terms of electron delocalization. The n→π* interaction generally occurs between two neighboring carbonyl groups (n→π*-amide) or a carbonyl group and an aryl ring (n→π*-aromatic) through delocalization of lone-pair electrons (*n*) on oxygen atom into a π* orbital of the acceptor group. In the literature, the presence of the n→π* interaction has been substantiated mostly through X-ray crystallography and NMR spectroscopic studies. For the first time, we have provided gas phase IR spectroscopic evidence for both n→π*-amide and n→π*-aromatic interactions.[4] In this talk, I will discuss exploration of the C=O…C=O n→π*-amide interaction in the monomeric building block of collagen, the most abundant protein in animals. Collagen has a unique triple helical structure consisting of three parallel left-handed polyproline II (PPII) strands while each of the strands consists of a repeating sequence of X-Y-Gly, where X=proline (Pro) and Y=4-hydroxyproline (Hyp). It has been reported that individual polypeptide strand in collagen is stabilized by n→π* interaction as intrastrand hydrogen bonding interaction in the polypeptide chains is absent. We have observed conformation specific IR spectroscopic signature for n→π*-amide interaction in a capped Hyp residue, the most important monomer building block of collagen, using isolated gas phase IR spectroscopy and quantum chemistry calculations.

References and Notes:

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Bio-Sketch of Speaker

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Aloke Das obtained his PhD from Indian Institute of Technology Kanpur in 2002. He worked with Professor Tapas Chakraborty for his PhD work on optical spectroscopy of aromatic clusters in a supersonic jet. After finishing his PhD, he moved to Purdue University for doing postdoctoral research with Professor Timothy S. Zwier and worked on conformation-specific UV and IR spectroscopy of flexible aromatic hydrocarbons, which are isomeric products in fuel combustion processes. During 2004-2007, he worked with Professor Erwin D. Poliakoff of the Louisiana State University to study vibrationally resolved Vacuum-Ultraviolet (VUV) photoelectron spectroscopy of polyatomic molecules in the gas phase using synchrotron radiation at the Advanced Light Source of the Lawrence Berkeley National Laboratory. In 2007, he joined Indian Institute of Science Education and Research (IISER) Pune as an Assistant Professor in the Department of Chemistry and presently, he is an Associate Professor there. His research includes molecular level understanding of non-covalent interactions through gas phase laser spectroscopy of molecules and complexes relevant to biomolecules and materials using laser desorption as the vaporization source. At present, major focus of his research is on understanding of $n \rightarrow \pi^*$ non-covalent interaction, Selenium (Se) hydrogen-bonding, sequence dependent folding motifs of peptides, conformation-specific electronic circular dichroism spectroscopy etc.