MIMICKING TRIMERIC INTERACTIONS IN THE AROMATIC SIDE CHAINS OF THE PROTEINS: A GAS PHASE STUDY OF INDOLE...(PYRROLE)$_2$ HETEROTRIMER

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

Aromatic trimeric interactions are extremely important in the stabilization of the specific structures of the proteins as well as protein-protein, and protein-ligand interactions. Here I will present a direct evidence of the observation of a cyclic asymmetric structure of indole...(pyrrole)$_2$ trimer bound by three N-H...π hydrogen bonding interactions in a supersonic jet. The experiment has been performed by using resonant two-photon ionization (R2PI), IR-UV, and UV-UV double resonance spectroscopic techniques. Density functional theory (DFT) calculations nicely corroborate the experimental results showing one weakly allowed IR-active band due to symmetric stretch of the N-H bonds and two strongly allowed IR-active bands due to two types of asymmetric stretches of the N-H bonds in the trimer. The most significant finding of the present investigation is that there is a direct IR spectral signature for the determination of the geometry of a trimer if it has a cyclic asymmetric structure.