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Measurement of dissociation energies for π-π stacked dimers of aromatic hydrocarbons

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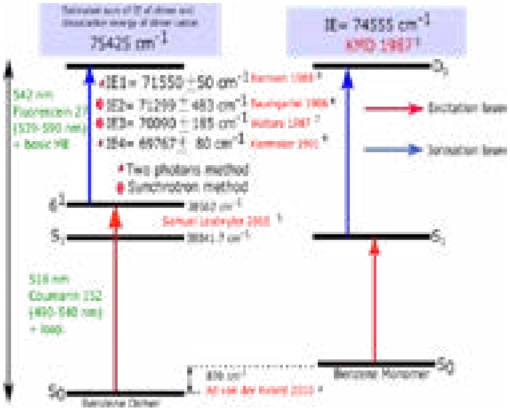
Non-covalent interactions such as aromatic π-π stacked interactions play an important role in the stabilisation and structure of various organic and biological molecules. The aromatic π-π interactions are mainly found in biological molecules such as DNA, proteins and nucleic acids. The work in this research will be focused on π-π stacking, i.e. the interaction of aromatic rings. High-precision measurements of the dissociation energies (D0) are going to be obtained by Mass Analysed Threshold Ionisation (MATI) and Zero-Electron Kinetic Energy (ZEKE) spectroscopy compared to high level Coupled Cluster *ab initio* theory (CC). The focus is to analyse the benzene dimer, naphthalene dimer and anthracene dimer. The experimental set-up consists of two nanosecond laser systems for excitation and ionisation energies coupled to a reflectron and linear time-of-flight mass spectrometer (TOF-MS) to study molecular clusters based on their mass detection. The IR OPO laser system is used to study vibrational levels of the excited states. All the samples will be prepared in the gas phase by utilising the supersonic free-jet expansion technique. SIMION, a simulation software package, will be used to fine tune the experimental conditions in the TOF spectrum. We are achieving high-precision measurements of the dissociation energies of polycyclic aromatic dimers and are applying (with Pavel Hobza's group) the most advanced level of theory to such dimers in order to determine their stabilisation energies (= negative dissociation energies). For the theory side, the Hobza group has made major progress towards a better understanding of the π-π interactions in overcoming the main difficulty: take proper account of the zero-point vibrational energy within the full space of the dimer. This is leading to a much more reliable comparison of the theoretical stabilisation enthalpy with the experimental dissociation enthalpy. The scheme shows the transition energies for the benzene monomer and the dimer, and recent ionisation energy measurements.



Scheme of ionisation energies of the benzene monomer and dimer

Biography

Ali Alessa is a PhD student researcher in University of Manchester. He has an experience using laser system to measure the dissociation energies of polycyclic aromatic dimers.

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