Conformationally-selected ions for reactions with conformationally-selected molecules

Content

The different effective dipole moment of conformational isomers allows for their spatial separation by means of electrostatic deflection, enabling their individual reactivity to be investigated [1]. Recently, the conformer-specific polar cycloaddition of dibromobutadiene (DBB) with trapped propene ions has shown that both gauche and s-trans DBB conformers display capture-limited reaction rates [2]. The reaction was found to occur through both a concerted and a stepwise reaction mechanism, despite the spatial rearrangement of atoms necessary in s-trans DBB for the latter to take place. These results were obtained by selectively aiming the molecular beam containing either one of the two conformers at a static target of propene ions embedded within a laser-cooled Coulomb crystal of calcium ions. In order to gain further control over the reaction partners, we now wish to also select the conformational isomer of the ionic reactant. Here, we discuss the generation of conformationally-selected ionic targets of 3-aminostyrene to enable the study of fully-conformationally-selected ion-molecule reactions. Following the detailed study of the isomer-selective ionisation of the two different 3-aminostyrene conformers, we aim to individually load them into a Coulomb crystal to determine their stability to such environment.

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