

Trapping and sympathetic cooling of conformationally selected ions

L. Xu¹, J. Toscano¹, S. Willitsch^{1*}

¹Department of Chemistry, University of Basel, Klingelbergstrasse 80, 4056 Basel, Switzerland

The different effective dipole moment of conformational isomers allows for their spatial separation by means of electrostatic deflection, enabling their individual reactivity to be investigated¹. 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 rates². 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 also wish to select the conformational isomer of the ionic reactant.

Here, we demonstrate for the first time the sympathetic cooling of different conformational isomers within a Coulomb crystal, setting the scene for fully conformationally selected ion-molecule reaction studies. Following the successful isomer-selective ionisation and loading of the two *m*-aminostyrene conformers into Coulomb crystals of trapped and laser-cooled calcium ions, we now aim to investigate their isomer-specific reactivity.

[1] Y.-P. Chang, K. Długołęcki, J. Küpper, D. Rösch, D. Wild and S. Willitsch, *Science*, **2013**, 342, 98.

[2] A. Kilaj, J. Wang, P. Straňák, M. Schwilk, U. Rivero, L. Xu, O. A. von Lilienfeld, J. Küpper and S. Willitsch, *Nat. Commun.*, **2021**, 12, 6047.