

Institutsseminar

Conformationally selected ions react differently with neutrals

Lei Xu

Department of Chemistry
University of Basel – Switzerland

The conformation of a molecule plays an important role in the chemistry of complex molecular systems, necessitating the development of experimental methods for the characterization of the chemical reactivity of individual conformers. Previously, the *cis* and *trans* conformers of neutral 3-aminophenol have been spatially separated in the gas phase based on their different dipole moment and reacted with a ‘Coulomb crystal’ of calcium ions [1]. These crystals are structures formed by trapped, laser-cooled ions and they can be used to ‘sympathetically cool’ other trapped ionic species. Building up on these methodologies, ionic Diels-Alder reactions were studied between conformationally selected neutral dibromobutadiene (DBB) molecules and sympathetically cooled propene ions. These studies provided new insights into conformationally dependent reaction mechanisms of cycloaddition reactions [2].

In order to gain an even deeper understanding of conformational effects of chemical reactions, conformational control of not only the neutral, but also the ionic reactants in ion-molecule reactions would be beneficial. To this end, we used a two-color (1+1') resonance-enhanced multiphoton ionization (REMPI) scheme [3] to selectively ionize the *cis* and *trans* conformers of *meta*-aminostyrene (mAS) molecules inside the ion trap and sympathetically cool them using calcium Coulomb crystals [4]. Following the developed ion loading scheme, conformationally selected mAS⁺ ions were individually reacted with calcium atoms and with 1,3-cyclohexadiene molecules. Different reactivities of

cis and *trans* mAS⁺ ions were observed, expanding the scope of conformational selectivity to ionic species and paving the way towards fully conformationally controlled chemistry.

Acknowledgments: This work was supported by Swiss National Science Foundation (SNSF), grant number IZCOZ0_189907

References

- [1] Chang, Yuan-Pin, et al. *Science* **342**.6154 (2013): 98-101.
- [2] Kilaj, Ardita, et al. *Nature Communications* **12**.1 (2021): 6047.
- [3] Dong, Changwu, et al. *Journal of Molecular Structure* **1058** (2014): 205-212.
- [4] Xu, Lei, et al. *Physical Review Letters* **132**.8 (2024): 083001.

HS C

15:30 Uhr

22.09.2025