Universität Basel

Research Project

Conformationally Controlled Chemistry

Third-party funded project

Project title Conformationally Controlled Chemistry
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Department
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The relationship between structure and reactivity is one of the central tenets of chemistry. In particular, many molecules exhibit structural isomers that interconvert over low barriers through rotations about covalent bonds (conformers). Conformers are the dominant isomers of complex molecules, and the conformation of a molecule can have pronounced effects on its chemical reactivity. Despite the eminent importance of conformational isomers in chemistry, very few studies have been reported thus far characterising conformational effects in chemical reactions under single-collision conditions. Consequently, the role of molecular conformations in fundamental reactions is only poorly understood. This striking lack of data reflects the experimental challenges to isolate und control specific conformers.

In a recent proof-of-principle study [Science 342 (2013), 98], we have spatially separated specific conformers in a molecular beam through electrostatic deflection and directed them at a spatially localized reaction target of cold ions in a trap. This approach allowed us to study conformation-specific effects in ion-molecule reactions under precisely controlled experimental conditions in the gas phase. Here, we pro- pose a wide-ranging research programme aiming at extending our method to neutral reactions and applying it to a range of chemically relevant problems in order to explore the relationship between structure and reactivity in unprecedented detail. These methodological advances will enable for the first time detailed and systematic studies of the reaction mechanisms and dynamics of isolated conformers. The fundamental mechanistic insights gained will benefit a wide range of fields as diverse as fundamental reaction dynamics, organic synthesis, catalysis, atmospheric chemistry and rational molecule design.

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Add publication

Published results

3720344, Rösch, Daniel; Gao, Hong; Kilaj, Ardita; Willitsch, Stefan, Design and characterization of a linear quadrupole ion trap for high-resolution Coulomb-crystal time-of-flight mass spectrometry, 2195-7045, EPJ Techniques and Instrumentation, Publication: JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

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