Universität Basel

Research Project

Controlled reactive collision with trapped ions

Third-party funded project

Project title Controlled reactive collision with trapped ions
Principal Investigator(s) Willitsch, Stefan ;
Organisation / Research unit
Departement Chemie / Chemische Physik (Willitsch)
Department
Project start 01.01.2020
Probable end 31.12.2023
Status Completed

Studies of the dynamics of chemical reactions have made impressive advances in recent years owing to the development of techniques for the cooling and manipulation of the motion of molecules in the gas phase. These methods have enabled new insights into the microscopic mechanisms, the quantum nature and the detailed dynamics of chemical processes which were not accessible before.

By combining trapped, sympathetically cooled molecular ions with electrostatically deflected molec- ular beams, we have recently established a new experimental approach for studying reactive collisions of trapped molecular ions with state- and conformationally controlled neutral molecules. While we have so far achieved state, collision-energy and conformational control for the neutral reactants using the electrostatic deflection technique, the quantum state and conformation of the ionic co-reactant has not been specified in our previous experiments. To achieve a comprehensive control over a reactive process by predetermining its most important dynamical parameters, it is necessary to specify the quantum state and conformation of both reactants. In the present grant application, we propose to additionally generate polyatomic molecular ions in the vibrational ground state of specific conformational isomers in order to realise a fully vibrationally, conformationally and collision-energy-controlled ion-molecule reaction experiment for the first time. This will be achieved by preparing the ions using conformer-selective photoionisation techniques in combination with sympathetic cooling of their translational motion in an ion trap. Our new methodology will be applied to study conformationally and state-specific dynamics in a range of pertinent model systems including the reactions of rotationally state-selected water molecules and of conformationally selected 3-aminophenol molecules with conformationally selected phenylalanine and 3-aminophenol ions. The experimental results on the kinetics and reaction dynamics of these systems will be complemented and analysed by quasiclassical-trajectory simulations on accurate ab-initio potential energy surfaces.

We expect that these advancements will take the study of ion-molecule chemistry of polyatomic systems to a new level and enable insights into their state- and geometry-specific reaction dynamics, kinetics and mechanisms in unprecedented detail. The present grant application is thematically fully embedded in the COST Action CA17113 - TIPICQA ”Trapped Ions: Progress in classical and quantum applications” and capitalises on scientific synergies through collaborations and scientific exchanges within Workgroup 4 ”Hybrid Systems” of this Action.

Financed by
Swiss Government (Research Cooperations)

Add publication

Add documents

Specify cooperation partners