Universität Basel

Research Project

Collisional and Half-Collisional Dynamics of Conformationally Selected Molecules

Third-party funded project

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The reaction rates and dynamics of chemical reactions and molecular energy transfer are often influenced by the structure of the involved molecules. Even subtle changes of the molecular geometry can make significant differences in chemical reactivity. Both intramolecular and intermolecular processes need to be understood on the quantum level in molecular systems with well-defined geometries in order to establish a detailed understanding of structure- reactivity relationships. The present project aims at establishing a comprehensive characterisation of these relationships in selected model systems by studying both collisional and half-collisional reactions by pooling the expertise of the Korean and Swiss partners. Combined structural and quantum aspects of chemical reaction dynamics will be studied under precisely controlled conditions in the gas phase. State-of-the-art experimental techniques such as Stark deflection, double-resonance, stimulated-emission pumping and hole-burning will be employed in order to spatially or spectroscopically isolate specific conformational isomers of the molecules in the gas phase. This will enable the study of half-collisional reactions such as photodissociation, intramolecular tunnelling, and isomerization as well as state-selective full collisional reactions in a conformer-specific manner. Measurements of conformationally resolved spectra and reaction-rate constants will be complemented by frequency and/or time resolved velocity-map ion/electron imaging experiments to elucidate fine details of the reaction dynamics. The systems targeted in this study are hydroquinone, resorcinol and oxalyl chloride and their reactions with free radicals such as F, Cl and OH which have been selected for their prototypical character and experimental amenability. In addition to the bare conformationally selected molecules, investigations will also be performed with their conformationally selected clusters with water in order to study the effects of incipient solvatisation on the reactivity and dynamics. Moreover, vibrationally state-selected studies will be performed to gain insights into the interplay between mode- and structure-specific reactive effects. The experiments will be complemented by ab-initio and reactive molecular dynamics calculations to analyse and interpret the data.

Spectroscopic characterization of conformers and their half-collisional dynamics will be studied at KAIST in Korea, whereas full collisional dynamics involving conformer-specific neutral-radical will be investigated at University of Basel in Switzerland. The partner groups constitute an ideal match to carry out the present research programme by sharing similar research interests, but contributing complementary scientific expertise, techniques and equipment. The project relies on harvesting the synergies between the groups through the exchange of knowledge, of experimental techniques and of data as well as through the joint training of PhD students and regular scientific visits of the involved personnel between Switzerland and Korea.

By for the first time contrasting intra- with inter-molecular dynamics in selected geometry- selected model systems, we expect that the present project will yield new and valuable insights into structure-reactivity relationships in chemistry. We expect that the present results will not only be of immediate relevance for

the advancement of molecular and chemical physics, but will also contribute to the general understanding of chemical reactivity and be of specific benefit to a wider range of disciplines such as synthetic chemistry and catalysis.

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