

**Conformational effects in radical reactions**P. Stranak<sup>1</sup>, L. Ploenes<sup>1</sup>, H. Gao<sup>1</sup>, S. Willitsch<sup>1\*</sup><sup>1</sup>Department Chemie, Universität Basel, Klingelbergstrasse 80, 4056 Basel

Revealing the dynamics of hydrocarbons reacting with free radicals is of major relevance for understanding atmospheric processes and combustion chemistry [1]. Despite their significance demonstrated by the vast body of literature, the conformational dependence of radical reactions still remains largely unexplored. Only a few studies demonstrate conformational effects in these reactions [2, 3]

To gain detailed insights into reaction dynamics, a crossed-molecular-beam apparatus with integrated conformer-selector is being built. The molecular beam technique allows us to study single-collision events under well controlled initial conditions. Due to different dipole moments, conformers can be spatially separated in a molecular beam using an inhomogeneous electric field. This technique of separation has been previously successfully implemented to study conformationally resolved reactions of 3-aminophenol with Ca<sup>+</sup> ions [4].

We are now extending this approach to neutral reactions. Our first target is the reaction of conformationally selected 1,2-bis(trifluorosilyl)ethane with chlorine radicals [5]. Calculations of the potential energy surface suggest that the abstraction of hydrogen by chlorine is more favourable from the gauche-conformer because of the sterical hinderance exerted by the SiF<sub>3</sub> groups. In a first stage, we aim to measure conformer-specific reaction rates which yield information about the activation energies of different conformational reaction pathways. At a later stage, the experiments will be extended for measurements of product state and angular distributions and different radical species, e.g., fluorine.

[1] R. I. Kaiser, A. M. Mebel, *Int. Rev. Phys. Chem.*, **2002**, 21, 307-356.

[2] V. L. Orkin et al., *J. Phys. Chem. A*, **2011**, 115, 6568-6574.

[3] C. A. Taatjes et al., *Science*, **2013**, 340, 177-180.

[4] D. Rösch et al., *Science*, **2013**, 342, 98-101.

[5] P. Klæboe et al., *J. Raman Spectrosc.*, **2009**, 40, 2111-2122.