

# State-of-the-art laboratory experiments combined with quantum chemistry to study reactive ion-molecule collisions under interstellar conditions

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Astronomical observations have revealed a rich chemical complexity in the close galactic molecular clouds of the interstellar medium (ISM) [1]. So far, more than 250 molecules have been detected in these environments. Most of them are stable neutral species, but there is plenty of radicals and molecular ions among them as well. The variety of the observed cations has grown rapidly in recent years, with the detection of species like  $\text{ArH}^+$ ,  $\text{C}_3\text{H}^+$ ,  $\text{C}_2\text{N}_2\text{H}^+$ ,  $\text{NO}^+$ ,  $\text{NS}^+$ , *etc.* While the majority of the neutral interstellar species are not highly reactive, the ionic species are usually efficiently involved in chemical reactive processes and thus initiate – or contribute to – the growth of molecular complexity. The study of reactive collisions however induces many challenges both from experimental as well as from theoretical side. What is the nature and internal state of the reaction products? What is their relative abundance? What kind of side species and isomers are formed? To understand the reactive molecular processes and answer these questions, a global approach is required, which involves state-of-the-art laboratory measurements from one hand along with in-depth theoretical analysis of the reaction kinetics on the other hand. At Institut de Physique de Rennes we have realized this unique combination of experimental and theoretical methods to investigate reactive ion–molecule collisions.

In our laboratory, we have developed an original method which combines a uniform supersonic flow reactor (CRESU) apparatus with a mass-selective source capable to produce stable ionic species at thermal energies (down to about 10 K) [2]. The apparatus is equipped with a quadrupole mass spectrometer which allows the detection of ionic products in the range of 0-100 amu in reactive collisions between molecular ions and neutral species [2]. In parallel, we combine high-level *ab initio* theories with molecular dynamics and transition state theory-based methods to explore the possible reaction paths and calculating reaction rates for the individual channels. The association of such experimental and theoretical tools allows one to follow reaction kinetics and derive precise branching ratios. We have recently studied the reaction of  $\text{N}_2^+$  with  $\text{C}_3\text{H}_4$  [3] and of  $\text{Ar}^+$  with  $\text{C}_2\text{H}_4$ , where for both of them we found a significant temperature dependence of the branching ratios. These findings initiate further investigation of ion–molecule collisions. We have now started to examine key interstellar reactions for rapid carbon chain elongation (*i.e.* all C atoms end up in the products) such as the one of  $\text{CH}_3^+$  with a range of hydrocarbons.

## References

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