



The Astrochemical Week

COST Action CM1401

Faro / Olhão

Portugal

16-20 January 2017

<https://astrochem2017.sciencesconf.org/>



# DISSOCIATIVE CHARGE TRANSFER OF INTERSTELLAR DIMETHYL ETHER AND METHYL FORMATE IN COLLISIONS WITH He<sup>+</sup>

A. Cernuto<sup>1</sup>, D. Ascenzi<sup>1</sup>, F. Pirani<sup>2</sup> and P. Tosi<sup>1</sup>

<sup>1</sup>Department of Physics, University of Trento, Italy  
e-mail: andrea.cernuto@unitn.it; daniela.ascenzi@unitn.it; paolo.tosi@unitn.it

<sup>2</sup>Dept. Chemistry, Biology & Biotechnology, University of Perugia, Italy  
e-mail: fernando.pirani@unipg.it

Collisions with He<sup>+</sup> are an important pathway for the decomposition of complex organic molecules in the interstellar medium (ISM). We have carried out dissociative charge transfer reactions of He<sup>+</sup> with two O-containing organic molecules, ubiquitous in ISM: dimethyl ether CH<sub>3</sub>OCH<sub>3</sub> (DME) and methyl formate HCOOCH<sub>3</sub> (MF). Since they have a prebiotic relevance, several models were developed to explain how these molecules are formed and destroyed in the ISM [1].

The reactions have been investigated by using the home-built Guided-Ion Beam Mass Spectrometer (GIB-MS) apparatus. Absolute cross sections and product branching ratios have been measured as a function of the collision energy in the hyperthermal energy range (i.e. from about 0.1 to 7 eV). The presence of the molecular ion was not observed among the products for these reactions, which means that the nascent DME and MF radical cations are formed in a dissociative state. Insights on the charge transfer process for the system DME–He<sup>+</sup> have been obtained by investigating the nature of the nonadiabatic transitions between the reactant and product potential energy surfaces. The PES has been represented by using a semi-empirical method in order to model the intermolecular interactions [2]. The observed crossings confirm the experimental conclusion: He<sup>+</sup> captures an electron from an inner valence orbital of the organic molecule, having binding energies about 12 eV higher than the HOMO. An improved Landau-Zener model has been developed in order to obtain the total integral cross section to be compared with the experimental results. Intermolecular interaction and electron densities of the orbitals involved in the reaction turned out to be key points to describe the dynamics of the dissociative charge transfer. A remarkable agreement is obtained between the experimental and calculated total cross sections at low collision energy, which is the most relevant range for the interstellar environment. These results represent a significant starting point to estimate rate constants for destruction of DME by collisions with He<sup>+</sup> ions in the ISM at low temperatures.

Implementation of the same model on the experimental results for MF is in progress.

## REFERENCES

- [1] N. Balucani, C. Ceccarelli, and V. Taquet, *MNRAS* **449**, L16 (2015).
- [2] F. Pirani, G. S. Maciel, D. Cappelletti, and V. Aquilanti, *Int. Rev. Phys. Chem.* **25**, 165 (2006).