Funded by the Horizon 2020 Framework Programme of the European Union

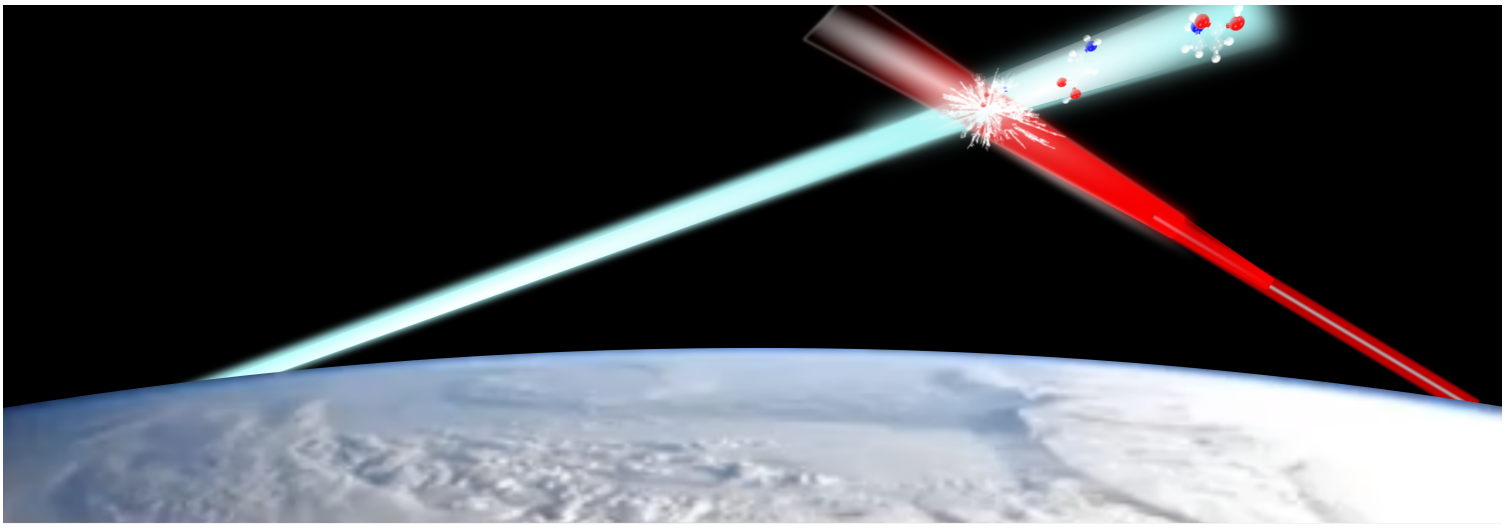
COST Action CA18212
MD-GAS
Molecular Dynamics in the GAS phase

cost
EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Working Group 1 & Working Group 2
Online Meeting

Book of Abstracts

15th-19th March 2021



MD-GAS COST ACTION

Molecular Dynamics in the Gas Phase

POSTER LIST

Tuesday 16th March

EXPERIMENTAL CHARA CTERIZATION AND ION OPTICS SIMULATION OF AN IN-VACUUM ELECTROSPRAY IONIZATION APPARATUS

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The ElectroSpray Ionization (ESI) is a technique to produce isolated molecular ions in gas phase by spraying a low concentration solution of the molecule of interest. This technique can be applied to a wide range of compounds, from oligopeptides to entire proteins, strands of DNA and nanoparticles [1]. In our laboratory at CNR-ISM, an ESI source has been coupled to a non-commercial apparatus to transport the molecular ion beam in vacuum. The apparatus, Fig. 1a, consists of several stages to achieve removal of neutral species, ions selection and analysis by mass/charge ratio and deposition by 'soft landing'.
The source parameters that affect the transmission and/or the composition of a molecular beam of Rhodamine 6G (from a 10^{-5} M of a water : ethanol, 1:1, solution) have been investigated by a combination of experimental measurements and ion optics simulations, Fig. 1b and c, respectively. These start-to-end ion optics simulations provide reliable information on the behavior and operation of the apparatus even though, due to the collisions with the buffer gas in the initial stages, the results concerning the kinetic energy of the ion beam must be treated with care. [2].

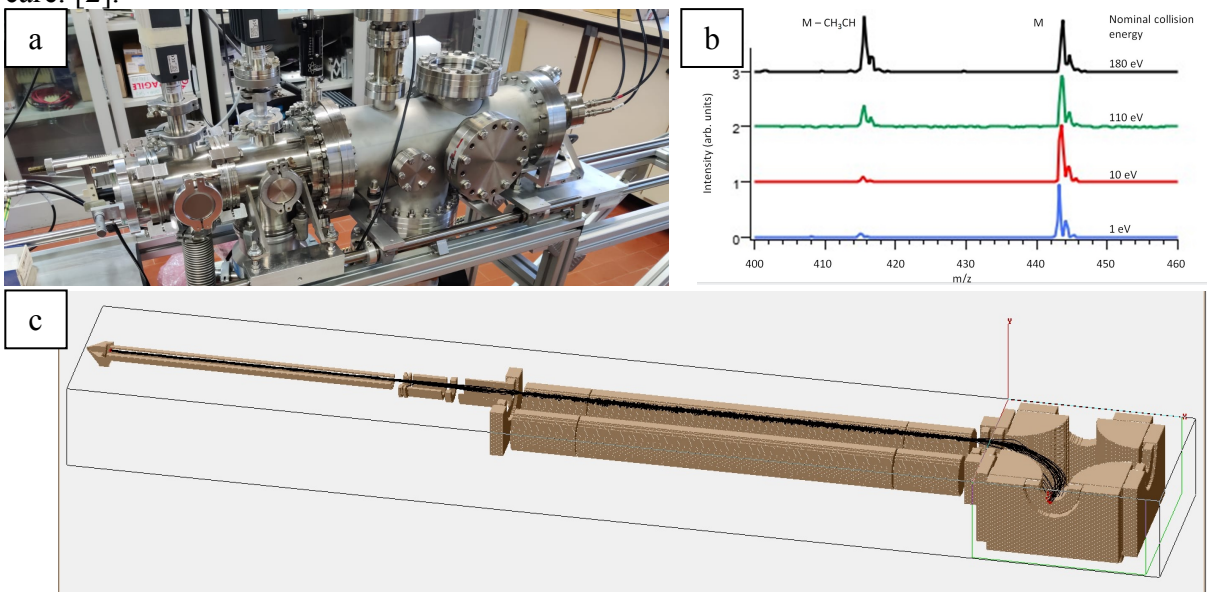

Figure 1: A) Pictures of the apparatus. B) Mass spectra of the Rhodamine 6G at increasing collision energy in the first stage of the apparatus. C) Snapshot of the simulation of the ion trajectories.

Acknowlegments

MAECI Italia-Svezia Project *Novel molecular tools for the exploration of the nanoworld* and Progetto Gruppi di Ricerca Regione Lazio *DESIR*.

References

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