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An electrospray ionisation apparatus for gas phase study of biomolecules

J Chiarinelli[1,2], P Bolognesi [1 *], J M Ramillon[3], P Rousseau[3], A Domaracka[3], M C Castrovilli[1] and L Avaldi[1]

[1]Istituto di Struttura della Materia, ISM-CNR, 00016 Monterotondo Scalo, Roma, Italy
[2]Dipartimento di Scienze, Università di Roma Tre, Roma, Italy
[3]Normandie Univ, ENSICAEN, UNICAEN, CEA, CNRS, CIMAP, Caen, France

Synopsis A set-up to study large biomolecules in the gas phase based on an ElectroSpray Ionisation source has been installed at CNR-ISM in Rome, and it is currently under commissioning. Accurate ion optics simulation provide crucial feedback in the understanding and optimisation of its performance.

The ElectroSpray Ionization (ESI) [1] allows to bring large organic molecules (proteins, enzymes etc) as intact and isolated units in the gas phase. The technique is based on the use of a low-concentration solution of the molecule of interest flowing in a small capillary held at high voltage with respect to a grounded counter electrode. Driven by the electric field from the Taylor cone formed at the tip of the noozle, the charged droplets undergo a fast decrease in their size as the solvent evaporates, and a gas of molecular ions is formed. Transported towards the high vacuum stage of the set-up, after mass-over-charge filtering, the selected molecular ions can finally be used for soft-landing applications as well as for gas phase experiments.

The ElectroSpray Ionisation (ESI) set-up recently installed at the CNR-ISM laboratory in Rome, presently consists of i) a heated capillary to transport the charged species in vacuum, ii) a first differential pumping stage equipped with an octupole ion guide, iii) a quadrupole mass filter and quadrupolar deflector to direct the ion beam towards either a diagnostic or application stages (see Figure 1).

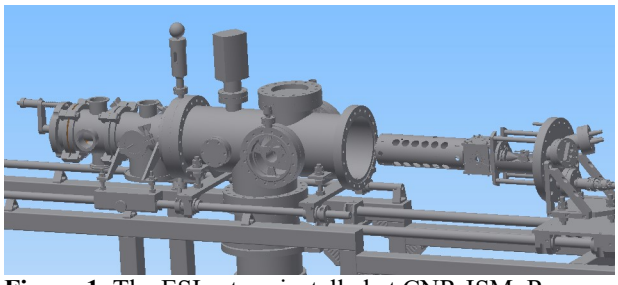

Figure 1. The ESI set-up installed at CNR-ISM, Rome.

The newly developed apparatus is currently under commissioning. Computer simulations by SIMION software [2] are being performed to optimise ion transmission through the numerous optical elements in the set-up.
The comparison of the simulated results with the ion current and ion kinetic energy distribution measured at different check-points in the apparatus provides a valuable feedback for the simulations and deep insights on the behaviour of the apparatus. These are crucial for the optimisation of its performances as well as for further improvements of the set-up.

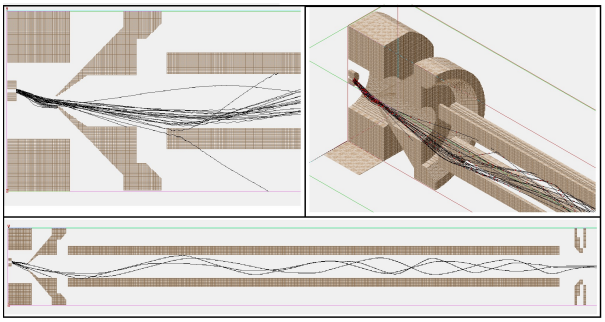

Figure 2. Snapshots of ion optics simulations of the first stage of the apparatus (capillary, skimmer and octupole) performed with Simion software.

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References

[1] Fenn J B *et al* 1989 *Science* **4926** 64
[2] https://simion.com/

* E-mail: paola.bolognesi@cnr.it