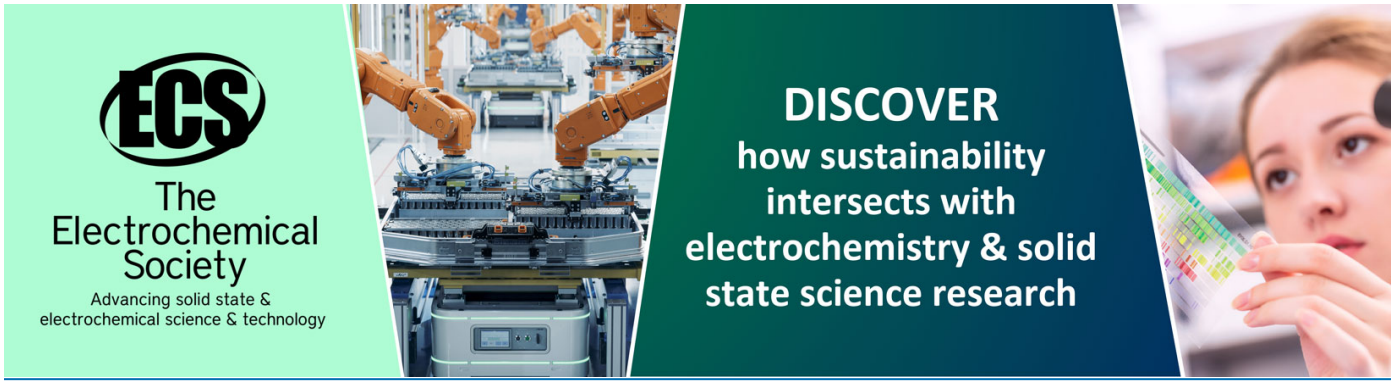
Ionization of pyrimidine molecule induced by proton



Ionization of pyrimidine molecule induced by proton

M A Quinto[1 *], J M Monti[1] and R D Rivarola[1]

[1]Instituto de Física Rosario, CONICET and Universidad Nacional de Rosario, Rosario, S2000EKF, Argentina

Synopsis In the present study will be investigated the ionization of isolated pyrimidine molecules induced by ions. The total and differential cross section have been computed with a quantum mechanical method within the continuum distorted wave-eikonal initial state (CDW-EIS) approximation. A comparison with the available data is presented.

The studies of the ionization processes induce by ion on molecules of biological interest has a great importance in radiobiology and medicine. In this context, the electron emission processes induced by charged particles on DNA components – including the nucleobases as well as the sugar-phosphate group – have been extensively studied on both experimental and theoretical sides [1,2]. However, some secondary biological molecules such as purine and pyrimidine have recived a particular interest of study since they are considered as a precursor of some DNA/RNA nucleobases (namely cytosine, thymine and uracil). Thus, pyrimidine has become a target of interest for radiobiology and it has been the subject of numerous electron and proton studies [3,4].

In the present work, we study the ionization of a isolated pyrimidine molecule induced by ions with a quantum mechanical framework within the CDW-EIS approximation [5]. A full set of total and differential cross sections will be present during the conference. A comparison with available experimental results will be made in every possible case (see Figure 1). The orbitals of the pyrimide molecular targer are described by linear combinations of their atomic compound orbitals (LCAOs). The corresponding binding energies and effective occupation electron analysis of each molecular orbital are obtained by using the GAUSSIAN09 software at the RHF/3-21G.

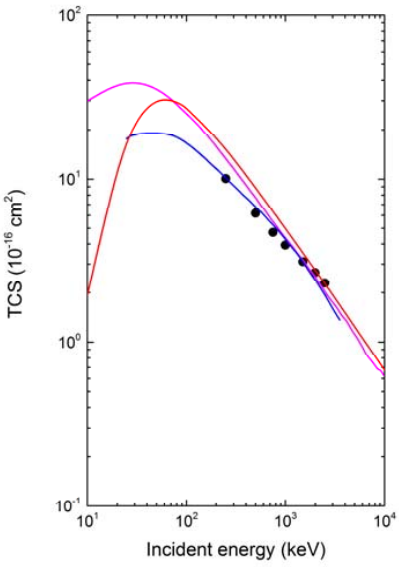


Figure 1. Total cross sections for single ionization of pyrimidine induced by proton. Theroretical calculations solid lines: CDW-EIS (red) and FBA (magenta) [3] . Semi-empirical results (blue) and experimental data are token from [4].

References

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* E-mail: quinto@ifir-conicet.gov.ar