

PAPER • OPEN ACCESS

Ionization of pyrimidine molecule induced by proton

To cite this article: M A Quinto *et al* 2020 *J. Phys.: Conf. Ser.* **1412** 212002

View the [article online](#) for updates and enhancements.

You may also like

- [Synthesis and biological activity of aza and deaza analogues of purine nucleosides](#)
Elena S. Matyugina, Sergey N. Kochetkov and Anastasia L. Khandazhinskaya
- [Efficiency and potential synthesis of pyrimido \[4,5-d\] pyrimidine derivatives by iodine catalyst as antioxidant agent](#)
A H Cahyana, A R Liandi and M Z R Zaky
- [Methods for the synthesis of aza\(deaza\)xanthines as a basis of biologically active compounds](#)
D A Babkov, A N Geisman, A L Khandazhinskaya et al.



The
Electrochemical
Society

Advancing solid state &
electrochemical science & technology



DISCOVER
how sustainability
intersects with
electrochemistry & solid
state science research



Ionization of pyrimidine molecule induced by proton

M A Quinto¹*, J M Monti¹ and R D Rivarola¹

¹Instituto 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 induced 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 received 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 pyrimidine molecular target 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.

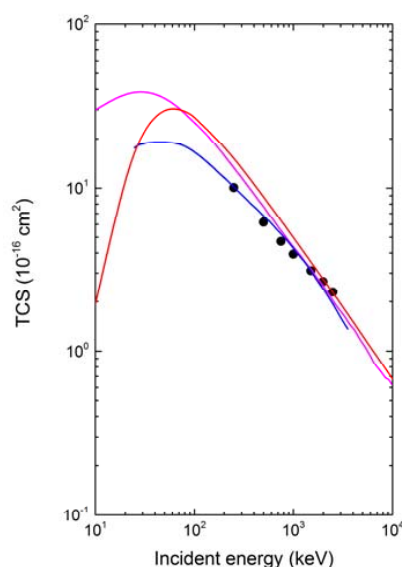


Figure 1. Total cross sections for single ionization of pyrimidine induced by proton. Theoretical calculations solid lines: CDW-EIS (red) and FBA (magenta) [3]. Semi-empirical results (blue) and experimental data are taken from [4].

References

- [1] Galassi M E *et al* 2012 *Phys. Med. Biol.* **57** 2081
- [2] Champion C *et al* 2012 *Phys. Med. Biol.* **57** 3039
- [3] Champion C *et al* 2015 *Eur. Phys. J. D* **69** 127
- [4] Wolff W *et al* 2014 *J. Chem. Phys.* **140** 064309
- [5] Monti J M *et al* 2014 *Appl Radiat Isot.* **83** 105–108

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