# Electron impact ionization of pyrimidine: differential and total cross sections

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**Synopsis** We provide theoretical cross sections for the ionization of pyrimidine by electron impact. The theoretical framework is based on a quantum approach making use of particular tools to overcome the computing challenges. The developed methodology allows to determine not only the total but also the triple, double and simple differential cross sections. This approach was previously used to calculate the triple differential cross sections of many molecules. Here, we demonstrate that it can be used to calculate more integrated cross sections of a molecule of biological interest: pyrimidine.

Providing cross sections for the electron impact ionization of biological molecules has become an urgent requirement for valid investigations of particle interactions within the biological medium. Due to the lack of cross section data for complex biological molecules, interaction cross sections with water are often used to model interactions in living tissue. However, recent studies show that using water to mimic biological systems is not quantitatively correct [1]. We propose a methodology to calculate differential and more integrated cross sections for the ionization of biologically relevant molecules by electron impact [2, 3]. It is based on a distorted wave model (DW) within the framework of the First Born Approximation. We show here the resultant cross sections for pyrimidine: a structural unit of DNA and RNA bases thymine, cytosine and uracil. In figure 1 we compare the triple differential cross sections (TDCS) obtained with the present model (solid line) to those computed using the orientation averaged molecular orbital (OAMO) approximation (dashed line) and the experimental data from [4]. The OAMO approximation was proposed as a solution to overcome the difficulty of calculating cross sections for an average molecular orientation by performing this average on the level of the molecular wave functions. It was used to determine the TDCSs for many molecules but was found to deplete important information about the molecular orbital structure. Figure 1 shows that the cross sections calculated with the DW model are in better agreement with the experimental data.

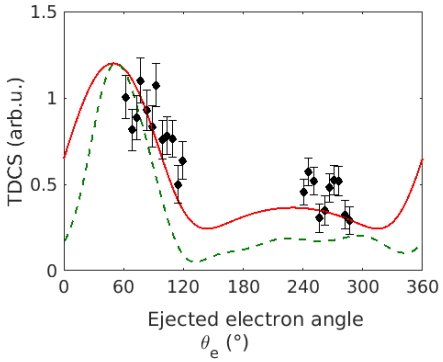


**Figure 1**. Summed TDCSs for the electron ionization of pyrimidine orbitals $10a_1$, $1b_1$ and $6b_2$ calculated with the DW (solid line) approach, compared to OAMO TDCSs (dashed line) and experimental data (solid circles) from [4].

## References

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