Ionization of thymine by electron impact

S. Nehaoua[1] , S. Houamer[1] and C. Dal Cappello[2]

[1] Laboratoire de Physique Quantique et Systèmes Dynamiques, Département de physique, Faculté des Sciences,Université Ferhat Abbas, Sétif, 19000, Algeria
[2]Université de Lorraine, Laboratoire de Physique Moléculaire et des Collisions, UMR

CNRS 7565, 1 Boulevard Arago, 57078 Metz Cedex 3, France

Email : s_houamer@univ-setif.dz

The single ionization of molecules by charged particles remains up to now a difficult problem when we want to treat it by an ab-initio quantum model. The difficulty is due to the multicenter character of the target wave function. One way to avoid this difficulty is to use a single center wave function for the initial (or excited) state of the molecule. The single center is just the center of the molecule. We have shown in a recent paper [1] that the valence electrons can be described by single center wave functions with few partial waves. We apply here the first and second Born approximation to study the triple differential cross sections for the ionization of the thymine molecule by electrons where an accurate single center wave function is used to describe the initial state in the case of the ionization of valence electrons. Our results are compared to the recent experiments for the ionization of thymine by electrons [2] recently used to describe the ionization process in the case of thymine. A good agreement between our results and the experiments of Bellm et al [2] is generally observed. As an example we can see in figure1 the TDCS of the single ionization process corresponding to the 1a' orbital of thymine. The TDCS is displayed at impact energy (E_i=250 eV) versus the ejection angle in the case of first and second Born. It is clearly observed that the data are correctly reproduced especially in the case of the second Born case where the peak is shifted towards greater angles. Our model is thus able to describe the process in the case if thymine and can be extended to other DNA molecules.

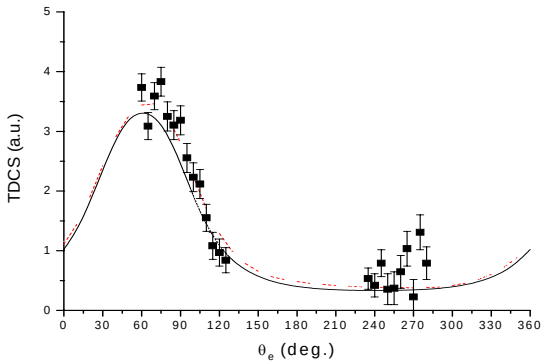

Figure 1. Triple differential cross section for 250eV electron-impact ionization of the 1a'' orbital of the thymine (ionization energy: I_i=16.08 eV). The energy of the ejected electron is E_e=20 eV and the scattered angle is 10^0. The theoretical calculations are performed in the first Born approximation (solid line) and in the second Born approximation (dashed line). Solid rectangles represent the experimental data [2].

References

[1] C Dal Cappello et al. Phys. Rev. A. **84** 032711 (2011)
[2] S M Bellm et al., Phys. Rev. A. . *A* **85** 022710 (2012)