

## Double Ionization DNA bases by electron impact

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**Synopsis** (e,3e) fivefold differential cross sections for the DNA bases are studied. The molecular wave functions are obtained by the multicenter wave functions from the Gaussain 03 program. To describe the correlations between ejected electron in the exit channel, we use the Ward-Macek method. The first order mechanisms involving the reaction are identified.

The ionization of biological molecules by electron impact is a fundamental step to understand the radiation damage in biological molecules and precisely in the DNA and RNA bases. It is well known that low energy electrons (less than 20 eV), resulting from the (e,3e) reaction are responsible for the main damage in biological systems[1].

We investigate here the double ionization of DNA molecules by electron impact in the experimental conditions of Casagrande et al. [2] where the scattered electron energy is fixed at 500 eV and the scattered angle  $\theta_s = -6^\circ$ . The ejected electron energies are chosen to be  $(E_1, E_2) = (12\text{eV}, 12\text{eV}), (37\text{eV}, 12\text{eV}), (37\text{eV}, 37\text{eV})$ . Fivefold cross sections(FDCS) are then calculated in the first Born approximation where the correlations between ejected electrons are described by the Ward-Macek method [3].

Firstly we calculate cross sections as a function of ejected energies and scattered angle for the DNA bases. We represent in (figure1) the thymine cases. the FDCS is maximum for small scattered angles and for  $12\text{ eV} < (E_1 + E_2) < 17.5\text{ eV}$ . In fact this corresponds to the energy range of the electrons that cause most damages in the branches of the DNA[1]. In a second step, we calculate cross section by considering experimental conditions [2], as a function of ejected angles. The method is applied to study the FDCS for adenine, cytosine, guanine and thymine.

The results show that the two first order mechanisms TS1 and SO are identified in the structures of all four molecules sometimes with the same intensity, which means that TS1 mechanism is also present both with the SO. This is due to the softer description of the repulsion between ejected electrons during the reaction by the Ward-Macek method. As an example, we report in (figure2) the FDCS for the adenine molecule in the situation:  $(E_1, E_2) = (37\text{eV}, 12\text{eV})$ .

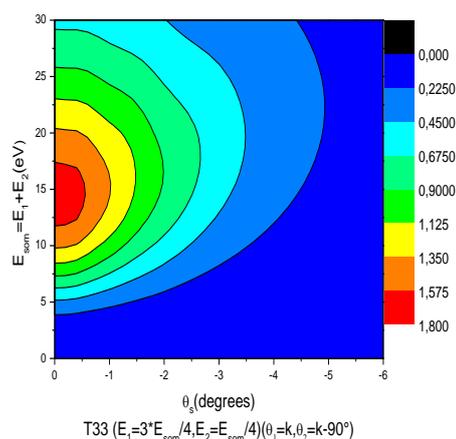
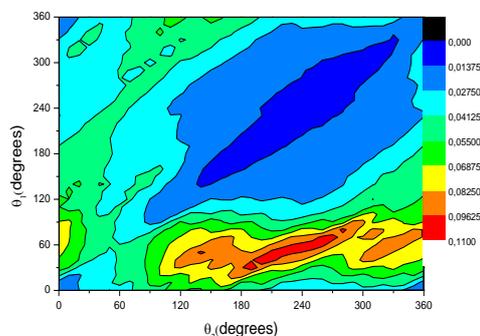


figure1: FDCS for thymine molecule .The scattered electron energy  $E_s = 500\text{ eV}$  and the scattering angle  $\theta_s = -6^\circ$ .



### References

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