

Ionization and fragmentation of the biomolecular analogue tetrahydrofuran by impact of electrons and protons

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Sinopse. The ionization and fragmentation of a chemical analogue to the sugar molecule in the DNA, tetrahydrofuran, was investigated by impact of electrons and protons at velocities ranging from of 3 to 7 and 4 to 20 Bohr velocities, respectively. The study shows the higher fragility of sugar molecule under the impact of light or heavy particles when compared to the analogue to the DNA bases, pyrimidine, supporting evidence that this molecule is the weak point of the DNA.

The motivation of the study is based on the evidence that the fragmentation of DNA and its constituents is the most important process associated with cell damage induced by ionizing radiation. The charged particles interact with living biological cells, for example cations in hadron-therapy, can produce structural and chemical modifications leading to bonds breaks in the DNA double helix.

The experimental study was carried out in the electron impact laboratory and laboratory of atomic and molecular collisions of the UFRJ at the Physics Institute and the PTB, the National Metrology Institution of Germany. The ionization and fragmentation processes have been investigated for tetrahydrofuran (THF) in gas phase induced by collisions with electrons and protons applying Time of Flight Mass spectrometry technique. The selected collision velocities are in the range of 3 to 7 v_0 and v_0 4 to 20, respectively. (v_0 corresponds to the Bohr velocity). Figure 1 shows the ratio of non-dissociative ionization in relation to all ionization processes of THF by electron and proton impact as function of incident particle's velocity.

The experimental results associated with the rupture the molecular bonds were analyzed in comparison to the stable ionized parent molecule (THF⁺) in order to verify the fragility of the molecule in dependence with the nature (light negatively charged and heavy positively charged particle) and velocity of the incident ionizing particle. In this study up to 45 fragments were identified and the abundance relative to the parent molecule determined. A previous study of DNA fragmentation with the base analogue pyrimidine identified a different velocity dependence for this ratio at specific ionic fragments by impact of light and heavy particles [1].

This contribution also reviews the recent systematic measurements on the total and partial dissociation cross sections for electron and proton impact on polyatomic molecules of biological interest with emphasis on tetrahydrofuran [2-5]. The aim is to quantify the radio-stability of relevant biomolecules under particle impact.

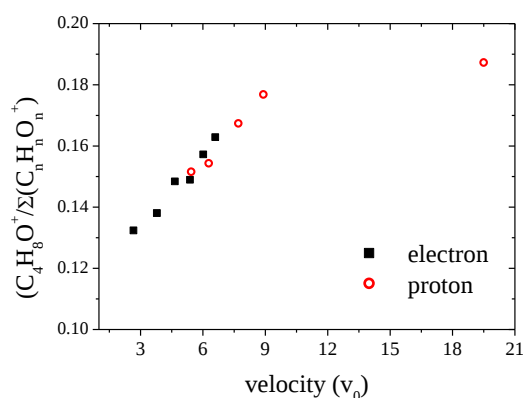


Figure 1. Fraction of non-dissociative ionization to the sum of non-dissociative ionization and dissociation processes in collisions of electrons and protons on THF as function of the incident particle velocity

Referências

- [1] W. Wolff, et al, *J. Chem Phys.* **140**, 064309 2014.
- [2] B. Rudek et al, *Eur. Phys J D* **69**:237 2015.
- [3] Fuss et al, *Phys. Rev A* **80**, 3 2009.
- [4] Mozejko et al, *Phys. Rev. A* **74**, 12708 2006.
- [5] W. Y. Baek et al *Phys. Rev A* **86**, 032702 2012.

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