

Conformation analysis and semiclassical dynamics study of charge exchange process induced by collision of C^{2+} ions with tetrahydrofuran

Ewa Erdmann* and Marta Łabuda^{1*}

* Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Narutowicza 11/12, 80233 Gdańsk, Poland

Synopsis We present the results of recent investigations of charge transfer process in the collision of C^{2+} ions with heterocyclic molecule of tetrahydrofuran.

Charge transfer (CT) in atomic and molecular collisions has been intensively studied by us in the past decade. [1-3] The importance of this process is evident in different fields of science such as chemistry, material science, astrophysics, laser research, biophysics and many others. For instance, the understanding of the CT mechanism is essential to address radiation damage in DNA. Important damage is due to secondary particles: low-energy electrons, radicals, or singly and multiply charged ions generated along the track after the interaction of the ionizing radiation with the biological medium. In this regard, we present a complete theoretical study of a fundamental CT process occurring in collision between multiply charged carbon ions and the tetrahydrofuran molecule. Tetrahydrofuran (THF, C_4H_8O) heterocyclic molecule is a model molecule which can be considered as a simple analog of the deoxyribose sugar and also structural unit for the DNA or RNA building blocks. A detailed analysis of the electronic structure of the THF molecule by employing several accurate quantum chemistry approaches is presented to determine the geometry of the molecule and to define the most important orbitals which are included in the process. The planar ($\theta=0^\circ$) and perpendicular ($\theta=90^\circ$) attacks of the C^{2+} projectile on the THF target molecule (being in envelope C_{2v} and twisted C_s symmetry orientation) were investigated using *ab initio* potential energy curves and non-adiabatic couplings calculated along internuclear distance R followed by a semi-classical collisional treatment with the impact energy range from eV to keV. Single and double electron capture channels have been identified in the potential energy curves. A strong delocalization of the π electrons of the THF ring towards the C^{2+} ion leading to the creation of a chemical bond between the oxygen atom and the colliding ion has been observed.

The presence of the cluster of the $[C^+-C_4H_8O]^+$ temporary formed during the interaction has been noticed, which confirms the experimental prediction [4] for the C^+ -THF system. Another important conclusion of our work concerns the calculated values of CT cross sections, which strongly depend on the orientation of the THF molecule.

It has been pointed out that change of the symmetry of the THF from C_{2v} to C_s in the collision with C^{2+} ions leads to the significant increase of the cross sections values even by three orders of magnitude (Figure 1).

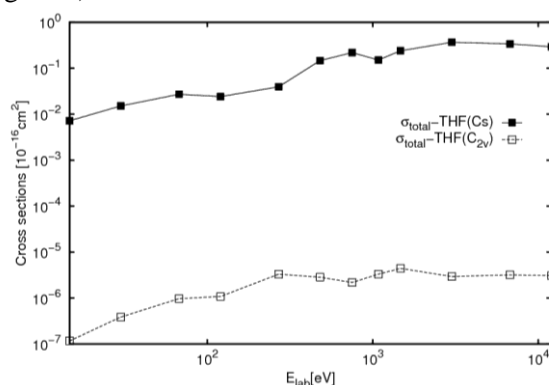


Figure 1. Averaged charge transfer cross sections for different orientations of the C^{2+} projectile toward the THF molecule at C_{2v} and C_s symmetry.

Taking into account the dependence between the fragmentation and electron capture processes, this would suggest that the CT process seems to be the most efficient and playing the most significant role when the carbon ion is colliding the THF in C_s symmetry with displaced orientation of $\alpha=23^\circ$ along C-O bond. Our work is a basis to study the fragmentation processes induced by the collision of ions and protons with the biologically relevant biomolecules and their analogs which we plan to present in future.

Acknowledgments: We thank the COST Action XLIC, Erasmus Plus Programme (M.Ł.) for financial support. Calculations were done at the Wrocław Centre for Networking and Supercomputing and Academic Computer Centre in Gdańsk.

References

- [1] M. C. Bacchus-Montabonel, M. Łabuda, Y. Tergiman, J. Sienkiewicz, 2005 *Phys. Rev. A*, **72**, 052706
- [2] M. Łabuda, J. González-Vázquez, L. González 2010 *Phys. Chem. Chem. Phys.* **12**, 5439
- [3] M. Łabuda, J. González-Vázquez, F. Martin and L. González. 2012 *Chemical Physics* **400**, 165
- [4] T. Wąsowicz, B. Pranszke 2015 *J. Phys. Chem. A* **119** 581

¹E-mail: marta.labuda@pg.gda.pl