Electron-impact ionization cross section calculations for selected ribonucleosides

Electron-impact ionization cross section calculations for selected ribonucleosides

P Możejko[1] *

[1]Department of Atomic, Molecular and Optical Physics, Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gabriela Narutowicza 11/12, 80-233 Gdańsk, Poland

Synopsis Total cross sections for the single electron-impact ionization of selected ribonuclosides (guanosine, adenosine, cytidine and uridine) have been calculated for electron energies ranging from the ionization threshold up to 5 keV.

Accurate data concerning electron collisions with matter are of great importance in many fields of science including space sciences, astrobiology and radiation physics and chemistry. It is well established now, that low- and intermediate-energy electron interactions should be taken into account in the studies of the processes induced within biological material by primary ionizing radiation [1]. Thus qualitative and quantitative studies and description of the electron interaction with components of biomolecules are strongly desired.

In the present work we have studied positive ionization of selected ribonucleosides (guanosine, adenosine, cytidine and uridine) by electron impact. Ribonuleosides consists simply of a nucleobase and a five-carbon sugar-ribose.

Total cross sections for the single electron-impact ionization of the studied targets have been derived using the binary-encounter-Bethe (BEB) model [2] for energies between the ionization threshold up to 5 keV. Due to the (BEB) method the electron-impact ionization cross section of a given molecular orbital can be calculated according to:

$$\sigma = \frac{S}{t+u+1}\left[\frac{\ln t}{2} - \frac{\ln t}{2t^2} + \frac{t-1}{t} - \frac{\ln t}{t+1}\right],$$

where $u = U/B$, $t = T/B$, $S = 4\pi a_0^2 N R^2/B^2$, $a_0 = 0.5292$ Å, $R = 13.61$ eV, U is the kinetic energy of the given orbital, B is the electron binding energy, T is the energy of impinging electron and N is the orbital occupation number. The total cross section for electron-impact ionization can be obtained as a sum of ionization cross sections calculated for all molecular orbitals. The used theoretical approaches and computational procedures are described in detail in our previous works [3, 4]. The BEB method provides usually ionization cross sections which are in quite good agreement (within ±15%) with experimental data [5]. The resulting total ionization cross sections for the single-ionization of guanosine ($C_{10}H_{13}N_5O_5$), adenosine ($C_{10}H_{13}N_5O_4$), cytidine ($C_9H_{13}N_3O_5$) and uridine ($C_9H_{12}N_2O_6$) are shown in figure 1.

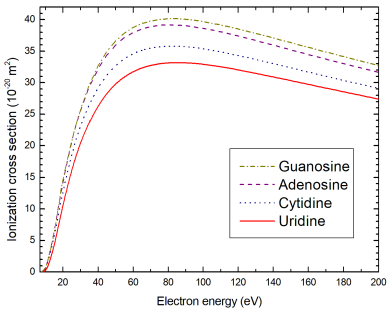

Figure 1. Comparison of ionization cross sections claculated in the present work for studied targets.

This work has been partially supported by the Polish Ministry of Science and Higher Education. Numerical computations have been performed at the Academic Computer Center (TASK) in Gdańsk.

References

[1] Sanche L 2005 *Eur. Phys. J. D* **35** 367
[2] Hwang W *et al* 1996 *J. Chem. Phys.* **104** 2956
[3] Możejko P *et al* 2003 *Radiat. Environ. Biophys.* **42** 201
[4] Możejko P *et al* 2005 *Radiat. Phys.Chem.* **73** 77
[5] Karwasz G P *et al* 2014 *Int. J. Mass Spectrom.* **365-366** 232

*E-mail: paw@pg.edu.pl