Eur. Phys. J. B (2017) 71: 35
DOI: 10.1140/epjd/e2017-70652-6

THE EUROPEAN
PHYSICAL JOURNAL B

Regular Article

Single ionization and capture cross sections from biological molecules by bare projectile impact[⋆]

Michele A. Quinto[1,a], Juan M. Monti[1], Pablo D. Montenegro[1], Omar A. Fojón[1], Christophe Champion[2], and Roberto D. Rivarola[1]

[1] Instituto de Física Rosario, CONICET and Universidad Nacional de Rosario, Rosario, Argentina
[2] Université de Bordeaux, CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux Gradignan, Gradignan, France

Received 19 October 2016 / Received in final form 9 December 2016

Abstract. We report calculations on single differential and total cross sections for single ionization and single electron capture from biological targets, namely, vapor water and DNA nucleobasese molecules, by bare projectile impact: H^+, He^{2+}, and C^{6+}. They are performed within the Continuum Distorted Wave – Eikonal Initial State approximation and compared to several existing experimental data. This study is oriented to the obtention of a reliable set of theoretical data to be used as input in a Monte Carlo code destined to micro- and nano- dosimetry.

1 Introduction

Electron ionization and electron capture from atoms and molecules by charged particle impact are of relevance in many areas like astrophysics, plasma physics, and radiobiology. In particular, in medical physics they are the main mechanisms leading to energy loss for swift ions in the living matter at medium and high impact energies.

In order to model the radiobiological damages induced by ionizing particles traversing the living matter, a precise knowledge of the full radiation history is required. Different electronic reactions must be properly characterized in order to give an accurate description of the cell-damaging processes and the dose deposition. Monte-Carlo (MC) track structure codes are among the best-suited tools to investigate these magnitudes since they provide an adequate description of the radio-induced energetic pattern at the finest scale. To this end the MC codes must be supplied with a full set of cross sections data for all the involved electronic reactions. On the other hand, biological tissue is usually modeled simply as water since this molecule represents about 80% of its composition.

The main physical reactions involved in the energy deposition process are usually studied by means of classical and semiempirical models [1–4]. We propose to use the state-of-the-art quantum-mechanical models, such as the Continuum Distorted Wave-Eikonal Initial State (CDW-EIS) one, to investigate electron ionization and electron capture when different molecular targets are irradiated by single and multiple charged ions at intermediate and high collision energies [5]. In particular we will focus our interest on the more frequently ion beams employed in hadrontherapy, namely, protons, helium and carbon ions. Previous calculations of doubly differential, single differential and total cross sections for water vapor and DNA nucleobases were done using the CDW-EIS and the first Born approximation with correct boundary conditions (CB1) [6–12].

In this work we present single differential and total cross sections for single electron ionization and single electron capture. The results are thoroughly compared with existing experimental data. We focus our interest in the cases of water vapor and DNA nucleobases, namely, adenine, cytosine, guanine and thymine. As a result, these calculations will be incorporated in a near future into the *TILDA-V* Monte Carlo code to determine the energy deposition patterns at the micro- and nano-meter scales in a simplified description of the cellular nucleus [13].

Atomic units will be used unless otherwise stated.

2 Theory

Let us consider an incident bare ion of charge Z_P impinging on a molecular target with a velocity $\mathbf{v}$. The impact velocities involved are high enough, so that we can consider the times associated to the vibration and rotation of the molecules to be much larger than the characteristic times of the collision. It is then possible to assume that the molecular nuclei remain fixed in their initial positions during the reaction. With regard to the multielectronic

---

[⋆] Contribution to the Topical Issue "Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces", edited by A.N. Grum-Grzhimailo, E.V. Gryzlova, Yu V. Popov, and A.V. Solov'yov.

[a] e-mail: `quinto@ifir-conicet.gov.ar`

problem, it is reduced to the analysis of a one-active electron system by considering that all the other electrons (the passive ones) remain frozen in their initial orbitals during the collision and that the active electron evolves independently of them in an effective mean field of the residual target. This approximation was first formulated with success to study electron capture [14] and ionization [15] (see also Refs. [16,17] for the case of atomic targets). It was then extended to molecular targets for both reactions, electron capture [18] and ionization [19].

Therefore, within the independent electron model and considering that there is just one active electron, the multielectronic Hamiltonian can be reduced to:

$$H_{el} = -\frac{1}{2}\bigtriangledown^2 + V_T(\mathbf{x}) + V_P(\mathbf{s}) + V_s(\mathbf{R}) \tag{1}$$

where $\mathbf{x}$ ($\mathbf{s}$) is the active electron coordinate in the target (projectile) reference frame, $V_T(\mathbf{x})$ is an effective one-electron target potential, $V_P(\mathbf{s}) = -Z_P/s$ is the interaction between the bare projectile and the active electron, and $V_s(\mathbf{R})$ is the interaction of the projectile with the target nuclei and the passive electrons. This last potential depends only on the internuclear coordinate $\mathbf{R}$ and thus, within the straight-line version of the impact-parameter approximation gives rise to a phase factor which only affects the projectile scattering [15]. In the following as we are not interested in the angular projectile distribution we will drop this term.

We perform the calculations by means of the CDW-EIS approximation that was first introduced by Crothers and McCann to study the single ionization of H by bare ion impact [20]. The CDW-EIS approximation was proposed to improve the large overestimation of the total cross sections, at intermediate impact energies obtained with the Continuum Distorted Wave (CDW) model [21], which was originated by the lack of normalization of at least one of the distorted wave functions in the initial and final channels. Using the same argument, the CDW-EIS approximation was introduced to investigate the electron capture [22]. This approximation solves the above mentioned problem, both for ionization and electron capture and exhibits, in general, a very good agreement with existing experimental data for differential and total cross sections.

CDW-EIS is the first order of a distorted wave series in which the initial and final distorted waves in case of ionization are proposed as:

$$\chi_i^+(\mathbf{x},t) = \varPhi_i(\mathbf{x},t)\,\mathcal{L}_i^+(\mathbf{s}) \tag{2}$$

$$\chi_f^-(\mathbf{x},t) = \varPhi_f(\mathbf{x},t)\,\mathcal{L}_f^-(\mathbf{s}), \tag{3}$$

respectively. In equations (2) and (3), $\varPhi_i(\mathbf{x},t) = \phi_i(\mathbf{x})\exp(-\imath\varepsilon_i t)$ and $\varPhi_f(\mathbf{x},t) = \phi_f(\mathbf{x})\exp(-\imath\varepsilon_f t)$ are initial and final target orbitals, respectively, solutions of the time-dependent Schrödinger equation. Also, ε_i is the electron energy of each one of the molecular orbitals and ε_f is the electron energy in the final state. The initial-bound wave function, $\phi_i(\mathbf{x})$, of each molecular orbital is considered as a linear combination of the atomic orbitals of its compounds (see Appendix A).

For the case of target ionization, considering an effective coulomb target potential $V_T(\mathbf{x}) = -\tilde{Z}_T/x$ in the exit channel, the target final-continuum state is written as:

$$\phi_f(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}}\exp(\imath\,\mathbf{k}\cdot\mathbf{x}) \times N^*(\lambda)\,{}_1F_1\left[-\imath\,\lambda, 1, -\imath\,(kx + \mathbf{k}\cdot\mathbf{x})\right], \tag{4}$$

with energy $\varepsilon_f = k^2/2$, being $\mathbf{k}$ the ejected electron momentum in the target reference frame, $N(a) = \exp(\pi a/2)\varGamma(1-\imath a)$ (with $\varGamma$ being the Euler's Gamma function) is the normalization factor of the ${}_1F_1$ hypergeometric function, and $\lambda = \tilde{Z}_T/k$ with $\tilde{Z}_T$ an effective charge. This charge is chosen in correspondence with the energy of each molecular orbital as $\tilde{Z}_T = \sqrt{-2n^2\varepsilon_i}$, being n the principal quantum number of each atomic orbital used to describe the molecular orbitals.

The initial distortion is proposed as:

$$\mathcal{L}_i^+(\mathbf{s}) = \exp\left[-\imath\nu\ln(vs + \mathbf{v}\cdot\mathbf{s})\right], \tag{5}$$

whereas the final distortion is chosen as:

$$\mathcal{L}_f^-(\mathbf{s}) = N^*(\zeta)\,{}_1F_1\left[-\imath\zeta; 1; -\imath\,(ps + \mathbf{p}\cdot\mathbf{s})\right] \tag{6}$$

where $\mathbf{v}$ is the projectile velocity, $\nu = Z_P/v$, $\zeta = Z_P/p$ and $\mathbf{p} = \mathbf{k} - \mathbf{v}$ is the ejected electron momentum in the projectile reference frame.

In the case of electron capture the initial distortion and the active electron initial orbital remain unchanged with respect to the case of ionization (see Eq. (2)). On the other hand, the final distortion wave is considered as:

$$\chi_f^-(\mathbf{s},t) = \varPhi_f(\mathbf{s},t)\,\mathcal{L}_f^-(\mathbf{x}), \tag{7}$$

where $\varPhi_f(\mathbf{s},t) = \phi(\mathbf{s})\exp\left(-\imath\varepsilon_f t + \imath\mathbf{v}\cdot\mathbf{x} - \imath\frac{v^2}{2}t\right)$ is the final projectile state and ε_f is the corresponding electron energy. Besides, the final distortion is chosen as:

$$\mathcal{L}_f^-(\mathbf{x}) = N^*(\xi)\,{}_1F_1\left[-\imath\xi; 1; -\imath\,(vx + \mathbf{v}\cdot\mathbf{x})\right] \tag{8}$$

with $\xi = \tilde{Z}_T/v$, whereas the active electron final state, $\phi_f(\mathbf{s})$, is a hydrogenic projectile bound state with charge Z_P and energy $\varepsilon_f = -Z_P/(2n_P^2)$, being n_P its principal quantum number.

The *prior*-version of the transition amplitude for the CDW-EIS approximation can be written as:

$$\mathcal{A}_{if}^-(\rho) = -\imath\int_{-\infty}^{+\infty} dt\left\langle \chi_f^-\left|\left[\left(H_{el} - i\frac{\partial}{\partial t}\right)\right|\chi_i^+\right\rangle\right] \tag{9}$$

provided now that the initial distorted wavefunction χ_i^+ does not contribute to the transition amplitude as $t \to +\infty$.

3 Results and discussions

We show in Figure 1 the single differential cross sections (SDCS) for single ionization of an isolated water molecule

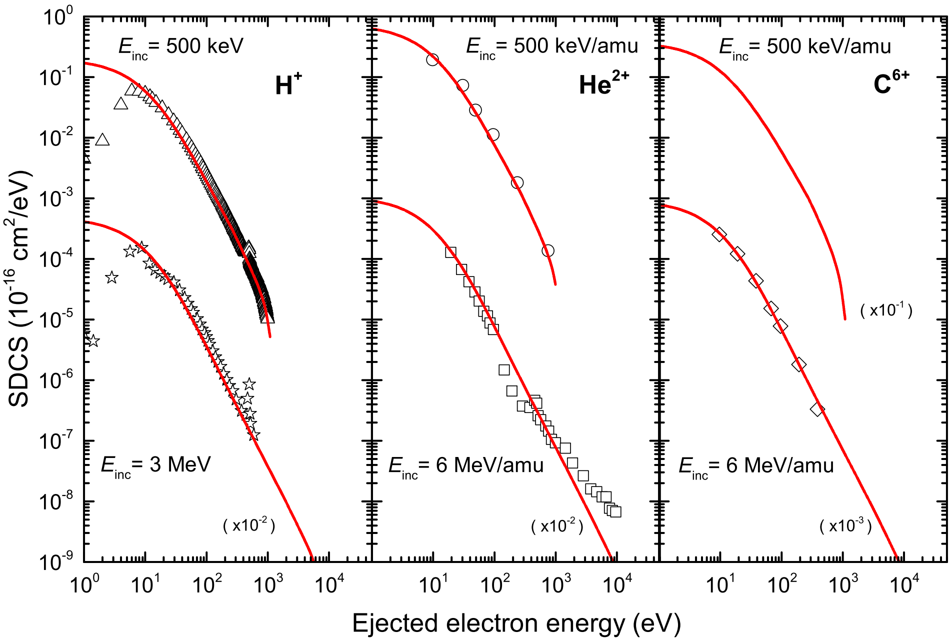

Fig. 1. Single differential cross sections for single electron ionization of water vapor molecules by bare-ion impact as a function of the ejected electron energy for different projectile–incident energy combinations. Left panel: 500 keV and 3 MeV H^+ projectiles; center panel: 500 keV/amu and 6 MeV/amu He^{2+} projectiles; right panel: 500 keV/amu and 6 MeV/amu C^{6+} projectiles. Solid line: present *prior* CDW-EIS calculations. Experimental data: △, ☆, ○ Toburen and Wilson [34]; □ Ohsawa et al. [35]; ◇ Dal Cappello et al. [36].

impacted by three different bare projectiles, H^+, He^{2+}, and C^{6+}, as a function of the ejected electron energy at fixed impact energies. As mentioned, CDW-EIS calculations are obtained in its *prior*-version, which is known to take into account approximately the dynamical interaction of the passive electrons on the ejected one in the exit channel [10,23]. For all projectiles the agreement with experimental data is remarkable in almost all the considered energy range above ∼10 eV. The large discrepancies found for proton impact in the energy range below 10 eV could be mainly due to experimental limitations [24]. For larger emission energies, above ∼1 keV, a small underestimation of the experimental results is found for protons. In the proton and alpha particle cases the experiments show evidence of the Auger electron emission, which is not included in the present theoretical model.

In Figure 2, we present the total cross sections (TCS) for electron ionization and electron capture of an isolated water molecule by impact of the same ions, above mentionated, as a function of the incident energy. For all of them a good agreement with experimental data is found in almost all the presented energy range. In the case of electron ionization by C^{6+}, only one experimental result is available in the literature, which is obtained as a result of the numerical integration of SDCS [25]. Besides, no experimental data are available for electron capture. We must also indicate that the theorical calculations overestimate the experimental data at collision energies lower than 150 keV/amu for alpha particle impact. Also, for the proton case, the recent theoretical calculations performed with CDW-EIS Molecular Orbital (CDW-EIS-MO) model have been reported [26]. In the case of ionization, a slight discrepancy, of the order of 20%, between theories come out in the medium energy range, while for hight impact energy, they show a very good agreement. The discrepancy in the medium energy range could be due to the different description of the target. In the present calculations a monocentric CNDO description is used. On the contrary, in [26] the geometric distribution of the compounding atoms of the molecule was considered. Moreover, in CDW-EIS-MO the influence of the inner orbital of H_2O is neglected. Further, for the capture process a good agreement between theories is found for all the presented impact energies range.

In Figure 3, we show the different molecular orbital contributions to the TCS for electron ionization and electron capture of an isolated water molecule by alpha particle impact. The contribution to ionization total cross sections is dominated by the outermost orbitals being decreasing their contributions according to the strength of the binding energy. It is well-known for electron capture from atomic targets, that the corresponding total cross section is dominated when the projectile momentuum approches the electron orbital momenta. Therefore the reaction is preferable from outer orbitals to inner ones as the collision energy increases. For the present molecular case the same behavior is observed, so that capture from the inner orbitals governs the TCS at enough high impact velocities.

In Figure 4, we present theoretical predictions of TCS for single ionization of DNA nucleobases interacting with alpha particle. To the best of our knowledge there are still

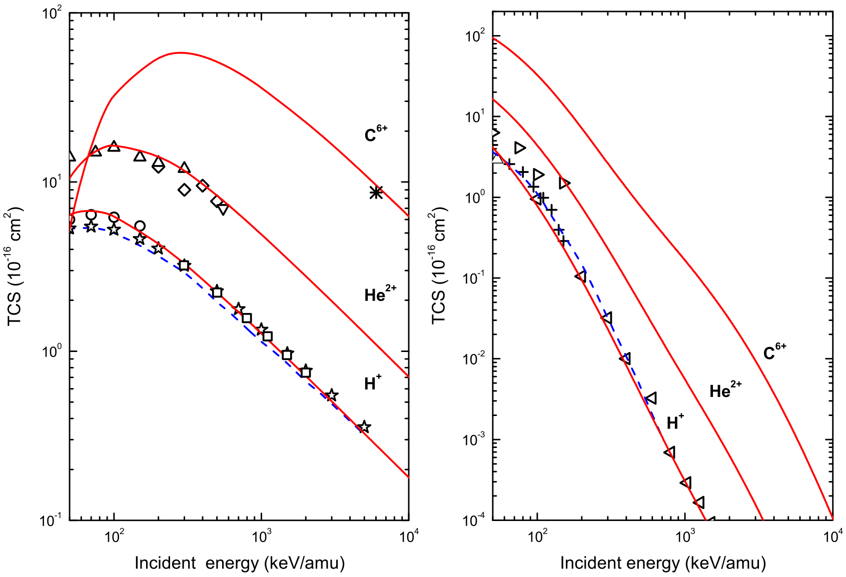

Fig. 2. Total cross sections for single electron ionization (left panel) and single electron capture (right panel) of water vapor by bare-ion impact as a function of the incident projectile energy. Solid line: present *prior* CDW-EIS calculations, dashed line: CDW-EIS-MO calcultations [26]. Experimental data: ☆ Rudd et al. [37]; ○ Bolorizadeh and Rudd [38]; □ Tavares et al. [39]; ◇ Rudd et al. [40]; △ Toburen et al. [41]; ▽ Rudolph and Melton [42]; ∗ Liamsuwan and Nikjoo [25]; ◁ Toburen et al. [43]; + Gobet et al. [44]; ▷ Rudd et al. [40].

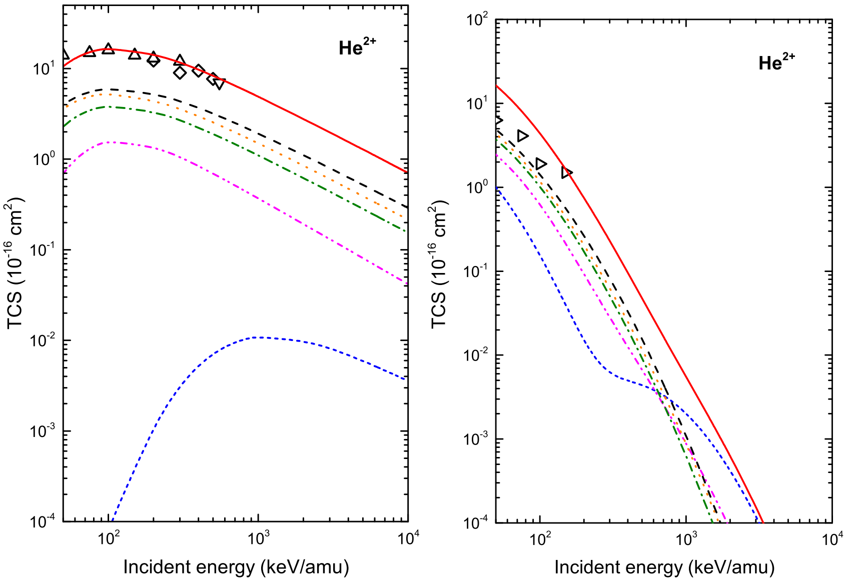

Fig. 3. Total cross sections for single electron ionization (left panel) and single electron capture (right panel) of water vapor by alpha particle impact as a function of the incident projectile energy. Lines: present *prior* CDW-EIS calculations showing the contribution of each individual molecular orbital: $1b_1$ (dashed line), $3a_1$ (dotted line), $1b_2$ (dash-dotted line); $2a_1$ (dash-dot-doted line); $1a_1$ (short-dashed line), sum of all molecular orbitals (solid line). Experimental data: same as in Figure 2.

no available experimental data for these systems. Present results are compared with other theoretical ones obtained employing a simpler approximation where a Classical Trajectory Monte Carlo (CTMC) and a Coulomb Over Barrier models (CTMC-COB) where combined [1,2]. It considers that at a distance where the maximum of the potential resulting from the combination of the projectile and target ones reaches the level corresponding to a certain initial bound state, an electron is "created" and then its trajectory is classicaly followed [1,2]. The maxima of CTMC-COB TCS appear at lower impact energies that CDW-EIS ones. At larger collision velocities CTMC-COB results underestimate the CDW-EIS ones by a factor of the order of ∼1.6.

Figure 5 shows the same results obtained for single ionization of DNA nucleobases compared to water vapor by alpha particle impact all normalized to the total number of electrons (N_e) of each molecule. The close agreement

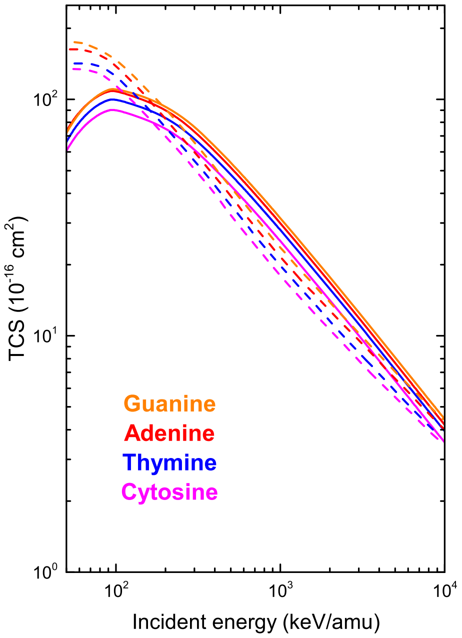

Fig. 4. Solid lines: present *prior* CDW-EIS calculations of TCS for single electron ionization of DNA nucleobases as a function of the incident alpha particle energy. Dashed lines: CTMC-COB calculations from Lekadir et al. [2] for ionization are shown.

found at high enough energies for all the targets shows that there is a clear and strong dependence on N_e (see also Figs. 2 and 4). This behavior was already investigated by Champion and coworkers for the case of proton impact on DNA nucleobases and water vapor [11].

4 Conclusions

Single differential and total cross sections for single electron ionization and single electron capture for water vapor and DNA nucleobases by bare ions are presented. A thorough comparison with existing experimental data was made. A very good agreement with experiments was found, showing the robustness and versatility of the theoretical model. A prediction of the TCS for single ionization of DNA nucleobases by alpha particle impact is presented. As no experimental data are available for these systems, the DNA nucleobases results are compared with the vapor water ones in order to investigate the dependence of TCS on the molecular number of electrons. Total and single differential cross sections presented here as well as the double differential cross sections reported in [10] partially constitute the input data for the MC code *TILDA-V* that is being prepared to investigate micro- and nano-dosimetry in biological matter [13].

The authors M.A.Q., J.M.M., P.D.M., O.A.F. and R.D.R. acknowledge financial support from the Agencia Nacional de Promoción Científica y Tecnológica through the project PICT 2011-2145 and from Consejo Nacional de Investigaciones Científicas y Técnicas through the project PIP 1026, both institutions from República Argentina.

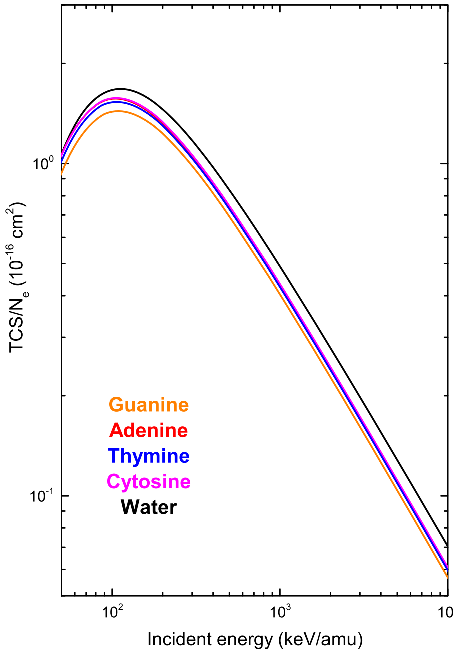

Fig. 5. Present *prior* CDW-EIS calculations of TCS for single electron ionization of DNA nucleobases and water vapor molecules by alpha particle impact as a function of the incident projectile energy. The results are divided by the number of electrons (N_e) of each molecule.

Appendix A: Calculation of the molecular initial bound state ϕ_i

The initial wavefunction ϕ_i of the active electron bound to a particular molecular orbital MO is described employing a CNDO approximation originally developed by Pople et al. [27] and Pople and Segal [28,29]. To simplify the computation of the cross sections, we make use of the method proposed by Senger et al. [30] and Senger and Rechenmann [31]. In this treatment the resulting cross sections for any MO is then reduced to a weighted sum of atomic cross sections corresponding to the atomic constituents of the molecule.

For the particular case of water, whose electronic configuration in the fundamental state is $(1a_1)^2\ (2a_1)^2\ (1b_2)^2\ (3a_1)^2\ (1b_1)^2$, cross section for the complete molecule can be calculated as [10]:

$$\sigma_{\mathrm{H_2O}} = \sigma_{1a_1} + \sigma_{2a_1} + \sigma_{1b_2} + \sigma_{3a_1} + \sigma_{1b_1} \tag{A.1}$$

where:

$$\sigma_{1a_1} = 2 \times \sigma_{\mathrm{O}_{1s}} \tag{A.2}$$
$$\sigma_{2a_1} = 1.48 \times \sigma_{\mathrm{O}_{2s}} + 0.52 \times \sigma_{\mathrm{H}_{1s}} \tag{A.3}$$
$$\sigma_{1b_2} = 1.18 \times \sigma_{\mathrm{O}_{2p}} + 0.82 \times \sigma_{\mathrm{H}_{1s}} \tag{A.4}$$
$$\sigma_{3a_1} = 0.22 \times \sigma_{\mathrm{O}_{2s}} + 1.44 \times \sigma_{\mathrm{O}_{2p}} + 0.34 \times \sigma_{\mathrm{H}_{1s}} \tag{A.5}$$
$$\sigma_{1b_1} = 2 \times \sigma_{\mathrm{O}_{2p}} \tag{A.6}$$

The vapor water molecule initial bound orbitals energies are given by: $\varepsilon_i(1a_1) = -19.842$ a.u., $\varepsilon_i(2a_1) = -1.18$ a.u., $\varepsilon_i(1b_2) = -0.67$ a.u., $\varepsilon_i(3a_1) = -0.54$ a.u., and $\varepsilon_i(1b_1) = -0.46$ a.u.

The atomic orbital populations presented in equations (A.2)–(A.6), which were calculated within the CNDO approach, were taken from reference [32]. In the calculation of the atomic cross sections that appear in (A.2)–(A.6), the initial bound wavefunctions were described by Roothaan-Hartree-Fock orbitals [33].

The same method is applied in the case of the DNA nucleobases initial bound orbitals. We refer the interested reader to a previous work by Galassi et al. [6], where all the quantum numbers and coefficients needed for expressing the target molecular wave functions are reported.

References

1. I. Abbas, C. Champion, B. Zarour, B. Lasri, J. Hanssen, Phys. Med. Biol. **53**, N41 (2008)
2. H. Lekadir, I. Abbas, C. Champion, O. Fojón, R.D. Rivarola, J. Hanssen, Phys. Rev. A **79**, 062710 (2009)
3. P. de Vera, R. Garcia-Molina, I. Abril, Phys. Rev. Lett. **114**, 018101 (2015)
4. H. Nikjoo, D. Emfietzoglou, T. Liamsuwan, R. Taleei, D. Liljequist, S. Uehara, Rep. Prog. Phys. **79**, 116601 (2016)
5. J.M. Monti, C.A. Tachino, J. Hanssen, O.A. Fojón, M.E. Galassi, C. Champion, R.D. Rivarola, Appl. Radiat. Isotopes **83**, 105 (2014)
6. M.E. Galassi, C. Champion, P.F. Weck, R.D. Rivarola, O. Fojón, J. Hanssen, Phys. Med. Biol. **57**, 2081 (2012)
7. C. Champion, P.F. Weck, H. Lekadir, M.E. Galassi, O.A. Fojón, P. Abufager, R.D. Rivarola, J. Hanssen, Phys. Med. Biol. **57**, 3039 (2012)
8. S. Nandi, S. Biswas, A. Khan, J.M. Monti, C.A. Tachino, R.D. Rivarola, D. Misra, L.C. Tribedi, Phys. Rev. A **87**, 052710 (2013)
9. D. Ohsawa, H. Tawara, F. Soga, M.E. Galassi, R.D. Rivarola, Phys. Scr. **T156**, 014039 (2013)
10. C.A. Tachino, J.M. Monti, O.A. Fojón, C. Champion, R.D. Rivarola, J. Phys. B **47**, 035203 (2014)
11. C. Champion, M.A. Quinto, J.M. Monti, M.E. Galassi, P.F. Weck, O.A. Fojón, J. Hanssen, R.D. Rivarola, Phys. Med. Biol. **60**, 7805 (2015)
12. S. Bhattacharjee, S. Biswas, C. Bagdia, M. Roychowdhury, S. Nandi, D. Misra, J.M. Monti, C.A. Tachino, R.D. Rivarola, C. Champion, L.C. Tribedi, J. Phys. B **49**, 065202 (2016)
13. M.A. Quinto, J.M. Monti, M.E. Galassi, P.F. Weck, O.A. Fojón, J. Hanssen, R.D. Rivarola, C. Champion, J. Phys.: Conf. Ser. **583**, 012049 (2015)
14. R.D. Rivarola, R.D. Piacentini, A. Salin, Dž. Belkic, J. Phys. B **13**, 2601 (1980)
15. P.D. Fainstein, V.H. Ponce, R.D. Rivarola, J. Phys. B **21**, 287 (1988)
16. P.D. Fainstein, V.H. Ponce, R.D. Rivarola, J. Phys. B **24**, 3091 (1991)
17. N. Stolterfoht, R.D. DuBois, R.D. Rivarola, *Electron Emission in Heavy Ion-Atom Collisions* (Springer, Berlin, 1997)
18. S.E. Corchs, R.D. Rivarola, J.H. McGuire, Phys. Rev. A **47**, 3937 (1993)
19. M.E. Galassi, R.D. Rivarola, P.D. Fainstein, Phys. Rev. A **70**, 032721 (2004)
20. D.S.F. Crothers, J.F. McCann, J. Phys. B **16**, 3229 (1983)
21. Dž. Belkic, J. Phys. B **11**, 3529 (1978)
22. A.E. Martínez, G.R. Deco, R.D. Rivarola, P.D. Fainstein, Nucl. Instrum. Methods B **34**, 32 (1988)
23. J.M. Monti, O.A. Fojón, J. Hanssen, R.D. Rivarola, J. Phys B **46**, 145201 (2013)
24. L.C. Tribedi, Private communication (2016)
25. T. Liamsuwan, H. Nikjoo, Phys. Med. Biol. **58**, 641 (2013)
26. L. Gulyás, S. Egri, H. Ghavaminia, A. Igarashi, Phys. Rev. A **93**, 032704 (2016)
27. J. Pople, D. Santry, G. Segal, J. Chem. Phys. **43**, S129 (1965)
28. J. Pople, G. Segal, J. Chem. Phys. **43**, S136 (1965)
29. J. Pople, G. Segal, J. Chem. Phys. **44**, 3289 (1966)
30. B. Senger, E. Wittendorp-Rechenmann, R.V. Rechenmann, Nucl. Instrum. Methods Phys. Res. B **194**, 437 (1982)
31. B. Senger, R.V. Rechenmann, Nucl. Instrum. Methods Phys. Res. B **2**, 204 (1984)
32. K. Siegbahn, C. Nordling, G. Johansson, H. Hedman, P.F. Hedén, K. Hamrin, U. Gelius, T. Bergmark, L.O. Werme, R. Manne, Y. Baer, *ESCA Applied to Free Molecules* (North Holland, Amsterdam, 1969)
33. E. Clementi, C. Roetti, Atomic Data, Nuclear Data Tables **14**, 177 (1974)
34. L.H. Toburen, W.E. Wilson, J. Chem. Phys. **66**, 5202 (1977)
35. D. Ohsawa, Y. Sato, Y. Okada, V.P. Shevelko, F. Soga, Phys. Rev. A **72**, 062710 (2005)
36. C. Dal Cappello, C. Champion, O. Boudrioua, H. Lekadir, Y. Sato, D. Ohsawa, Nucl. Instrum. Methods Phys. Res. B **267**, 781 (2009)
37. M.E. Rudd, T.V. Goffe, R.D. DuBois, L.H. Toburen, Phys. Rev. A **31**, 492 (1985)
38. M.A. Bolorizadeh, M.E. Rudd, Phys. Rev. A **33**, 888 (1986)
39. A.C. Tavares, H. Luna, W. Wolff, E.C. Montenegro, Phys. Rev. A **92**, 032714 (2015)
40. M.E. Rudd, T.V. Goffe, A. Itoh, Phys. Rev. A **32**, 2128 (1985)
41. L.H. Toburen, W.E. Wilson, R.J. Popowich, Rad. Res. **82**, 27 (1980)
42. P.S. Rudolph, C.E. Melton, J. Chem. Phys. **45**, 2227 (1966)
43. L.H. Toburen, M.Y. Nakai, R.A. Langley, Phys. Rev. **171**, 114 (1968)
44. F. Gobet, B. Farizon, M. Farizon, M.J. Gaillard, Phys. Rev. Lett. **86**, 3751 (2001)