Molecular mechanisms for electron-induced damage to biocomponents: cross sections and temporary anionic states for monosaccharides

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Abstract. The electron-molecule collision process for β-D-ribose and β-D-deoxyribose in gas-phase is here characterized in the range 0-20 eV. The description of the ensuing dissociative electron attachment in terms of the Transient Negative Ions (TNIs) is complemented by new calculations on the integral cross sections which show significant differences between ribose and deoxyribose in their furanosic, 5-member-ring conformers. Such finding could suggest a similar response of RNA versus DNA to secondary electrons in the condensed phase with interesting implications for the radiation damage research field.

1. Introduction

There is a variety of processes initiated by the primary radiation impinging on DNA which can induce serious genetic effects, such as mutation [1]. At energies below the DNA ionization threshold the main mechanism responsible for single- and double-strand-breaks (SSBs and DSBs) has been linked to the action of low energy electrons (LEEs) [2, 3, 4] which have been proven to be the most abundant among the secondary species produced by the primary radiation [5]. The essential intermediates between the initial electron collision and the final molecular break-up have been identified as the Transient Negative Ions (TNIs), i.e. metastable states occurring in the scattering process which originate from the temporary trapping of the incident electron in the molecular potential field. The TNIs show a strong ‘local’ character in the sense that they can essentially be associated to quantum resonances of the single DNA basic constituents (see, e.g. [6, 7]).

The characterization of these anionic intermediates is crucial in order to gather critical data for the analysis of the biological consequences of the electron interaction with the complex structures of the living tissues.

The present contribution reviews our most recent advances in the study of electron induced molecular damage as applied to two monosaccharides, the 2-deoxy-D-ribose and the D-ribose. Such basic constituents occupy a central position in the chemical
structure of, respectively, the deoxyribonucleic acid (DNA) and the ribonucleic acid (RNA) by binding the phosphate groups into the formation of the well-known backbone structures which provide a link between neighboring nucleotides bases of the single strand of RNA/DNA. We will also complement the analysis of the TNIs arising in the electron-sugar collision by presenting our new results on the corresponding elastic cross sections, which have been obtained by a computational procedure (see Section 2) which solves the same scattering equation by means of a different algorithm.

For both monosaccharides we analysed the two most important conformers [8] identified as the pyranosic, six-member-ring structure and the furanosic, five-member-ring structure. The pyranosic is the predominant structure in the gas-phase and, hence, the most relevant in order to compare our theoretical findings with the available experimental results. The second conformer, the furanosic, might also be present (in a much smaller percentage) in the gas phase according to the purity of the sample powder vaporized in the experimental chamber [9]. Furthermore, the sugars in the backbones of DNA and RNA are in their furanosic structure, so that the investigation of such conformer of the isolated molecules could provide valuable information for the further analysis of the condensed phase.

The work is organized as follows: the next Section illustrates our two computational procedures, Section 3 reviews our results on the resonance states of both monosaccharides, Section 4 discusses our findings on the elastic cross sections and, finally, Section 5 summarizes our conclusions.

2. The Computational Procedure

2.1. Scattering equations in a single center expansion

The approach we follow to model the electron-molecule interaction is based on a single-centre expansion of the molecular and incident electron wavefunctions about the centre of mass of the molecule (further details on our theoretical procedure when applied to biological systems can be found in Ref. [10]). The expansion basis is given by symmetry-adapted angular functions \{X_{h\mu}(\theta, \phi)\} determined by the point group of the molecule [11]. Hence, for instance, the one-electron bound orbitals \(\phi_k\) of the target molecule can be expanded as

\[
\phi_k^{pp}(r) = \frac{1}{r} \sum_{h\mu} u_{h\mu}^{k}(r) X_{h\mu}(\theta, \phi),
\]

where the index \(k\) labels a specific, multicenter occupied orbital which belongs to one specific irreducible representation (IR) of the point group of the molecule. The indices \((p\mu)\) label a relevant IR \(p\) and one of its components \(\mu\). The index \(h\) labels a specific basis function, for a given partial wave \(l\), used within the \(\mu\)th component of the \(p\)th IR. Finally, the radial coefficients are numerically computed on a grid[12, 13]. In the same fashion all the potential functions modelling the electron-molecule interactions will be expanded in a symmetry-adapted angular basis.
In order to perform the expansion in equation (1) one needs to start from the multicentre wavefunction which describes the target molecule and then generate by quadrature each of the $u^k_{hl}$ coefficients. We generate the bound molecular wavefunction by means of a standard quantum chemistry code, like Gaussian [14]; the explicit expression of the quadrature used to compute the $u^k_{hl}$ coefficients for multicentre Gaussian Type Orbitals (GTOs) has been given in [15].

The Born-Oppenheimer (BO) approximation is assumed to hold and the geometry of the molecular target is kept fixed to the optimized equilibrium geometry for the ground electronic state. We further approximate the target electronic wave function at the Static-Exchange (SE) level with the ground electronic state given by a single Hartree-Fock (HF) determinant in the self-consistent field (SCF) model. The post HF correlation and polarization corrections are included by means of model potentials (later referred to as $\hat{V}^{cp}$ in Eq. 3 and 4) added to the SE description [16, 12].

The total wave function of the “target + e−” is then represented as an antisymmetrized product of electronic wave functions which depend on the positions of the fixed nuclei

$$\Psi(r, X; R) = \mathcal{A}\{F(r)\psi(X; R)\}.$$  \hspace{1cm} (2)

where $r$ is the position of the continuum electron, $X$ represents collectively the coordinates $x_i$ ($i = 1, \ldots, N$) of the target electrons, $R$ corresponds to the set of frozen nuclear coordinates $R_\gamma$ ($\gamma = 1, \ldots, M$) of the target molecule acting as fixed parameters and, finally, $\mathcal{A}$ is the antisymmetrization operator which operates on the coordinates of the target electrons and of the incident electron. Inserting expression 2 into the Schrödinger equation for the electronic motion and integrating over the target electrons degrees of freedom $X \equiv \{x_i\}$ leads to the following integro-differential equation (in a.u.)

$$\left[-\frac{1}{2} \nabla^2 - \frac{1}{2} \mathbf{k}^2 + \hat{V}^{st} + \hat{V}^{cp} + \hat{V}^{model\ exc}\right] F(r) = \int \hat{V}^{exch}(r, r') F(r')dr'.$$  \hspace{1cm} (3)

where $r'$ generically represents the coordinate $x_i$ of one of the target electrons, $\hat{V}^{st}$ defines the static part of the potential in the scattering process (given by the attractive interaction between the scattering electron and the positive nuclei plus the local part of the repulsive interaction with the target electrons), $\hat{V}^{cp}$ is the model correlation-polarization potential and $\hat{V}^{exch}$ is the non-local part of the potential.

2.2. Cross section calculation: solution of Volterra equations

If the exchange term is approximated by a local potential we can rewrite the scattering equation in an homogeneous form to obtain the static-model-exchange correlation-polarization (SMECP) approximation for the scattering equation:

$$\left[-\frac{1}{2} \nabla^2 - \frac{1}{2} \mathbf{k}^2 + \hat{V}^{st} + \hat{V}^{cp} + \hat{V}^{model\ exc}\right] F(r) = 0.$$  \hspace{1cm} (4)

As in several previous works, we chose to approximate the exchange interaction by an energy-dependent local function of the electron density of the target by employing the
where the expansion coefficients are solutions to the matrix eigenvalue equation
\[
\left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right] F_{lh}^{\mu}(r) = 2 \sum_{l'h'} V_{lh,l'h'}^{\mu}(r) F_{l'h'}^{\mu}(r),
\]
and the potential coupling elements are given as
\[
V_{lh,l'h'}(r) = \langle X_{lh}^{\mu}(\hat{r}) | V(r) | X_{l'h'}^{\mu}(\hat{r}) \rangle = \int d\hat{r}' X_{lh}^{\mu}(\hat{r}) V(r) X_{l'h'}^{\mu}(\hat{r}).
\]
The upper limit of the integral on the right-hand side of the previous equation is a variable (integral equations with this property are called Volterra equations) and the integral vanishes for \( r' > r \) because the regular Green’s function \( g_{lh}(r, r') \) is used
\[
g_{lh}(r, r') = \frac{1}{k} \left[ \hat{j}_l(kr) \hat{n}_l(kr') - \hat{n}_l(kr) \hat{j}_l(kr') \right],
\]
where \( \hat{j}_l(kr) \) and \( \hat{n}_l(kr) \) are Riccati-Bessel and Riccati-Neumann functions.

The four structures under study show no symmetry elements, i.e. they belong to the \( C_1 \) symmetry group; hence, no reduction of the size of the problem into subgroups corresponding to the appropriate irreducible representations can be carried out. In our calculations we include the contribution of all the partial waves up to \( l_{\text{max}}=30 \) for the scattering wavefunction (giving a total number of 961 coupled channels) while the potential is expanded up to \( L_{\text{max}}=60 \) (corresponding to 3721 partial waves). For each scattering energy, from the K matrix obtained after the Volterra integration we derive the transition T matrix and, finally, the integral cross section (ICS) at that collision energy.

### 2.3. Resonances calculation: the piece-wise diabatic model

An alternative expansion basis to that of Eq.(1) is provided by the eigenfunctions obtained from diagonalizing the angular Hamiltonian at each radius \( r \) \([19, 20]\). These new angular eigenstates are referred to as the adiabatic angular functions (AAFs) \( Z_k^{\mu}(\theta, \phi, r) \) which are distance-dependent, linear combinations of the symmetry-adapted “asymptotic” harmonics mentioned before
\[
Z_k^{\mu}(\theta, \phi, r) = \sum_{lh} X_{lh}^{\mu}(\theta, \phi) C_{lh,k}(r),
\]
where the expansion coefficients are solutions to the matrix eigenvalue equation
\[
\sum_{lh} V_{l'h',lh}(r) C_{lh,k}(r) = V_k^{\lambda}(r) C_{l'h',k}(r).
\]
The eigenvalues $V_k^A(r)$ of the angular Hamiltonian now form an adiabatic radial potential for each index value $k$ over the selected range of the $e^-\text{-molecule}$ distances [12, 21].

Solving the scattering equations using these new $V_k^A(r)$ potentials allows the expansion of the scattering wave function in adiabatic angular states to converge more rapidly than the corresponding expansion in angular momentum eigenstates [19]. Thus, the number of coupled radial equations which must be solved with the adiabatic basis set is usually much smaller. Furthermore, the numerical instabilities in the solution of the standard momentum eigenfunction expansion when very large angular momentum values have to be considered (as in the present molecules) are greatly reduced. On the other hand, the non-adiabatic radial coupling introduces additional terms in the radial differential equations for which the standard integration method is not directly applicable.

In order to avoid the non-adiabatic coupling terms we actually employ a piecewise diabatic (PD) representation for the potential [12] where the radial coordinate is divided into a number of regions. In each radial region we average the coupling potential $V_{l'h',lh}(r)$ over $r$ and the resulting averaged potential is diagonalized to yield a set of angular functions $Z_{l'i}^\mu(\theta, \phi)$ for each region $i$ thereby transforming the scattering potential into a new representation in which it is nearly diagonal. The resulting equations are then solved using the full scattering potential in each region with the further approximation of ignoring the off-diagonal couplings within the region (for further details see Ref. [20, 12]).

A narrow and isolated resonance in a scattering process at an energy $E_R$ and width $\Gamma$ is associated to a pole in the scattering (S) matrix which has been analytically continued into the complex plane at an energy $E = E_R - i\Gamma/2$ [22]. The S matrix is obtained from a scattering wavefunction by finding a solution with the asymptotic form

$$\lim_{r \to \infty} \Psi_{l'h',lh}(r) = h_z^{-}(kr)\delta_{l'h'} \delta_{h'lh} - S_{l'h',lh} h_z^{+}(kr)$$

where $h_z^{+}(kr)$ and $h_z^{-}(kr)$ are the appropriate Hankel functions. Then it is possible to compute directly the S matrix at complex energies by computing the solution using the standard numerical procedure with a complex valued energy and by matching the solution to the Hankel functions with the appropriate complex argument. A resonance energy in the scattering process can be located by finding those energies at which $0 = 1/\det S$.

As already mentioned, the use of adiabatic angular functions enables us to solve for a smaller number of coupled equations so that we can attain a good degree of convergence in a reduced expansion basis. However, the computational weight of the electron scattering problem for the large, low-symmetry biological molecules sets a limit to the dimension of the final expansion basis. Furthermore, the use of adiabatic angular functions implies a simplification in the evaluation of the radial coupling elements. Hence, we expect some possible shifts in the energy location of the complex S-matrix poles with respect to the resonance peaks shown by our computed cross sections. In fact, as illustrated in the previous Section 2.2, the elastic scattering probabilities are found...
by solving the full scattering problem. For both approaches we need instead to consider possible effects caused by the use of a simplified, local potential and dipole effects at low energies. However, the main focus of the present paper, as well as of our previous work, is to examine in some detail the mechanism and the qualitative characteristics of low-energy one-electron resonances. The analysis requires a model which is simple enough to be applied to large molecules with very few symmetry elements (even none as in the present work) but includes sufficient details of the full scattering problem to accurately reproduce the essential features of the more accurate exact-exchange calculations. Although it is possible that the nonlocality of the exchange potential could provide an additional mechanism for resonant trapping, the good qualitative agreement between results obtained using exact exchange and local model exchange potentials in the resonance analysis (see, e.g. Ref. [23]), gives us confidence on the reliability of the present work. The threshold region is, on the other hand, more critical as for the role of the exact exchange potential on the cross sections, so that in the present work we will limit our discussion of the ICSs to the energy range beyond 2 eV.

3. Resonances and fragmentation channels

We review here our main results concerning electron attachment to isolated ribose [24] and deoxyribose [25] in the collisional energy range 0-20 eV. The four optimized structures for the furanosic and pyranosic structures of the $\beta$-D-ribose and the $\beta$-D-deoxyribose are reported in Figure 1.
Table 1. Position (in eV), width $\Gamma$ (in eV), associated lifetime (in fs) $\tau = h/\Gamma$ and time $t_{\text{e-}}$ required by a non-attaching electron travelling at the resonance energies to pass through a molecular box of 6 Å for the TNIs found for the $\beta$-D-Ribose and the $\beta$-D-Deoxyribose in the range 0-20 eV. In italic the poles added with respect to our previous works [24, 25].

| Ribofuranose | Ribopyranose | Deoxyribofuranose | Deoxyribofuranose |
|--------------|--------------|-------------------|-------------------|
| **E (eV)**   | **$\Gamma$ (eV)** | **$\tau$ (fs)** | **$t_{\text{e-}}$ (fs)** | **E (eV)**   | **$\Gamma$ (eV)** | **$\tau$ (fs)** | **$t_{\text{e-}}$ (fs)** | **E (eV)**   | **$\Gamma$ (eV)** | **$\tau$ (fs)** | **$t_{\text{e-}}$ (fs)** |
| 6.41         | 0.90         | 4.60              | 0.400             | 7.98         | 1.59         | 2.60              | 0.358             |
| 8.46         | 1.93         | 2.14              | 0.348             | 8.23         | 2.84         | 1.46              | 0.353             |
| 9.48         | 2.41         | 1.72              | 0.329             | 8.67         | 1.35         | 3.06              | 0.344             |
| 10.63        | 2.37         | 1.75              | 0.310             | 9.49         | 3.14         | 1.32              | 0.328             |
| 12.40        | 2.14         | 1.93              | 0.287             | 11.17        | 2.66         | 1.55              | 0.303             |
| 12.77        | 2.49         | 1.66              | 0.283             | 11.46        | 1.85         | 2.24              | 0.299             |
|              |              |                   |                   | 14.09        | 2.79         | 1.48              | 0.270             |
| 7.13         | 0.92         | 4.50              | 0.379             | 8.56         | 1.57         | 2.63              | 0.346             |
| 8.76         | 2.12         | 1.95              | 0.342             | 8.86         | 2.71         | 1.53              | 0.340             |
| 9.79         | 2.22         | 1.86              | 0.323             | 9.05         | 3.29         | 1.26              | 0.336             |
| 9.95         | 2.68         | 1.54              | 0.321             | 10.10        | 2.81         | 1.47              | 0.318             |
| 12.30        | 2.91         | 1.42              | 0.288             | 10.76        | 4.23         | 0.98              | 0.308             |
| 12.88        | 2.44         | 1.69              | 0.282             | 11.22        | 2.60         | 1.59              | 0.302             |
|              |              |                   |                   | 11.87        | 4.16         | 0.99              | 0.294             |
|              |              |                   |                   | 14.54        | 4.15         | 1.00              | 0.265             |

In the ribose case [24] we had limited ourselves to characterize the energy range around 8 eV, where new experimental findings were discussed together with our theoretical investigation; in the present work we extend such range up to 20 eV in order to properly compare the previous results to our new calculations for the cross sections. With respect to [25] we also add here three poles with width larger than 4 eV (which we had arbitrarily taken as the upper limit in the selection of acceptable poles) since the associated lifetime is in the same order of magnitude with respect to the other chosen resonances. In any case it is longer than the time needed by a free electron (moving at the energies given by the resonances’ locations) to go across a molecular box of 6 Å as can be seen in Table 1 where we report, for all the four structures we studied, the positions, widths, associated lifetimes and corresponding residence time of a ‘transient’ electron. Hence, in spite of the large widths, the computed poles can be associated to metastable states once the associated lifetimes are compared to the time that a non-attaching electron would spend in the neighborhood of the molecule.

For both monosaccharides all the computed poles fall in the energy range which corresponds to OH$^-$/O$^-$ detection in the gas-phase experiments reported in [24, 26]. The analysis of the spatial features of the resonance wavefunctions [24, 25] revealed that the excess charge is localized, in different fashions according to the specific TNI under study, on the oxidrilic groups, on the ring oxygen atoms and on some of the carbon atoms.
of the rings. The simultaneous presence of antibonding nodal planes across selected bonds of the TNIs suggests, at least in the case of direct, single-break mechanism, what fragments would originate from the TNI dissociation. Such an analysis shows indeed for most TNIs a selective electron attachment to well identified oxydrilic groups which can then be released as anionic fragments due to the antibonding character of the related C-OH bond. However, due to the overlap among the observed resonances, the selective fragment release might be eventually observed, upon isotopic substitution, only for the lowest resonance of the furanosic conformer of both monosaccharides (located at 6.41 eV in ribofuranose case and at 7.13 for its deoxygenated analogue, see Table 1). Considering a possible energy shift in the locations of the S-matrix poles caused by the approximations discussed in Section 2.3, we could also take the lowest-energy resonances as reasonable candidates to be associated with the ring fragmentation observed between 5 and 7 eV, but the complex dynamics associated to multiple ring breaks is largely beyond our level of characterization of the TNIs. Hence, we did not analyse possible ring-breaking mechanisms leading to the heavier fragments experimentally observed around 6 eV for both monosaccharides [24, 26].

Our calculations do not indicate any resonant structures near threshold while the experiments reveal intense signals from threshold and up to about 1.5 eV [26, 27, 28] leading to hydrogen and water molecule abstractions. We might hence suggest that such resonances do not originate from simple dynamical trapping by the shape of the potential and would need a post-HF description of the target molecule.

4. Cross sections

Following the procedures discussed in Section 2.2 we computed the ICS for the electron scattering by the two monosaccharides in their two conformational structures. In order to compare our findings with the only available data found in literature [29], we also repeated the calculations, in the deoxyribofuranose case, at the lower Static Model Exchange (SME) level, hence neglecting the short-range correlation and the long-range polarization contributions to the electron-molecule interaction and approximating the exchange term by a local model potential. We notice that at the SME level the ICS shows a monotonic, structureless decrease with increasing energy (see the insert in the left panel of Fig. 2). The addition of \( V^{\text{sp}} \) does not substantially change the magnitude of the scattering but tunes the shape of the total interaction enabling the trapping of the incident electron at several collision energies in the range 0-20 eV. With respect to the findings reported in [29] our SME cross section for the deoxyribofuranose is globally larger than the SE cross section of [29] and also qualitatively different in the sense that we do not observe the broad minimum found in [29] around 6 eV.

In the left panel of Fig. 2 we compare the ICS for electron scattering by the furanosic conformers of the two monosaccharides. Both compounds show marked resonant characters in their ICS between 5 and 20 eV in the ribose case and between 3 and 20 eV in the deoxyribose case. For the ribofuranose molecule we can distinguish five
peaks in both cases: at about 5 eV, 7 eV, 9.5 eV, 13.5 eV and 18 eV in the ribofuranose case and at about 3 eV, 5 eV, 8 eV, 10 eV and 16 eV in the deoxyribofuranose case. Excluding for the present the very low energy range, (see Section 2.3) we immediately notice that the two methods we employed to locate the S-matrix poles and to calculate the cross sections, both indicate the 5-15 eV as the interesting region for electron attachment. Furthermore, this is the region where the two monosaccharides differ the most in their ICS, suggesting the ribofuranose to be more reactive towards the electron scattering and attachment in such energy region. Considering that monosaccharides present in the backbones of RNA and DNA are in the furanosic structure, and that we expect some of the features exhibited by the isolated molecules to be carried along in the condensed phase [25], the present finding might provide an interesting piece of information to the wider community working in the radiation damage field.

As for the pyranosic structures, which represent the dominant configurations in the gas-phase, we notice small differences at low energies while the two ICSs are practically indistinguishable over 7 eV.

We are at present carrying on a high-level Breit-Wigner analysis of the computed cross sections in order to establish a more quantitative connections between the resonant peaks found in the ICSs and the TNIs already characterized by means of the different
computational procedure based on the S-matrix poles calculation in the piece-wise diabatic potential. In such a way we will be able to offer a complete description of the process by 'measuring' the probability for the electron scattering (and attachment) to occur and by analysing the spatial features of the transient anions in order to suggest possible break-up routes.

5. Conclusions

In the present work we complemented our characterization of the electron attachment process by low-energy electrons on the isolated ribose and 2-deoxyribose molecules with the calculations of the elastic scattering integral cross sections in the range 0-20 eV.

The comparison of the computed TNIs and of the peaks shown by the ICSs indicates a substantial agreement in the description of the process at the molecular level. Furthermore, the data on the furanosic, 5-member-ring conformers, show a significative difference which could have important implications in the condensed phase.

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