

# Ionization of molecules by multicharged bare ions by using the stoichiometric model

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## Abstract

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## I. INTRODUCTION

The damage caused by the impact of multicharged heavy projectile has become a field of interest because of the use in ion-beam cancer therapy. The effectiveness of the radiation depends on the choice of the ions. In particular theoretical and experimental studies with different projectiles arrived to the conclusion that charged Carbon ions could be the most convenient ion to use. This opens a new challenge for the theoretical point of view, since multicharged ions at not-so-high-velocities departs from the first Born approximation which is the most popular theory used in this field. The first Born approximation as any perturbative direct calculation warrants the  $Z^2$  laws where  $Z$  is the projectile charge. However the concentrated damage in the vicinities of the Bragg peak correspond to energies of hundreds of Kev/amu, that is in the intermediate energy region. Precisely in this region the Born approximation starts to fail. There is another serious problem from the theoretical point of view and this is that we are dealing with complex molecules. This article deals precisely with these two items. First, we perform more appropriate calculations on the main damage mechanism -i.e. atomic ionization by multicharged ions which can replace the Born results. And secondly we use and inspect the stoichiometric model which reduces a molecule to a sum of atomic processes quantities weight by the numbers of a that atom in the molecule.

As we have to deal with multicharged ions we resort to the Continuum Distorted Wave-Eikonal Initial State (CDW for short) which includes higher perturbative corrections. We start from the premise that ionization process is the mechanism that deposit the largest primary energy. This process produces an electron-energy spectrum that we need to be integrated. In addition these ejected electrons becomes a new source of local damage which needs to be investigated because this quantities are used in MonteCarlo simulations. With this end in mind we not only calculate ionization cross section but also energy and angular mean values of the emitted electrons

To deal with the molecules we resort to the simplest stoichiometric model (SSM): this is to consider that the molecule is composed of independent isolated atoms. In all cases that the total cross section is simply the sum of cross section of each individual atoms.

With this two tools in mind, i.e. CDW instead of Born approximation and the SSM, we calculate ionization cross section of different molecules (see Table(2)) by the impact of antiprotons,  $H^+$ ,  $He^{2+}$ ,  $Be^{4+}$ ,  $C^{6+}$ , and  $O^{8+}$ . In particular in section 3, we are interested in

ADN molecules such as Adenine, Timine, Cytosine, Guanine, Uracil, and DNA backbone.

The results are processed to test the Toburen scaling rule which states that the ratio of the ionization cross section divided by the number valence electrons (outer electrons) plotted in terms of the projectile velocity can be **grouped** in a narrow universal band. We have also applied this rule to several hydrocarbons and pirimide molecules. We will prove that the resulting universal band can be greatly sharpened (**angostada**) if we redefine effective valence electrons as developed in Section 3.2

It is well known the biological damage caused by the electron emerging after the ionization process. To inspect this mechanism, in section 3.3 AND 3.4 we have calculated the mean electron energy an angular values. To our surprise we found a substantial dependence of the projectile charged, totally unexpected in first Born approximation.

To deal with large projectile charge we resort to the CDW but the simplest stoichiometric model used seems to be very simplistic since consider each atom as neutral, which is not correct. In section 3.5 we run the chemistry code GAMES to calculate the excess or defect of electron density one each atoms. With these knowledge we modify the simple stoichiometric model to account for the departure of the neutrality. We find that, for the ADN molecules this modification does not introduce a substantial change.

## II. THEORY: IONIZATION OF ATOMS

For our interest we require just six atoms  $\alpha = \text{H, C, N, O, P and S}$ . Most of the organic molecules are composed by these atoms. Some particular molecules include also halogen atoms such as Fluor and Bromine; ionization cross sections for these elements in its ion form were already published [2, 3].

Total ionization cross sections of these atoms were calculated using the CDW The initial bound and final continuum radial wave functions were obtained by using the RADIALF code developed by Salvat and co-workers using a Hartree Fock potential obtained the Depurated Inversion Model [5, 6] . The number of pivots used to solve the Schrödinger equation rounds a few thousands of points, depending on the number of oscillations of the continuum state. The radial integration was performed using the cubic spline technique. The number of angular momenta considered varied between 8, at very low ejected-electron energies, up to 30, at the largest energies considered. The same number of azimuth angles were required to

obtain the four fold differential cross section. The calculation so performed does not display prior-post discrepancies at all. Each atomic total cross section in Eq. (1) was calculated using 35 to 100 momentum transfer values, 28 fixed electron angles and around 45 electron energies depending on the projectile impact energy. Details of the calculation can be seen in [10]. In parallel we will be reporting state to state ionization cross sections for these cases in Ref.[[11]] which will be very useful to estimate molecule fragmentation.

In Figure 1 we report our results of total ionization of the six basic elements by impact of six different projectile, i.e.: antiprotons,  $H^+$ ,  $He^{2+}$ ,  $Be^{4+}$ ,  $C^{6+}$ , and  $O^{8+}$ . To bring all these 36 magnitudes to a consistent figure we exploit the property that in first Born approximation, the ionization cross section scales with the projectile charge to square, i.e.  $Z^2$ . The values of impact energies considered range between 0.1 to 10 MeV/amu, i.e. where the CDW is supposed to hold. In fact for the highest projectile charges the minimum impact energy where the CDW is expected to be valid could be larger than 100 KeV. From some MeV/amu on, the first the Born approximation provides quite reliable results and using a much simpler formalism; we check it. We keep the same color to indicate the projectile charge along the all figures of this work : dashed-red, solid-red, blue, magenta, olive and orange for antiprotons,  $H^+$ ,  $He^{2+}$ ,  $Be^{4+}$ ,  $C^{6+}$ , and  $O^{8+}$ , respectively. It is notable that there is no complete tabulation of ionization of atoms by impact of multiple charge ions. We hope that the ones presented in this article will be very useful.

### III. IONIZATION OF MOLECULES

#### A. The stoichiometric model

Lets us consider a molecule  $M$  composed by  $n_\alpha$  atoms of the element  $\alpha$ , the SSM describes the total ionization cross section of the molecule  $\sigma_M$  as a simple sum of ionization cross sections of the isolated atoms  $\sigma_\alpha$ . i.e.

$$\sigma_M = \sum_{\alpha} n_{\alpha} \sigma_{\alpha} \quad (1)$$

We divided sixteen molecular targets of our interest in 3 families, namely

CH	CH <sub>4</sub> , C <sub>2</sub> H <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> , C <sub>2</sub> H <sub>6</sub> , and C <sub>6</sub> H <sub>6</sub> .
CHN	C <sub>5</sub> H <sub>5</sub> N, C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> , C <sub>2</sub> H <sub>7</sub> N <sub>1</sub> , and C <sub>1</sub> H <sub>5</sub> N <sub>1</sub>
ADN	Adenine(C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> ), Timine(C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> ), Cytosine(C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O), Guanine(C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O), Uracilo(C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> ), DNA backbone (C <sub>5</sub> H <sub>10</sub> O <sub>5</sub> P <sub>1</sub> ) dry DNA(C <sub>20</sub> H <sub>27</sub> N <sub>7</sub> O <sub>13</sub> P <sub>2</sub> )

(2)

In Figure 2 we report total ionization cross sections by the impact of multicharged ions for the four basic ADN component that is: Adenine, Timine Cytosine, and Guanine, and in Figure 3 we report results on Uracil and ADN Backbone containing P. For Adenine the agreement with the three experiments available in our range of validity are quite good. For Uracil there is a conflicting situation, we have a good agreement with the experiments by proton impact of itoh et al [1], but for the same target our theory fails by a factor of two for impact of C<sup>4+</sup> and O<sup>6+</sup> ions. Anyway should be said that our theoretical results coincide with the ones of Champion Rivarola and collaborators [7, 8], indicating a possible misstep of the experiments.

## B. Scaling rule

The first attempt to develop a simple but comprehensive phenomenological model for electron ejection from large molecules was posed by Toburen and collaborators [9, 12]. These authors found convenient to scale the experimental ionization cross section in terms of the number of outer or weakly bound valence electrons (total number of electrons minus the inner-shell ones). We then introduce the cross section per weakly bound electron  $\sigma_e$ , or simply ionization cross section per valence electron as

$$\sigma_e = \frac{\sigma_M}{N_M} = \frac{\sum_{\alpha} n_{\alpha} \sigma_{\alpha}}{\sum_{\alpha} n_{\alpha} v_{\alpha}} = \sigma_e(v), \text{ with} \quad (3)$$

$$v_{\alpha} = \begin{cases} 4, & \text{for C,} \\ 5, & \text{for N and P} \\ 6, & \text{for O and S} \end{cases} \quad (4)$$

and  $v_H = 1$  The Toburen rule can be stated by saying that  $\sigma_e$  is an *universal* parameter independent on the molecule and depending only on the impact velocity. In Ref. [[12]] it was found experimentally that for proton impact on some simple molecules  $\sigma_e$  result

$$\begin{array}{cccc} E(\text{MeV}) & 0.25 & 1.00 & 2.00 \\ \sigma_e \text{ (in } 10^{-16} \text{ cm}^2) & 0.39 & 0.17 & 0.11 \end{array} \quad (5)$$

with an estimated error of about 20%. A similar ratio was found in Ref.[[1]] dealing with protons on uracil and adenine. Figure 5a shows  $\sigma_e$  calculated with the CDW as a function of the impact velocity for different projectile charges calculated with the SSM for the sixteen molecular targets displayed in (2). The universality with  $Z$  is the one provided by Born approximation, i.e.  $\sigma_e(Z) = Z^2 \sigma_e(Z = 1)$  and it holds for large impact velocities, as shown Figure 5a. Obviously, for lower impact velocities the distorted wave CDW breaks this behavior discarding the rule  $Z^2$ . Although the Toburen rule holds for high energies, its performance is still not satisfactory: the universal band is quite wide. This departure of our theoretical results from the Toburen rule can be explained by the simple fact that our atomic cross sections  $\sigma_\alpha$  behaves differently for each atom in terms of the projectile charges. By inspecting Figure 1 one can easily see that the rule  $\sigma_\alpha/v_\alpha \sim \sigma_e$  is not well satisfied by the CDW. A much better theoretical atomic rule is given by

$$\sigma_e^{CDW} = \frac{\sum_{\alpha} n_{\alpha} \sigma_{\alpha}^{CDW}}{\sum_{\alpha} n_{\alpha} v_{\alpha}^{CDW}}, \quad \text{with} \quad (6)$$

$$v_{\alpha}^{CDW} \sim \begin{cases} 4, & \text{for C, N, and O,} \\ 4.5, & \text{for P and S} \end{cases} \quad (7)$$

and obviously  $v_H^{CDW} = 1$ .  $\sigma_e^{CDW}$  is plotted in Figure 5b where we can observe a much better sharp band, specially at high energy where the theory is expected to work. Experiments will be interesting to tune up this theoretical prediction

### C. Emitted electron energies

In a given biological medium, ion direct ionization account for just a fraction of the overall damage. Secondary electrons as well as recoil target ions also contribute substantially to

the total damage. We can consider the magnitude  $d\sigma_{\alpha nl}/dE$  -i.e. the single differential cross section of the shell  $nl$  of the atom  $\alpha$  as a function of the ejected electron energy  $E$ - as a simple distribution function ?? . We can therefore define the mean value  $\overline{E}_\alpha$  simply as Ref.[[? ]]

$$\overline{E}_\alpha = \frac{\langle E_\alpha \rangle}{\langle 1 \rangle} = \frac{1}{\sigma_\alpha} \sum_{nl} \int dE E \frac{d\sigma_{\alpha, nl}}{dE} \quad (8)$$

$$\langle 1 \rangle = \sigma_\alpha = \sum_{nl} \int dE \frac{d\sigma_{\alpha, nl}}{dE} \quad (9)$$

where  $\Sigma_{nl}$  takes into account the sum of the different sub-shells contribution of the element  $\alpha$ .

Figure 5 shows  $\overline{E}_i$  for our six elements of interest. Our range of impact velocities in this figure was shorten up to  $v = 10$  and this so because of a numerical limitation of our spherical harmonics expansion. In our theoretical treatment we expand our final continuum wave function in the usual form

$$\psi_{\vec{k}}^-(\vec{r}) = \sum_{l=0}^{l_{\max}} \sum_{m=-l}^l R_{kl}^-(r) Y_l^m(\hat{r}) Y_l^{m*}(\hat{k}), \quad (10)$$

We are confident with our calculations up to  $l_{\max} \sim 30$ . As the impact velocity  $v$  increases  $\langle E_\alpha \rangle$  also increases, and therefore  $l_{\max}$  should also increases, including in this way very oscillatory functions in the integrand. Furthermore, as the integrand of  $\langle E_\alpha \rangle$  includes the kinetics-energy variable  $E$  ( see Eq.(8)), it cancels the small energy region and reinforces the large one making the result more sensible lo large angular momenta. Anyway for  $v > 10$ , the first Born approximation holds.

In Figure 5 we can estimate  $\overline{E}_\alpha$  in the range 0.5-2 in a.u. or equivalently in between 15-50 eV for all the targets in accordance with the experimental findings ?? but what it surprising is the sensible dependence with the projectile charge  $Z$  which can duplicate the proton results. This effect can be attributed to the depletion caused by the multicharged ions to the yields of low energy electrons. In the high electron energy regime the CDW falls on the simple first Born approximation surviving the simple  $Z^2$  law which the ratio in Eq.(8) cancels out, becoming then  $\overline{E}_\alpha$  an universal value independent on  $Z$ .

Extending the simple stoichiometric model for the mean electron energy calculation, it

results

$$\overline{E}_M = \frac{\sum_{\alpha} n_{\alpha} \overline{E}_{\alpha}}{\sum_{\alpha} n_{\alpha} \sigma_{\alpha}}. \quad (11)$$

For impact of  $H^+$  and  $He^{2+}$  on water at 1 MeV/amu we obtain of  $\overline{E}_{H_2O} = 43.7$  and 45 eV, while the experiments on liquid water Pimblott and LaVerne [ ] found 51.5 and 52.2 eV, respectively. Just to stress the importance of the projectile charge, for  $O^{8+}$  on water at the same impact energy 1 MeV/amu we, obtain  $\overline{E}_{H_2O} = 54.7$  eV, i.e. 25% larger than proton impact. We recall here that there should not be any difference if the calculation is carried in first Born approximation. We will come back on this issue

#### D. Emitted electron angles

As mentioned before, secondary electrons contribute to the total damage. It is important not only the ejection energy but also the angle of emission. In similar fashion, we can consider the magnitude  $d\sigma_{\alpha,nl}/d\Omega$  -i.e. the single differential cross section in terms of the ejected electron solid angle  $\Omega$  - as a distribution function, and define the mean angle  $\overline{\theta}_{\alpha}$  as

$$\overline{\theta}_{\alpha} = \frac{\langle \theta_{\alpha} \rangle}{\langle 1 \rangle} = \frac{1}{\sigma_{\alpha}} \sum_{nl} \int d\Omega \theta \frac{d\sigma_{\alpha,nl}}{d\Omega} \quad (12)$$

Figure 6 shows  $\overline{\theta}_{\alpha}$  for our six elements of interest. Again here we observe an important dependence of  $\overline{\theta}_{\alpha}$  with  $Z$ . It is the common view [18] that the angular dispersion of emitted electrons are nearly isotropic due to the fact that angular anisotropy of sub-50-eV yield is not significant. A typical used value of ejection angle is about  $\overline{\theta}_{\alpha} \sim 70$  degrees [13] and this quite correct in the range of validity of the first Born approximation for any target. But when a distorted wave approximation is used as observed in Figure 6,  $\overline{\theta}_{\alpha}$  decreases substantially with  $Z$  in the intermediate energy region. For example for  $C^{6+}$  impact the Bragg peak occurs at 0.3 MeV/amu where  $\overline{\theta}_{\alpha}$  calculated in CDW is about the half of the one calculated with the First Born approximation. This correction should close the damage to the forward direction.

The only responsible of this correction is the capture to the continuum effect: the larger the charge  $Z$  the smaller  $\overline{\theta}$  will be, of course at intermediate energies, not at high impact energies where the Born approximation rules. One illustrative observation is the behavior of



antiprotons: the projectile in this case repels the electrons making the distribution almost symmetric. Note the opposite effect of proton and antiprotons, they run one oppose to the other one, as compared with the first Born approximation.

### E. A modified stoichiometric model

One can correctly argue that the SSM considers an assembly of isolated neutral atoms which is definitively unrealistic. A first improvement is to consider that the atoms are not neutral and within the molecule they have more or less electrons given by a charge  $q_\alpha$ . One parameter that measures  $q_\alpha$  is the Mulliken charge. This is not the only one, there is a large variety of charges such as the net or natural atomic charge [15], the lowin charge, etc.

Consider that the total amount of electrons  $Q_\alpha$  on element  $\alpha$  are equally distributed on all the atoms  $\alpha$ , therefore each element  $\alpha$  will have a an additional charge:  $q_\alpha = Q_\alpha/n_\alpha$ . positive or negative depending on the relative electronegative value respect to the other ones [16]. Instead of the integer number of elements  $n_\alpha$  of the atom  $\alpha$ , It could be argued that we have now an continuous number of atoms given by

$$n'_\alpha = n_\alpha - \frac{q_\alpha}{v_\alpha^{CDW}} \quad (13)$$

In the case of neutral atoms  $q_\alpha = 0$ , we obviously recover  $n'_\alpha = n_\alpha$  as before.

To inspect the effect of the  $q_\alpha$  we have run GAMES for.... In the table ( 14) we display  $q_\alpha$  of the different ADN basis and in the last column we rewrite the new stoichiometric expression.

Element	H	C	N	O	New stoichiometry
Adenine					$C_5H_5N_5$
Timine	+0.14	+0.07	-0.22	-0.38	$C_{4.91}H_{5.16}N_{2.09}O_{2.13}$
Cytosine					$C_{3.81}H_{4.46}N_{3.12}O_{1.11}$
Guanine					$C_5H_5N_5O$

(14)

All the previous formula holds with the simple replacement of integer value  $n_\alpha$  by the continuous values  $n'_\alpha$  to produce a new ionization cross section  $\sigma'$

In Figure 7, we displays the relative difference of ionization cross sections

$$e = \frac{\sigma' - \sigma}{\sigma} \times 100 \quad (15)$$

for the four ADN basis. The difference is just very few percents. Indicating that the SSM is a quite robust model to treat the type of molecule we are dealing with, and of course within the range error that one can expect from the SSM.

We now return to the calculation of the mean electron energy of  $H^+$  and  $He^{2+}$  in water  $\overline{E}_{H_2O}$ . If we consider that the residual charge of each hydrogen in water is  $q_H = +0.35$  [16] which implies that on Oxygen we have a residual charge of  $q_O = -0.7$ , we could rewrite the formula of water using (15) as  $H_{1.3}O_{1.17}$  considering  $n_O^{CDW} \simeq 4$  and  $n_H^{CDW} \simeq 1$ . Recalculating mean electron energy by impact of  $H^+$  and  $He^{2+}$  on water at 1 MeV/amu we obtain:  $\overline{E}_{H_2O} = 46.2$  and 47.6 eV which compared a little better with the experiments: 51.5 and 52.2 eV [17], respectively. i.e. within 10% of the experiments which is not bad accounting for the simplicity of our method.

Another parameter that we can calculate in our model is the fraction of energy carried by the electron  $f$  defined as

$$f = \frac{\sum_{\alpha} n_{\alpha} \sigma_{\alpha} \overline{E}_{\alpha}}{\sum_{\alpha} n_{\alpha} (\sigma_{\alpha} \overline{E}_{\alpha} + \sum_{nl} \sigma_{\alpha nl} E_{\alpha nl})} \quad (16)$$

Using our shell-to-shell ionization cross sections  $\sigma_{\alpha nl}$  [11] and atomic binding energies of the atom  $\alpha$ ,  $E_{\alpha nl}$  [? ], we obtain  $f = 0.70$  and 0.71 for  $H^+$  and  $He^{2+}$  on water at 1 MeV/amu, which differ from the experiments  $f = 0.81$  and 0.80, respectively.

This difference with the experiment could be attributed to the difference of binding energy between the molecular water 12.65 eV and the atomic component H (13.6 eV) and O (17.19 eV), which is an issue beyond our independent atom approximation and so our model cannot not accounted for. We could estimate this contribution resorting, once more to the stoichiometric, model, we can arrivesgar a upper-limit difference per molecule of water as

$$\delta E = (13.6 - 12.65)1.17 + (17.19 - 12.65)1.3 = 7 \text{ eV} \quad (17)$$

Most of this energy should be transfer to the kinetics energy of the emitted electron. Thus we can add 7 eV to the previous values to give  $\overline{E}_{H_2O} = 53.2$  and 54.6 eV for  $H^+$  and  $He^{2+}$  on water at 1 MeV/amu, respectively, much near to the experiments: 51.5 and 52.2 eV. If we add  $\delta E$  to the numerator of Eq.(16) we obtain  $f = 0.81$  and 0.80 in perfect agreement with the experiments (see Table 1 of Ref.([17])

## IV. CONCLUSIONS

We have calculated ionization cross sections by impact of antiprotons,  $H^+$ ,  $He^{2+}$ ,  $Be^{4+}$ ,  $C^{6+}$ , and  $O^{8+}$  with molecule involved in biological basis containing H, C, N, O, P and S with the CDW method. The importance of the influence of  $Z$  was observed in the mean energy  $\bar{E}_\alpha$  and angle  $\bar{\theta}_\alpha$ . For a given target  $\alpha$ , as  $Z$  increases  $\bar{E}_\alpha$  increases but  $\bar{\theta}_\alpha$  decreases. At high impact energy, say larger than 1 MeV/amu these values tend to the ones of the Born approximation which embodies the simple  $Z^2$  law. Sixteen molecules were investigated using the simple stoichiometric model. Results for the six ADN basis were presented and compared with the sparse available experiments. We explore the rule of Toburen which scales all the molecular ionization cross section when divided by the number of weakly bound valence electrons  $\nu_\alpha$  given by Eq.(3). We have found the rule scales much better when normalizing our theoretical ionization cross sections to the number  $\nu'_\alpha$  given by Eq.(7). And finally we attempt to improve the stoichiometric model by the use of the Mulliken charge to redefine a new stoichiometric model containing continuum rather than integer proportions. NO substantial correction was found indicating that the SSM works quite well.

Our aim in this article is to provide the tools to estimate any inelastic parameter parameter -such as the emission angle, the emitted mean energy and cross section- by the impact of any multicharged ion on any molecule containing H, C, N, O, P and S, with the help of the stoichiometrical model. Our goal was quite **pretencioso**, considering the simplicity of our proposal. However we think our results could be used to estimate the ionization magnitude with an acceptable level of uncertainties.

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