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The mean ionization potential of DNA and Liquid water

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ABSTRACT

The Partial Stopping Power Effective Charge (PSPEC) ζ(q), the mean excitation energy I(eV), have been determined in target DNA and H_2O in the present work we use the Drude-dielectric formalism to calculate the effects of contribution of inner and outer-electron shell to energy-loss of protons in two targets of high biological interest, namely, H_2O and DNA. For a better control and understanding of the effects of radiation damage in living tissues, it is necessary to advance an accurate description of the energy loss from the ion beam to the target. The results show that the charged particles (protons) with energy between 0.05 MeV to 2.5 MeV are very efficient in producing secondary electrons in dry DNA, which are able to produce strand breaks and could be very effective for the biological damage of malignant cells. An effort to study the interaction of energetic ion beams with liquid water H_2O at intermediate energies has been carried out recently, since water represents over 80% of the content of the cells of soft tissues. Screening length effects has been taken in the consideration and good agreement is achieved with previous work using Isabel Abril [1] for numerical calculations in the program.

***Keywords*:** Outer and inner shells; Dielectric formalism; Energy-loss function (ELF); Drude-dielectric function; Partial Stopping Power Effective Charge (PSPEC); properties of the targets (H_2O and DNA)

1. INTRODUCTION

When a proton (One of the types of ionizing radiations) moving inside living tissues, such as: liquid water H_2O and DNA which are the most relevant biological materials, we'll get energy distribution of the electronic excitations in this process, hence the focus will be on these materials as targets. Several models have been proposed to describe the electronic response of the targets. By studying energy distribution will be calculated the mean energy of the electronic excitations induced by a proton moving in liquid water and DNA [2]. In another area the space radiation health, whereas research on proton and heavier ion effects on human tissues is important for the radiological protection of human crew in long-duration deep space missions. It is very important to study of interaction between ion-beams with biological materials for predicting the effects of radiation in living tissues [3].

It is worth mentioning the dielectric formulation $\in(k,\omega)$ which was obtained by Lindhard (1954) for a free electron gas had been the basis of many applications and had become one of the most used methods to describe the interaction of swift ions and other charged particles with matter. Lindhard dielectric function is the basic of many applications and because it is applicable to only a limited number of so-called nearly-free-electron materials like aluminum.

The use of this formalism is to study the energy loss of charged particles was introduced by Fermi (1940) in his classical treatment of the density effect in the stopping power of relativistic particles in dense media. Secondary electrons which produced by ionizations induced in the living tissues by a fast projectile also contribute to the cellular damage. These electrons are able to travel and produce further ionizations in the DNA, eventually leading to the cellular death [4]. The lethal efficiency of each secondary electron depends on its energy [5,6], therefore it is very important to have information about the energy and number of the electrons generated by the projectile in the target.

2. THEORETICAL MODEL

2. 1. Interaction of heavy charged particle with matter

When a fast projectile which represents one of the types of the ionizing radiation and by using an incident proton as a projectile passes through material, energy of this incident proton after the collision with the atomic electrons will be loss than the target material (DNA and liquid water) , the energy loss of the projectile per unit distance in the target material is called the stopping power of the material $\left(-\frac{\mathrm{dE}}{\mathrm{dX}}\right)$. It depends on the velocity, charge of the projectile and, of course, the target material. And will be a loss of energy in the DNA ($\mathrm{C_{20}H_{27}N_7O_{13}P_2}$) of more filling because of that more complex elements of Liquid water ($\mathrm{H_2O}$), after that, apply Bragg rule in calculation [7]. The stopping power can be divided into two parts are *:-* electronic stopping and nuclear stopping.

2. 2. dielectric function

The dielectric formalism $\varepsilon(k,\omega)$ as a function of each wave vector (k) and frequency ***(ω)*** has significant consequences for physical properties of solids. The dielectric formulation had become one of the most used methods since it describes the interaction of swift ions and other charged particles with material. This formalism has been used for studying the energy loss of charged particles since then, this has been a subject of continuous and growing interest.

The dielectric function consisting of the imaginary part, for this reason it's considered to be very important since the imaginary part of dielectric function or dielectric constant of valence electrons in material has known as the mutant energy and momentum variable (k) where unilateral dispersion occurs is flexible, dielectric function is used and the imaginary part depending on the type of polarization caused by falling on the target ion. The presence of the imaginary part in dielectric function is very important and that what its content of detailed information on the energy levels of the valence electrons in materials, called exchange loss or (energy loss), can also be brokered account energy ground level [8,9].

Drude-model one of the most important types of the dielectric-function, which has been used in calculation. Drude-model ELFs can be written as follow equation:

$$Im\left[\frac{-1}{\in(k,\omega)}\right] = \sum_i \frac{A_i\gamma_i}{(w-w_i)^2+(w\gamma)^2} \qquad (1)$$

where $A_{i,D}$, ω_i , γ_i **:** are the intensity **,** position **,** width **,** and the subscript D stands for Drude. Later this model was extended to finite values of k namely the extended-Drude model [13], the improved extended-Drude model [10].

2. 3. Partial Stopping Power Effective Charge (PSPEC)

The formula of Partial Stopping Power Effective Charge (PSPEC) have derived by Brandt and Kitagawa for projectiles ionization q(v) in a variational statistical approximation [11]. At low frequency, this approximation is used to construct energy loss function i.e.

$$\left\{\text{imaginary part } \mathrm{Im}\left[\frac{-1}{\in(\mathrm{k},\omega)}\right]\right\}$$

or the dielectric function. This approximation is applicable in the well- known Lindhard-function [12].

This function also can gives an exact description of the dielectric function for a low velocity ion in a non-relativistic free electron gas with high density at zero temperature [13]. With the dielectric function formalism, the energy loss cross-section of a singly charged projectile with velocity v can be expressed as follow

$$S_{(q)} = \frac{2}{N\pi v^2}\int_0^\infty \frac{dk}{k}|\rho(k)|^2 \int_0^{kv} d\omega\, \omega\, Im\left[\frac{-1}{\epsilon(k,\omega)}\right] \qquad (2)$$

where N : is the atomic density of the medium.

$$\rho(k) = z_1 \frac{q+(k\Lambda)^2}{1+(k\Lambda)^2} \qquad (3)$$

where: Λ : is the screening length, q : the degree of ionization.

In eq. (2) the imaginary part $\mathrm{Im}\left[\frac{-1}{\in(\mathrm{k},\omega)}\right]$ will be divided into two parts one of them for the outer electron excitations of the targets (liquid water and dry DNA) which is calculated by using Drude-model energy loss function.

The (PSPEC) fraction of energy loss is given by

$$\zeta(q) = \frac{S(q)}{S(q=1)} \qquad (4)$$

and ($S_{q=1}$) which represents the energy loss for the bare nucleus of the projectile.

$$S_{(q=1)} = \frac{2}{N\,\pi\,v^2} \int_0^\infty \frac{dk}{k} \int_0^{kv} d\omega\; \omega\; Im\left[\frac{-1}{\epsilon(k,\omega)}\right] \qquad (5)$$

The dielectric-function at low velocities is described as:

$$\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right] \simeq \begin{cases} \dfrac{2k\omega}{(k^2+k_D^2)^2} & \text{for } k \le 2k_F \\ 0 \;\; \text{for } k > 2k_F\,, \end{cases} \qquad (6)$$

Now, by inserting eq. (6) and eq.(3) into eq. (2), the stopping power cross section is obtained as:

$$\mathrm{S(q)} = \frac{2}{\pi\, v_1^2} \int_0^\infty \frac{dk}{k} \left| Z_1 \frac{q+(k\Lambda)^2}{1+(k\Lambda)^2} \right|^2 \int_0^{kv_1} d\omega\; \omega\; \frac{2K\,\omega}{(K^2+K^2{}_D)^2} \qquad (7)$$

$$= \frac{4v_1}{3\pi} \int_0^{2K_F} dK\, \frac{K^3}{(K^2+K^2{}_D)^2} \left| Z_1 \frac{q+(k\Lambda)^2}{1+(k\Lambda)^2} \right|^2 \qquad (8)$$

The solution of *eq. (7)* is given by the following equation

$$S(q) = \frac{2Z_1^2 v_1}{3\pi}\, I(\pi K_F) \times \zeta^2(q) \qquad (9)$$

$$S(q) = S_{(q=1)} \times \zeta^2(q) \qquad (10)$$

where
$(S_{q=1})$ is gives as follows:

$$S_{(q=1)} = \frac{2Z_1^2 v_1}{3\pi}\, I(\pi K_F) \qquad (11)$$

$$I(\pi K_F) = In(1+\pi K_F) - \frac{\pi K_F}{1+\pi K_F} \qquad (12)$$

In general the function *I(z)* is given as:

$$I(z) = In(1+z)\frac{z}{z+1} \qquad (13)$$

The stopping power of charged particle *S(q)* of individual element given in DNA ($C_{20}H_{27}N_7O_{13}P_2$) has been calculated numerically and used to find the (PSPEC) of DNA. By using Bragg's additivity-rule, for DNA

$$S_{DNA}(q) = 20S_C(q) + 27S_H(q) + 7S_N(q) + 13\, S_O(q) + 2S_P(q) \qquad (14)$$

For water H_2O :-

$$S_{H2O}(q) = 2S_H(q) + \ S_O(q) \qquad (15)$$

where
$S_i(q)$ refers to the (PSPEC) of each elements in DNA in *eq.(14)* and for each elements in liquid water in *eq.(15).*

3. RESULTS AND DISCUSSION

A program has been written in (FORTRAN - 90) for the numerical calculations given in previous section. By using the parameterization which uses Bragg's additivity rule for compound targets (DNA and Liquid water) over all possible charge states (q = 0 and 1 for H) in order to obtain the energy distribution, the mean energy, P(T,E) and ⟨E(T)⟩ of the electronic excitations produced in the target (DNA and Liquid water), therefor the calculation of the previous magnitudes requires to the description of the projectile charge density and to the target excitation spectrum by means of its energy-loss function (ELF), Im $\left[\frac{-1}{\epsilon(k,\omega)}\right]$.

Each parameter in liquid water or in DNA are important for calculating S(q), for this reason we calculate numerically S(q) of individual element then apply Bragg's rule, we can notice Eq.(14) for DNA and for liquid water H_2O in Eq. (15), which has been used to find the (PSPEC). A program has been written in Fortran-90 and the results were as (Figs 1-5).

The Figures (1-5) show that the starting point at y-axis's is different as a function of incident H-ions energy. On the other hand, the values of the mean excitation energy I eV for biological materials like:- DNA or H_2O are desirable because a difference in this amounts (I values) of only a few percent might cause a large changes in the range and stopping maximum of therapeutic ion beams [14,15]. I(eV) value of the target can calculate as a function of the transferred energy ħω as follows

$$\ln I(\omega) = \frac{\int_0^{\omega} d\omega'\omega' \ln(\omega') Im[-1/\epsilon(k=0,\omega')]}{\int_0^{\omega} d\omega'\omega' \, Im[-1/(k=0,\omega')]} \qquad (16)$$

The magnitude of the variation at mean excitation energy I(eV) as a function of the transferred energy, which produced in (a) DNA (b) H_2O with the energy E in eV, has been calculated by using Drude- dielectric function in Eq.(16). The results show how the atomic shell structure is evident in the mean excitation energy and illustrates that inner- and outer-shell electrons contribute to the mean excitation energy in almost the same proportion.

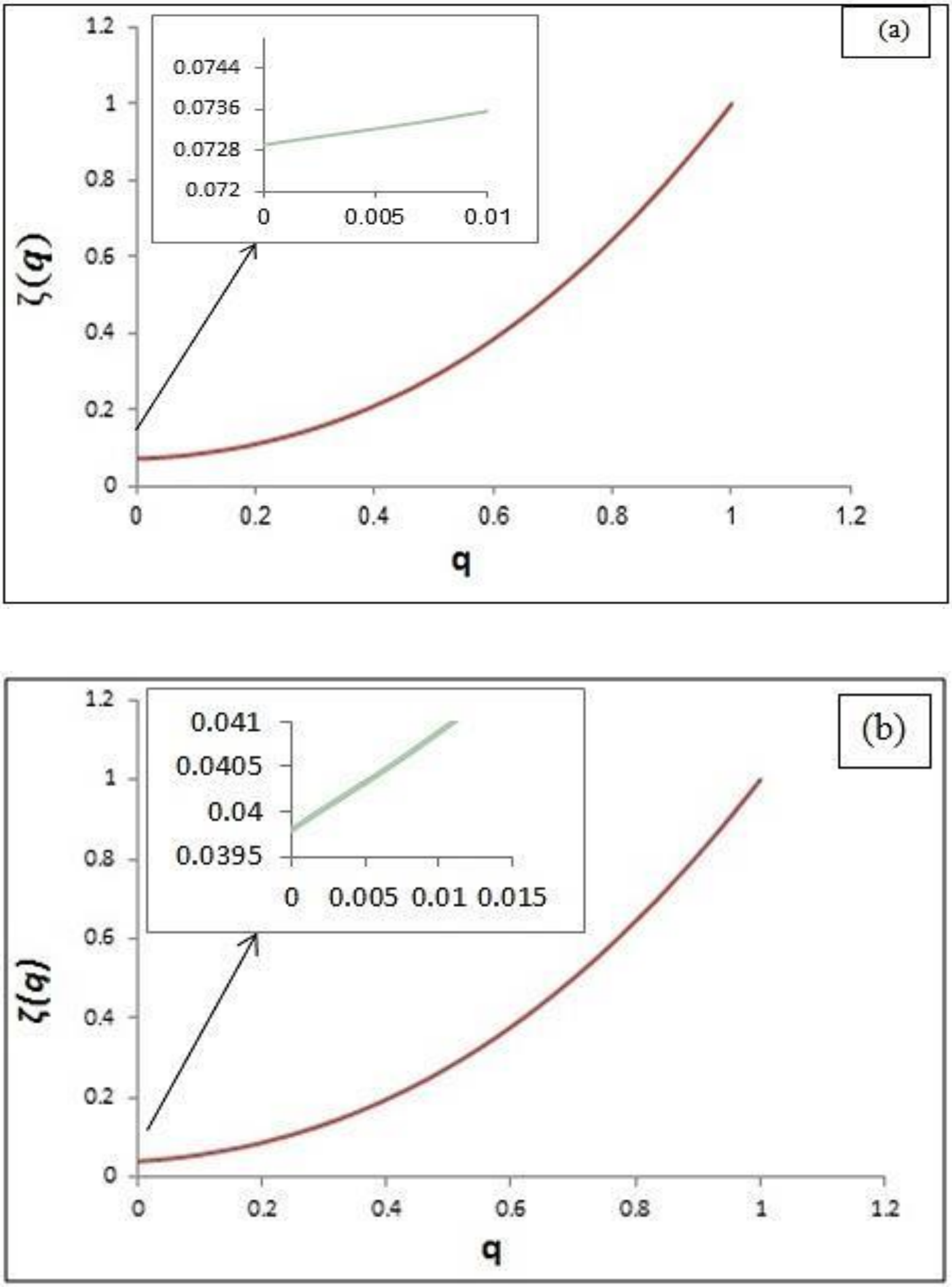


Fig. 1. Total PSPEC of Sub-shells, ζ_{shell} (q) with charge fraction (q) at incident H-ions energy T = 0.05 MeV/u in (a) DNA , (b) H_2O at Λ.

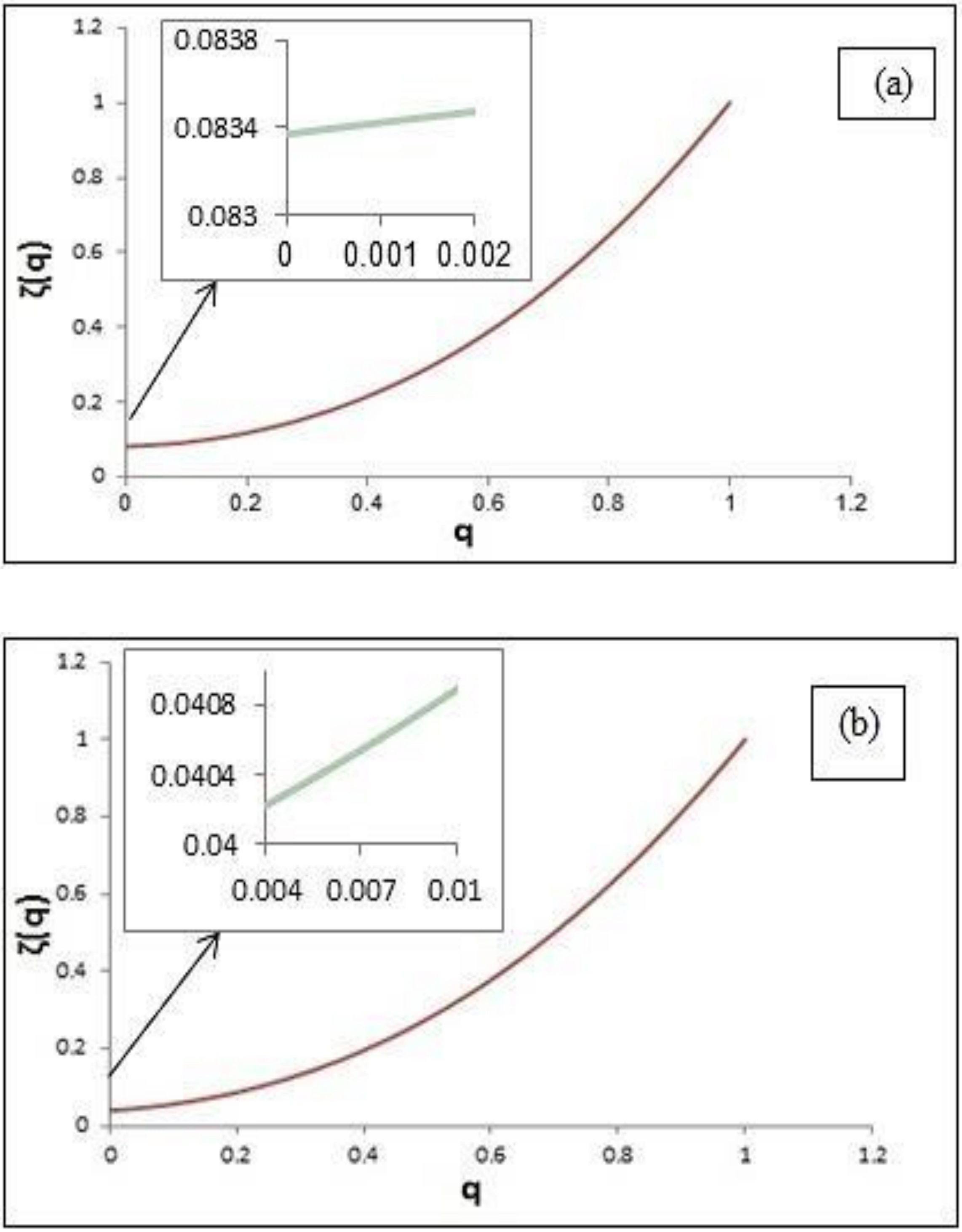


Fig. 2. Total PSPEC of Sub-shells, $\zeta_{shell}(q)$ with charge fraction (q) at incident H-ions energy T = 0.25 MeV/u in (a) DNA, (b) H_2O at ʌ.

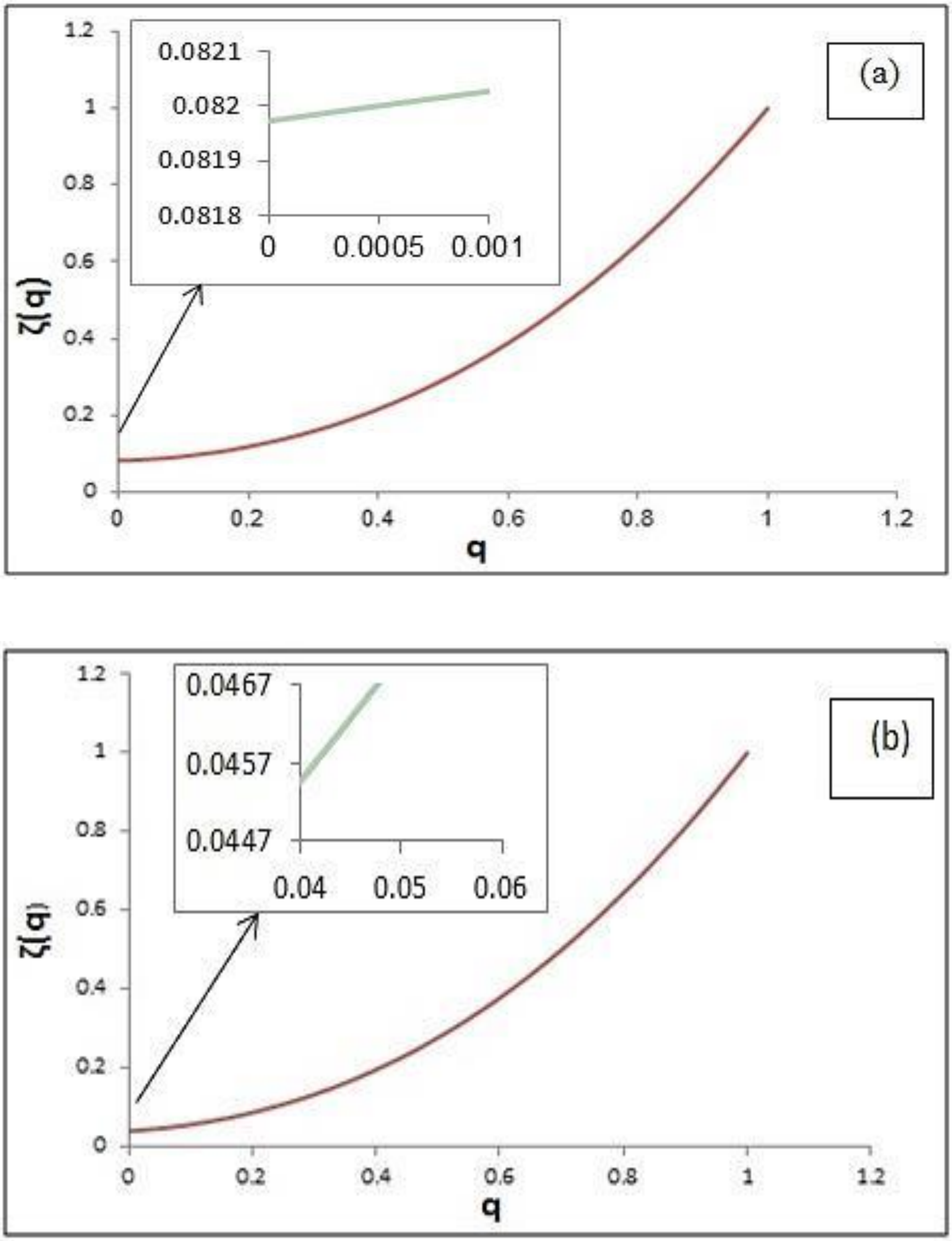


Fig. 3. Total PSPEC of Sub-shells, $\zeta_{shell}(q)$ with charge fraction (q) at incident H-ions energy T =1 MeV/u in (a) DNA , (b) H_2O at ʌ .

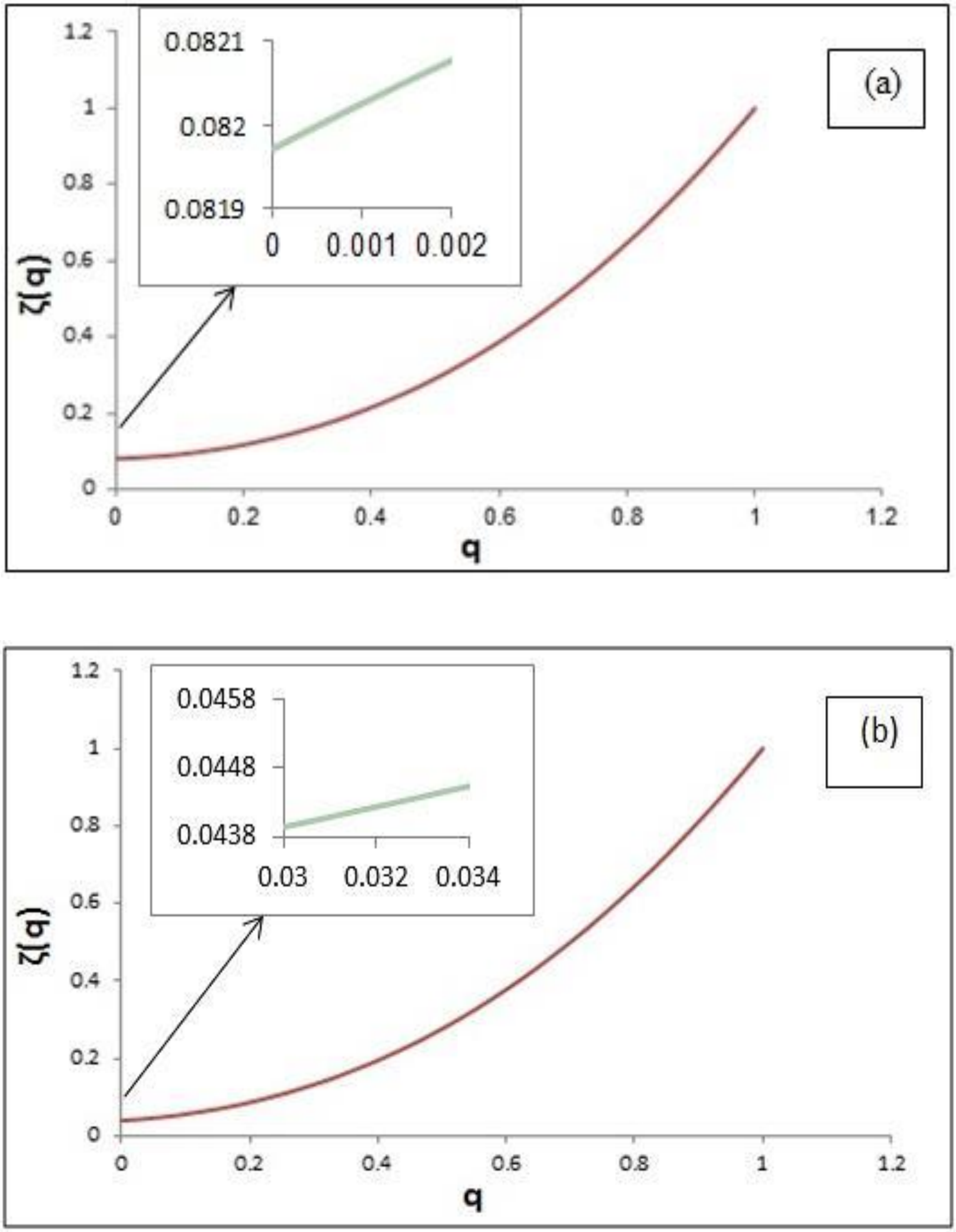
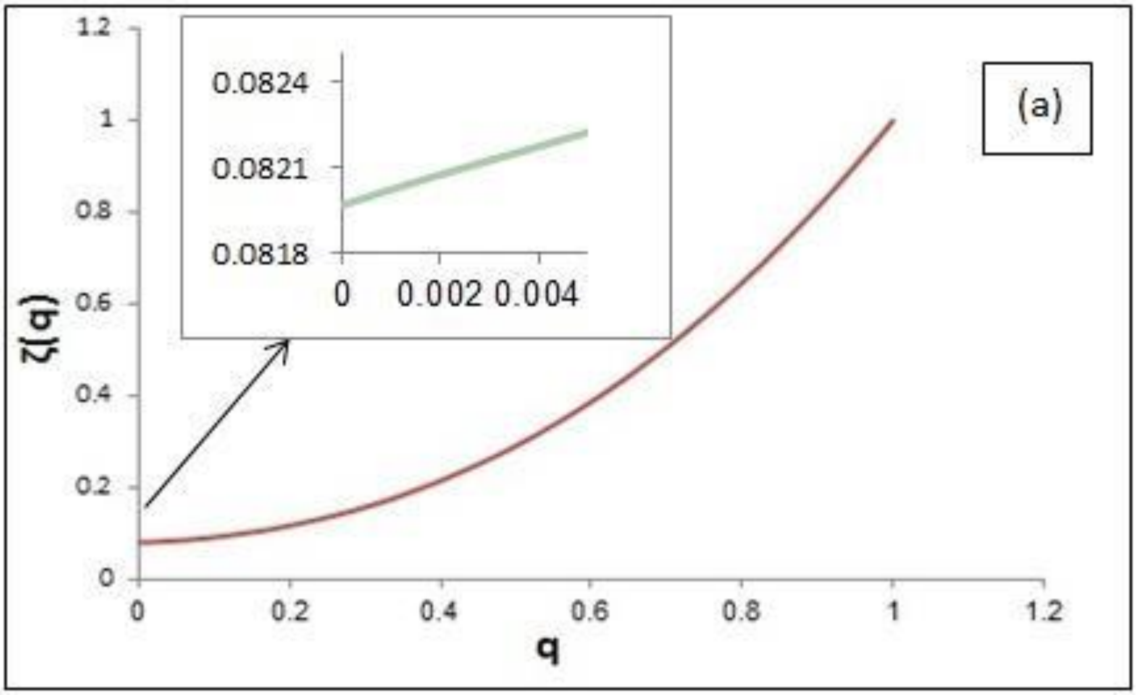


Fig. 4. Total PSPEC of Sub-shells, $\zeta_{shell}(q)$ with charge fraction (q) at incident H-ions energy T = 2 MeV/u in (a) DNA , (b) H_2O at $\wedge$.



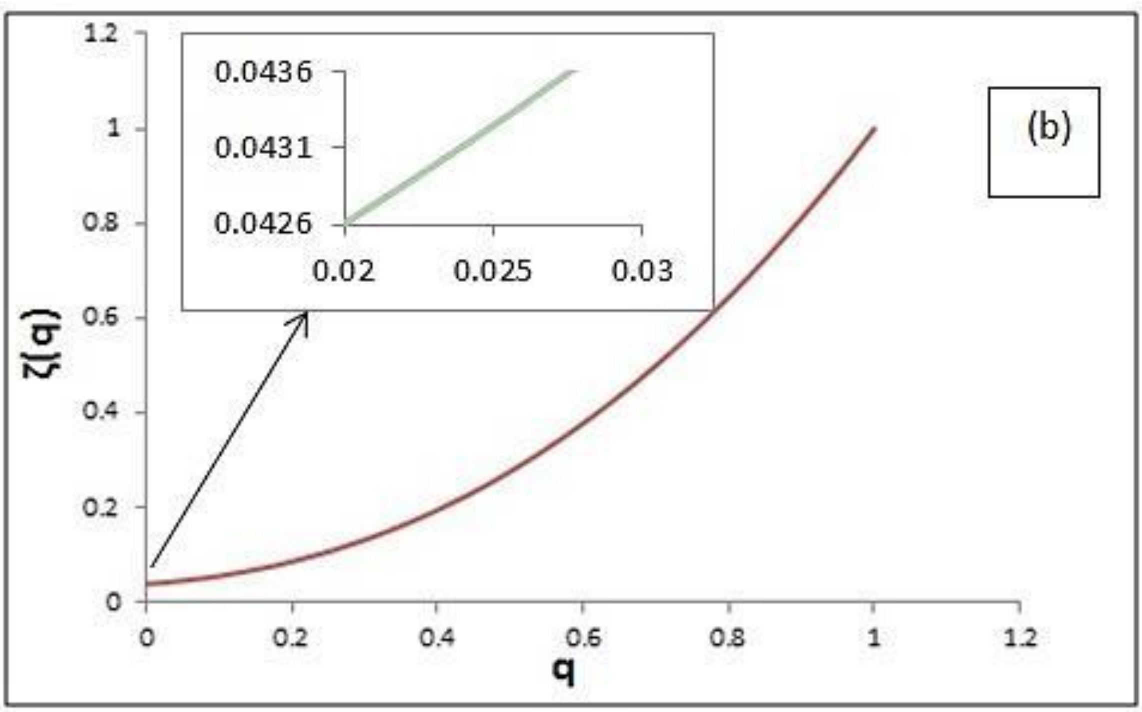


Fig. 5. Total PSPEC of Sub-shells, $\zeta_{shell}(q)$ with charge fraction (q) at incident H-ions energy T =2.5 MeV/u in (a) DNA , (b) H_2O at Λ .

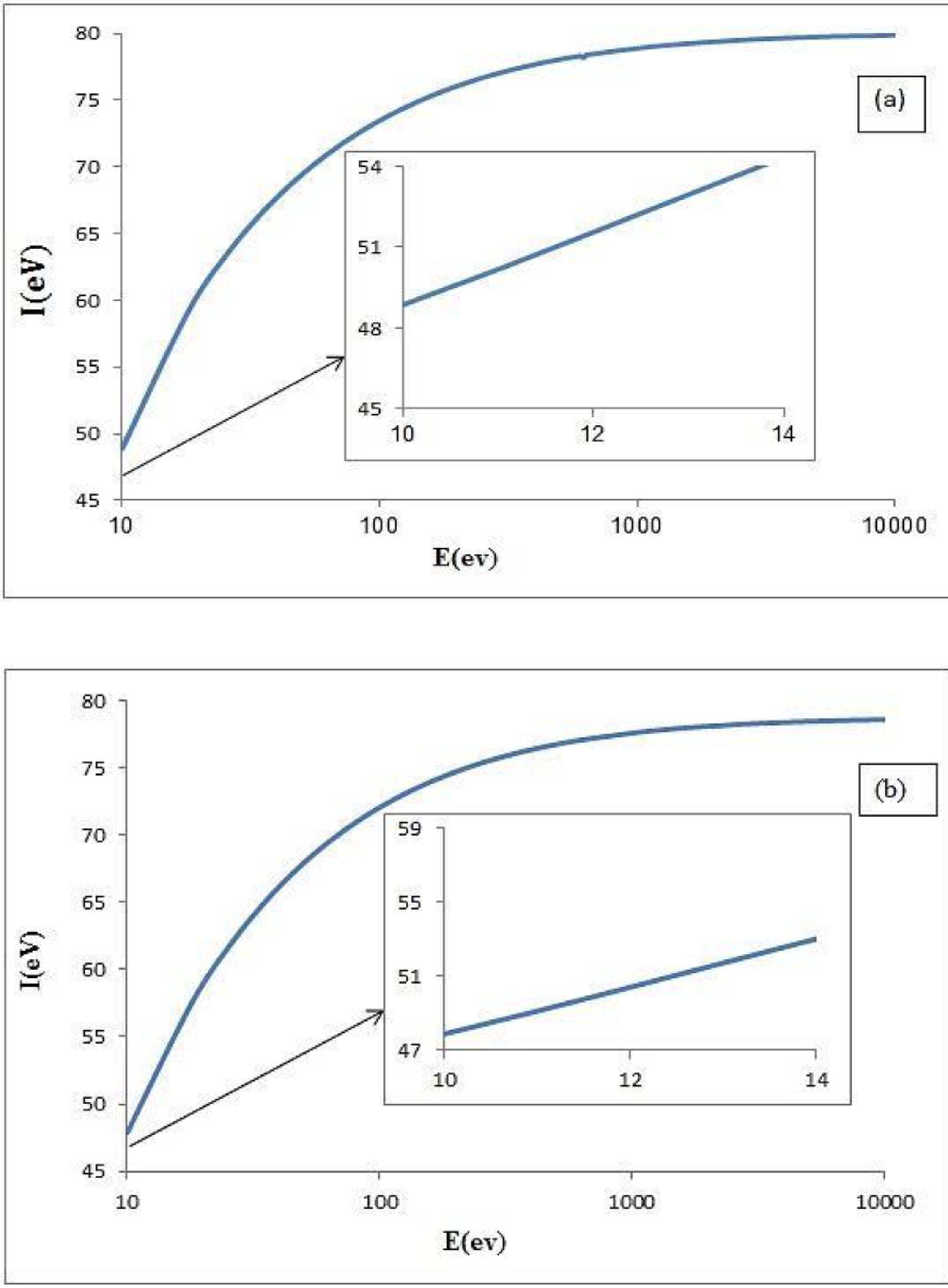


Fig. 6. The variation of mean ionization energy for (a) DNA, (b) H_2O by using Drude-dielectric function.

4. CONCLUSIONS

In the present work we have applied the Drude-dielectric formalism to calculate the main significant magnitudes in the energy loss of hydrogen- ion beams in a dry DNA and H_2O targets, namely, the stopping power, the effects of ionization fraction of Partial Stopping Power Effective Charge (PSPEC) in two targets of high biological interest, namely, DNA and H_2O, the mean ionization potential I in eV. The calculations have been done taking into account the charge-state fractions of the projectile, which vary as a function of the incident energy. The excitation spectrum of the DNA and H_2O has been described accurately by means of the Drude - GOS method [16], which uses Drude-type energy-loss functions for the outer electron excitations and generalized oscillator strengths for the inner-shell excitations.

The main points in the present work are listed below:

1- When charged particles such as: - (protons) pass through a targets (dry DNA and liquid water), these particles (protons) energy transmitted gradually to the target atoms, mainly transmitted by inelastic collisions with electrons target atoms and then the result of this process occurs ionizations and excitations for atoms of the target.

2- Figs. (1-5) show the stopping parameter $\zeta(q)$ of Sub-shells with ionization fraction q for different incident proton energy on elements of two targets (DNA and H_2O) at Λ by using Drude-dielectric function. At $q \rightarrow 0$, $\zeta(q)$ has less dependence on incident proton energy, whereas at $q \rightarrow 1$, $\zeta(q) \rightarrow 1$ at different incident proton energy.

3- The values of $\zeta(q)$ have a significant dependence on velocity at low charge state ($q = 0$) while the dependence become less important at high charge state ($q > 0$).

4- The formula of the Partial Stopping Power Effective Charge (PSPEC) has been obtained according to the BK- model with the dielectric-function method and a modified screening length of the projectile.

5- The mean excitation energy IeV has been calculated as a function of the transferred energy with the energy E in eV, which produced in (a) DNA (b) H_2O by using Drude-dielectric function in Eq. (16). The results of I for Drude-dielectric functions are when $\hbar\omega \rightarrow \infty$, we obtain I = 80 eV in (a) DNA, whereas, I = 78 eV in (b) liquid water see Fig. (6).

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