

PROTON IMPACT OF BIMOLECULAR TARGETS



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ABSTRACT

Article History

Received: 19 June 2017
Revised: 18 July 2017
Accepted: 3 August 2017
Published: 10 August 2017

Keywords

Hadron therapy
Organic compounds
Electronic excitation
DNA
Proton beams
Energy loss function.
Liquid water

For a better control and understanding of the effects of radiation damage in living tissues by using the irradiation of biological systems by energetic ion beams have multiple applications in medical physics and space radiation health, such as hadron therapy for cancer treatment and it is necessary to advance an accurate description of the energy loss from the ion beam to the target. In the present work the dielectric formalism like Drude has been used to calculate the probability for an energetic proton and to produce electronic excitations in five targets of high biological interest, namely, liquid water, DNA, PMMA, Adenine and Guanine. Also, the effects of ionization fraction on the mean excitation energy, average energy and Inelastic mean free path studied taking in to consideration electronic excitation in the target. Good agreement achieved with previous work.

Contribution/ Originality: This study document an empirical method of obtaining the energy loss function which is the key quantity to study the energy deposited in targets of biological interest by swift projectiles such as protons, so it contains all the information about the electron excitation spectrum of the target.. The model used through (ELF), namely the extended-Drude ELF. Each term in the sum of Drude-type functions has three adjustable parameters. The parameters a, b and c can be obtained by a fit of Eq. (1) to the ELF for compounds. Table 1 presents the determined three parameters in Eq. (1) for 5 compounds have been taken from reference [9]. The energy delivered by a swift proton beam in materials of interest to hadron therapy in 5 compounds is investigated.

1. INTRODUCTION

When high-energy radiation interacts with living tissue it produces a range of structural and chemical modifications that can affect biological function. These modifications occur via the production of intermediate species, which include excited atoms and molecules, radicals, ions, and secondary electrons [1]. To characterize energy delivered by the swift ions as a function of the depth by the Bragg curve, with a notorious peak nearly at the end of the trajectory, whose position and height based on projectile energy and target nature [2].

Besides the application to inert substances, the study of energetic projectiles interacting with materials of biological interest is also useful because they can be utilized in a controlled manner to kill malignant tumor cells [3].

The use heavier ion such as proton beams for treating tumors lies in the reduced amount of energy deposited into healthy tissue in contrast with the higher dose delivered at the tumor location, and the well-defined range reached by the beam. Both characteristics are embodied in the depth–dose curve (commonly referred to as the Bragg curve), which represents the amount of energy delivered by the projectile as a function of the depth in the target [4].

In this paper we epitomize the formalism used to calculate, from the condensed matter point of view, the target probability, these analytical results are employed as input into the simulation in section 2.3 to enumerate Average electronic excitation energy and inverse inelastic mean free path in section 2.5 think out mean excitation energy. Which are the main features of the energy deposited by a proton beam in materials currently used in hadron therapy treatment planning, such as liquid water, DNA, Poly (methyl methacrylate) (PMMA), Adenine and Guanine. Which are frequently utilized in hadron therapy remediation plans as tissue phantoms.

2. THEORETICAL BACK GROUND

2.1. Energy Loss Function

The dielectric approach has been acclimatized for describing the electron emission from liquid water and another compound induced by ion beams [5] its protraction to other relevant biological targets only was achieved very recently. The advantage of the dielectric formalism is that, provided that the ELF is experimentally known, many-body interactions and target physical-state effects are naturally included in the subsequent calculations [6].

The formula of dielectric function has a lot of importance to the content of the important guaranteed by the imaginary part that can be brokered account the energy lost of the different levels [7]. They can calculate the energy loss function ELF [8]:

$$\text{Im} \left[\frac{-1}{\epsilon(k=0, E)} \right] = \frac{a(Z_2)E}{[E^2 - b(Z_2)]^2 + c(Z_2)^2 E^2} \quad (1)$$

Where $\text{Im} \left[\frac{-1}{\epsilon(k=0, E)} \right]$ is ELF with single-Drude function and the parameters, $a(Z_2)$ (in eV³), $b(Z_2)$ (in eV), and $c(Z_2)$ (in eV) describe the height, position, and width of the single-Drude ELF. Whereas, $b(Z_2)$ and $c(Z_2)$ are parameterized as a function of the mean atomic number of the target, Z_2 , $a(Z_2)$ is simply obtained by imposing the accomplishment of the f-sum rule [6].

$$\left. \begin{aligned} b &= 19.927 + 0.9807 \bar{Z}_2 \\ c &= 13.741 + 0.3215 \bar{Z}_2 \end{aligned} \right\} \quad (2)$$

\bar{Z}_2 is the no of electrons per formula divided by the no of atoms.

$$\bar{Z}_2 = \frac{\sum_i n_i z_i}{\sum_i n_i}$$

In present work we recommended extend Drude-formula [9]

$$Im \left[\frac{-1}{\epsilon(k, \omega)} \right] = \sum_i \frac{A_{Di} c(k) E}{(E^2 - b^2)^2 + c^2 E^2} \quad (3)$$

Where the subscript ‘D’ stands for Drude; A_{Di} is the intensity. The extended form of Drude-formula is as follow [Abril, et al. \[10\]](#):

The ELF of the material, $Im \left[-1/ \epsilon(k, \omega) \right]$ is a key parameter to obtain reliable results for the inelastic energy-loss magnitudes, for the whole $k-\omega$ plane [\[11\]](#).

Table-1. The fitted parameters a, b and c, mean atomic number \bar{Z} , B binding energy, ρ density and the source of optical data for 4 organic compounds and water [\[9\]](#).

Compound	formula	a(eV) ^s	b(eV)	c(eV)	\bar{Z}	B(eV)	ρ (g/cm ³)
Water	H ₂ O	3856.3	22.71	14.61	3.333	18.13	1.00
DNA	C ₂₀ H ₂₇ N ₇ O ₁₃ P ₂	5156.2	23.70	15.24	5.185	20.00	1.35
PMMA	C ₅ H ₈ O ₂	5399.2	23.70	15.57	3.600	20.00	1.188
Guanine	C ₅ H ₅ O ₁ N ₅	6704.5	25.31	15.11	4.875	21.09	1.58
Adenine	C ₅ H ₅ N ₅	4885.7	24.32	12.78	4.667	20.44	1.35

Source: [Tan, et al. \[9\]](#)

2.2. Probability Per Unite Length

When fast projectile (proton) moves in substance material such as (liquid water, DNA and another compound) with mass M_1 , atomic mass Z_1 , kinetic energy T , and charge, it induces electronic excitations and ionizations in the material, losing energy in the process [\[12\]](#). The probability per unite path length $P_q(T, \omega)$ that a projectile with charge state q and energy T produces in the target an excitation of energy $E = \hbar\omega$ irrespective of its momentum, $\hbar k$, (in a.u $\hbar=1$) is given by [Sabin and Oddershede \[13\]](#).

$$P_q(T, \omega) = \frac{d\lambda^{-1}(T, \omega)}{d\omega} = \frac{M_1 e^2}{\pi \hbar^2 T} \int_{k_{min}}^{k_{max}} \frac{dk}{k} [\rho_q(k)]^2 Im \left[\frac{-1}{\epsilon(k, \omega)} \right] \quad (5)$$

Where λ^{-1} is the inverse inelastic mean free path.

For heavy projectiles, when $M_1 \gg m_e$ (where m_e is the electron mass), the integration limits can be approximated

$$k_{max} \approx \infty \quad k_{min} = \omega / \sqrt{2T/M_1} \quad [13].$$

Where e is the absolute value of the electron charge $\rho_q(k)$ is the Fourier transform of the projectile electronic charge density [\[14\]](#).

$$\rho(q) = Z_1 \frac{q + (k\Lambda)^2}{1 + (k\Lambda)^2} \quad (6)$$

Where Λ is the screen length and given in the following Eq. [\[15\]](#):

$$\Lambda = \frac{0.48 N^{2/3}}{Z_1 - N/7} \quad (7)$$

N: is the number of bound electrons and q is charge state of the projectile inside the target can be change through capture and loss processes. When charge equilibrium is reached, the probability $\phi_q(T)$ of finding the projectile in charge state remains constant for each incident energy T [16].

$$P(T, E) = \sum_{q=0}^{Z_1} \phi_q(T) P_q(T, E) \quad (8)$$

where the charge-state fractions, $\phi_q(T)$, which do not only depend on the projectile energy, but also on its nature as well as on the target characteristics, are obtained from a parameterization to the experimental equilibrium charge fractions [17]. They can evaluate through the expression [15]:

$$\phi_q = \frac{f_q}{\sum_{q=0}^{Z_1} f_q} \quad (9)$$

We assume that they are proportional to the Gaussian charge-state distribution:

$$f_q = \frac{1}{\sqrt{2\pi d^2}} \exp\left[-\frac{(q-\langle q \rangle)^2}{2d^2}\right] \quad (10)$$

$\langle q \rangle$ and d are mean the equilibrium charge and the standard deviation of the distribution [18].

Where $\langle q^2 \rangle = d^2 + \langle q \rangle^2$

2.3. Mean Excitation (Ionization) Energy

The mean excitation energy describes how easily a target, typically a molecule or atom can absorb kinetic energy from the projectile, primarily as electronic (inclusive ionization) and vibrational (including fragmentation) excitation. The mean excitation energy is characteristic of the target only, and has no dependence on the properties of the projectile ion. (One should note parenthetically that if the target is in an excited electronic state before the collision, the projectile might absorb energy from the target [18]). As the mean excitation energy enters the stopping power expression under the logarithm and in atomic units, small changes in mean excitation energies do not produce major changes in the stopping cross section [19].

Mean ionization energy required to remove a given electron from its atomic orbit and place it at rest at an infinite distance. The mean excitation is defined to be the mean value of the minimum energy transfer in a proton – atomic electron collision which produces an ionization event [20]. I is the ionization potential which, for considered system, is defined by Emfietzoglou, et al. [21]:

$$\ln I = \frac{\int_0^\infty E \ln(E) \text{Im}[-1/\epsilon(E,0)] dE}{\int_0^\infty E \text{Im}[-1/\epsilon(E,0)] dE} \quad (11)$$

2.4. Average Electronic Excitation Energy E_{av}

To appreciate the possible damage induced in biological materials due to the irradiation with energetic particles, another interesting magnitude is the average energy $E_{av}(T)$ transferred by a projectile of energy T to the target producing electronic excitations and ionizations, which is defined by Pimblott and LaVerne [22]:

$$E_{av}(T) = \frac{\sum_{q=0}^{Z_1} \phi_q(T) \int_0^\infty d\omega (\hbar\omega) P_q(T, \omega)}{\sum_{q=0}^{Z_1} \phi_q(T) \int_0^\infty d\omega P_q(T, \omega)} \quad (12)$$

The average over all possible charge states ($q = 0$ and 1) in order to obtain the energy distribution, $P(T, E)$, and the average energy E_{av} , of the electronic excitations produced in the target.

2.5. Inverse Inelastic Mean Free Path λ^{-1}

Proton inelastic mean free path is a characteristic quantity to describe the inelastic interactions of a charged proton with organic materials. It is essential importance this quantity in many fields of fundamental and applied research, like space radiation, shielding, radiation biology, and radiotherapy [23]. Monte Carlo track-structure calculations of charged particles represent a useful tool for the investigation of radiation effects on the radiated materials [24].

The calculations are based in the dielectric formalism, with a realistic description of the electronic properties of the target by the single Drude function,

$$\lambda_q^{-1}(T) = \int d(\hbar\omega) P_q(T, \omega) \quad (13)$$

and taking into account charge-exchange processes of the projectile.

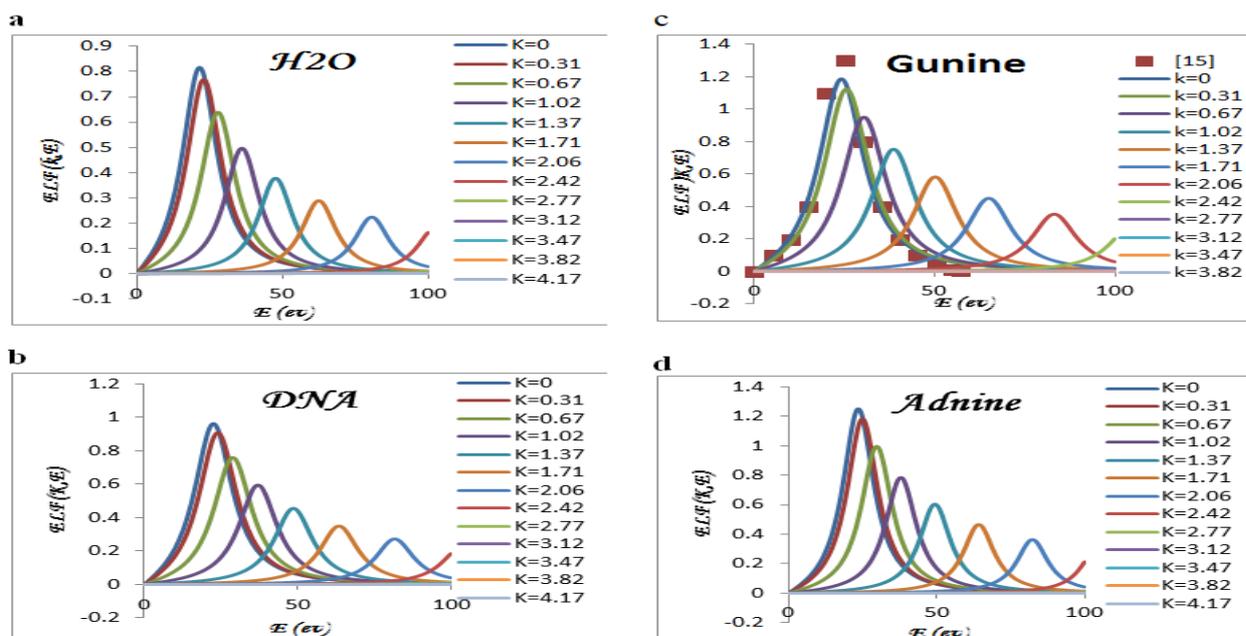
$$\lambda^{-1}(T) = \sum_{q=0}^{Z_1} \phi_q(T) \lambda_q^{-1}(T) \quad (14)$$

3. RESULTS AND DISCUSSION

In this work (Eq. (3)) has been used as the key equation for all calculations. Additionally FORTRAN program has been written for our data analysis.

All parameters in (eq. (3)) are helped to evaluate the energy loss as function of incident proton in five compounds.

Fortunately, experimental information about the ELF in the optical limit, $k = 0$, exists for important biological materials, such as liquid water, DNA, PMMA, adenine, or Guanine. The Energy loss function ELF with different wave no $k=0$ to $k=4.17$ is show in fig. (1) for (a) liquid water (b) DNA (c) Guanine (d) Adenine and (e) PMMA.



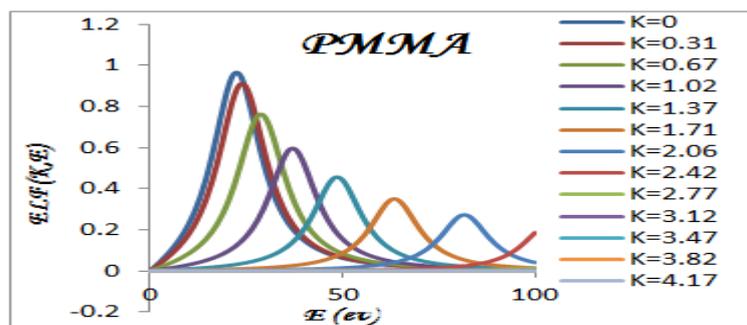


Fig-1. Energy loss function (ELF) of (a) H2O, (b) DNA, (c) Guanine (d) Adenine and (e) PMMA as a function of the transferred energy hw , for several values of the momentum transfer hk .

Source: this is our presentation work

Fig 2 shows the calculated probability per unit path length $P(E, T)$, Eq. (3), for a proton beam (having incident energies T (0.25, 0.5, 2.5, 5, 10 MeV)) at and of producing an electronic excitation of energy E in (a) H2O, (b) DNA, (c) Guanine (d) Adenine and (e) PMMA, and PMMA. The probability $P(E, T)$ decreases as the proton energy T increases, indicating that a larger number of electronic excitations are produced when lower incident energies T are used, and at energy less than 20 eV, the probability $P(T, E)$ increases as the excitation energy E increases as well.

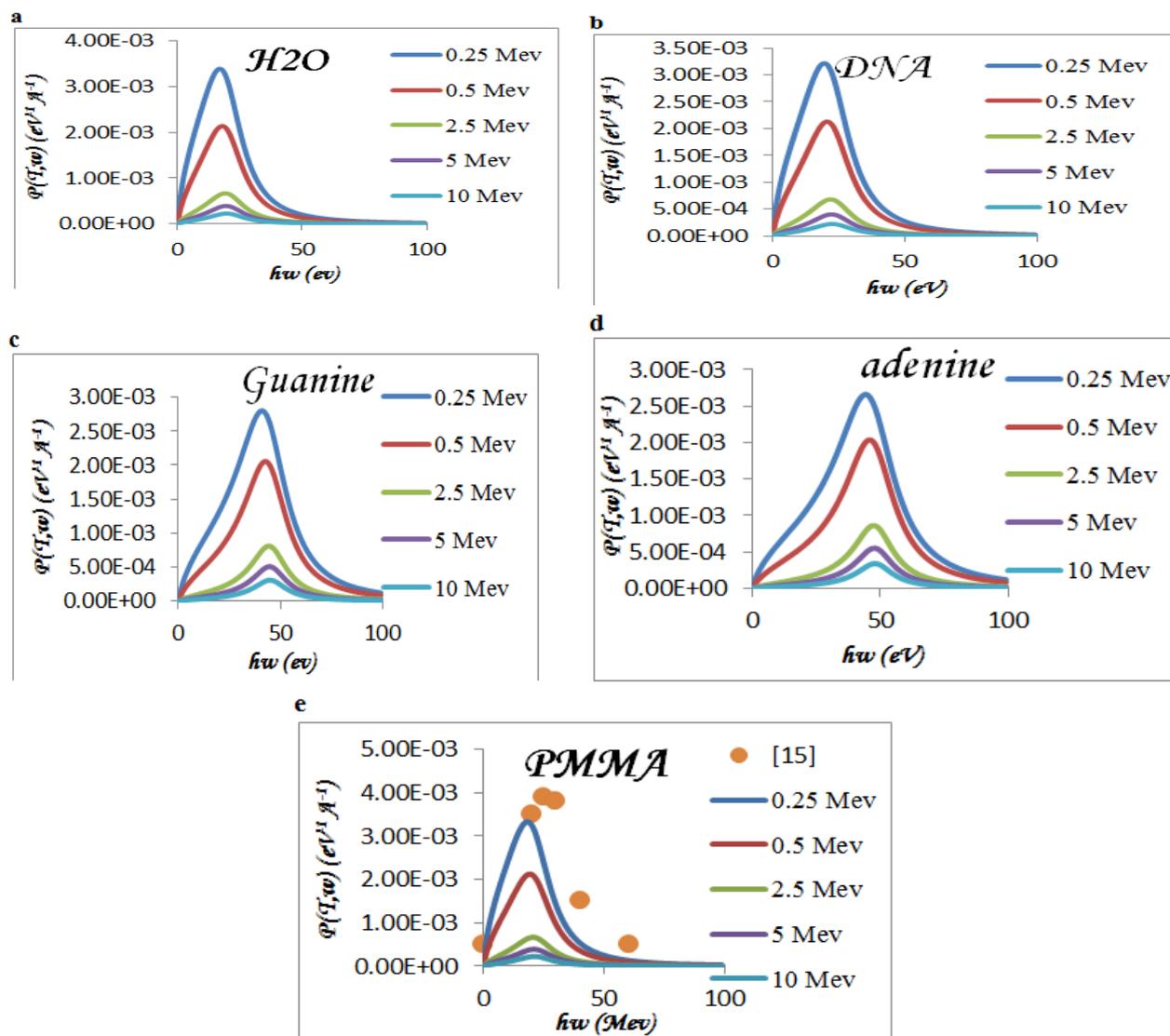


Fig-2. Probability per unit path P for projectile induces electronic excitation of energy E in (a) H2O, (b) DNA, (c) Guanine (d) Adenine and (e) PMMA at energy $T=(0.25-10)$ MeV, previous work [19].

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The ionization potential (*I*-value) of (a) H₂O, (b) DNA, (c) Guanine (d) Adenine and (e) PMMA, are shown in table (2).

Our present results of ionization potential are compared with available previous work for dry DNA (*I*= 81.02 eV) [8] good agreement is achieved in previous work [16].

Table-2. The mean excitation energy for projectile induces electronic excitation of energy *T* in H₂O, DNA, Guanine, Adenine and (e) PMMA.

Material	I (eV) calculated	I (eV) Expected	I (eV) Present work
DNA	86.64 [25]	90 [9]	81.02
Adenine	73.90 [25]	71.4 [9]	76.26
Guanine	78.25 [25]	75 [9]	77.01
PMMA	68.37 [9]	74 [9]	79.55
H ₂ O	72.5 [9]	75 [9]	76.32

Source: this is our presentation work

Figure 3 shows $E_{av}(T)$ as a function of the energy of a proton beam in liquid water, DNA, PMMA, adenine and Guanine with available previous data. We can observe that $E_{av}(T)$ is rather similar for liquid water and DNA.

The mean energy $E_{av}(T)$, given in Eq. (12), of the electronic excitations produced by a proton in DNA and another compound is depicted in Fig. (4). It is seen that $E_{av}(T)$ increases with the proton energy *T*, being around 9-10 MeV in DNA and H₂O, PMMA, Adenine or Guanine and around 69.48 eV for DNA, ≈66.3 eV, for H₂O, ≈68.02 eV for PMMA, ≈ 69.09 eV for Adenine and ≈ 72.2 eV for Guanine. As the number of electronic excitations, the mean energy of the excitation increase with *T*. The results granted in Figs. (3) and table 3 agree with available previous work [10].

Table-3. The average energy for projectile induces electronic excitation of energy *T* in H₂O, DNA, Guanine, Adenine and (e) PMMA

Material	E _{av} (eV) Present work	E _{av} (eV) Previous work
DNA	69.48	63 [14]
Adenine	69.09	----
Guanine	72.2	----
PMMA	68.02	----
H ₂ O	67.3	----

Source: this is our presentation work

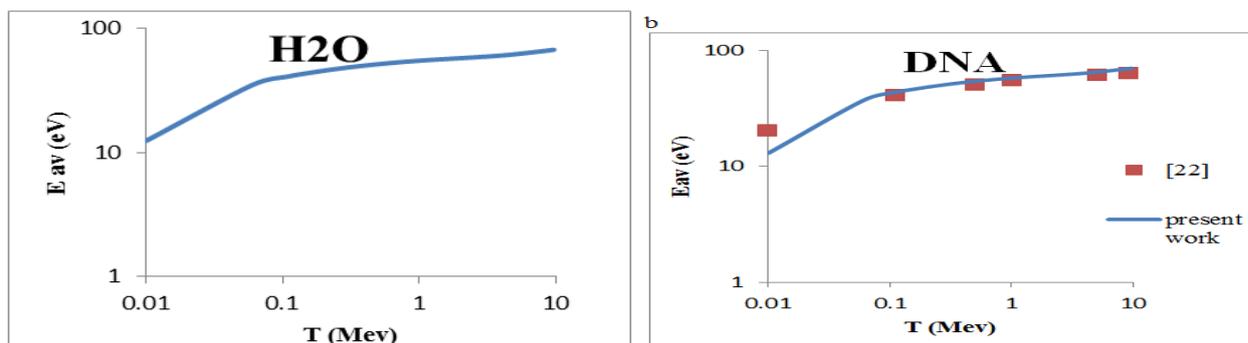


Fig-3. Average energy E_{av} transferred by the projectile producing electronic excitations and ionizations in (a) H₂O, (b) DNA, induced by a proton beam as a function of its energy. The calculations were obtained with the dielectric formalism the single Drude function. Circles correspond to results for ionization processes from a proton beam in DNA from Pimblott and LaVerne [22].

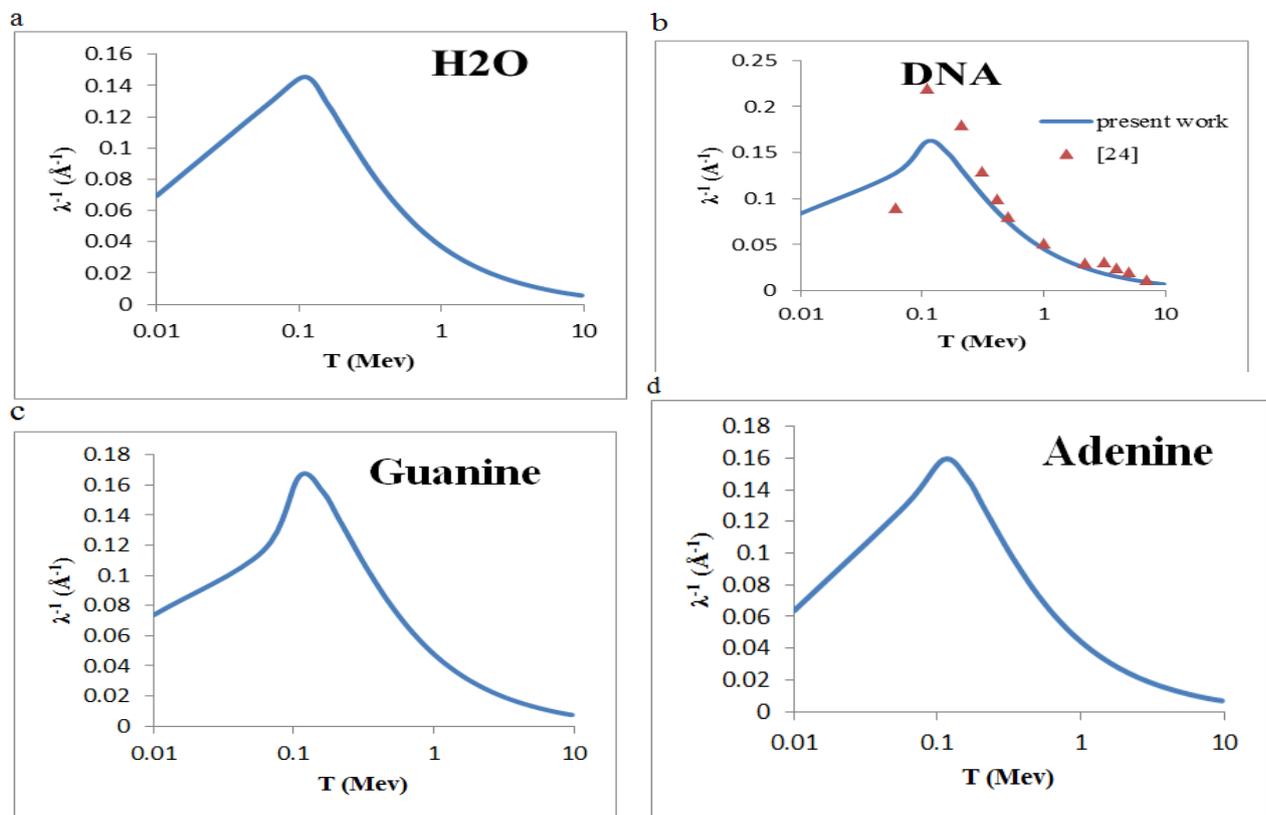
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We offered a methodology of estimating the IMFP of energetic proton in organic materials. Using this methodology we have performed the systematic calculations for the IMFP of 0.01–10MeV protons in a group of eleven important organic compounds, i.e. DNA, liquid water, PMMA, Adenine and Guanine.

The results in figure 4 obtain the inverse inelastic mean free path, or IIMFP, for protons in liquid water, and four organic compounds by using dielectric formalism in Eqs. (1). At proton energies lower than 1 MeV, sizeable differences between the inelastic mean free path corresponding to the five materials.

The maximum value of the inelastic mean free path, corresponding to proton energy ~ 0.1 MeV for the five biological materials DNA, H₂O and Guanine, Adenine, and PMMA. The IIMFP in DNA is larger than in liquid water, whereas the IIMFP in PMMA is greater than in liquid water and compounds. IIMFP for H₂O (0.145\AA^{-1}), DNA (0.162\AA^{-1}), Guanine is (0.165\AA^{-1}), for adenine is (0.159\AA^{-1}) and for PMMA is (0.147\AA^{-1}).

The results granted in Figs. (4)b for DNA agree with available previous work [26]. The purpose of this work is to give the proton inelastic MFP for these organic materials because of their importance in related radiation effect research and in space research. The data presented here are the first results of proton inelastic MFP for these bioorganic compounds over the energy range of 0.01–10MeV.



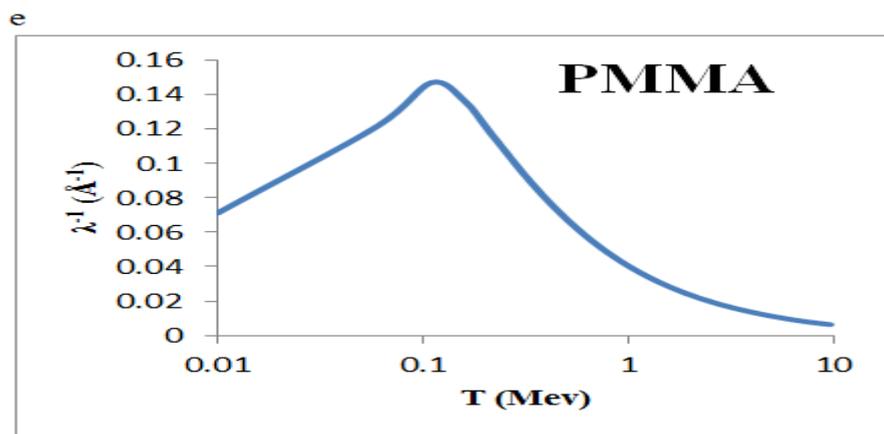


Fig-4. Inelastic mean free path (IMFP) results as a function of proton energy for (a) H₂O, (b) DNA, (c) Guanine (d) Adenine and (e) PMMA.

Source: this is our presentation work

4. CONCLUSIONS

We have calculated the spectral distribution of the electronic excitations induced by a proton in liquid water, dry DNA and three compounds. For this purpose we use the dielectric formalism and obtain the target energy-loss function, $\text{Im}[-1/\epsilon(\mathbf{k}, \omega)]$, from optical data to describe its extension to arbitrary values of momentum-transfer k , namely the extended-Drude. We find that, regardless of the proton energy, the probability distribution P , of the electronic excitations has a maximum around 20 eV. Besides, $P(E, T)$, which is related to the number of electronic excitations of a given energy E , decreases with the proton energy T . On the other hand the mean energy E_{av} of the electronic excitations increases monotonically with the proton energy T ranging from (10–20) eV at $T = 0.01$ MeV and around 10 eV for $T = 10$ MeV the mean energy of the excitation increases with T . This model examined agree in the calculation of $P(T, E)$ and E_{av} at large values of the proton energy. At lower projectile energies important differences arise among the model. The mean excitation energy (I) of liquid water is estimated to be 72.5 eV. The inelastic MFPs for 0.05–10 MeV protons in a group of 4 organic materials and water have been performed. The calculations are based on the method described in our previous work. The aim of this work is to present the proton IMFP for these organic compounds because of their importance in related radiation effect research and in space science.

Funding: This study received no specific financial support.

Competing Interests: The authors declare that they have no competing interests.

Contributors/Acknowledgement: All authors contributed equally to the conception and design of the study.

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