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Shell Correction, Bloch Correction and Barkas Effects in Biological Materials

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Abstract:
The proton has special advantage in radiation thereby because of its deep Brag peak which provides unaffected tissues. Five compounds organic and inorganic included liquid water, DNA, Adenine, Guanine and PMMA have been used in present work. The description to interactionis by dielectric formalism through Drude dielectric function for outer electrons and by general oscillator strength to describe the inner contribution,Brag rules has been applied hear for element in compounds. The investigations included shell correction, Barkas effect, Bethe and Born. The results give the influence of inner shell and Block correction. In this work Bethe correction (Barkas effect, shell, Born and Bloch correction) has been evaluated for first time for compounds under work except for Liquid water and not clearly way for DNA. The work has been programing by Fortran- 90.

Keywords: *Dielectric function, General oscillator strength, Shell correction, Barkas effect, Bloch correction.*

Introduction

The important ways to understand how the interaction between the projectile and target has been happened (any type of target solid, gas and biological material) is studying Bethe equation and correction on it.

The study of collision and its mathematical relations take the researchers interest, in this field addition to is acts original study of physics, it important when study the radiation thereby. That included treatment different type of tumors cancer in any part of human body by using charged particle as projects which consists electrons protons and its anti-particles, alpha particles and other heavy ions. What special in those ways in treatment particularly by protons is that gives least damages in around healthy cells and (that for protons) goes directly to goal tissue, so the study of collision and stopping power and other titles has been taken a large interest in our work.

Hadron therapy acts the one of an influence treatment way to deals with cancer, that belong to providing tumors by a high and enough transfer dose and as mention above resultless damage into healthy cells(Surdutovich and Solov'yov 2014).

The stopping power of charged particles and matter is the more part have alarge important in the interaction between target and projectile in applied physics. Stopping power can be calculated by use the known theory that is the Bethe theory which used to wide range of energy of swift particle(Bichsel and Porter 1982),actually Bethe- Bloch formula and additions corrections . as we will see in the present work.

The dielectric formalism or in origin expression the dielectric constant which is complex numberrepresents the important physical method to gain the information of structure matters, spatially that materials which had no enough details about it such like biological materials . That formalism in framework of first order penetration theory is depended on constructing of the model dielectric response function.(Abril, et al. 1998) The dielectric benefit, some material had been no practically suffices information, so the using of dielectric function is so useful to accurate this order. The dielectric function depends on the momentum and the angular frequency or the energy on incident particles.There are many models to express the dielectric response, Lindhard (Abril, et al. 1998) model represents the base of the other models to structure the expressions.Present work depends on Drude dielectric response function which called single Drude function which belongs to harmonic oscillator case, andcase of free electron gas that about polarization(Lindhard 1976). The present work interest into the effective of electron in inner shells of target and evaluating the influence of bothvelance and inner electrons equally.

The influence of inner shells on present work calculated into general oscillator strength method (GOS)(Dingfelder 2014; Dingfelder, et al. 2000). present work includes evaluating the corrections of Bethe-Bloch equation (Barkas effect, shell correction and Bloch correction) for five compounds organic and inorganic that involved liquid water, DNA, Adenine, Guanine and PMM, in term of dielectric function and taking into account the influences of inner shells that calculation by used general oscillator strength (GOS).

Theory

The nature of atoms structure makes the electrons in outer shells in the front of when the interaction (collision) has been done. The more interaction happened in the velance electrons, one must doesn't forgets an important thing, that is the collision is random process and the projectiles come in different energies ,so the big part of contribution in collision and stopping action is come from the outer shells, there is many ways to evaluate the effectiveness of outer shells, one of its, which acts empirical formula single Drude function which describes the response of dielectric response of matter, it takes the following expression from(Abril, et al. 2010):

$$\eta_{out}(\omega,k) = \mathrm{Im}[-1/\epsilon(\omega)] = \frac{a(\hbar\omega)}{[(\hbar\omega)^2-b]^2+c^2(\hbar\omega)^2} \quad (1)$$

Where $a(Z_2)$ in $(eV)^3$, $b(Z_2)$ in (eV) and $c(Z_2)$ in (eV) representing an intensity, position and width of the single-Drude ELF; a, b and c are parameters. ω is angular frequency or in general it used to express the incident energy; a, b and c for five interesting compounds show in table (1):

Table (1): The values of fitted parameters for semi empirical Drude function (Tan, et al. 2004)

Compound	Chemical formula	$a(eV)^3$	b(eV)	c(eV)
Liquid water	H_2O	3856.3	22.71	14.61
DNA	$C_{20}H_{27}N_7O_{13}P_2$	5156.2	23.70	15.24
Adenine	$C_5H_5N_5$	4885.7	24.32	12.78
Guanine	$C_5H_5N_5O$	6704.5	25.31	15.11
PMMA	$C_5H_8O_2$	5399.2	23.70	15.57

Letimaginary part of dielectric function in convenient title

$$\eta_r(\omega,k) = \mathrm{Im}[-1/\varepsilon(\omega,k)] \quad (2)$$

Im[-1/є (ω,k)] is the imaginary part of the argument.$\eta_r(\omega,k)$is related to the outer shell $\eta_{out}(\omega,k)$and inner shell$\eta_{shl}(\omega,k)$(Dingfelder 2014):

$$\eta_r(\omega,k) = \eta_{out}(\omega,k) + \eta_{shl}(\omega,k) \quad (3)$$

Inner shells have different influence because of the higher binding energy of this shells, that effective calculated from different method.One of those methods is generalized-oscillator strength (GOS),Oscillator strength can be defined according to (Hilborn 1982) as "the ratio between the quantum mechanical transition rate and the classical absorption/emission rate of a single electronoscillator with the same frequency as the transition". Oscillator strength in spectroscopy acts amount without dimension and it represented the probability of absorption or emission of electromagnetic radiation in transitions between energy levels of an atom or molecule(Liston, et al. 1996).The inelastic scattering between the swift projectile and targets which is inside first Born approximation (FBA) has been described by GOS, where the differential scattering cross section is commensurate together with generalized oscillator strength. When the momentum equal to zero that mean the work at optical limit, GOS become OOS pointed to optical oscillator strength(Garcia-Molina, et al. 2009) The inner-shell electrons are described in GOS by the hydrogenic approach which uses to analytically GOS. One can express of general oscillator strength as shown in(Dingfelder 2014; Dingfelder, et al. 2000) on the following:

$$\frac{df(\omega,k)}{d\omega} = 2\xi \frac{df^H(\omega,k)}{d\omega} \quad (4)$$

Where:

$$\frac{df^H(E,K)}{dE} = 2^7 \frac{E}{R_y{}^2 Z_{eff}{}^4} \frac{1}{Z_{eff}{}^2}\left((Ka_\circ)^2 + \frac{E}{3R_y}\right) \times \frac{Z_{eff}{}^{12}}{[(Ka_\circ+ka_\circ)^2+Z_{eff}{}^2]^3[(Ka_\circ-ka_\circ)^2+Z_{eff}{}^2]^3} \times exp\left\{-\frac{2Z_{eff}{}^2}{ka_\circ} arctan\left(\frac{2ka_\circ Z_{eff}}{(Ka_\circ)^2-(ka_\circ)^2+Z_{eff}{}^2}\right)\right\} \times \left(1-exp\left\{\frac{2\pi Z_{eff}}{ka_\circ}\right\}\right)^{-1} \quad (5)$$

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$ka_\circ = \sqrt{E/R_y - Z_{eff}}^{\,2}$,Ry represents the Rydberg energy which$me^4/(2\hbar^2) = 13.606\ eV$

Eq.(3) work under the condition,$E > Ry\, Z_{eff}^2$ for the rang of energy $I_{k\text{-shell}} < E < Ry\, Z_{eff}^2$, eq.(3) becomes:

$$\frac{df^{(H)}(E,K)}{dE} = 2^7 \frac{E}{Ry^2 Z_{eff}^4} \frac{1}{Z_{eff}^2}\left((Ka_\circ)^2 + \right.$$
$E3RyZeff12Ka_\circ 2 - ERy2 + 4Ka_\circ 2Zeff231 - b1 + bZeffZeff2 - ERy$ (6)

Where:

$$b = \frac{2Z_{eff}\sqrt{Z_{eff}^2 - E/Ry}}{(Ka_\circ)^2 - E/Ry + 2Z_{eff}^2}$$
(7)

Where $a_\circ$is Bohr radius,Z_{eff}=Z-0.3 is the effective nuclear charge inclusive the effects of screening from the other electrons, for more details, see (Dingfelder 2014)

The relevant or the connect between the express above of GOS and the dielectric function is through the following expression in optical limit (Dingfelder, et al. 2000):

$$\eta_{shl}(\omega,0) = [Im(-1/\varepsilon(\omega,0))]_{shl} = \frac{\pi}{2}\frac{\omega_p^2}{Z}\frac{1}{\omega}\frac{df}{d\omega}$$
(8)

Where ω_p and $\frac{df}{d\omega}$ are the Plasmon energy and GOS,

$\omega_p = 28.816(\rho Z/A)^{1/2}$ eV.

Bohr, Bethe and Bloch and them important work about interaction of ions with matter, give corner stone of many later works in this field(Arista 2002).

Bohr as theoretical work in classical model of term called stopping power of charged particle in the non-relativistic velocities written as(Kadhim and Hussien 2016)

$$-\frac{dE}{dx} = \frac{4\pi Z_1^2 Z_2 e^2}{m_e v^2} L_{Bohr} \qquad (9)$$

Where$L_{Bohr} = ln\left(\frac{Cm_e V^3}{Z_1 e^2 w}\right)$, C is Euler's constant $C = 2e^{-d}$, d=0.5772, $Z_1$and $Z_2$are the atomic number of projectile and target, e, $m_e$charge and mass of electron, L in general called the stopping number.Bethe formula at high energy is derived from quantum mechanics (Emfietzoglou, et al. 2009):

$$-\frac{dE}{dx} = \frac{Z^2 E_p^2}{2a_\circ T} ln\left(\frac{4T}{I}\right) \qquad (10)$$

Where I is the excitation energy, evaluated by dependent on different ways, one of them is by dielectric function which takes form(Emfietzoglou and Nikjoo 2005):

$$\ln[I(\omega)] = \frac{\int_0^\infty d\omega'\omega'\ln(\omega')\eta_r(\omega,0)}{\int_0^\infty d\omega'\omega'\eta_r(\omega,0)} (11)$$

Where $\eta_r(\omega,0)$take from eq.(3)

The stopping power driving from firs order perturbation and first Born approximation (FBA), is correct valid at$K_B = \frac{2Z_1 v_\circ}{v} < 1$, to asymptotic form of Bethe formula, Eq.(10), correction need to be applied. The corrected stoppingnumber of Bethe formula becomes:

$$L = L_\circ + z_1 L_1 + z_1^2 L_2 (12)$$

The correctionZ_1L_1 is Barkas effect, Z_1L_2 is Bloch correction.Bloch correction consisted the bounded between the classic concept and that of quantum mechanics, from another hand the Bloch correction gives the different between the obvious conceptions. Bichsel and Porter 1982 have been used what is named standard parametrization (Bichsel and Porter 1982):

$Z_2^2 L_2 = -y^2[1.202 - y^2(1.042 - 0.855\, y^2 +$
$0.343\, y4(13)$
Where$y = \frac{Z_1 v_\circ}{v}$
.
can be written as what it called stopping number(Porter and Lin 1990), $L_\circ$ represents Born correction which has following express(Fano 1963):

$$L_\circ = L_{Born} = \left(\frac{2mv^2}{I}\right) + \left(\frac{c}{z_2}\right) + \delta/2 (14)$$

And the term$\left(\frac{c}{z_2}\right)$represents shell correction and$\delta/2$is density correction (which is ignored in this work.

Shell correction arises from dipole approximation, that go to idea of I-value that make (C/Z) connected to momentum dependence of DF(dielectric function).The shellcorrection acts the greatest important under energy 1MeV of protons in Bethe formula correction evaluate in term of dielectric function (Basbas 1984). The important of shell correction is increasing when

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the other correction who work in not high energy (Barkas and Bloch correction) being sizeable.Fano 1963(Fano 1963)assumed theoretical mathematic formula deals with non-relativistic velocity for shell correction term, these allowed to outer and inner shells to contribution in term belongs to shell correction at independently way (Emfietzoglou, et al. 2009):

$$\frac{C_1}{Z_2} = \frac{2}{\pi E_p^2}\int_0^{E_{max}} E.\,dE \int_0^{k_{min}} \frac{1}{k}\{\mathrm{Im}\,[-1/\in(E,k)] - \mathrm{Im}\,[-1/\in(E,0)]\}\,dk \quad (15\ a)$$

$$\frac{C_2}{Z_2} = -\frac{2}{\pi E_p^2}\int_0^{E_{max}} E.\,dE \int_0^{k_{min}} \frac{1}{k}\,\mathrm{Im}\,[-1/\in(E,k)]\,dk \quad (15\ b)$$

$q_{min} \approx E/v$, at this value, term of shell correction rises during the velocity of projectile is decreasing(Oddershede, et al. 2005).

Shell correction $\frac{C}{Z_2}$ can be written as (Fano 1963):

$$\frac{C}{z_2} = \frac{c_1}{z_2} + \frac{c_2}{z_2} \quad (16)$$

The direction of using Born or Bethe limits, which mean classic or quantum deals is determines by or dependent on Bohr parameter:

$$k_B = \frac{2Z_1 v_\circ}{v} \quad (17)$$

The other correctionpart is Barkas effects, Z_1L_1, Barkas effect causes of: duringthe charged particle Passes through the matter polarization has been happened to the target charged (the electrons of the target have been polarized by the projectle), in other word what happened is loss or capture to the electrons z,that gives different in opposite particles' rang or in rate of the energy loss(Lindhard 1976)

Many researchers calculated Barkas effect like J. C. Ashley ,R. H. Hitchie Wsterner and Brandt (Ashley, et al. 1972), their pointed to binding force, Lindhard formula(Lindhard 1976) for Barkas effect calculated it by inter the infleuance of distant collesion , Jackson and Macarthy (JM)(Jackson and McCarthy 1972) using harmonic oscillator raduse in detalise of evaluate the Barkas effects.

The refinement to the ARP model has been propoused by Ashly 1991(Ashley 1991), that make the actual absorption spectrum of the material is known. So the Barkas effects as approximation from Ashly 1991 is(Ashley 1991):

$$L_{Barkas} = \frac{2}{\pi E_p^2}\int_0^{E_{max}} E\, Im[-1/\varepsilon\,(E,0)]L_1(E;\xi)dE \quad (18)$$

$$L_1(E;\xi) = \left(\sqrt{Ry}/2\right)\frac{E}{T^{3/2}}H(\xi) \quad (19)$$

Where $\xi = 0.1356a\left(E/T^{1/2}\right)$, a is minimum distance of glancing collision, H(ξ)being a tabulated function which has been analytically approched that was by Ashley at 1991(Ashley 1991).

$$H(\xi) = \begin{cases} (3\pi/2)In(1/\xi) - 2.417 - 2\pi\xi^2[(In\xi)^2 + 1.14In\,\xi - 0.33] & \xi < 0.25 \\ \left(-0.5986 + \frac{0.9962}{\xi} - 0.1233/\xi^2\right)\xi^{-3/4} & 0.25 \le \xi < 1 \\ 9.052\,exp\,(-3.72\,\xi + 0.217\,\xi^2 & 1 \le \xi \le 2 \end{cases} \quad (20)$$

The analytic form for small ω was derived (see (Ashley 1991)) and reproduces tabulated values to Within 1% for ξ ≤ 0.2 increasing to 1.7% at ξ= 0.25 The other terms were found by fitting the tabulated values-to within 2% for 0.25 ≤ξ <1 and within 0.2% for 1≤ ξ ≤ 1.

So the stopping power given the Bethe formula will contains three corrections to the first Born approximation

The present work includes evaluating the above corrections (Barkas, shell and Bloch correction) for five compounds organic and inorganic that involved liquid water, DNA, Adenine, Guanine and PMM, in term of dielectric function and taking into account the influences of inner shells that calculation by used general oscillator strength (GOS).

Result and discussion

In addition to the influences of the outer electrons shell when calculated the corrections, the focus her on the inner shell and its effects on the calculates as essentially way that by evaluate the effects of K, L or other shells (according the compounds and its atomic number) that happens by calculated the general oscillator strength approximation eq.(3,4) as a conditions above according the energy in terms of dielectric function. In this work use Bragg's rule (see (Bragg and Kleeman 1905)) to summation the effects of each element in single compounds into applied the GOS.

The dependence of shell correctionon momentum is appeared from equation (14) and the influence of ionization spectrum included by ELF(Basbas 1984).

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Figure (1) shows the shell correction present in equation (15a,15b) with energy proton (Ep (KeV)) for five interest compounds, shell corrections explain how the electrons of inner shells contribution in stopping process. From figures a, b, c, d, and e, one can see two curves to each compound, one belong to valence or outer electronsand the other pointedto total contribution of inner and outer shells.Contributions, inner and outer, in general whole contribution and all action in this part happened below 1 MeV

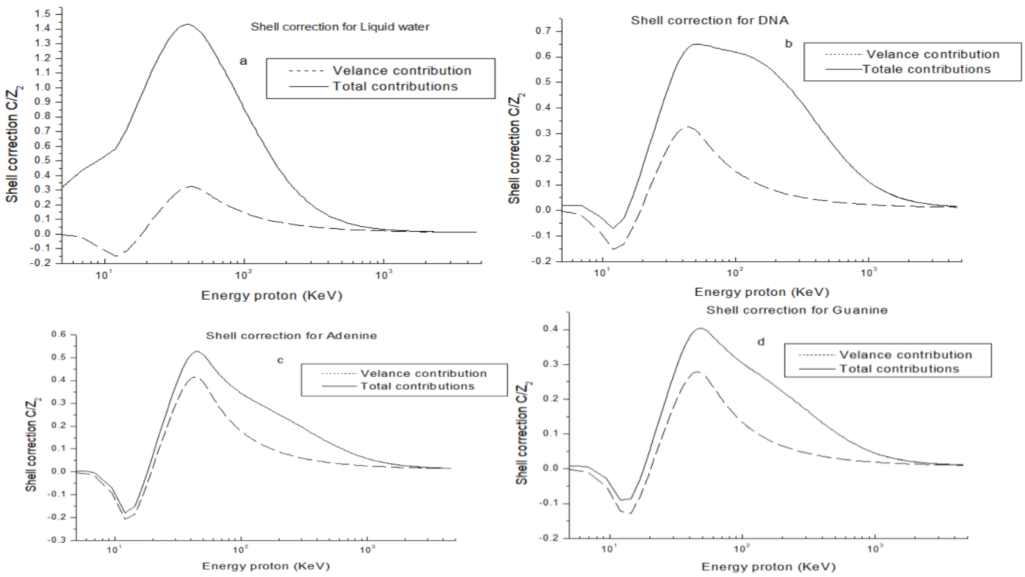
The curves of total contribution of shells prove a large contribution of nuclear electrons. The binding energy of inner electrons is strong than that of valence, that givesexplanation the high position and widely of peak of total curves appearing in high values of energy. The large part of valance is represented on positive equation that also dependent on the momentum as mention above.

Generally the sittings of peaks on x-axis act the most contribution of electronsin stopping number or stopping power or higher absorption. One can notesfrom velance curve, to Guanine was less beak, and DNA, H_2O, PMMA respectively, Adenine recorded higherpeak. All $(C/Z_2)V$ curves started with negative values because of the nature of shell correction equation, the bigger value in negative was to DNA -0.975,the rest compounds started from about -0.1, the minimum value was belongto Guanine which records -0.0647.Fig.(1) included also part g which acts Table (1) containsvalues of maximum contribution of outer shells forfive compounds.One can note, what it characterize shell correction is that it is appear as clear in different energy values.

Eq.(18) acts Barkas correctionwhich represents expression the polarization happened to the target electrons by projectile (proton in our work), this correction is important addition on the Bethe equation of stopping power and that make different between particle and anti-particle(Pions) cross sectionsby exists Z_1.Barkas effects evaluated in term of dielectric response by single Drude dielectric function as the rest ofpresent work is. Figure (2) shows the correction of Barkas with Proton energy in KeV for five compounds. According to the concept of Barkas effect the almost interaction is happened with outer electrons which give many polarized most likely because of numbers of outer electrons. That gives clear, higher and larger curves of L1 belonging to valenceelectrons in medium and low velocity of projects H2O has higher peak in outer curveswhich is 0.6445 and lower one was from PMMA; Figure (3)is showing the five compounds together in outer shells and totally contributions including indeed the influence of inner shells. Top of the outercurves acts the larger polarized happened, that means the most validity of Barkas effect that in the low energy of incident proton. Table (2) contain the values of Barkas effect from the present work.

Eq. (14) evaluates the stopping number or Born correction which acts the result of the difference between Bethe expression and shell correction.This term also dependent on the atomic number of target as its showing in Fig.(4), one can see the difference . Eq.(14) represents stopping power at high proton energy.

Which is worth mentioning that, due to Bragg's rule which neglects bond effects the calculations of inner shells is less than valance electrons, and need more work to do about type of bonds (single, double and triple).



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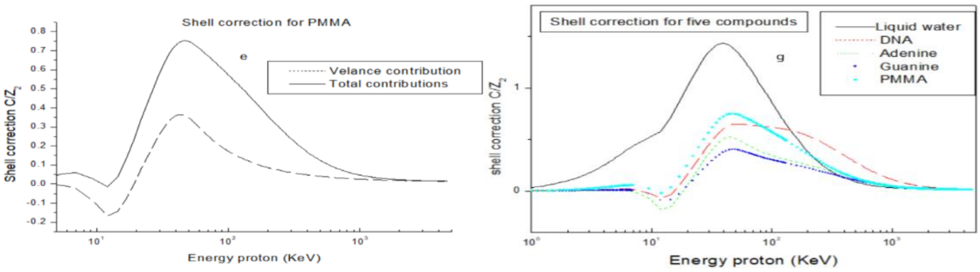

Fig.(1) Shell correction evaluated from eq.(14 and 15) in term of dielectric function by single Drude function and general oscillator strength. (a) Liquid water,(b) DNA, (c) Adenine, (d) Guanine and (e) PMMA.(Dashed line) for valance contribution, (full line) represents total contribution including influence. (g) acts the total contribution for five interest compounds together.

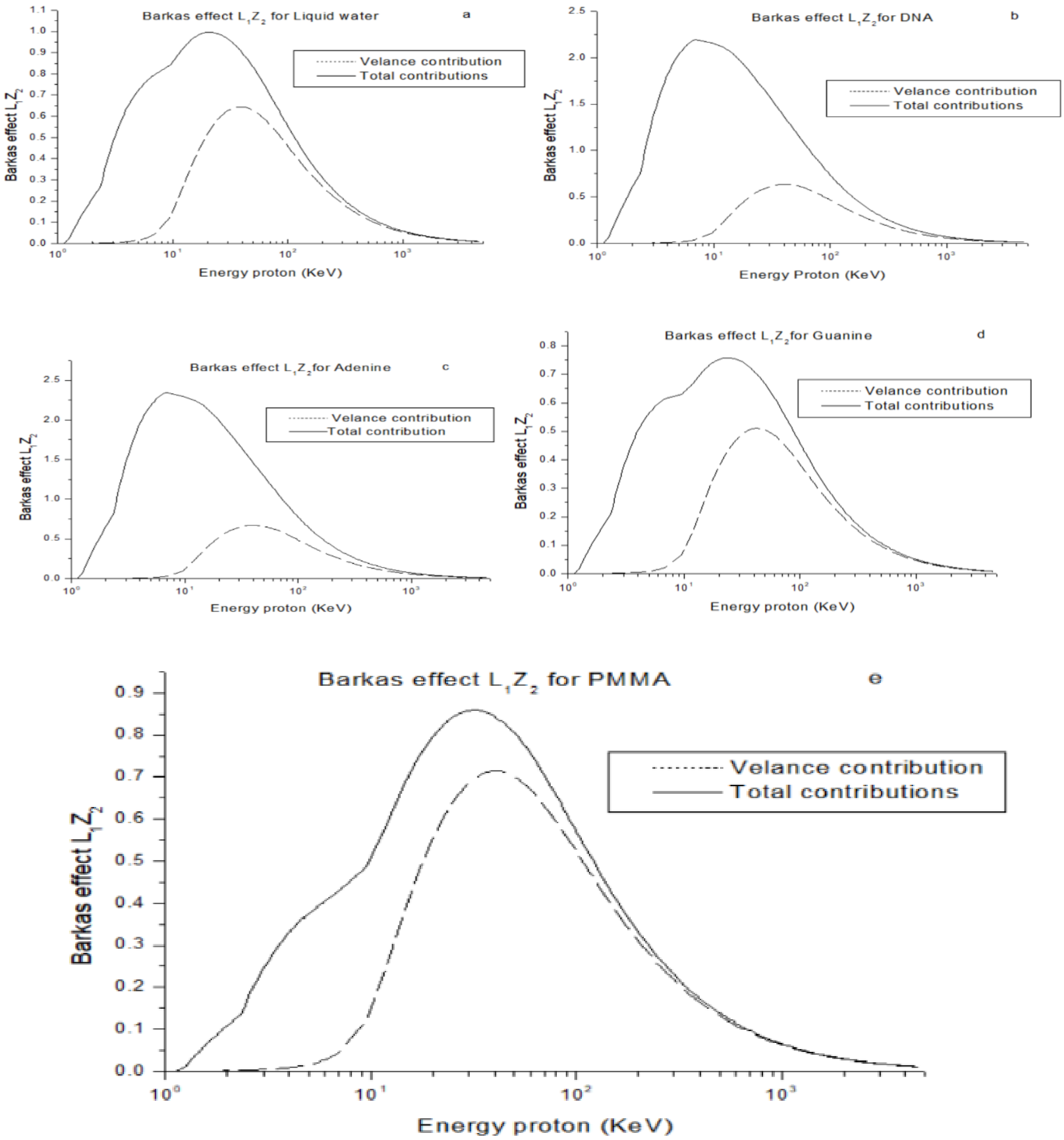

Fig.(2): Barkas effect evaluated from eq.(17) in term of dielectric function by single Drude function and general oscillator strength. (a) Liquid water,(b) DNA, (c) Adenine, (d) Guanine and PMMA.(Dashed line) for valance contribution, (full line) represents total contribution including inner contributions.

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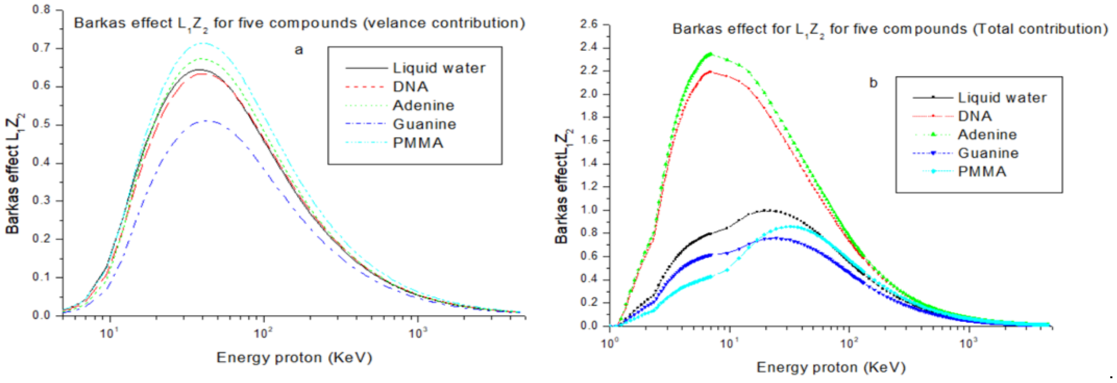

Fig.(3) :Barkas effect for five compounds in splitting form (a):curves act the valance contribution for five compound as explain inside figure ,which appear smooth, (b): curves represent totally contribution and showing the influence of inner shells. In both a and b the dependent on atomic number of targets is clear.

Table (2): Maximum values of shell correction for outer electrons for five organic and inorganic compounds, the comparison to Liquid water of (Emfietzoglou, et al. 2009)

compounds	Outer shell correction		Totally shell correction
	Present work	Previous work	
Liquid water	0.3246	0.38 (Ritchie) 0.41 (Penn) 0.28(Emfietzoglou)	1.433
DNA	0.3269	-----	0.6505
Adenine	0.4153	-----	0.5236
Guanine	0.2736	-----	0.4002
PMMA	0.3594	-----	0.751

Table (3): Maximum values of Barkas effect for outer electrons and totally contribution for five organic and inorganic compounds

compounds	Barkas effect (outer)	Barkas effect (totally)
Liquid water	0.6445	0.995
DNA	0.5296	2.1929
Adenine	0. 6396	2.3469
Guanine	0.5103	0.7571
PMMA	0.3641	0.8589

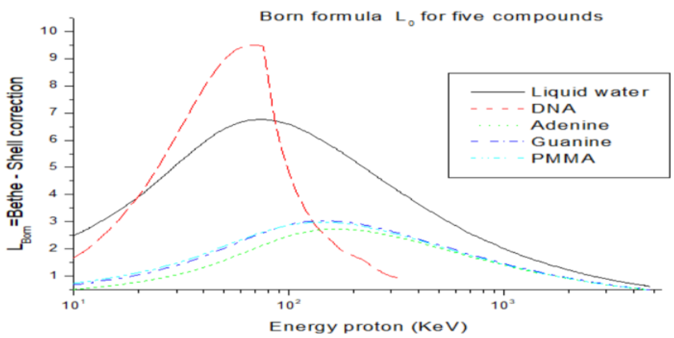

Fig.(4): Born formula eq.(14) for five compounds as appear in marking in team of dielectric function and its including the excitation spectrum, there are different according to atomic number of targets.

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Conclusion

Fortran 90 has been used to programming the work. In term of dielectric response which acts the imaginary part of single Drude dielectric function and GOS method, the corrections of Bethe equation has been calculated in present work in more accuracy because of the study interest the contribution of inner shells (nuclear electrons) addition to outer electrons ,that involved in the total part of work . Values of Shell correction for Liquide water record the heights value in totally contribution which are 1.433 while Guanine has lower value which was0.4002. Largest value of Barkas effect was from Adenine which 2.3469, lowest one of Guanine was 0.7571. Born term also discussed and DNA recordheights peak .shell correction and Barkas effect in totally contribution has been effected by the included the inner shell they evaluated by GOS. In this work Bethe correction (Barkas effect, shell, Born and Bloch correction) has been evaluated for first time for compounds under work except for Liquid water and not clearly way for DNA.

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