International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064
Index Copernicus Value (2013): 6.14 | Impact Factor (2013): 4.438

Calculation of Protons Stopping Power in Some Organic Compounds for Energies (0.02-1000)MeV

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Abstract: ***The stopping power in heavy charged particles is an important parameter in determining the energy loss. In this paper we calculated the stopping power of proton in Some Organic Compounds like Chloroform ($CHCl_3$) , Polyving Holuene (C_9H_{10}) , Propanediol ($C_3H_8O_2$) , Alanine ($C_3H_7N_1O_2$) , Protein ($C_{107}H_{197}N_{29}O_{49}S_2$). The Stopping Power calculated by using SRIM2013 program fitting equations , Semi Empirical Relation written by Mathlab language ,and we calculated the rate error and correlation coefficient between Stopping Power(SRIM2013) and Stopping Power(Semi Empirical) . These relations are also used to find the stopping power for compound targets by using the Bragg's additivity rule. We compared the results with SRIM2013 program . The obtained results are in satisfactory agreement with results SRIM2013 program.***

Keywords: Protons Stopping Power

1. Introduction

The subject of penetration of energetic heavy ions through matter has captivated generations of physicists over the past many decades because of its applications to basic and applied sciences as well as to manufacturing. As a result, there has been a continuous effort among the scientific public to improve the understanding of various complex physical processes that are involved in such beam-matter interactions. These include the debauchery of energy of the projectile ions due to interaction with bound and free electrons of the target matter, elastic and inelastic nuclear collisions and evolution of the charge-state distribution of the projectile ions[1]. When charged particle pass through a medium it will lose energy while passing through matter due to ionization and excitation of the atoms in the material[2].

2. Stopping Power

The stopping power of a material for a fast ion is the energy deposited per unit pathlength of the ion through the target, $-dE/dx$[3]. The stopping power depends on the type and energy of the particle and on the properties of the material it passes[4].

$$-\frac{dE}{dX} = NS(v) \tag{1}$$

Where
E is the means energy and X is the path length
N : atomic density ($N=N_A\rho/A$)
N_A : Avogadro´s number = $6.022\times10^{23} mole^{-1}$
ρ : Density of material
A : mass number of target .

At low energies, the slowing down of ions (stopping power) is usually separated into two distinct processes: electronic and nuclear slowing down or stopping power[4].

3. Stopping Power in Compounds

The mass collision stopping power, the mass radiation stopping power , and their sum the mass stopping power can all be well approached for intimate mixtures of elements, or for chemical compounds, through the assumption of Bragg's Rule . it states that atoms contribute nearly independently to the stopping power, and hence their effects are additive . In terms of the weight fractions fz_{22}, fz_{21} of elements of atomic numbers Z_{21},Z_{22},…etc. present in a compounds or mixture, the mass stopping power $(dE/\rho\, dx)_{mix}$ can be written as[5]

$$\left(\frac{dE}{\rho dx}\right)_{mix} = \left[f_{Z2_1}\left(\frac{dE}{\rho dx}\right)_{Z_{21}} + f_{Z_{22}}\left(\frac{dE}{\rho dx}\right)_{Z_{22}} + \cdots\right] \tag{2}$$

Where all stopping powers refer to a common kinetic energy and type of charged particle.

Let n_j be the number of the jth kind of atom in a compound (it need not be an integer for a mixture), and f_j its weight fraction[6]:

$$f_{2j} = \frac{n_j A_{2j}}{\sum_k n_k A_{2k}} \tag{3}$$

1) **Mean Excitation Energies**

Mean excitation energies, I, have been calculated using the quantum mechanical approach or measured in experiments. The following approximate empirical formulas can be used to estimate the I value in eV for an element with atomic number Z_2 [1,7]:

$$I \approx \begin{cases} 19.0\ \mathrm{eV};\ Z_2 = 1\ (\mathrm{Hydrogen}) \\ 11.2\ \mathrm{eV} + (11.7)(Z_2)\ \mathrm{eV};\ (2 \le Z_2 \le 13) \\ 52.8\ \mathrm{eV} + (8.71)(Z_2)\mathrm{eV};\ (Z_2 > 13) \end{cases} \tag{4}$$

For compounds or mixtures, the contributions from the individual components must be added[7].

In this way a composite lnI value can be obtained that is weighted by the electron densities of the various elements[7]. The following example is for water (and is probably sufficient for tissue) [7].

$$n \ln I = \sum_i N_i Z_{2i} \ln I_i \tag{5}$$

Where n is the total number of electrons in the material ($n = \Sigma_i N_i Z_i$) [7].

4. Results and Discussion

We have done the calculation stopping power of proton for five organic compounds with energies (0.02-1000)MeV and by using a program written with Mathlab .

a-Fitting equation

By using the SRIM2013 program, which have been written in the Mathlab2011 program and by using accident implement (curve fitting tool), we attained to find an equations (6,7,8) with its constants (q_1,q_2,q_3,q_4,q_5), (p_1,p_2,p_3,p_4,p_5) and (a,b,c) respectively it is shown in the table (2) in any medium of five organic compounds it is shown in the table (1) . Which represent the stopping power equations of proton .

$$S(E) = q_1E^4 + q_2E^3 + q_3E^2 + q_4E^1 + q_5 \quad (6)$$

Equation (6) using in energy range (0.02-0.09)MeV

$$S(E) = p_1E^4 + p_2E^3 + p_3E^2 + p_4E^1 + p_5 \quad (7)$$

Equation (7) using in energy range (0.1-2)MeV

$$S(E) = aE^b + c \quad (8)$$

Equation (8) using in energy range (2.02-1000)MeV

Where S(E) is the stopping power , E is the kinetic energy of proton .

Table 1: Shown the organic compounds[6,8].

Compounds	Formulas Chemical	(I) Ionization potential (eV)	(ρ) Density (g/cm^3)
Alanine	*C3H7N1O2*	*71.52*	*1.401*
Protein	*C107H197N29O49S2*	*72.45*	*1.3*
Chloroform	*CHCl3*	*174*	*1.48*
Polyvinyl Toluene	*C9H10*	*63.43*	*1.03*
Propanediol	*C3H8O2*	*48.91*	*1.0597*

Table 2: Shown constants used in fitting equations(6,7,8).

Compounds	*(0.02-0.09)MeV*	*(0.1-2)MeV*	*(2.02-1000)MeV*
C3H7N1O2	*q1 = 1.417×105* *q2 = -4.822×104* *q3 = 7025* *q4 =-595.7* *q5 =29.68*	*p1 =-0.3861* *p2 = 2.228* *p3 = -4.984* *p4 =5.556* *p5 = -3.318*	*a = 0.265* *b = -0.8017* *c = 0.0009708*
C107H197N29O49S2	*q1 = -9304* *q2 = 2960* *q3 = -394* *q4 = 24.78* *q5 = 0.2854*	*p1 = 0.6429* *p2 = -2.794* *p3 = 4.274* *p4 = -2.998* *p5 = 1.12*	*a = 0.288* *b =-0.8173* *c =0.0006739*
C9H10	*q1 = 2.286×105* *q2 = -7.564×104* *q3 = 1.039×104* *q4 =-796.1* *q5 =35.04*	*p1 = -0.6327* *p2 = 3.352* *p3 =-6.83* *p4 = 6.964* *p5 = -3.852*	*a = 0.3001* *b = -0.8213* *c = 0.0006994*
CHCL3	*q1 = 514.6* *q2 = -142.1* *q3 = 12.7* *q4 = 0.1952* *q5 = 0.521*	*p1 =0.4857* *p2 =-2.074* *p3 = 3.072* *p4 = -2.044* *p5 =0.7315*	*a =0.2066* *b = -0.7822* *c = 0.0004388*
C3H8O2	*q1 = 1.046×104* *q2 = -1.618×104* *q3 =4171* *q4 =-484.1* *q5= 27.79*	*p1 = -0.488* *p2 = 2.684* *p3 = -5.716* *p4 = 6.101* *p5 = -3.508*	*a =0.3041* *b =-0.8213* *c=0.0007268*

b-Semi Empirical formula for proton stopping power

We get a semi empirical formula for five compounds by replacement the energy, ionization potential , Density of material and weight fraction in equation (3) of organic compounds .

$$S(E) = \frac{2.11AB}{A+B} \times \frac{\sum_j f_{2j}}{\left(\rho \log\left(\frac{I}{4}\right)\right)} \quad (9)$$

Where

$A = 6.019E^{0.6} + 5.6$

$$B = \left(\frac{0.2389}{E}\right) \log\left(1.59 + \left(\frac{0.596}{E} + 4.532E^{0.7}\right)\right)$$

Where S(E) stopping power of proton ,E energy of proton ,I Ionization potential in unit (eV) calculated from equation (5), fj weight fraction of compound calculated from equation (3) and ρ is Density of compound .

Through the semi empirical formula we get results agreement with SRIM2013program. Figures (1),(2),(3),(4) and (5) shows the relationship between the stopping power and energy of protons in organic compound and we concluded that the results are very good agreement with SRIM2013 program.

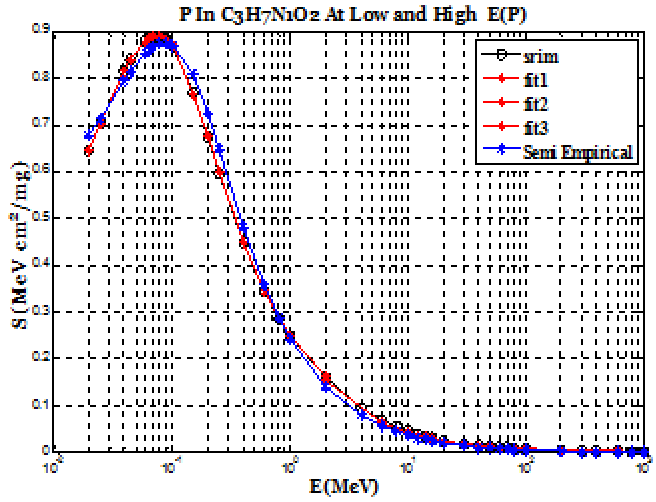

Figure 1: Shows the relationship between the stopping power and energy of protons in compound C3H7N1O2 the correlation coefficient (0.99869) and the error ration (0.018779)

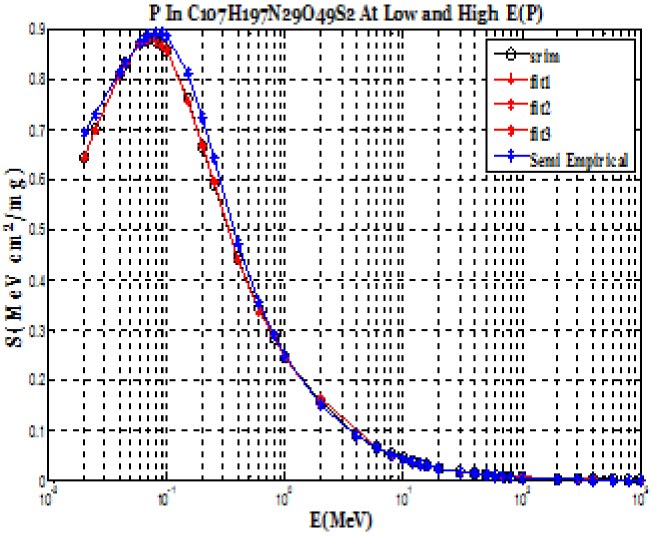

Figure 2: shows the relationship between the stopping power and energy of protons in compound C107H197N29O49S2 the

correlation coefficient (0.999245) and the error ration (0.014145)

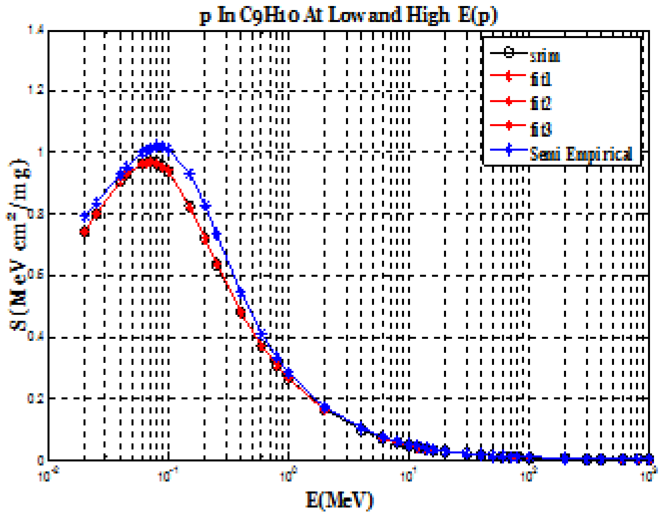

Figure 3: shows the relationship between the stopping power and energy of protons in compound C_9H_{10} the correlation coefficient (0.99885) and the error ration (0.019312) .

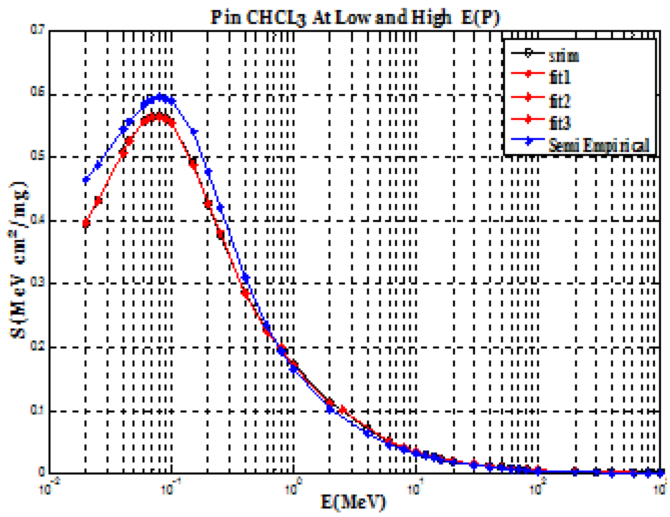

Figure 4: shows the relationship between the stopping power and energy of protons in compound $CHCL_3$ the correlation coefficient (0.993051) and the error ration (0.010983)

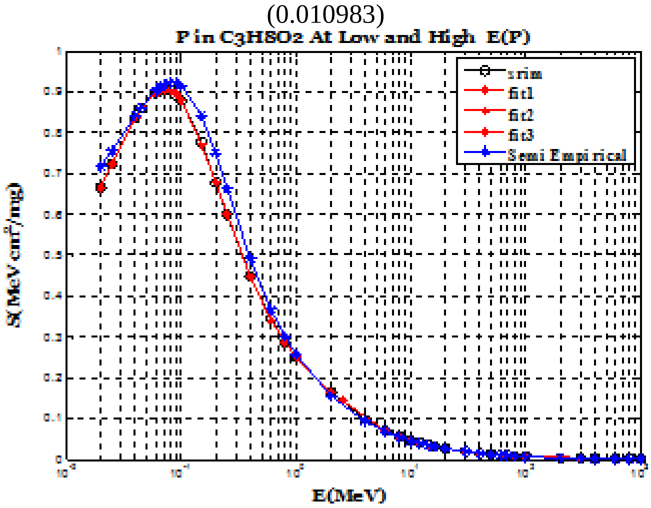

Figure 5: shows the relationship between the stopping power and energy of proton in compound $C_3H_8O_2$ the correlation coefficient (0.999005) and the error ration (0.016646)

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