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Calculation of Proton Range in some organic Compounds Energies (10-900) keV

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Abstract: ***Theoretical study have been done to calculated the Range for protons in ten organic compounds which is: [polypropylene(C_3H_6) ,Polycarbonate ($C_{16}H_{14}O_3$), Mylar ($C_{10}H_8O_4$), Polyvinylalcohol (C_2H_4O), Polyoxymethylene (CH_2O), Polyacrylonitrile (C_3H_3N), Polyvinylpyrro-lidone (C_6H_9NO), Polyvinylacetate ($C_4H_6O_2$), Kapton ($C_{22}H_{10}N_2O_5$) , Bakelite ($C_{44}H_{36}O_6$)], by using SRIM 2013 program written by Mathlab language. the range calculated to protons for energy (10-900) keV , by using fitting equations and the semi empirical equation (Devise two equation), and we calculated the rate error and correlation coefficient between Range(SRIM) and Range(semi-emp) as seen in tables by using Excel program. The results are agreed with the SRIM 2013 program, so our results showed to be good.***

Keyword: proton Range, organic compound.

1. Introduction

Niels Bohr published a seminar paper on the theory of charged particle penetration in matter, based solely on classical physics. Bohr's early work is instructive because for the first time a unified theory of stopping was attempted [1]. He evaluated the classical stopping of a fast heavy charged particle to an electron bound in a harmonic potential [2]. Consider a charge particle entering into a medium with kinetic energy. Then the average value of the distances that a particle travels before coming to rest, is called the "Range". The range of a proton in an absorbing medium will be somewhat smaller than the path length as measured from the original angle of incidence into the material, because the proton will undergo multiple coulomb scattering [3]. The charged particles when passing in the material medium losing part of its kinetic energy at any collision operation with the target matter as it is known. The continuous of this operation on the particle path in the medium causing decreasing kinetic energy for charged particles until reaching to zero, its losing all the kinetic energy and reaching to the rest state in the certain point. So the total range for charged particles passing in the material medium can be define as the length path that the particle passing before reaching to the rest , and depending on the matter target and the type of the incident particle in addition to its energy [4]. Range- energy relations for protons have been obtained by several authors, such as Livingston and Bethe, Sternheiner, Bichsel, etc. Sternheimer has carried out calculations [5], to determine range energy relations for some of the commonly used materials Aluminum, copper, Carbon, Beryllium and lead for proton energy from 2 MeV to 100GeV. Bichsel has also obtained range energy relation for the same substances from 1MeV to 100MeV [6].

In similar fashion, empirical range relations have been developed for other charged particles. The proton is range in air [7]:

$$R_{air} = \left(\frac{E_p}{9.3}\right)^{1.8} \quad (1)$$

Where Ep is the proton energy < 200 MeV.

Bichsel has measured the range of protons in aluminum, and his results can be presented by [8]:

$$R_{Al} = \begin{cases} 14.21E^{1.5874} & 1\text{MeV} < E_P \leq 2.7\text{MeV} \\ \frac{10.5E_p^2}{0.68+0.434\ln(E_P)} & 2.7\text{MeV} < E_P \leq 20\text{MeV} \end{cases} \quad (2)$$

The range in the compound is given by [9]:

$$R_{com} = \frac{M_{com}}{\sum_i n_i \left(\frac{A_i}{R_i}\right)} \quad (3)$$

2. Results and Discussion

We have done the calculation range of protons for ten organic compounds with energies (10-900) keV and by using a program written with Mathlab.

*Fitting equations**:** By using the SRIM_2013 program, which have been written in the Mathlab_2011 program and by using coincidence tool (curve fitting tool), we achieved to find an equation (4) with its Constants (p1, p2, p3) it is shown in the table (1) and (2) in any medium of ten organic compounds. Which represent the range equations of protons.

$$R(E) = E^2 + p_2E + p_3) \quad (4)$$

Where R is the Range; E is the kinetic energy of proton. Unit range meter.

*Semi Empirical formula for protons range: In this research achieved the suggestion about semi empirical formula for ten organic compounds. We have calculated Range by semi empirical equation (5) by using a program have been written by Mathlab language, also we calculated the rate error and correlation coefficient between Range(SRIM) and Range(semi emp) by using Excel program. As follows:

The Energy (10 keV - 900 keV) we got an semi empirical formula for ten organic compounds by substitution energy, ionization potential and atomic number for target which is:

$$R=\frac{E^{1.375} * \log Z_2^X}{5.075*10^8(\log I)} \quad (5)$$

Where:

R is the range (m); E is the energy of proton; Z is atomic number of target; I is ionization potential of target; X is the variable

$$X = \begin{cases} 1.00 \text{ at } 16 \leq Z_2 < 55 \\ 0.73 \text{ at } 56 \leq Z_2 < 150 \\ 0.60 \text{ at } 151 \leq Z_2 < 400 \end{cases}$$

Through the figures (1), (2), (3), (4), (5), (6), (7), (8), (9) and (10) note the semi empirical formula results agree with SRIM-2013 results. We concluded that our results are very good.

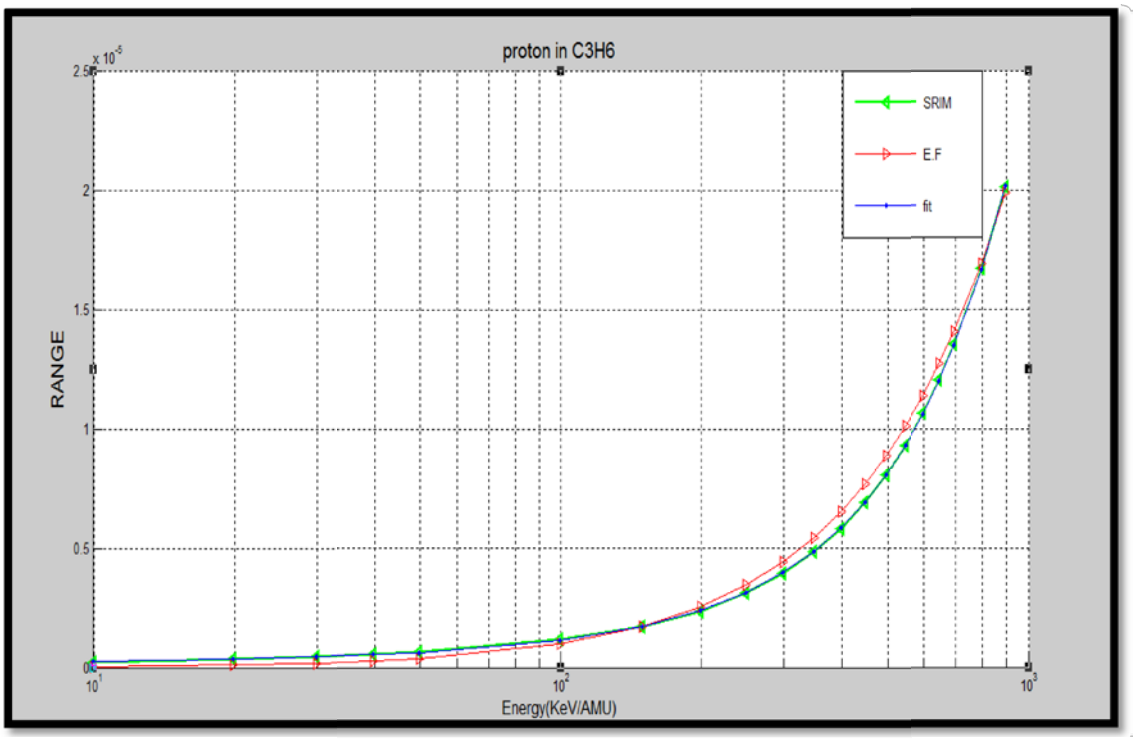

Figure 1: Shows the relationship between the range and energy of compound C3H6 was the correlation coefficient (0.997873) and the error rate ($3.97*10^{-7}$)

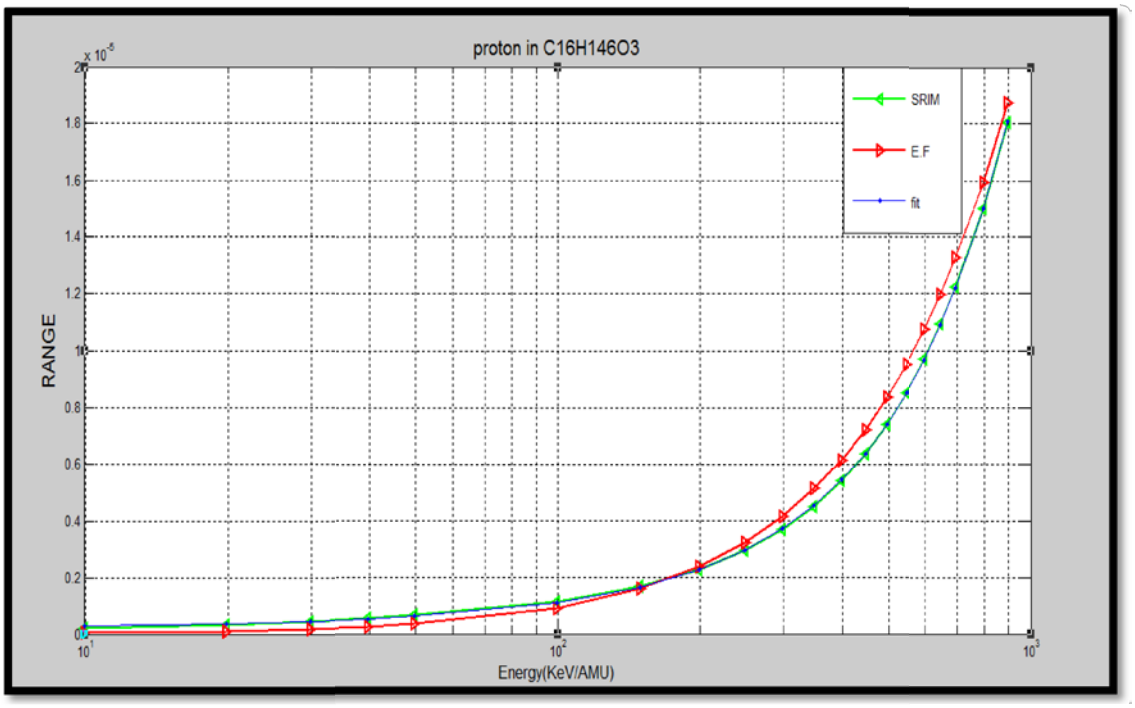

Figure 2: Shows the relationship between the range and energy of compound C16H14O3 was the correlation coefficient (0.998514) and the error rate ($3.23*10^{-7}$)

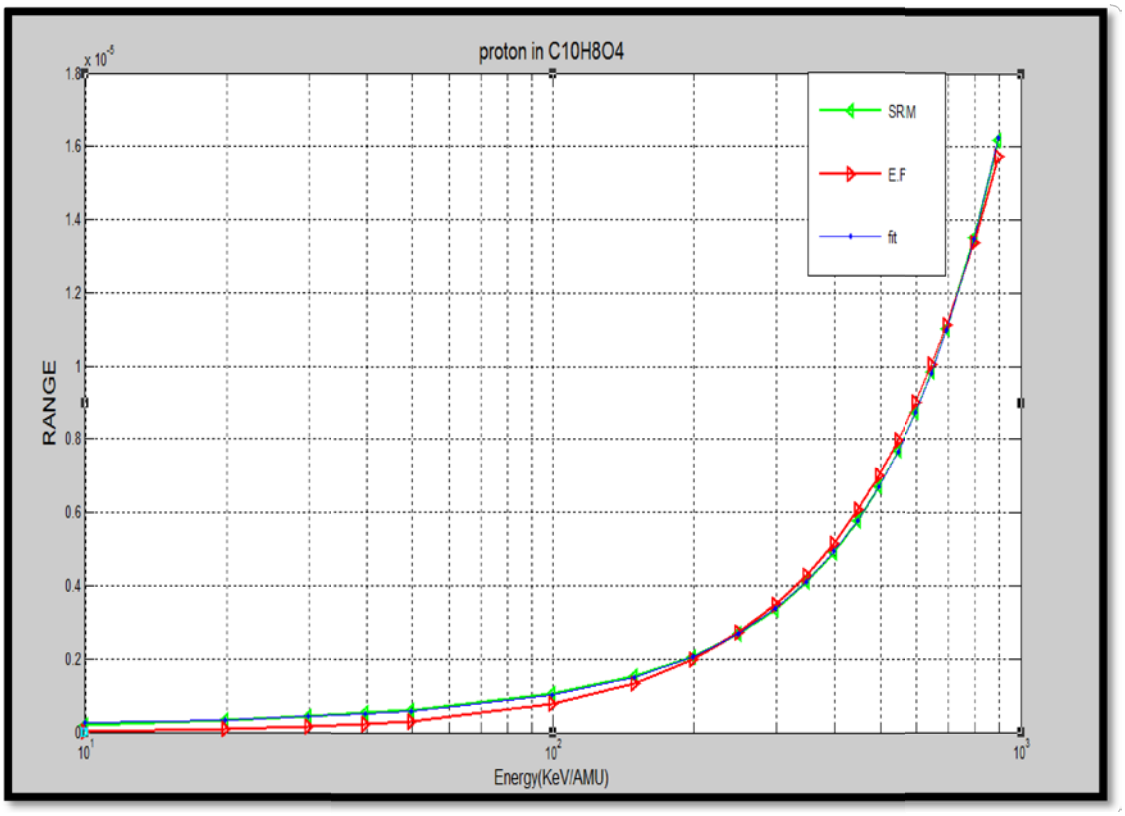

Figure 3: Shows the relationship between the range and energy of compound C10H8O4 was the correlation coefficient (0.99865) and the error rate ($2.45*10^{-7}$)

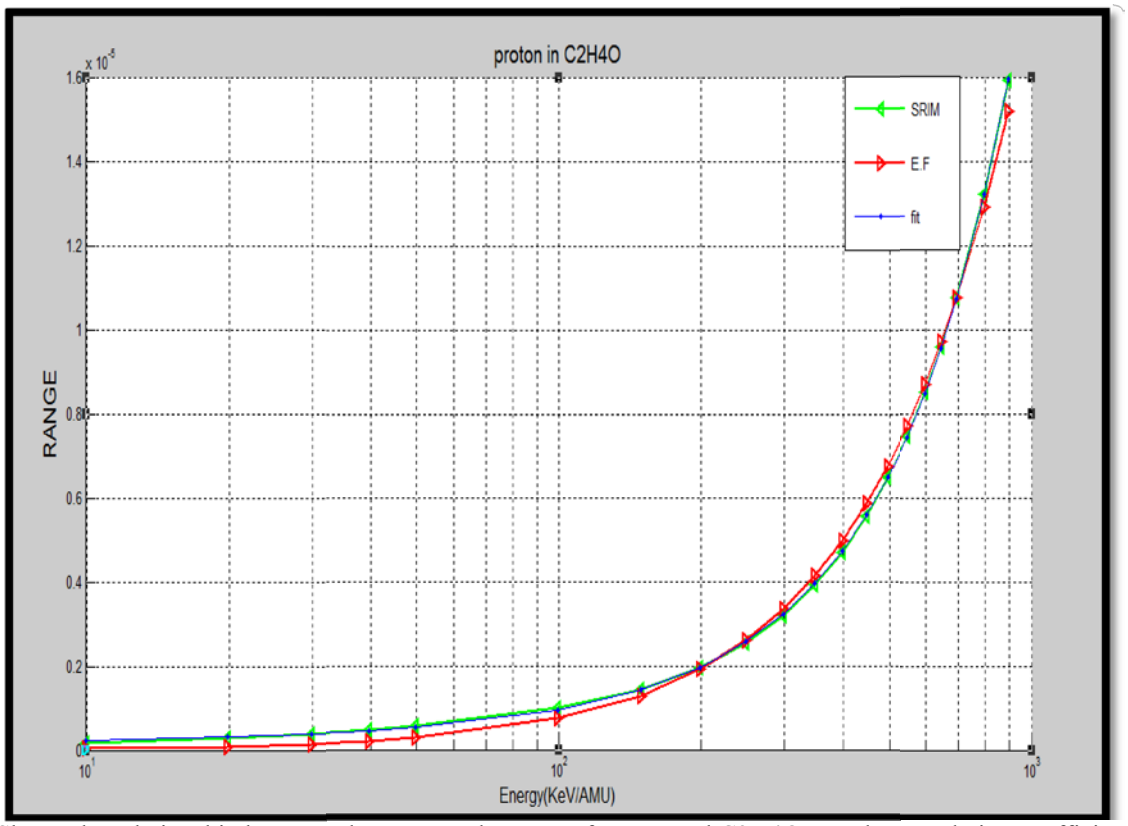

Figure 4: Shows the relationship between the range and energy of compound C2H4O was the correlation coefficient (0.9983) and the error rate ($3.23*10^{-7}$)

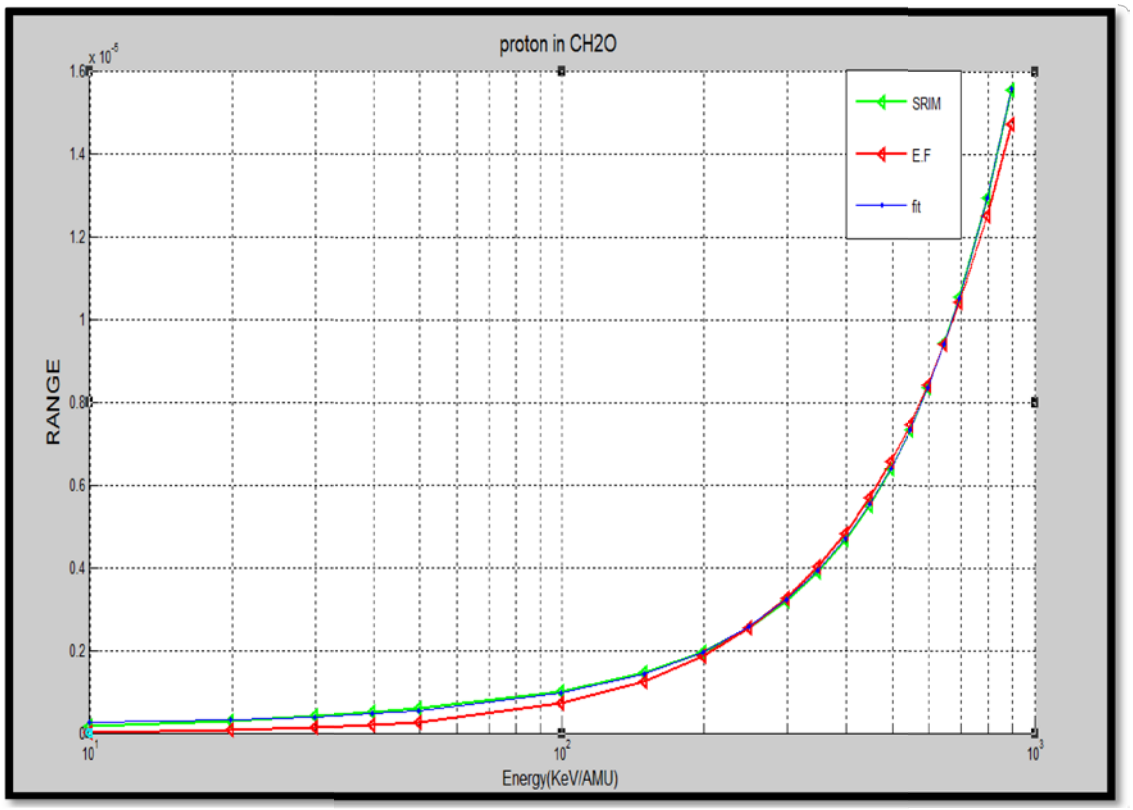

Figure 5: Shows the relationship between the range and energy of compound CH2O was the correlation coefficient (0.9985) and the error rate ($2.56*10^{-7}$)

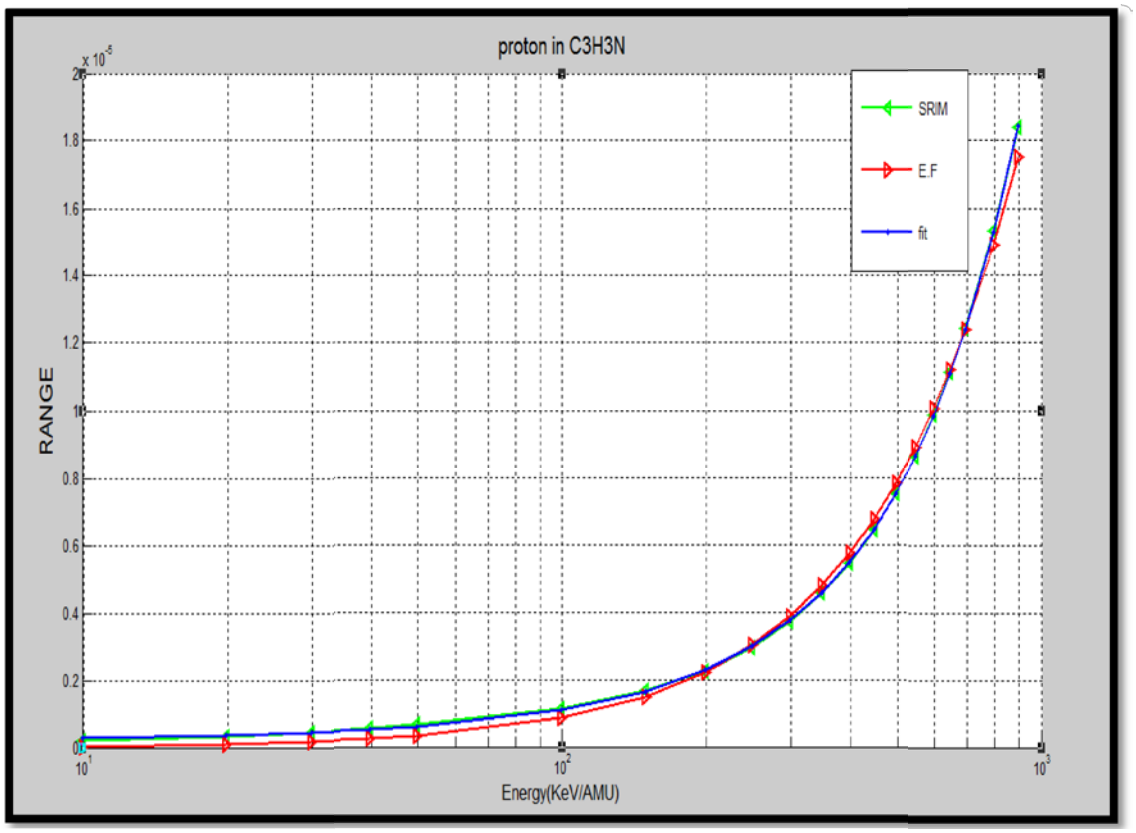

Figure 6: Shows the relationship between the range and energy of compound C3H3O was the correlation coefficient (0.99836) and the error rate ($3.18*10^{-7}$).

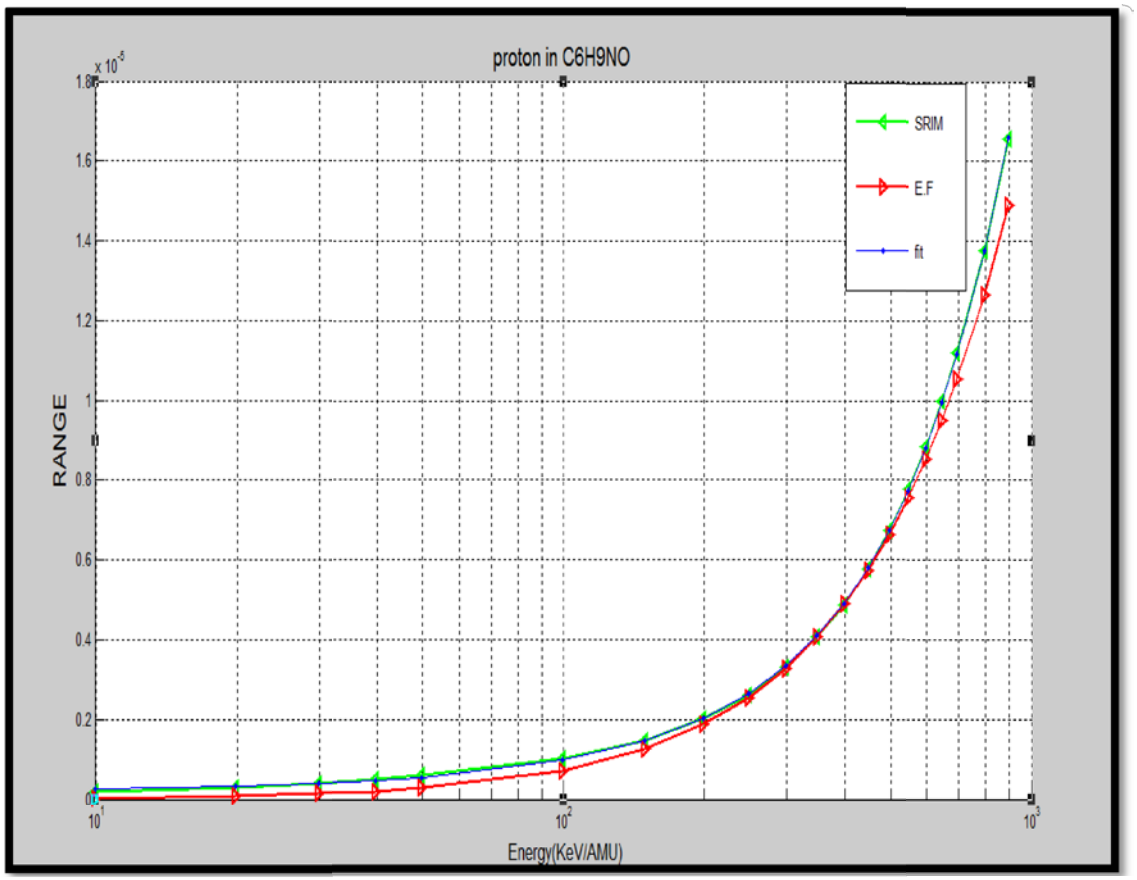

Figure 7: Shows the relationship between the range and energy of compound C6H9NO was the correlation coefficient (0.998265) and the error rate ($2.95*10^{-7}$)

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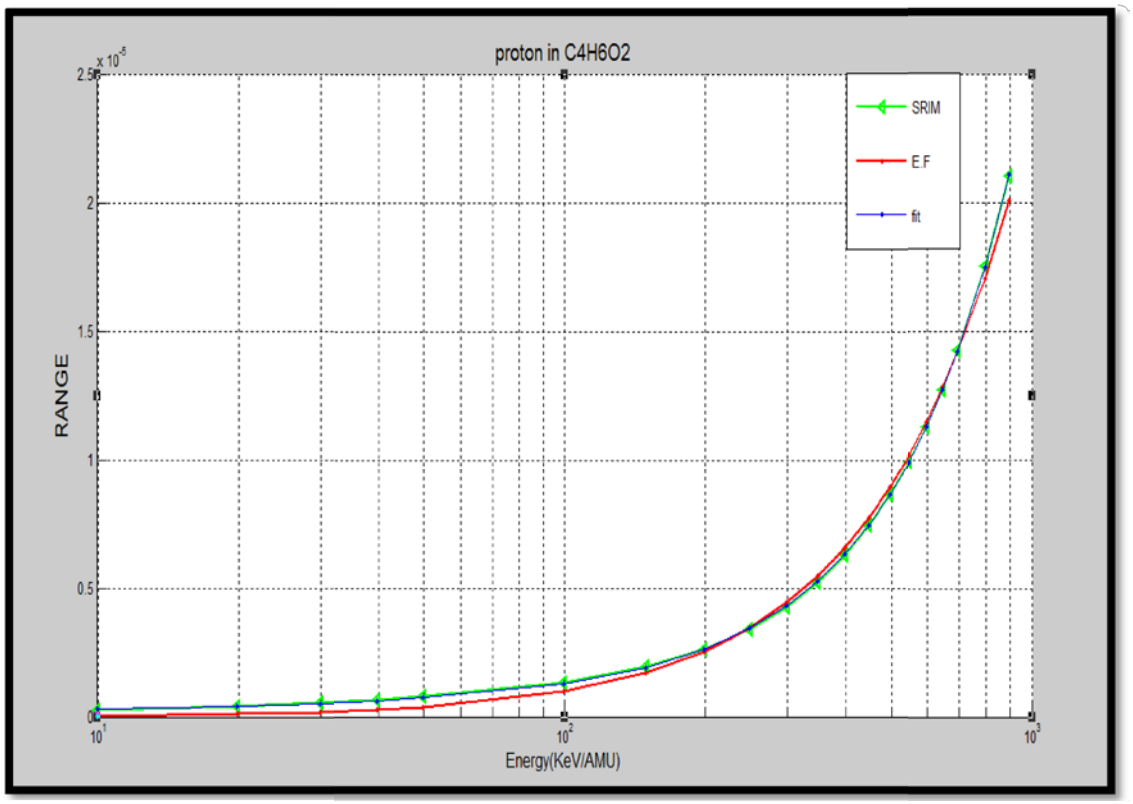

Figure 8: Shows the relationship between the range and energy of compound C4H6O2 was the correlation coefficient (0.9985) and the error rate ($2.56*10^{-7}$).

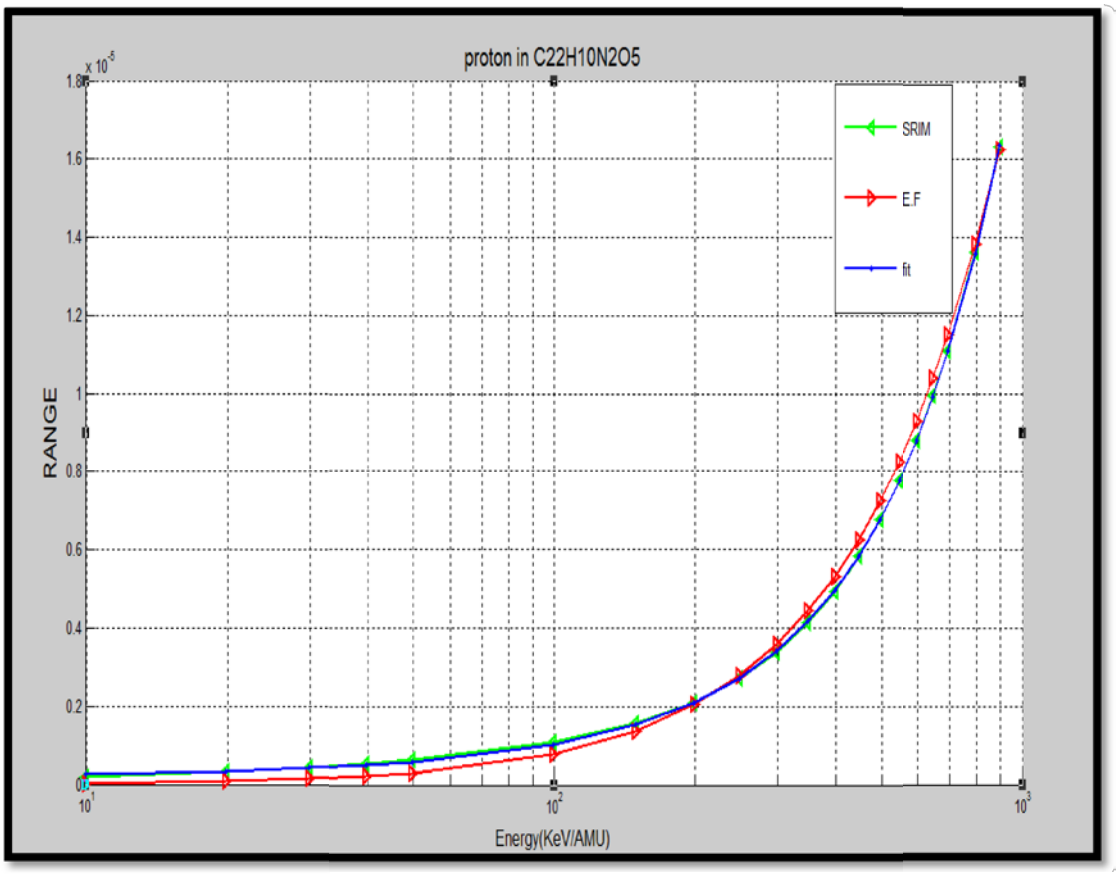

Figure 9: shows the relationship between the range and energy of compound C4H6O2 was the correlation coefficient (0.9985) and the error rate ($2.48*10^{-7}$).

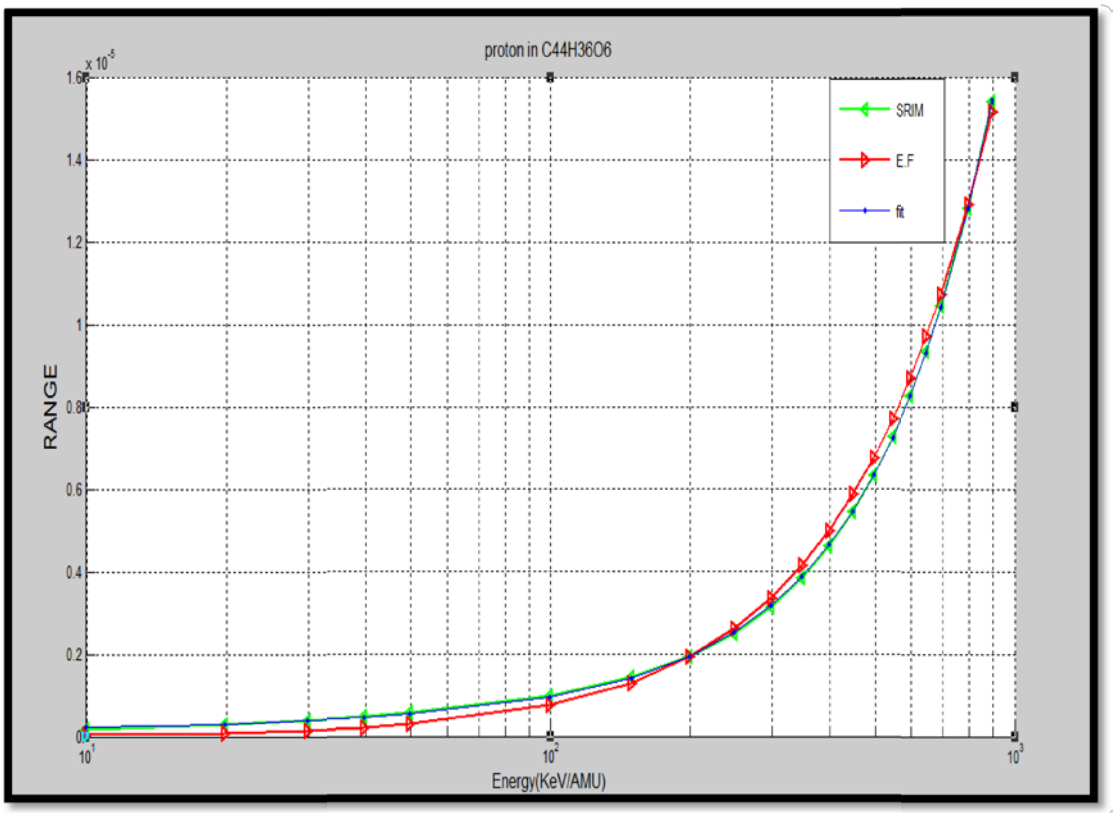

Figure 10: shows the relationship between the range and energy of compound C44H36O6 was the correlation coefficient (0.998507) and the error rate ($2.55*10^{-7}$).

Table 1

Energy	function	compound	Constants
(10 - 900) keV	polynomial Degree 2	Polypropylene (PP) C3H6	RMSE=3.878*10^{-8} p1=1.646 e-011 p2=7.667 e-009 p3=1.995 e-007
	$F(x) = x^2 + p_2x + p_3$ or $R(E) = E^2 + p_2E + p_3$	Polycarbonate C16H14O3	RMSE=3.409*10^{-8} p1 =1.386e-011 p2 =7.64e-009 p3 =2.052e-007
		Mylar C10H8O4	RMSE=3.36*10^{-8} p1 = 1.223e-011 p2 = 7.031e-009 p3 = 1.957e-007
		Polyvinyl alcohol C2H4O	RMSE=3.878*10^{-8} p1=1.249e-011 p2=6.485e-009 p3=1.799e-007
		Polyoxymethylene CH2O	RMSE=3.482*10^{-8} p1=1.192e-011 p2=6.581e-009 p3=1.905e-007

Table 2

Energy	function	compound	constants
(10 - 900) keV	polynomial Degree 2	Polyacrylonitrile C3H3N	RMSE=3.605*10^{-8} p1=1.437e-011 p2=7.591e-009 p3=2.022e-007
	$F(x) = x^2 + p_2x + p_3$ or $R(E) = E^2 + p_2E + p_3$	Polyvinylpyrrolidone C6H9NO	RMSE=3.386*10^{-8} p1 = 1.306e-011 p2 = 6.718e-009 p3 = 1.811e-007

			Polyvinyl acetate $C_4H_6O_2$	RMSE=$3.374*10^{-8}$ p1=1.626e-011 p2=8.809e-009 p3=2.449e-007
			Kapton $C_{22}H_{10}N_2O_5$	RMSE=$3.366*10^{-8}$ p1= 1.22e-011 p2= 7.188e-009 p3= 1.963e-007
			Bakelite $C_{44}H_{36}O_6$	RMSE=$3.056*10^{-8}$ p1= 1.184e-011 p2= 6.507e-009 p3= 1.727e-007

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