



GLOBAL JOURNAL OF SCIENCE FRONTIER RESEARCH: B  
CHEMISTRY

Volume 14 Issue 5 Version 1.0 Year 2014

Type : Double Blind Peer Reviewed International Research Journal

Publisher: Global Journals Inc. (USA)

Online ISSN: 2249-4626 & Print ISSN: 0975-5896

## Calculation of Proton Range in Some Organic Compounds Energies (1000-100000) keV

By Abothur G. Mohammed, Rashid. A . Kadhum & Dhia. A . Aljouher

*Kufa University, Iraq*

**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 ( $CH_2O$ ), by using SRIM2013 program written by Matlab language. the range calculated to protons for energy (1000-100000) 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.

**Keywords:** proton Range, organic compound.

**GJSFR-B Classification :** FOR Code: 030599



*Strictly as per the compliance and regulations of :*



# Calculation of Proton Range in Some Organic Compounds Energies (1000-100000) keV

Abothur. G. Mohammed <sup>α</sup>, Rashid. A. Kadhum <sup>σ</sup> & Dhia. A. Aljouher <sup>ρ</sup>

**Abstract-** Theoretical study have been done to calculated the Range for protons in ten organic compounds which is: [ polypropylene(C<sub>3</sub>H<sub>6</sub>) ,Polycarbonate (C<sub>16</sub>H<sub>14</sub>O<sub>3</sub>), Mylar (C<sub>10</sub>H<sub>8</sub>O<sub>4</sub>), Polyvinylalcohol (C<sub>2</sub>H<sub>4</sub>O), Polyoxymethylene (CH<sub>2</sub>O), by using SRIM2013 program written by Matlab language. the range calculated to protons for energy (1000-100000) keV , by using fitting equations and the semi empirical equation (Devise two equation), and we calculated the rate error and correlation coefficient betweenRange(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.

**Keywords:** proton Range, organic compound.

## I. 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]:

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

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

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

## II. RESULTS AND DISCUSSION

We have done the calculation range of protons for ten organic compounds with energies (1000-100000) keV and by using a program written with Matlab.

### a) Fitting equation

By using the SRIM\_2013 program, which have been written in the Matlab\_2011 program and by using coincidence tool (curve fitting tool), we achieved to find an equation (4) with its Constants (a, b) it is shown in the table (1) and (2) in any medium of ten organic compounds. Which represent the range equations of protons.

$$R(E) = aE^b \quad (4)$$

Where R is the Range; E is the kinetic energy of proton. Its unit meter.

### b) Semi Empirical formula for protons range

We got a semi empirical formula for ten compounds by substitution the energy, Atomic number and ionization potential

$$R = \frac{E^{1.75} * \log Z^2}{2.1875 * 10^{9.5} (\log I)} \quad (5)$$

The unit of R is m

R is the range

E is the energy of proton

Author <sup>α σ ρ</sup>: Kufa University, Education College of girls, Dep. of Physics. Najaf, Iraq. e-mails: abothur7899@yahoo.com, abothur7899@gmail.com

Z is atomic number of target  
 I is ionization potential of target  
 X is the variable

Through the semi empirical formula we got results agreement with the program SRIM 2013. From these figures (1), (2), (3), (4)(5), (6), (7), (8), (9), and (10) we concluded that the results are very good.

$$x = \begin{cases} 1.05 & \text{at } (16 \leq Z \leq 46) \\ 0.84 & \text{at } (47 \leq Z \leq 65) \\ 0.78 & \text{at } (66 \leq Z \leq 195) \\ 0.66 & \text{at } (195 \leq Z \leq 350) \end{cases}$$

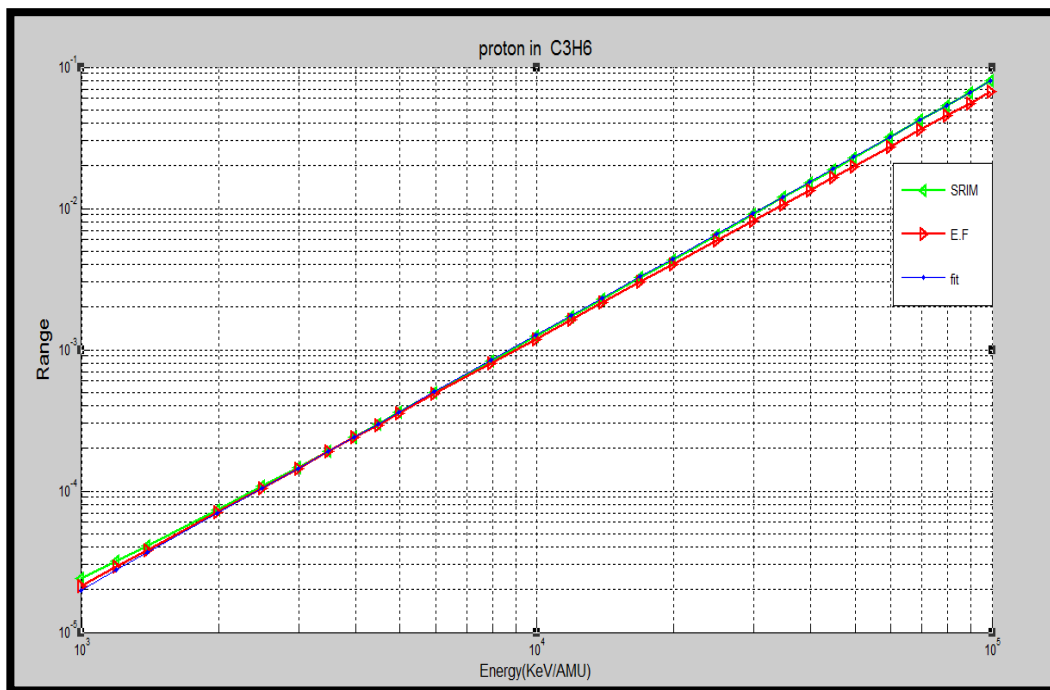


Figure 1 : shows the relationship between the range and energy of compound C3H6 was the correlation coefficient (0.99998) and the error ratio(0.000263)

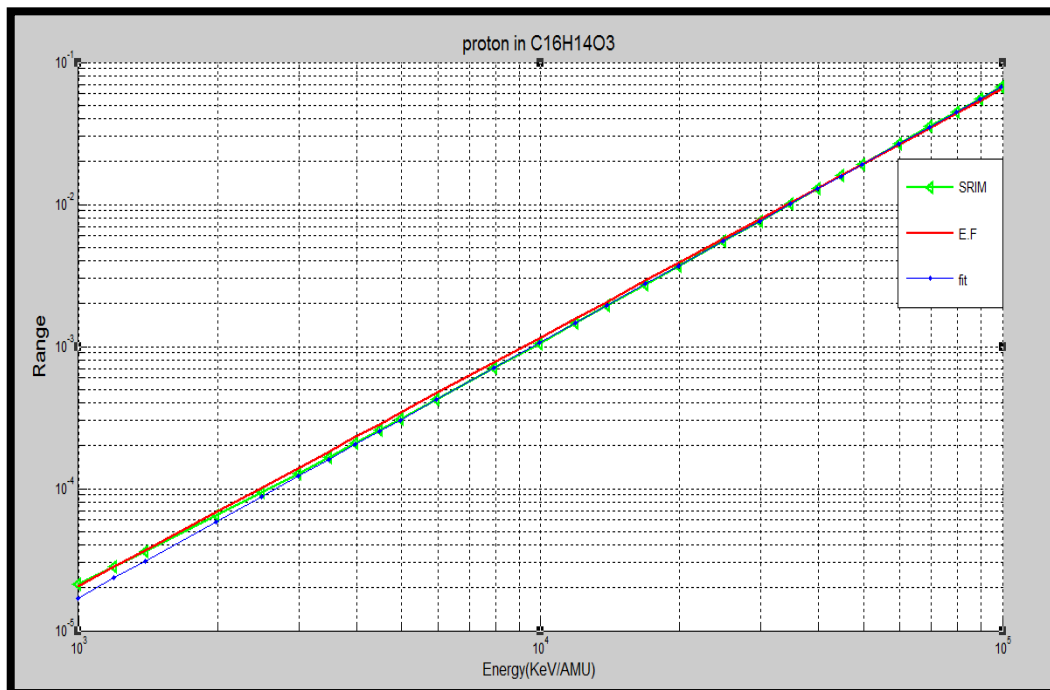


Figure 2 : shows the relationship between the range and energy of compound C16H14O3 was the correlation coefficient (0.999912) and the error ratio(0.000201)

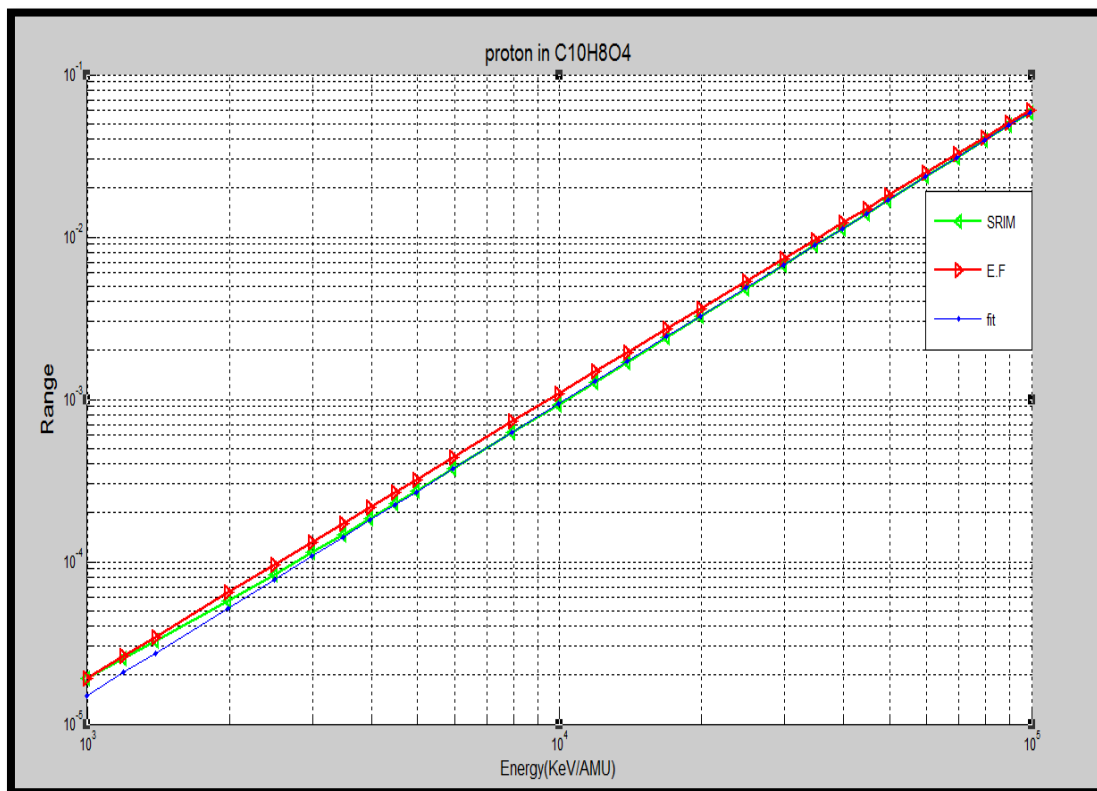


Figure 3 : shows the relationship between the range and energy of compound C10H8O4 was the correlation coefficient (0.999917) and the error ratio(0.000172)

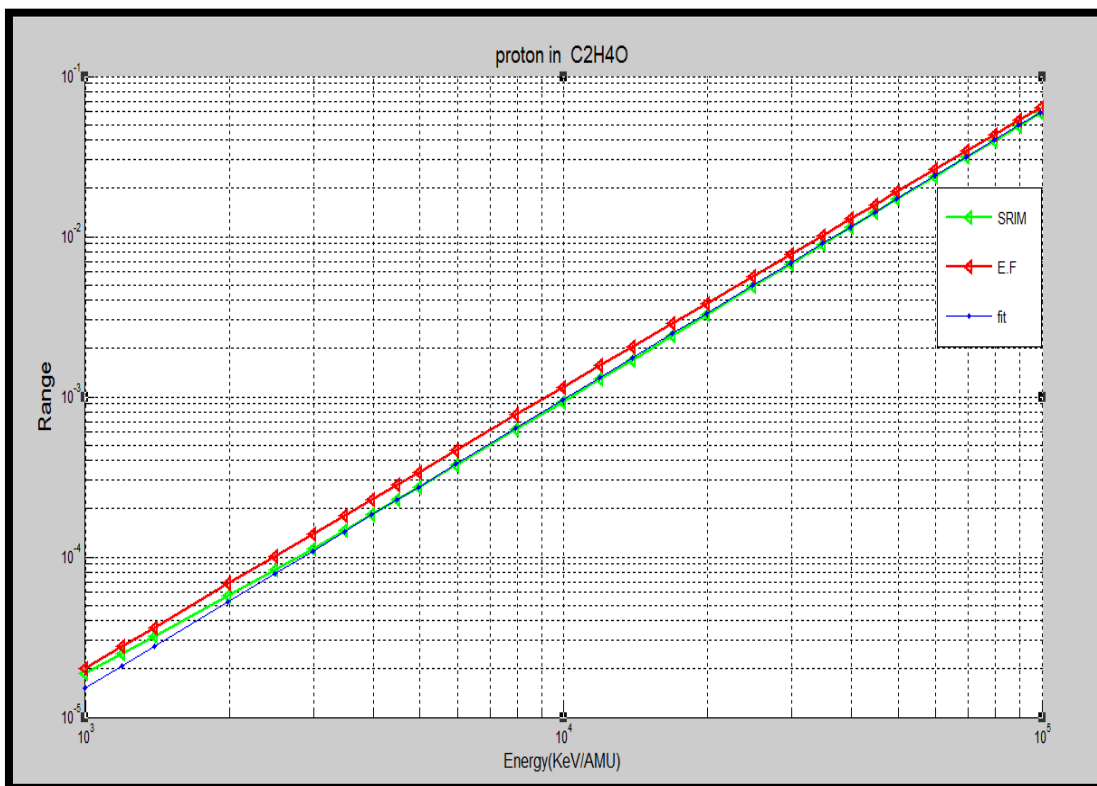


Figure 4 : shows the relationship between the range and energy of compound C2H4O was the correlation coefficient (0.999909) and the error ratio(0.000182)

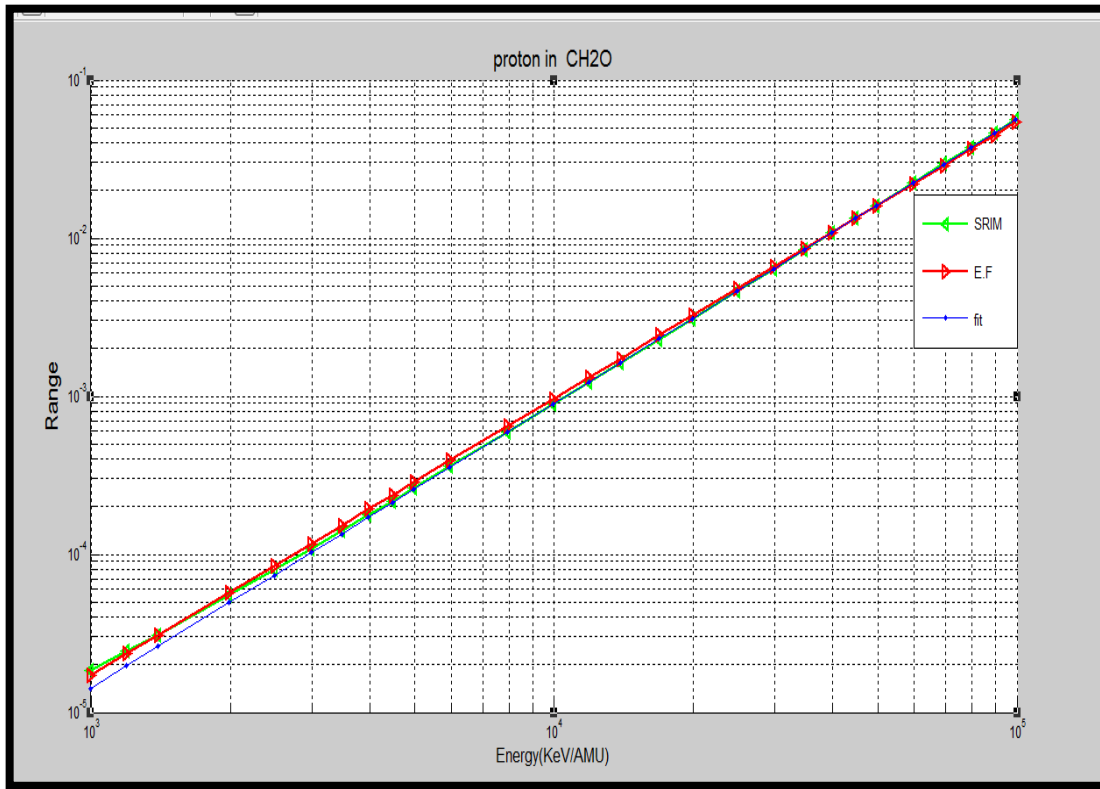


Figure 5 : shows the relationship between the range and energy of compound CH2O was the correlation coefficient (0.999915) and the error ratio(0.000166)

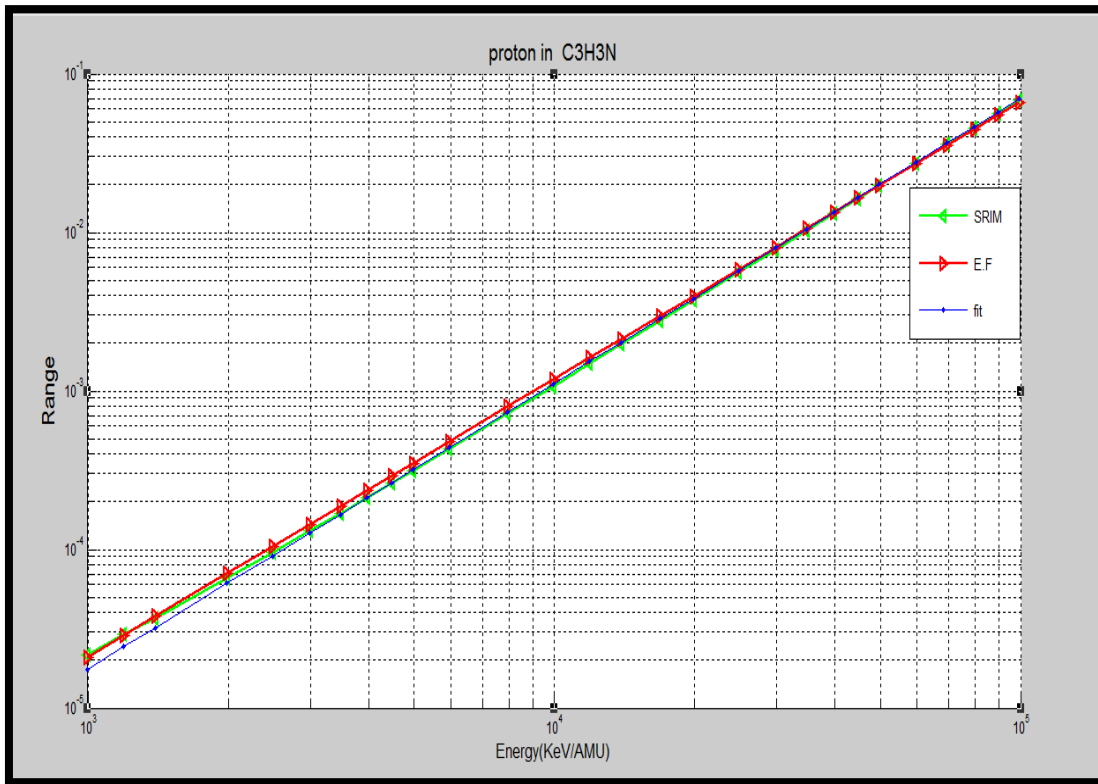


Figure 6 : shows the relationship between the range and energy of compound C3H3N was the correlation coefficient (0.999912) and the error ratio(0.000207)

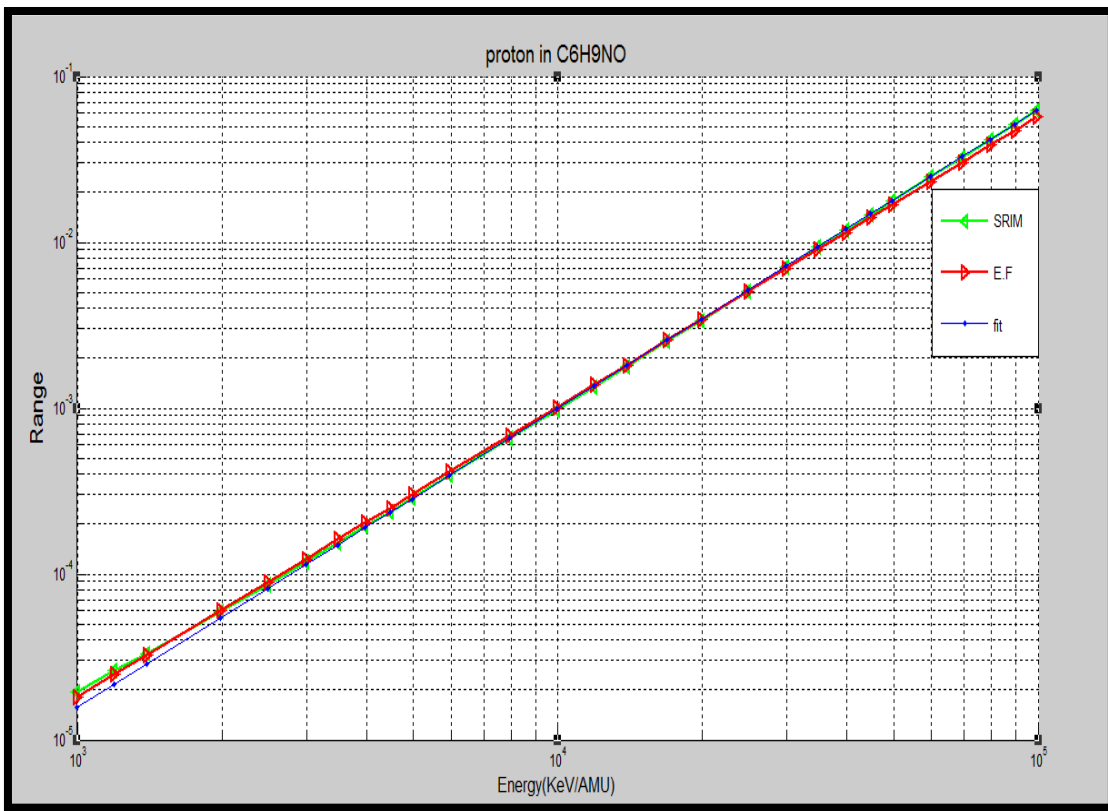


Figure 7 : shows the relationship between the range and energy of compound C6H9NO was the correlation coefficient (0.999909) and the error ratio(0.000191)

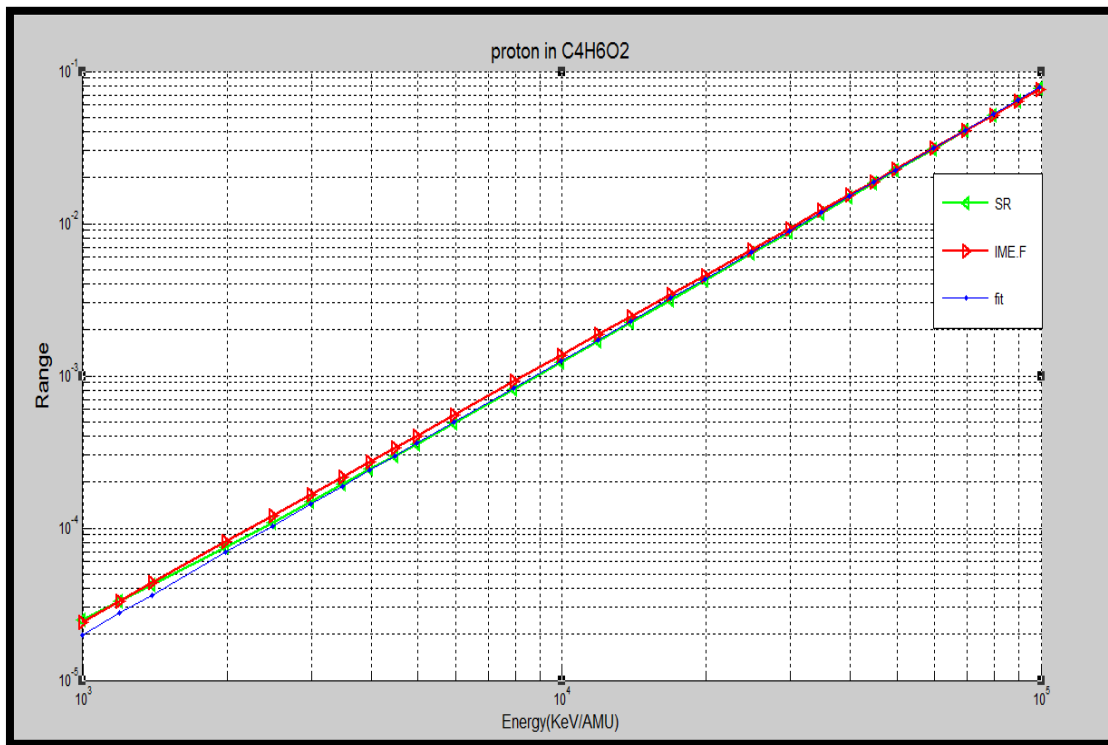


Figure 8 : shows the relationship between the range and energy of compound C4H6O2 was the correlation coefficient (0.999913) and the error ratio(0.000232)

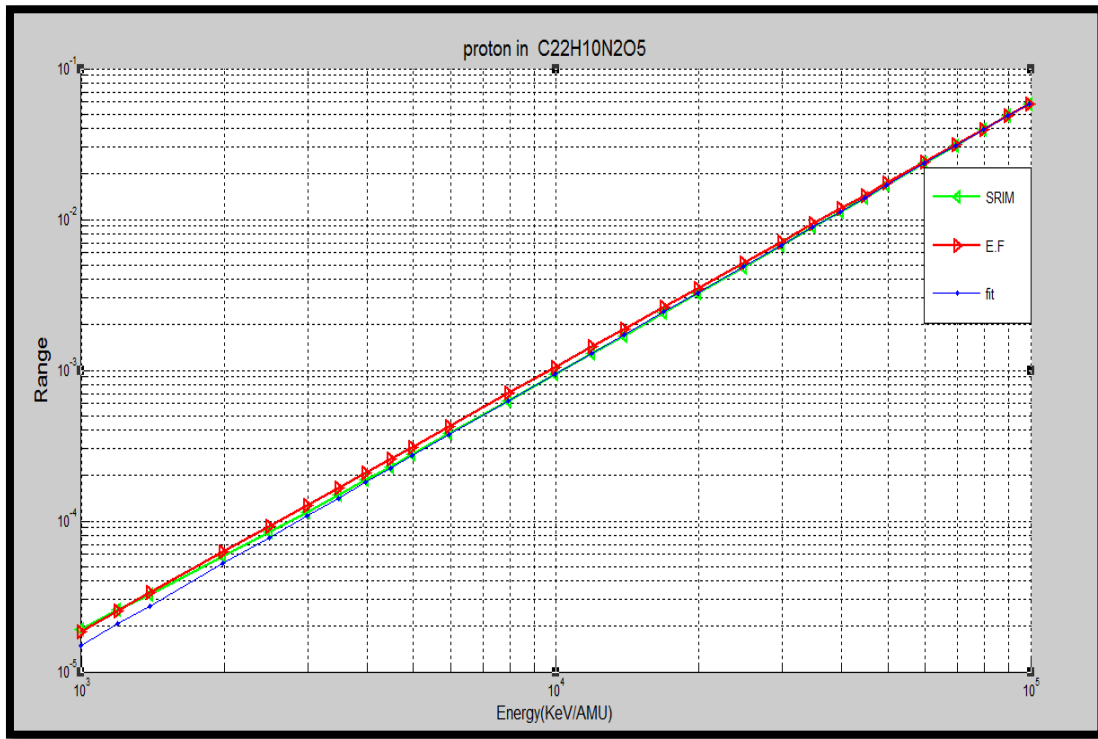


Figure 9 : shows the relationship between the range and energy of compound C22H10N2O5 was the correlation coefficient (0.999919) and the error ratio(0.00017)

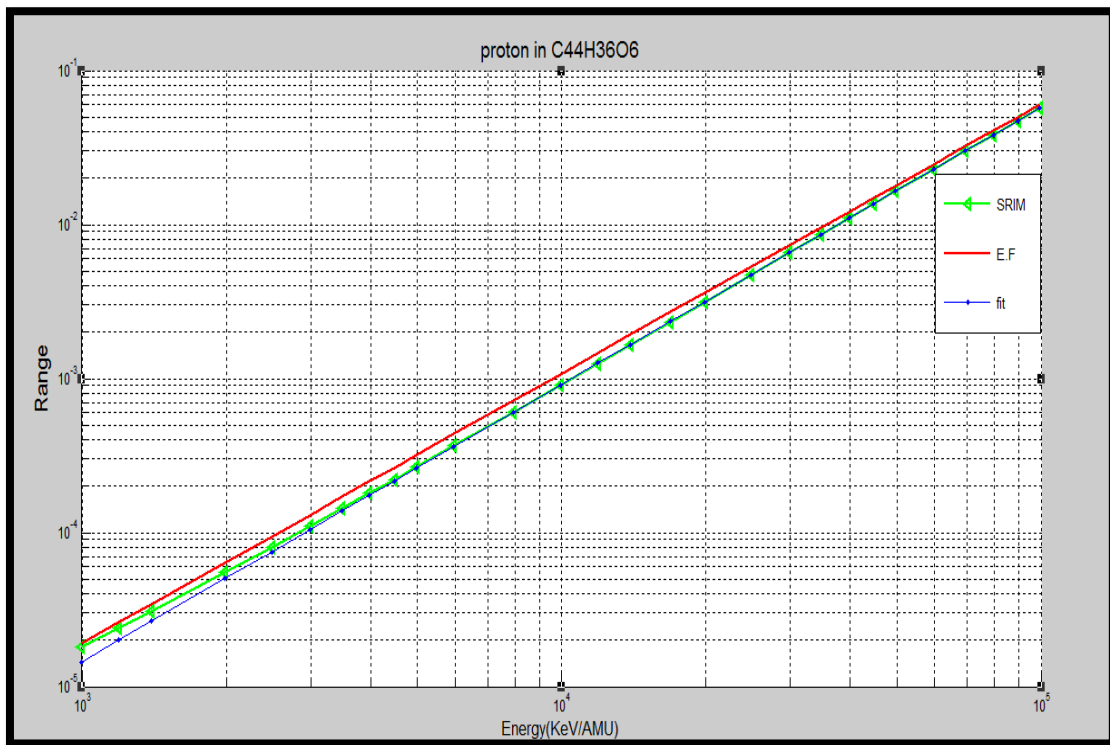


Figure 10 : shows the relationship between the range and energy of compound C44H36O6 was the correlation coefficient (0.999913) and the error ratio(0.000172)

Table (1)

Energy	function	compound	constants
(1000 - 100000) keV	Power Number 1	$F(x) = ax^b$ or $R(E) = aE^b$	Polypropylene <chem>C3H6</chem> RMSE=4.057*10 <sup>-5</sup> a= 7.763*10 <sup>-11</sup> b=1.803
			Polycarbonate <chem>C16H14O3</chem> RMSE=3.125*10 <sup>-5</sup> a=9.05*10 <sup>-11</sup> b=1.798
			Mylar <chem>C10H8O4</chem> RMSE=2.795*10 <sup>-5</sup> a=6.14*10 <sup>-11</sup> b=1.797
			Polyvinyl alcohol <chem>C2H4O</chem> RMSE=2.937*10 <sup>-5</sup> a=6.032*10 <sup>-11</sup> b=1.799
			Polyoxymethylene <chem>CH2O</chem> RMSE=2.714*10 <sup>-5</sup> a=5.854*10 <sup>-11</sup> b=1.797



Table (2)

Energy	function		ompound	constants
(1000 - 100000) keV	Power Number 1	$F(x) = ax^b$ or $R(E) = aE^b$	Polyacrylonitrile C <sub>3</sub> H <sub>3</sub> N	RMSE=3.196*10 <sup>-5</sup> a= 7.028*10 <sup>-11</sup> b=1.803
			Polyvinylpyrrolidone C <sub>6</sub> H <sub>9</sub> NO	RMSE=3.018*10 <sup>-5</sup> a=6.32*10 <sup>-11</sup> b=1.8
			Polyvinylacetate C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	RMSE=3.77*10 <sup>-5</sup> a=8.003*10 <sup>-11</sup> b=1.798
			Kapton C <sub>22</sub> H <sub>10</sub> N <sub>2</sub> O <sub>5</sub>	RMSE=2.788*10 <sup>-5</sup> a=6.216*10 <sup>-11</sup> b=1.769
			Bakelite C <sub>44</sub> H <sub>36</sub> O <sub>6</sub>	RMSE=2.64*10 <sup>-5</sup> a=5.921*10 <sup>-11</sup> b=1.798

## REFERENCES RÉFÉRENCES REFERENCIAS

1. H. D. Betz , "Behr's Adiabatic Criterion and Effective Charge of Heavy Ions", Nucl. Inst. and Math.132 (1976).
2. N Bohr, philos. Mag. Vol.25, pp.10(1913) cited by J. F. Ziegler, J. Appl. phys. Rev. Appl. phys., Vol.85, (1999).
3. Joseph F. Janni "Calculations of Energy Loss, Range, Pathlength, Straggling, Multiple Scattering, and the Probability of Inelastic Nuclear Collision for 0.1- to 1000-MeV Protons", Technical Report no. AFWL-TR-65-150, (1966).
4. A. K. Chaubey and H. V. Gupta," New empirical relations for stopping power and range of charged particles", revue de physique appliquée, Vol. 12, (1977).
5. David W. Anderson, Absorption of ionizing Radiation, Universitt park press, (1984).
6. E. Segre, Experimental Nuclear Physics, vol. 1, (1953).
7. N. Tsoufanidis, Measurement and Detection of Radiation, Hemisphere Publishing Corp, (1983).
8. Glenn F. Knoll, "Radiation Detection and Measurements", Third edition, John, Wiley and Sons, Inc.), University of Michigan, p (41), (2000).
9. Paul J. flory, "Principles of polymer Chemistry", cornell university, (1995).