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Stopping Power and Range Calculation of Electrons in NH_3, PH_3, AsH_3, SbH_3 Molecules

Ahlam K. Yassir and Alaa A. Khalaf

Department of Physics, College of Science, University of Basrah

Abstract: The research included a theoretical study in calculating the electronic stopping power of light particles (electrons) with an energy range of (0.01 -100) MeV for NH_3, PH_3, AsH_3 and SbH_3 molecules. The equations were programmed in mathematical ways and implemented in a mathematical program written in MATLAB2021 to obtain the required theoretical results, illustrated in graphs. The theoretical results obtained from this study were compared with the experimental results of the E-STAR program for electrons. The results showed a good agreement by calculating the correlation coefficient (r) of not less than 0.9. The range of electrons in molecules has also been calculated in the same energy range, In general, our calculations showed a good agreement with the other data, which we compared with it.

Keywords: Stopping power; Stopping range; Beth-Bloch equation; Molecules; E-STAR program; correlation coefficient..

INTRODUCTION

When charged particles enter molecules, they collide or interact with their atoms, resulting in electromagnetic forces between the charged particles and the material's atoms. Irritation and ionization of the target atoms occur in the inelastic process. Energy dissipation at a constant rate during an elastic response is the nuclear stopping power, whereas energy dissipation at a constant rate during an inelastic reaction is the electronic stopping power. [Almutairi, A.S. *et al*., 2022].For many years, scientists have debated the cessation of energetic ions in matter. It is critical for theoretical and experimental physicists. To put it another way, the stopping power (-dE/dX) is the rate at which a particle with a certain energy loses energy within the substance per unit of distance. As charged particles descend through a medium, they transfer some of their kinetic energy to the medium's atoms, causing them to become ionized and irritated[Krane, E. *et al*., 1988-Liu, W, 2001]. The discontinuous power of a medium may be seen clearly as the typical energy loss fraction learned from the elements of charge per unit pathway distance in the middle [Todreas, N. E. *et al*., 2021-El-Ghossain, M. O, 2017]. Energy and impact are the two primary components of stopping power. Often used to lessen the average mass dependency (ρ),[Saleh, A. J, 1987] impact-preventing power is the primary outcome of interaction between event units and nuclear electrons. (SRIM-2003)[Khaleel, M. A, 1987]. Suggests that the stopping power of matter may be quantified using a quantum mechanical approach of ion atom collisions, providing a possible basis for deriving absolute discontinuing power. When charged particles pass through material mediums, they continuously lose energy in a large number of collisions. The interactions that occur between falling particles and the atoms of these media are referred to as liquids and solids, and these interactions are classified as follows [Thompson, W, 1971; Khaleel, M. A, 1987 - Al Rubyi, A. A, 1999] Interactions of heavy charged particles with matter, namely: Heavy charged particles with atomic number (Z1< 2) greater than or $Z_1 \geq 2$, such as protons, alpha particles, and fission fragments And the interaction of light particles such as electrons. The stopping power (-dE/dX) is an important quantity in our research. The process of energy loss from charged particles captured and continues to capture widespread interest in equations of atomic physics and other fields of science[Al Rubyi, A. A, 1999]. The first to develop a general theory for calculating the stopping power charged particle collisions were Beth in 1930-1932 and Bohr in 1948[Holbert, K, 2012] The passage of electrons through physical media is similar to the passage of heavy charged particles through physical media, implying that the Coulomb reaction is dominant. There are three distinctions, however [Singh, H. *et al*., 2013]

1. Falling electrons are typically relativistic particles.
2. Typically, scattering occurs between particles that are similar but not compatible.
3. Interact with active nuclei, and the direction of electrons can change to the opposite direction, when it collides with a heavy nucleus

The interaction of electrons with matter is more complicated than the interaction of heavy charged particles with matter [Hadi, H. S. *et al*., 2017], for the reasons: Because the incident electron and the electrons inside the material have the same mass,

***Corresponding Author:** Ahlam K. Yassir

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the incident electron will scatter more (it cannot be known which of them was the incident electron). As a result, the length of the path through the material can be much greater than the length of the line, while the charge of the falling object remains constant. For energies approaching the limits of electron volts, the loss of energy through ionization is very large, resulting in gaps at the end of the electron path and electrons with a certain kinetic energy moving faster than heavy particles of the same energy. [Liu, W, 2001] . This study aims to Calculate the total electronic stopping power and the rang of the electrons falling in NH_3,PH_3,$AsH_3$and SbH_3 molecules.

THE THEORY

Because of two physical variables, the collisional stopping strength of beta particles differs from that of heavy charged particles. For starters, a beta particle may lose a significant portion of its energy in a single collision with an atomic electron of identical mass. Second, aβ^- particle is the same as the atomic electron with which it collides, while a β^+ particle is the electron's antiparticle [Turner, J. E, 2008]. The identity of the particles in quantum mechanics means that the incident and impacted electrons cannot be distinguished empirically after a collision. Energy loss is defined such that the electron with the lowest energy following a collision is considered the impacted particle. In contrast to heavy charged particles, the identity of β^- and the relationship of β^+ to atomic electrons puts symmetry constraints on the equations that explain their collisions with atoms. [Tanuma, S. *et al*., 2005]

It is possible to write collisional stopping-power formulae for electrons [Turner, J.E, 2007];

$$\left(-\frac{dE}{dx}\right)_{col} = \frac{4\pi k_0^2 e^2 n}{mc^2\beta^2}\left[\ln\frac{mc^2\tau\sqrt{\tau+2}}{\sqrt{2}\,I} + F(\beta)\right] \quad (1)$$

Where,

$$F(\beta) = \frac{1-\beta^2}{2}\left[1 + \frac{\tau^2}{8} - (2\tau+1)\ln 2\right] \quad (2)$$

$$\tau = \frac{T}{mc^2} \quad (3)$$

T is kinetic energy of electron in material, mc^2 electron rest energy, $k_0 = 8.99\times10^9\ Nm^2\ C^{-2}$, e is magnitude of electron charge n is number of electrons per unit volume in the medium, m is electron rest mass, c is speed of light in vacuum, $\beta = v/c$ is speed of particle relative to speed of light in vacuum, and I is mean ionization potential of medium.

The total stopping power for electrons is the sum of the collisional and radiative contributions:

$$\left(-\frac{dE}{dx}\right)_{tot} = \left(-\frac{dE}{dx}\right)_{coll} + \left(-\frac{dE}{dx}\right)_{rad} \quad (4)$$

The ratio of radiative and collisional stopping powers for an electron of total energy E, expressed in MeV, in an element of atomic number Z the Following approximate formula gives [Turner, J.E, 2007].

$$\left(-\frac{dE}{dx}\right)_{rad} \approx \frac{ZE}{800}\left(-\frac{dE}{dx}\right)_{col} \quad (5)$$

$$\left(-\frac{dE}{dx}\right)_{tot} = \left(-\frac{dE}{dx}\right)_{coll}\left(1 + \frac{EZ_2}{800}\right) \quad (6)$$

A charged particle's range is the distance it travels before coming to rest. The distance traveled per unit energy lost is given by the reciprocal of the Stopping power , The range R(E) of a particle of Kinetic energy E is the integral of the quantity down to Zero energy

$$R(E) = \int_0^E \left(\frac{dE}{dx}\right)^{-1} dE \quad (7)$$

FITTING

We took the data of E-STAR program and applied it in the MATLAB-2021 program, using the curve fitting tool, and extracted an equation of the following objectives (NH3, PH3, AsH3, and SbH3) suit mentioned in Table 1, equation represents the ability to hold electrons in the

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energy range (0.01 – 100 MeV). The fitting coefficient was calculated for all.

Table 1: Formula of Curve fitting for electron stopping power in NH_3, PH_3, AsH_3, and SbH_3 molecules

$S_{fit} = 10^{a+bx+cx^2+dx^3}$ $where\ x = \log E$				
target	A	b	c	d
NH_3	0.3321	-0,1028	0.1888	-0.0226
PH_3	0.2401	-0.1018	0.2051	-0.0101
AsH_3	0.1497	-0.0630	0.2329	0.0013
SbH_3	0.1150	-0.0259	0.2486	0.0045

DISCUSSION AND RESULTS

Figures 1 and 2 display the findings for the overall stopping power correspondingly. Equations 1, 5, 6, and 7 in MATLAB 2021 provide these values for the energy range (0.01 – 100) MeV for the molecules NH_3, PH_3, ASH_3, and SbH_3.

exhibit strong agreement with the E-star [physics.nist.go] code up to 3 MeV, but start to diverge in terms of stopping power over that threshold (0.9). An electron's momentum is reduced when it enters a field. When the electron reaches the nuclear domain of the target atom, its course will be severely distorted by the frequent reversals in direction it experiences. Interaction of the electric fields of the two electrons causes the collision interaction between the incident electrons and orbital electrons. There is no physical contact between the orbital electrons as the incident electron approaches; instead, they interact like magnetic poles. The value of S_{Rad} is proportional to the incident electron's energy, and this is because low-energy electrons (slow electrons) use up most of their potential during this phase. They have a high likelihood of connecting with atomic electrons because of their interactions with orbital electrons, while fast electrons have a low probability of engaging with atomic electrons and crossing the coulombic barrier. As this has no effect on electrons, it forces electrons to create new pathways for the loss of radiant energy. We observed that $S_{Coll's}$ results are more influential on the S_{tot} value than $S_{Rad's}$ because S_{Coll} operates at a smaller power range. Figures 1 and 2 show that, at energies more than 1.5 MeV, there is a discrepancy between the present data and the Ester results. This might be because the computations in this paper employed the Bethe-Bloch Relative Formula.

In figure 1(a, b ,c , d) shows the calculations for the total stopping power of the (NH_3 PH_3,AsH_3 ,SbH_3) molecules .

Fig. two (a, b ,c , d) demostrates the calculations for the Range of the (NH_3 PH_3,AsH_3 ,SbH_3) molecules

CONCLUSION

The findings of this study make it possible to draw conclusions:

For incident particles with energies between 0.1 and 10^2 MeV, the following calculations show that the total stopping power lowers as the particle rises because of the impact of the collision stopping power, but that it rises for incident electrons with energies above 10^2 MeV because of the actual stopping force of the radiation; the exact value of this evaluated based on the speed molecules that limit the type of interactions with the target. The nature of the particles' interactions with their target is dependent on their speed. S_{tot} is affected by the transverse particle's energy, but very slightly by the target's atomic number. The findings of the curve fit are close to the results of the procedure, leading us to infer that the Beth-Bloch equation is good for determining the stopping power of electrons in the examined molecules. And we noticed with increasing the energy the range increases and the results calculated for the range according to the Bethe equation, that the value of the range is greater than its value according to E-STAR and the matching tool when the energy is greater than 10 MeV and because of this difference that the equation needs to be developed at high energies and also we noticed that the range of electrons Increases with energy The stopping power according to the Beth-Bloch equation differed, and instead of increasing, as in the results of the E-STAR program and the matching tool, the stopping power continued to decrease with the increase in energy, and this is attributed to the Beth-Bloch equation. Additional corrections are needed to improve the results in the high energy region.

From the results of this research work, we can conclude the following:

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1. The calculations show that the total stopping force, S_{tot}, lowers as the energy of the falling particle increases from $(0.01\text{-}10^2)$ MeV because of the impact of the collision stopping force and then rises as the energy of the incident electrons increases attributable to the radiation stopping power effectively; this energy varies with the velocity of the molecules that limits the type of interactions with the target. How particles interact with their target depends on their velocities. $S_{tot'}$ value is affected by the transverse particle's energy, but only slightly affected by the target's atomic number. The findings of the curve are similar to the results of the procedure, leading us to believe that the Beth-Bloch equation is useful for determining the stopping power of electrons in the examined molecules

2. With the increase in energy the range increases and the results calculated for the range according to the Bethe equation, that the value of the range is greater than its value according to the E-STAR and matching tool when the energy is greater than 10 MeV, as we know that electrons' radii expand as their energies grow. Application of the E-STAR system and modifications to accommodate it.

3. We find that the Beth-Bloch equation requires further modifications to enhance the results for estimating stopping power and range in the high energy zone since stopping power continues to drop with rising power.

4. Table 2 shows calculations for one of the molecules used in the research, ammonia, and includes calculations for collision, radiation, total electron stopping force, stopping range, and beta values. In the same way, values were calculated for the rest of the molecules.

Table 2: Electron Collisional, Radiative, Total Mass stopping powers; and Range in NH_3 molecule

E (MeV)	β^2	$\left(-\frac{dE}{dx}\right)_{col}$	$\left(-\frac{dE}{dx}\right)_{rad}$	$\left(-\frac{dE}{dx}\right)_{tot}$	**Range (cm)**
		$(MeV.cm^2/g)$			
0.01	0.0380	25898.07	1.68	25899.75	2.02×10^{-5}
0.0125	0.0472	21706.95	1.76	21708.72	0.0001
0.1	0.3005	4606.82	2.99	4609.82	0.0138
0.5	0.7445	2243.49	7.29	2250.78	0.1758
1	0.8856	2049.92	13.32	2063.24	0.4363
5	0.9914	2104.24	68.45	2172.69	2.5087
10	0.9976	2051.50	134.40	2185.90	4.9998
20	0.9994	1967.51	258.46	2225.98	9.8440
30	0.9997	1911.32	376.78	2288.10	14.5012
40	0.9998	1870.71	491.82	2362.53	18.9606
50	0.9999	1839.07	604.49	2443.56	23.2248
60	0.9999	1813.13	715.27	2528.40	27.3032
70	0.9999	1791.15	824.48	2615.63	31.2088
80	1.0000	1772.08	932.34	2704.43	34.9531
90	1.0000	1755.23	1039.03	2794.27	38.5476
100	1.0000	1740.15	1144.67	2884.82	42.0035

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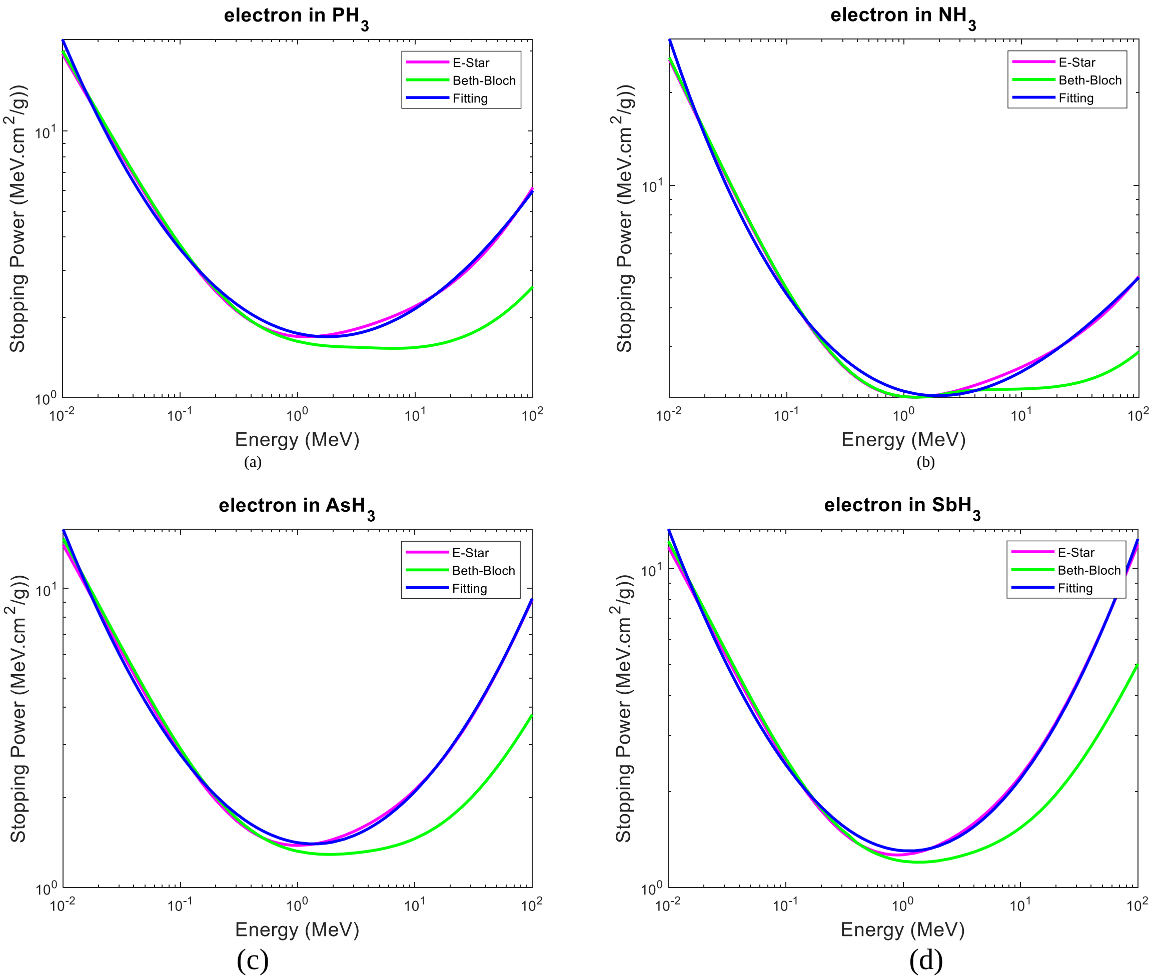
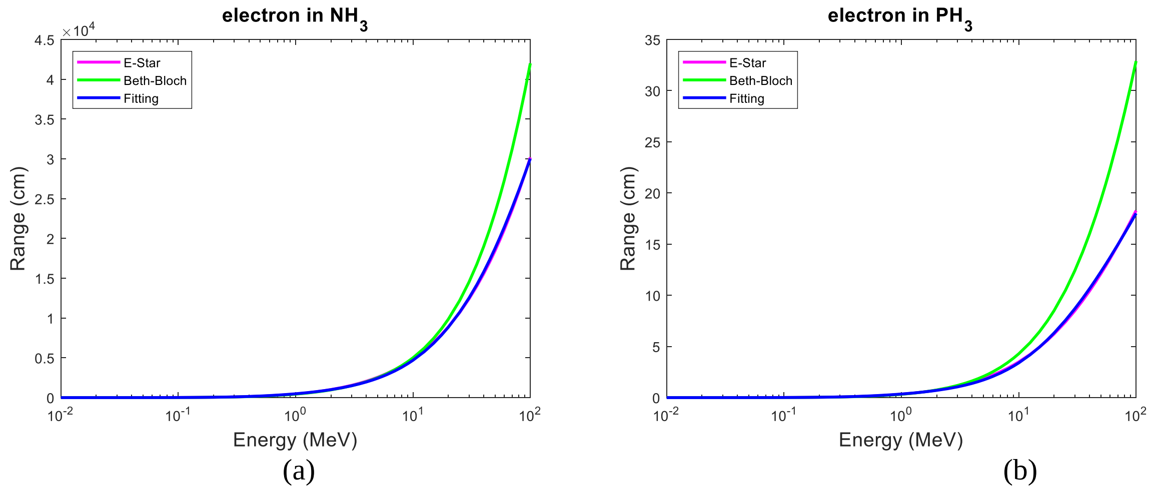


Fig. 1 (a, b, c , d) demostrates the calculations for the total stopping power of the (NH3, PH3,AsH3, SbH3) molecule



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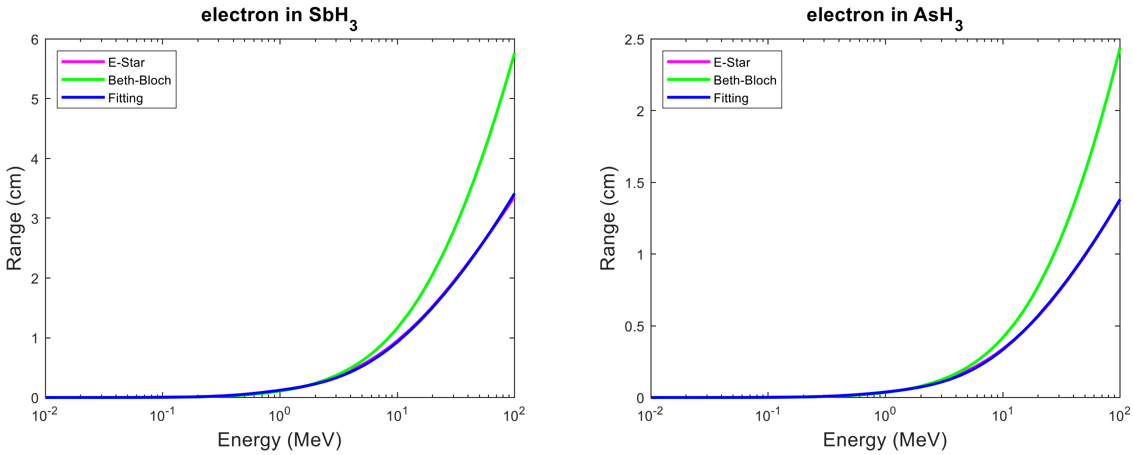

(c) (d)

Fig. 2 (a, b,c , d) demostrates the calculations for the Range of the (NH_3 PH_3,AsH_3 ,SbH_3) molecules

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