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Calculation of Mass Stopping Power of Alpha Particles in (C16H14O and CH3OH)

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ABSTRACT

In this research, we calculated the mass total stopping power (in MeV cm2/g) of Alpha particles in two compounds(C16H14O and CH3OH) in the range of energy (0.01-1000)MeV. By using the Bethe and Bohr and Ziegler equations and Bragg rule. The calculations were compared with experimental data from the SRIM 2013 program and ASTAR code, and the equations were programmed using MATLAB. The outcome demonstrated good agreement between SRIM and ASTAR code.

1. Introduction:

The The energy loss of charge particle in matter has been described with excellent theoretical background based on the theory developed by Bohr, Bethe and Bloch, and improved upon by numerous empirical and semi-empirical contributions derived from charge particle-matter interaction. The interest in the quantification of the energy loss of swift charge particles primarily due to the needs of basic physics research, studies in applied sciences gained importance over the years. In addition to that, accurate determination of the stopping powers of organic materials has long been recognized very important for applications in radiation physics and, and recently, medicine and biology[1]. The average energy loss per unit path length is used to describe a material's stopping power, and the sum of the stopping powers of electronic and nuclear components is the total stopping power:

$$\left(\frac{-dE}{dx}\right)_{total} = \left(\frac{-dE}{dx}\right)_{ele} + \left(\frac{-dE}{dx}\right)_{nuc} \qquad (1)$$

The majority of the total stopping power for heavy charged particles comes from the electronic stopping power, which is based on inelastic collision with the target's electrons. The least amount of stopping power is provided by nuclear stopping power, which comes from elastic coulomb collisions with target nucleons and is only significant at very low energies. For instance, for protons in water, the nuclear stopping power contributes more than 1% to the total stopping power only at energies below 0.02MeV.[2]. Some of the processes that can cause the ions penetrating the material to lose energy include excitation and ionization of the target atoms, capture of the electron, ionization, or excitation of the projectile.[3].

2. Experimental

2.1 Energy Loss in compound and mixture

We have calculated the stopping power for all element in compound, by a linear combination of the constituent stopping powers (Bragg's additivity rule) found the total stopping power, as

$$\left(\frac{-dE}{dx}\right) = \sum_i w_i \left(\frac{\left(\frac{-dE}{dx}\right)}{\rho}\right)_i \qquad (2)$$

Where ω_i is the fraction by weight, and $\left(\frac{\left(\frac{-dE}{dx}\right)}{\rho}\right)_i$,is the mass total stopping power of the i constituent[4].

2.2. Bohr theory

Bohr "treated the energy loss of an energetic heavy charged particle due to collisions with individual atomic electrons , the occasional nuclear scattering as seen in Rutherford's experiments does not play a significant role in stopping power unless the ions in moving very slowly"[5]. Bohr derived an expression of the stopping cross section per target electron of a material[6].

$$\left(\frac{-dE}{dx}\right) = \frac{4\pi z_1^2 e^4}{mv^2} \log \frac{Cmv^3}{z_1 e^2 w} \qquad (3)$$

Where: ν and Z_1 are the projectile velocity and atomic number respectively e, m are the electron charge and mass, ω is resonance frequency of electron and C=1.1229 .

2.3. Bethe equation

The Bethe equation can be used to determine the stopping power of charged particles (quantum mechanics)[7].

$$\left(\frac{-dE}{dx}\right) = K \frac{Z_2 Z_1^2}{A\beta^2} L_{Bethe} \qquad (4)$$

Where:

$$L_{Bethe} = \ln\left[\frac{2m_e\, c^2\, \beta^2}{1-\beta^2}\right] - \beta^2 - \ln\langle I\rangle \qquad (5)$$

$K = 4\pi r_\circ^2 m_e\, c^2 = 0.307075$ MeV.cm^2/g

r_o : the classical radius of electron $\frac{e^2}{m_e\, c^2}$ = 2.818* 10^{-15} m

Z_2: the target atomic number, β: is relative velocity = ν/c and c are light velocity

I: ionization potential in eV.

2.4. Ziegler formula

Ziegler collected the experimental stopping powers of He ions in all materials, as well as calculated the stopping powers of all energies using the local Oscillator Model, characterized by its simple calculation, and the free electron gas model, both theories are based on the perturbation approximation, and the Bethe stopping power theory, Ziegler has constructed tables of stopping power of helium for all elements. Where Ziegler was able to consolidate theoretical data closely related to other calculations[8]. Ziegler came up with semi-experimental equations for calculating both the nuclear and electronic stopping power of alpha particles

2.4.1. The nuclear stopping power

The semi empirical nuclear stopping power for Alpha particles energies is given by the relations[8]:

When be the energy ($\varepsilon < 0.01$) we used[7]:

$$\left(\frac{-dE}{\rho dx}\right)_{nuc} = 1.593\varepsilon^{1/2} \qquad (6)$$

When be the energy ($0.01 \le \varepsilon \le 10$) we used:

$$\left(\frac{-dE}{\rho dx}\right)_{nuc} = 1.7\left(\varepsilon^{1/2}\right)\left[\frac{\ln(\varepsilon+exp1)}{1+6.8\varepsilon+3.4\varepsilon^{3/2}}\right] \qquad (7)$$

When be the energy ($\varepsilon > 10$) we used:

$$\left(\frac{-dE}{\rho dx}\right)_{nuc} = \frac{\ln 0.47\varepsilon}{2\varepsilon} \qquad (8)$$

Where the reduced ion energy defined as:

$$\varepsilon = \frac{32.53M_2E}{Z_1Z_2(M_1+M_2)\left(Z_1^{2/3}+Z_2^{2/3}\right)^{1/2}} \qquad eV/atom/cm^2 \qquad (9)$$

E is initial proton kinetic energy (keV)

M_1 and M_2 are the projectile and target mass numbers

Z_1 and Z_2 are the projectile and target atomic numbers

2.4.2 The electronic stopping power

Ziegler was able to come up with semi-experimental equations to calculate the electronic stopping power of alpha particles and energy regions based on the formula proposed by Varelas and Biersack, where this formula combines sufficient flexibility in shape and simplicity in formulation. The mass Electronic stopping power ($\left(\frac{-dE}{\rho dx}\right)_{ele}$) in low energy (below 10 MeV) we used [8]:

$$\left(\left(\frac{-dE}{\rho dx}\right)_{ele}\right)^{-1} = \left(\left(\frac{-dE}{\rho dx}\right)_{LOW}\right)^{-1} + \left(\left(\frac{-dE}{\rho dx}\right)_{HIGH}\right)^{-1} \qquad (10)$$

$$\left(\frac{-dE}{\rho dx}\right)_{LOW} = A_1E^{A_2} \qquad (11)$$

$$\left(\frac{-dE}{\rho dx}\right)_{HIGH} = \left(\frac{A_3}{E/1000}\right)\ln\left[1+\left(\frac{A_4}{E/1000}+\frac{A_5E}{1000}\right)\right] \qquad (12)$$

When high energy ($E > 10MeV$) we used formula :

$$\left(\frac{-dE}{\rho dx}\right)_{ele} = \exp(A_6 + A_7EE + A_8EE^2 + A_9EE^3) \qquad (13)$$

Where E is particle energy(MeV)

$$EE=\ln(1/E) \qquad (14)$$

Where from A_1 to A_9 is constants shown in table 2 of the hydrogen and oxygen and carbon.

3. Results and Discussions

The Bohr Equation, the Bethe Equation and the Ziegler Equations, which were programmed using the MATLAB program, were used to calculate the mass stopping power of alpha particles in the two compounds ($C_{16}H_{14}O_3$, CH_3OH) In the energy range (0.01-1000mev) the Figures (1,2) shows the comparison of the theoretically calculated results of these equations with the practical results of the SRIM2013 program and the practical data of the ASTAR program using the MATLAB program . The correlation coefficient CORREL was calculated for each target as

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shown in Table (1).

As for the Bohr equation(3), we note its departure from the practical values of the SRIM program and the ASTAR program at low energies, the reason for this is due to the origin of the classical Bohr equation and it is not valid for high energies. Figure (1,2) shows the stopping power as a function of the energy of alpha particles. when applying the Bohr Equation (3), at low energies, the mass stopping power reaches the cut-off limit within the energy (0.01 < E< 0.3)MeV. The reason for this cutting is that the particle velocity is very low, so the Bohr stopping number L_{Bohr} is negative and less than zero $(\ln \frac{cMv^3}{Z_1 e^2 w} < 0)$.

The maximum value of the mass stopping power resulting from the application of the Bohr Equation (3) shown in Figure (1,2) is at Energy E=0.7 MeV. Then the stopping power decreases with increasing energy.

As for the results of the Beth Equation (4) we note that in the case of low energies the cut-off limit (cut off) in the Figure (1,2) is within the energies (0.01< E< 0.2)MeV, The reason for this cat off is due to the fact that the speed of the charged particle is very low, so the stopping number of the L_{Bethe} is a negative value. The validity of Beth's theory also depends on the hypothesis that the velocity of the incident particle is much greater than the orbital motion of electrons of the atoms of the target. We note that the greatest value of the mass stopping power of alpha particles when applying the Beth Equation(4) in Figure (1,2) is at Energy E=0.3 MeV, Then after these maximum values of the mass stopping power of alpha particles the stopping power decreases as the energy of the incident particle increases. And the reason for this rapid decrease when applying Beth's equation is due to the fact that the energy loss is inversely proportional to the square of the velocity of the incident particle ($1/v^2$). We note that the results of the Beth equation deviate from the experimental values of the SRIM2013 program and the ASTAR program at low energies and agree with these experimental values of the two programs when the energy is high because the Beth equation is quantitative and suitable for high energies.

Using the nuclear and electronic Ziegler equations(6,7,8,9,10,11,12,13,14) to calculate the total mass stopping power of the alpha particles programmed using the MATLAB program and compare the results calculated in this research with the practical data of the SRIM2013 program as in the two tables(2,3). The correlation coefficient CORREL was calculated for each target as shown in Table (1).

We note from Figures (1 and 2) that the values of the mass total stopping powers at the first region for energy (0.01-10 MeV), which is divided into two regions: 1) the low region, their increase is very small due to the very low speed, but in the second region the stopping power begins to increase rapidly and clearly until it reaches its greatest value due to the ionization and excitation of atoms of matter. in Figure (1,2) the stopping power reaches its peak(the maximum value) at energy E= 0.6MeV.

As for the second region of the Ziegler regions of the range energies (E > 10MeV) the range of energies in which we observe through Figures 1 and 2, the values of the stopping powers gradually decrease as the energy of the incident particle increases, because the energy loss is inversely proportional to the square of the velocity of the incident particle. and these results are good agreements with the practical data of the SRIM2013 program.

4. Conclusion

demonstrated good agreement between the mass stopping power values calculated using the Bohr and Bethe equations. with SRIM2013 and ASTAR results at energies greater than (0.3 MeV), We also note a very good agreement of the values the mass total stopping power computed using the Ziegler formula with the results SRIM2013. with correlation coefficients shown in the Table (1). The calculation of the stopping power has useful applications as the design of radiation technology systems and in shielding and the selection of the appropriate thickness for the target, it also has applications in several important fields including in the field of studies, scientific research, diagnosis and medical treatment.

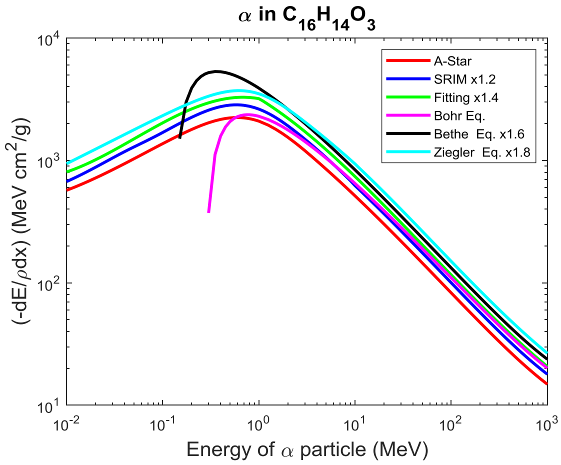

Fig.1. Show the mass stopping power and energy for Alpha particle in $C_{16}H_{14}O_3$

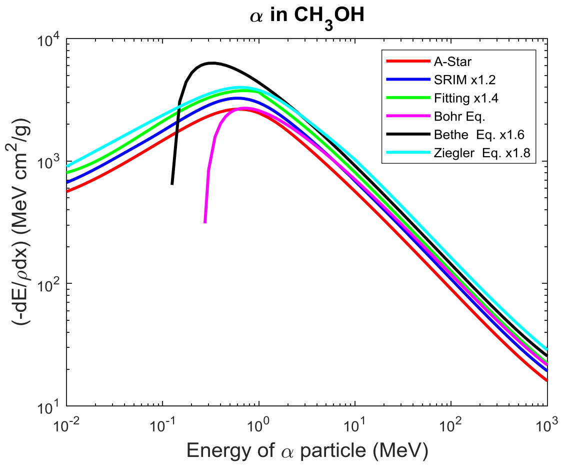

Fig. 2. show the mass stopping power and Energy for Alpha particle in CH_3OH

Table 1. showing correlation coefficients values when comparing the Alpha particle mass stopping power resulting from Bohr and Bethe and Ziegler equations and ASTAR and SRIM2013

Equation	Bohr with ASTAR	Bethe with ASTAR	Zeigler with SRIM2013
Correlation coefficient of $C_{16}H_{14}O_3$	0.9174	0.9780	0.9995
Correlation coefficient of CH_3OH	0.9139	0.9759	0.9995

Table 2. showing the values of coefficients for Alpha particles stopping[8]

Element	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9
H solid	0.9661	0.4126	6.92	8.831	2.582	2.371	0.5462	-0.0793	-0.00685
H gas	0.39	0.63	4.17	85.55	19.55				
O solid	1.766	0.5261	37.11	15.24	2.804	3.782	0.3734	-0.1011	-0.00787
O gas	2.717	0.4858	32.88	25.88	4.336				
C solid	4.232	0.3877	22.99	35	7.993	3.588	0.3921	-0.0993	-0.00780
C gas	3.47	0.4485	22.37	36.41	7.993				

Table 2. showing the values of the mass stopping power for Alpha particle in $C_{16}H_{14}O_3$

E(MeV)	A-star	Bohr	Bethe	SRIM	Ziegler
0.01	569.3694	-604514	-312711	559.42	521.7935
0.02	717.9919	-239521	-114531	732.34	686.0738
0.03	837.4084	-135215	-60043.7	870.35	805.7175
0.035	890.0908	-107930	-46151.0	928.71	856.4696
0.04	939.1556	-88392.9	-36353.5	981.107	902.9478
0.045	985.3170	-73834	-29156.0	1028.3	945.951
0.05	1028.841	-62635.8	-23697.1	1071.2	986.058
0.055	1069.8	-53805	-19452.0	1110.8	1023.7
0.06	1109.181	-46696	-16080.5	1148.7	1059.2
0.07	1182.854	-36039	-11125.8	1219	1124.797
0.08	1249.669	-28512.7	-7720.77	1285.2	1184.406
0.09	1312.061	-22975.7	-5283.59	1348.2	1239.096
0.1	1370.199	-18771	-3483.75	1408.9	1289.639
0.2	1789.916	-3112.01	2440.625	1874.3	1650.339
0.3	2029.249	371.8852	3258.244	2144.1	1858.8
0.4	2161.663	1580.865	3311.742	2291.1	1979.591
0.5	2223.373	2072.634	3188.094	2357	2041.76
0.6	2239.422	2277.343	3023.571	2369.9	2063.192
0.7	2224.036	2350.731	2857.499	2348.4	2056.32
0.8	2190.334	2359.128	2701.85	2304.9	2030.155
0.9	2144.326	2333.994	2559.679	2248.3	1991.277
1	2091.62	2291.408	2430.956	2185.9	1944.5
1.25	1941.739	2156.477	2160.405	2052.7	1839.742
1.5	1794.197	2017.283	1947.211	1862.1	1681.1
1.75	1661.138	1888.736	1775.514	1747.5	1583.7
2	1543.583	1773.677	1634.308	1597.1	1454.3
2.25	1441.291	1671.526	1516.042	1489.8	1361.5
2.5	1351.873	1580.818	1415.437	1396.6	1280.7
2.75	1272.519	1499.994	1328.719	1315.3	1209.9
3	1202.995	1427.638	1253.118	1244.1	1147.7
3.5	1085.113	1303.671	1127.474	1123.7	1043.4
4	990.4617	1201.377	1027.029	1026.5	959.22
4.5	912.9324	1115.491	944.6885	945.993	889.73
5	848.1235	1042.292	875.8232	878.157	831.158
5.5	792.93	979.1013	817.278	820.1	780.961
6	745.4332	923.9438	766.8248	769.67	737.344
6.5	703.6956	875.3361	722.843	725.48	699.00
7	667.0397	832.1416	684.1238	686.49	664.98
8	605.0597	758.6374	618.9964	620.426	607.094
9	554.7117	698.31	566.2368	566.317	559.529
10	512.9671	647.8074	522.5355	517.97	519.617
15	377.2337	481.7218	381.7131	381.42	382.048
20	301.7607	388.0802	304.2365	305.1322	305.7012
30	219.0492	284.2726	219.9836	223.0547	221.6004
40	173.9241	227.1005	174.3458	176.7079	175.6966
50	145.2265	190.4976	145.4309	147.3828	146.5424
60	125.3026	164.8886	125.3501	127.038	126.2858

70	110.5093	145.8855	110.5333	111.9383	111.3442
80	99.15191	131.1798	99.11889	100.3802	99.84135
90	90.09452	119.4355	90.03709	91.15358	90.69638
100	82.68923	109.8234	82.62759	83.6365	83.24123
200	47.29064	63.46931	47.22862	47.72794	47.7064
300	34.4205	46.41379	34.37178	34.70402	34.80221
400	27.67567	37.41873	27.64089	27.88619	28.01179
500	23.50153	31.82804	23.48038	23.6742	23.78144
600	20.66563	28.00489	20.64853	20.8036	20.87475
700	18.60689	25.22092	18.59529	18.72623	18.74506
800	17.04101	23.10131	17.03852	17.15142	17.11213
900	15.81954	21.43291	15.8182	15.91365	15.81698
1000	14.82583	20.0853	14.83666	14.91698	14.76248

Table 3. showing the values of the mass stopping power for Alpha particle in CH_3OH

E(MeV)	$-\frac{dE}{\rho dx}(MeV.cm^2/g)$				
	A-star	Bohr	Bethe	SRIM	Ziegler
0.01	562.2862	-631016	-319945	556.117	500.6628
0.02	716.9862	-248630	-115387	718.200	668.7671
0.03	847.5537	-139672	-59537	854.197	793.4599
0.035	906.4714	-111220	-45366	914.238	846.8527
0.04	961.8347	-90875.8	-35400	969.859	895.9947
0.045	1014.5	-75728	-28100	1021.6	941.6658
0.05	1064.528	-64088.8	-22579	1070.0	984.4304
0.055	1112.2	-54919	-18297	1116.0	1024.7
0.06	1158.047	-47543.7	-14906.7	1160.1	1062.8
0.07	1244.542	-36502.3	-9944.13	1243.3	1133.6
0.08	1324.579	-28718.6	-6553.81	1321.7	1198.2
0.09	1399.707	-23002.3	-4142	1396.1	1257.9
0.1	1470.351	-18669	-2372.36	1467.4	1313.288
0.2	2002.439	-2646.76	3272.511	2026.1	1716.268
0.3	2327.645	843.6149	3920.556	2377.3	1957.068
0.4	2519.219	2020.642	3865.806	2583.7	2101.568
0.5	2616.386	2477.813	3666.925	2684.7	2180.129
0.6	2648.736	2651.327	3446.827	2711.8	2212.004
0.7	2635.714	2697.623	3237.853	2690.3	2210.933
0.8	2594.25	2682.622	3047.973	2637.4	2187.088
0.9	2534.377	2637.199	2877.785	2566.9	2148.017
1	2463.745	2576.897	2725.659	2487.6	2099.3
1.25	2264.657	2406.229	2410.416	2330.7	1987.7
1.5	2072.551	2239.96	2165.26	2086.7	1816.1
1.75	1903.286	2090.15	1969.452	1950.3	1710.3
2	1756.718	1957.912	1809.341	1772.7	1569.8
2.25	1630.957	1841.564	1675.814	1648.0	1469.2
2.5	1523.122	1738.906	1562.605	1541.3	1381.8
2.75	1429.447	1647.867	1465.283	1448.7	1305.5
3	1347.926	1566.669	1380.626	1367.6	1238.6
3.5	1212.017	1428.129	1240.298	1232.4	1126.8

4	1103.799	1314.291	1128.43	1124.0	1037.1
4.5	1015.293	1219.007	1036.927	1034.7	963.068
5	941.5257	1137.995	960.5337	959.84	900.803
5.5	878.8785	1068.192	895.684	896.05	847.479
6	825.1841	1007.361	839.8672	840.744	801.155
6.5	778.0632	953.8236	791.2616	792.4290	760.429
7	736.7396	906.303	748.5118	749.892	724.267
8	667.1125	825.5501	676.6888	677.88	662.679
9	610.7697	759.3764	618.5826	621.435	611.977
10	564.154	704.0488	570.5053	569.83	569.354
15	413.3367	522.5255	415.9134	417.74	417.143
20	330.0288	420.4654	331.0856	337.0922	333.1412
30	239.0534	307.568	239.034	242.9439	240.9443
40	189.5818	245.5031	189.2651	192.1486	190.7795
50	158.1702	205.8127	157.7702	160.1149	158.9807
60	136.3577	178.0657	135.9165	137.8752	136.9164
70	120.2145	157.4885	119.802	121.4339	120.6577
80	107.8207	141.5722	107.3944	108.852	108.1507
90	97.93596	128.8662	97.52668	98.8097	98.21355
100	89.85452	118.4704	89.47892	90.63574	90.11683
200	51.30551	68.3852	51.07216	51.64191	51.57867
300	37.31591	49.98019	37.14307	37.52027	37.60766
400	29.99336	40.27965	29.85619	30.14099	30.26123
500	25.46623	34.25296	25.35411	25.58253	25.68636
600	22.38561	30.13287	22.29078	22.47765	22.54376
700	20.15459	27.13335	20.07023	20.23162	20.24162
800	18.45665	24.85003	18.38692	18.5277	18.47667
900	17.13406	23.05302	17.06759	17.19561	17.07693
1000	16.06175	21.60172	16.00652	16.11644	15.93733

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