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ELASTIC ELECTRON–ATOM TOTAL SCATTERING CROSS SECTIONS FOR THE ALKALINE EARTH METALS

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ABSTRACT

Total Cross-Sections (TCS) of elastic electron-atom scattering for the Alkaline Earth Metals Beryllium (Be), Magnesium (Mg), Calcium (Ca), Strontium (Sr), Barium (Ba) and Radium (Ra) are presented. The computed TCS were calculated using Born, Eikonal and the Optical Theorem approximation methods with the Lenz-Jensen potential, at electron incident energies between 1 to 1000 eV. Results obtained are in good agreement with experimental TCS data.

Keywords: Total Cross-Section, elastic scattering, alkaline earth metals, Optical theorem, Born approximation, Eikonal approximation

INTRODUCTION

Electron-atom and electron-molecule collision processes play an important role in many systems such as solar plasmas, aurorae, discharge or electron-beam lasers, plasma processing devices, etc. According to Tanaka and Inokuti (2000) electron collisions with molecules initiate the first step in plasma generation.

In scattering theory, the Total Cross-Section (TCS) is a measure of the probability that an interaction occurs; the larger the cross section, the greater the probability that an interaction will take place when a particle is incident on a target (Abdu, 2018a; Abdu, 2018b; Anchaver, 2003).

Elastic electron-atom scattering takes place if the final state of an atom after the interaction coincides with the initial one (Winitzki, 2004). Total and differential cross-sections for such a process can be calculated in various approximations — Born (Merzbacher, 1970)), Eikonal (Innanen, 2010; Shajesh, 2010), optical theorem (Lokajicek & Kundrat, 2009; Ronniger, 2006), partial wave method (Cox & Bonham, 1967), etc. In this work, the total cross-sections of the alkaline earth metals (Halka & Nordstrom, 2010) Beryllium (Be), Magnesium (Mg),Calcium (Ca), Strontium (Sr), Barium (Ba) and Radium (Ra) were computed using the Born, Eikonal and Optical Theorem approximation methods for comparison.

The six alkaline earth metals are in group two of the periodic table and have very important and have strategic uses. They are shiny, slivery-white somewhat reactive metals at standard temperature and pressure. They are soft or semisoft metals, insoluble in water and generally harder and less reactive than the metals in group one. Their uses include: Beryllium is used as a component in aircraft disc breaker, high speed computers, audio components, rocket propellants, navigational systems, nuclear weapons, fuel containers, mirrors, nuclear reactors, neutron reflections, etc; Magnesium is used to produce lightweight products such as car seats, luggage, laptops, cameras and power tools; Calcium is used as a reducing agent in preparing other metals such as thorium and uranium, and also used as an alloying agent; Barium is mostly used in drilling fluids for oil and gas wells, as well as in paint and glass making; Strontium is used for producing cathode ray tubes for colour televisions, as well as in producing ferrite ceramic magnets and in refining zinc. The world's most accurate atomic clock, accurate to one second in 200 million years, was developed using strontium atoms; Radium is used to treat cancer, and its radiation is used to study the composition of metals, plastics, and other materials.

MATERIALS AND METHODS

We used the FORTRAN code program developed by Koonin & Meredith (1989) which takes the relativistic differential cross-section as a sum of squared modules of the real and imaginary scattering amplitudes. The amplitudes can be calculated through the phase shifts of spherical waves, which are obtained by integration of equations for radial wave functions (Koonin & Meredith, 1989). In these computations the analytical approximation for the atomic electrostatic potential given by Lenz and Jensen, called the Lenz-Jensen potential (Blister & Hautala, 1978), based on the Thomas-Fermi model, is used.

Scattering Theory

For particles of mass m and energy

$$E = \frac{\hbar^2 k^2}{2m} > 0 \qquad (1)$$

scattering from a central potential, V(r) is described by a wave function, ψ(r) that satisfies the Schrodinger Wave Equation (SWE)

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \quad (2)$$

with the boundary condition at large distance

$$\psi_{r\to\infty} \to e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \quad (3)$$

Equation (3) holds for a beam of electrons incident along z-axis, and the scattering angle, θ is the angle between r and $\hat{z}$ while f is the complex scattering amplitude, which is the basic function we seek to determine (Babaji, Abdu & Taura, 2012). The differential cross-section is given by:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \quad (4)$$

The total cross-section is

$$\sigma = \int d\Omega \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = 2\pi \int_0^{\pi} \mathrm{d}\theta \sin\theta |\mathrm{f}(\theta)|^2 \quad (5)$$

f is a function of both E and θ (Koonin & Meredith, 1989).

Approximation Methods

Approximations play a very important role in our understanding of processes that cannot be solved exactly. The calculation of scattering cross sections is one of the most important uses of Fermi's Golden Rule (Wacker, 2011). Fermi's rule involves only one matrix element of the interaction which makes it a first order approximation to the exact result. This approximation suggests an approximation to the complex scattering amplitude. The Born approximation involves an approximation to the complex scattering amplitude (Merzbacher, 1970). It has been extensively used to study low energy as well as high energy scattering processes. The Eikonal approximation is a technique for estimating the high energy behaviour of a forward scattering amplitude (Innanen, 2010). It was originally developed for potential scattering in quantum mechanics, where one approximates the classical trajectory corresponding to forward scattering by a straight line and uses a WKB approximation for the wavefunction (Sakuri, 1985). The optical theorem relates the forward scattering amplitude to the cross section (Lokajicek & Kundrat, 2009).

The Lenz-Jensen Potential

One practical application of the theory discussed above is the calculation of the scattering of electrons from neutral atoms. In general this is a complicated multi-channel scattering problem since there can be reactions leading to final states in which the atom is excited. However, the reaction probabilities are small in comparison to those for elastic scattering, thus the problem can be modeled by the scattering of an electron from a central potential (Koonin & Meredith, 1989). This potential represents the combined influence of the attraction of the central nuclear charge (Z) and the screening of this attraction by the Z atomic electrons. For a neutral target atom, the potential vanishes at large distances faster than r^{-1}(Koonin & Meredith, 1989). An accurate approximation to this potential can be obtained by solving for the self-consistent Hartree-Fock potential of the neutral atom. However, a much simpler estimate is obtained using an approximation to the Thomas-Fermi model of the atom given by Lenz and Jensen (Blister & Hautala, 1978)

$$V = -\frac{Ze^2}{r}e^{-x}(1 + x + b_2x^2 + b_3x^3 + b_4x^4); \quad (6)$$

with

$$e^2 = 14.409;\ b_2 = 0.3344;\ b_3 = 0.0485;\ b_4 = 2.647 \times 10^{-3};\ \text{and}$$
$$x = 4.5397Z^{\frac{1}{6}}r^{\frac{1}{2}} \quad (7)$$

This potential is singular at the origin. If the potential is regularized by taking it to be a constant within some small radius r_{min} (say the radius of the atom's 1s shell), then the calculated cross-section will be unaffected except at momentum transfers large enough so that $qr_{min} \gg 1$. The incident particle is assumed to have the mass of the electron, and, as is appropriate for atomic systems, all lengths are measured in angstrom (Å) and all energies in electronvolt (eV). The potential is assumed to vanish beyond 2Å. Furthermore, the r^{-1} singularity in the potential is cutoff inside the radius of the 1s shell of the target atom.

RESEARCH METHODOLOGY

A FORTRAN program developed by Koonin & Meredith (1989) was the main program used for all the computations. The

program is made up of four categories of files: common utility programs, physics source code, data files and include files. The physics source code is the main source code which contains the routine for the actual computations. The data files contain data to be read into the main program at run-time and have the extension .DAT.

The first thing done was the successful installation of the FORTRAN codes in the computer. This requires familiarity with the computer's operating system, the FORTRAN compiler, linker, editor, and the graphics package to be used in plotting. The program runs interactively. The main menu below is displayed:

1. Change physical parameter
2. Change numerical parameters
3. Change output parameters
4. Display physical and numerical parameters
5. Display output parameters
6. Run the program
7. Stop the program

We made a menu choice of (1) and the following options were displayed:

1. Lenz-jensen potential: electron and neutral atom
2. Square well
3. Gausian well

We made a menu choice of (1) and it then displayed "Enter charge of the atomic nucleus" where we entered the nuclear charge (atomic number) of the first alkaline earth metal. It then displayed "Enter energy <ev>" where we entered the energy (1.0 eV) for the metal. It then displayed the numerical parameter which is the quadrature point with default value of 20 which we accepted. We then chose to display text output on the screen and save a copy. We then returned to the main menu and chose to run the program. This procedure is repeated for all the alkaline earth metals with various electron energies.

RESULTS AND DISCUSSION

Results were generated for several electron incident energies as presented in tables 1-3 below and plotted as given in figures 1-6:

Table 1: Computed Total Cross-Sections for Elastic Electron-Atom Scattering for Be, Mg, Ca, Sr, Ba and Ra using the Born Approximation Method with the Lenz-Jensen Potential.

Energy (eV)	TOTAL CROSS SECTION ($Å^2$)					
	Be	Mg	Ca	Sr	Ba	Ra
1.0	68.810	202.300	316.400	532.200	718.100	1000.700
5.0	39.100	131.300	218.200	395.000	555.800	815.600
10.0	24.410	90.210	157.000	300.600	437.200	665.700
20.0	14.040	56.510	102.600	207.900	313.200	496.900
30.0	9.911	41.570	77.140	160.800	247.000	401.200
40.0	7.637	32.900	61.930	131.600	204.700	337.900
50.0	6.210	27.260	51.820	111.600	175.300	292.800
60.0	5.235	23.300	44.610	97.070	153.500	258.700
70.0	4.524	20.300	39.190	85.940	136.700	232.100
80.0	3.980	18.070	34.950	77.140	123.700	210.500
90.0	3.551	16.240	31.540	69.990	112.300	192.800
100.0	3.205	14.750	28.750	64.080	103.100	177.800
200.0	58.560	7.708	15.290	34.890	57.160	101.000
300.0	50.540	5.216	10.430	24.030	39.660	70.850
400.0	0.811	3.941	7.914	18.330	30.390	54.640
500.0	0.649	3.165	6.377	14.820	24.650	44.490
600.0	0.541	2.645	5.340	12.440	20.730	37.530
700.0	0.464	2.271	4.593	10.720	17.890	32.470
800.0	0.406	1.990	4.029	9.417	15.730	28.610
900.0	0.361	1.770	3.589	8.396	14.040	25.570
1000.0	0.325	1.594	3.235	7.575	12.680	23.120

From Figures 1-6 and table 1, the calculated TCS using the Born approximation method are significantly higher than those obtained using the two other approximation methods. This is in agreement with Babaji *et al.* (2012). As observed in Fig. 1, the calculated

TCS of all the alkaline earth metals decrease with increasing incident energies from 1 to 1000 eV except those for Beryllium which reduced to its minimum, 3.205 Å^2 at 100 eV, then rose sharply to 58.560 Å^2 at 200 eV. Thereafter it continued to decrease with increasing electron incident energy. Also, the calculated TCS increased with increasing atomic number (Z) for the alkaline earth metals as can be seen from tables 1-3 and Figures 1-6. Radium has the largest value of TCS of 1000.700 Å^2 at 1 eV (Table 1 and Fig. 6), while Beryllium recorded the smallest, 0.325 Å^2 at 1000 eV (Table 1 and Fig. 1).

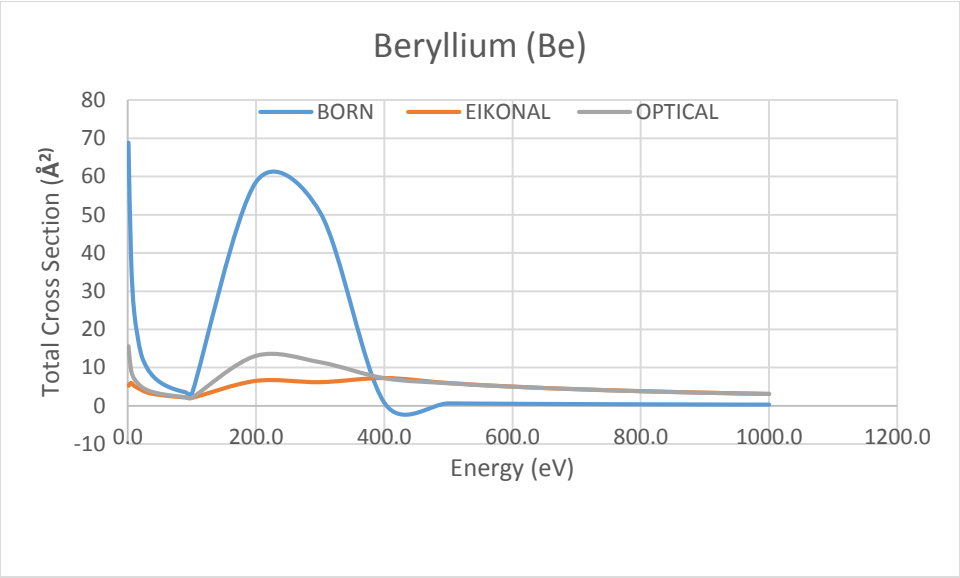

Fig. 1: TCS for Beryllium using Born, Eikonal and Optical Theorem approximations

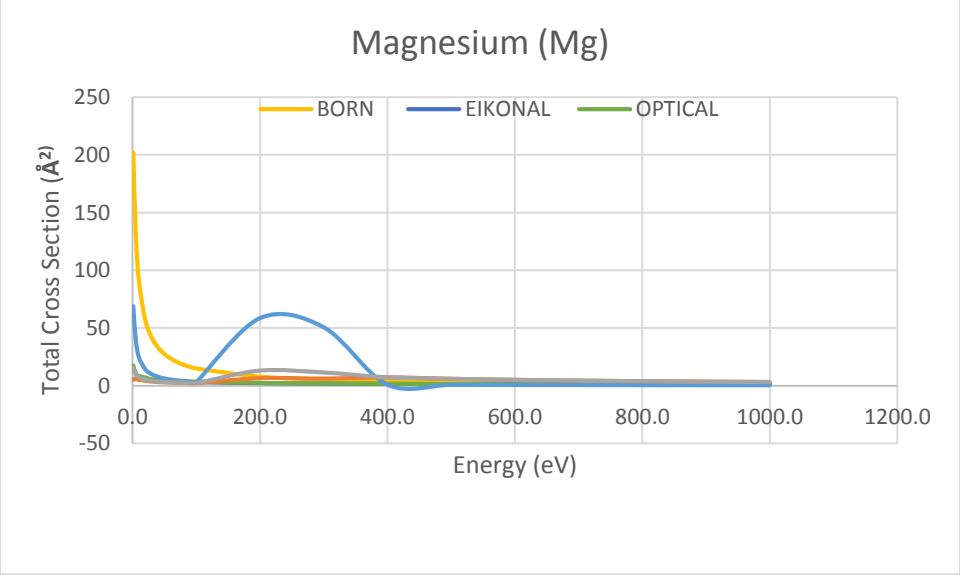

Fig. 2: TCS for Magnesium using Born, Eikonal and Optical Theorem approximations

Table 2: Computed Total Cross-Sections for Elastic Electron- Atom Scattering for Be, Mg, Ca, Sr, Ba and Ra using the Eikonal Approximation Method with the Lenz-Jensen Potential.

Energy (eV)	TOTAL CROSS SECTION (Å^2)					
	Be	Mg	Ca	Sr	Ba	Ra
1.0	5.215	5.654	4.016	4.198	5.032	4.476
5.0	5.941	5.891	6.845	5.048	4.953	3.151
10.0	5.191	5.474	6.474	4.813	7.206	5.227
20.0	4.245	5.409	4.673	5.752	4.114	2.999
30.0	3.471	4.316	5.330	4.301	5.087	4.330
40.0	3.080	4.419	4.535	3.931	4.609	4.542
50.0	2.832	4.119	4.001	3.980	3.581	4.283
60.0	2.635	3.720	3.773	4.184	3.653	3.963
70.0	2.466	3.439	3.773	4.455	3.475	3.311
80.0	2.318	3.304	3.820	4.143	3.636	2.991
90.0	2.184	3.229	3.723	3.783	3.772	3.614
100.0	2.062	3.152	3.537	3.501	3.807	3.132
200.0	6.494	2.301	2.656	2.994	2.691	3.114
300.0	6.152	1.913	2.298	2.674	2.660	2.411
400.0	7.229	1.642	2.007	2.214	2.560	2.449
500.0	5.917	1.446	1.800	2.057	2.363	2.375
600.0	5.008	1.300	1.648	1.973	2.056	2.262
700.0	4.340	1.186	1.529	1.924	1.927	2.265
800.0	3.829	1.095	1.431	1.885	1.874	2.180
900.0	3.426	1.019	1.346	1.759	1.807	2.102
1000.0	3.100	0.954	1.273	1.655	1.743	1.970

From table 2 and Figures 1-6, using the Eikonal method, the TCS for the alkaline earth metals are significantly lower than those calculated using the other two methods. The calculated TCS for Berrilium fluctuated between 1 to 400 eV, where it reached its maximum value of 7.229 Å^2 (Fig. 1). It then decreased steadily thereafter to its minimum value of 3.100 Å^2 at 1000 eV. The TCS for Magnesium fluctuated between 1 to 40 eV and thereafter decreased steadily with increase in electron incident energy (Fig. 2); those for Calcium fluctuated between 1 to 80 eV and thereafter decreased steadily with increasing incident energy (Fig. 3); those for Strontium fluctuated between 1 to 70 eV and thereafter decreased steadily with increasing incident energy (Fig. 4); those for Barium fluctuated between 1 to 100 eV and thereafter decreased steadily with increasing incident energy (Fig. 5); and those for Radium fluctuated between 1 to 400 eV and thereafter decreased steadily with increasing incident energy (Fig. 6). From Table 2, Beryllium has the largest value of TCS of 7.229 Å^2 at 400 eV, while Magnesium recorded the smallest, 0.954 Å^2 at 1000 eV.

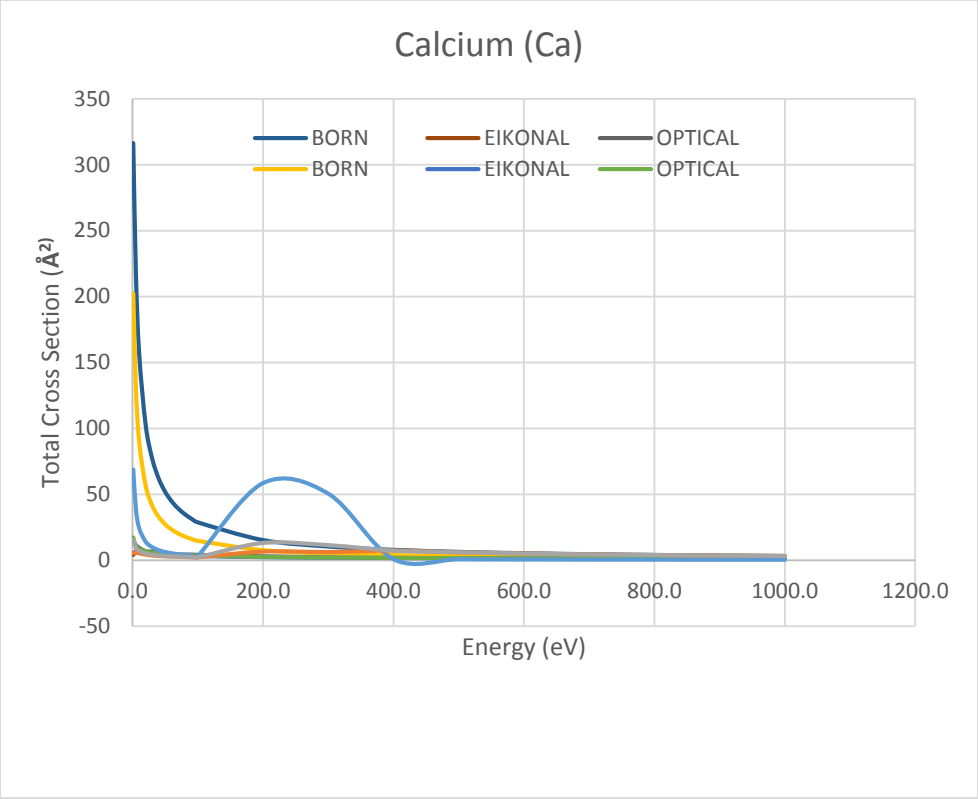

Fig. 3: TCS for Calcium using Born, Eikonal and Optical Theorem approximations

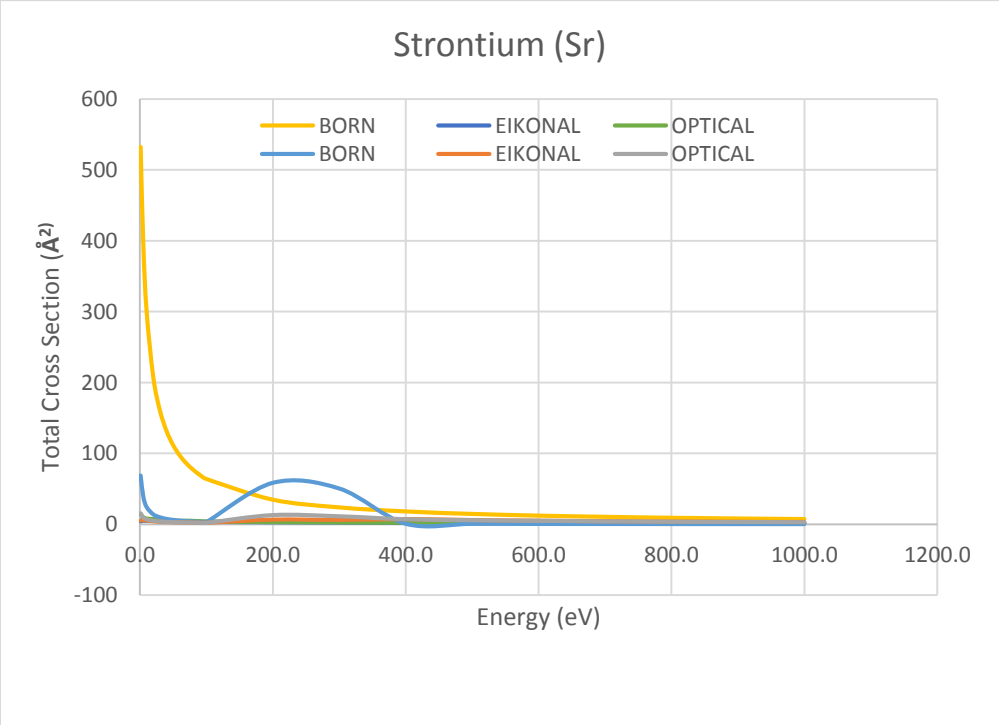

Fig. 4: TCS for Strontium using Born, Eikonal and Optical Theorem approximations

Table 3: Computed Total Cross-Sections for Elastic Electron- Atom Scattering for Be, Mg, Ca, Sr, Ba and Ra using the Optical Theorem with the Lenz-Jensen Potential.

Energy (eV)	TOTAL CROSS SECTION (Å^2)					
	Be	Mg	Ca	Sr	Ba	Ra
1.0	15.610	17.390	14.340	14.710	15.260	14.760
5.0	9.388	10.710	11.320	10.130	9.727	7.304
10.0	7.091	8.364	9.382	8.247	9.834	8.542
20.0	5.162	7.008	6.795	7.565	6.593	5.314
30.0	4.133	5.615	6.544	6.654	6.741	6.214
40.0	3.553	5.279	5.754	5.443	6.029	5.991
50.0	3.167	4.536	5.063	5.148	4.800	5.591
60.0	2.877	4.423	4.614	5.112	4.798	5.591
70.0	2.643	4.045	4.393	5.250	4.582	4.386
80.0	2.447	3.791	4.351	4.972	4.483	3.749
90.0	2.279	3.625	4.277	4.529	4.600	3.925
100.0	2.133	3.496	4.105	4.132	4.539	3.992
200.0	13.100	2.479	2.870	3.358	3.142	3.683
300.0	11.410	2.011	2.489	2.853	2.936	2.620
400.0	7.232	1.714	2.118	2.402	2.814	2.595
500.0	5.919	1.500	1.869	2.202	2.504	2.547
600.0	5.009	1.340	1.706	2.085	2.154	2.469
700.0	4.341	1.216	1.583	2.006	1.994	2.414
800.0	3.830	1.116	1.481	1.909	1.918	2.256
900.0	3.426	1.035	1.393	1.797	1.854	2.102
1000.0	3.100	0.966	1.314	1.687	1.802	1.937

From table 3 and Fig. 1, using the Optical theorem method, the calculated TCS for Beryllium decreased steadily between 1 to 100 eV, where it reached its minimum value of 2.133 Å^2. It then rose sharply to 13.100 Å^2 at 200 eV, then decreased steadily thereafter; those for Strontium decreased steadily to 5.112 Å^2 at 60 eV, rose to 5.250 Å^2 at 70 eV and then decreased steadily with increasing incident energy (Fig. 4); those for Barium decreased steadily to 6.593 Å^2 at 20 eV, rose to 6.741 Å^2 at 30 eV and then decreased steadily with increasing incident energy (Fig. 5); and those for Radium fluctuated between 1 to 30 eV, remained the same at 50 and 60 eV, and thereafter decreased steadily with increasing incident energy (Fig. 6). Barium has the largest value of TCS of 15.610 Å^2 at 1 eV, while Magnesium recorded the smallest, 0.966 Å^2 at 1000 eV.

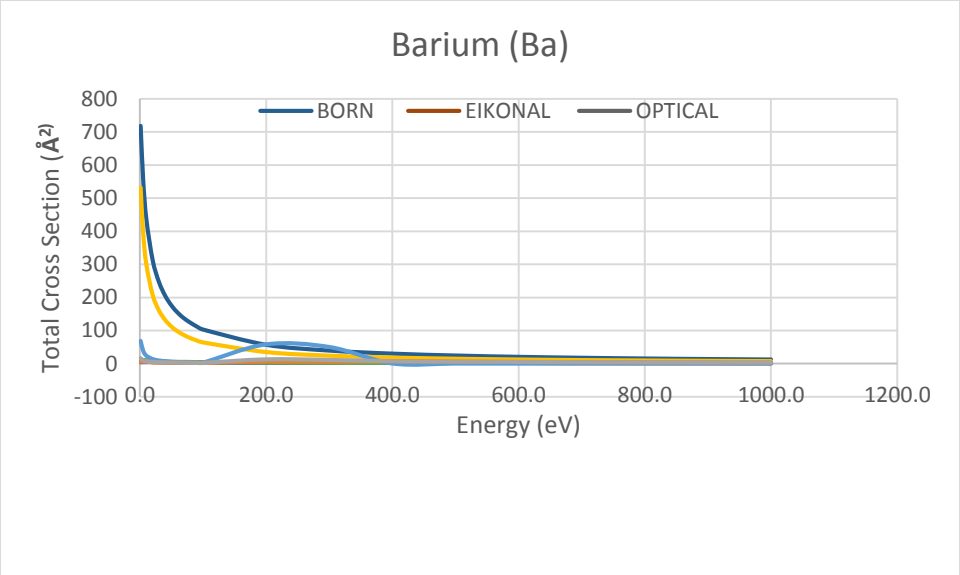

Fig. 5: TCS for Barium using Born, Eikonal and Optical Theorem approximations

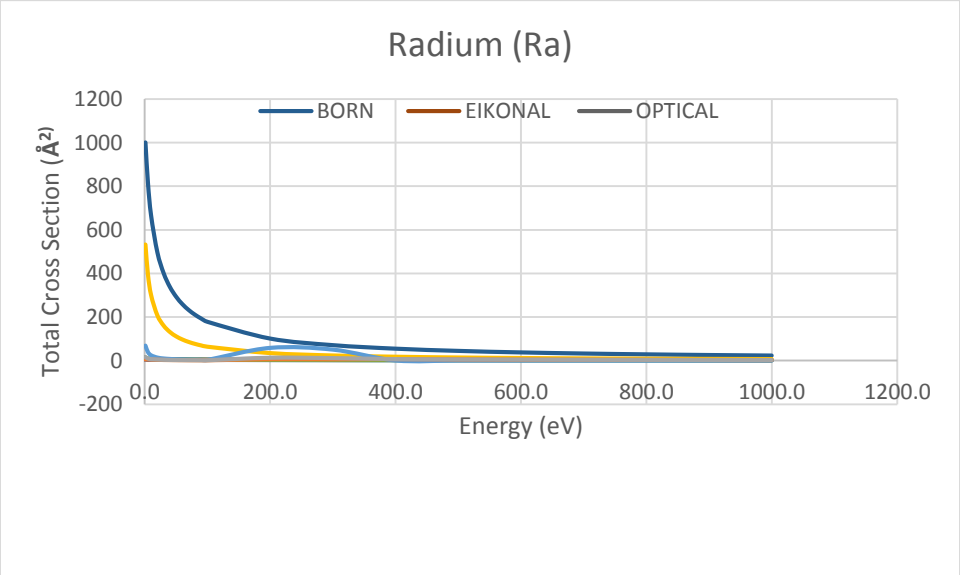

Fig. 6: TCS for Radium using Born, Eikonal and Optical Theorem approximations

The calculated TCS using Eikonal and Optical theorem approximation methods are in good agreement with the TCS calculated by Cox and Bonham (1967). However TCS calculated using the Born approximation method are much higher than the values for the energy range considered. This is because the Born approximation is only valid at high electron incident energies (Babaji *et al.*, 2012). Results obtained using the Eikonal and Optical theorem methods are in good agreement with the experimental TCS values (NIST SRD 64, 2016).

CONCLUSION

Computed Total Cross-Sections (TCS) of elastic electron-atom scattering for the alkaline earth metals have been computed using the Born, Eikonal and the Optical theorem approximation methods with the Lenz-Jensen potential, at incident energies of 1to1000 eV. Results obtained using the Eikonal and Optical theorem methods are in good agreement with the experimental TCS values.

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