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Computations of Scattering Cross Sections for He, Ne, Ar, Kr, Xe and Rn

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ABSTRACT

Calculated Total Cross-Sections (TCS) of elastic electron-atom scattering for He, Ne, Ar, Kr, Xe and Rn are presented. The computed TCS were calculated using the partial wave, Eikonal, Born, and the optical theorem approximation methods with the Lenz-Jensen potential, at electron incident energies between 1to1000 eV. Results obtained using the partial wave, Eikonal and optical theorem approximation methods are in good agreement with experimental TCS data of Van den Biesen *et al* (1982).

Keywords: Total Cross-Sections, elastic scattering, noble gases, partial wave, Eikonal, optical theorem, Born approximation.

INTRODUCTION

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 (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 noble gases He, Ne, Ar, Kr, Xe and Rn (Halka *&* Nordstrom, 2010; Ramazanov *et al,* 2007) were computed using the four approximation methods listed above.

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. 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

$$E = \frac{\hbar^2 k^2}{2m} > 0 \qquad 1.0$$

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

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \qquad 2.0$$

with the boundary condition at large distance

$$\psi_{r\to\infty} \to e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \qquad 3.0$$

Equation (3.0) 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. The differential cross-section is given by:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \qquad 4.0$$

The total cross-section is

$$\sigma = \int d\Omega \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = 2\pi \int_0^{\pi} \mathrm{d}\theta \sin\theta |f(\theta)|^2 \qquad 5.0$$

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).

Partial Wave Method

The method of partial wave expansion is a special trick to simplify the calculation of the scattering amplitude, f (Newton, 1982). The standard partial wave decomposition of the scattering wave function ψ is

$$\psi(r) = \sum_{l=0}^{\infty}(2l+1)i^l e^{i\sigma}\frac{R_l(r)}{kr}P_l(cos\theta) \qquad 6.0$$

When equation (2.6) is substituted into the SWE (2.0) the radial wave functions, R_l are found to satisfy the radial differential equations:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right]R_l(r) = 0 \qquad 7.0$$

This is the same equation as that satisfied by a bound state wave function but the boundary conditions are different. In particular, R vanishes at the origin, but it has the large-r asymptotic behaviour

$$R_l \to kr[cos\delta_l j_l(kr) - sin\delta_l n_l(kr)] \qquad 8.0$$

Where j_l and n_l are the regular and irregular spherical Bessel functions of order l.
The scattering amplitude is related to the phase shifts δ_l by [9]:

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}sin\delta_l P_l(cos\theta) \qquad 9.0$$

From equations (5.0) and (9.0) the total cross-section is given by

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)sin^2\delta_l \qquad 10.0$$

Although the sums in equations (9.0) and (10.0) extend over all l, they are in practice limited to only a finite number of partial waves. This is because for large l, the repulsive centrifugal potential in equation (7.0) is effective in keeping the particle outside the range of the potential and so the phase shift is very small.

If the potential is negligible beyond a radius r_{max}, an estimate of the highest partial wave that is important is had by setting the turning point at this radius:

$$\frac{l_{max}(l_{max}+1)\hbar^2}{2mr_{max}^2} = E \qquad 11.0$$

$$\Rightarrow l_{max} \approx kr_{max} \qquad 12.0$$

This estimate is usually slightly low since the penetration of the centrifugal barrier leads to non-vanishing phase shifts in partial waves somewhat higher than this (Koonin & Meredith, 1989).

The Phase shifts

To find the phase shift in a given partial wave, we must solve the radial equation (7.0). The equation is linear, so that the boundary condition at large r can be satisfied simply by appropriately normalizing the solution.

If we put $R_l(r=0) = 0$ and take the value at the next lattice point, $R_l(r=h)$, to be any convenient small number we then use

$$f'' \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2} \qquad 13.0$$

for $R_l''(h)$, along with the known values $R_l(0)$, $R_l(h)$, and $k(h)$ to find $R_l(2h)$.
Now we can integrate outward in r to a radius $r^{(1)} > r_{max}$. Here, V vanishes and R must be a linear combination of the free solutions, $krj_l(kr)$ and $krn_l(kr)$:

$$R_l^{(1)} = Akr^{(1)}\left[cos\delta_l j_l(kr^{(1)}) - sin\delta_l n_l(kr^{(1)})\right] \qquad 14.0$$

Although the constant, A above, depends on the value chosen for $R(r=h)$, it is largely irrelevant for our purposes; however, it must be kept small enough so that overflows are avoided. Now we continue integrating to a larger radius $r^{(2)} > r^{(1)}$:

$R_l^{(2)} = Akr^{(2)}[cos\delta_l j_l(kr^{(2)}) - sin\delta_l n_l(kr^{(2)})]$ 15.0

Equations (14.0) and (15.0) can then be solved for δ_l to obtain

$tan\delta_l = \frac{Gj_l^{(1)} - j_l^{(2)}}{Gn_l^{(1)} - n_l^{(2)}}; G = \frac{r^{(1)}R_l^{(2)}}{r^{(2)}R_l^{(1)}}$ 16.0

where $j_l^{(1)} = j_l(kr^{(1)}$ etc. Equation (16.0) determines δ_l only within a multiple of π but this does not affect the physical observables [see equations (9.0) and (10.0)]. The correct multiple of π's at a given energy can be determined by comparing the number of nodes in R and in the free solution, krj_l which occur for $r < r_{max}$. The phase shift in each partial wave vanishes at high energies and approaches $N_l\pi$ at zero energy, where N_l is the number of bound states in the potential in the l'th partial wave (Koonin & Meredith, 1989).

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, as the reaction probabilities are small in comparison to elastic scattering, for many purposes 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}**.** A very accurate approximation to this potential can be had by solving for the self-consistent Hartree-Fock potential of the neutral atom. However, a much simpler estimate can be obtained using an approximation to the Thomas-Fermi model of the atom given by Lenz and Jensen (Blister & Hautala, 1978)

$V = -\frac{Ze^2}{r}e^{-x}(1 + x + b_2x^2 + b_3x^3 + b_4x^4);$ 17.0

with

$e^2 = 14.409;\ b_2 = 0.3344;\ b_3 = 0.0485;\ b_4 = 2.647 \times 10^{-3};$ 18.0

and

$x = 4.5397Z^{\frac{1}{6}}r^{\frac{1}{2}}$ 19.0

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. It begins with a title page describing the physical problem to be investigated and the output that will be produced. Next, the menu is displayed, giving the choice of entering parameter values, examining parameter values, running the program, or terminating the program. When the calculation is finished, all values are zeroed (except default parameters), and the main menu is re-displayed, giving us the opportunity to redo the calculation with a new set of parameters or to end execution. Data generated from the program were saved in files which were later imported into the graphics software *Origin 5.0* for plotting.

RESULTS

Results were generated for several electron incident energies as presented in the tables below:

From table 1 below, using the partial wave method, we observed that the TCS for He decrease with increasing electron incident energies from 1 to 1,000 eV. The TCS for Ne, Ar, Xe and Rn exhibited a number of minima and maxima between 1 to 100 eV, but decrease with increasing incident energies between 100 to 1,000 eV. Also, the TCS increase with increasing atomic number for all elements considered. The differences in TCS for He, in the energy range of about 70 to 1,000 eV, are substantially higher than differences in TCS for other noble gases. This might have resulted from the fact that He has an "S" valance shell only while all the others have "P" valence shells.

Table 1: Computed Total Cross-Sections for Elastic Electron- Atom Scattering for He, Ne, Ar, Kr, Xe and Rn using the Partial Wave Method with the Lenz-Jensen Potential.

	ELEMENT					
E (eV)	He	Ne	Ar	Kr	Xe	Rn
1.0	7.553	8.651	27.289	34.350	1.065	2.615
5.0	7.532	2.023	36.882	25.574	44.328	3.328
10.0	6.728	3.184	19.513	14.571	5.089	5.091
20.0	4.686	4.815	11.903	7.024	10.461	13.309
30.0	3.577	5.154	9.844	4.825	5.900	12.120
40.0	2.879	5.086	8.559	3.917	5.238	9.873
50.0	2.400	4.882	7.468	3.526	5.285	8.611
60.0	2.058	4.629	6.599	3.381	5.547	7.870
70.0	1.803	4.380	5.936	3.354	5.854	7.375
80.0	1.604	4.152	5.418	3.371	6.107	6.997
90.0	1.444	3.943	5.001	3.403	6.260	6.679
100.0	1.313	3.751	4.664	3.436	6.298	6.401
200.0	0.687	2.571	3.137	3.278	4.344	4.768
300.0	0.463	2.010	2.548	2.903	3.366	4.001
400.0	0.350	1.679	2.197	2.608	2.910	3.410
500.0	0.281	1.452	1.950	2.379	2.620	2.967
600.0	0.234	1.286	1.764	2.197	2.409	2.656
700.0	0.201	1.157	1.617	2.047	2.245	2.436
800.0	0.176	1.054	1.497	1.923	2.113	2.274
900.0	0.156	0.969	1.396	1.818	2.002	2.149
1,000.0	0.141	0.897	1.311	1.727	1.908	2.049

From table 2 , using the Eikonal method, the TCS for He also decrease with increasing electron incident energies from 1 to 1,000 eV. The TCS for Ne, Ar, kr, Xe and Rn exhibited a number of minima and maxima between 1 to 30 eV, but decrease with increasing incident energies between 30 to 1,000 eV. Also, the TCS increase with increasing atomic number for all elements considered. The differences in TCS for He, in the energy range of about 50 to 1,000 eV, are substantially higher than differences in TCS for other noble gases.

Table 2: Computed Total Cross-Sections for Elastic Electron- Atom Scattering for He, Ne, Ar, Kr, Xe and Rn using the Eikonal Approximation Method with the Lenz-Jensen Potential..

	ELEMENT					
E (eV)	He	Ne	Ar	Kr	Xe	Rn
1.0	4.784	6.203	3.797	4.691	4.951	4.424
5.0	4.755	6.686	6.448	4.914	4.991	3.083
10.0	4.335	5.490	6.526	5.079	7.331	5.188
20.0	3.440	4.809	4.602	6.267	3.990	3.103
30.0	2.698	4.632	5.066	4.305	5.156	4.289
40.0	2.191	4.268	4.330	3.949	4.300	4.689
50.0	1.834	3.740	3.913	4.103	3.600	4.386
60.0	1.573	3.538	3.895	4.444	3.614	3.908
70.0	1.376	3.424	3.962	4.393	3.519	3.269
80.0	1.222	3.286	3.799	3.989	3.756	2.990
90.0	1.098	3.130	3.566	3.643	3.799	3.042
100.0	0.997	2.981	3.379	3.423	3.873	3.221
200.0	0.518	2.164	2.640	3.046	2.717	3.101
300.0	0.350	1.746	2.211	2.575	2.704	2.388
400.0	0.264	1.486	1.927	2.197	2.570	2.466
500.0	0.212	1.308	1.735	2.055	2.305	2.348
600.0	0.177	1.175	1.589	1.986	2.018	2.283
700.0	0.152	1.070	1.469	1.920	1.925	2.254
800.0	0.133	0.983	1.369	1.825	1.864	2.178
900.0	0.119	0.910	1.283	1.716	1.799	2.083
1,000.0	0.107	0.848	1.208	1.610	1.734	1.932

From table 3, using the Born method, the calculated TCS are significantly higher than the TCS obtained using the three other approximation methods. This is as a result of the fact that the Born approximation is only valid at high electron incident energies. As previously observed, the calculated TCS decrease with increasing incident energies but no minima and maxima were observed for all the elements considered.

Table 3: Computed Total Cross-Sections for Elastic Electron- Atom Scattering for He, Ne, Ar, Kr, Xe and Rn using the Born Approximation Method with the Lenz-Jensen Potential..

	ELEMENT					
E (eV)	He	Ne	Ar	Kr	Xe	Rn
1.0	30.950	171.100	289.500	510.100	698.500	990.400
5.0	16.070	108.600	197.200	376.300	538.500	800.300
10.0	9.415	73.420	140.600	285.000	422.300	652.000
20.0	5.121	45.300	91.110	196.200	301.600	485.700
30.0	3.518	33.080	68.170	151.400	237.400	391.600
40.0	2.665	26.060	54.570	123.600	196.500	329.600
50.0	2.143	21.520	45.580	104.700	168.100	285.400
60.0	1.791	18.350	39.180	91.000	147.100	252.100
70.0	1.538	16.000	34.380	80.510	130.900	226.000
80.0	1.346	14.180	30.630	72.220	118.000	205.000
90.0	1.197	12.730	27.630	65.500	107.400	187.600
100.0	1.078	11.550	25.160	59.940	98.640	173.100
200.0	0.539	5.995	13.340	32.570	54.580	98.170
300.0	0.359	4.046	9.086	22.400	37.840	68.820
400.0	0.270	3.051	6.890	17.080	28.990	53.060
500.0	0.216	2.448	5.549	13.810	23.500	43.190
600.0	0.180	2.044	4.646	11.590	19.760	36.440
700.0	0.154	1.754	3.995	9.982	17.050	31.510
800.0	0.134	1.536	3.504	8.767	14.990	27.760
900.0	0.120	1.366	3.120	7.816	13.380	24.810
1,000.0	0.108	1.230	2.812	7.051	12.080	22.430

From table 4 and fig. 4, using the optical theorem method, the calculated TCS for Kr, Xe and Rn exhibited a number of minima and maxima in the energy range of 1 to 100 eV. No minima or maxima were observed for He, Ne and Ar. Here also, the calculated TCS decrease with increasing electron incident energies.

The calculated TCS using the partial wave, Eikonal and optical theorem approximation methods are generally in good agreement with the experimental TCS obtained by Van den Biesen et al (1982). However TCS calculated using the Born approximation method are much higher than the experimental values for the energy range considered. This is because the Born approximation is only valid at high electron incident energies.

Table 4: Computed Total Cross-Sections for Elastic Electron- Atom Scattering for He, Ne, Ar, Kr, Xe and Rn using the Optical Theorem with the Lenz-Jensen Potential.

	ELEMENT					
E (eV)	He	Ne	Ar	Kr	Xe	Rn
1.0	14.100	17.970	14.720	15.650	15.030	14.780
5.0	7.362	11.110	10.930	10.040	9.741	7.424
10.0	5.558	8.350	9.390	8.464	9.859	8.527
20.0	3.760	6.477	6.622	7.953	6.482	5.435
30.0	2.810	5.683	6.430	6.072	6.788	6.237
40.0	2.236	5.115	5.550	5.362	5.767	6.063
50.0	1.854	4.494	4.900	5.217	4.802	5.668
60.0	1.583	4.126	4.592	5.266	4.864	5.117
70.0	1.381	3.893	4.539	5.262	4.563	4.269
80.0	1.224	3.692	4.402	4.823	4.613	3.837
90.0	1.100	3.500	4.165	4.353	4.606	3.997
100.0	0.998	3.321	3.932	4.076	4.596	4.062
200.0	0.518	2.310	2.862	3.408	3.188	3.690
300.0	0.350	1.834	2.381	2.763	2.978	2.598
400.0	0.264	1.541	2.019	2.384	2.812	2.662
500.0	0.212	1.343	1.800	2.193	2.436	2.536
600.0	0.177	1.198	1.646	2.095	2.121	2.491
700.0	0.152	1.085	1.522	1.995	1.997	2.402
800.0	0.133	0.994	1.416	1.874	1.918	2.242
900.0	0.119	0.918	1.324	1.751	1.856	2.078
1,000.0	0.107	0.853	1.244	1.640	1.803	1.904

CONCLUSION

Computed Total Cross-Sections (TCS) of elastic electron-atom scattering for the elements He, Ne, Ar, Kr, Xe and Rn are presented. The TCS were calculated using the partial wave, Eikonal, Born, and the optical theorem approximation methods with the Lenz-Jensen potential, at incident energies of 1to1000 eV. Results obtained using the partial wave, Eikonal and optical theorem methods are in good agreement with the experimental TCS values.

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