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Full Length Research Article

COMPUTATION OF THE TOTAL SCATTERING CROSS SECTIONS FOR THE HALOGENS

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ABSTRACT
Calculated Total Cross-Sections (TCS) of elastic electron-atom scattering for F, Cl, Br, I and At 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 1to1000 eV. Results obtained are in good agreement with experimental TCS data.

Keywords: Total Cross-Section, elastic scattering, halogens, optical theorem, Born approximation, Eikonal 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 halogens Flourine (F), Chlorine (I), Bromine (Br), Iodine (I) and Astatine (At) (Halka & Nordstrom, 2010) were computed using the three approximation methods named 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 (Babaji, Abdu & Taura, 2012). The differential cross-section is given by:

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

The total cross-section is

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

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 behavior

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

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:

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

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

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 $krn_l(kr)$:

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

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 $r^{(2)} > r^{(1)}$:

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

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

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

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)

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

with

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

and

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

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.

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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.

RESULTS AND DISCUSSION

Results were generated for several electron incident energies as presented in tables 1-3 below:

Table 1: Computed Total Cross-Sections for Elastic Electron-Atom Scattering for F, Cl, Br, I and At Using the Born Approximation Method with the Lenz-Jensen Potential.

	TOTAL CROSS SECTION (ANGSTROMS**2)				
E (eV)	F	Cl	Br	I	At
1.0	155.100	275.700	521.200	688.800	981.900
5.0	97.240	186.600	385.700	529.900	792.500
10.0	65.130	132.300	292.800	414.900	645.100
20.0	39.860	85.370	202.000	295.700	480.100
30.0	28.990	63.730	156.100	232.500	386.800
40.0	22.780	50.940	127.600	192.400	325.500
50.0	18.780	42.500	108.200	164.500	281.700
60.0	15.990	36.510	94.030	143.900	248.800
70.0	13.930	32.010	83.220	128.000	223.000
80.0	12.330	28.510	74.670	115.400	202.200
90.0	11.060	25.700	67.740	105.000	185.100
100.0	10.030	23.400	62.000	96.410	170.700
200.0	5.192	12.390	33.730	53.300	96.760
300.0	3.499	8.430	23.210	36.940	67.810
400.0	2.637	6.391	17.710	28.290	52.270
500.0	2.115	5.146	14.310	22.930	42.550
600.0	1.765	4.307	12.010	19.280	35.890
700.0	1.514	3.703	10.350	16.630	31.040
800.0	1.326	3.248	9.091	14.630	27.340
900.0	1.179	2.892	8.105	13.050	24.440
1,000.0	1.061	2.607	7.312	11.780	22.090

From table 1, using the Born method, the calculated TCS are significantly higher than those obtained using the two other approximation methods as reported by Babaji *et al.* (2012). This is as a result of the fact that the Born approximation is only valid at high electron incident energies. As observed, the calculated TCS of all the Halogens (F, Cl, Br, I and At) decrease with increasing incident energies from 1 to 1000 eV. Also, the calculated TCS increase with increasing atomic number (Z) for all the Halogens.

Table 2: Computed Total Cross-Sections for Elastic Electron-Atom Scattering for F, Cl, Br, I and At Using the Eikonal Approximation Method with the Lenz-Jensen Potential.

	TOTAL CROSS SECTION (ANGSTROMS**2)				
E (eV)	F	Cl	Br	I	At
1.0	6.071	4.250	4.431	5.049	4.557
5.0	6.891	6.587	5.028	4.836	3.207
10.0	5.842	6.442	4.851	7.456	5.353
20.0	4.689	4.902	6.137	4.004	3.159
30.0	4.681	4.982	4.258	5.208	4.228
40.0	3.993	4.219	3.906	4.216	4.792
50.0	3.704	3.918	4.038	3.627	4.418
60.0	3.525	4.031	4.295	3.587	3.908
70.0	3.340	3.957	4.447	3.561	3.251
80.0	3.165	3.705	4.062	3.787	2.999
90.0	3.012	3.485	3.714	3.831	3.049
100.0	2.879	3.313	3.455	3.893	3.267
200.0	2.052	2.164	3.081	2.733	3.104
300.0	1.650	2.161	2.622	2.716	2.383
400.0	1.410	1.889	2.204	2.581	2.483
500.0	1.240	1.701	2.055	2.276	2.333
600.0	1.110	1.555	1.979	2.004	2.293
700.0	1.006	1.434	1.925	1.992	2.247
800.0	0.919	1.332	1.842	1.862	2.175
900.0	0.847	1.245	1.738	1.793	2.072
1,000.0	0.785	1.171	1.633	1.730	1.911

From table 2, using the Eikonal method, the TCS for F exhibited a single maxima 5 eV, then decrease with increasing incident energy between 5 to 1000 eV. The TCS for Cl, Br and I exhibited a number of minima and maxima between 1 to 100 eV, then decrease with increasing incident energy between 100 to 1000 eV. Those for At exhibited a number of minima and maxima between 1 to 400 eV, then decrease with increasing incident energy. Here, the calculated TCS increase with increasing atomic number (Z) for all the Halogens only for incident energies greater than 400 eV.

Table 3: Computed Total Cross-Sections for Elastic Electron-Atom Scattering for F, Cl, Br, I and At Using the Optical Theorem with the Lenz-Jensen Potential.

	TOTAL CROSS SECTION (ANGSTROMS**2)				
E (eV)	F	Cl	Br	I	At
1.0	16.940	15.850	15.080	15.110	15.170
5.0	11.100	11.030	10.090	9.616	7.612
10.0	8.497	9.312	8.288	9.886	8.634
20.0	6.299	6.775	7.814	6.437	5.512
30.0	5.661	6.344	6.041	6.803	6.212
40.0	4.853	5.432	5.374	5.703	6.138
50.0	4.370	4.834	5.178	4.806	5.695
60.0	4.054	4.670	5.165	4.842	5.125
70.0	3.789	4.573	5.279	4.555	4.193
80.0	3.557	4.332	4.897	4.668	3.868
90.0	3.357	4.073	4.440	4.622	4.012
100.0	3.185	3.847	4.092	4.617	4.116
200.0	2.190	2.845	3.382	3.213	3.698
300.0	1.723	2.316	2.805	2.991	2.596
400.0	1.449	1.973	2.392	2.809	2.639
500.0	1.263	1.765	2.196	2.402	2.532
600.0	1.123	1.612	2.090	2.112	2.500
700.0	1.014	1.485	2.003	1.997	2.394
800.0	0.924	1.377	1.893	1.919	2.234
900.0	0.850	1.284	1.775	1.856	2.064
1,000.0	0.787	1.204	1.664	1.804	1.886

From table 3, using the Optical theorem method, the calculated TCS for F, Cl, and Br decrease with increasing incident energy between 1 to 1000 eV, except for Br at 70 eV. Those for I exhibited a number of minima and maxima in the energy range 1 to 80 eV, then decrease with increasing incident energy between 80 to 1000 eV. The TCS for At exhibited a number of minima and maxima in the energy range 1 to 400 eV, then decrease with increasing incident energy between 400 to 1000 eV.

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).

Conclusion

Computed Total Cross-Sections (TCS) of elastic electron-atom scattering for the halogens 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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