A Thesis

entitled

Calculation of Total Electron Excitation Cross-Sections and Partial Electron Ionization Cross-Sections for the Elements

by

T. J. Greene

as partial fulfillment of the requirements of the Doctor of Philosophy Degree in Physics and Astronomy

The University of Toledo
December, 1973
A Thesis

entitled

Calculation of Total Electron Excitation Cross-Sections and Partial Electron Ionization Cross-Sections for the Elements

by

T. J. Greene

as partial fulfillment of the requirements of the Doctor of Philosophy Degree in Physics and Astronomy

Advisor

Dean of the Graduate School

The University of Toledo
December, 1973
ABSTRACT

Computer programs are used to calculate the total electron excitation cross-section for atoms and the partial ionization cross-section. The calculation is done in the following manner. Each of the approximations listed below results in an expression for a scattering amplitude, involving the atomic wave function of the target. These amplitudes are simply related to the differential cross-sections which are integrated to give the total excitation (or partial ionization) cross-section for the collision.

The approximations to the scattering amplitude used are:

Non-Exchange Excitation:
1) Born
2) Bethe
3) Modified Bethe

Exchange Excitation
1) Ochkur

Non-Exchange Ionization
1) Coulomb - Born.

The atomic wave functions used are Hartree-Fock-Slater, (HFS) functions for bound states and the coulomb wave function for the continuum.

The programs are presented and some results are examined.
ACKNOWLEDGEMENTS

It is a great pleasure to thank Dr. William Williamson for introducing me to this problem and for his continued guidance, criticism, and patience. The funds provided by NASA Contract No. NGR 36-010-017 in support of this research are gratefully acknowledged. The encouragement and assistance of Dr. Y. Kondo and Dr. R. Kovar and other people of the M.S.C. group during the work done at Houston was of great assistance.

Finally, I wish to thank my wife, Edna, for her constant support, encouragement, patience, and assistance during the many difficulties encountered in this research.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Number</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>i</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>ii</td>
</tr>
<tr>
<td>TABLE OF CONTENTS</td>
<td>iii</td>
</tr>
<tr>
<td>I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1. History and Significance of the Problem</td>
<td>1</td>
</tr>
<tr>
<td>II. WAVE FUNCTIONS</td>
<td>5</td>
</tr>
<tr>
<td>1. Bound State Wave Functions</td>
<td>6</td>
</tr>
<tr>
<td>2. Continuum Wave Functions</td>
<td>14</td>
</tr>
<tr>
<td>III. EXCITATION CROSS-SECTIONS</td>
<td>17</td>
</tr>
<tr>
<td>1. The General Problem</td>
<td>17</td>
</tr>
<tr>
<td>2. The Born-Approximation Solution</td>
<td>20</td>
</tr>
<tr>
<td>3. The Bethe-Approximation Solution</td>
<td>25</td>
</tr>
<tr>
<td>4. The Modified-Bethe Approximation</td>
<td>27</td>
</tr>
<tr>
<td>5. The Ochkur Approximation</td>
<td>32</td>
</tr>
<tr>
<td>6. Summary of the Excitation Cross-Section Expressions Used in the Computer Programs</td>
<td>38</td>
</tr>
<tr>
<td>IV. IONIZATION CROSS-SECTION</td>
<td>41</td>
</tr>
<tr>
<td>1. Relationship Between Ionization and Excitation Expressions</td>
<td>41</td>
</tr>
<tr>
<td>2. The Born-Coulomb Approximation</td>
<td>41</td>
</tr>
<tr>
<td>3. The Expression Used in the Computer Programs</td>
<td>45</td>
</tr>
<tr>
<td>V. COMPUTER PROGRAMS</td>
<td>47</td>
</tr>
<tr>
<td>1. Wave-Function Program</td>
<td>47</td>
</tr>
<tr>
<td>a) Listing</td>
<td>47</td>
</tr>
<tr>
<td>b) Discussion</td>
<td>65</td>
</tr>
<tr>
<td>Number</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>------</td>
</tr>
<tr>
<td>i) Herman-Skillman Program</td>
<td>65</td>
</tr>
<tr>
<td>ii) Modifications for This Calculation</td>
<td>68</td>
</tr>
<tr>
<td>2. Excitation Cross-Section Program</td>
<td>69</td>
</tr>
<tr>
<td>a) Listing</td>
<td>69</td>
</tr>
<tr>
<td>b) Discussion</td>
<td>80</td>
</tr>
<tr>
<td>3. Ionization Cross-Section Program</td>
<td>84</td>
</tr>
<tr>
<td>a) Listing</td>
<td>84</td>
</tr>
<tr>
<td>b) Discussion</td>
<td>91</td>
</tr>
</tbody>
</table>

VI. SOME SAMPLE RESULTS FOR EXCITATION | 93 |
| 1. Table | 93 |
| a) Alkali | 93 |
| b) Inert | 121 |
| 2. Discussion | 129 |

VII. SAMPLE RESULTS FOR IONIZATION | 132 |
| 1. Table | 132 |
| 2. Discussion | 141 |

VIII. CONCLUSIONS AND FUTURE RESEARCH | 143 |

IX. REFERENCES | 145 |

X. APPENDIXES | 149 |
| Appendix I - Notation | 150 |
| Appendix II - Atomic Units | 151 |
| Appendix III - 3-j Symbol Identity | 153 |
| Appendix IV - Equivalent Bethe Approximations | 155 |
| Appendix V - Partial Wave Analysis | 158 |
| Appendix VI - Ochkur Expression of $f_e(n)$ | 163 |
| Appendix VII - User Manual | 166 |
I. INTRODUCTION

1. History and Significance of the Problem.

The purpose of this research is to calculate the total electron excitation cross-section and the partial ionization cross-section for atoms. Symbolically the excitation process is written:

\[ Z(n_i l_i m_i) + e \rightarrow Z(n_f l_f m_f) + e \]  \hspace{1cm} (1)

The problems of computing excitation and ionization cross-sections have been of interest for some time. An attempt to compute cross-sections for excitations to the continuum (i.e. ionization) was made by Thomson in (1912). His classical theory of ionization of atoms has been recently restudied by Rudge (1968) as a result of a renewal of interest in semiclassical calculations as approximations to more elaborate quantum mechanical calculations.

Some of the early papers in Quantum Mechanics were also concerned with the problem of atomic excitation calculations. The papers of Born in (1926) and Oppenheimer in (1928) are particularly noteworthy.

As the field of astrophysics has advanced in sophistication interest in atomic cross-section calculations has further increased. Bates mentioned in (1950) that quantitative information on the cross-section associated with excitation and ionization by electrons is necessary in connection with several astrophysical problems. In particular such information is necessary for an understanding of the observed spectral characteristics of aurorae and in connection with investigations of the solar corona and gaseous nebulae. The subject
of gaseous nebulae is discussed by Cyszak (1968) who mentions that accurate transition probabilities and collisional cross-sections are necessary for proper interpretation of the properties of nebulae.

These are some of the needs for excitation cross-sections. There are two methods of determining such cross-sections: experimental measurements or theoretical calculations.

Certain inelastic collisions of electrons with atoms have been studied experimentally and some cross-section information has been obtained (Kieffer (1967)), but experimental measurements, particularly of the absolute values of the excitation cross-sections, are in general very difficult. Furthermore, exceptional difficulties are encountered in the experimental measurements in many cases of particular interest (Heddle (1968)).

Three main categories of experimental methods have been used (see Moiseiwhitsch and Smith (1968)). In the first method intensities of spectral lines excited by an electron beam are measured. The measurements in this case effectively determine an optical excitation function as opposed to the desired electron excitation cross-section. The fundamental differences between these two quantities arise due to the effects in the photon measurements of cascades from higher levels with several channels for decay, which produce an anisotropic radiation pattern. A principal problem in these measurements is absolute calibration of the optical system.

A second method is based on the deactivation of "metastable" states at a metal target. The electrons ejected from the metal target provide information. The difficulties of this method are connected with determining the efficiency of collection and conversion of metastable atoms at
the metal target.

The third experimental method involves a study of the energy loss spectrum of scattered electrons. Here an electron beam of definite energy is passed through a gas and the energy spectrum of electrons scattered at a particular angle with respect to the beam axis is measured by use of an electron energy analyzer. The principal difficulties here arise from the necessity of taking data at many angles as well as over a range of energies.

As is pointed out by Bely (1970), reviews of experimental methods have been written by Fite (1962), Moiseiwitsch and Smith (1968), and Hedde and Kessing (1968).

The difficulties encountered in a theoretical approach are immediately obvious in view of the fact that an electron target atom system is essentially a many-body system. The particular difficulties involved and the approximations made in an attempt to overcome these difficulties will be one of the concerns of the present research.

At the outset we are forced to recognize that the problem of electron impact excitation of atoms is so complex that, even for the case of electron collisions with atomic hydrogen, there is no exact solution known for the excitation cross-section of the two lowest states. Therefore, to assess the accuracy of various approximate calculations the only method available is that of comparing the cross-sections obtained in the various calculations with one another and with the limited experimental data available.

The data that is available, both experimental and theoretical, has recently been collected by the Information Center of the Joint Institute
of Laboratory Astrophysics (JILA), and the Oak Ridge Atomic and Molecular Information Center. A series of reports published by JILA emphasize that for many elements and transitions there is in fact no data available (see Kieffer (1967)).

This fact is again emphasized in a recent article by Athay (1972). The author states, "We have no information either experimental or theoretical of collision cross-sections for (these) forbidden transitions."

Motivated by the need (expressed in particular by astrophysicists) but restricted by the complexity of the problem, the present research obtains inexact but reasonable excitation cross-section values for all elements by use of various approximations.
II. WAVE FUNCTIONS

A fundamental difficulty in any problem involving atoms is that of obtaining accurate atomic wave functions. These are the solutions to the problem:

\[ H\phi_A = E_A\phi_A \]  

(2)

where \( H \) is the Hamiltonian operator incorporating all of the interactions of the constituents of the atom and the \( \phi_A \) are the eigensolutions of this operator for the eigenvalues \( E_A \).

The exact treatment of this problem requires the use of the proper Dirac Hamiltonian (i.e. the inclusion of relativistic effects) but this problem is so complex that the following assumptions are commonly made:

I. It is assumed that the Dirac Hamiltonian can be approximated by the Schröedinger Hamiltonian. (This allows the wave function to be represented by a single function rather than the matrix of four functions required by the Dirac equation.)

II. It is assumed that the particles move independently. (This allows the total wave function for the system of particles to be written as a product of one particle wave functions).

III. It is assumed the electrons move in a central field due to the nucleus and all other electrons. (This allows the one particle wave functions to be separated into radial and angular components).
The separation of the radial and angular parts of the wave functions allowed by assumption III gives two equations. The spherical harmonics are the solutions of the angular equation. Thus the problem is reduced to finding the radial wave functions which solve the remaining radial equation.

We would expect these assumptions would be less valid and therefore our wave functions less accurate where

- relativistic effects are significant (i.e. Large Z)
- electron - electron interactions are more significant
  (i.e. large occupation numbers for given orbitals).

These expectations are confirmed by the comparison of experimental and theoretical energy values given by Herman and Skillman (1963) in Chapter (3) of their work.

1. Bound State Wave Functions

A technique for finding the radial wave functions for bound state electrons was developed by Hartree. His treatment involves assuming a form for the central field, solving the radial equations for the one particle wave functions, finding the field due to these wave functions and then comparing the calculated field with the assumed field. Where the two fields agree, to within some previously specified tolerance, the problem is considered solved. Otherwise, where the two fields do not sufficiently agree, the calculation is begun again using the computed field as the assumed field and computing a new field. The procedure is repeated until the desired agreement is obtained.

The Schröedinger Hamiltonian for an n-electron atom is given in atomic units (see Appendix II) as:
\[ H = -\frac{1}{2} \sum_{i=1}^{n} \nabla_i^2 - \sum_{i=1}^{n} \frac{Z}{r_i} + \sum_{ij} \frac{1}{r_{ij}} \]  

The prime indicates that the summation is over all pairs, each pair being included once and the term \( i=j \) being omitted.

In the Hartree model the total wave function for the system is assumed to be a product of single electron wave functions.

\[ \phi = \phi_a(\vec{r}_i) \cdots \phi_z(\vec{r}_n) \]  

The third term in \( H \) represents the electron-electron interaction. The charge density of the \( j \)th-electron is \( |\phi(r_j)|^2 \). We can then make the replacement

\[ \sum_{i} \frac{1}{r_{ij}} \rightarrow \sum_{i} \left\{ \sum_{j} \int dr_j \frac{|\phi(r_j)|^2}{r_{ij}} = U(r_i) \right\} \]  

The Schrödinger equation for this system is then

\[ \sum_{i=1}^{n} \left( -\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} + U(r_i) \right) \prod_{k} \phi_{a_k}(\vec{r}_k) = \prod_{k} \phi_{a_k}(\vec{r}_k) \]  

This equation separates into the set of \( n \)-equations

\[ \left[ -\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} + U(r_i) \right] \phi_{a_i}(\vec{r}_i) = E_{a_i} \phi_{a_i}(\vec{r}_i) \]  

(A rigorous derivation of this approximation using a variational principle is given by Slater (1957)).

Let us notice that as assumed in Eq. (5) the spherical harmonics solve the angular equation and the problem remaining is the radial equation:

\[ \left[ \frac{d^2}{dr^2} + (E_n e + \frac{Z}{r} - U(r)) - \frac{\ell(\ell+1)}{r^2} \right] P(N\ell;r) = 0 \]  

For computational ease in the numerical procedures required by the
Hartree model, this equation is traditionally written:

\[
\left\{ \frac{d^2}{dr^2} + \frac{2}{r} \left[ Y(r) + \gamma_o(n\lambda:n\lambda:0) \right] - e_{n\lambda,n\lambda} - \frac{\lambda(\lambda+1)}{r^2} \right\} P(n\lambda:r) = 0 \quad (9)
\]

where

\[
Y(r) = Z - \sum_{n'\lambda'} q(n'\lambda') \gamma_o(n'\lambda':n'\lambda':r)
\]

(10)

and where \(q(n\lambda)\) represents the number of electrons in each shell. \(\gamma_o(n'\lambda':n'\lambda':r)\) is a spherically symmetric charge distribution of radial charge density \(|P(n'\lambda':r)|^2\). Eq. (9) is the Hartree self consistent field equation without exchange (H-EQ).

The Hartree equation may also be derived from the variational principle. For the present purpose the principle is expressed by the statement that if \(\psi\) is an approximate wave function for the ground state of a system described by the Hamiltonian \(H\), the closer \(\psi\) approaches the true eigenfunction of the Hamiltonian the lower the approximate eigenenergy becomes; i.e.

\[
E \leq \int \psi^H \psi \, d\tau / \int \psi^\dagger \psi \, d\tau \quad .
\]

(11)

(For a more detailed statement of the principle see Landau (1958), Hartree (1957) or Gottfried (1966)).

The derivation is then the result of assuming the approximate wave function form \(\psi = \psi_1(\vec{r}_1)\cdots\psi_n(\vec{r}_n)\) and finding the best solutions of the Schrödinger equation by minimizing \(\int \psi^H \psi \, d\tau / \int \psi^\dagger \psi \, d\tau\) subject to the condition \(\int d\vec{r}|\psi(\vec{r})|^2 = 1\). This procedure again results in the Hartree equation and assures us that the Hartree eigenfunctions are the best for the assumed analytic form.

Since the Hartree model assumes that the total wave function, \(\psi_{\lambda}\), is represented by a simple product of single electron wave functions,
it neglects the Pauli principle. Fock improved on the model by requiring that the total wave function be antisymmetric under exchange of any two of the electrons. (See Fock (1930)). The resulting Hartree-Fock model postulates $\Phi_A$ to be a Slater determinant of the form

$$\Phi_A = \frac{1}{n!} \epsilon_{\alpha\beta...\pi} \phi_\alpha(1) \phi_\beta(2) ... \phi_\pi(n)$$

(12)

where the $\phi(i)$ represents products of electron space and spin functions of the form

$$\phi(i) = \psi(\mathbf{r}_i) \chi(\sigma_i)$$

(13)

By application of the variational principle in the Hartree-Fock model, a Hartree-Fock self-consistent field equation (H-F-EQ), is derived which is analogous to the Hartree equation obtained above. The (H-F) equation is: (See Cyszak (1968).)

$$\left[ \frac{d^2}{dr^2} + \frac{2}{r} Y(r) - \epsilon_{n\ell,n\ell} - \frac{\ell(\ell+1)}{r^2} \right] P(n\ell;r) = -2 \int_0^\infty K(n\ell;r,s) P(n\ell;s) ds$$

$$+ \sum_{n'\neq n} \epsilon_{n\ell,n'\ell} P(n'\ell;r)$$

(14)

where $Y(r)$ is defined in Eq. (10). The function $K(n\ell;r,s)$ occurring in this equation is defined by the following relations

$$U_k(r,s) = r^{k+1}$$

where $r^k$ refers to $r$ or $r'$

$$K_k(n'\ell';rs) = P(n'\ell';r) U_k(r,s) P(n'\ell';s)$$

$$K(n\ell;rs) = \sum_{n'\ell'\neq n\ell} K_k(n'\ell';rs) + \sum_{k} a_{k\ell} K_k(n\ell;rs)$$

(15)

where the $a's$ are constants depending on the $P(n\ell;r)$ of interest.
A detailed discussion of the derivation and interpretation of these terms is given by several authors. (In particular the work of Hartree (1957) is useful and the discussion of the Hartree-Fock equation by Cyszak (1968) includes a sample calculation.) For our purpose, it is sufficient to note that the inclusion of exchange couples the equations for the single electron wave functions by introducing the second term on the right-hand side of Eq. (14). Thus, the Hartree-Fock model requires the solution of a coupled set of differential equations and the problem has significantly increased in complexity.

A third model for atomic wave functions which is sometimes used allows for so called "configuration interaction". Recall one of the basic assumptions of the Hartree model is that electrons move independently. Actually the electrons are correlated (see Leighton (1959) or Stevenson (1965)). The correlations are of two types; statistical correlations due to the Pauli Exclusion Principle and coulomb correlations due to the non-central nature of the $1/r_{ij}$ term. The Hartree-Fock model includes statistical correlations by use of determinantal wave functions but ignores coulomb correlations. The coulomb non-central effects together with a spin-spin correlation are discussed in many texts as Russel-Saunders or LS Coupling (see Schiff (1968)). The configuration interaction model is the adoption of an approximate wave function consisting of a linear combination of determinantal wave functions. Since the operators $\hat{L}^2$, $\hat{S}^2$ and Parity commute with the Hamiltonian containing the non-central $1/r_{ij}$ term, (see Condon (1935)), only those configurations of the same $L$, $S$ and Parity are included in
the approximate wave function. This model increases the complexity of
the calculation of the wave functions still further.

Since each of the atomic models involves a self-consistent calcu-
lation, the computations, as might be expected are laborious. The early
computations were done by hand, and a compilation of these calculations
through 1958 is given by Slater (1960).

In the mid 1950's with the advent of relatively high speed comput-
ers Piper (1956) and Vainshtein (1957) made separate attempts to use
the Hartree-Fock model to calculate large numbers of atomic wave func-
tions. In 1963 two authors, Herman and Skillman, produced a calculation
of all ground state atomic wave functions for all elements. Other cal-
culations have since been made by other authors (as referenced in
Cyszak (1968)). These other calculations in general involve two types
of procedures; either an analytic procedure or a numerical procedure.

In the analytic procedure the radial wave functions, $P(n_i \ell_i : r) =
P_i(r)$ are taken to have the general form:

$$P_i(r) = \sum_j c_{ij} \left[ \frac{(2Z_j)^{2l+2}A_j^{+3}}{(2Z_j + 2A_j + Z_j)^{3/2}} \right] r^{l+1} A_j + 2 e^{-Z_j r}$$

subject to the normalization condition, $\int |P_i(r)| dr = 1$. Here the
$Z_j$'s are screening constants and the $A_j$'s are the parameters which de-
fine the basis functions. A set of $P$'s are chosen by defining the $A_j$'s
and the best of this set is determined by minimizing $\int \psi^+ H \psi \, dx$ with
respect to variations in the $P$'s. This determines the $Z_j$'s. The
Hartree-Fock equation is then solved by determining the eigenvectors
$C_{ij}$. (A sample calculation using this technique is discussed by
Winterbon (1968)).
In the numerical procedure a straightforward numerical integration of the Hartree-Fock equation is carried out and the $P(n\xi;r)$ are obtained as tabulated numerical functions. Analytic programs have been developed by Nesbet and Watson (1960), Roothan (1960), Watson and Freeman (1961). Numerical programs such as the Herman and Skillman work, have been also written by Froese (1963) and by Mayers and Hersh (1963). All the above mentioned calculations use the (HF)-model. A program to include configuration interactions has been developed by Mayers and Obrien (1963), and a program to calculate atomic wave functions by use of the Dirac equation has been written by Liberman, Waber, and Cramer (1965).

Since the review of Cyszak (1968), additional wave function calculations have appeared in the literature; Smith (1967) provided numerical solutions to the Dirac equation, Cowan (1967), (1968a), (1968b), using the Herman-Skillman as a starting point has developed calculations of atomic transition probabilities. Other recent works of interest are:

C. (Froese) Fisher (1967), (1968) has expanded her earlier work (see Froese (1963)) to include configuration-interactions; Mayers (1971) with his collaborator Obrien have continued the relativistic wave function work they began in the 60's (see Mayers (1963)); Seaton (1970) has reviewed some of the basic principles of Hartree-Fock calculations.

The work of Herman and Skillman is of interest for the present calculation. Recall that the Hartree-Fock equations Eq. (14) are coupled by the exchange term,

$$\sum_{n' \neq n} \epsilon_{n\xi,n'\xi} P(n'\xi;r) .$$
These equations can be decoupled by means of a simplifying assumption due to Slater (1951), who suggested that the Hartree-Fock exchange potentials for different occupied orbitals could be replaced by an averaged exchange potential obtained from the theory of a free-electron gas.

In a free-electron gas, which is a uniform system, the averaged exchange potential is proportional to the cube root of the electronic charge density (see Slater (1960)),

\[ v^{\text{exch}}(r) = - 6\left[3/8\pi \rho(r)\right]^{1/3} \]

The Slater assumption is that in the atom, which is a non-uniform system, the averaged exchange potential depends only on the local charge density \( \rho(r) \).

Collecting all potential energy terms into \( V(r) \), the Hartree-Fock equation with the Slater assumption may be written:

\[
\left[ \frac{d^2}{dr^2} - \frac{e(\ell+1)}{r^2} - V(r) - \epsilon_{n\ell,n\ell} \right] p(n\ell;r) = 0 \quad (17)
\]

The function \( V(r) \) is as follows:

\[
V(r) = -2Z/r - 2\int_0^r \sigma(t) dt - 2\int_r^\infty \frac{\sigma(t)}{t} dt - 6\left[\frac{3}{8\pi} \rho(r)\right]^{1/3}
\]

\[
\sigma(r) = \sum_{\ell \geq 0} q_{n\ell} |P(n\ell;\ell)|^2 \rho(r) = 4\pi r^2 \sigma(r) \quad \text{and} \quad q_{n\ell} = \left[ \text{occupation number} \right]
\]

Eq. (17) is the Hartree-Fock Slater (HFS) equation. This approximation decouples the wave equation.

Herman and Skillman wrote a Fortran Program for the IBM 7090 Computer to solve the (HFS) equation and obtain ground state wave functions for all atoms. Their results are given in terms of sets of tabulated orbital radial wave functions for specified configurations. It is
these ground state wave functions (and their eigenenergies) that are used in this calculation. They have been chosen because they have the desired accuracy, can be generated on the available IBM 370/145, and are well-known.

The excited state wave functions which are also needed in the present work were obtained by a modification of the Herman-Skillman program (H-S). Let us note that the decoupling of the wave equations discussed here for the target wave functions is consistent with the cross-section approximations presented in Chapter III (i.e. the approximations to the cross-section do not involve coupled channels). This modification is discussed in Chapter III, Section 2 and the program listing is given in Chapter V, Section 1. From this discussion it will be made clear that the wave functions have been isolated from the cross-section calculation. This has been done so that different wave function programs may be used with the cross-section program used here.

2. Continuum Wave Functions

In addition to the bound state wave functions obtained from the modified Herman-Skillman program, this calculation will require continuum wave functions for use in the calculation of ionization cross-sections. These wave functions will be "coulomb" wave functions. These are the solutions to the problem of an electron moving in a field of charge $Z$ with $1/r$ dependence. The functions are discussed in most standard texts. (For example see Landau (1965) or Schiff (1968)).

The coulomb wave function is a particular form of the confluent hypergeometric function. Since the evaluation of this function requires
elaborate mathematical techniques, two approaches to removing the need for numerically evaluating this function are commonly made in atomic structure calculations.

The first approach is to use bound state wave function of the "analytic" type discussed earlier. This technique allows the evaluation of matrix elements by analytic evaluation of integrals of the form

\[ \int_0^\infty e^{-\lambda Z} Z^a F(\alpha, \gamma, kZ) F(\alpha', \gamma', kZ) \, dZ \]  

(19)

where \( F(\alpha, \gamma, kZ) \) is the confluent hypergeometric function. See Landau (1958), Peach (1968), and Omidvar (1972).

A second approach is to use numerical bound state wave functions (as we have selected here), and to use some reasonable approximation for the coulomb wave function such as the following one.

The wave function we seek is to describe an electron moving away from a point charge \( Z = +1 \) with a wave vector \( \hat{k} \) and a position vector \( \vec{r} \). This function must satisfy the ionization boundry condition (rather than the scattering condition) of an outgoing "plane" wave and an ingoing "spherical" wave. This system of functions may be obtained from the more common system that are solutions to the scattering problem by applying the time-reversal operator to the scattering solution, (see Landau (1957)). The solutions of interest are of the form

\[ \Psi_c(\vec{r}) = \frac{1}{4\pi K} \sum_{j=0}^\infty i^j (2l+1) e^{-i\delta \lambda} R_{K\lambda}(r) P_{\lambda}(\hat{\vec{r}} \cdot \hat{\vec{j}}) \]  

(20)

where \( \delta \lambda = \text{ARG} (z+1-i/k) \), \( P_{\lambda} \) is the Legendre Polynomial \( \hat{\lambda} \) a unit vector and
\[ R_{KL}(r) = \frac{C_{KL}}{(2l+1)!} (2Kr) e^{-iKr} \frac{1}{\Gamma(i)} \left( \frac{i}{K} + l + 1, 2l + 2, 2iKr \right) \]  

where

\[ C_{KL} = \frac{2\sqrt{\pi}}{(1 - \exp(-2\pi/K))} \frac{\Gamma(l+1)}{\Gamma(l+1)} (S^2 + 1/K^2)^{1/2} \]

and where \( \text{if}_{1}(a,b,c) \) is the confluent hypergeometric (i.e. Kummer's) function, (see McGuire (1973)). These wave functions have the asymptotic form

\[ \Psi_c(r) \sim \frac{1}{Kr} \sin \left[ kr - \frac{\pi}{2} + \frac{1}{K} \ln(2Kr) \right] \]

These are the continuum wave functions used in this calculation.

The evaluation of these wave function in the present work is done using the relation

\[ e^{-iKr} \frac{1}{\Gamma(i)} \left( \frac{i}{K} + l + 1, 2l + 2, 2iKr \right) = \sum_{N,l+1} A^l_N(k) (Kr)^{N-l-1} \]

where

\[ A^l_{l+1}(k) = 1 \] \[ A^l_{l+2}(k) = -\frac{1}{K} (l + 1) \]

and

\[ (N+l)(N-l-1)A^l_N(k) = -(2/K)A^l_{N-1}(k) - A^l_{N-2}(k) \]

This expression is given by Abramowitz (1964). The convergence of this series over the range of \( l,k,r \) of interest is such that a maximum of 30 terms is needed to evaluate the wave function.

The criteria for truncation of the sum may be seen in the subroutine FLNR (L,RHO,ETA) listed in Chapter 5, Section 3 of this paper.
III. EXCITATION CROSS-SECTIONS

1. The General Problem

The total electron excitation cross-section, \( Q(n_{1f} \rightarrow n_{2f}) \), we are interested in calculating may be obtained from the scattering amplitude \( f(\theta, \phi) \). The general expression is developed below.

The Schrödinger equation for a system of an incident electron with coordinate \( \vec{r}_o \), and an atomic target with nuclear charge \( Z \) and atomic electrons at positions \( \vec{r}_s \) is given in atomic units as:

\[
\left( -\frac{1}{2} \sum_{s} \nabla^2_s - \sum_{s} \frac{Z}{r_s} + \sum_{st} \frac{1}{r_{st}} \right) + \left( -\frac{1}{2} \nabla^2_o + \sum_{s} \frac{1}{r_{os}} \right) \Psi(\vec{r}_o, \vec{r}_1, \ldots, \vec{r}_z) = E \Psi(\vec{r}_o, \vec{r}_1, \ldots, \vec{r}_z) \tag{26}
\]

The atomic wave functions are the solutions \( \Psi_A \) of the equation:

\[
\left( -\frac{1}{2} \sum_{s} \nabla^2_s - \sum_{s} \frac{Z}{r_s} + \sum_{st} \frac{1}{r_{st}} \right) \Psi_A(\vec{r}_1, \ldots, \vec{r}_z) = E_A \Psi_A(\vec{r}_1, \ldots, \vec{r}_z) \tag{27}
\]

Assuming the solutions \( \Psi_A \) to be known, they can be chosen as orthonormal basis functions in terms of which the total wave function can be expanded.

\[
\Psi(\vec{r}_o, \vec{r}_1, \ldots, \vec{r}_z) = \int \Psi_F(\vec{r}_o) \bar{\Psi}(\vec{r}_1, \ldots, \vec{r}_z) \tag{28}
\]

Substituting the expansion into Eq. (26), multiplying the result by \( \Psi_F(\vec{r}_1, \ldots, \vec{r}_z) \) and integrating over \( d\vec{r}_1 \cdots d\vec{r}_z \) we find,

\[
\left[ \left( -\frac{1}{2} \nabla^2 + k_r^2 \right) \Psi_F(\vec{r}_o) \right] = 2 \int d\vec{r}_1 \cdots d\vec{r}_z \Psi_F(\vec{r}_1, \ldots, \vec{r}_z) V(\vec{r}_o, \vec{r}_1, \ldots, \vec{r}_z) \bar{\Psi}(\vec{r}_o, \vec{r}_1, \ldots, \vec{r}_z) \tag{29}
\]

where
\[
V(r_0, \ldots, r_N) = \sum_{i=0}^{N} \frac{1}{r_{di}} - \sum_{i} \frac{Z}{r_i}
\]  
(30)

and

\[
k_F^2 = 2(E - E_F);
\]

\[E = \text{total energy of system};\]

\[E_F = \text{final energy of atomic target}.\]

Assuming the incoming electron is incident with wave vector \(k_I\), then our problem requires the asymptotic boundary condition

\[
F_F(r_o) = \exp\left[ik_I \cdot r_o\right] \delta_{F_1} + r_o^{-1} \exp\left[ik_F r_o\right] f_F(\theta, \phi)
\]  
(31)

Since our equation for \(F_F(r_o)\) is of the Helmholtz form with a source term, we may write the solution in terms of a Green's function \(G(r_o, \cdot)\)

\[
F_F(r_o) = \exp\left[ik_F^2 \cdot r_o\right] \delta_{F_1} + 2 \int d\vec{r}'d\vec{r}_2\ldots d\vec{r}_Z \Psi_F(\vec{r}_1) \Psi_F(\vec{r}_2) \ldots \Psi_F(\vec{r}_Z).
\]  
(32)

Here \(G\) satisfies the equation

\[
\left[V^2 + k_F^2\right] G(r_o, \vec{r}) = \delta(r_o - \vec{r})
\]  
(33)

To satisfy the asymptotic boundary condition Eq. (31), we choose

\[
G(r_o, \vec{r}) = -\exp\left[ik_F \cdot (r_o - \vec{r})\right] / (4\pi |r_o - \vec{r}|)
\]  
(34)

Then expanding equation \(G\) for large \(r_o\) and using

\[
k_F \cdot (r_o - \vec{r}) = k_F r_o - k_F^* \cdot \vec{r'}, \quad \text{where} \quad \vec{k}_F = \hat{r}_o
\]
we can compare the asymptotic expression for Eq. (32) with that given in Eq. (31) to obtain the result

\[ f_r(\theta, \phi) = -\left(\frac{2}{4\pi}\right) \int d^3r_1 \cdots d^3r_2 \exp[-i K_I r_i \cdot r_j] \left< \hat{\psi}(r_i) \right| \hat{\psi}(r_j) \right> \tag{35} \]

The differential cross-section is defined to be the flux scattered into the direction \((\theta, \phi)\) per unit incident flux. Since the current density is given by

\[ S(r_i) = \frac{1}{2i} \left[ \hat{\psi}^+(r_i) \nabla \cdot \hat{\psi}(r_i) - \nabla \cdot \hat{\psi}^+(r_i) \hat{\psi}(r_i) \right] \tag{36} \]

it follows from Eq. (31) that the incident flux has the value \((1/2i) (2k_i)\) while the scattered flux in the direction \((\theta, \phi)\) can be written \((-ik_F)|f(\theta, \phi)|^2/r^2\). The differential cross-section \(dQ/d\Omega\) therefore is given by

\[ \frac{dQ}{d\Omega} = (K_F/K_i) |f(\theta, \phi)|^2 \tag{37} \]

The total cross-section, \(Q\), results from the integration of \(dQ/d\Omega\) over all angles, i.e.

\[ Q = (K_F/K_i) \int d\Omega |f_r(\Omega)|^2 \tag{38} \]

It can be seen from Eq. (35) that the scattering amplitude involves the total wave function for the incident electron and the atomic target, \(\hat{\psi}(r_i)\). But since this total wave function is not known, it is clear that some additional approximation is necessary in order to evaluate an atomic cross-section. Many different approximations have been made in this connection. These can be categorized in terms of those that allow for exchange between the incident electron and the target atom electrons and those that do not. The present calculation computes cross-
sections in three non-exchange approximations and one exchange approximation.

2. Born-Approximation

The simplest approximation is the first Born-Approximation. Here the wave function of the total system is approximated for all \( |\vec{r}_0| \) by the correct wave function in the asymptotic region of large \( |\vec{r}_0| \), i.e.

\[
\Psi(|\vec{r}_0, \vec{r}_1, \ldots, \vec{r}_2|) = \exp\left[ i \frac{\vec{R}_1 \cdot \vec{r}_0}{\hbar} \right] \Psi(\vec{r}_1, \ldots, \vec{r}_2).
\]

This approximation leads immediately to the following form for the scattering amplitude;

\[
\tilde{f}_{\text{Born}}(d\omega) = -(1/2\pi) \int d\vec{r}' \exp[i(\vec{K}_1 - \vec{R}_F) \cdot \vec{r}'] \Psi(\vec{r}'). \tag{40}
\]

where

\[
\Psi(\vec{r}') = \int d\vec{r}_1 \ldots d\vec{r}_2 \Psi(\vec{r}_1, \ldots, \vec{r}_2) \exp \left[ -\frac{\vec{r}'}{R_{\text{opt}}} + \sum_s \frac{1}{2 \alpha_s^2} \right] \Psi(\vec{r}_1, \ldots, \vec{r}_2). \tag{41}
\]

This approximation is most valid for high incident energies. Classically, at low incident energies, the incoming electron spends more time in the interaction region and, clearly, a free particle description is not accurate.

Using the Bethe integral, (see Schiff (1968))

\[
\int d\vec{r}' \exp[i(\vec{K}_1 - \vec{r}') \cdot \vec{r}_s] = (4\pi/k^2) \exp[i(\vec{K}_1 \cdot \vec{r}_s)] \tag{42}
\]

where \( \vec{K} = \vec{K}_1 - \vec{K}_F \), the first Born Scattering amplitude can be rewritten

\[
f_{\text{Born}}(\omega) = -(2/k^2) \int F \Psi(\vec{r}_1, \ldots, \vec{r}_2), \quad F \neq I \tag{43}
\]

where
A further simplification results from the following argument. Recall that a Hartree-Fock wave is an antisymmetrized product wave function of the form

\[ \Phi_A = \frac{1}{\sqrt{Z!}} \mathcal{E}_{\alpha \gamma \cdots \gamma} \psi_1(1) \psi_2(2) \cdots \psi_Z(Z). \]  

(45)

For the atomic systems considered in the present calculation the assumption is made that the atomic core electrons are unchanged. Then only the wave function of the "active" electron is assumed to differ in the initial and final states of the atom. (The Herman-Skillman program is modified to compute the excited state wave function by solving the HFS equation for the excited state using the self-consistant potential of the ground state configuration.) With this assumption the expression for \( I_{FI} \) can be reduced via the relation, (inserting the spin wave function \( \chi(\sigma_1 \cdots \sigma_Z) \))

\[
\sum_{s=1}^{Z} \int d\mathbf{r}_1 \cdots d\mathbf{r}_Z \psi^s_f(\mathbf{r}_1 \cdots \mathbf{r}_Z) \psi(\mathbf{r}_1 \cdots \mathbf{r}_Z) \chi(\sigma_1 \cdots \sigma_Z) \chi(\sigma_1 \cdots \sigma_Z) =
\left( \frac{4}{Z!} \right) \sum_{s=1}^{Z} \mathcal{E}_{\alpha \gamma \cdots \gamma} \mathcal{E}_{\alpha \gamma \cdots \gamma} \int d\mathbf{r}_1 \cdots d\mathbf{r}_Z \psi_{s_f}^s(\mathbf{r}_1 \cdots \mathbf{r}_Z) \psi_{s_f}^s(\mathbf{r}_1 \cdots \mathbf{r}_Z) \chi(\sigma_1 \cdots \sigma_Z) \chi(\sigma_1 \cdots \sigma_Z) \]

and by use of the following property of the Levi-Chivita symbol;

\[ \mathcal{E}_{\alpha \gamma \cdots \gamma} \mathcal{E}_{\alpha \gamma \cdots \gamma} = (Z-1)! \delta_{\alpha \gamma \cdots \gamma}. \]  

(47)

(where \( Z \) is the number of indices). Consider the \( p \)th term of the sum over \( s \) in Eq. (44).
\[ J_p' = \left[ \varepsilon_{\alpha_1} \ldots \varepsilon_{\alpha_m} / m \right] \int d\hat{p}_1 \ldots d\hat{p}_m \\phi^{(i)}_{\alpha_1}(\hat{r}_{\alpha_1}) \ldots \phi^{(f)}_{\alpha_m}(\hat{r}_{\alpha_m}) \]

\[ C \exp [i \hat{K} \cdot \hat{r}_p] \phi^{(i)}_{\alpha_1} \ldots \phi^{(f)}_{\alpha_m} = \left[ \varepsilon_{\alpha_1} \ldots \varepsilon_{\alpha_m} / m \right] \quad (48) \]

\[ \int d\hat{p}_1 \phi^{(i)}_{\alpha_1}(i^{(1)}) \ldots \int d\hat{p}_m \phi^{(f)}_{\alpha_m}(i^{(m)}) \exp [i \hat{K} \cdot \hat{r}_p] \phi^{(i)}_{\alpha_1} \ldots \int d\hat{p}_m \phi^{(f)}_{\alpha_m}(i^{(m)}) \]

which, by use of the orthogonality of the \( \phi \)'s reduces to

\[ J_p' = \left[ \varepsilon_{\alpha_1} \ldots \varepsilon_{\alpha_m} / m \right] \int d\hat{p}_p \phi^{(i)}_{\alpha_1}(i^{(1)}) \ldots \phi^{(f)}_{\alpha_m}(i^{(m)}) \exp [i \hat{K} \cdot \hat{r}_p] \phi^{(i)}_{\alpha_1} \ldots \phi^{(f)}_{\alpha_m} \quad (49) \]

which gives

\[ J_p' = \frac{(Z-1)\frac{1}{Z}}{Z} \quad \delta_{\alpha \beta} \int d\hat{p}_p \phi^{(i)}_{\alpha_1}(i^{(1)}) \ldots \phi^{(f)}_{\alpha_m}(i^{(m)}) \exp [i \hat{K} \cdot \hat{r}_p] \quad (50) \]

where \( \phi^{i}_{\alpha} \) and \( \phi^{f}_{\alpha} \) denote the initial and final state wave functions of the excited electron. (Since spin does not appear in the Hamiltonian the spin-space and the \( r \)-space are decoupled. Let us factor out the spin function and neglect it in further discussions, \( \phi(\hat{r}_p, \sigma_p) = \psi(\hat{r}_p) \chi(\sigma_p) \). Since \( J_p \) is clearly independent of \( p \) (after integration over \( \hat{r}_p \)) the sum in \( \text{IF}_I \) results only in a factor of \( Z \), and the expression for \( f_{\text{Born}} \) reduces to the form,

\[ f_{\text{Born}}(\Delta) = -\frac{(2/k^2)}{Z} \int d\hat{r} \psi^{(i)}_{\alpha}(\hat{r}) \exp [i \hat{K} \cdot \hat{r}] \psi^{(f)}_{\alpha}(\hat{r}) \quad (51) \]

where the initial and final state single electron wave functions are denoted by \( \psi_i \) and \( \psi_f \) for clarity. This expression for \( f_{\text{Born}} \) will be of use in discussion of other approximations.

By choosing the \( z \)-axis in the \( \vec{k}_l \)-direction, so that \( \vec{k} \) depends only on the polar angle of \( \vec{k}_F \) with respect to \( \vec{k}_l \),

\[ k^2 = k^2_l + k^2_r - 2 k_l k_r \cos \Theta; \quad k d k = k_l k_r \sin \Theta d \Theta \quad (52) \]
and the total cross-section can be expressed in the form
\[ Q = \left( \frac{K_I}{K_F} \right) \int_{K_{\text{min}}}^{K_{\text{max}}} |f_{\text{BORN}}(K)|^2 \sin \theta d\theta \]
\[ = \left( \frac{2n}{K_F^2} \right) \int_{K_{\text{min}}}^{K_{\text{max}}} |A(K)|^2 dK ; \quad K_{\text{min}} = K_I + K_F \]

If the cross-sections are measured in units \( \pi a_B^2 \) instead of \( a_B^2 \) (as is implied by atomic units) this is rewritten
\[ Q[\pi a_B^2] = \int_{K_{\text{min}}}^{K_{\text{max}}} |f_{\text{BORN}}(K)|^2 K dK \]

Since the single electron wave functions are designated by the quantum numbers \( n \geq m \), while the cross-sections of interest in the present calculation are for transitions of the type \((n\ell' - n\ell')\) independent of \( m \), we require for what follows the average of the above expression over \( m_\ell \) and its sum over \( m_F \).

Consider.
\[ \sum_{m_\ell, m_F} \left| \frac{j_{\ell}(K)}{\sqrt{\ell + 1}} \right|^2 = \frac{4}{K^4(2\ell + 1)} \sum_{m_\ell, m_F} \left| \int d\vec{r} \psi_{n\ell}(\vec{r}) \psi_{n'\ell'}(\vec{r}) \exp[i\ell k \cdot \vec{r}] \right|^2 \]

For the integration over \( \vec{r} \) choose the z-axis along the \( \vec{k} \)-direction and recall, (Jackson (1962))
\[ \exp[i\ell k \cos \Theta] = \sum_{\ell} j_{\ell}(Kr) Y_{\ell,0}(\hat{\Theta}) \]

Since \( \psi_{n\ell m}(\vec{r}) \) can be written as \( \frac{P_{\ell m}(\hat{r})}{\ell} Y_{\ell m}(n) \)

we may write
In appendix III the sum involving the angular integrals is evaluated in terms of 3j-symbols. By using the result of that appendix we obtain,

\[
\sum_{m_-m_+} \left| \int d^3r \, \Psi^*_f(r) \exp[iK_r \cos \Theta] \Psi_f(r) \right|^2 = \sum_{\lambda, \lambda'} \left| \sum_{m_-m_+} [4\pi(2\lambda+1)]^{1/2} \cdot \nonumber \right.
\]
\[
\times \int dr \, P_i(r) \, j_{\lambda'}(K_\alpha) \, P_i(1) \int d\Omega \, Y_{m_-,m_+}^{*}(\hat{n}) \, Y_{\lambda_0}(\hat{n}) \, Y_{m_-,m_+}(\hat{n}) \right|^2 = \nonumber \]
\[
\sum_{\lambda, \lambda'} \left( \sum_{i} \langle i | Y_{\lambda'}(\hat{n}) | 4\pi \rangle (2\lambda+1) \right)^{1/2} \int dr \, P_i(r) \, j_{\lambda'}(K_\alpha) \, P_i(1) \int d\Omega \, Y_{m_-,m_+}^{*}(\hat{n}) \, Y_{\lambda_0}(\hat{n}) \, Y_{m_-,m_+}(\hat{n}) \right)^2 \nonumber \]
\[
(57) \nonumber \]

Since the triangle rule, \( \Delta(\mathbf{\epsilon}_\alpha \mathbf{\epsilon}_\lambda) \), requires \( \lambda(\text{minimum}) = |\mathbf{\epsilon}_\alpha - \mathbf{\epsilon}_\lambda| \) and \( \lambda(\text{maximum}) = \mathbf{\epsilon}_\alpha + \mathbf{\epsilon}_\lambda \), we obtain for the required sum the result

\[
\left| f_{\text{BORN}}'(K) \right|^2 = \sum_{m_-m_+} \left| f_{\text{BORN}}'(K) \right|^2 \left( 2\lambda + 1 \right) = \frac{4}{K^2} \sum_{\lambda = \lambda_{\text{min}}}^{\lambda = \lambda_{\text{max}}} (2\lambda + 1)^2 \left| \sum_{m_-m_+} [4\pi(2\lambda+1)]^{1/2} \cdot \nonumber \right.
\]
\[
\times \int dr \, P_{m_-m_+}(r) \, j_{\lambda}(K_\alpha) \, P_{m_-m_+}(r) \right|^2 \Delta(\mathbf{\epsilon}_\alpha \mathbf{\epsilon}_\lambda) \nonumber \]
section program.

3. Bethe Approximation

A simplification of the Born-Approximation is due to Bethe. Recall the expression for the Born scattering amplitude

\[ |f_{\text{Born}}(K)|^2 = \left| -\left( \frac{2}{\kappa} \right) \int d\mathbf{p} f_\mathbf{k}(\mathbf{p}) \exp[i\mathbf{K} \cdot \mathbf{p}] \psi_\mathbf{i}(\mathbf{r}) \psi_\mathbf{f}(\mathbf{r}) \right|^2 \]  

(61)

When the z-axis is chosen in the K-direction for the integration and \( \exp[iKr \cos \phi] \) is expanded, the following series is obtained

\[ |f_{\text{Born}}(K)|^2 = \left( \frac{4}{\kappa^2} \left| \mathbf{\alpha} \right| \left| \mathbf{\beta} \right| \right)^2 + \left( \frac{4}{\kappa^4/4} \right) \left| \mathbf{\alpha} \right|^2 \left| \mathbf{\beta} \right|^2 + \ldots \]  

(62)

where

\[ \left( \mathbf{\alpha} \cdot \mathbf{\beta} \right)_{\mathbf{f}, \mathbf{i}} = \int \psi_{\mathbf{f}}^*(\mathbf{r}) \left( i \cos \Theta \right)^{\mathbf{\alpha}} \psi_{\mathbf{i}}(\mathbf{r}) d\mathbf{r} \]  

(63)

This series converges provided \( \kappa a_B << 1 \) where \( a_B \), the Bohr radius, is the approximate range of the atomic wave functions. For \( \kappa a_B >> 1 \) \( |f(K)|^2 \) is small and contributes negligibly to the excitation cross-section (This is discussed in detail by Mott and Massey (1965) in Chapter XVI of their text.).

Approximating the square of the scattering amplitude by the first non-zero term of this series is the Bethe approximation.

The Legendre polynomial \( P_2(X) \) has \( X^2 \) as its highest power of \( X \), the next highest being \( X^0 \), and so on. This may be seen by the power series solution of the Legendre equation, (Jackson (1962)). Recall that
\[
\chi_{\mu}(\Theta, \Phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \Theta)
\]

Hence (see Abramowitz (1964))

\[
(c \cos \Theta)^S = \sum_{r=0}^{S} a_r Y_r(\mathbf{n})
\]

Using \( Y_{nlm}(r) = P_{nl}(r) Y_{lm}(\mathbf{n}) / r \),

we may write

\[
(\mathcal{S})_{if} = \int_0^\infty dr(r) P_{nl}(r) P_{n'l'}(r) \sum_{r=0}^{S} a_r \langle l_i, m_i | t o | l_{i'}, m_{i'} \rangle
\]

Once again we must average over \( m_i \) and sum over \( m_{i'} \):

\[
\sum_{m_i m_{i'}} \langle l_i, m_i | t o | l_{i'}, m_{i'} \rangle \langle l_{i'}, m_{i'} | t' o | l_f, m_f \rangle = \left( \frac{4}{K^*} \right) (2l_i + 1) \sum_{m_i m_{i'}} (K)^{2s} | (\mathcal{S})_{if} |^2
\]

\[
= \left[ \frac{4 K^{2s}}{K^* (2l_i + 1)} \right] \int_0^\infty dr(r)^3 P_{nl}(r) P_{n'l'}(r) \int_0^\infty dr'(r')^3 P_{nl}(r') P_{n'l'}(r')
\]

Again using the result of Appendix III we may rewrite the final sum in terms of the 3-j symbol and find:

\[
| f'_{i, l, m, t} \rangle = \left( \frac{4 K^{2s}}{K^*} \right) \int_0^\infty dr(r)^3 P_{nl}(r) P_{n'l'}(r) \langle l_i, m_i | t o | l_{i'}, m_{i'} \rangle
\]

where \( s \) is the first non-zero term in the expansion given in Eq. (62).

The cross-section \( Q_{\text{Bethe}}(n_{il} \rightarrow n_{il'}) \) is:
Noting that the \( K \)-dependence is isolated, we may write

\[
Q_{\text{Bethe}} = \left( \frac{2}{K} \right) \int_{\frac{k}{k}}^{k} \left| f_{\text{Bethe}}(K) \right|^2 K \, dK. \tag{69}
\]

To evaluate \( a_4 \) we note the following expression from the power series solution of the Legendre Equation given in Kreyzig (1963)

\[
P_\ell(x) = \sum_{t=0}^{\frac{\ell}{2}} \frac{\ell - t}{\ell} x^t \quad \text{where} \quad a_4 = \frac{(2t)!}{2^t (t!)^2} \tag{71}
\]

4. Modified Bethe Approximation

The results of the Bethe approximation can be improved for the case of low incident energy electrons by the use of a cut-off procedure developed by Seaton (1955). This approximation is called the Modified Bethe (M.B.) approximation and was first stated as follows:

"The total cross-section \( Q \) is the sum of the components \( Q^\ell \) arising from the components of the incident wave with angular momentum \( \hbar \ell (\ell + 1) \). For these (components) a limiting value of \( Q_{\text{max}}^\ell \) is set by the requirement of charge conservation (the continuity equation for the optical model). The approximation adopted is to calculate \( Q^\ell \) using the Bethe approximation, to accept the values obtained if \( Q_{\text{Bethe}}^\ell < \frac{1}{2} Q_{\text{max}}^\ell \) and to put \( Q^\ell = \frac{1}{2} Q_{\text{max}}^\ell \) if \( Q_{\text{Bethe}}^\ell \geq \frac{1}{2} Q_{\text{max}}^\ell \)."
To clarify further discussion of the approximation it is useful to examine three concepts relating to the approximation.

A. In many standard textbooks, (Shiff (1968), Landau (1957)) the scattering problem is discussed from the position of resolving the initial state into states of definite orbital angular momentum. For elastic scattering by a spherically symmetric potential it may be shown that the scattering amplitude can be decomposed in terms of angular momentum states in the form

$$f(\theta) = (2i\hbar) \sum_{L=0}^{\infty} (2L+1) (\exp[2i\delta_L] - 1) P_L(\cos \theta)$$  \hspace{1cm} (72)

where $\delta_L$ is termed the phase shift.

Inelastic scattering may be described by use of a complex potential (i.e. an optical model potential). Applying the method of partial waves to such a model results in complex phase shift $\delta_L = \alpha_L + i\beta_L$. The elastic, absorption, and total cross-sections may be written in terms of these phase shifts. Introducing $s_L = \exp[2i\delta_L]$ the expression for the absorption cross-section is:

$$Q_{abs} = \left( \frac{\pi}{K_x} \right)^2 \sum_{L=0}^{\infty} (2L+1) (1 - |S_L|^2)$$  \hspace{1cm} (73)

Since $|s_L|^2$ cannot be less than zero the partial absorption cross-section $Q_L$ has a limiting value expressed by the relation

$$Q_L \leq \left[ \left( \frac{\pi}{K_x} \right) (2L+1) \right]$$  \hspace{1cm} (74)

(If a scattering-matrix formulation of the problem is made, the same condition is contained in the requirement of unitarity of the $S$-matrix.)
Hence Eq. (74) is sometimes referred to as "the unitarity condition." 

B. Recall from earlier discussion, the Bethe approximation is obtained by considering the Born scattering amplitude in the form

\[ f_{\text{Born}}(n) = -\left(\frac{2}{k^2}\right) \int d\vec{r}^* \psi_f(\vec{r}) \exp\left[i \vec{K} \cdot \vec{r}\right] \psi_i(\vec{r}) \]  

(75)

and expanding the exponential. In the "exponential statement" of the Bethe approximation, the approximation is said to result from retention of the first non-zero term in the resulting series for the amplitude

\[ f(n) = -\left(\frac{2}{k^2}\right) \int d\vec{r}^* \psi_f(\vec{r}) \left(\sum_\lambda \frac{(i \vec{K} \cdot \vec{r}^*)^\lambda}{\lambda!}\right) \psi_i(\vec{r}) \]  

(76)

Although this is the most common statement of the Bethe approximation, an alternate statement of the approximation can be presented as follows. Consider the Born scattering amplitude in the form,

\[ f_{\text{Born}}(n) = -\left(\frac{1}{2\pi}\right) \int d\vec{r}_o \exp\left[i \vec{K} \cdot \vec{r}_o\right] \left\{ \int d\vec{r}_1 \frac{\psi_f^*(\vec{r}_1) \psi_i(\vec{r}_1)}{|\vec{r}_o - \vec{r}_1|}\right\} \]  

(77)

The asymptotic form for the potential

\[ \sqrt{\left|\vec{r}_o - \vec{r}_1\right|} = \frac{1}{\left|\vec{r}_o - \vec{r}_1\right|} \]

for large \(|\vec{r}_o|\) is obtained from the expression

\[ \frac{1}{\left|\vec{r}_o - \vec{r}_1\right|} = \sum_{\lambda=0}^{\infty} \frac{r_{\lambda}^{\lambda}}{r_o^{\lambda+1}} L^\lambda (\cos \left[\vec{r}_o \cdot \vec{r}_1\right]) ; \quad r_S \text{ is } r_o \text{ or } r_1 \]  

(78)

That is

\[ \sqrt{\left|\vec{r}_o - \vec{r}_1\right|} \equiv \lim_{r_o \to \infty} \left(\frac{1}{\left|\vec{r}_o - \vec{r}_1\right|}\right) = \sum_{\lambda=0}^{\infty} \frac{r_{\lambda}^{\lambda}}{r_o^{\lambda+1}} L^\lambda (\cos \left[\vec{r}_o \cdot \vec{r}_1\right]) \]  

(79)

The so called "potential statement" of the Bethe approximation results
from approximating the scattering amplitude of Eq. (77) by the first non-zero term in the series resulting from the replacement of the potential by Eq. (79) i.e. the first non-zero term in the series

\[ f(m) = -\left(\frac{1}{2\pi}\right) \int d^2 r e^{i\mathbf{R} \cdot \mathbf{r}} \sum_{l=0}^{\infty} \int d^2 q e^{i\mathbf{q} \cdot \mathbf{r}} \left| \psi_{l+1}^r(q) \right|^2 \left| \psi_l(q) \right|^2 \left\{ \cos \left[ \hat{r}_0 \cdot \hat{r}_1 \right] \right\} \]  

(80)

The equivalence of the exponential statement and the potential statement of the Bethe approximation is demonstrated in Appendix IV.

C. A partial wave analysis of the first Born approximation scattering cross-section, \( Q_{\text{Born}} \), is given in Appendix V. The resulting expression for the partial cross-section is:

\[ Q_{\text{Born}}^\lambda = (18) \left( 2 \ell_+^l + 1 \right) \frac{K_F}{K_0} \sum_{l''} \left( \frac{2 \ell'' + 1}{2 \ell + 1} \right)^2 \left( \frac{\ell''+1}{\ell+1} \right) \int \frac{d r_0}{r_0} \frac{d r_1}{r_1} \left( r_0 + r_1 \right)^2 |R^\text{Born}_{\lambda} (r_0) |^2 |J^{\text{Born}}_{\lambda} (r_0) |^2 \]  

(81)

where

\[ R^\text{Born}_{\lambda} (r_0) = \int \frac{d r_1}{r_1} \frac{r_1}{r_0} \left( \frac{r_1}{r_0} \right) R_{\eta_{\lambda}^{\text{Born}}} (r_1) \]  

(82)

Notice that since the Born expression explicitly contains the term \( r_{<}/r_{>^2+1} \), we may apply the "potential statement" of the Bethe approximation and obtain the Bethe partial cross-section \( Q^\lambda_{\text{Bethe}} \) by the replacement of \( R^\text{Born}_{\lambda} (r_0) \) with \( R^\text{Bethe}_{\lambda} (r_0) = \int P(\eta) P(i) \frac{r_1}{r_0} \frac{r_1}{r_0} d r_1 \) in Eq. (81).

Then

\[ Q^\lambda_{\text{Bethe}} = (18) \left( 2 \ell_+^l + 1 \right) \frac{K_F}{K_0} \sum_{l''} \left( \frac{2 \ell'' + 1}{2 \ell + 1} \right)^2 \left( \frac{\ell''+1}{\ell+1} \right) \int \frac{d r_0}{r_0} \frac{d r_1}{r_1} \left( r_0 + r_1 \right)^2 |R^\text{Bethe}_{\lambda} (r_0) |^2 |J^{\text{Bethe}}_{\lambda} (r_0) |^2 \]  

(83)

Returning to our statement of the Modified Bethe (MB) approximation,
the approximation involves enforcement of the unitarity condition for
those Bethe partial cross-sections that violate that condition.

Let \( \lambda_0 \) be a value of \( \lambda \) such that

\[
Q^\lambda_{\text{Bethe}} < \left[ \frac{1}{2} \right]^{\lambda} Q^{\lambda}_{\text{max}} = \left( \frac{1}{2 \, K^2} \right) \left( 2 \, \lambda + 1 \right) \quad \text{for} \quad (\lambda \geq \lambda_0) \tag{84}
\]

\[
Q^\lambda_{\text{Bethe}} > \left[ \frac{1}{2} \right]^{\lambda} Q^{\lambda}_{\text{max}} \quad \text{for} \quad (\lambda < \lambda_0)
\]

Then the Modified Bethe approximation to the cross-section is expressed
by the relation

\[
Q_{MB} = \sum_{\lambda = \lambda_0}^{\lambda_0} \frac{1}{2} Q^{\lambda}_{\text{max}} + \sum_{\lambda = \lambda_0 + 1}^{\infty} Q^\lambda_{\text{Bethe}} \tag{85}
\]

To compute the cross-section it is convenient to rewrite this
expression. Notice the following

\[
Q^\lambda_{\text{Bethe}} = \sum_{\lambda = \lambda_0}^{\lambda_0} Q^\lambda_{\text{Bethe}} + \sum_{\lambda = \lambda_0 + 1}^{\infty} Q^\lambda_{\text{Bethe}} \tag{86}
\]

or

\[
\sum_{\lambda = \lambda_0 + 1}^{\infty} Q^\lambda_{\text{Bethe}} = Q_{\text{Bethe}} - \sum_{\lambda = \lambda_0}^{\infty} Q^\lambda_{\text{Bethe}} \tag{87}
\]

Also notice

\[
\sum_{\lambda = \lambda_0}^{\lambda_0} \frac{1}{2} Q^{\lambda}_{\text{max}} = \left( \frac{1}{2 \, K^2} \right) \sum_{\lambda = \lambda_0}^{\lambda_0} (2 \, \lambda + 1) = \left( \frac{1}{2 \, K^2} \right) \left( \lambda_0^2 + 1 \right) \tag{88}
\]

Applying Eq. (87) and Eq. (88) to Eq. (85) we write

\[
Q_{MB} = Q_{\text{Bethe}} + \left( \frac{1}{2 \, K^2} \right) \left( \lambda_0^2 + 1 \right) - \sum_{\lambda = \lambda_0}^{\infty} Q^\lambda_{\text{Bethe}} \tag{89}
\]

The computer program of the present calculation computes \( Q^\lambda_{\text{Bethe}} \)
using the "exponential statement", Eq. (76), of the Bethe approximation
for use in Eq. (89). Only optically allowed transitions are computed
in this approximation, (i.e. the initial and final states must be s-p, p-d, etc.).

With the restriction to optically allowed transitions the cross-section expressions used in the computer programs are:

$$Q_{\text{Bethe}}^{(\text{optical})} = \left( \frac{8\pi}{3k^2} \right) (2l_f + 1) \left( \frac{l_f l_i}{o o o} \right)^2 \ln \left[ \frac{k_{\text{med}}}{k_{\text{min}}} \right] \, (90)$$

$$x \left[ \int_0^\infty dr \, P_{l_i, l_f}(r) \, P_{l_i, l_f}(r) \right] = |< r >_{i f}|^2$$

$$Q_{\text{Bethe}}^{(\text{optical})} = (72\pi)(2l_f + 1) \left( \frac{l_f l_i}{o o o} \right)^2 |< r >_{i f}|^2$$

$$x \left( 2l^2 + 1 \right) \left( \frac{l^2}{o o o} \right) J^2(l - 1) + \left( \frac{l l l}{o o o} \right) J^2(l + 1) \, (91)$$

where

$$J^2(l' \pm 1) \equiv \int_0^\infty dr \, j_{l'}(k r) \, j_{l' \pm 1}(k r) \, (92)$$

(It is of interest to notice that the scheme of imposing the unitarity condition to cross-section calculations was applied to the Born approximation in 1961, (Seaton (1961)). This resulted in the "Unitarized Born Approximation", since used in calculations found in the literature).

5. The Ochkur Approximation

In our discussion so far we have ignored the indistinguishability of the incident electron from the target electron. These have been "non-exchange" approximations. To examine how exchange effects cross-sections let us return to a general formulation of the problem.

The problem of exchange (i.e. the effects of particle identity
and spin) is discussed in most standard texts in quantum mechanics (e.g. Schiff (1968), Landau (1958), and Gottfried (1966)). For our purposes here let us note

1) If the interaction of a system of particles does not depend on spin, then it is possible to write the total wave function for the system as a product of a spatial eigenfunction and a spin eigenfunction.

2) Properly symmetrized solutions can be constructed from a general unsymmetrized solution.

3) For the case of 2 spin (1/2) - particles there are 3 symmetric (the triplet) and 1 antisymmetric (the singlet) spin eigenfunctions.

For simplicity, let us examine the case of an atom with one valence electron outside a closed shell (i.e. Hydrogen or an Alkali atom). With our inert-core assumption this is a two electron system. Recall from Chapter III Section 1 Eq. (28) the total unsymmetrized spatial wave function for this system may be written

$$\Psi(\vec{r}_o, \vec{r}_1) = \int_{\mathcal{P}} F_p(\vec{r}_o) \tilde{\Psi}_p(\vec{r}_1)$$

(93)

where \(\vec{r}_o\) and \(\vec{r}_1\) are the position vectors of the scattered electron and the valence electron respectively. The summation \(\mathcal{P}\) in Eq. (93) is over the complete set of states (continuous and discrete) of the atomic target.

Following the procedure of Chapter III Section 1 we find the scattering amplitude (and from it the cross-section) by examining the
asymptotic behavior of the total wave function of the system. Since there are two electrons we require asymptotic forms for the exact unsymmetrized wave function $\psi(\vec{r}_o, \vec{r}_1)$ when $r_0$ is large and when $r_1$ is large. These asymptotic behaviors are:

$$\Psi(r_0, r_1) \xrightarrow{r \to \infty} \psi_x(r) \exp(i k_x \cdot \vec{r}) + r_0^{-1} \exp(i k_r r_0) f_d(\langle N \rangle) \Psi_f(\vec{r})$$  \hspace{1cm} (94)$$

$$\Psi(\vec{r}_o, \vec{r}_1) \xrightarrow{r_1 \to \infty} \psi_x(r) \left[ r_1^{-1} \exp(i k_r r_1) f_e(\langle N \rangle) \right]$$  \hspace{1cm} (95)$$

where $f_d$ and $f_e$ are the direct and exchange scattering amplitude respectively. (Schiff (1968))

Using the singlet and triplet spin wave functions it is clear that the triplet is symmetric and must be multiplied by an antisymmetric spatial wave function $(\psi(\vec{r}_o, \vec{r}_1) - \psi(\vec{r}_1, \vec{r}_0))$. Similarly the antisymmetric singlet spin eigenfunction must be multiplied by the symmetric spatial function $(\psi(\vec{r}_o, \vec{r}_1) + \psi(\vec{r}_1, \vec{r}_0))$.

The asymptotic form for large values of one of the arguments (because of the symmetrization either will do) say $r_0$, is given by

$$\Psi(\vec{r}_o, \vec{r}_1) \pm \psi(\vec{r}_1, \vec{r}_0) \xrightarrow{r \to \infty} \exp(i k_x \cdot \vec{r}_0) \psi_x(\vec{r}_0) + r_0^{-1} \exp(i k_r r_0) \left[ f_d(\langle N \rangle) \pm f_e(\langle N \rangle) \right] \psi_f(\vec{r}_1).$$  \hspace{1cm} (96)$$

Using the fundamental postulate of quantum mechanics (see Huang (1963)) that all spin states are equally likely to appear in the collision, the differential cross-section must be computed with the symmetric spatial function in $1/4$ of the collisions and with the antisymmetric spatial function in $3/4$ of the collisions. That is
\[ \frac{dQ}{d\lambda} = \frac{1}{4} \left| f_d(\lambda) + f_e(\lambda) \right|^2 + \frac{3}{4} \left| f_d(\lambda) - f_e(\lambda) \right|^2. \]  

(97)

With this general understanding of the exchange problem let us now examine an approximation due to Oppenheimer (1928). Analagous to the Born approximation given in Chapter III, Section 2 Eq. (39), Oppenheimer assumed that the exact expression:

\[ \Psi_\text{ex} \left( \vec{r}_p, \vec{r}_q \right) = \int \left[ F_p(\vec{r}_p) \Psi_p(\vec{r}_p) \pm F_p(\vec{r}_q) \Psi_p(\vec{r}_q) \right] \]

(98)

could be approximated

\[ \Psi_\text{ex} \left( \vec{r}_p, \vec{r}_q \right) \approx \exp(i K_p \cdot \vec{r}_p) \Psi_p(\vec{r}_p) \pm \exp(i K_p \cdot \vec{r}_q) \Psi_p(\vec{r}_q) \]

(99)

With this approximation it may be shown (see Bates (1950) that the direct amplitude \( f_d \) may be written

\[ f_d(\lambda) = -\left( \frac{1}{2\pi} \right) \int d\vec{r}_p \exp(i [K_x - K_p] \cdot \vec{r}_p) V_{FI}(\vec{r}_p) \]

(100)

where

\[ V_{FI}(\vec{r}_p) = \int d\vec{r}_q \Psi_\text{f}^\dagger(\vec{r}_q) \frac{1}{|\vec{r}_p - \vec{r}_q|} \Psi_\text{f}(\vec{r}_q) \]

(101)

and the exchange amplitude \( f_e \) may be written

\[ f_e(\lambda) = \left( \frac{1}{2\pi} \right) \int d\vec{r}_p d\vec{r}_q \exp(i K_p \cdot \vec{r}_q) \Psi_\text{f}(\vec{r}_q) \]

\[ \times \frac{1}{|\vec{r}_p - \vec{r}_q|} \exp(-i K_p \cdot \vec{r}_p) \Psi_\text{f}^\dagger(\vec{r}_p) \]

(102)

The extension of the above formulae to the 3 electron case is straightforward but tedious. The 8 spin eigenfunctions for a three...
electron system and a derivation of the scattering amplitude for an elastic collision of an electron with a Helium atom is given by Schiff (1968) in Chapter 10 of his book.

The direct and exchange scattering amplitudes for a Helium-like system are:

\[
f_d = -\left(\frac{1}{2\pi}\right) \int d\vec{r}_e \exp \left(i\left[K_z^2 - K_r^2\right] \cdot \vec{r}_e\right) V_{FI}(\vec{r}_e)
\]

and

\[
f_e = \left(\frac{1}{2\pi}\right) \int d\vec{r}_e d\vec{r}_1 d\vec{r}_2 \left[\frac{1}{|r_0 - r_1|} + \frac{1}{|r_0 - r_2|}\right] \Psi^*(\vec{r}_1, \vec{r}_2) \exp \left(-iK_r \cdot \vec{r}_1\right)
\]

This Born-Oppenheimer approximation to the exchange scattering amplitude, \( f_e \), gives rise to cross-sections which violate the requirement of detail balancing, (i.e. \(|H_{FI}|^2 = |H_{IF}|^2\)). (see Segre (1965)). In the literature this has been referred to as the "post-prior" discrepancy. It has been shown that this problem arises from the non-orthogonality of the initial and final state wave functions (see Rudge (1965)).

The Ochkur-approximation is an improvement on the Born-Oppenheimer exchange amplitude which removes this discrepancy. In his original work Ochkur (1964) examines the exchange amplitude for Helium, Eq. (105), and notes that "the collision of an electron with an arbitrary atom can
be carried out in a completely analogous manner."

Briefly Ochkur expands the exchange amplitude in a power series in \((1/k_l)\) and retains only the leading term. (This expansion is given in Appendix VI). The resulting approximation to the exchange amplitude is:

\[
\tilde{f}_e (\Omega) = \left( \frac{\mathbf{r}_l}{K_x^2} \right) d \mathbf{r}_1 d \mathbf{r}_2 \mathfrak{P}_f^+(\mathbf{r}_1, \mathbf{r}_2) \exp(i[\mathbf{K}_x - \mathbf{K}_s] \cdot \mathbf{r}_l) \mathfrak{P}_I (\mathbf{r}_1, \mathbf{r}_2) \tag{106}
\]

Notice that the "direct" scattering amplitude \(f_d\) given in Eq. (103) is the Born scattering amplitude, \(f_{\text{Born}}\), discussed earlier in Chapter III, Section 2 Eq. (51). Further the Ochkur exchange amplitude, \(f_e\), of Eq. (106) may be written in terms of the Born amplitude as:

\[
f_e = \frac{K_x^2}{K_s^2} f_{\text{Born}} \tag{107}
\]

where \(\mathbf{K}_s = \mathbf{K}_x - \mathbf{K}_s\).

Recall Chapter III, Section 2 that in the present calculation we are making the inert-core-active-electron approximation. In this approximation all target atoms are treated as one valence electron systems. Returning then to our earlier discussion we define

\[
\frac{dQ^+}{d\Omega} = |f_d (\Omega)|^2 + \left| f_e (\Omega) \right|^2 \left| \left( 1 + \frac{K_x^2}{K_s^2} \right) f_{\text{Born}} (\Omega) \right|^2 \tag{108}
\]

and use Eq. (97) to write

\[
\frac{dQ}{d\Omega} = \left( \frac{1}{4} \right) \frac{dQ^+}{d\Omega} + \left( \frac{3}{4} \right) \frac{dQ^-}{d\Omega} \tag{109}
\]

Then in the usual manner (see Chapter III, Section 2) we may write

\[
Q = \frac{K_x}{K_s} \int d\Omega \frac{dQ}{d\Omega} = \left( \frac{2\pi}{K_x^2} \right) \int_{K_{\text{min}}}^{K_{\text{max}}} K dK \frac{dQ}{dK} \tag{110}
\]
where
\[
\frac{dQ}{dK} = \left( \frac{1}{4} \right) \frac{dQ^+}{dK} + \left( \frac{3}{4} \right) \frac{dQ^-}{dK} \tag{111}
\]

Let us again measure cross-sections in units of \( \pi a_b^2 \). Then the total cross-section is written
\[
Q_{\text{Ochkur}} = \left( \frac{2}{K_x^2} \right) \int_{K_{\text{min}}}^{K_{\text{max}}} \frac{dK}{K} \left\{ \left( \frac{1}{4} \right) \left( 1 + \frac{2 K_x^2}{K_x^2 + K_s^2} + \frac{K_s^4}{K_s^2} \right) \right\} \left( 1 - \frac{2 K_x^2}{K_x^2 + K_s^2} + \frac{K_s^4}{K_s^2} \right) \left| f_{\text{Born}}(\kappa) \right|^2 \tag{112}
\]

This is the Ochkur expression used in the present calculation.

Let us note here that it has been observed by Rudge (1965a) that the approximation of Ochkur is "in a certain sense incorrect". Specifically, Rudge has shown that the Ochkur expression cannot be obtained from a variational principle. However, the Ochkur approximation does overcome some of the difficulties of the Born-Oppenheimer approximation. For that reason it is still used to incorporate exchange. Rudge himself provides Ochkur calculations in his ionization review paper (see Rudge (1968)). He observes, "The derivation of Ochkur's result is of an ad hoc nature and it is not altogether clear why it yields a marked improvement over the Born-Oppenheimer method."

6. Summary of the Excitation Cross-Section Expressions Used in the Computer Programs.

In summary, the final form of each of the four approximations discussed in this chapter and used in the calculation are given below. Some of the Fortran variable names will also be given for reference.
A) Born

\[ Q_{\text{born}} = \left( \frac{2}{k_x} \right) \frac{1}{k_x - k_{p_x}} \int dK \leq K \mid \frac{f_{\text{born}}'(K)}{f_{\text{born}}(K)} \right|^2 \]  \hspace{1cm} (113)

where

\[ \left| \frac{f_{\text{born}}'(K)}{f_{\text{born}}(K)} \right|^2 = \left( \frac{4}{k_y} \right)^2 \sum_{\lambda = \ell} \int dK \leq K \mid \frac{2 \lambda + 1}{2 \lambda + 1} \left( \frac{\ell}{\ell} \right)^2 \int dr P^n_{\ell} (r) \left( \frac{\ell}{\ell} \right) \right|^2 \]  \hspace{1cm} (114)

B) Bethe

\[ Q_{\text{Bethe}} = \left( \frac{6}{k_x} \right) \frac{1}{k_x - k_{p_x}} \int dK \leq K \mid \int_0^{\infty} dr r^3 P^n_{\ell} (r) \left( \frac{\ell}{\ell} \right) \right|^2 \]  \hspace{1cm} (115)

\[ \times \sum_{\lambda = \ell} \left( \frac{2 \lambda + 1}{4 \pi} \right) \left( \frac{\ell}{\ell} \right)^2 \left( \frac{2 \ell + 1}{2 \ell + 1} \right)^2 \]  \hspace{1cm} (116)

C) Modified Bethe

\[ Q_{\text{modified Bethe}} = Q_{\text{Bethe}} + \left( \frac{1}{2 k_x^2} \right) (\lambda + 1) \int \sum_{\ell = 0}^{\infty} Q_{\ell}^{\text{Bethe}} \]  \hspace{1cm} (117)

D) Ochkur

\[ \left( \frac{2}{k_x} \right) \int dK \leq K \right)^2 \frac{1}{k_x - k_{p_x}} \int dK \leq K \mid \frac{f_{\text{born}}'(K)}{f_{\text{born}}(K)} \right|^2 \]  \hspace{1cm} (118)

where \( f_{\text{born}}(K) \) is as given above.

The program listings and a discussion are given in Chapter V, Section 2. Some of the Fortran names used for the variables in the
above expressions are:

\[ Q \rightarrow \Sigma G \]
\[ K_T \rightarrow X \mathcal{I} N \]
\[ K_F \rightarrow X F \]
\[ \lambda_f \rightarrow \mathcal{L} \]
\[ \lambda_e \rightarrow \mathcal{L} \]
\[ P_{\frac{n}{n'}} \rightarrow PF \]

\[
\int_0^\infty dr \left[ \mathcal{I}_{\frac{n}{n'}}^{(r)} \mathcal{P}_{\frac{n}{n'}}^{(r)} \mathcal{P}_{\frac{n}{n'}}^{(r)} \right] \rightarrow \text{RDINT} (BJ, LAM, X)
\]

It may be shown (Gottfried 1966) that for a potential \( U(r) \) the criterion for validity of the Born approximation is

\[
\frac{1}{K_T} \left| \int_0^\infty \exp(iK_Tr) sm(K_Tr) U(r) \, dr \right| < 1
\]

Gottfried argues that for a neutral atom of charge \( Z \) (in some cases an effective charge) this condition is equivalent to

\[
Z \sqrt{E_H} \ll \sqrt{E}
\]

where \( E_H \) is the Rydberg. An upper limit of \( E \) is set by the fact that we are considering non-relativistic electrons and therefore \( E \ll mc^2 \). Hence the region of validity for the Born approximation in eV is

\[
(Z)^{3/2} \ll \sqrt{E} \ll 7.1 \times 10^5 \quad \text{or} \quad Z \ll 200
\]

Gottfried notes that "the Born approximation actually leads to considerably more accurate inelastic cross-sections at low energies than one would surmise from this inequality."

The Bethe approximation assumes the above condition is satisfied and furthermore assumes that

\[
\left[ \left( K \mathcal{Z} \right)_{zf}^s / s! \right] / \left[ \left( \mathcal{K} \mathcal{Z} \right)_{zf}^{s-1} / (s-1)! \right] \ll 1
\]
s is the power of the first non-zero term in the Bethe series (Eq. 62).

The Ochkur approximation must satisfy the Born criterion, and the Modified Bethe approximation must satisfy both the Born and Bethe criteria.

The expected validity of the results for the specific calculations of this paper will be given after some of the results are considered.
IV. IONIZATION CROSS-SECTION

1. Relationship to Excitation Expressions

The problem of electron collisions with neutral atoms causing ionization is both similar and dramatically different from the problem of excitation. It is similar insofar as we can state ionization as "excitation to the continuum". Having noted this, much of the earlier discussion of the excitation problem (and many of the expressions derived) may be applied to ionization, but with caution.

The ionization problem is dramatically different for two reasons. First, the continuum state wave functions only have specific states associated with specific wave-vectors $\mathbf{k}_e$. Therefore, an ionization cross-section is excited to a state with specific direction. Second, the electron that is ionized (secondary electron) is indistinguishable from the scattering electron and this must be accounted for in the computation.

2. The Born-Coulomb Approximation

The most commonly used approximation to the cross-section for electron impact ionization of neutral atoms is the Born-Coulomb approximation. This is an approximation of the cross-section by the Born-approximation derived earlier, with the final state of the atom (the ionized electron) described by a Coulomb wave.

Consider the system of an electron with a wave vector $\mathbf{k}_I$ incident on an atom described by the atomic wave function $\psi_i$. In this system the electron is scattered into a direction ($\Omega_F$) with a wave vector $\mathbf{k}_F$ and the
atom is ionized, emitting a secondary electron into a direction \( (\Omega_e) \) with a wave vector \( \vec{k}_e \). Let us derive the cross-section for this collision.

Using the Born approximation (i.e. describe the primary electron by the plane waves \( \exp(i\vec{k}_I \cdot r) \) and \( \exp(-i\vec{k}_F \cdot r) \) and the inert-core approximation recall:

\[
\frac{d\Omega}{d\vec{k}_e} [\Omega_\theta, \phi] = \left( \frac{2}{\kappa_2^2} \right) \int_{\kappa_2, \kappa_1} d\vec{k} \ d\Omega \left| \int \sigma_{\text{Born}} (\vec{k}, \vec{k}_e) \right|^2
\]

(120)

where

\[
\sigma_{\text{Born}} (\vec{k}_e, \vec{k}) = \left( \frac{2}{\kappa_2} \right) \int d\vec{r} \ \Psi^*_t (\vec{k}_e, \vec{r}) \ \exp(i\vec{k}_e \cdot \vec{r}) \ \Psi_t (\vec{r})
\]

(121)

Let us assume the atomic wave functions are of the form:

\[
\Psi_t (\vec{r}) = \mathcal{R}_{m_i l_i m_i} (\vec{r}) \ Y_{l_i m_i} (\Omega_t)
\]

(122)

\[
\Psi_f (\vec{k}_e, \vec{r}) = \sum_{\ell \ell_e m_e} \mathcal{R}_{\ell_e l_e m_e} (\kappa_e, \vec{r}) \ Y_{\ell_e m_e} (\Omega_{\kappa_e})
\]

(123)

To integrate Eq. (121), choose the \( z \)-axis along the \( \vec{k} \)-direction and recall

\[
\exp(i\vec{k} \cdot \vec{r} \cos \theta) = \sum_{\lambda = \ell} \left[ + \pi (z \lambda + 1) \right]^{1/2} j_{\lambda} (kr) \ Y_{\lambda} (\Omega_r)
\]

(124)

Using the addition theorem to write

\[
\Psi_f (\vec{k}_e, \vec{r}) = \sum_{\ell_e, l_e m_e} \left\{ \frac{4\pi}{(2\ell_e + 1)} \mathcal{R}_{\ell_e l_e m_e} (\kappa_e, \vec{r}) \ Y_{\ell_e m_e}^* (\Omega_{\kappa_e}) \right\} Y_{\ell_e m_e} (\Omega_{\ell_e})
\]

(125)

then Eq. (121) may be expanded as
To find the cross-section we require

$$f_{\text{Born}}(\mathbf{K}_e, K) = \left( \frac{2}{K^2} \right)^{\frac{1}{2}} \sum_{l_e m_e} \left[ \frac{4\pi}{2\lambda + 1} \right]^{\frac{1}{2}} \left( \frac{2\pi (2\lambda + 1)}{2\lambda + 1} \right) \gamma^2 = C(\lambda_e, \lambda)$$

$$\times \left\{ \int_0^\infty d\Omega \left[ Y_{l_e m_e}^{\dagger}(\Omega_{l_e}) Y_{\lambda_e}^{\dagger}(\Omega_{\lambda_e}) Y_{l_i m_i}(\Omega_{l_i}) \right] \right\}$$

$$x \left\{ \int_0^\infty d\nu \left[ R_{l_e}(\mathbf{k}, \nu) j_\lambda(\mathbf{k}\nu) R_{l_i}^{\dagger}(\nu) \right] \right\}$$

$$= -\left( \frac{2}{K^2} \right)^{\frac{1}{2}} \sum_{l_e m_e} C(\lambda_e, \lambda) \left( Y_{l_e m_e}^{\dagger}(\Omega_{l_e}) \langle l_e m_e | \lambda_0 l_i m_i \rangle R_{l_e}(\lambda_e, \lambda, l_i) \right)$$

To find the cross-section we require

$$\left| f_{\text{Born}}(\mathbf{K}_e, K) \right|^2 = \left( \frac{2}{K^2} \right)^{\frac{1}{2}} \sum_{l_e m_e} \sum_{l_i m_i} C(\lambda_e, \lambda) C^{\dagger}(\lambda_0, \lambda) Y_{l_i m_i}^{\dagger}(\Omega_{l_i}) Y_{l_e m_e}(\Omega_{l_e})$$

$$\times \langle l_e m_e | \lambda_0 l_i m_i \rangle \langle l_e \lambda_0 l_i m_i \rangle R_{l_e}(\lambda_e, \lambda, l_i) R_{l_e}(\lambda_0, \lambda, l_i)$$

This would allow us to calculate the cross-section $\frac{dQ}{dK_e}$ for the collision. But the total ionization cross-section would be for all allowed values of the secondary wave-vector. That is

$$Q_{\text{Born}}^{\text{ionization}} = \int_{\frac{2}{K_e^2}}^{\frac{2}{K_{e0}^2}} \frac{dQ}{dK_e} = \int_{\frac{2}{K_{e0}^2}}^{\frac{2}{K_e^2}} K_e^2 dK_e \int_{\Omega_{l_e}} d\Omega_{l_e} \int_{\Omega_{l_i}} d\Omega_{l_i} \int_{K_{min}}^{K_{max}} dK \int_{K_{min}}^{K_{max}} dK_e \left| f_{\text{Born}}(\mathbf{K}_e, K) \right|^2$$

where for a given initial state of the atom and a given incident energy of the primary electron $K_e$ is determined by the conservation of energy for the condition of the primary electron at rest. That is,

$$E_e^{\text{max}} = E_i - E_{\text{ionization}}$$

We may rewrite Eq. (128) as

$$Q_{\text{Born}}^{\text{ion}} = \left( \frac{2}{K_e^2} \right)^{\frac{1}{2}} \int_{\frac{2}{K_{e0}^2}}^{\frac{2}{K_e^2}} K_e^2 dK_e \int_{\Omega_{l_e}} d\Omega_{l_e} \int_{K_{min}}^{K_{max}} dK \int_{K_{min}}^{K_{max}} dK_e \left| f_{\text{Born}}(\mathbf{K}_e, K) \right|^2$$
Using Eq. (127) and noting

\[ \int d \Omega_{\kappa_e} \, Y_{L \lambda e}^*(\Omega_{\kappa_e}) \, Y_{L \lambda e}^\dagger(\Omega_{\kappa_e}) = \delta_{L \lambda e} \delta_{m_e m_e} \]  

(130)

we can sum over \( L \lambda e \) and write

\[ |f(\Omega_{\kappa_e}|^2 = \int d \Omega_{\kappa_e} \, |f(\Omega_{\kappa_e})|^2 = \left( \frac{4}{K^*} \right) \sum_{L \lambda e m_e} C(L \lambda e) C^\dagger(L \lambda e) \]

(131)

\[ x \langle l_l m_e | \lambda \lambda | l_l m_l \rangle \langle l_l m_l | \lambda \lambda | l_l m_e \rangle \mathcal{R}(L \lambda e L_l m_l) \mathcal{R}(L \lambda e L_l m_e) \]

averaging over \( m_l \) we write

\[ |f'(\Omega_{\kappa_e})|^2 = \sum_{m_l} |f(\Omega_{\kappa_e})|^2 = \left( \frac{4}{K^*} \right) \sum_{L \lambda e} C(L \lambda e) C^\dagger(L \lambda e) \]

(132)

\[ x \mathcal{R}(L \lambda e L_l) \mathcal{R}(L \lambda e L_l) \sum_{m_l m_e} \langle l_l m_e | \lambda \lambda | l_l m_l \rangle \langle l_l m_l | \lambda \lambda | l_l m_e \rangle \]

With Appendix III we can write

\[ \sum_{m_l m_e} \langle l_l m_e | \lambda \lambda | l_l m_l \rangle \langle l_l m_l | \lambda \lambda | l_l m_e \rangle = (2l_l + 1) \frac{(2l_l + 1)}{4\pi} \]

(133)

\[ x \left( \begin{array}{c} \lambda_l \varepsilon_l \lambda \varepsilon \end{array} \right) \delta(2\lambda + 1) \delta(l_l l_l) \]

For the Born Approximation is:

\[ Q^{\text{ion}}_{\text{Born}} = \int_0^{\kappa_e^{**}} \kappa_e^2 \, d\kappa_e \, dQ \frac{dQ}{d\kappa_e} \]  

(135)

\[ \frac{dQ}{d\kappa_e} = \left( \frac{2}{\kappa_e^2} \right) \int_{K_{K_F}}^{K_{K_{e}}} k \, dk \left| f(\text{Born} \, (K, \kappa_e)) \right|^2 \]  

(136)
\[ |f_{\text{Born}}'(K, \kappa_e)|^2 = \left( \frac{4\pi r^2}{K^4} \right) \sum_{\lambda \kappa_e, \ell \kappa_e} (\ell_i \ell_{\kappa_e} \lambda)^2 \frac{(2\lambda + 1)}{(2\ell + 1)} \int_0^\infty dr \, P_{\lambda} \, j_\lambda (Kr) \, P_{\ell \kappa_e} (r) \] (137)

where \( K_{\text{max}}^{\text{max}} \) in atomic units is
\[ K_{\text{max}}^{\text{max}} = \sqrt{(K_e - 2\mathcal{I})} \quad \mathcal{I} = \text{Ionization Energy} \]

However, as mentioned earlier we must account for the secondary electron being indistinguishable from the primary electron. As discussed by Rudge (1968), this may be approximated by setting \( E_{\text{max}}^{\text{max}} \) equal to \( E_{\text{max}}^{\text{max}}/2 \). Then
\[ K_{\text{max}}^{\text{max}'} = \sqrt{2(K_e - 2\mathcal{I})} \] (138)

3. The Expression Used in the Computer Programs.

In summary, the expressions used in the calculation are given below. Some of the Fortran variable names are also given.

\[ Q_{\text{Born}} = \int_0^{K_{\text{max}}^{\text{max}}} K_e^2 \, dK_e \, \frac{dQ}{dK_e} \] (139)

\[ \frac{dQ}{dK_e} = (2\mathcal{I}K_e) \int_{K_e - K_e}^{K_e + K_e} \kappa \, d\kappa \left| f_{\text{Born}}'(K, \kappa_e) \right|^2 \] (140)

\[ \left| f_{\text{Born}}'(K, \kappa_e) \right|^2 = \left( \frac{4\pi r^2}{K^4} \right) \sum_{\lambda \kappa_e, \ell \kappa_e} (\ell_i \ell_{\kappa_e} \lambda)^2 \frac{(2\lambda + 1)}{(2\ell + 1)} \int_0^\infty dr \, P_{\lambda} \, j_\lambda (Kr) \, P_{\ell \kappa_e} (r) \] (141)
The program listing and discussion is presented in Chapter V, Section 3.

Some of the Fortran variable names are:

\[ K_e + KAPA \]
\[ \pi + PI \]
\[ \kappa_e + L2 \]
\[ p_{\kappa_e}(K_e, r) \rightarrow PF \]
V. COMPUTER PROGRAMS

In this chapter the programs themselves will be presented. For each of the three programs used in the calculation (HFSWF, EXCSCT, IONCST) a program listing is given, and some details of the program are discussed. The information on how to run the program is given in Appendix VII--User Manual.

1. Wave Function Program

This program, named HFSWF, is a self-consistent field calculation of radial atomic wave functions. The program consists of a main routine and a subroutine SCHEQ.

a) Listing
PROGRAM HFSWF(INPUT)

==-------------------------------------------------------------==
* *
* HFSWF * *
* *
* A FORTRAN PROGRAM TO CALCULATE HARTREE-FOCK-SLATER NUMERICAL WAVE FUNCTIONS AS PUNCHED CARD OUTPUT. ITERATION NUMBER, MEASURE OF SELF-CONSISTENCY AND ATOMIC NUMBER Z ARE ALWAYS PRINTED ON-LINE.
* *
* IF KEY=0 NORMALIZED NUMERICAL ATOMIC POTENTIAL IS READ IN AS 110 VALUES, EVERY 4TH MESH POINT 1 TO 437.
* *
* IF KEY=1 COMPLETE ATOMIC POTENTIAL IS READ IN (437PT)
* IF KEY=2 EXTRAPOLATE STARTING POTENTIAL
* *
* MAXIT=MAXIMUM NO. OF ITERATIONS (MAXIT=0 IMPLIES 20).
* *
* IF KUT=0, MODIFIED H~F~S POTENTIAL IS USED IN Wv~EQ.
* IF KUT=1, UNMODIFIED H~F~S POTENTIAL IS USED IN Wv~EQ.
* *
* IF NOCOPY=0, ACTIVE ELECTRON WAVE FUNCTIONS ARE PUNCHED.
* IF NOCOPY=1 ALL Wv, FNCTS. AND SELF-CONSISTENT POTENTIAL ARE PRINTED ON-LINE.
* *
* =======
* *
* PROGRAM AND SUBROUTINES ORIGINALLY WRITTEN BY SHERWOOD SKILLMAN, RCA-LAB, PRINCETON NJ, SPR 1961
* MODIFIED BY (1) F. HERMAN, RCA-LAB, PRINCETON NJ, SUMMER 1961
* (2) R. KORTUM, LCKHEED RSCH-LAB, PALO ALTO, SUM 1962
* (3) T. GREENE, UNIV. TOLEDO, TOLE, CHIC, FALL 1971.
* *
* DIMENSION X(521), RSCORE(521), RUINL1(521), RU2(521), RU(521), NNL 1Z(24), R(521), RVAL(521), RUFLN1(521), RU3(521), XI(521), WWNL(2 24), V(521), RATOM(521), RUINL2(521), XNUM(521), XIJ(521), NKKK(24) 3, EE(24), RUXCH(521), RUFLN2(521), DENM(521), SLN(10,521), SNL(5 421), A(4,5)
COMMON V,SNL,R,RSCORE,RVAL,R,RUXCH,XI,XJ,RSATOM,SNL,RUINLI,RU 1,FLN1,RUINL2,FLN2,RU3,NNLZ,WWNL,NKKK,EE,A EQUIVALENCE (RSCORE,XNUM), (RVAL,DENM), (EQ,RSATOM)
NFILES=0
1 CONTINUE

READ HEADING CARD.

READ (5,138)
WRITE (6,138)

READ CONTROL CARDS AND INPUT POTENTIALS. CALCULATE TRIAL POTENTIAL

NCARDS=50
PRINT 132, KEY
READ (5,131) KEY, TOL, THRESH, MEsh, IPRAT, MAXIT, NOCOPY, KUT, IP, IM, IR, IC, DEFOLT, JE
IF (DEFOLT) 2, 2, 3
 KEY=0
 TOL=.001
 THRESH=.0001
 MESH=441
 IPRATT=1
 MAXIT=20
 NCOPIY=1
 KUT=0
 IP=6
 IM=6
 IR=5
 IC=7
 JE=1
 GC TO 5
 IF (MAXIT) 4, 4, 5
 MAXIT=20
 CONTINUE
 NBLOCK=(MESH)/40

CC CONSTRUCT X MESH AND R MESH

I=1
 X(I)=0.0
 R(I)=0.0
 DELTAX=0.0025
 CO 7 J=1, NBLOCK
 DD 6 K=1,40
 I=I+1
 X(I)=X(I-1)+DELTAX
 7 CELTAX=DELTAX+DELTAX
 IF (KEY=1) 9, 10, 8
 8 READ (IR, 129) (RU2(M), M=1, 441)
 READ (IR, 129) (RU3(M), M=1, 441)
 ZE2=RU2(1)/2.0
 ZE3=RU3(1)/2.0
 GO TO 11

READ IN ATOMIC POTENTIAL

9 READ (IR, 124) (RU2(M), M=1, 437, 4)
 GO TO 11
 10 READ (IR, 129) (RU3(M), M=1, 441)
 ZE3=RU3(1)/2.0
 11 READ (IR, 125) Z, NCORES, NVALES, ION
 IF (Z) 120, 1, 12
 12 NFILES=NFILES+1
 NZ=Z
 13 R(I)=C*X(I)
 READ (IR, 127) (NNLZ(I), WWN(I), E(I), I=1, NCSNVS)
 WW=0.0
 CC 14 I=1, NCSNVS
14 \texttt{WWW=WWW+HWNL(I)}
   \texttt{IF (ABS(Z+1.0=WWW-ZZ)=0.001) 16,15,15}
15 \texttt{PRINT 126, WWW,ZZ, Z, NCORES, NVALES, NCSPWS}
   \texttt{CALL EXIT}
16 \texttt{CONTINUE}
   \texttt{IF (KEY=1) 21,26,17}
17 \texttt{CONSTRUCT ATOMIC POTENTIAL}
18 \texttt{IF (ABS(ZE3-ZE2-Z+Z2F3)=0.001) 19,19,18}
19 \texttt{WRITE (IP,139) Z, ZE2, ZE3}
   \texttt{CALL EXIT}
20 \texttt{CONTINUE}
21 \texttt{GO TO 21}
22 \texttt{2WOZ=Z*Z}
23 \texttt{RUI(I)=RU3(I)*2WOZ}
24 \texttt{RU(I+1)=RU2(I)*2WOZ}
25 \texttt{RU(I+2)=RU2(I)*2WOZ}
26 \texttt{RU(I+3)=RU2(I)*2WOZ}
27 \texttt{CONTINUE}
28 \texttt{GO TO 31}
29 \texttt{Z=Z/ZE3}
30 \texttt{DO 30 I=1,441}
   \texttt{RUI(I)=RU3(I)*Z}
31 \texttt{CONTINUE}
32 \texttt{GO TO 31}
33 \texttt{V(I)=RU(I)/R(I)}
34 \texttt{IF (MESH=M) 32,37,36}
35 \texttt{V(I)=2WOI/N/R(I)}
36 \texttt{LIMIT=M}
37 \texttt{CONTINUE}
   \texttt{ICUT=MESH}
   \texttt{IC=MESH}
   \texttt{GO TO 47}
38 \texttt{CONTINUE}
   \texttt{ICUT=0}
39 \texttt{GO 42 I=2,M}
IF (ICUT) 38, 38, 40
38 IF (TWOZZZ*RU(I)) 41, 41, 39
39 ICUT=1
40 V(I)=TWOZZZ/R(I)
   GO TO 42
41 V(I)=RU(I)/R(I)
42 CONTINUE
   IF (ICUT) 43, 43, 44
43 ICUT=M
44 LIMIT=ICUT
   IF (MESH=M) 47, 47, 45
45 CONTINUE
   DO 46 I=44, MESH
46 V(I)=TWOZZZ/R(I)
47 CONTINUE
   DELTA=1000000
   NITER=0
   NCOREN=3
   IPRSH=0
   PRINT 133
   C  START ITERATION
   C
48 MCARDS=50
   IF (MAXIT=NITER) 49, 51, 51
49 CONTINUE
   WRITE (IP, 140)
   DO 50 I=1, MESH
   WRITE (IP, 141) I, X(I), RU(I), RU(II), RU(III), RU(IV), RU(V)
50 CONTINUE
   GO TO 11
51 DO 52 I=1, MESH.
   RSCORE(I)=0.0
52 RSVALE(I)=0.0
   C  SOLVE SCHROEDINGER EQUATION FOR EACH ORBITAL IN TURN
   C  CALCULATE CORE AND VALENCE ELECTRONIC DENSITIES
53 M=1, NCSPVS
   E=EE(M)
   NN=NNLZ(M)/100
   LAM=NNLZ(M)/1000*NN
   XL=LAM
   CALL SCHEQ (Z, E, LAM, NN, KKK, MESH, C, THRESH)
   IF (M=NCORES) 53, 53, 55
54 RSCORE(I)=RSCORE(I)+WWNL(M)*SNL(I)**2
   GO TO 57
55 RSCORE(I)=RSCORE(I)+WWNL(M)*SNL(I)**2
56 RSVALE(I)=RSVALE(I)+WWNL(M)*SNL(I)**2
57 DO 58 I=1, KKK
58 SNL(M,I)=SNL(I)
   KKK(M)=KIKK
   MCARDS=MCARDS+2+((KKK-1)/40)*9
59 EE(M)=E
   C
C CALCULATE TOTAL ELECTRONIC DENSITY AND ATOMIC EXCHANGE POTENTIAL

C DO 60 I=1,MESH
RSATOM(I)=RSCORE(I)+RSVALE(I)
60 RUEXCH(I)=6.0*((3.0*R(I)*RSATOM(I))/315.82724)**(1.0/3.0)

C CALCULATE ATOMIC COULOMB POTENTIAL

A1=0.0
ASUM=0.0
B1=0.0
BSUM=0.0
T=0.0025*C
I=1
XI(I)=0.0
XJ(I)=0.0

C DO 62 J=1,NI
62 XI(I)=XI(I)+RUEXCH(I)
XJ(I)=XJ(I)+T

C CONTINUE

I=I+1
A2=RSATOM(I)/2.0
A1=A1+A2
B2=RSATOM(I)/2.0*R(I)
B1=B1+B2
XI(I)=ASUM*A1+H
XJ(I)=BSUM*B1+H
A1=A1+A2
B1=B1+B2
ASUM=XI(I)
BSUM=XJ(I)
A1=A2
B1=B2

C DO 63 I=1,MESH
63 XI(I)=2.0*Z2*2.0*(XI(I)+R(I)*(XJ(MESH)-XJ(I)))
XJ(I)=XI(I)+RUEXCH(I)

C CONTINUE

I=I+1
RSATOM(I)=RSCORE(I)+RSVALE(I)

C DO 64 J=1,NI
64 RUFNL2(I)=XJ(I)

C CONTINUE

NITER=NITER+1
PCELTA=DELTA
CELTA=0.0
DO 66 I=1,LIMIT
66 XI(I)=ARS(SNLO(I))
XJ(I)=ARS(RU(I))
IF (XI(I)=DELTA) 66,66,65
65 CELTA=XI(I)
IDELTA=I
C IF SCF CRITERION NOT SATISFIED, CALCULATE NEXT TRIAL POTENTI
IF (IPRSW) 68, 68, 73
69 RU(I) = 0.5*(RU(I)+XJ(I))
    IF (MESH=LIMIIT) 72, 72, 7C
70 RUZM=XJ(MESH)
    RATIO=(RUZM=RU(LIMIT))/(RUZM=XJ(LIMIT))
CC 71 I=LIMIT, MESH
71 RU(I)=RUZM=RATIO*(RUZM=XJ(I))
    LIMIT=MESH
72 IPRSW=IPRATT
CC TO 93
73 CONTINUE
    IF (NONMON) 68, 68, 74
74 IF (PDELTA=DELTA) 75, 75, 76
C
C    IF DELTA IS NOT MONOTONIC DECREASING FOUR TIMES, BYPASS
C PRATT IMPROVEMENT SCHEME
C
75 AGNON=NONMON=1
    IF (NONMON) 68, 68, 76
76 ALPH=0.5
C
C PRATT IMPROVEMENT SCHEME
C
CC 84 I=2, ICUT
CC XNUM(I)=RUINL(I)*RUFLN I(I)*RUINL2(I)*RUFLN2(I)
CC CENM(I)=RUFLN(I)=RUINL2(I)*RUFLN2(I)
    IF (ABS(CENM(I)/RUINL2(I))=0.0001) 77, 77, 78
77 CONTINUE
    ALPH=0.5
    GO TO 83
78 ALPH=XNUM(I)/DENM(I)=RUINL2(I)/SNLO(I)
    IF (ALPH) 79, 82, 8C
79 ALPH=0.0
    GO TO 83
80 IF (0.5=ALPH) 81, 82, 82
81 ALPH=0.5
82 CONTINUE
83 XI(I)=ALPH
84 CONTINUE
    IPRSW=IPRAT=1
    IF (KUT) 87, 87, 87
85 CONTINUE
    I0=ICUT+20
    IC1=ICUT+1
    ACEL=XI(1)/ICUT/20.
CC 86 I=IC1, IC
    XI(I)=XI(I-1)=ACEL
86 XI(I)=XI(I)
87 CONTINUE
    XJ(I)=0.5
    XJ(2)=XI(2)
    ASUM=XI(2)+XI(3)+XI(4)+XI(5)
CC 88 I=3, ICUT
    XJ(I)=ASUM*0.2
88 ASUM=ASUM+XI(I-2)+XI(I+3)
    IF (KUT) 91, 89, 91
89 CONTINUE
    IC1=IC+1
CO 90 I=1C1, MESH
XJ(I)=0.0
90 RI(I)=RUFNL2(I)
91 CONTINUE
CO 92 I=2, IC
92 RI(I)=RUFNL2(I)+XJ(I)*SALG(I)
93 CONTINUE
IF (KUT) 94, 96, 94
94 ICUT=MESH
LIMIT=MESH
CO 95 I=2, MESH
VLAST=V(I)
V(I)=RI(I)/R(I)
95 XI(I)=V(I)=VLAST
GC TO 102
96 CONTINUE
ICUT=0
CO 101 I=2, MESH
VLAST=V(I)
IF (ICUT) 97, 97, 97
97 IF (THOZZZ+RUI(I)) 100, 100, 98
98 ICUT=1
99 V(I)=THOZZZ/R(I)
GC TO 101
100 V(I)=RI(I)/R(I)
101 XI(I)=V(I)=VLAST
102 CONTINUE
XI(I)=0.0
C
NEXT TRIAL EIGENVALUES PREDICTED BY PERTRUPTION THEOERY.
C
NCARDS=9C
C 105 N=1, NCSPVS
K=(NKK(M)=1)/40
H=0.0025*C
ASUM=0.0
A1=0.0
I=1
CO 104 J=1, K
CC 103 L=1, 4C
I[I+1]
A2=XI(I)*SNL(M, I)*2
103 A1=A1+A2*H
ASUM=ASUM+A1=(A2/2, 0)*H
H=H^H
104 A1=(A2/2, 0)*H
EE(M)=EE(M)+ASUM
105 NCARDS=NCARDS+8*K+2
GC TO 4E
C
WHEN NOCOPY=1 ALL RESULTS TRANS FROM INTERN MEMORY TO PRINT.
C
WHEN NOCOPY=0 OUTPUT IS LAST ORBITAL WY, FNCT, ONLY
C
106 CONTINUE
IF (NOCOPY) 107, 114, 107
107 CONTINUE
PRINT 130, NCARDS, MCARDS
NC=1
WRITE (IM,136) Z,NC,RES,NVALES,ION,IZ,NC
CC 110 I=1,441
IF (TWOION+RUINL2(I)) 110,112,108
108 CC 108 M=1,441
109 RUINL2(I)=TWOION
GO TO 111
110 CONTINUE
111 CONTINUE
CC 112 MIN=I,440+5
MAX=MIN+4
NC=NC+1
WRITE (IM,136) (RUINL2(M),M=MIN,MAG),IZ,NC
112 CONTINUE
NC=NC+1
WRITE (IM,137) RUINL2(441),IZ,NC
CC 114 M=1,NC,SPV,S
NLZ=NNLZ(M)
KKK=NNKKK(M)
XL=NLZ/10=10*(NLZ/100)
NC=NC+1
WRITE (IM,134) NLZ,XL,EFF(M),WWNL(M),KKK,IZ,NC
K1=KKK+1
CC 113 MIN=I,K1,5
NC=NC+1
MAX=MIN+4
WRITE (IM,136) (SNL(M,I),I=MIN,MAG),IZ,NC
113 CONTINUE
WRITE (IM,137) SNL(M,KKK),IZ,NC
114 CONTINUE
IF (KEY=1) 115,116,118
115 KEY=1
116 CC 117 I=1,MESH
117 RU3(I)=RU(I)
ZE2=ZE
GO TO 11
118 CC 119 I=1,MESH
RU2(I)=RU3(I)
119 RU3(I)=RU(I)
ZE2=ZE
GO TO 11
120 CONTINUE
C PUNCH GROUND STATE WAVE FUNCTIONS
C
Z=AZ
NC=0
M=NC,SPV,S
NLZ=NNLZ(M)
KKK=NNKKK(M)
XL=NLZ/10=10*(NLZ/100)
NC=NC+1
WRITE (ID,142) NLZ,XL,EFF(M),WWNL(M),KKK,IZ,NC
K1=KKK+1
CC 121 MIN=I,K1,5
NC=NC+1
MAX=MIN+4
WRITE *(ID,136) (SNL(M,I),I=MIN,MAX),IZ,NC
121 CONTINUE
NC=NC+1
WRITE *(ID,137) SNL(M,KKK),IZ,NC

C CALCULATE EXCITED STATE WAVE FUNCTIONS

DC 123 KC=1,JE
M=NCSPVS+1
READ *(IR,127) NNLZ(M),WWNL(M),EE(M)
WWW=0.0
WWW=WWW+WWNL(M)
E=EE(M)
NN=NNLZ(M)/100
LAM=NNLZ(M)/100=NN
XL=LAM
CALL SCHEQ (Z,EE,LAM,NN,KKK,MESH,C,THRESH)

C PUNCH EXCITED STATE WAVE FUNCTIONS

NC=0
M=NCSPVS+1
NLZ=NNLZ(M)
XL=NLZ/100=NLZ/100
NC=NC+1
WRITE *(IC,142) NLZ,XL,EE(M),WWNL(M),KKK,Z,IZ,NC
K1=KKK+1
DO 122 MIN=1,K1,5
NC=NC+1
MAX=MIN+4
WRITE *(IC,136) (SNL(I),I=MIN,MAX),IZ,NC
122 CONTINUE
NC=NC+1
WRITE *(IC,137) SNLO(KKK),IZ,NC
123 CONTINUE
CALL EXIT

C FFORMAT (F8.5,9F7.5)
124 FORMAT (F4.0,314)
125 FORMAT (F4.0,314)
126 FORMAT (16H WWW= F4.0,6H ZZZ= F4.0,6H Z= F4.0,10H NCORES=I4,11W
1 NVALE= I4,11H NCSPVS= I4/25H CONTROL CARDS INCORRECT,1)
127 FORMAT (I4.0,F4.0,F8.4)
128 FORMAT (I7.0,F7.0,1PE14.7)
129 FORMAT (1PE15.7,1PE14.7)
130 FORMAT (10H NCARDS= I4,10H MCARDS=I4)
131 FORMAT (I4,2F8.6,11I4)
132 FORMAT (8H KEY = I4)
133 FORMAT (16H ITER,7X,1H7,4X5HDELTA,7X,3OH(DEL) X(DEL) X(1CUT))
134 FORMAT (I4,1P3E14.7,14,1PE14.7,8X,1HZ,I3,14)
135 FORMAT (F4.0,314,56X,1HZ,I3,14)
136 FORMAT (1PE15.7,1PE14.7,1X,1HZ,I3,14)
137 FORMAT (1PE15.7,57X,1HZ,I3,14)
138 FORMAT (72H)
139 FORMAT (27HOSTARTING POTENTIALS AND Z=,F4.0,9H IN ERROR,2F4.0)
140 FORMAT (40H11,X,RU3,RUINL1,RUFNL1,PUINL2,RUFNL2,RU )
141 FORMAT (18,F10.4,1PE16.7)
142 FORMAT (I4,1P3E14.7,14,CPF4.0,C,1AX,1HZ,I3,14)
SUBROUTINE SCHEQ (ZZ, EN, LAMBD, NOFL, KKK, MESS, SCF, THRESH)

SUBROUTINE SCHEQ

COMPUTE ENERGY EIGENVALUE AND WAVE FUNCTION

ORIGINALLY WRITTEN BY SHERWOOD SKILLMAN

RCA LABORATORIES, PRINCETON, NEW JERSEY, SPRING 1961

MODIFIED BY FRANK HERMAN, SUMMER 1961

FURTHER MODIFIED BY RICHARD KORTUM AND PAUL KELLY, LOCKHEED

RESEARCH LABORATORIES, PALO ALTO, CALIFORNIA, SUMMER 1962

POTENTIAL AVAILABLE IN COMMON STORAGE AT START. WAVE FUNCTION, COMputed EIGENVALUE, AND KKK LOCAATED IN COMMON STORAGE AT RETURN FROM SCHEQ.

NOTATION: ATOMIC NUMBER (ZZ=Z); TRIAL EIGENVALUE (EN=E); ORBIT.

QUANT. NO. (LAM=XL); PRINC. QUANT. NO. (NCFL=N); NO. OF MESH PTS. USED FOR WV. FNCT. (KKK); NO. OF INTEGRATION MESH PTS.

(MESS=MESS); SCALE FACTOR (SCF); EIGENVALUE ACCUR. CRIT. (THRESH)

DIMENSION P(5), Q(5), T(5), D(5)

DIMENSION R(521), PSCORE(521), RUINL1(521), RU2(521), RU(521), NNL(241), RSVALE(521), RUFLN1(521), RU3(521), XI(521), WWNL(241), V(521), RSATML(521), RUINL2(521), XNUM(521), XJ(521), NNK(241), EE(241), RUFLN2(521), DENM(521), SNL(10,521), SNLO(521), QQ(4521)

COMMON V, SNLO, RSATML, RSCORE, RSVALE, RU, RUFLN2, RU3, RU2, RU, NNL, RUINL1, RUFLN1, NKKK, EE

EQUIVALENCE (RSCORE, XNUM), (RSVALE, DENM), (QQ, RSATML)

SET UP CONSTANTS AND INITIALIZE

IR=5
IP=6
IM=6
Z=ZZ
LAM=LAMBD
NN=NOFL
MESS=MESS
SCF=MANY=20C
EN=E
MOREV=0
LESSV=0
EMORE=C
ELESS=C
MORE=0
LESS=0
CE=0
0
NN=NN=LAM
0=LAM*LAMP
0C=R42
FSQ=H*H

B3=(V(3)-V(2))/H=7/HSQ
Y=H+H
FLPS=4*LAM+6
SLPT=6*LAM+12
ELPT=8*LAM+20
A1=Z/XLP
YSP=Y+Y
B1=Z=Z
AB1=A1+B1
AB3=A1+B3

C C RAISE H AND Y TO LAM+1
C

FTLH
YTL=Y
IF (LAM) 6,3,1
1 DO 2 I=1,LAM
2 YTL=FTL#Y
3 H1=HSQ
BCHS=B/HSQ
EO=F1/E1
PT=F1#E1
EQ3=BCHS+BOH*BTH
EQ4=BCHS/4.0+BOH/2.0+BTH+BTH
EPL=E+LAM
FPL=5+LAM
XIFC=C+21701389E=4

C C START OUTWARD INTEGRATION
C

4 NPRINT=NPRINT+1
EPS=E=E
EG=F
IF (MANy=NPRINT) 5,8,8
5 WRITE (IP,55) NN,LAM,Z
CALL EXIT
6 NSTOP=77
7 WRITE (IP,96) NSTOP
CALL EXIT
8 DO 9 I=1,MESH
9 SNLO(I)=C
IF (NPRINT=1) 6,10,17
10 CONTINUE
CO 11 I=4,MESH
GQ(I)=V(I)+B/(R(I)*R(I))=E
11 CONTINUE
12 M=MESH
CO 14 I=4,MESH
IF (QQ(M)) 13,14,14
13 IK=M+1
CO TO 15
14 M=M+1
NSTOP=521

C C Q IS EVERYWHERE POSITIVE
C

CO TO 7
15 IF (Q(MESH>IK)) 16,16,19
16 EPS=QQ(MESH=40)
E = E + EPS

17 CONTINUE
CC 18 I=4,MESH
18 Continue = QQ(I)=EPS
GO TO 12
19 CONTINUE
NCROSS = 0
SIGN = 1.0
H = OC.
Y = H
1
C B = LAM*(LAM+1)
C B1 = -2.0*Z
B2 = 3.0*H/E + 2.0*V(2) - V(3)
C B3 = (V(3) - V(2))/H = Z/HSQ
C A1 = -Z/(LAM+1)
A2 = (AB1+B2)/FLPS
C A2 = (A1*B1+B2)/(4*LAM+6)
A3 = (A3*B1+A2*B2+B3)/SLPT
C A3 = (A2*B1+A1*B2+B3)/(6*LAM+12)
A4 = (A3*B1+A2*B2+AB3)/ELPT
C A4 = (A3*B1+A2*B2+AB3)/(8*LAM+20)
P(3) = { 1.0*(1.0*A1+H2*B2+A3+H3+4.0)*H2**2*(XL+1.0)}
P(4) = { 1.0*(1.0+C*(A1+Y*(A2+Y*(A3+Y*A4))))}*YTL
C P(4) = { 1.0+C*(A1+Y*(A2+Y*3+4.0+A4))*Y**4}**2*(XL+1.0)
Q(3) = BQ3*B2
Q(3) = (B*B1+H2*B2+A3+H3+3.0)/H2**2
Q(4) = BQ4*B2
C Q(4) = (B*B1+Y*B2+Y**2+3.0+Y**3)/Y2**2
SNLO(2) = P(3)
SNLO(3) = P(4)
1=3
DX = OC
H1 = H2 = 2
H2 = H1/12.0
T(3) = P(3) = (1.0*H2*Q(3))
T(4) = P(4) = (1.0*H2*Q(4))
C(4) = T(4) = T(3)
NCOUNT = 3
NINT = 2
20 I = I+1
C IF END OF MESH IS REACHED, MODIFY TRIAL EIGENVALUE
C IF (I=MESH) 22,21,21
21 IF (NDCS=NCROSS) 37,44,44
C RETURN TO BEGINNING OF OUTWARD INTEGRATION IF NECESSARY
C 22 Q(5) = QQ(I)
IF (I=I) 34,34,23
23 Q(5) = Q(4)*H1*Q(4)*P(4).
T(5) = D(T(5))*T(4)
IF (1.0=ABS(H2*Q(5))) 21,21,24
24 P(5) = T(5)/(1.0*H2*Q(5))
SNLO(1) = P(5)
IF (SIGN) 25,6,26
25 IF (P(5)) 28,28,27
26 IF (P(5)) 27,28,28


27 NCROSS = NCROSS + 1

COUNT CHANGES IN SIGN

SIGN = -SIGN

28 NCOUNT = NCOUNT + 1

IF (7 = NCOUNT) 6, 29, 30

29 NCOUNT = 2

30 NINT = NINT + 1

IF (10 = NINT) 6, 31, 32

31 CX = DX + DX

T = CX

H1 = H**2

H2 = H1/12.0

NINT = 0

T(5) = P(5)*{1.0 + H2*Q(5)}

T(3) = P(3)*{1.0 + H2*Q(3)}

C(5) = T(5) = T(3)

32 CC 33 K = 1, 4

P(K) = P(K+1)

T(K) = T(K+1)

D(K) = D(K+1)

33 Q(K) = Q(K+1)

GO TO 20

34 IF (NCOUNT = 2) 6, 25, 23

35 IF (NINT = 4) 23, 22, 36

MATCHING RADIUS HAS BEEN REACHED GOING OUT

IF NOCR NOT EQUAL TO NCROSS, MODIFY TRIAL EIGENVALUE

36 EIGEN = E

IF (NOCR = NCROSS) 37, 52, 44

37 MORE = 1

TOO MANY CROSSINGS, INCREASE ABSF(E)

MOREV = MOREV + 1

IF (MOREV = 1) 38, 40, 35

38 NSTOP = 50

GO TO 7

39 IF (E = EMORE) 40, 41, 41

40 EMORE = E

41 IF (LESS) 42, 43, 51

42 NSTOP = 55

GO TO 7

43 E = 1.25*EG

GO TO 4

44 LESS = 1

TOO FEW CROSSINGS, DECREASE ABSF(E)

LESSV = LESSV + 1

IF (LESSV = 1) 45, 47, 46

45 NSTOP = 57

GO TO 7

46 IF (ELESS = E) 47, 48, 48

47 ELESS = E

48 IF (MORE) 49, 50, 51
49 NSTOP=62
  CC TO 7
50 E=0.75*EG
  CC TO 4
51 E=0.5*(EMORE-LESS)
  CC TO 4
52 IF (ABS(SNLO(I-1))=ABS(SNLO(I+2))) 53, 56, 56.

CHECK TO SEE THAT WAVE IS IN THE DAMPED REGION (ABSOLUTE VALUE DECREASING AND SIGNS ALIKE)

53 IF (P(1)) 54, 23, 55
54 IF (SNLO(I-21)) 57, 23, 23
55 IF (SNLO(I-21)) 23, 23, 57
56 IF (1.0E-25=ABS(P(5))) 44, 44, 23

LARGE ABSOLUTE VALUE OF P IN WHAT SHOULD BE THE DAMPED REGION. INDICATES TOO FEW PEAKS, DECREASE ABSF(E)

NOW NDCR = NCROSS AND MATCHING RADIUS LIES IN DAMPED REGION

57 IMATCH=I+2
  XMATCH=R(I+1)
  PP0UT={(T(4)-T(2)+0.5*(P(4)-P(2)))/H
  S2=PP0UT/P(3)

INTEGRATION IS BY 8 APPLICATIONS OF NEWTON-COTES CLOSED QUADRATURE FOR FIVE INTERVALS ON EACH BLOCK

XIFC=(5*H(BLOCK-1)/288)/2, H(1)=0.0025*SCALE FACTOR

SUM1=0.0
  XIF=XIFC
  I=1
  VALUE=C.0 C
58 MM=A
  SUM2=0.0
  XIF=XIF+XIF
59 Y=VALUE
  VALUE=SNLO(I+5)**2
  SUM2=SUM2+1.0*(VALUE+Y)+75.0*(SNLO(I+4)**2+SNLO(I+1)**2)+50.0*(SNL0(I+2)**2+SNLO(I+3)**2)
  I=I+5
  IF (IMATCH==I) 6, 62, 6C
60 MM=MM+1
  IF (MM) 6, 61, 55
61 SUM1=SUM2*XIF+SUM1
  CC TO 58
62 SUM1=SUM1+SUM2*XIF
  S1=SUM1/P(3)**2
  PMATCH=P(3)
  IF (NN==1) 6, 63, 64
63 XINW=EPL*XMATCH

FOR N =1, START INWARD INTEGRATION AT 8+LAP*XMATCH OR X MAX

CC TO 65
64 XINW=FPL*XMATCH
FOR N NOT=1, START AT (5*LAM)*X MATCH OR X MAX (END OF MESH)

65 DO 67 I=41,MESH,40
   IF (XINH=R(I)) 66,66,67
66 KKK=I
   GO TO 68
67 CONTINUE
   KKK=MESH
68 I=KKK
   DX=R(I-I)=R(I)
   H=DX
   IF(Q* 1736 1111=1*DX)
   H=SQ=H*H
   F=SQ12=HSQ/120
   C(3)=QQ(1)
   P(3)=EXP(R(I)*SQR(T(Q(3))))
   SUM3=P(3)/Q(3)
   I=I=1
   Q(4)=QQ(1)
   P(4)=EXP(R(I)*SQR(T(Q(4))))
   IF (ARS(P(4))=100 CE=35) 69,69,71
69 KKK=KKK+40
   IF (KKK=IMATCH) 70, 70, 68
70 WRITE (IP,97) 2, NN, LAM, KKK
   KKK=KKK+40
   P(4)=1.0.E=35
   P(3)=1.0.E=35
71 IF (PMATCH) 72,6,73
72 P(3)==P(3)
   P(4)==P(4)
73 SNLO(I+1)=P(I)
   SNLO(I)=P(I)
   T(3)=P(3)*(1.0=HSQ12*Q(3))
   T(4)=P(4)*(1.0=HSQ12*Q(4))
   C(4)=T(4)=T(3)
74 CC 76 M=2,40
   I=I=1
   Q(5)=QQ(I)
   C(5)=HSQ*Q(4)*P(4)+D(4)
   T(5)=D(5)*T(4)
   P(5)=T(5)*1.0=HSQ12*Q(5)
   IF (I=IMATCH+1) 67,74,75
75 SNLO(I)=P(5)
   CC 76 K=1,4
   P(K)=P(K+1)
   T(K)=T(K+1)
   C(K)=D(K+1)
76 Q(K)=QQ(K+1)
   G(5)=QQ(I=2)
   C(5)=HSQ*Q(4)*P(4)+D(4)
   T(5)=D(5)*T(4)
   P(5)=T(5)*1.0=HSQ12*Q(5))
   P(5)=C,9375*P(4)+C,2734375*P(5)=0.546875*P(3)+0.21875*P(2)=0.0390
1625*D(I)
   I=I=1
   DX=DX/2.0
   Q(5)=QQ(1)
   H=DX
   H=SQ=H*H
\[ H SQ12 = H SQ / 12.0 \]
\[ T(5) = P(5) \times 1.0 = H SQ12 \times Q(5) \]
\[ T(4) = P(4) \times 1.0 = H SQ12 \times Q(4) \]
\[ C(5) = T(5) / T(4) \]
\[ SNLO(I) = P(I) \]
\[ DO \ 77 \ L = 1, 4 \]
\[ P(L) = P(L + 1) \]
\[ T(L) = T(L + 1) \]
\[ C(L) = C(L + 1) \]
\[ 77 \ Q(L) = Q(L + 1) \]
\[ GO \ TO \ 74 \]

MATCHING RADIUS HAS BEEN, REACHED COMING IN

\[ 78 \ K = K K K \]
\[ VALUE = SNLO(K) \times 2 \]
\[ GO \ TO \ 80 \]
\[ 79 \ CONTINUE \]
\[ SUM3 = 0 \]
\[ XIF = XIF \times C \]
\[ 80 \ MM = 8 \]
\[ SUM4 = 0 \]
\[ Y = VALUE \]
\[ VALUE = SNLO(K = 5) \times 2 \]
\[ SUM4 = 0 \]
\[ 81 \ IF \ (K = IMATCH) \]
\[ MM = MM + 1 \]
\[ 82 \ SUM3 = SUM3 + XIF \times SUM4 \]
\[ S3 = SUM3 / P(4) \times 2 \]
\[ PIN = T(5) \times C \times 5 \times (P(5) = P(3)) / H \]
\[ S4 = PIN / P(4) \]
\[ CE = (S2 - S4) / (S1 - S3) \]
\[ IF \ (ABS(CE/E) = THRESH) \]
\[ 86 \ E = E \times DE \]
\[ IF \ (E) \]
\[ E = E \times DE \]
\[ CE = DE / 2 \times C \]
\[ GO \ TO \ 84 \]

IMPROVE TRIAL EIGENVALUE BY PERTURBATION THEORY IF NECESSARY

CALCULATE THE NORMALIZED WAVE FUNCTIONS

\[ 86 \ FC = FC / P(4) \]
\[ GO \ 87 \ J = IMATCH, K K K \]
\[ 87 \ SNLO(J) = SNLO(J) \times FC \]
\[ SUM1 = 0 \]
\[ J = 1 \]
\[ XIF = XIF \times XIF \]
\[ VALUE = 0 \]
\[ MM = 8 \]
\[ XIF = XIF \times XIF \]
\[ SUM2 = 0 \]
\[ 88 Y = VALUE \]
\[ VALUE = SNLO(J + 5) \times 2 \]
\[ SUM2 = SUM2 \times 15.0 \times (VALUE \times Y) \times 75.0 \times (SNLO(J + 4) \times 2 + SNLO(J + 1) \times 2) + 50.0 \times (SNL) \]
\[ 10(J + 2) \times 2 + SNLO(J + 3) \times 2) \]
J=J+5
MM=MM=1
IF (MM) 6, 90, 89
90 SUM1=SUM1+XIF*SUM2
IF (KKK=J) 6, 91, 88
91 C1=SORT(SUM1)
   IF (SNLO(1)) 92, 6, 93
92 C1=SI
93 DO 94 I=1, KKK
94 SNLO(I)=SNLO(I)/C1
EN=E
RETURN
C
95 FORMAT (20H NO CONVERGENCE ON, I4, I1, F4.0)
96 FORMAT (5HOSTOP, I4, 8HIN SCHEQ)
97 FORMAT (6HOSTOP Z=, F6.0, 6H NL=, I3+I1, 7H KKK =, I5, 23H IS LESS THAN I IMATCH =, I5, 43H INWARD INTEGRATION WILL BE TRIED AT KKK+40)
END
b) Discussion

This program, HFSWF, is a modification to the program written by Herman and Skillman (1963), H+S. The original work contains subroutines not presented here. However, the two principle components of H+S, the main program "Hartree-Fock-Slater Self-Consistent Atomic Field Program" and the principle subroutine "Schröedinger Equation Subroutine" (SCHEQ) are used. The text H+S gives several hundred pages of discussion and tables concerning these calculations and should be consulted for further discussion. The material here will be an overview of the principle logic of the program as highlighted by the "comment" cards in the program listing.

This program computes numerical radial wave functions for the elements by solving the H-F-S equation

\[ \left[ \frac{d^2}{dr^2} - \frac{\lambda (1+\frac{1}{r})}{r^2} - \gamma(t) - \varepsilon \eta(t) \right] P_{\alpha \lambda}(r) = \omega \]  

(142)

for each orbital in a given configuration of an atom using the self-consistent field technique. A reading of the program listing will be useful for the discussion that follows.

Let us examine those sections of the program developed by H+S and separately consider the modifications made for use in this work.

i) Herman and Skillman Program

Initially let us note that in order to have a common mesh for all atoms in the periodic table the
parameter \( x \), was used as the independent variable in place of \( r \), the true radial distance. This parameter \( x \) is defined

\[
x = \frac{f}{\mu} \quad \text{where} \quad \mu = \left( \frac{1}{2} \right) \left( \frac{3\pi}{4} \right)^{3/2} \left( \frac{1}{2} \right)^{3/2}\]

References will be made to the "x-mesh" and "r-mesh" in the following discussion.

The program begins by reading a heading card and some control parameters (KEY, TOL, THRESH, etc.) that determine the form of the potential, define the self-consistency criteria, and provide other control information. The allowed values and meanings of these control parameters are reviewed in the "User-Manual" (Appendix VII). After constructing the "x-mesh" array some, or all, of the normalized potentials \( RU(M) \) are read depending on the value of KEY.

The configuration information (\( Z \), number of core orbitals (NCORES), etc.) is read and for each orbital the number of electrons (WWNL) and starting eigenvalue is read. If only some of the starting values of the potential have been read (\( KEY = 0 \)) or if the potential is to be constructed from other potentials (\( KEY = 2 \)), the calculation of the full 441 point normalized potential \( RU(M) \) is carried out.

From the normalized potential \( RU(M) \) the starting potential \( V(M) \) to be used in the HFS equation is constructed in either the modified (\( KUT = 1 \)) or un-modified (\( KUT = 0 \)) form by use of the relations

\[
V(M) = \min \left[ \frac{RU(M)}{R(M)} - \frac{Z}{R(M)} \right] \quad \text{or} \quad V(M) = \frac{RU(M)}{R(M)} \quad (143)
\]

where \( R(M) \) is the true radial distance. After initializing some counting parameters, (e.g. MITER, number of iterations; LIMIT, mesh value \( M \)) where
RU(M) = -2Z) the iteration is begun. If the test (MAXIT - NITER) shows that the number of iterations has exceeded the chosen limit, MAXIT, an error message is printed and the program ends. If the test succeeds (i.e. MAXIT < ITER) the following occurs for the iteration.

For each orbital, the Schrödinger equation is solved using the constructed potential V(M). By calling SCHEQ the electronic densities for each orbital (RSCORE(M) and RVALE(M)) and the total electronic density (RSATOM(M) = RSCORE(M) + RVALE(M)) are calculated.

The atomic exchange potential (RUEXCH(M)), the total coulomb potential XI(M) and the final potential XJ(M) are calculated. Defining DELTA as the maximum difference between the starting potential, RU(M), and the potential calculated from this set of wave functions, XJ(M), that is

\[ \text{DELTA} = \max \left| XJ(M) - RU(M) \right| \]  

(144)

a comparison with the required tolerance for self-consistency, TOL, is made. If \( \text{DELTA} < \text{TOL} \), self-consistency has been reached and transfer to the output routine is made. Otherwise an improved starting potential RU(M) is calculated and another iteration is begun.

The improved starting potential is calculated from the initial and final potentials by a simple arithmetic average

\[ RU(M) = \frac{RU1(M) + XJ(M)}{2} \]  

(145)

or by use of the Pratt improvement scheme,

\[ RU(M) = 2 \ RH(M) + (1 - a) \ XJ(M) \]  

(146)

where \( 0 \leq \alpha \leq 0.5 \) below \( M = \text{LIMIT} \), \( \alpha = 0 \) above limit. (For more discussion of the Pratt improvement scheme see Herman and
Skillman (1963), Chapter 4 or Pratt (1952)).

New trial eigenvalues for each orbital are calculated using perturbation theory,

\[ E = E + \langle M | H' | M \rangle \]  \hspace{1cm} \text{(147)}

With the improved potential and the new eigenvalues the next iteration is begun.

The output routine is either all the radial wave functions and the self-consistent potential (NOCOPY=1) or just the last orbital (NOCOPY = 0) as punched cards.

ii) Modifications for This Calculation.

As discussed earlier we seek the appropriate radial wave functions that are consistent with our simplifying assumptions of the inert-core-active electron approximation used in developing the cross-section expressions used in this calculation.

Having achieved a self-consistent set of radial wave functions and a self-consistent potential we enforce our simplifying assumptions by solving for the excited state orbital in the given potential. This is done by reading the eigenvalue of the excited state and the number of electrons in the excited state and solving the wave equation in the ground-state self-consistent potential by calling SCHEQ.

The wave function achieved is punched as output.

Using the IBM 360/75 computer, the program HFSWF had a run time of 29 sec for the CESIUM 6s and 6p wave function calculation.
2. Excitation Cross-Section Program

This program, named EXCSCT, is a calculation of total electron atom excitation cross-sections for a range of incident electron energies using one of four possible approximations to the scattering amplitude. The program consists of a main routine and six subroutines.

a) Listing
PROGRAM EXCSCT(INPUT)

* A FORTRAN PROGRAM TO CALCULATE EXCITATION CROSS-SECTIONS FOR THE ELECTRON IMPACT EXCITATION OF ATOMS.
* ENERGY IS MEASURED IN UNITS OF THRESHOLD ENERGY, EPSIL.
* EPSIL IS MEASURED IN UNITS OF TWICE THE RYDBERG.
* IPROX=THE APPROXIMATION USED; ALLOWED VALUES ARE:
  * (1=BORN; 2=OCHKUR; 3=BETHE; 4=MODIFIED BETHE).
* N=0; *** MODIFIED BETHE (IPROX=4) MAY ONLY BE USED FOR
  * OPTICALLY ALLOWED TRANSITIONS***

REAL*8 AQ,8044),80i
CIMENSION ZN(25), SIG(25), FX(1001), XMSh(1001), SG(8), EPSL(4), N
1L1(4), NL2(4), SIGM(25), SIG2(254)
COMMON PINf(521), PF(521), C,vANsY(521), KKK
EXTERNAL BJR, RN
DATA N,ZN(1),ZN(2),ZN(3),ZN(4),ZN(5),ZN(6),ZN(7),ZN(8),ZN(9),20,1.
120,1.35,1.50,1.75,2.00,2.33,2.67,3.0,3.50,ZN(10),ZN(11),ZN(12),ZN(13),
213,ZN(14),ZN(15),ZN(16),ZN(17),ZN(18),ZN(19),ZN(20)/4.00,5.00,6.0
3C7.00,8.00,10.00,12.00,15.00,18.00,21.00,24.00/ 
NCC=O
IP=6
IN=5
IR=5

READ CONTROL CARD; N=NO. OF VALUES OF INCIDENT ENERGY;
  NTC=TYPE OF SERIES; NC=NO. OF SERIES; NOTP=OUTPUT OPTION;
  A=ELEMENT NAME.
  NTC: 1=SINGLE CASE; 2=MULTIPLE APPROX; 3=MULTIPLE WV. FNCT.
  NOTP: 1=PUNCHED CARD; 2=SINGLE LIST; 3=MULTIPLE LIST;

READ (IM,46) N,NTC, NC, NOTP, AQ

READ ENERGY RANGE
ZN(N)=VALUES OF INCIDENT ENERGY IN THRESHOLD UNITS.

IF (N.NE.1) GO TO 1
N=19
GO TO 2
1 READ (IR,47) (ZN(I),I=1,N)
2 CONTINUE
READ INPUT WAVE FUNCTIONS
READ (IR,49) PIN(I),I=MIN,MAX
READ (IR,50) PIN(KKK1)
READ (IR,48) NLZ2, XL2, EE2, WNL2, KKK2, Z
K21=KKK2-1
DO 5 MIN=1,K21,5
MAX=MIN+4
READ (IR,49) PF(I),I=MIN,MAX
READ (IR,50) PF(KKK2)
KKK=AMINO(KKK1,KKK2)
C=0.885341381/Z**(-0.333333333)
EPSIL=ABS(EE2-EE1)/2.
N1=NLZ1/10
N2=NLZ2/10
C READ THE APPROXIMATION IPROX.
C IPROX VALUES ARE; 1=BORN; 2=OCKHUR; 3=BETHE; 4=MODIFIED BETHE.
6 READ (IM,51) IPROX, BQ
C TRANSFER TO THE APPROPRIATE APPROXIMATION.
MWTCH=2
IF (IPROX.EQ.1.OR.IPROX.EQ.2) MWTCH=1
GO TO (260) MWTCH
C BETHE APPROXIMATION
C FIND RDMO
7 CONTINUE
XLAM=ABS(XL2-XL1)
LAM=XLAM
IF (((IPROX.EQ.4).AND.(LAM.NE.1)) GO TO 35
C CALL RDINT (RN,LAM,1.0)
C RDMO=(RANS**2)
C FIND ANCFCT
ANCFCT=(2.0*XL2+1.0)*((TJ(XL1,XL2,XLAM)*(2.0**XLAM)*(FACT(XLAM)/F 12.0**XLAM))**2)/(2.0**XLAM+1.)
C FIND CUTOFF FOR BETHE
ZW=30.
WMAX=SQRT(2.*ZW*EPSIL)*SQRT((ZW=1.0)/ZW)
WMIN=SQRT(2.*ZW*EPSIL)*SQRT((ZW=1.0)/ZW)
WKIN=2.*ZW*EPSIL
LAMIN=LAM
LAMAX=XL2*EPSIL
C FIND SBRNW
WSUM=0.0
HANS=0.0
DELW=(WMAX-WMIN)/100.
W=WMIN+DELW
KW=1
CO 11 IW=1,101
W=W*DELW
FW=0.0
CO 8 I=LAMIN,LAMAX
IF=0
CALL RDINT (BJ,I,W)
FW=(FW+(2.*XL2+1.0)*(2.*WI+1.0)*((TJ(XL1,XL2, WI)*RANS)**2))/W**3
8 CONTINUE
KW=KW
IF ((IW=1)*(IW=101)*KW) .9,11,10
9 WSUM=WSUM+2.*FW
10 WSUM=WSUM+FW
11 WSUM=WSUM+FW
WANS=WSUM*DELW/3.
SGBRN=8.*WANS/WKIN
C CORRECTION FOR DEL=LAM=0 IN BETHE APPROX.
IF (LAM=NE.0) GO TO 12
XLAM=2.
LAM=2
CALL RDINT (RN,LAM,1.0)
RCMO=(RANS**2)
ANGFCT=(2.*XL2+1.0)*((TJ(XL1,XL2,XLAM)*(2.**XLAM)*(FACT(XLAM)/FACT(12.*XLAM)))**2)/(2.*XLAM+1.0)
C 12 WFF=8.*RDMO*ANGFCT/WKIN
IF (LAM.EQ.1) GO TO 13
XLAM=2.*XLAM=2.
WKUT=(XLAM2*SGB RN/WFF+WMIN**XLAM2)**(1./XLAM2)
GO TO 14
13 WKUT=(EXP(SGBRN/WFF)*WMIN)**XLAM2
GO TO 14
C CONTINUE
C FINE ENGFC
CC 17 I=1,N
XMAX=WKUT
XMIN=SQR(2.*ZNI*EPSIL)*(1.=SQR((ZNI**1)/ZNI**1))
ZKIN=2.*ZNI*EPSIL
IF (Xlam.EQ.1.0) GO TO 15
XXINT=(XMAX**(2.*XLAM=2.)**(2.*XLAM=2.)**(2.*X**
XLAM=2.)
GO TO 16
15 XXINT=ALOG(XMAX/XMIN)
16 ENFCT=(8.*XXINT)/ZKIN
C 17 SIG(I)=RDMO*ANGFCT*ENFCT
IF (IPROX.EQ.3) GO TO 36
C MODIFIED BETHE CALCULATION
CC 25 I=1,N
IF (ZNI(LT.1.5) GO TO 23
ZKIN=2.*ZNI*EPSIL
SZ=(ZNI**1)/ZNI**1)
STUFF=RDMO*ANGFCT*4.0/(3.*ZKIN)
CC 20 LP1=1.
LP=LP1
IF (LP.EQ.0) GO TO 18


\[ ZETA = ((XLP + 1) \times F((1, LP, ZN) \times (SZ / 2)) + XLP \times (SZ / 2)) / (2 + XLP / 1) \]

\[ REST = \text{REST} / (XLP \times (XLP + 1)) \]

18 \[ REST = (SZ^{1.5} \times (F((2, LP, ZS) \times (SZ / 2))) \]

19 \[ SG(LP1) = \text{STUFF} \times \text{REST} \]

C

FIND SGML
SGML = (2 + XLP / 1) / ZKI 

C

IF (LP \text{EQ.} 0) \text{GO C}
XLO = LO

C

FIND L0-TERM
TRM0 = ((XLO/1) \times (ZS / 2)) / (2 + ZKI)

C

FIND SUM-TERM
TRMSM = 0.0
DO 22 LS = 1, LP
TRMSM = TRMSM + SG(LS)

C

FIND MOD. BETH THE C-SECTION
GO TO 24

23 SIG(I) = 0.0
GO TO 25

24 SIG(I) = SIG(I) + TRM0 = TRMSM
GO TO 26

C

PORN \times OCHKUR
C

26 CONTINUE
XMN = SQRT((2 + ZN(N)) \times EPSIL) \times \{(SZ / 1) / ZKN(N)) \}
XMN = SQRT((2 + ZN(N)) \times EPSIL) \times \{(SZ / 1) / ZKN(N)) \}
CELX = (XMN = XMNN) / 1000.
X = XMNN = CELX
DO 28 IX = 1, 1001
X = X + DELX
LAMIN = \text{ABS}(XL2 - XL1)
LAMAX = XL2 + XL1
DO 27 I = LAMIN, LAMAX
XI = I
FX(I) = 0.0

C

CALL RINT (B1J, I, X)
C

FX(I) = FX(I) + (2 + XL2/1) \times (2 + XI/10) \times ((XL1 \times XL2 \times XI) \times RANS \times (SZ / 2)) / (1 \times 3)

27 CONTINUE
XMSH(I) = X

28 CONTINUE

C

FIND K-LIMITS AND COMPUTE SIG
DO 24 I=1,N
  XM=SQRT(1.0+Z(N(I))*EPSIL)*SQR((Z(N(I))=1.0)/Z(N(I)))
  XM=SQRT(1.0+Z(N(I))*EPSIL)*SQR((Z(N(I))=1.0)/Z(N(I)))
  Z(N)=Z(N)+EPSIL
  CALL RINT (RJ,J,XMAX)
  FM=FM+(Z(N)+1.0)*(Z(N)+1.0)+(TJ+XL+XL)*RANS)**2)/XMAX
  CALL RINT (B1,J,SMIN)
  FM=FM+(Z(N)+1.0)*(Z(N)+1.0)+(TJ+XL+XL)*RANS)**2)/XMIN
  CONTINUE

29 CONTINUE

C BEGIN K=INTEGRATION
  XSUM=0.0
  XANS=0.0
  LP=(XMIN-XMN)/DELX
  LQ=(XMAX-XMIN)/DELX
  TEST FOR NO. OF INTG. PTS. EVEN FOR SIMSON'S RULE INTEGRATION
  XLP=LP
  XLQ=LQ
  T1=(LP=LQ)/2
  T2=(XLQ=XLQ)/2
  IF (T1=T2 EQ 0.0) GO TO 30
  LC=LQ=1

C FIND CORRECTION (C1) USING TRAPEZOID INTEGRATION APPROXIMATE.

30 DLX1=XMIN-XMIN/LDLX1
  C1=(FX(LP)+FXMIN)*DLX1/2
  X=XMIN+DELX
  X=X+DELX
  A=(1.0-(Z(N)+2/ZKIN)**(Z(N)+2/ZKIN)**2)
  IF (IPROX.EQ.1.0) A=1.0
  DSIG=FX(I)*A
  KX=1
  DO 33 IX=LPLQ
    X=IX
    X=X+DELX
    A=(1.0-(Z(N)+2/ZKIN)**(Z(N)+2/ZKIN)**2)
    IF (IPROX.EQ.1.0) A=1.0
    DSIG=FX(I)*A
    KX=KX
    IF (IX=LP)*0.0 (IX=LQ)*KX 31,33,32
  31 XSUM=XSUM+2.0*DSIG
  32 XSUM=XSUM+DSIG
  33 XSUM=XSUM+DSIG
  XANS=XSUM/DELX/3
  DLX2=XMAX-X
  C2=(FX(I)+FXMAX)*DLX2/2
  XANS=XANS+C1+C2
  34 SIG(I)=(6.0*XANS)/ZKIN
  GO TO 36

C OUTPUT ROUTINES

35 WRITE (6,53)
  CALL EXIT
  IF (NOTP=2) 37,39,41
  NOTP=1;PUNCHED CARDS
  NCC=NCC+1
CC 38 I=1,N
WRITE (IP,54) ZN(I),SIG(I),BQ,Z,AQ,N1,N2,EPSIL
38 CONTINUE
IF (NCC.EQ.NC) GO TO 45
GO TO (45,6,4), NTC
C
C NOTP=2; SINGLE LIST
39 NCC=NCC+1
WRITE (IP,60) AQ,BQ
WRITE (IP,61)
WRITE (IP,62)
WRITE (IP,63)
WRITE (IP,57) Z,EPSIL,N1,N2
WRITE (IP,55)
WRITE (IP,56)
40 CONTINUE
IF (NCC.EQ.NC) GO TO 45
GO TO (45,6,4), NTC
C
C NOTP=3; MULTIPLE LIST
41 NCC=NCC+1
CO 42 I=1,N
42 SIGM(I,NCC)=SIG(I)
EPSL(NCC)=EPSIL
BQ(NCC)=BQ
NL1(NCC)=N1
NL2(NCC)=N2
IF (NCC.NE.NC) GO TO 44
WRITE (IP,66) A,Z
WRITE (IP,61)
WRITE (IP,62)
WRITE (IP,63)
WRITE (IP,67)
43 CONTINUE
WRITE (IP,69) B0(1),BO(2),BO(3),BO(4)
WRITE (IP,68) NL1(1),NL2(1),NL1(2),NL2(2),NL1(3),NL2(3),NL1(4),NL2(4)
44 CONTINUE
WRITE (IP,65) EPSL(1),EPSL(2),EPSL(3),EPSL(4)
GO TO 45
44. GO TO (45,6,4), NTC.
C
45 CONTINUE
STOP
C
46 FORMAT (4I3,A8)
47 FORMAT (12F6.2)
48 FORMAT (I4,1P3E14.7,I4,0F4.0,C)
49 FORMAT (1PE15.7,1P4E14.7)
50 FORMAT (1PE15.7)
51 FORMAT (I3,A8)
52 FORMAT (2X,**ERROR**,LP1 HAS EXCEEDED VALUE OF 8.0)
SUBROUTINE RDINT (GRND, LAM, X)

C CO INTEGRATION OVER WAVE FUNCTIONS

C COMMON PIN(521), PF(521), CRANS, Y(521), KKK
YSUM=0.0
YANS=0.0
DELY=0.0
CC25
Y(1)=0.0
YMIN=0.0
YMAX=0.0
KY=1
L=1
JY=41
1 CO 10 IV=L, JY
  IF (IV=1) 2, 4, 2
  IF (IV=L) 5, 3, 5
3 Y(IV)=YMIN
  GO TO 6
4 SMTX=0.0
  GO TO 7
5 Y(IV)=Y(IV-1)+DELY
6 CONTINUE
W=C*Y(IV)*X
F=GRND(LAM, W)
SMTX=PF(IV)*F*PIN(IV)
7 KY=KY
  IF (IV=L)*(IV=JY)*KY 8 10, 9
8 YSUM=YSUM+2*SMTX
9 YSUM=YSUM+SMTX
10 YSUM=YSUM+SMTX
YANS=DELY*YSUM/3+YANS
DELY=DELY+DELY
L=JY
JY=JY+40
YSUM=0.0
YMIN=YMAX
YMAX=YMAX+40*DELY
KY=1
IF (JY=KKK=1) 1, 11, 11
11 RANS=YANS*C
RETURN
ENC
FUNCTION BJ {L, W)
SW=SIN(W)
CW=COS(W)
L1=L*1
GO TO (1, 2, 3, 4, 5, 6, 7, 8), L1
1 BJ=SW/W
RETURN
2 BJ=SW/(W**2)=CW/W
RETURN
3 BJ=3.0*SW/(W**3)=3.0*CW/(W**2)=SW/W
RETURN
4 BJ=15.0*SW/(W**4)=15.0*CW/(W**3)=6.0*SW/(W**2)*CW/W
RETURN
5 BJ=105.0*SW/(W**5)=105.0*CW/(W**4)=45.0*SW/(W**3)=10.0*CW/(W**2)=SW/W
RETURN
6 BJ=945.0*SW/(W**6)=945.0*CW/(W**5)=420.0*SW/(W**4)=105.0*CW/(W**3)=15.0
1*SW/(W**2)=CW/W
RETURN
7 BJ=12285.0*SW/(W**7)=12285.0*CW/(W**6)=7140.0*SW/(W**5)=2140.0*CW/(W**4)
140.0*SW/(W**3)=230.0*CW/(W**2)=SW/W
RETURN
8 BJ=184275.0*SW/(W**8)=184275.0*CW/(W**7)=108045.0*SW/(W**6)=4095.0*CW/
W**5=4020.0*SW/(W**4)=450.0*CW/(W**3)=30.0*SW/(W**2)=CW/W
RETURN
END
FUNCTION RN {L, W)
RN=W*W
RETURN
END
FUNCTION TJ {X1, X2, X3)
C
CALCULATE 3*J SYMBOL
A=X1+X2+X3
AF=FACT(A)
B=X1+X2
BF=FACT(B)
C=X2+X3
CF=FACT(C)
C=X1*X2+X3+1.
CF=FACT(C)
E=(X1+X2+X3)/2.
EF=FACT(E)
E1=E=X1
E1F=FACT(E1)
E2=E=X2
E2F=FACT(E2)
E3=E=X3
E3F=FACT(E3)
TJ=(SQRT(AF*BF*CF/DF)) *(EF/(E1F*E2F*E3F))
RETURN
END
FUNCTION FACT {A)
C
CALCULATE FACTORIAL OF A NUMBER (A).
FACT = 1.0
IF (A. EQ. 0.0) A = 1.0
J = A
CC 1  I = 1, J
B = I
1 FACT = FACT * B
RETURN
ENC
FUNCTION F (M, N, Z)
DIMENSION AL (8, 8)
C
AL (1, 1) = 1.0
AL (1, 2) = 1.0
AL (2, 2) = 1.0
AL (1, 3) = 0.5
AL (2, 3) = 1.0
AL (3, 3) = 1.0
AL (1, 4) = 0.5
AL (2, 4) = 0.5
AL (3, 4) = 1.0
AL (4, 4) = 2.0
AL (1, 5) = 0.625
AL (2, 5) = 0.5
AL (3, 5) = 0.75
AL (4, 5) = 2.0
AL (5, 5) = 4.375
AL (1, 6) = 0.875
AL (2, 6) = 0.625
AL (3, 6) = 0.75
AL (4, 6) = 1.25
AL (5, 6) = 4.375
AL (6, 6) = 7.875
AL (1, 7) = 1.3125
AL (2, 7) = 0.875
AL (3, 7) = 0.9375
AL (4, 7) = 1.25
AL (5, 7) = 2.1875
AL (6, 7) = 7.875
AL (7, 7) = 14.4375
AL (1, 8) = 2.0625
AL (2, 8) = 1.3125
AL (3, 8) = 1.3125
AL (4, 8) = 1.5625
AL (5, 8) = 2.1875
AL (6, 8) = 3.9375
AL (7, 8) = 14.4375
AL (8, 8) = 26.8125
C
XN = N
A = XN / (2.0 ** (XN - 1.0))
C
e = 0.5 * ALOG((1.0 + SQRT(Z)) / (1.0 - SQRT(Z)))
C
FINC E, C * C
C
N1 = N + 1
CC TO (L, 8) W
C
FIN E
1 CONTINUE
IF (N=1) 2, 2, 3
2 E=0.
GO TO 6
3 E=0.
CC 5 IP1=3, N1
S=0.
IP1M2=IP1=2
CO 4 IN1=1, IP1M2
XIN1=IN1
4 S=S+(Z***(IN1=1))/(2.0*(XIN1=1.0)+1.0)
5 E=E+AL(N1=IP1+1, N1) *(Z**(IP=IP1+2)) * S
6 C=FIND D
7 C=AL(N1, N1)
8 C=FIND C
C=0.
CO 7 IP1=1, N1
XIP1=IP1
7 C=C+AL(N1=IP1+1, N1) *(Z**(IP=IP1+2))
GO TO 15
8 C=FIND E
9 CONTINUE
IF (N=1) 9, 10, 10
9 E=0.
GO TO 13
10 E=0.
CO 12 IP1=2, N1
S=0.
IP1M1=IP1=1
CO 11 IN1=1, IP1M1
XIN1=IN1
11 S=S+(Z***(IN1=1))/(2.0*(XIN1=1.0)+1.0)
12 E=E+AL(IP1, N1) *(Z**(IP=IP1+1)) * S
13 CONTINUE
C FIND D
C=0.
C FIND C
C=0.
CO 14 IP1=1, N1
XIP1=IP1
14 C=C+AL(IP1, N1) *(Z**(IP=IP1))
C C
15 F=A*(B+C=D=E)
RETURN
C ENC
b) Discussion

This program calculates electron impact excitation atomic cross-sections for a given range of incident energies using one of the following approximations to the scattering amplitude; Born, Bethe, Modified Bethe, or Ochkur.

The program begins by initializing the incident energy matrix ZN(N) to a standard set of 20 values, and by assigning values to the read-write parameters IP, IM, IR. A control card is then read to control parameters whose meaning and allowed values are discussed in the User Manual—Appendix VII.

Depending on the value of N the incident energy values specified by the user are read in (N ≠ -1), or the standard values are retained (N = -1). The initial and final state wave functions and related data (i.e. eigenenergies, EE; orbital quantum number, XLI; etc.) are then read. The approximation to be used for this calculation is then read and the calculation begins.

Control is transferred to one of two major sections of the program depending on the approximation used. If the Born or Ochkur is used a "switch" parameter MWTCH is set to 1 and the control moves to statement 26. Otherwise MWTCH is set to 2 and the program continues at statement 7. Statement 7 begins the Bethe, Modified Bethe section of the program. After testing to determine whether or not the Modified Bethe approximation is being used, the transition is checked to see if it is optically allowed (Δλ = 1), then the radial integral

\[ \int_0^\infty dr \, r^2 R_{n_f\ell_f} (r)^2 R_{n_i\ell_i} \]

is calculated by calling the subroutine RDINT. (If the Modified
Bethe optical allowed test fails an error message is printed and the program ends. The angular factor ANGFCT is then calculated by calling the 3-j symbol subroutine TJ(XLI, XLZ, XLAM).

As is usually done in Bethe calculations the limits on the momentum transfer integral are cut-off by fitting the Bethe curve to a Born cross-section for a particular value of incident energy at high energy. This is done by using an incident energy value of 30 threshold units, and computing the Born cross-section for that value and finding a cut-off value for KMAX of WKUT. In the Bethe calculation, if the change in angular momentum, LAM is 0 the quadrapole moment is the first non-zero term in the Bethe series. The test is made and if necessary LAM is set equal to 2.

A particular value of the incident energy is next chosen and the energy term ENGFCT of the Bethe calculation is obtained.

The Bethe cross-section SIG(I) for the chosen energy value ZN(I) is calculated and the next energy value is chosen.

If the Bethe approximation is being used transfer to the output routine (statement 36) occurs after a cross-section for each energy has been computed. If the Modified Bethe approximation is being used, the additional terms for approximation are calculated as follows. An energy value is selected, ZN(1) a value of the final angular momentum LP is selected and the partial cross-section SG(LP1) is calculated. The "unitarity limit", $Q_L^{max}$, cross-section for this value of LP is found and a test of $Q_L$ is made. When the value of LP is
such that \( Q_L < \frac{1}{2} r_L^{\max} \) this value of \( LP \) is designated \( L_O \). The two correction terms for the Modified Bethe approximation TRMLO, TRMSM are then found and subtracted from the Bethe Cross-section (as discussed in Chapter III). When this procedure is complete for all energy values transfer to the output routine (Statement 36) is made.

The next section of the program is for calculation of Born or Ochkur cross-sections.

For efficiency in the program the scattering amplitude \( f_{\text{born}}(k) \) is found over the range \( K_{\text{MAX}}(ZN(N)) \) to \( K_{\text{MIN}}(ZN(N)) \) (where \( ZN(N) \) is the largest incident energy) and tabulated for 1000 values of \( f(k) \). The integration for the final cross-section for each energy value is then done by use of this table.

This section begins by calculating \( K_{\text{MAX}}(ZN(N)) = XMXN \) and \( K_{\text{MIN}}(ZN(N)) = XMNN \). Then for a selected value within this range \( f(k) \) is found. This involves calling the radial integration subroutine RDINT which includes the spherical Bessel function subroutine BJ. When the table of values of \( f(k) \) (i.e. \( FX(IX) \)) is found, the calculation of the cross-sections for a particular value of the energy begins.

The limits on the \( K \)-integration (\( XMAX, XMIN \)) for the selected value of the energy \( ZN(I) \) are found. The value of the scattering amplitude at these limits \( FXMAX, FXMIN \) is found, and the integration over the range of \( K \) is begun. The closest value of \( XMAX, XMIN \) to the tabulated values are found, and those tabulated values are labeled \( LP \) and \( LQ \) respectively.
Since a Simpson's rule formula is used for the integration the number of integration points must be even. The value of LQ is adjusted to guarantee this and the integration $\int_{k_{\ell_{LP}}}^{k_{\ell_{LP}+1}} \frac{1}{d\kappa}$ is carried out using Simpson's rule, and selecting either the Ochkur (A $\neq$ 1) or Born (A = 1) expression.

The correction terms

$$\int_{k_{\ell_{LP}}}^{k_{\ell_{LP}+1}} \frac{d\theta}{d\kappa} \, d\kappa \quad \text{and} \quad \int_{k_{\ell_{LP}}}^{k_{\ell_{LP}+1}} \frac{d\varphi}{d\kappa} \, d\kappa$$

are found using a trapezoid integration and these correction terms are added to the tabular integration to obtain the cross-section $\Sigma(I)$. Transfer to the output routine (Statement 36) is then made.

At Statement 36 control is transferred to one of the three output routines discussed in the user's manual.

When output has been completed, a test for the number of cases to be run is made and the program either ends or transfers back to read a new final state-wave function and approximation (Statement 4) or a new approximation (Statement 6).

Using the IBM 360/75 computer, the program EXCST for the CESIUM 6s-6p transition (where the radial integral has 441 points) had the following run times:

- Single Born case = 2 min 3 sec
- Single Ochkur case = 2 min 2 sec
- Single Bethe case = 25 sec
- Single Modified Bethe case = 24 sec
- 4 approximations = 4 min 18 sec
3. Ionization Cross-Section Program

This program, named IONCST, is a calculation of the ionization cross-section for a single value of Incident Electron Energy. The program consists of a main program and five subroutines.

a) Listing
program ioncst(input)

* * * * ioncst * * *

* a fortran program to calculate partial cross-sections *
* for neutral atoms ionized by incident electrons *
* the calculation uses numerical wave functions for the *
* atom and the born-coulomb approximation *

*******************************************************************************

program

* and subroutines by *
* tom j greene *
* university of toledo *
* 1977 *

*******************************************************************************

real*4 kappa,kamanx
real*8 aq
dimension zn(21),sggl(6),z12(6)
external bj,rn,fact
common pin(521),pf(521),c,rans,y(521),kkk
etamax=10.
etamin=10.
rhomax=0.
rhomin=10.
ip=6
im=5
ir=5

do 15 igt=1,1

read bound state wave function

read (im,17) aq
read (ir,18) nl21,kl1,ff1,wwnl1,kkk1,z
k11=kkk1=1
do 1 min=1,k11,5
max=min+4
read (ir,19) (pin(t),t=vin,max)
1 continue
read (ir,20) pin(kkk1)
epsil=(abs(ee1)/2.)
p=3.1415927

c=0.805341381/333333333333)
kkk=kkk1

build y(i1)

nalert=kkk1/40
ii=1
y(i1)=0.0
deltay=.0025
10 do j1=1,nalert,1
   do k1=1,40

program ioncst(input)
\[
X_F = \sqrt{\pi \kappa A^{-2} + 2 \cdot (N(1) = 1) \cdot \varepsilon}
\]
\[
X_{\text{MIN}} = X_{\text{IN}} - X_F
\]
\[
X_{\text{MAX}} = X_{\text{IN}} + X_F
\]
\[
\Delta X = \frac{(X_{\text{MAX}} - X_{\text{MIN}})}{20}
\]
\[
X_{\text{SUM}} = 0.0
\]
\[
X_{\text{ANS}} = 0.0
\]
\[
X = X_{\text{MIN}} - \Delta X
\]
\[
KX = 1
\]
\[
\text{DO } 1 0 \quad IX = 1, 21
\]
\[
X = X + \Delta X
\]
\[
FPR = 0.0
\]
\[
X_{\text{INTG}} = 0.0
\]
\[
\text{DO } 7 \quad LAM = LAM_{\text{MIN}} \cdot LAM_{\text{MAX}}
\]
\[
LAM = LAM_1 = 1
\]
\[
X_{\text{LAM}} = LAM
\]
\[
\text{CALL } \text{ROINT } (BJ, LAM, X)
\]
\[
X_T = T \cdot (X_{\text{LAM}}), X_{\text{LAM}})
\]
\[
7 \quad FLP = (2 \cdot X_{\text{LAM}} + 1.0) \cdot ((X_T \cdot X_{\text{RANS}})^{2}) / (2 \cdot X_{L2} + 1.0) \cdot FLP
\]
\[
FPR = FLP
\]
\[
X_{\text{INTG}} = FPR / (X^{2})
\]
\[
KX = KX
\]
\[
\text{IF } \{ (IX = 1) \cdot (IX = 2C1) \cdot KX \} 9, 10, 9,
\]
\[
8 \quad X_{\text{SUM}} = X_{\text{SUM}} + 2 \cdot X_{\text{INTG}}
\]
\[
9 \quad X_{\text{SUM}} = X_{\text{SUM}} + X_{\text{INTG}}
\]
\[
10 \quad X_{\text{SUM}} = X_{\text{SUM}} + X_{\text{INTG}}
\]
\[
X_{\text{ANS}} = X_{\text{SUM}} / \Delta X / 3.
\]
\[
DSG = \{128 \cdot X_{\text{ANS}} \cdot \{1 \cdot (\kappa \cdot X_{\text{IN}})^{2}\} \}
\]
\[
KS = KX
\]
\[
\text{IF } \{ (IKS = 1) \cdot (IKS = 11) \cdot KX \} 11 + 13, 12
\]
\[
11 \quad S C L S U M = S G L S U M + 2 \cdot D S G L
\]
\[
12 \quad S C L S U M = S G L S U M + D S G L
\]
\[
13 \quad S C L S U M = S G L S U M + D S G L
\]
\[
S C L = S G L S U M / D E L K A P / 3.
\]
\[
Z N L G = A L O G 1 \cdot (Z N(1))
\]
\[
N 1 = N 2 \cdot 1 / 10
\]
\[
S G L G L (1 X 2 P 1) = S G L
\]
\[
Z L 2 (1 X 2 P 1) = X_{L2}
\]
\[
14 \quad S G = S G + S G L
\]
\[
15 \quad \text{CONTINUE}
\]
\[
C \quad \text{OUTPUT ROUTINE}
\]
\[
\text{WRITE } (I P, 22) \quad A Q
\]
\[
\text{WRITE } (I P, 27)
\]
\[
\text{WRITE } (I P, 28)
\]
\[
\text{WRITE } (I P, 29)
\]
\[
\text{WRITE } (I P, 26) \quad Z, \varepsilon, N 1
\]
\[
\text{WRITE } (I P, 24)
\]
\[
\text{WRITE } (I P, 25)
\]
\[
\text{DO } 1 6 \quad I = 1, 6, 3
\]
\[
\text{WRITE } (I P, 24)
\]
\[
\text{WRITE } (I P, 32)
\]
\[
\text{WRITE } (I P, 31) \quad Z L 2 (1 \cdot S G L (1) \cdot Z L 2 (1 \cdot 1) \cdot S G L (1 + 1) \cdot Z L 2 (1 + 2) \cdot S G L (1 + 2)
\]
\[
\text{WRITE } (I P, 32)
\]
\[
16 \quad \text{CONTINUE}
\]
\[
\text{WRITE } (I P, 24)
\]
\[
\text{WRITE } (I P, 23)
\]
\[
\text{WRITE } (I P, 30) \quad Z N(1), Z N L G, S G
\]
\[
\text{WRITE } (I P, 23)
\]
\[
\text{WRITE } (I P, 24)
\]
WRITE (IP,34) RHOMAX,ETAMAX
WRITE (IP,33) RHOMIN,ETAMIN
WRITE (IP,24)
RETURN

C
17 FORMAT (A8)
18 FORMAT (14,E14.7,14,E14.7)
19 FORMAT (1PE15.7,1P4E14.7)
20 FORMAT (1PE15.7)
21 FORMAT (I12F6.2)
22 FORMAT (32X,AP2**COUL=BOHR**/)
23 FORMAT (1X,AP2**RHOX,AP2**)
24 FORMAT (1X,O**RHO**ETAX)
25 FORMAT (1X,O**RHO**ETAX)
26 FORMAT (3X,O*AT. NO.=F4.0)O,13X,O (EPSIL=*,1PE10.3,0),10X,0(NL
1=N**L**0.0,0(2.0=CONTINUUM)0)
27 FORMAT (6X,O*CROSS=SECTIONS ARE IN UNITS OF PI*(BOHR RADII)**2)
28 FORMAT (6X,O*INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (E
1PSIL))
29 FORMAT (6X,O*EPSIL IS IN UNITS OF TWICE THE RYDBERG)
30 FORMAT (1X,O*9,SIG(N)=OPF8.3,8X,O*1LOG(N)=1PE10.3,8X,
31 FORMAT (1X,O*9,XO*1PE10.3,9X)
32 FORMAT (1X,O*9,OPE8.3,2X,0,3X,1PE10.3,2X,0,9)
33 FORMAT (1X,O*9,OPE14.7,34X,0,ETA(MIN)=0,1PE14.7,0***)
34 FORMAT (1X,O*9,OPE14.7,34X,0,ETA(MAX)=0,1PE14.7,0***)

END
FUNCTION FLNR (L,RHO,ETA)
XL=L
PI=3.14159265
C
FLNR=CLN*(RHO**(L+1))*PHI
C
FIND CLN=PROD*(2.0**L)*SQRT(2.0**P(*ETA))FACT(2.0**XL+1.0)*SQRT(1.0-E
C
(2.0**PI**ETA))
A=2.0**PI**ETA
B=2.0**XL+1.0
C=ABS(1.0=EXP(A))
FCT=FACT(B)
PROD=1.0
IF (L.EQ.0) GO TO 2
CONTINUE
2 CONTINUE
C
PROD=PROD*SQRT(S**2+ETA**2)
1 CONTINUE
2 CONTINUE
C
CLNPROD*(2.0**L)*SQRT(1/A)/(FACT(2.0**XL+1.0)*SQRT(1.0-E
C
(2.0**PI**ETA))
FIND PHI=AKL*(RHO**K=L=1)
AKM2=1.0
AKM1=ETA/(XL+1.0)
CSUM=1.0*AKM1*RHO
TCSUM=0.0
L3=L+3
L30=L+30
DO 3 K=L3,L30
XK=K
AK=(2.0*ETA**AKM1=AKM2)/(XK+XL)**(XK=XL=1.0)
IF ((RHO**K(K=L=1))LT(1.E=40)AND.(AKLT1.E=20)) GO TO 4
CSUM=CSUM+AK*RHO**K(K=L=1)
TCSUM=CSUM

C
AKM2=AKM1
AKM1=AK
3 CONTINUE
4 CONTINUE
5 PHI=CSUM
6 FLNR=CLN*(RHO**((L+1))*PHI
7 RETURN
8 END
9 SUBROUTINE RDINT (GRND, LAM, X)
10 DO INTEGRATION OVER WAVE FUNCTIONS
11 COMMON PIN(521), PF(521), C, RANS, Y(521), KKK
12 YSUM=0.0
13 YANS=0.0
14 DELY=0.025
15 Y(1)=0.0
16 YMIN=0.0
17 YMAX=0.1
18 KY=1
19 L=1
20 JY=41
21 C CONTINUE
22 IF (IY=1) 2, 4, 2
23 IF (IY=1) 5, 3, 5
24 Y(IY)=YMIN
25 GO TO 6
26 SMTX=0.0
27 GO TO 7
28 Y(IY)=Y(IY-1)*DELY
29 CONTINUE
30 W=C*Y(IY)*X
31 F=GRND(LAM, W)
32 SMTX=PF(IY)*F*PIN(IY)
33 IF=6
34 KY=1
35 IF (IY=L)* (IY=JY)*KY) 8, 10, 9
36 YSUM=YSUM+2.0*SMTX
37 YSUM=YSTY+SUBO
38 YANS=DELY*YSUM/3.+YANS
39 DELY=DELY*DELY
40 L=JY
41 JY=JY+40
42 YSUM=0.0
43 YMIN=YMAX
44 YMAX=YMAX+4O,6=DELY
45 KY=1
46 IF (JY=KKG=1) 1, 11, 11
47 RANS=YANS*C
48 RETURN
49 END
50 FUNCTION BJ (L, W)
51 IF (W<LT.1.) GO TO 8
52 SN=SIN(W)
53 CN=COS(W)
54 LI=L+1
55 GO TO (1, 3.4, 5.6, 7), LI
56 BJ=SN/W
57
RETURN
2 BJ=SW/(W**2)-CW/W
RETURN
3 BJ=3.0*SW/(W**3)-3.0*CW/(W**2)-SW/W
RETURN
4 BJ=15.0*SW/(W**4)-15.0*CW/(W**3)-6.0*SW/(W**2)+CW/W
RETURN
5 BJ=105.0*SW/(W**5)=105.0*CW/(W**4)-455.0*SW/(W**3)+105.0*CW/(W**2)-SW/W
RETURN
6 BJ=945.0*SW/(W**6)=945.0*CW/(W**5)-420.0*SW/(W**4)-105.0*CW/(W**3)+15.0
1*SW/(W**2)=CW/W
RETURN
7 BJ=10395.0*SW/(W**7)=10395.0*CW/(W**6)-4725.0*SW/(W**5)+1260.0*CW/(W**4)+210.0*SW/(W**3)-21.0*CW/(W**2)=SW/W
RETURN
8 XL=L
   XN=XL+1.
   A=(W**2)/(2.0*(2.0*XN+3.0))
   B=(W**4)/(8.0*(2.0*XN+3.0)*(2.0*XN+5.0))
   BJ=(W**XL)*(12.0*XN)*FACT(XN)/FACT(2.0*XN))*11.0=A+B
RETURN
END
FUNCTION RN (L,W)
   RN=W**L
RETURN
END
FUNCTION TJ (X1,X2,X3)
   CALCULATE 3=J. SYMBOL
   A=XL*X2=X3
   AF=FACT(A)
   B=XL*X3=X2
   BF=FACT(B)
   C=X2*X3=X1
   CF=FACT(C)
   C=XL*X2*X3+1.
   DF=FACT(C)
   E=(XL*X2*X3)/2.
   EF=FACT(E)
   E1=E-X1
   E1F=FACT(E1)
   E2=E-X2
   E2F=FACT(E2)
   E3=E-X3
   E3F=FACT(E3)
   TJ=(SQR(T(AF*BF*CF/DF))*EF/(E1F*E2F*E3F))
RETURN
END
FUNCTION FACT (A)
   CALCULATE FACTORIAL OF A NUMBER (A).
   FACT=1.
   AA=A
   IF (A.EQ.0.0) AA=1.0
   J=AA
   DO 1 I=1,J
   B=1
1  FACT=FACT*B
RETURN
END
b) Discussion

This program calculates the first five partial-wave electron impact ionization cross-sections for a value of the incident energy using the Coulomb-Born approximation. The program consists of a main program and six subroutines.

It begins by reading the initial state radial wave function PIN and related parameters (eigenenergy, orbital angular momentum, etc.) whose values are discussed in the User Manual—Appendix VII. After constructing the x-mesh (called Y[I]) the incident energy is read.

The final state angular momentum quantum number (XLZ) is selected. For the particular value of the incident energy ZN(I), the maximum allowed value of the wave vector for the secondary electron KAPAMX is found. Within the range 0 to KAPAMX, a value of KAPA is selected, and the integration over KAPA is begun. For these values of XLZ and KAPA the final state Coulomb wave function is found by calling the function FLNR.

If the initial orbital angular momentum XLI and the final angular momentum are the same the final state radial wave function is forced to be orthogonal to the initial state radial wave function, i.e. PF = PF - \[ \int dr(PF)(PIN) \] PIN]

The limits on the momentum transfer integral XMAX, XMIN, are found and the integral over the momentum transfer for this value of the secondary electron wave number is carried out. This is done by calling the radial integration routine RDINT, and by use of the 3-j symbol routine TJ.
Another value of the secondary electron wave number is selected and the process repeated until the maximum allowed value of KAPAMX is reached, giving the partial cross-section \( Q_L \) for this value of the final angular momentum.

The next value of the final angular momentum is selected and the process is repeated until the Partial Cross-Section \( Q(L) \) for \( L = 0, 5 \) are found. These partial cross-sections are added together to give the "total" ionization cross-section, \( SG \), for this value of the incident energy.

The partial cross-section and the total cross-section are then printed out in the form shown in the User Manual.

Using the IBM 360/75 computer, the program IONCST had a run time of (7 min 6 sec) for the Helium case for one value of the incident energy. In this case the additional time is primarily due to the evaluation of the Coulomb wave function.
VI. SOME SAMPLE RESULTS FOR EXCITATION

In this chapter some results of the excitation cross-section calculations will be presented. Recall (Page 3) that for assessing the accuracy of various calculations the only methods available are those of comparing the cross-sections obtained in the various calculations with one another and with the limited experimental data available.

The tables presented will include reference data from other calculations and experimental work so that a comparison can be made. The two families of elements selected for presentation here were chosen to demonstrate what I expect to be the best and worst cases for the calculation. The Alkali family, which is an excellent approximation to the one-electron model, and the Inert family, where the inert-core-active electron assumption is weakest.

1) Tables

The two sets of tables will now be presented and a discussion of the results will follow.

a) Alkali Excitation Tables.

To establish a straight-forward comparison of the results of this calculation with the literature I chose to calculate cross-sections for the Alkali elements using the energy values of Vainshtein (1964). Vainshtein and his co-workers carried out a study of the Alkali family using the Born approximation that was reprinted in the classic work of Moiseiwitsch and Smith (1968). The organization of the Vainshtein tables has been used here. First the resonance (ns-np) transitions of the Alkalids are examined.
Then for each of the elements of the Alkali family, the first few transitions are calculated.

The Vainshtein* values are designated Born (1) in the tables that follow. The Born calculation of the present work is designated Born (2).

The energy range $N$ is given in threshold units; the transition energy $\varepsilon$ is in units of twice the Rydberg; and the cross-sections are measured in units of $\pi a_B^2$.


and

ALKALI ELEMENT C-SECTION TABLES

Li: 2s-2p Born(1), Born(2), Ochkur, Bethe, Mod. Bethe
Na: 3s-3p Born(1), Born(2), Ochkur, Bethe, Mod. Bethe*
K: 4s-4p Born(1), Born(2), Ochkur, Bethe, Mod. Bethe
Rb: 5s-5p Born(1), Born(2), Ochkur, Bethe, Mod. Bethe
Cs: 6s-6p Born(1), Born(2), Ochkur, Bethe, Mod. Bethe

For the remaining transitions Born(1), Bethe, and Ochkur results are given:

Na: 3s-4p 3s-4s 3s-3d 3s-7d
3s-5p 3s-5s 3s-4d
3s-6p 3s-6s 3s-5d
3s-7p 3s-7s 3s-6d
K: 4s-5p 4s-5s 4s-3d 4s-6d
4s-6p 4s-6s 4s-4d
4s-7p 4s-7s 4s-5d
Rb: 5s-6p 5s-6s 5s-4d 5s-7d
5s-7p 5s-7s 5s-5d
5s-8p 5s-8s 5s-6d
Cs: 6s-7p 6s-7s 6s-5d 6s-8d
6s-8p 6s-8s 6s-6d
6s-9p 6s-9s 6s-7d

Note (1): The use of the cut-off parameter in the Bethe calculation can lead to negative cross-section when $K_{\text{max}} < K_{\text{min}}$ for low values of the incident energy. These non-physical values have been set equal to zero.

*Note (2): Since the well-known sodium 3s-3p transition was recently the subject of a careful experimental study, the data from that study is given.
<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>OCHKUR</th>
<th>BETHE</th>
<th>MODBETHE</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>OCHKUR</th>
<th>BETHE</th>
<th>MODBETHE</th>
<th>EXP*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>4.14(1)</td>
<td>4.07(1)</td>
<td>3.99(1)</td>
<td>6.96(0)</td>
<td>0.0</td>
<td>3.07(1)</td>
<td>3.08(1)</td>
<td>3.00(1)</td>
<td>0.0</td>
<td>0.0</td>
<td>1.75(1)</td>
</tr>
<tr>
<td>1.04</td>
<td>5.71(1)</td>
<td>5.62(1)</td>
<td>5.54(1)</td>
<td>2.43(1)</td>
<td>0.0</td>
<td>4.26(1)</td>
<td>4.27(1)</td>
<td>4.14(1)</td>
<td>0.0</td>
<td>0.0</td>
<td>1.81(1)</td>
</tr>
<tr>
<td>1.08</td>
<td>7.71(1)</td>
<td>7.58(1)</td>
<td>7.55(1)</td>
<td>4.68(1)</td>
<td>0.0</td>
<td>5.78(1)</td>
<td>5.79(1)</td>
<td>5.62(1)</td>
<td>0.0</td>
<td>0.0</td>
<td>1.94(1)</td>
</tr>
<tr>
<td>1.16</td>
<td>9.98(1)</td>
<td>9.81(1)</td>
<td>9.55(1)</td>
<td>7.36(1)</td>
<td>0.0</td>
<td>7.56(1)</td>
<td>7.58(1)</td>
<td>7.07(1)</td>
<td>2.50(1)</td>
<td>0.0</td>
<td>2.20(1)</td>
</tr>
<tr>
<td>1.32</td>
<td>1.20(2)</td>
<td>1.18(2)</td>
<td>1.14(2)</td>
<td>1.00(2)</td>
<td>0.0</td>
<td>9.32(1)</td>
<td>9.32(1)</td>
<td>8.45(1)</td>
<td>5.87(1)</td>
<td>0.0</td>
<td>2.72(1)</td>
</tr>
<tr>
<td>1.64</td>
<td>1.31(2)</td>
<td>1.28(2)</td>
<td>1.19(2)</td>
<td>1.18(2)</td>
<td>5.55(1)</td>
<td>1.04(2)</td>
<td>1.04(2)</td>
<td>9.14(1)</td>
<td>8.56(1)</td>
<td>1.80(1)</td>
<td>3.30(1)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.24(2)</td>
<td>1.22(2)</td>
<td>1.10(2)</td>
<td>1.18(2)</td>
<td>6.38(1)</td>
<td>1.02(2)</td>
<td>1.03(2)</td>
<td>9.04(1)</td>
<td>9.56(1)</td>
<td>3.76(1)</td>
<td>3.52(1)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.03(2)</td>
<td>1.01(2)</td>
<td>0.97(2)</td>
<td>0.98(1)</td>
<td>6.14(1)</td>
<td>8.84(1)</td>
<td>8.85(1)</td>
<td>8.07(1)</td>
<td>8.66(1)</td>
<td>4.43(1)</td>
<td>3.65(1)</td>
</tr>
<tr>
<td>6.12</td>
<td>7.53(1)</td>
<td>7.35(1)</td>
<td>6.92(1)</td>
<td>7.38(1)</td>
<td>5.06(1)</td>
<td>6.66(1)</td>
<td>6.66(1)</td>
<td>6.33(1)</td>
<td>6.67(1)</td>
<td>4.11(1)</td>
<td>3.56(1)</td>
</tr>
<tr>
<td>11.24</td>
<td>5.01(1)</td>
<td>4.89(1)</td>
<td>4.74(1)</td>
<td>4.93(1)</td>
<td>3.66(1)</td>
<td>4.54(1)</td>
<td>4.53(1)</td>
<td>4.42(1)</td>
<td>4.57(1)</td>
<td>3.17(1)</td>
<td>3.15(1)</td>
</tr>
<tr>
<td>21.48</td>
<td>3.12(1)</td>
<td>3.04(1)</td>
<td>3.00(1)</td>
<td>3.07(1)</td>
<td>2.40(1)</td>
<td>2.87(1)</td>
<td>2.87(1)</td>
<td>2.84(1)</td>
<td>2.90(1)</td>
<td>2.17(1)</td>
<td>2.42(1)</td>
</tr>
<tr>
<td>41.96</td>
<td>1.86(1)</td>
<td>1.81(1)</td>
<td>1.80(1)</td>
<td>1.83(1)</td>
<td>1.48(1)</td>
<td>1.73(1)</td>
<td>1.73(1)</td>
<td>1.72(1)</td>
<td>1.75(1)</td>
<td>1.37(1)</td>
<td>1.66(1)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>OCHKUR</th>
<th>BETHE</th>
<th>MODBETHE</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>OCHKUR</th>
<th>BETHE</th>
<th>MODBETHE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>5.47(1)</td>
<td>5.51(1)</td>
<td>5.36(1)</td>
<td>0.0</td>
<td>0.0</td>
<td>5.85(1)</td>
<td>5.66(1)</td>
<td>5.47(1)</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>1.04</td>
<td>7.57(1)</td>
<td>7.65(1)</td>
<td>7.39(1)</td>
<td>0.0</td>
<td>0.0</td>
<td>8.11(1)</td>
<td>7.86(1)</td>
<td>7.54(1)</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>1.08</td>
<td>1.03(2)</td>
<td>1.04(2)</td>
<td>1.00(2)</td>
<td>0.0</td>
<td>0.0</td>
<td>1.10(2)</td>
<td>1.07(2)</td>
<td>1.02(2)</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>1.16</td>
<td>1.35(2)</td>
<td>1.37(2)</td>
<td>1.26(2)</td>
<td>2.77(1)</td>
<td>0.0</td>
<td>1.46(2)</td>
<td>1.42(2)</td>
<td>1.29(2)</td>
<td>1.11(0)</td>
<td>0.0</td>
</tr>
<tr>
<td>1.32</td>
<td>1.66(2)</td>
<td>1.69(2)</td>
<td>1.51(2)</td>
<td>9.58(1)</td>
<td>0.0</td>
<td>1.80(2)</td>
<td>1.78(2)</td>
<td>1.55(2)</td>
<td>8.33(1)</td>
<td>0.0</td>
</tr>
<tr>
<td>1.64</td>
<td>1.87(2)</td>
<td>1.91(2)</td>
<td>1.65(2)</td>
<td>1.52(2)</td>
<td>8.85(0)</td>
<td>2.03(2)</td>
<td>2.04(2)</td>
<td>1.73(2)</td>
<td>1.53(2)</td>
<td>0.0</td>
</tr>
<tr>
<td>2.28</td>
<td>1.86(2)</td>
<td>1.91(2)</td>
<td>1.67(2)</td>
<td>1.75(2)</td>
<td>4.80(1)</td>
<td>2.02(2)</td>
<td>2.07(2)</td>
<td>1.80(2)</td>
<td>1.86(2)</td>
<td>3.59(1)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.59(2)</td>
<td>1.66(2)</td>
<td>1.51(2)</td>
<td>1.62(2)</td>
<td>6.92(1)</td>
<td>1.76(2)</td>
<td>1.82(2)</td>
<td>1.66(2)</td>
<td>1.76(2)</td>
<td>6.59(1)</td>
</tr>
<tr>
<td>6.12</td>
<td>1.20(2)</td>
<td>1.26(2)</td>
<td>1.20(2)</td>
<td>1.26(2)</td>
<td>6.86(1)</td>
<td>1.33(2)</td>
<td>1.39(2)</td>
<td>1.33(2)</td>
<td>1.39(2)</td>
<td>7.10(1)</td>
</tr>
<tr>
<td>11.24</td>
<td>8.21(1)</td>
<td>8.60(1)</td>
<td>8.41(1)</td>
<td>8.67(1)</td>
<td>5.54(1)</td>
<td>9.13(1)</td>
<td>9.60(1)</td>
<td>9.39(1)</td>
<td>9.67(1)</td>
<td>5.94(1)</td>
</tr>
<tr>
<td>21.48</td>
<td>5.20(1)</td>
<td>5.47(1)</td>
<td>5.41(1)</td>
<td>5.52(1)</td>
<td>3.89(1)</td>
<td>5.80(1)</td>
<td>6.13(1)</td>
<td>6.07(1)</td>
<td>6.19(1)</td>
<td>4.25(1)</td>
</tr>
<tr>
<td>41.96</td>
<td>3.14(1)</td>
<td>3.31(1)</td>
<td>3.29(1)</td>
<td>3.34(1)</td>
<td>2.51(1)</td>
<td>3.51(1)</td>
<td>3.72(1)</td>
<td>3.71(1)</td>
<td>3.76(1)</td>
<td>2.77(1)</td>
</tr>
<tr>
<td>N</td>
<td>BORN(1)</td>
<td>BORN(2)</td>
<td>OCHKUR</td>
<td>BETHE</td>
<td>MODBETHE</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>---------</td>
<td>---------</td>
<td>--------</td>
<td>-------</td>
<td>----------</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.02</td>
<td>7.50(1)</td>
<td>7.06(1)</td>
<td>6.81(1)</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.04</td>
<td>1.04(2)</td>
<td>9.82(1)</td>
<td>9.38(1)</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.08</td>
<td>1.41(2)</td>
<td>1.35(2)</td>
<td>1.27(2)</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.16</td>
<td>1.86(2)</td>
<td>1.79(2)</td>
<td>1.60(2)</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.32</td>
<td>2.30(2)</td>
<td>2.26(2)</td>
<td>1.95(2)</td>
<td>8.78(1)</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.64</td>
<td>2.60(2)</td>
<td>2.62(2)</td>
<td>2.21(2)</td>
<td>1.88(2)</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.28</td>
<td>2.60(2)</td>
<td>2.69(2)</td>
<td>2.34(2)</td>
<td>2.39(2)</td>
<td>2.63(1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.56</td>
<td>2.26(2)</td>
<td>2.39(2)</td>
<td>2.19(2)</td>
<td>2.31(2)</td>
<td>7.27(1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.12</td>
<td>1.72(2)</td>
<td>1.85(2)</td>
<td>1.77(2)</td>
<td>1.84(2)</td>
<td>8.56(1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11.24</td>
<td>1.17(2)</td>
<td>1.28(2)</td>
<td>1.25(2)</td>
<td>1.29(2)</td>
<td>7.45(1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>21.48</td>
<td>7.46(1)</td>
<td>8.21(1)</td>
<td>8.14(1)</td>
<td>8.29(1)</td>
<td>5.46(1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>41.96</td>
<td>4.52(1)</td>
<td>5.00(1)</td>
<td>4.98(1)</td>
<td>5.05(1)</td>
<td>3.61(1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**LITHIUM**

**2s-3p**

\[ \text{\text{EPSIL}} = 1.41 \times (\text{-1}) \]

<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>BETHE</th>
<th>OCHKUR</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>9.67(-1)</td>
<td>9.74(-1)</td>
<td>2.76(-0)</td>
<td>9.72(-1)</td>
<td>2.24(-1)</td>
<td>2.27(-1)</td>
<td>3.24(-1)</td>
<td>2.28(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.30(0)</td>
<td>1.32(0)</td>
<td>2.72(-0)</td>
<td>1.34(-1)</td>
<td>3.01(-1)</td>
<td>3.05(-1)</td>
<td>3.30(-1)</td>
<td>3.14(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>1.68(0)</td>
<td>1.70(0)</td>
<td>2.64(-0)</td>
<td>1.79(-0)</td>
<td>3.84(-1)</td>
<td>3.90(-1)</td>
<td>3.35(-1)</td>
<td>4.16(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>2.01(0)</td>
<td>2.03(0)</td>
<td>2.48(-0)</td>
<td>2.15(-0)</td>
<td>4.49(-1)</td>
<td>4.56(-1)</td>
<td>3.33(-1)</td>
<td>4.95(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>2.11(0)</td>
<td>2.15(0)</td>
<td>2.21(-0)</td>
<td>2.29(-0)</td>
<td>4.67(-1)</td>
<td>4.67(-1)</td>
<td>3.18(-1)</td>
<td>5.10(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>1.87(0)</td>
<td>1.92(0)</td>
<td>1.80(-0)</td>
<td>1.90(-0)</td>
<td>3.91(-1)</td>
<td>4.02(-1)</td>
<td>2.82(-1)</td>
<td>4.04(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.39(0)</td>
<td>1.43(0)</td>
<td>1.33(-0)</td>
<td>1.27(-0)</td>
<td>2.84(-1)</td>
<td>2.93(-1)</td>
<td>2.26(-1)</td>
<td>2.56(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>8.91(-1)</td>
<td>9.22(-1)</td>
<td>8.71(-1)</td>
<td>7.34(-1)</td>
<td>1.84(-1)</td>
<td>1.89(-1)</td>
<td>1.62(-1)</td>
<td>1.56(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>5.20(-1)</td>
<td>5.37(-1)</td>
<td>5.19(-1)</td>
<td>4.66(-1)</td>
<td>1.13(-1)</td>
<td>1.13(-1)</td>
<td>1.05(-1)</td>
<td>9.76(-2)</td>
</tr>
<tr>
<td>11.24</td>
<td>2.88(-1)</td>
<td>2.94(-1)</td>
<td>2.90(-1)</td>
<td>2.69(-1)</td>
<td>6.67(-2)</td>
<td>6.55(-2)</td>
<td>6.39(-1)</td>
<td>5.99(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>1.55(-1)</td>
<td>1.56(-1)</td>
<td>1.56(-1)</td>
<td>1.49(-1)</td>
<td>3.85(-2)</td>
<td>3.69(-2)</td>
<td>3.69(-2)</td>
<td>3.53(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>8.23(-2)</td>
<td>8.16(-1)</td>
<td>8.19(-2)</td>
<td>7.95(-2)</td>
<td>2.19(-2)</td>
<td>2.05(-2)</td>
<td>2.07(-2)</td>
<td>2.00(-2)</td>
</tr>
</tbody>
</table>

**2s-4p**

\[ \text{\text{EPSIL}} = 1.66 \times (\text{-1}) \]
### Lithium

#### 2s-5p

<table>
<thead>
<tr>
<th>( N )</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>8.95(-2)</td>
<td>9.07(-2)</td>
<td>7.90(-2)</td>
<td>9.12(-2)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.20(-1)</td>
<td>1.21(-1)</td>
<td>8.43(-2)</td>
<td>1.26(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>1.52(-1)</td>
<td>1.54(-1)</td>
<td>9.03(-2)</td>
<td>1.66(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>1.76(-1)</td>
<td>1.79(-1)</td>
<td>9.58(-2)</td>
<td>1.97(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>1.77(-1)</td>
<td>1.82(-1)</td>
<td>9.81(-2)</td>
<td>2.00(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>1.50(-1)</td>
<td>1.55(-1)</td>
<td>9.35(-2)</td>
<td>1.56(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.09(-1)</td>
<td>1.12(-1)</td>
<td>8.00(-2)</td>
<td>9.78(-2)</td>
</tr>
<tr>
<td>3.56</td>
<td>7.21(-2)</td>
<td>7.32(-2)</td>
<td>6.09(-2)</td>
<td>6.02(-2)</td>
</tr>
<tr>
<td>6.12</td>
<td>4.54(-2)</td>
<td>4.51(-2)</td>
<td>4.15(-2)</td>
<td>3.89(-2)</td>
</tr>
<tr>
<td>11.24</td>
<td>2.78(-2)</td>
<td>2.69(-2)</td>
<td>2.62(-2)</td>
<td>2.47(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>1.65(-2)</td>
<td>1.56(-2)</td>
<td>1.56(-2)</td>
<td>1.50(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>9.63(-3)</td>
<td>8.89(-3)</td>
<td>8.99(-3)</td>
<td>8.71(-3)</td>
</tr>
</tbody>
</table>

#### 2s-3s

<table>
<thead>
<tr>
<th>( N )</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>1.21(0)</td>
<td>1.23(-0)</td>
<td>1.03(0)</td>
<td>1.20(-0)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.66(0)</td>
<td>1.68(-0)</td>
<td>1.83(0)</td>
<td>1.64(-0)</td>
</tr>
<tr>
<td>1.08</td>
<td>2.21(0)</td>
<td>2.24(-0)</td>
<td>2.72(0)</td>
<td>2.17(-0)</td>
</tr>
<tr>
<td>1.16</td>
<td>2.79(0)</td>
<td>2.83(-0)</td>
<td>3.55(0)</td>
<td>2.62(-0)</td>
</tr>
<tr>
<td>1.32</td>
<td>3.25(0)</td>
<td>3.27(-0)</td>
<td>4.04(0)</td>
<td>2.91(-0)</td>
</tr>
<tr>
<td>1.64</td>
<td>3.33(0)</td>
<td>3.32(-0)</td>
<td>3.94(0)</td>
<td>2.83(-0)</td>
</tr>
<tr>
<td>2.28</td>
<td>2.90(0)</td>
<td>2.88(-0)</td>
<td>3.23(0)</td>
<td>2.45(-0)</td>
</tr>
<tr>
<td>3.56</td>
<td>2.12(0)</td>
<td>2.10(-0)</td>
<td>2.25(0)</td>
<td>1.86(-0)</td>
</tr>
<tr>
<td>6.12</td>
<td>1.34(0)</td>
<td>1.33(-0)</td>
<td>1.37(0)</td>
<td>1.23(-0)</td>
</tr>
<tr>
<td>11.24</td>
<td>7.68(0)</td>
<td>7.55(-1)</td>
<td>7.66(-1)</td>
<td>7.24(-1)</td>
</tr>
<tr>
<td>21.48</td>
<td>4.12(0)</td>
<td>4.05(-1)</td>
<td>4.06(-1)</td>
<td>3.96(-1)</td>
</tr>
<tr>
<td>41.96</td>
<td>2.14(0)</td>
<td>2.10(-1)</td>
<td>2.10(-1)</td>
<td>2.08(-1)</td>
</tr>
</tbody>
</table>
### LITHIUM

#### 2s-4s

<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>2.13(-1)</td>
<td>2.17(-1)</td>
<td>4.43(-1)</td>
<td>2.11(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>2.91(-1)</td>
<td>2.96(-1)</td>
<td>5.31(-1)</td>
<td>2.86(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>3.86(-1)</td>
<td>3.91(-1)</td>
<td>6.24(-1)</td>
<td>3.76(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>4.84(-1)</td>
<td>4.88(-1)</td>
<td>7.00(-1)</td>
<td>4.47(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>5.55(-1)</td>
<td>5.56(-1)</td>
<td>7.24(-1)</td>
<td>4.86(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>5.58(-1)</td>
<td>5.56(-1)</td>
<td>6.64(-1)</td>
<td>4.64(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>4.76(-1)</td>
<td>4.71(-1)</td>
<td>5.25(-1)</td>
<td>3.96(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>3.42(-1)</td>
<td>3.37(-1)</td>
<td>3.57(-1)</td>
<td>2.97(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>2.13(-1)</td>
<td>2.09(-1)</td>
<td>2.15(-1)</td>
<td>1.93(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>1.20(-1)</td>
<td>1.18(-1)</td>
<td>1.19(-1)</td>
<td>1.13(-1)</td>
</tr>
<tr>
<td>21.48</td>
<td>6.43(-2)</td>
<td>6.30(-2)</td>
<td>6.31(-2)</td>
<td>6.15(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>3.32(-2)</td>
<td>3.25(-2)</td>
<td>3.25(-2)</td>
<td>3.22(-2)</td>
</tr>
</tbody>
</table>

#### 2s-5s

<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>7.81(-2)</td>
<td>7.89(-2)</td>
<td>1.83(-1)</td>
<td>7.65(-2)</td>
</tr>
<tr>
<td>1.07(-1)</td>
<td>1.08(-1)</td>
<td>2.10(-1)</td>
<td>1.04(-1)</td>
<td></td>
</tr>
<tr>
<td>1.41(-1)</td>
<td>1.42(-1)</td>
<td>2.36(-1)</td>
<td>1.36(-1)</td>
<td></td>
</tr>
<tr>
<td>1.76(-1)</td>
<td>1.76(-1)</td>
<td>2.59(-1)</td>
<td>1.60(-1)</td>
<td></td>
</tr>
<tr>
<td>2.01(-1)</td>
<td>2.00(-1)</td>
<td>2.62(-1)</td>
<td>1.73(-1)</td>
<td></td>
</tr>
<tr>
<td>2.00(-1)</td>
<td>1.98(-1)</td>
<td>2.37(-1)</td>
<td>1.65(-1)</td>
<td></td>
</tr>
<tr>
<td>1.60(-1)</td>
<td>1.67(-1)</td>
<td>1.85(-1)</td>
<td>1.40(-1)</td>
<td></td>
</tr>
<tr>
<td>1.21(-1)</td>
<td>1.18(-1)</td>
<td>1.25(-1)</td>
<td>1.04(-1)</td>
<td></td>
</tr>
<tr>
<td>7.50(-2)</td>
<td>7.32(-2)</td>
<td>7.52(-2)</td>
<td>6.76(-2)</td>
<td></td>
</tr>
<tr>
<td>4.23(-2)</td>
<td>4.12(-2)</td>
<td>4.17(-2)</td>
<td>3.94(-2)</td>
<td></td>
</tr>
<tr>
<td>2.25(-2)</td>
<td>2.19(-2)</td>
<td>2.20(-2)</td>
<td>2.14(-2)</td>
<td></td>
</tr>
<tr>
<td>1.16(-2)</td>
<td>1.13(-2)</td>
<td>1.13(-2)</td>
<td>1.12(-2)</td>
<td></td>
</tr>
</tbody>
</table>

**EPSIL = 1.60(-1)**

**EPSIL = 1.75(-1)**
## LITHIUM

### 2s-3d

\[ \text{EPSIL} = 1.43 \times 10^{-1} \]

<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>BETHE</th>
<th>OCHKUR</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>1.38(0)</td>
<td>1.31(-0)</td>
<td>0.0</td>
<td>1.26(-0)</td>
<td>4.09(-1)</td>
<td>3.91(-1)</td>
<td>0.0</td>
<td>3.79(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.90(0)</td>
<td>1.80(-0)</td>
<td>0.0</td>
<td>1.73(-0)</td>
<td>5.62(-1)</td>
<td>5.36(-1)</td>
<td>0.0</td>
<td>5.16(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>2.56(0)</td>
<td>2.43(-0)</td>
<td>0.0</td>
<td>2.31(-0)</td>
<td>7.56(-1)</td>
<td>7.15(-1)</td>
<td>0.0</td>
<td>6.83(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>3.31(0)</td>
<td>3.13(-0)</td>
<td>0.0</td>
<td>2.83(-0)</td>
<td>9.53(-1)</td>
<td>9.07(-1)</td>
<td>2.60(-1)</td>
<td>8.25(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>3.96(0)</td>
<td>3.73(-0)</td>
<td>9.82(-1)</td>
<td>3.24(-0)</td>
<td>1.11(0)</td>
<td>1.06(-0)</td>
<td>7.26(-1)</td>
<td>9.22(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>4.19(0)</td>
<td>3.94(-0)</td>
<td>2.81(-1)</td>
<td>3.32(-0)</td>
<td>1.14(0)</td>
<td>1.08(-0)</td>
<td>9.54(-1)</td>
<td>9.10(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>3.77(0)</td>
<td>3.52(-0)</td>
<td>3.18(-0)</td>
<td>3.01(-0)</td>
<td>9.86(-1)</td>
<td>9.35(-1)</td>
<td>9.00(-1)</td>
<td>7.94(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>2.82(0)</td>
<td>2.63(-0)</td>
<td>2.56(-0)</td>
<td>2.35(-0)</td>
<td>7.16(-1)</td>
<td>6.79(-1)</td>
<td>6.72(-1)</td>
<td>6.02(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>1.81(0)</td>
<td>1.69(-0)</td>
<td>1.67(-0)</td>
<td>1.58(-0)</td>
<td>4.50(-1)</td>
<td>4.26(-1)</td>
<td>4.25(-1)</td>
<td>3.96(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>1.04(0)</td>
<td>9.70(-1)</td>
<td>9.69(-1)</td>
<td>9.35(-1)</td>
<td>2.56(-1)</td>
<td>2.42(-1)</td>
<td>2.42(-1)</td>
<td>2.32(-1)</td>
</tr>
<tr>
<td>21.48</td>
<td>5.62(-1)</td>
<td>5.23(-1)</td>
<td>5.23(-1)</td>
<td>5.13(-1)</td>
<td>1.37(-1)</td>
<td>1.30(-1)</td>
<td>1.30(-1)</td>
<td>1.26(-1)</td>
</tr>
<tr>
<td>41.96</td>
<td>2.92(-1)</td>
<td>2.72(-1)</td>
<td>2.72(-1)</td>
<td>2.69(-1)</td>
<td>7.08(-2)</td>
<td>6.71(-2)</td>
<td>6.71(-2)</td>
<td>6.63(-2)</td>
</tr>
</tbody>
</table>
LITHIUM

2s-5d

\[ \text{EPSIL} = 1.78 \times (-1) \]

<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BORN(2)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>1.79(-1)</td>
<td>1.71(-1)</td>
<td>0.0</td>
<td>1.66(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>2.45(-1)</td>
<td>2.35(-1)</td>
<td>0.0</td>
<td>2.26(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>3.26(-1)</td>
<td>3.12(-1)</td>
<td>2.23(-2)</td>
<td>2.98(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>4.10(-1)</td>
<td>3.93(-1)</td>
<td>2.14(-1)</td>
<td>3.58(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>4.73(-1)</td>
<td>4.52(-1)</td>
<td>3.65(-1)</td>
<td>3.95(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>4.78(-1)</td>
<td>4.57(-1)</td>
<td>4.25(-1)</td>
<td>3.84(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>4.08(-1)</td>
<td>3.90(-1)</td>
<td>3.82(-1)</td>
<td>3.30(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>2.93(-1)</td>
<td>2.80(-1)</td>
<td>2.78(-1)</td>
<td>2.47(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>1.82(-1)</td>
<td>1.74(-1)</td>
<td>1.74(-1)</td>
<td>1.61(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>1.03(-1)</td>
<td>9.85(-2)</td>
<td>9.85(-2)</td>
<td>9.43(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>5.50(-2)</td>
<td>5.26(-2)</td>
<td>5.26(-2)</td>
<td>5.14(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>2.85(-2)</td>
<td>2.72(-2)</td>
<td>2.72(-2)</td>
<td>2.69(-2)</td>
</tr>
</tbody>
</table>
SODIUM

<table>
<thead>
<tr>
<th>N</th>
<th>BORN (1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
<th>BORN (1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
<th>BORN (1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>1.43(0)</td>
<td>6.61(-0)</td>
<td>1.40(-1)</td>
<td>3.85(-1)</td>
<td>1.66(-0)</td>
<td>3.75(-1)</td>
<td>1.64(-1)</td>
<td>6.77(-1)</td>
<td>1.59(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.95(0)</td>
<td>6.56(-0)</td>
<td>1.91(-0)</td>
<td>5.23(-1)</td>
<td>1.64(-0)</td>
<td>5.11(-1)</td>
<td>2.22(-1)</td>
<td>6.66(-1)</td>
<td>2.16(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>2.58(0)</td>
<td>6.42(-0)</td>
<td>2.53(-0)</td>
<td>6.83(-1)</td>
<td>1.59(-0)</td>
<td>6.68(-1)</td>
<td>2.89(-1)</td>
<td>6.44(-1)</td>
<td>2.82(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>3.20(0)</td>
<td>6.10(-0)</td>
<td>3.03(-0)</td>
<td>8.37(-1)</td>
<td>1.49(-0)</td>
<td>7.88(-1)</td>
<td>3.51(-1)</td>
<td>6.30(-1)</td>
<td>3.30(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>3.63(0)</td>
<td>5.52(-0)</td>
<td>3.28(-0)</td>
<td>9.25(-1)</td>
<td>1.33(-0)</td>
<td>8.32(-1)</td>
<td>3.84(-1)</td>
<td>5.34(-1)</td>
<td>3.44(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>3.60(0)</td>
<td>4.60(-0)</td>
<td>3.06(-0)</td>
<td>8.90(-1)</td>
<td>1.09(-0)</td>
<td>7.46(-1)</td>
<td>3.65(-1)</td>
<td>4.35(-1)</td>
<td>3.04(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>3.06(0)</td>
<td>3.45(-0)</td>
<td>2.53(-0)</td>
<td>7.30(-1)</td>
<td>7.97(-1)</td>
<td>5.92(-1)</td>
<td>2.96(-1)</td>
<td>3.17(-1)</td>
<td>2.37(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>2.22(0)</td>
<td>2.32(-0)</td>
<td>1.88(-0)</td>
<td>5.13(-1)</td>
<td>5.22(-1)</td>
<td>4.26(-1)</td>
<td>2.05(-1)</td>
<td>2.06(-1)</td>
<td>1.68(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>1.42(0)</td>
<td>1.42(-0)</td>
<td>1.26(-0)</td>
<td>3.18(-1)</td>
<td>3.11(-1)</td>
<td>2.75(-1)</td>
<td>1.26(-1)</td>
<td>1.22(-1)</td>
<td>1.08(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>8.39(-1)</td>
<td>8.10(-1)</td>
<td>7.62(-1)</td>
<td>1.82(-1)</td>
<td>1.73(-1)</td>
<td>1.63(-1)</td>
<td>7.10(-2)</td>
<td>6.73(-1)</td>
<td>6.30(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>4.68(-1)</td>
<td>4.45(-1)</td>
<td>4.32(-1)</td>
<td>9.91(-2)</td>
<td>9.30(-2)</td>
<td>9.00(-2)</td>
<td>3.83(-2)</td>
<td>3.58(-2)</td>
<td>3.47(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>2.54(-1)</td>
<td>2.39(-1)</td>
<td>2.36(-1)</td>
<td>5.25(-2)</td>
<td>4.88(-2)</td>
<td>4.81(-2)</td>
<td>2.01(-2)</td>
<td>1.86(-2)</td>
<td>1.84(-2)</td>
</tr>
<tr>
<td></td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
</tr>
<tr>
<td>-----</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>1.02</td>
<td>8.65(-2)</td>
<td>3.47(-1)</td>
<td>8.38(-2)</td>
<td>1.27(0)</td>
<td>6.92(-1)</td>
<td>1.32(-0)</td>
<td>2.25(-1)</td>
<td>4.60(-1)</td>
<td>2.32(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.17(-1)</td>
<td>3.41(-1)</td>
<td>1.14(-1)</td>
<td>1.75(0)</td>
<td>1.70(0)</td>
<td>1.81(-0)</td>
<td>3.08(-1)</td>
<td>5.70(-1)</td>
<td>3.14(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>1.52(-1)</td>
<td>3.30(-1)</td>
<td>1.48(-1)</td>
<td>2.33(0)</td>
<td>2.83(0)</td>
<td>2.39(-0)</td>
<td>4.09(-1)</td>
<td>6.89(-1)</td>
<td>4.12(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>1.84(-1)</td>
<td>3.08(-1)</td>
<td>1.73(-1)</td>
<td>2.96(0)</td>
<td>3.89(0)</td>
<td>2.89(-0)</td>
<td>5.15(-1)</td>
<td>7.89(-1)</td>
<td>4.90(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>2.01(-1)</td>
<td>2.73(-1)</td>
<td>1.78(-1)</td>
<td>3.47(0)</td>
<td>4.57(0)</td>
<td>3.23(-0)</td>
<td>5.96(-1)</td>
<td>8.29(-1)</td>
<td>5.37(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>1.90(-1)</td>
<td>2.21(-1)</td>
<td>1.57(-1)</td>
<td>3.58(0)</td>
<td>4.54(0)</td>
<td>3.19(-0)</td>
<td>6.06(-1)</td>
<td>7.67(-1)</td>
<td>5.24(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.53(-1)</td>
<td>1.61(-1)</td>
<td>1.21(-1)</td>
<td>3.15(0)</td>
<td>3.76(0)</td>
<td>2.82(-0)</td>
<td>5.21(-1)</td>
<td>6.10(-1)</td>
<td>4.58(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.06(-1)</td>
<td>1.04(-1)</td>
<td>8.54(-2)</td>
<td>2.32(0)</td>
<td>2.63(0)</td>
<td>2.17(-0)</td>
<td>3.76(-1)</td>
<td>4.17(-1)</td>
<td>3.46(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>6.47(-2)</td>
<td>6.13(-2)</td>
<td>5.43(-2)</td>
<td>1.47(0)</td>
<td>1.61(0)</td>
<td>1.44(-0)</td>
<td>2.35(-1)</td>
<td>2.52(-1)</td>
<td>2.27(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>3.65(-2)</td>
<td>3.38(-2)</td>
<td>3.17(-2)</td>
<td>8.43(-1)</td>
<td>9.00(-1)</td>
<td>8.51(-1)</td>
<td>1.33(-1)</td>
<td>1.40(-1)</td>
<td>1.32(-1)</td>
</tr>
<tr>
<td>21.48</td>
<td>1.96(-2)</td>
<td>1.79(-2)</td>
<td>1.73(-2)</td>
<td>4.53(-1)</td>
<td>4.78(-1)</td>
<td>4.66(-1)</td>
<td>7.11(-2)</td>
<td>7.40(-2)</td>
<td>7.21(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>1.03(-2)</td>
<td>9.30(-3)</td>
<td>9.16(-3)</td>
<td>2.35(-1)</td>
<td>2.46(-1)</td>
<td>2.44(-1)</td>
<td>3.68(-2)</td>
<td>3.81(-2)</td>
<td>3.77(-2)</td>
</tr>
<tr>
<td>N</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
</tr>
<tr>
<td>------</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>1.02</td>
<td>8.02(-2)</td>
<td>1.96(-1)</td>
<td>8.40(-2)</td>
<td>3.94(-2)</td>
<td>1.00(-1)</td>
<td>4.07(-2)</td>
<td>1.94(0)</td>
<td>0.0</td>
<td>1.80(-0)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.10(-1)</td>
<td>2.30(-1)</td>
<td>1.14(-1)</td>
<td>5.40(-2)</td>
<td>1.16(-1)</td>
<td>5.50(-2)</td>
<td>2.67(0)</td>
<td>0.0</td>
<td>2.46(-0)</td>
</tr>
<tr>
<td>1.08</td>
<td>1.46(-1)</td>
<td>2.65(-1)</td>
<td>1.48(-1)</td>
<td>7.16(-2)</td>
<td>1.31(-1)</td>
<td>7.17(-2)</td>
<td>3.60(0)</td>
<td>0.0</td>
<td>3.28(-0)</td>
</tr>
<tr>
<td>1.16</td>
<td>1.83(-1)</td>
<td>2.94(-1)</td>
<td>1.76(-1)</td>
<td>8.99(-2)</td>
<td>1.44(-1)</td>
<td>8.46(-2)</td>
<td>4.62(0)</td>
<td>0.0</td>
<td>4.02(-0)</td>
</tr>
<tr>
<td>1.32</td>
<td>2.11(-1)</td>
<td>3.01(-1)</td>
<td>1.91(-1)</td>
<td>1.03(-1)</td>
<td>1.46(-1)</td>
<td>9.19(-2)</td>
<td>5.49(0)</td>
<td>0.0</td>
<td>4.60(-0)</td>
</tr>
<tr>
<td>1.64</td>
<td>2.14(-1)</td>
<td>2.73(-1)</td>
<td>1.86(-1)</td>
<td>1.04(-1)</td>
<td>1.32(-1)</td>
<td>8.93(-2)</td>
<td>5.76(0)</td>
<td>4.00(-0)</td>
<td>4.70(-0)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.83(-1)</td>
<td>2.15(-1)</td>
<td>1.62(-1)</td>
<td>8.87(-2)</td>
<td>1.03(-1)</td>
<td>7.75(-2)</td>
<td>5.13(0)</td>
<td>4.50(-0)</td>
<td>4.25(-0)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.31(-1)</td>
<td>1.46(-1)</td>
<td>1.22(-1)</td>
<td>6.34(-2)</td>
<td>6.96(-2)</td>
<td>5.81(-2)</td>
<td>3.82(0)</td>
<td>3.60(-0)</td>
<td>3.31(-0)</td>
</tr>
<tr>
<td>6.12</td>
<td>8.17(-2)</td>
<td>8.79(-2)</td>
<td>7.92(-2)</td>
<td>3.94(-2)</td>
<td>4.18(-2)</td>
<td>3.77(-2)</td>
<td>2.44(0)</td>
<td>2.36(-0)</td>
<td>2.22(-0)</td>
</tr>
<tr>
<td>11.24</td>
<td>4.61(-2)</td>
<td>4.88(-2)</td>
<td>4.62(-2)</td>
<td>2.22(-2)</td>
<td>2.32(-2)</td>
<td>2.20(-2)</td>
<td>1.40(0)</td>
<td>1.36(-0)</td>
<td>1.31(-0)</td>
</tr>
<tr>
<td>21.48</td>
<td>2.46(-2)</td>
<td>2.58(-2)</td>
<td>2.53(-2)</td>
<td>1.18(-2)</td>
<td>1.23(-2)</td>
<td>1.19(-2)</td>
<td>7.56(-1)</td>
<td>7.35(-1)</td>
<td>7.21(-1)</td>
</tr>
<tr>
<td>41.96</td>
<td>1.27(-2)</td>
<td>1.33(-2)</td>
<td>1.31(-2)</td>
<td>6.11(-3)</td>
<td>6.30(-3)</td>
<td>6.24(-3)</td>
<td>3.93(-1)</td>
<td>3.82(-1)</td>
<td>3.78(-1)</td>
</tr>
<tr>
<td>N</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
</tr>
<tr>
<td>-----</td>
<td>----------</td>
<td>-------</td>
<td>--------</td>
<td>----------</td>
<td>-------</td>
<td>--------</td>
<td>----------</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>1.02</td>
<td>5.45(-1)</td>
<td>0.0</td>
<td>5.11(-1)</td>
<td>2.34(-1)</td>
<td>0.0</td>
<td>2.19(-1)</td>
<td>1.22(-1)</td>
<td>0.0</td>
<td>1.16(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>7.46(-1)</td>
<td>0.0</td>
<td>6.96(-1)</td>
<td>3.19(-1)</td>
<td>0.0</td>
<td>2.98(-1)</td>
<td>1.67(-1)</td>
<td>3.28(-2)</td>
<td>1.57(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>9.92(-1)</td>
<td>0.0</td>
<td>9.16(-1)</td>
<td>4.22(-1)</td>
<td>1.53(-1)</td>
<td>3.92(-1)</td>
<td>2.20(-1)</td>
<td>1.26(-1)</td>
<td>2.06(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>1.25(0)</td>
<td>5.30(-1)</td>
<td>1.11(-0)</td>
<td>5.28(-1)</td>
<td>3.60(-1)</td>
<td>4.69(-1)</td>
<td>2.75(-1)</td>
<td>2.18(-1)</td>
<td>2.46(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>1.44(0)</td>
<td>1.06(-0)</td>
<td>1.23(-0)</td>
<td>6.02(-1)</td>
<td>5.15(-1)</td>
<td>5.14(-1)</td>
<td>3.11(-1)</td>
<td>2.83(-1)</td>
<td>2.67(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>1.46(0)</td>
<td>1.30(-0)</td>
<td>1.20(-0)</td>
<td>6.00(-1)</td>
<td>5.62(-1)</td>
<td>4.94(-1)</td>
<td>3.07(-1)</td>
<td>2.96(-1)</td>
<td>2.54(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.25(0)</td>
<td>1.20(-0)</td>
<td>1.04(-0)</td>
<td>5.05(-1)</td>
<td>4.90(-1)</td>
<td>4.89(-1)</td>
<td>2.57(-1)</td>
<td>2.52(-1)</td>
<td>2.14(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>9.01(-1)</td>
<td>8.77(-1)</td>
<td>7.82(-1)</td>
<td>3.59(-1)</td>
<td>3.52(-1)</td>
<td>3.11(-1)</td>
<td>1.81(-1)</td>
<td>1.79(-1)</td>
<td>1.57(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>5.62(-1)</td>
<td>5.51(-1)</td>
<td>5.12(-1)</td>
<td>2.22(-1)</td>
<td>2.18(-1)</td>
<td>2.02(-1)</td>
<td>1.12(-1)</td>
<td>1.10(-1)</td>
<td>1.02(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>3.18(-1)</td>
<td>3.13(-1)</td>
<td>3.00(-1)</td>
<td>1.25(-1)</td>
<td>1.23(-1)</td>
<td>1.18(-1)</td>
<td>6.27(-1)</td>
<td>6.20(-2)</td>
<td>5.93(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>1.70(-1)</td>
<td>1.67(-1)</td>
<td>1.63(-1)</td>
<td>6.65(-2)</td>
<td>6.56(-2)</td>
<td>6.40(-2)</td>
<td>3.33(-2)</td>
<td>3.30(-2)</td>
<td>3.22(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>8.79(-2)</td>
<td>8.65(-2)</td>
<td>8.55(-2)</td>
<td>3.44(-2)</td>
<td>3.39(-2)</td>
<td>3.35(-2)</td>
<td>1.72(-2)</td>
<td>1.71(-2)</td>
<td>1.68(-2)</td>
</tr>
</tbody>
</table>
### SODIUM

#### 3s-7d

**\( \text{EPSIL} = 1.79 (-1) \)**

<table>
<thead>
<tr>
<th>(N)</th>
<th>BORN(1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>7.31(-2)</td>
<td>0.0</td>
<td>6.89(-2)</td>
</tr>
<tr>
<td>1.04</td>
<td>9.97(-2)</td>
<td>3.86(-2)</td>
<td>9.35(-2)</td>
</tr>
<tr>
<td>1.08</td>
<td>1.31(-1)</td>
<td>8.92(-2)</td>
<td>1.23(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>1.63(-1)</td>
<td>1.38(-1)</td>
<td>1.46(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>1.84(-1)</td>
<td>1.72(-1)</td>
<td>1.58(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>1.81(-1)</td>
<td>1.75(-1)</td>
<td>1.49(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.50(-1)</td>
<td>1.48(-1)</td>
<td>1.25(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.06(-1)</td>
<td>1.05(-1)</td>
<td>9.16(-2)</td>
</tr>
<tr>
<td>6.12</td>
<td>6.48(-2)</td>
<td>6.42(-2)</td>
<td>5.91(-2)</td>
</tr>
<tr>
<td>11.24</td>
<td>3.64(-2)</td>
<td>3.60(-2)</td>
<td>3.44(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>1.94(-2)</td>
<td>1.92(-2)</td>
<td>1.87(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>9.97(-3)</td>
<td>9.88(-3)</td>
<td>9.76(-3)</td>
</tr>
<tr>
<td>N</td>
<td>4s-5p BORN(1)</td>
<td>4s-5p BETHE</td>
<td>4s-5p OCHKUR</td>
</tr>
<tr>
<td>-----</td>
<td>---------------</td>
<td>-------------</td>
<td>-------------</td>
</tr>
<tr>
<td>1.02</td>
<td>2.24(0)</td>
<td>1.13(+1)</td>
<td>2.19(0)</td>
</tr>
<tr>
<td>1.04</td>
<td>3.06(0)</td>
<td>1.12(+1)</td>
<td>2.98(0)</td>
</tr>
<tr>
<td>1.08</td>
<td>4.03(0)</td>
<td>1.09(+1)</td>
<td>3.90(0)</td>
</tr>
<tr>
<td>1.16</td>
<td>5.01(0)</td>
<td>1.03(+1)</td>
<td>4.63(0)</td>
</tr>
<tr>
<td>1.32</td>
<td>5.69(0)</td>
<td>9.20(0)</td>
<td>5.00(0)</td>
</tr>
<tr>
<td>1.64</td>
<td>5.57(0)</td>
<td>7.60(0)</td>
<td>4.74(0)</td>
</tr>
<tr>
<td>2.28</td>
<td>4.84(0)</td>
<td>5.63(0)</td>
<td>4.02(0)</td>
</tr>
<tr>
<td>3.56</td>
<td>3.32(0)</td>
<td>3.73(0)</td>
<td>3.02(0)</td>
</tr>
<tr>
<td>6.12</td>
<td>2.25(0)</td>
<td>2.25(0)</td>
<td>2.00(0)</td>
</tr>
<tr>
<td>11.24</td>
<td>1.32(0)</td>
<td>1.27(0)</td>
<td>1.20(0)</td>
</tr>
<tr>
<td>21.48</td>
<td>7.34(-1)</td>
<td>6.90(-1)</td>
<td>6.71(-1)</td>
</tr>
<tr>
<td>41.96</td>
<td>3.97(-1)</td>
<td>3.66(-1)</td>
<td>3.62(-1)</td>
</tr>
</tbody>
</table>
### POTASSIUM

#### 4s-5s

\[
\text{EPSIL} = 9.58 \times 10^{-2}
\]

<table>
<thead>
<tr>
<th>N</th>
<th>BORN (1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>1.66(0)</td>
<td>0.0</td>
<td>1.81(0)</td>
</tr>
<tr>
<td>1.04</td>
<td>2.29(0)</td>
<td>9.14(-1)</td>
<td>2.60(0)</td>
</tr>
<tr>
<td>1.08</td>
<td>3.09(0)</td>
<td>3.22(0)</td>
<td>3.45(0)</td>
</tr>
<tr>
<td>1.16</td>
<td>3.96(0)</td>
<td>5.48(0)</td>
<td>4.19(0)</td>
</tr>
<tr>
<td>1.32</td>
<td>4.77(0)</td>
<td>7.08(0)</td>
<td>4.79(0)</td>
</tr>
<tr>
<td>1.64</td>
<td>5.06(0)</td>
<td>7.38(0)</td>
<td>5.00(0)</td>
</tr>
<tr>
<td>2.28</td>
<td>4.30(0)</td>
<td>6.28(0)</td>
<td>4.66(0)</td>
</tr>
<tr>
<td>3.56</td>
<td>3.42(0)</td>
<td>4.46(0)</td>
<td>3.69(0)</td>
</tr>
<tr>
<td>6.12</td>
<td>2.19(0)</td>
<td>2.75(0)</td>
<td>2.47(0)</td>
</tr>
<tr>
<td>11.24</td>
<td>1.26(0)</td>
<td>1.55(0)</td>
<td>1.47(0)</td>
</tr>
<tr>
<td>21.48</td>
<td>6.80(-1)</td>
<td>8.22(0)</td>
<td>8.04(-1)</td>
</tr>
<tr>
<td>41.96</td>
<td>3.53(-1)</td>
<td>4.24(-1)</td>
<td>4.22(-1)</td>
</tr>
</tbody>
</table>

#### 4s-6s

\[
\text{EPSIL} = 1.25 \times 10^{-1}
\]

<table>
<thead>
<tr>
<th>N</th>
<th>BORN (1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.01</td>
<td>2.90(-1)</td>
<td>5.38(-1)</td>
<td>3.24(-1)</td>
</tr>
<tr>
<td>1.39</td>
<td>4.00(-1)</td>
<td>7.56(-1)</td>
<td>4.39(-1)</td>
</tr>
<tr>
<td>1.87</td>
<td>5.38(-1)</td>
<td>9.95(-1)</td>
<td>5.77(-1)</td>
</tr>
<tr>
<td>2.41</td>
<td>6.93(-1)</td>
<td>1.21(0)</td>
<td>6.94(-1)</td>
</tr>
<tr>
<td>2.88</td>
<td>8.24(-1)</td>
<td>1.32(0)</td>
<td>7.89(-1)</td>
</tr>
<tr>
<td>3.02</td>
<td>8.66(-1)</td>
<td>1.26(0)</td>
<td>8.20(-1)</td>
</tr>
<tr>
<td>2.67</td>
<td>7.53(-1)</td>
<td>1.01(0)</td>
<td>7.52(-1)</td>
</tr>
<tr>
<td>1.94</td>
<td>5.60(-1)</td>
<td>6.98(-1)</td>
<td>5.82(-1)</td>
</tr>
<tr>
<td>1.44</td>
<td>3.53(-1)</td>
<td>4.24(-1)</td>
<td>3.83(-1)</td>
</tr>
<tr>
<td>6.90</td>
<td>2.01(-1)</td>
<td>2.36(-1)</td>
<td>2.25(-1)</td>
</tr>
<tr>
<td>8.21</td>
<td>1.26(0)</td>
<td>1.55(0)</td>
<td>1.47(0)</td>
</tr>
<tr>
<td>7.01</td>
<td>1.08(-1)</td>
<td>1.25(-1)</td>
<td>1.22(-1)</td>
</tr>
<tr>
<td>4.34</td>
<td>6.80(-1)</td>
<td>8.22(0)</td>
<td>8.04(-1)</td>
</tr>
<tr>
<td>2.24</td>
<td>3.53(-1)</td>
<td>4.24(-1)</td>
<td>4.22(-1)</td>
</tr>
</tbody>
</table>

#### 4s-7s

\[
\text{EPSIL} = 1.38 \times 10^{-1}
\]

<table>
<thead>
<tr>
<th>N</th>
<th>BORN (1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.01</td>
<td>1.01(-1)</td>
<td>2.58(-1)</td>
<td>1.17(-1)</td>
</tr>
<tr>
<td>1.39</td>
<td>1.39(-1)</td>
<td>3.25(-1)</td>
<td>1.57(-1)</td>
</tr>
<tr>
<td>1.87</td>
<td>1.87(-1)</td>
<td>3.96(-1)</td>
<td>2.06(-1)</td>
</tr>
<tr>
<td>2.41</td>
<td>2.41(-1)</td>
<td>4.57(-1)</td>
<td>2.47(-1)</td>
</tr>
<tr>
<td>2.88</td>
<td>2.88(-1)</td>
<td>4.82(-1)</td>
<td>2.81(-1)</td>
</tr>
<tr>
<td>3.02</td>
<td>3.02(-1)</td>
<td>4.48(-1)</td>
<td>2.92(-1)</td>
</tr>
<tr>
<td>2.67</td>
<td>2.67(-1)</td>
<td>3.57(-1)</td>
<td>2.66(-1)</td>
</tr>
<tr>
<td>1.94</td>
<td>1.94(-1)</td>
<td>2.44(-1)</td>
<td>2.04(-1)</td>
</tr>
<tr>
<td>1.44</td>
<td>1.44(-1)</td>
<td>1.48(-1)</td>
<td>1.34(-1)</td>
</tr>
<tr>
<td>6.90</td>
<td>6.90(-2)</td>
<td>8.21(-2)</td>
<td>7.01(-2)</td>
</tr>
<tr>
<td>4.34</td>
<td>4.34(-2)</td>
<td>4.25(-2)</td>
<td></td>
</tr>
<tr>
<td>2.24</td>
<td>2.24(-2)</td>
<td>2.22(-2)</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>BORN (1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
</tr>
<tr>
<td>-----</td>
<td>----------</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>1.02</td>
<td>7.64(0)</td>
<td>1.77(+1)</td>
<td>8.27(0)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.04(1)</td>
<td>9.86(+1)</td>
<td>1.14(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>1.38(1)</td>
<td>7.84(-1)</td>
<td>1.53(+1)</td>
</tr>
<tr>
<td>1.16</td>
<td>1.74(1)</td>
<td>8.50(0)</td>
<td>1.87(+1)</td>
</tr>
<tr>
<td>1.32</td>
<td>1.98(1)</td>
<td>1.59(+1)</td>
<td>2.10(+1)</td>
</tr>
<tr>
<td>1.64</td>
<td>1.97(1)</td>
<td>1.91(+1)</td>
<td>1.99(+1)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.67(1)</td>
<td>1.73(+1)</td>
<td>1.60(+1)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.20(1)</td>
<td>1.27(+1)</td>
<td>1.14(+1)</td>
</tr>
<tr>
<td>6.12</td>
<td>7.46(0)</td>
<td>7.98(0)</td>
<td>7.31(0)</td>
</tr>
<tr>
<td>11.24</td>
<td>4.23(0)</td>
<td>4.52(0)</td>
<td>4.29(0)</td>
</tr>
<tr>
<td>21.48</td>
<td>2.26(0)</td>
<td>2.42(0)</td>
<td>2.35(0)</td>
</tr>
<tr>
<td>41.96</td>
<td>1.17(0)</td>
<td>1.25(0)</td>
<td>1.23(0)</td>
</tr>
</tbody>
</table>
POTASSIUM

4s-6d

$$\varepsilon = 1.44 \times 10^{-1}$$

<table>
<thead>
<tr>
<th>N</th>
<th>Born (1)</th>
<th>Bethe</th>
<th>Ochkur</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>2.08(-1)</td>
<td>0.0</td>
<td>8.01(-3)</td>
</tr>
<tr>
<td>1.04</td>
<td>2.80(-1)</td>
<td>0.0</td>
<td>1.72(-2)</td>
</tr>
<tr>
<td>1.08</td>
<td>3.59(-1)</td>
<td>0.0</td>
<td>3.76(-2)</td>
</tr>
<tr>
<td>1.16</td>
<td>4.23(-1)</td>
<td>0.0</td>
<td>7.39(-2)</td>
</tr>
<tr>
<td>1.32</td>
<td>4.39(-1)</td>
<td>0.0</td>
<td>1.28(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>3.86(-1)</td>
<td>1.18(-2)</td>
<td>1.56(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>2.87(-1)</td>
<td>1.01(-1)</td>
<td>1.40(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.86(-1)</td>
<td>1.06(-1)</td>
<td>1.06(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>1.08(-1)</td>
<td>7.65(-2)</td>
<td>7.28(-2)</td>
</tr>
<tr>
<td>11.24</td>
<td>5.89(-2)</td>
<td>4.62(-2)</td>
<td>4.45(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>3.08(-2)</td>
<td>2.55(-2)</td>
<td>2.49(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>1.58(-2)</td>
<td>1.34(-2)</td>
<td>1.32(-2)</td>
</tr>
</tbody>
</table>
**RUBIDIUM**

<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
<th>BORN(1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
<th>BORN(1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>2.47(0)</td>
<td>1.32(+1)</td>
<td>2.36(0)</td>
<td>6.48(-1)</td>
<td>3.29(0)</td>
<td>6.29(-1)</td>
<td>2.79(-1)</td>
<td>1.35(0)</td>
<td>2.68(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>3.37(0)</td>
<td>1.31(+1)</td>
<td>3.20(0)</td>
<td>8.84(-1)</td>
<td>3.25(0)</td>
<td>8.48(-1)</td>
<td>3.80(-1)</td>
<td>1.33(0)</td>
<td>3.60(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>4.47(0)</td>
<td>1.28(+1)</td>
<td>4.20(0)</td>
<td>1.17(0)</td>
<td>3.15(0)</td>
<td>1.10(0)</td>
<td>5.01(-1)</td>
<td>1.28(0)</td>
<td>4.65(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>5.62(0)</td>
<td>1.21(+1)</td>
<td>5.01(0)</td>
<td>1.46(0)</td>
<td>2.96(0)</td>
<td>1.29(0)</td>
<td>6.23(-1)</td>
<td>1.20(0)</td>
<td>5.42(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>6.47(0)</td>
<td>1.10(+1)</td>
<td>5.51(0)</td>
<td>1.67(0)</td>
<td>2.64(0)</td>
<td>1.39(0)</td>
<td>7.08(-1)</td>
<td>1.07(0)</td>
<td>5.76(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>6.68(0)</td>
<td>9.15(0)</td>
<td>5.43(0)</td>
<td>1.68(0)</td>
<td>2.16(0)</td>
<td>1.33(0)</td>
<td>7.06(-1)</td>
<td>8.70(-1)</td>
<td>5.46(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>5.73(0)</td>
<td>6.86(0)</td>
<td>4.81(0)</td>
<td>1.44(0)</td>
<td>1.59(0)</td>
<td>1.14(0)</td>
<td>6.00(-1)</td>
<td>6.35(-1)</td>
<td>4.61(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>4.26(0)</td>
<td>4.60(0)</td>
<td>3.72(0)</td>
<td>1.05(0)</td>
<td>1.04(0)</td>
<td>8.50(-1)</td>
<td>4.33(-1)</td>
<td>4.13(-1)</td>
<td>3.39(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>2.77(0)</td>
<td>2.81(0)</td>
<td>2.51(0)</td>
<td>6.76(-1)</td>
<td>6.21(-1)</td>
<td>5.55(-1)</td>
<td>2.75(-1)</td>
<td>2.45(-1)</td>
<td>2.19(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>1.65(0)</td>
<td>1.60(0)</td>
<td>1.52(0)</td>
<td>3.98(-1)</td>
<td>3.47(-1)</td>
<td>3.28(-1)</td>
<td>1.50(-1)</td>
<td>1.36(-1)</td>
<td>1.28(-1)</td>
</tr>
<tr>
<td>21.48</td>
<td>9.29(-1)</td>
<td>8.83(-1)</td>
<td>8.60(-1)</td>
<td>2.22(-1)</td>
<td>1.87(-1)</td>
<td>1.82(-1)</td>
<td>8.86(-2)</td>
<td>7.25(-2)</td>
<td>7.06(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>5.08(-1)</td>
<td>4.74(-1)</td>
<td>4.69(-1)</td>
<td>1.20(-1)</td>
<td>9.81(-2)</td>
<td>9.70(-2)</td>
<td>4.47(-2)</td>
<td>3.78(-2)</td>
<td>3.74(-2)</td>
</tr>
</tbody>
</table>
### Rubidium

<table>
<thead>
<tr>
<th>N</th>
<th>Born(1)</th>
<th>Bethe</th>
<th>Ochkur</th>
<th>Born(1)</th>
<th>Bethe</th>
<th>Ochkur</th>
<th>Born(1)</th>
<th>Bethe</th>
<th>Ochkur</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>1.80(-1)</td>
<td>0.0</td>
<td>2.00(0)</td>
<td>2.78(-1)</td>
<td>4.80(-1)</td>
<td>3.35(-1)</td>
<td>1.06(-1)</td>
<td>2.54(-1)</td>
<td>1.20(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>2.51(0)</td>
<td>0.0</td>
<td>2.72(0)</td>
<td>3.85(-1)</td>
<td>1.48(-1)</td>
<td>4.54(-1)</td>
<td>1.47(-1)</td>
<td>3.36(-1)</td>
<td>1.62(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>3.38(0)</td>
<td>2.78(0)</td>
<td>3.62(0)</td>
<td>5.22(-1)</td>
<td>1.04(0)</td>
<td>6.01(-1)</td>
<td>1.99(-1)</td>
<td>4.25(-1)</td>
<td>2.14(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>4.38(0)</td>
<td>5.62(0)</td>
<td>4.43(0)</td>
<td>6.81(-1)</td>
<td>1.31(0)</td>
<td>7.31(-1)</td>
<td>2.58(-1)</td>
<td>5.03(-1)</td>
<td>2.60(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>5.27(0)</td>
<td>7.71(0)</td>
<td>5.15(0)</td>
<td>8.25(-1)</td>
<td>1.47(0)</td>
<td>8.50(-1)</td>
<td>3.12(-1)</td>
<td>5.40(-1)</td>
<td>3.03(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>5.64(0)</td>
<td>8.27(0)</td>
<td>5.52(0)</td>
<td>8.81(-1)</td>
<td>1.42(0)</td>
<td>9.11(-1)</td>
<td>3.31(-1)</td>
<td>5.07(-1)</td>
<td>3.25(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>5.10(0)</td>
<td>7.14(0)</td>
<td>5.27(0)</td>
<td>7.88(-1)</td>
<td>1.15(0)</td>
<td>8.52(-1)</td>
<td>2.92(-1)</td>
<td>4.07(-1)</td>
<td>3.02(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>3.84(0)</td>
<td>5.10(0)</td>
<td>4.22(0)</td>
<td>5.83(-1)</td>
<td>7.99(-1)</td>
<td>6.65(-1)</td>
<td>2.14(-1)</td>
<td>2.79(-1)</td>
<td>2.34(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>2.47(0)</td>
<td>3.16(0)</td>
<td>2.84(0)</td>
<td>3.69(-1)</td>
<td>4.86(-1)</td>
<td>4.40(-1)</td>
<td>1.35(-1)</td>
<td>1.69(-1)</td>
<td>1.54(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>1.42(0)</td>
<td>1.78(0)</td>
<td>1.69(0)</td>
<td>2.10(-1)</td>
<td>2.71(-1)</td>
<td>2.58(-1)</td>
<td>7.67(-2)</td>
<td>9.42(-2)</td>
<td>8.98(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>7.66(-1)</td>
<td>9.47(-1)</td>
<td>9.26(-1)</td>
<td>1.13(-1)</td>
<td>1.44(-1)</td>
<td>1.41(-1)</td>
<td>4.10(-2)</td>
<td>4.99(-2)</td>
<td>4.88(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>3.98(-1)</td>
<td>4.89(-1)</td>
<td>4.86(-1)</td>
<td>5.85(-2)</td>
<td>7.42(-2)</td>
<td>7.36(-2)</td>
<td>2.12(-2)</td>
<td>2.57(-2)</td>
<td>2.55(-2)</td>
</tr>
<tr>
<td>N</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
</tr>
<tr>
<td>----</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>1.02</td>
<td>1.04(+1)</td>
<td>0.0</td>
<td>1.15(+1)</td>
<td>1.24(0)</td>
<td>0.0</td>
<td>8.25(-1)</td>
<td>3.38(-1)</td>
<td>0.0</td>
<td>1.32(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.43(+1)</td>
<td>0.0</td>
<td>1.59(+1)</td>
<td>1.67(0)</td>
<td>1.43(-1)</td>
<td>1.16(0)</td>
<td>4.65(-1)</td>
<td>0.0</td>
<td>1.96(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>1.88(+1)</td>
<td>1.61(0)</td>
<td>2.13(+1)</td>
<td>2.15(0)</td>
<td>4.94(-1)</td>
<td>1.58(0)</td>
<td>5.83(-1)</td>
<td>0.0</td>
<td>2.85(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>2.35(+1)</td>
<td>1.35(+1)</td>
<td>2.61(+1)</td>
<td>2.58(0)</td>
<td>8.38(-1)</td>
<td>1.96(0)</td>
<td>6.89(-1)</td>
<td>0.0</td>
<td>3.86(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>2.66(+1)</td>
<td>2.28(+1)</td>
<td>2.92(+1)</td>
<td>2.71(0)</td>
<td>1.08(0)</td>
<td>2.13(0)</td>
<td>7.11(-1)</td>
<td>0.0</td>
<td>4.63(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>2.62(+1)</td>
<td>2.65(+1)</td>
<td>2.74(+1)</td>
<td>2.42(0)</td>
<td>1.13(0)</td>
<td>1.73(0)</td>
<td>6.18(-1)</td>
<td>5.08(-2)</td>
<td>4.08(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>2.18(+1)</td>
<td>2.38(+1)</td>
<td>2.18(+1)</td>
<td>1.81(0)</td>
<td>9.59(-1)</td>
<td>1.05(0)</td>
<td>4.62(-1)</td>
<td>1.84(-1)</td>
<td>2.74(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.54(+1)</td>
<td>1.73(+1)</td>
<td>1.54(+1)</td>
<td>1.17(0)</td>
<td>6.80(-1)</td>
<td>5.94(-1)</td>
<td>2.91(-1)</td>
<td>1.84(-1)</td>
<td>1.77(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>9.52(0)</td>
<td>1.08(+1)</td>
<td>9.90(0)</td>
<td>6.84(-1)</td>
<td>4.19(-1)</td>
<td>3.58(-1)</td>
<td>1.79(-1)</td>
<td>1.30(-1)</td>
<td>1.18(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>5.36(0)</td>
<td>6.12(0)</td>
<td>5.80(0)</td>
<td>3.72(-1)</td>
<td>2.36(-1)</td>
<td>2.11(-1)</td>
<td>9.29(-2)</td>
<td>7.82(-2)</td>
<td>7.26(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>2.86(0)</td>
<td>3.27(0)</td>
<td>3.17(0)</td>
<td>1.95(-1)</td>
<td>1.25(-1)</td>
<td>1.18(-1)</td>
<td>4.88(-2)</td>
<td>4.30(-2)</td>
<td>4.11(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>1.48(0)</td>
<td>1.69(0)</td>
<td>1.66(0)</td>
<td>9.98(-2)</td>
<td>6.47(-2)</td>
<td>6.25(-2)</td>
<td>2.50(-2)</td>
<td>2.25(-2)</td>
<td>2.20(-2)</td>
</tr>
</tbody>
</table>
RUBIDIUM

5s-7d

EPSIL = 1.38 (-1)

<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>1.23(-1)</td>
<td>0.0</td>
<td>3.74(-2)</td>
</tr>
<tr>
<td>1.04</td>
<td>1.66(-1)</td>
<td>0.0</td>
<td>5.87(-2)</td>
</tr>
<tr>
<td>1.08</td>
<td>2.12(-1)</td>
<td>0.0</td>
<td>9.28(-2)</td>
</tr>
<tr>
<td>1.16</td>
<td>2.61(-1)</td>
<td>0.0</td>
<td>1.38(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>2.60(-1)</td>
<td>0.0</td>
<td>1.82(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>2.27(-1)</td>
<td>7.54(-3)</td>
<td>1.77(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.38(-1)</td>
<td>9.14(-2)</td>
<td>1.33(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.10(-1)</td>
<td>9.68(-2)</td>
<td>9.50(-2)</td>
</tr>
<tr>
<td>6.12</td>
<td>6.68(-2)</td>
<td>7.01(-2)</td>
<td>6.51(-2)</td>
</tr>
<tr>
<td>11.24</td>
<td>3.66(-2)</td>
<td>4.24(-2)</td>
<td>4.01(-2)</td>
</tr>
<tr>
<td>21.48</td>
<td>1.93(-2)</td>
<td>2.34(-2)</td>
<td>2.26(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>9.97(-3)</td>
<td>1.23(-2)</td>
<td>1.21(-2)</td>
</tr>
</tbody>
</table>
### Cesium

<table>
<thead>
<tr>
<th></th>
<th>6s-7p</th>
<th>6s-8p</th>
<th>6s-9p</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>BORN(1) Bethe Ochkur</td>
<td>BORN(1) Bethe Ochkur</td>
<td>BORN(1) Bethe Ochkur</td>
</tr>
<tr>
<td>1.02</td>
<td>2.88(0) 1.69(1) 2.75(0)</td>
<td>7.64(-1) 4.11(0) 7.23(-1)</td>
<td>3.26(-1) 1.67(0) 3.06(-1)</td>
</tr>
<tr>
<td>1.04</td>
<td>3.95(0) 1.68(1) 3.72(0)</td>
<td>1.04(0) 4.05(0) 9.73(-1)</td>
<td>4.44(-1) 1.64(0) 4.11(-1)</td>
</tr>
<tr>
<td>1.08</td>
<td>5.25(0) 1.63(1) 4.88(0)</td>
<td>1.38(0) 3.92(0) 1.26(0)</td>
<td>5.84(-1) 1.58(0) 5.31(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>6.66(0) 1.54(1) 5.83(0)</td>
<td>1.74(0) 3.67(0) 1.49(0)</td>
<td>7.25(-1) 1.48(0) 6.21(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>7.78(0) 1.39(1) 6.50(0)</td>
<td>2.00(0) 3.26(0) 1.62(0)</td>
<td>8.20(-1) 1.31(0) 6.72(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>8.04(0) 1.15(1) 6.56(0)</td>
<td>2.03(0) 2.66(0) 1.60(0)</td>
<td>8.13(-1) 1.06(0) 6.54(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>7.12(0) 8.52(0) 5.90(0)</td>
<td>1.75(0) 1.94(0) 1.38(0)</td>
<td>6.84(-1) 7.70(-1) 5.60(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>5.36(0) 5.66(0) 4.56(0)</td>
<td>1.28(0) 1.26(0) 1.03(0)</td>
<td>4.88(-1) 4.99(-1) 4.11(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>3.53(0) 3.42(0) 3.05(0)</td>
<td>8.24(-1) 7.47(-1) 6.70(-1)</td>
<td>3.06(-1) 2.94(-1) 2.64(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>2.12(0) 1.94(0) 1.83(0)</td>
<td>4.84(-1) 4.15(-1) 3.92(-1)</td>
<td>1.76(-1) 1.62(-1) 1.53(-1)</td>
</tr>
<tr>
<td>21.48</td>
<td>1.21(0) 1.05(0) 1.03(0)</td>
<td>2.70(-1) 2.21(-1) 2.16(-1)</td>
<td>9.65(-2) 8.58(-2) 8.36(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>6.66(-1) 5.60(-1) 5.55(-1)</td>
<td>1.46(-1) 1.15(-1) 1.42(-1)</td>
<td>5.14(-2) 4.45(-2) 4.40(-2)</td>
</tr>
<tr>
<td>N</td>
<td>BORN(1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
</tr>
<tr>
<td>----</td>
<td>---------</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>1.02</td>
<td>1.83(0)</td>
<td>0.0</td>
<td>2.17(0)</td>
</tr>
<tr>
<td>1.04</td>
<td>2.54(0)</td>
<td>0.0</td>
<td>2.96(0)</td>
</tr>
<tr>
<td>1.08</td>
<td>3.46(0)</td>
<td>1.56(0)</td>
<td>3.96(0)</td>
</tr>
<tr>
<td>1.16</td>
<td>4.54(0)</td>
<td>5.75(0)</td>
<td>4.92(0)</td>
</tr>
<tr>
<td>1.32</td>
<td>5.57(0)</td>
<td>8.97(0)</td>
<td>5.93(0)</td>
</tr>
<tr>
<td>1.64</td>
<td>6.09(0)</td>
<td>1.01(+1)</td>
<td>6.67(0)</td>
</tr>
<tr>
<td>2.28</td>
<td>5.61(0)</td>
<td>8.97(0)</td>
<td>6.58(0)</td>
</tr>
<tr>
<td>3.56</td>
<td>4.27(0)</td>
<td>6.50(0)</td>
<td>5.36(0)</td>
</tr>
<tr>
<td>6.12</td>
<td>2.76(0)</td>
<td>4.05(0)</td>
<td>3.65(0)</td>
</tr>
<tr>
<td>11.24</td>
<td>1.60(0)</td>
<td>2.29(0)</td>
<td>2.17(0)</td>
</tr>
<tr>
<td>21.48</td>
<td>8.62(-1)</td>
<td>1.22(0)</td>
<td>1.20(0)</td>
</tr>
<tr>
<td>41.96</td>
<td>4.49(-1)</td>
<td>6.31(-1)</td>
<td>6.28(-1)</td>
</tr>
<tr>
<td>N</td>
<td>BORN (1)</td>
<td>BETHE</td>
<td>OCHKUR</td>
</tr>
<tr>
<td>-----</td>
<td>----------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>1.02</td>
<td>1.62(1)</td>
<td>1.24(+1)</td>
<td>1.52(+1)</td>
</tr>
<tr>
<td>1.04</td>
<td>2.21(1)</td>
<td>1.93(+1)</td>
<td>2.13(+1)</td>
</tr>
<tr>
<td>1.08</td>
<td>2.92(1)</td>
<td>2.71(+1)</td>
<td>2.90(+1)</td>
</tr>
<tr>
<td>1.16</td>
<td>3.64(1)</td>
<td>3.42(+1)</td>
<td>3.66(+1)</td>
</tr>
<tr>
<td>1.32</td>
<td>4.09(1)</td>
<td>3.82(+1)</td>
<td>4.23(+1)</td>
</tr>
<tr>
<td>1.64</td>
<td>3.97(1)</td>
<td>3.68(+1)</td>
<td>3.96(+1)</td>
</tr>
<tr>
<td>2.28</td>
<td>3.22(1)</td>
<td>3.00(+1)</td>
<td>2.92(+1)</td>
</tr>
<tr>
<td>3.56</td>
<td>2.22(1)</td>
<td>2.08(+1)</td>
<td>1.85(+1)</td>
</tr>
<tr>
<td>6.12</td>
<td>1.35(1)</td>
<td>1.27(+1)</td>
<td>1.13(+1)</td>
</tr>
<tr>
<td>11.24</td>
<td>7.52(0)</td>
<td>7.06(0)</td>
<td>6.54(0)</td>
</tr>
<tr>
<td>21.48</td>
<td>3.98(0)</td>
<td>3.74(0)</td>
<td>3.58(0)</td>
</tr>
<tr>
<td>41.96</td>
<td>2.05(0)</td>
<td>1.93(0)</td>
<td>1.88(0)</td>
</tr>
</tbody>
</table>
**CESIUM**

6s-8d

$$\text{EPSIL} = 1.27 \times 10^{-1}$$

<table>
<thead>
<tr>
<th>N</th>
<th>BORN(1)</th>
<th>BETHE</th>
<th>OCHKUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>2.18(-2)</td>
<td>0.0</td>
<td>6.56(-2)</td>
</tr>
<tr>
<td>1.04</td>
<td>3.38(-2)</td>
<td>0.0</td>
<td>9.61(-2)</td>
</tr>
<tr>
<td>1.08</td>
<td>5.46(-2)</td>
<td>0.0</td>
<td>1.52(-1)</td>
</tr>
<tr>
<td>1.16</td>
<td>8.74(-2)</td>
<td>0.0</td>
<td>2.37(-1)</td>
</tr>
<tr>
<td>1.32</td>
<td>1.28(-1)</td>
<td>0.0</td>
<td>3.74(-1)</td>
</tr>
<tr>
<td>1.64</td>
<td>1.58(-1)</td>
<td>4.04(-1)</td>
<td>5.00(-1)</td>
</tr>
<tr>
<td>2.28</td>
<td>1.57(-1)</td>
<td>5.39(-1)</td>
<td>5.20(-1)</td>
</tr>
<tr>
<td>3.56</td>
<td>1.28(-1)</td>
<td>4.56(-1)</td>
<td>4.29(-1)</td>
</tr>
<tr>
<td>6.12</td>
<td>8.69(-2)</td>
<td>3.05(-1)</td>
<td>2.92(-1)</td>
</tr>
<tr>
<td>11.24</td>
<td>5.17(-2)</td>
<td>1.78(-1)</td>
<td>1.74(-1)</td>
</tr>
<tr>
<td>21.48</td>
<td>2.83(-2)</td>
<td>9.67(-2)</td>
<td>9.54(-2)</td>
</tr>
<tr>
<td>41.96</td>
<td>1.48(-2)</td>
<td>5.04(-2)</td>
<td>5.00(-2)</td>
</tr>
</tbody>
</table>
b) Inert Gas Excitation Tables

An Inert-gas study such as the Vainshtein work for the Alkali family has not been done until the present work.

Furthermore with the exception of Helium, the literature does not reveal much data either experimental or theoretical. However, since the usefulness of such a study is clear, a systematic calculation of cross-section data for the inert elements is presented here, and comparison with data from the literature is presented where such data has been found.
## INERT ELEMENT C-SECTION TABLES

<table>
<thead>
<tr>
<th>Element</th>
<th>Transition</th>
<th>Reference(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>1s - 2p</td>
<td>Born, Ochkur, Bethe, Mod. Bethe</td>
</tr>
<tr>
<td></td>
<td>1s - 2s</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td></td>
<td>1s - 3s</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td>Ne</td>
<td>2p - 3p</td>
<td>Born, Ochkur, Bethe, Mod. Bethe</td>
</tr>
<tr>
<td></td>
<td>2p - 3p</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td></td>
<td>2p - 4s</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td>Ar</td>
<td>3p - 4s</td>
<td>Born, Ochkur, Bethe, Mod. Bethe</td>
</tr>
<tr>
<td></td>
<td>3p - 4p</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td></td>
<td>3p - 3d</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td>Kr</td>
<td>4p - 5s</td>
<td>Born, Ochkur, Bethe, Mod. Bethe</td>
</tr>
<tr>
<td></td>
<td>4p - 5p</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td></td>
<td>4p - 4d</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td>Xe</td>
<td>5p - 6s</td>
<td>Born, Ochkur, Bethe, Mod. Bethe</td>
</tr>
<tr>
<td></td>
<td>5p - 6p</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td></td>
<td>5p - 4d</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td>RN</td>
<td>6p - 7s</td>
<td>Born, Ochkur, Bethe, Mod. Bethe</td>
</tr>
<tr>
<td></td>
<td>6p - 7p</td>
<td>Born, Ochkur</td>
</tr>
<tr>
<td></td>
<td>6p - 6d</td>
<td>Born, Ochkur</td>
</tr>
</tbody>
</table>
## HELIUM

\[ \text{ls} - 2p \quad \text{ls} - 2s \quad \text{ls} - 3s \]

### \( \text{ls} - 2p \)  
**Epsilon = 7.74(-1)**

<table>
<thead>
<tr>
<th>( N )</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>BETHE</th>
<th>MODBETHE</th>
<th>LIT(1)</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT(2)</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>3.22(-2)</td>
<td>2.98(-2)</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>2.48(-2)</td>
<td>2.48(-2)</td>
<td>2.60(-2)</td>
<td>4.63(-3)</td>
<td>4.65(-3)</td>
<td></td>
</tr>
<tr>
<td>1.10</td>
<td>4.52(-2)</td>
<td>4.06(-2)</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>3.24(-2)</td>
<td>3.24(-2)</td>
<td>3.40(-2)</td>
<td>6.03(-3)</td>
<td>6.04(-3)</td>
<td></td>
</tr>
<tr>
<td>1.20</td>
<td>6.26(-2)</td>
<td>5.37(-2)</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>3.96(-2)</td>
<td>4.04(-2)</td>
<td>3.20(-2)</td>
<td>7.33(-3)</td>
<td>7.49(-3)</td>
<td></td>
</tr>
<tr>
<td>1.80</td>
<td>1.02(-1)</td>
<td>8.63(-2)</td>
<td>4.14(-2)</td>
<td>2.12(-1)</td>
<td>1.05(-1)</td>
<td>4.10(-2)</td>
<td>3.97(-2)</td>
<td>0.0</td>
<td>7.43(-3)</td>
<td>7.16(-3)</td>
<td></td>
</tr>
<tr>
<td>2.50</td>
<td>1.08(-1)</td>
<td>9.60(-2)</td>
<td>8.16(-2)</td>
<td>2.00(-1)</td>
<td>1.33(-1)</td>
<td>3.35(-2)</td>
<td>3.08(-2)</td>
<td>0.0</td>
<td>6.00(-3)</td>
<td>5.48(-3)</td>
<td></td>
</tr>
<tr>
<td>5.00</td>
<td>9.20(-2)</td>
<td>8.78(-2)</td>
<td>8.78(-2)</td>
<td>1.43(-1)</td>
<td>1.28(-1)</td>
<td>1.88(-2)</td>
<td>1.70(-2)</td>
<td>0.0</td>
<td>3.33(-3)</td>
<td>3.00(-3)</td>
<td></td>
</tr>
<tr>
<td>10.00</td>
<td>6.54(-2)</td>
<td>6.41(-2)</td>
<td>6.53(-2)</td>
<td>9.10(-2)</td>
<td>9.70(-2)</td>
<td>9.87(-3)</td>
<td>9.23(-3)</td>
<td>0.0</td>
<td>1.74(-3)</td>
<td>1.62(-3)</td>
<td></td>
</tr>
<tr>
<td>15.00</td>
<td>5.12(-2)</td>
<td>5.06(-2)</td>
<td>5.16(-2)</td>
<td>6.83(-2)</td>
<td>7.70(-2)</td>
<td>6.68(-3)</td>
<td>6.36(-3)</td>
<td>0.0</td>
<td>1.17(-3)</td>
<td>1.12(-3)</td>
<td></td>
</tr>
<tr>
<td>20.00</td>
<td>4.25(-2)</td>
<td>4.22(-2)</td>
<td>4.29(-2)</td>
<td>5.52(-2)</td>
<td>6.43(-2)</td>
<td>5.04(-3)</td>
<td>4.86(-3)</td>
<td>0.0</td>
<td>8.86(-4)</td>
<td>8.53(-4)</td>
<td></td>
</tr>
<tr>
<td>30.00</td>
<td>3.22(-2)</td>
<td>3.20(-2)</td>
<td>3.25(-2)</td>
<td>4.06(-2)</td>
<td>0.0</td>
<td>3.39(-3)</td>
<td>3.30(-3)</td>
<td>0.0</td>
<td>5.95(-4)</td>
<td>5.79(-4)</td>
<td></td>
</tr>
<tr>
<td>50.00</td>
<td>2.22(-2)</td>
<td>2.12(-2)</td>
<td>2.25(-2)</td>
<td>2.72(-2)</td>
<td>0.0</td>
<td>2.04(-3)</td>
<td>2.01(-3)</td>
<td>0.0</td>
<td>3.58(-4)</td>
<td>3.53(-4)</td>
<td></td>
</tr>
<tr>
<td>100.00</td>
<td>1.56(-2)</td>
<td>1.55(-2)</td>
<td>1.57(-2)</td>
<td>1.87(-2)</td>
<td>0.0</td>
<td>1.28(-3)</td>
<td>1.27(-3)</td>
<td>0.0</td>
<td>2.25(-4)</td>
<td>2.22(-4)</td>
<td></td>
</tr>
</tbody>
</table>


### NEON

#### 2p - 3s

\[ \text{EPSIL} = 6.12(-1) \]

<table>
<thead>
<tr>
<th>N</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>BETHE</th>
<th>MODBETHE</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>3.07(-3)</td>
<td>2.60(-3)</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>1.06(-3)</td>
<td>9.60(-4)</td>
<td></td>
<td>4.16(-4)</td>
<td>3.45(-4)</td>
<td></td>
</tr>
<tr>
<td>1.10</td>
<td>4.74(-3)</td>
<td>3.87(-3)</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>1.45(-3)</td>
<td>1.27(-3)</td>
<td></td>
<td>6.61(-4)</td>
<td>5.31(-4)</td>
<td></td>
</tr>
<tr>
<td>1.20</td>
<td>7.46(-3)</td>
<td>5.78(-3)</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>1.91(-3)</td>
<td>1.57(-3)</td>
<td></td>
<td>1.07(-3)</td>
<td>8.31(-4)</td>
<td></td>
</tr>
<tr>
<td>1.80</td>
<td>1.58(-2)</td>
<td>1.39(-2)</td>
<td>2.09(-3)</td>
<td>2.27(-1)</td>
<td></td>
<td>2.54(-3)</td>
<td>2.18(-3)</td>
<td></td>
<td>2.34(-3)</td>
<td>2.10(-3)</td>
<td></td>
</tr>
<tr>
<td>2.50</td>
<td>1.83(-2)</td>
<td>1.70(-2)</td>
<td>1.22(-2)</td>
<td>1.73(-1)</td>
<td></td>
<td>2.33(-3)</td>
<td>2.19(-3)</td>
<td></td>
<td>2.68(-3)</td>
<td>2.52(-3)</td>
<td></td>
</tr>
<tr>
<td>5.00</td>
<td>1.68(-2)</td>
<td>1.63(-2)</td>
<td>1.57(-2)</td>
<td>9.54(-2)</td>
<td></td>
<td>1.48(-3)</td>
<td>1.48(-3)</td>
<td></td>
<td>2.41(-3)</td>
<td>2.34(-3)</td>
<td></td>
</tr>
<tr>
<td>10.00</td>
<td>1.23(-2)</td>
<td>1.21(-2)</td>
<td>1.23(-2)</td>
<td>5.18(-2)</td>
<td></td>
<td>8.14(-4)</td>
<td>8.01(-4)</td>
<td></td>
<td>1.74(-3)</td>
<td>1.71(-3)</td>
<td></td>
</tr>
<tr>
<td>15.00</td>
<td>9.77(-3)</td>
<td>9.67(-3)</td>
<td>9.83(-3)</td>
<td>3.61(-2)</td>
<td></td>
<td>5.59(-4)</td>
<td>5.48(-4)</td>
<td></td>
<td>1.37(-3)</td>
<td>1.36(-3)</td>
<td></td>
</tr>
<tr>
<td>20.00</td>
<td>8.16(-3)</td>
<td>8.10(-3)</td>
<td>8.24(-3)</td>
<td>2.79(-2)</td>
<td></td>
<td>4.25(-4)</td>
<td>4.17(-4)</td>
<td></td>
<td>1.14(-3)</td>
<td>1.13(-3)</td>
<td></td>
</tr>
<tr>
<td>30.00</td>
<td>6.23(-3)</td>
<td>6.20(-3)</td>
<td>6.31(-3)</td>
<td>1.94(-2)</td>
<td></td>
<td>2.87(-4)</td>
<td>2.83(-4)</td>
<td></td>
<td>8.67(-4)</td>
<td>8.63(-4)</td>
<td></td>
</tr>
<tr>
<td>50.00</td>
<td>4.33(-3)</td>
<td>4.32(-3)</td>
<td>4.39(-3)</td>
<td>1.22(-2)</td>
<td></td>
<td>1.74(-4)</td>
<td>1.73(-4)</td>
<td></td>
<td>5.99(-4)</td>
<td>5.98(-4)</td>
<td></td>
</tr>
<tr>
<td>80.00</td>
<td>3.05(-3)</td>
<td>3.05(-3)</td>
<td>3.09(-3)</td>
<td>7.97(-3)</td>
<td></td>
<td>1.10(-4)</td>
<td>1.09(-4)</td>
<td></td>
<td>4.21(-4)</td>
<td>4.21(-4)</td>
<td></td>
</tr>
</tbody>
</table>

#### 2p - 3p

\[ \text{EPSIL} = 6.83(-1) \]

#### 3p - 4s

\[ \text{EPSIL} = 7.24(-1) \]
ARGON

<table>
<thead>
<tr>
<th>N</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>BETHE</th>
<th>MODBETHE</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>6.20(-3)</td>
<td>4.96(-3)</td>
<td>0.0</td>
<td>0.0</td>
<td>1.81(-3)</td>
<td>1.50(-3)</td>
<td>2.66(-3)</td>
<td>2.68(-3)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.10</td>
<td>1.07(-2)</td>
<td>8.46(-3)</td>
<td>0.0</td>
<td>0.0</td>
<td>2.79(-3)</td>
<td>2.24(-3)</td>
<td>3.42(-3)</td>
<td>3.47(-3)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.20</td>
<td>1.91(-2)</td>
<td>1.49(-2)</td>
<td>0.0</td>
<td>0.0</td>
<td>4.30(-3)</td>
<td>3.41(-3)</td>
<td>4.10(-3)</td>
<td>4.29(-3)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.80</td>
<td>4.85(-2)</td>
<td>4.37(-2)</td>
<td>0.0</td>
<td>3.08(-1)</td>
<td>7.60(-3)</td>
<td>7.60(-3)</td>
<td>3.91(-3)</td>
<td>3.96(-3)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.50</td>
<td>5.89(-2)</td>
<td>5.49(-2)</td>
<td>3.16(-2)</td>
<td>2.58(-1)</td>
<td>7.43(-3)</td>
<td>7.71(-3)</td>
<td>3.04(-3)</td>
<td>2.89(-3)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.00</td>
<td>5.69(-2)</td>
<td>5.50(-2)</td>
<td>5.22(-2)</td>
<td>1.62(-1)</td>
<td>4.90(-3)</td>
<td>4.79(-3)</td>
<td>1.59(-3)</td>
<td>1.42(-3)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.00</td>
<td>4.30(-2)</td>
<td>4.24(-2)</td>
<td>4.26(-2)</td>
<td>9.62(-2)</td>
<td>2.73(-3)</td>
<td>2.64(-3)</td>
<td>8.01(-4)</td>
<td>7.34(-4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15.00</td>
<td>3.45(-2)</td>
<td>3.42(-2)</td>
<td>3.47(-2)</td>
<td>7.00(-2)</td>
<td>1.89(-3)</td>
<td>1.83(-3)</td>
<td>5.35(-4)</td>
<td>5.01(-4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20.00</td>
<td>2.90(-2)</td>
<td>2.88(-2)</td>
<td>2.93(-2)</td>
<td>5.56(-2)</td>
<td>1.44(-3)</td>
<td>1.41(-3)</td>
<td>4.01(-4)</td>
<td>3.81(-4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30.00</td>
<td>2.23(-2)</td>
<td>2.22(-2)</td>
<td>2.26(-2)</td>
<td>4.00(-2)</td>
<td>9.75(-4)</td>
<td>9.59(-4)</td>
<td>2.67(-4)</td>
<td>2.58(-4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50.00</td>
<td>1.56(-2)</td>
<td>1.55(-2)</td>
<td>1.58(-2)</td>
<td>2.62(-2)</td>
<td>5.93(-4)</td>
<td>5.87(-4)</td>
<td>1.61(-4)</td>
<td>1.58(-4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>80.00</td>
<td>1.10(-2)</td>
<td>1.10(-2)</td>
<td>1.12(-2)</td>
<td>1.77(-2)</td>
<td>3.74(-4)</td>
<td>3.71(-4)</td>
<td>1.01(-4)</td>
<td>9.99(-5)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### KRYPTON

#### 4p - 5s

<table>
<thead>
<tr>
<th>( N )</th>
<th>BORN ( 10^{-2} )</th>
<th>OCHKUR ( 10^{-2} )</th>
<th>BETHE</th>
<th>MODBETHE</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>1.14</td>
<td>9.19</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>2.04</td>
<td>1.64</td>
<td></td>
<td>6.35</td>
<td>6.44</td>
<td></td>
</tr>
<tr>
<td>1.10</td>
<td>1.95</td>
<td>1.54</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>3.39</td>
<td>2.70</td>
<td></td>
<td>8.19</td>
<td>8.33</td>
<td></td>
</tr>
<tr>
<td>1.20</td>
<td>3.43</td>
<td>2.66</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>5.65</td>
<td>4.67</td>
<td></td>
<td>9.77</td>
<td>1.03</td>
<td></td>
</tr>
<tr>
<td>1.80</td>
<td>8.58</td>
<td>7.63</td>
<td>0.0</td>
<td>3.49</td>
<td>(-1)</td>
<td>1.10</td>
<td>1.16</td>
<td>(-2)</td>
<td>9.21</td>
<td>9.24</td>
<td>(-3)</td>
</tr>
<tr>
<td>2.50</td>
<td>1.04</td>
<td>9.57</td>
<td>5.66</td>
<td>3.15</td>
<td>(-1)</td>
<td>1.09</td>
<td>1.14</td>
<td>(-2)</td>
<td>7.10</td>
<td>6.61</td>
<td>(-3)</td>
</tr>
<tr>
<td>5.00</td>
<td>1.00</td>
<td>9.65</td>
<td>9.19</td>
<td>2.15</td>
<td>(-1)</td>
<td>7.22</td>
<td>6.96</td>
<td>(-3)</td>
<td>3.69</td>
<td>3.25</td>
<td>(-3)</td>
</tr>
<tr>
<td>10.00</td>
<td>7.55</td>
<td>7.43</td>
<td>7.49</td>
<td>1.34</td>
<td>(-1)</td>
<td>4.05</td>
<td>3.90</td>
<td>(-3)</td>
<td>1.86</td>
<td>1.70</td>
<td>(-3)</td>
</tr>
<tr>
<td>15.00</td>
<td>6.05</td>
<td>5.99</td>
<td>6.08</td>
<td>9.98</td>
<td>(-2)</td>
<td>2.80</td>
<td>2.72</td>
<td>(-3)</td>
<td>1.25</td>
<td>1.17</td>
<td>(-3)</td>
</tr>
<tr>
<td>20.00</td>
<td>5.08</td>
<td>5.05</td>
<td>5.13</td>
<td>8.02</td>
<td>(-2)</td>
<td>2.14</td>
<td>2.09</td>
<td>(-3)</td>
<td>9.48</td>
<td>9.02</td>
<td>(-3)</td>
</tr>
<tr>
<td>30.00</td>
<td>3.90</td>
<td>3.89</td>
<td>3.95</td>
<td>5.86</td>
<td>(-2)</td>
<td>1.45</td>
<td>1.43</td>
<td>(-3)</td>
<td>6.72</td>
<td>6.51</td>
<td>(-4)</td>
</tr>
<tr>
<td>50.00</td>
<td>2.73</td>
<td>2.72</td>
<td>2.77</td>
<td>3.90</td>
<td>(-2)</td>
<td>8.83</td>
<td>8.74</td>
<td>(-4)</td>
<td>3.77</td>
<td>3.69</td>
<td>(-4)</td>
</tr>
<tr>
<td>80.00</td>
<td>1.93</td>
<td>1.93</td>
<td>1.96</td>
<td>2.66</td>
<td>(-2)</td>
<td>5.57</td>
<td>5.53</td>
<td>(-4)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
</tr>
</tbody>
</table>

#### 4p - 5p

<table>
<thead>
<tr>
<th>( N )</th>
<th>BORN ( 10^{-1} )</th>
<th>OCHKUR ( 10^{-1} )</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>1.14</td>
<td>9.19</td>
<td></td>
<td>2.04</td>
<td>1.64</td>
<td></td>
<td>6.35</td>
<td>6.44</td>
<td></td>
<td>9.21</td>
<td>9.24</td>
<td></td>
</tr>
<tr>
<td>1.10</td>
<td>1.95</td>
<td>1.54</td>
<td></td>
<td>3.39</td>
<td>2.70</td>
<td></td>
<td>8.19</td>
<td>8.33</td>
<td></td>
<td>7.10</td>
<td>6.61</td>
<td></td>
</tr>
<tr>
<td>1.20</td>
<td>3.43</td>
<td>2.66</td>
<td></td>
<td>5.65</td>
<td>4.67</td>
<td></td>
<td>9.77</td>
<td>1.03</td>
<td></td>
<td>3.69</td>
<td>3.25</td>
<td></td>
</tr>
<tr>
<td>1.80</td>
<td>8.58</td>
<td>7.63</td>
<td></td>
<td>1.10</td>
<td>1.16</td>
<td>(-2)</td>
<td>9.21</td>
<td>9.24</td>
<td>(-3)</td>
<td>1.86</td>
<td>1.70</td>
<td>(-3)</td>
</tr>
<tr>
<td>2.50</td>
<td>1.04</td>
<td>9.57</td>
<td></td>
<td>1.09</td>
<td>1.14</td>
<td>(-2)</td>
<td>7.10</td>
<td>6.61</td>
<td>(-3)</td>
<td>1.25</td>
<td>1.17</td>
<td>(-3)</td>
</tr>
<tr>
<td>5.00</td>
<td>1.00</td>
<td>9.65</td>
<td></td>
<td>7.22</td>
<td>6.96</td>
<td>(-3)</td>
<td>3.69</td>
<td>3.25</td>
<td>(-3)</td>
<td>9.48</td>
<td>9.02</td>
<td>(-3)</td>
</tr>
<tr>
<td>10.00</td>
<td>7.55</td>
<td>7.43</td>
<td></td>
<td>4.05</td>
<td>3.90</td>
<td>(-3)</td>
<td>1.86</td>
<td>1.70</td>
<td>(-3)</td>
<td>6.72</td>
<td>6.51</td>
<td>(-4)</td>
</tr>
<tr>
<td>15.00</td>
<td>6.05</td>
<td>5.99</td>
<td></td>
<td>2.80</td>
<td>2.72</td>
<td>(-3)</td>
<td>1.25</td>
<td>1.17</td>
<td>(-3)</td>
<td>3.77</td>
<td>3.69</td>
<td>(-4)</td>
</tr>
<tr>
<td>20.00</td>
<td>5.08</td>
<td>5.05</td>
<td></td>
<td>2.14</td>
<td>2.09</td>
<td>(-3)</td>
<td>9.48</td>
<td>9.02</td>
<td>(-3)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
</tr>
<tr>
<td>30.00</td>
<td>3.90</td>
<td>3.89</td>
<td></td>
<td>1.45</td>
<td>1.43</td>
<td>(-3)</td>
<td>6.72</td>
<td>6.51</td>
<td>(-4)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
</tr>
<tr>
<td>50.00</td>
<td>2.73</td>
<td>2.72</td>
<td></td>
<td>8.83</td>
<td>8.74</td>
<td>(-4)</td>
<td>3.77</td>
<td>3.69</td>
<td>(-4)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
</tr>
<tr>
<td>80.00</td>
<td>1.93</td>
<td>1.93</td>
<td></td>
<td>5.57</td>
<td>5.53</td>
<td>(-4)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
</tr>
</tbody>
</table>

#### 4p - 4d

<table>
<thead>
<tr>
<th>( N )</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>1.14</td>
<td>9.19</td>
<td></td>
<td>2.04</td>
<td>1.64</td>
<td></td>
<td>6.35</td>
<td>6.44</td>
<td></td>
<td>9.21</td>
<td>9.24</td>
<td></td>
</tr>
<tr>
<td>1.10</td>
<td>1.95</td>
<td>1.54</td>
<td></td>
<td>3.39</td>
<td>2.70</td>
<td></td>
<td>8.19</td>
<td>8.33</td>
<td></td>
<td>7.10</td>
<td>6.61</td>
<td></td>
</tr>
<tr>
<td>1.20</td>
<td>3.43</td>
<td>2.66</td>
<td></td>
<td>5.65</td>
<td>4.67</td>
<td></td>
<td>9.77</td>
<td>1.03</td>
<td></td>
<td>3.69</td>
<td>3.25</td>
<td></td>
</tr>
<tr>
<td>1.80</td>
<td>8.58</td>
<td>7.63</td>
<td></td>
<td>1.10</td>
<td>1.16</td>
<td>(-2)</td>
<td>9.21</td>
<td>9.24</td>
<td>(-3)</td>
<td>1.86</td>
<td>1.70</td>
<td>(-3)</td>
</tr>
<tr>
<td>2.50</td>
<td>1.04</td>
<td>9.57</td>
<td></td>
<td>1.09</td>
<td>1.14</td>
<td>(-2)</td>
<td>7.10</td>
<td>6.61</td>
<td>(-3)</td>
<td>1.25</td>
<td>1.17</td>
<td>(-3)</td>
</tr>
<tr>
<td>5.00</td>
<td>1.00</td>
<td>9.65</td>
<td></td>
<td>7.22</td>
<td>6.96</td>
<td>(-3)</td>
<td>3.69</td>
<td>3.25</td>
<td>(-3)</td>
<td>9.48</td>
<td>9.02</td>
<td>(-3)</td>
</tr>
<tr>
<td>10.00</td>
<td>7.55</td>
<td>7.43</td>
<td></td>
<td>4.05</td>
<td>3.90</td>
<td>(-3)</td>
<td>1.86</td>
<td>1.70</td>
<td>(-3)</td>
<td>6.72</td>
<td>6.51</td>
<td>(-4)</td>
</tr>
<tr>
<td>15.00</td>
<td>6.05</td>
<td>5.99</td>
<td></td>
<td>2.80</td>
<td>2.72</td>
<td>(-3)</td>
<td>1.25</td>
<td>1.17</td>
<td>(-3)</td>
<td>3.77</td>
<td>3.69</td>
<td>(-4)</td>
</tr>
<tr>
<td>20.00</td>
<td>5.08</td>
<td>5.05</td>
<td></td>
<td>2.14</td>
<td>2.09</td>
<td>(-3)</td>
<td>9.48</td>
<td>9.02</td>
<td>(-3)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
</tr>
<tr>
<td>30.00</td>
<td>3.90</td>
<td>3.89</td>
<td></td>
<td>1.45</td>
<td>1.43</td>
<td>(-3)</td>
<td>6.72</td>
<td>6.51</td>
<td>(-4)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
</tr>
<tr>
<td>50.00</td>
<td>2.73</td>
<td>2.72</td>
<td></td>
<td>8.83</td>
<td>8.74</td>
<td>(-4)</td>
<td>3.77</td>
<td>3.69</td>
<td>(-4)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
</tr>
<tr>
<td>80.00</td>
<td>1.93</td>
<td>1.93</td>
<td></td>
<td>5.57</td>
<td>5.53</td>
<td>(-4)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
<td>1.47</td>
<td>1.46</td>
<td>(-3)</td>
</tr>
</tbody>
</table>

\( \text{EPSIL} = 3.66(-1) \)

\( \text{EPSIL} = 4.22(-1) \)

\( \text{EPSIL} = 4.48(-1) \)
### XENON

#### 5p - 6s

<table>
<thead>
<tr>
<th>N</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>BETHE</th>
<th>MODBETHE</th>
<th>LIT</th>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>1.26(-2)</td>
<td>9.86(-3)</td>
<td>0.0</td>
<td>0.0</td>
<td>2.30(-3)</td>
<td>1.82(-3)</td>
<td>2.36(-2)</td>
<td>2.42(-2)</td>
</tr>
<tr>
<td>1.10</td>
<td>2.34(-2)</td>
<td>1.84(-2)</td>
<td>0.0</td>
<td>0.0</td>
<td>4.31(-2)</td>
<td>3.52(-3)</td>
<td>3.03(-2)</td>
<td>3.14(-2)</td>
</tr>
<tr>
<td>1.20</td>
<td>4.42(-2)</td>
<td>3.50(-2)</td>
<td>0.0</td>
<td>0.0</td>
<td>7.94(-3)</td>
<td>7.13(-3)</td>
<td>3.61(-2)</td>
<td>3.93(-2)</td>
</tr>
<tr>
<td>1.80</td>
<td>1.21(-1)</td>
<td>1.09(-1)</td>
<td>0.0</td>
<td>3.85(-1)</td>
<td>1.68(-2)</td>
<td>1.85(-2)</td>
<td>3.35(-2)</td>
<td>3.50(-2)</td>
</tr>
<tr>
<td>2.50</td>
<td>1.50(-1)</td>
<td>1.38(-1)</td>
<td>7.19(-2)</td>
<td>3.76(-1)</td>
<td>1.68(-2)</td>
<td>1.74(-2)</td>
<td>2.56(-2)</td>
<td>2.42(-2)</td>
</tr>
<tr>
<td>5.00</td>
<td>1.48(-1)</td>
<td>1.43(-1)</td>
<td>1.34(-1)</td>
<td>2.77(-1)</td>
<td>1.13(-2)</td>
<td>1.07(-2)</td>
<td>1.32(-2)</td>
<td>1.15(-2)</td>
</tr>
<tr>
<td>10.00</td>
<td>1.13(-1)</td>
<td>1.11(-1)</td>
<td>1.12(-1)</td>
<td>1.80(-1)</td>
<td>6.35(-3)</td>
<td>6.11(-3)</td>
<td>6.74(-3)</td>
<td>6.12(-3)</td>
</tr>
<tr>
<td>15.00</td>
<td>9.09(-2)</td>
<td>9.01(-2)</td>
<td>9.13(-2)</td>
<td>1.36(-1)</td>
<td>4.40(-3)</td>
<td>4.27(-3)</td>
<td>4.63(-3)</td>
<td>4.33(-3)</td>
</tr>
<tr>
<td>20.00</td>
<td>7.66(-2)</td>
<td>7.61(-2)</td>
<td>7.73(-2)</td>
<td>1.10(-1)</td>
<td>3.36(-3)</td>
<td>3.29(-3)</td>
<td>3.80(-3)</td>
<td>3.62(-3)</td>
</tr>
<tr>
<td>30.00</td>
<td>5.90(-2)</td>
<td>5.88(-2)</td>
<td>5.98(-2)</td>
<td>8.13(-2)</td>
<td>2.28(-3)</td>
<td>2.25(-3)</td>
<td>3.22(-3)</td>
<td>3.14(-3)</td>
</tr>
<tr>
<td>50.00</td>
<td>4.14(-2)</td>
<td>4.13(-2)</td>
<td>4.20(-2)</td>
<td>5.48(-2)</td>
<td>1.39(-3)</td>
<td>1.38(-3)</td>
<td>1.18(-3)</td>
<td>1.15(-3)</td>
</tr>
<tr>
<td>80.00</td>
<td>2.94(-2)</td>
<td>2.93(-2)</td>
<td>2.98(-2)</td>
<td>3.77(-2)</td>
<td>8.77(-4)</td>
<td>8.72(-4)</td>
<td>3.92(-3)</td>
<td>3.91(-3)</td>
</tr>
</tbody>
</table>

#### 5p - 6p

<p>| EPSIL = 3.06(-1) |</p>
<table>
<thead>
<tr>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.30(-3)</td>
<td>1.82(-3)</td>
<td></td>
</tr>
<tr>
<td>4.31(-2)</td>
<td>3.52(-3)</td>
<td></td>
</tr>
<tr>
<td>7.94(-3)</td>
<td>7.13(-3)</td>
<td></td>
</tr>
<tr>
<td>1.68(-2)</td>
<td>1.85(-2)</td>
<td></td>
</tr>
<tr>
<td>1.13(-2)</td>
<td>1.07(-2)</td>
<td></td>
</tr>
<tr>
<td>6.35(-3)</td>
<td>6.11(-3)</td>
<td></td>
</tr>
<tr>
<td>4.40(-3)</td>
<td>4.27(-3)</td>
<td></td>
</tr>
<tr>
<td>3.36(-3)</td>
<td>3.29(-3)</td>
<td></td>
</tr>
<tr>
<td>2.28(-3)</td>
<td>2.25(-3)</td>
<td></td>
</tr>
<tr>
<td>1.39(-3)</td>
<td>1.38(-3)</td>
<td></td>
</tr>
<tr>
<td>8.77(-4)</td>
<td>8.72(-4)</td>
<td></td>
</tr>
</tbody>
</table>

#### 5p - 5d

<p>| EPSIL = 3.70(-1) |</p>
<table>
<thead>
<tr>
<th>BORN</th>
<th>OCHKUR</th>
<th>LIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.36(-2)</td>
<td>2.42(-2)</td>
<td></td>
</tr>
<tr>
<td>3.03(-2)</td>
<td>3.14(-2)</td>
<td></td>
</tr>
<tr>
<td>3.61(-2)</td>
<td>3.93(-2)</td>
<td></td>
</tr>
<tr>
<td>3.35(-2)</td>
<td>3.50(-2)</td>
<td></td>
</tr>
<tr>
<td>2.56(-2)</td>
<td>2.42(-2)</td>
<td></td>
</tr>
<tr>
<td>1.32(-2)</td>
<td>1.15(-2)</td>
<td></td>
</tr>
<tr>
<td>6.74(-3)</td>
<td>6.12(-3)</td>
<td></td>
</tr>
<tr>
<td>4.63(-3)</td>
<td>4.33(-3)</td>
<td></td>
</tr>
<tr>
<td>3.80(-3)</td>
<td>3.62(-3)</td>
<td></td>
</tr>
<tr>
<td>3.22(-3)</td>
<td>3.14(-3)</td>
<td></td>
</tr>
<tr>
<td>1.18(-3)</td>
<td>1.15(-3)</td>
<td></td>
</tr>
<tr>
<td>3.92(-3)</td>
<td>3.91(-3)</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>BORN</td>
<td>OCHKUR</td>
</tr>
<tr>
<td>-----</td>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>1.05</td>
<td>2.56(-2)</td>
<td>2.04(-2)</td>
</tr>
<tr>
<td>1.10</td>
<td>4.42(-2)</td>
<td>3.48(-2)</td>
</tr>
<tr>
<td>1.20</td>
<td>7.83(-2)</td>
<td>6.11(-2)</td>
</tr>
<tr>
<td>1.80</td>
<td>1.96(-1)</td>
<td>1.75(-1)</td>
</tr>
<tr>
<td>2.50</td>
<td>2.35(-1)</td>
<td>2.17(-1)</td>
</tr>
<tr>
<td>5.00</td>
<td>2.25(-1)</td>
<td>2.17(-1)</td>
</tr>
<tr>
<td>10.00</td>
<td>1.69(-1)</td>
<td>1.67(-1)</td>
</tr>
<tr>
<td>15.00</td>
<td>1.35(-1)</td>
<td>1.34(-1)</td>
</tr>
<tr>
<td>20.00</td>
<td>1.14(-1)</td>
<td>1.13(-1)</td>
</tr>
<tr>
<td>30.00</td>
<td>8.72(-2)</td>
<td>8.69(-2)</td>
</tr>
<tr>
<td>50.00</td>
<td>6.09(-2)</td>
<td>6.08(-2)</td>
</tr>
<tr>
<td>80.00</td>
<td>4.31(-2)</td>
<td>4.31(-2)</td>
</tr>
</tbody>
</table>
2) Discussion

A comparison of the Born calculations for the Alkalisc of Vainshtein with the results of the present work reveals agreement in all cases between the two calculations is within 5%.

As expected the incorporation of the exchange effect (by use of the Ochkur approximation) lowers the value of the cross-section. This is shown for a larger number of cases then previously considered with the Ochkur approximation. Furthermore, as expected, agreement between the Ochkur and Born calculations for large values of incident energy is confirmed.

Likewise, the Modified Bethe calculations decrease the peak value of the cross-section as expected.

Although the agreement between the Born and Bethe calculations in the high energy region is to be expected, since this agreement is forced by use of the Bethe cut-off, the 20% agreement in the upper energy region of the peak value (approximately 4 threshold units) confirms that Bethe approximations can be of significant use when calculations must be "quick". (The Bethe calculation is about 10 times faster than the Born calculation.)

For the Alkali tables two serious disagreements with the Vainshtein data were found. For the Li(2s-3s) case the Vainshtein values (as reprinted in Moiseiwitsch (1968)) for the last three energy values are too large by a factor of 10. This appears to be a typographical error since these values would give a "second" peak to the cross-section at 11 threshold energy units. Furthermore, division by 10 brings the Vainshtein values into agreement.
with the present Born calculation.

The second discrepancy is of a more serious nature. For the Potassium (4s-4d), (4s-5d), (4s-6d), the Vainshtein data is in serious disagreement with the present calculation. The difference of a factor of two between the Vainshtein Born calculation and my Ochkur calculation led me to perform a Born calculation for the 4s-4d case. The results of this calculation are:

<table>
<thead>
<tr>
<th>E</th>
<th>1.02</th>
<th>1.08</th>
<th>1.64</th>
<th>2.28</th>
</tr>
</thead>
<tbody>
<tr>
<td>Born(1)</td>
<td>1.36(0)</td>
<td>2.39(0)</td>
<td>3.11(0)</td>
<td>2.23(0)</td>
</tr>
<tr>
<td>Born(2)</td>
<td>5.77(-1)</td>
<td>1.00(0)</td>
<td>1.11(0)</td>
<td>8.31(-1)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>E</th>
<th>6.12</th>
<th>11.24</th>
<th>21.48</th>
<th>41.96</th>
</tr>
</thead>
<tbody>
<tr>
<td>Born(1)</td>
<td>8.86(-1)</td>
<td>4.88(-1)</td>
<td>2.57(-1)</td>
<td>1.32(-1)</td>
</tr>
<tr>
<td>Born(2)</td>
<td>3.28(-1)</td>
<td>1.83(-1)</td>
<td>9.70(-2)</td>
<td>5.11(-2)</td>
</tr>
</tbody>
</table>

This disagreement is peculiar because agreement between the present calculation and other series of the form ns-(n-1)d, ns-nd, ns-(n+1)d exists. Since other data for this transition was not found, a definitive resolution of the discrepancy does not seem possible. Further, the wave functions used by Vainshtein are not readily available. They are to be found in Vainshtein (1957) which is a journal reference before the A.P.S. began reprinting Russian articles. However, the Sodium paper Vainshtein L. A. (1965) Opt. Spectry. USSR 18, 538 indicates that the wave functions used were found using the "semi-empirical method taking
account of exchange" as discussed in the 1957 reference. The statement of semi-empirical wave functions suggests that perhaps the data Vainshtein used for the K(4d) (5d) (6d) wave functions was erroneous; hence the present work may be more accurate, since the wave functions used are straight-forward solutions of the HFS-equation.

Returning to the tables, the amount of Inert-gas data available from the literature for comparison with the present work was disappointingly small. The goal was to clearly establish the boundaries of accuracy for the present work by the criteria of comparison with the literature for the two extreme cases of the "inert-core active electron assumption". Although an exhaustive comparison of the Inert-gas study with the literature was not possible, the few cases of comparison with the literature do show reasonable agreement.

Therefore, the credibility of this calculation is firmly established by the detailed comparison with the literature for the Alkali study and the few cases available for the Inert study.

The conclusion is that order of magnitude validity for all cases of electron impact excitation of atoms can be expected from this calculation. The results will tend to be in better agreement with experiment for Alkali-like elements, and for elements of small charge. That is, since our assumptions for the cross-section expressions assume Hydrogen-like behavior for all elements, elements more Hydrogen like will give better results.
VII. SAMPLE RESULTS FOR IONIZATION

In this chapter some results of the ionization calculations will be presented. As indicated in earlier discussion the ionization cross-sections are computed by calculating the first six partial-wave cross-sections and adding them together to obtain the total C-section. The tables, and the normal output of the program IONCST, include the partial C-sections and the total C-section for the given incident energy. The limitations of this calculation will be illustrated by some of the results and this limitation examined in the discussion that follows the tables.

1) Tables

As in earlier tables, the energy range N is given in threshold units; the transition energy $\varepsilon$ is in units of twice the Rydberg; and the cross-sections (partial and total) are measured in units of $\pi a_B^2$. 

Ionization Cross-Section Tables

<table>
<thead>
<tr>
<th>Element</th>
<th>Transition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>(1s $\rightarrow$ Continuum)</td>
</tr>
<tr>
<td>Helium</td>
<td>(1s $\rightarrow$ Continuum)</td>
</tr>
<tr>
<td>Lithium</td>
<td>(2s $\rightarrow$ Continuum)</td>
</tr>
<tr>
<td>Sodium</td>
<td>(3s $\rightarrow$ Continuum)</td>
</tr>
<tr>
<td>Potassium</td>
<td>(4s $\rightarrow$ Continuum)</td>
</tr>
<tr>
<td>Rubidium</td>
<td>(5s $\rightarrow$ Continuum)</td>
</tr>
<tr>
<td>Cesium</td>
<td>(6s $\rightarrow$ Continuum)</td>
</tr>
</tbody>
</table>

The literature (Lit) data are referenced as follows:


The data given from these sources is graphically interpolated.
HYDROGEN (1s - ION)

\[ \text{EPSIL} = .500 \]

<table>
<thead>
<tr>
<th>ENERGY</th>
<th>LOG ( N = .301 )</th>
<th>LOG ( N = .398 )</th>
<th>LOG ( N = .439 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Q_e )</td>
<td>(This Paper)</td>
<td>Lit. (This Paper)</td>
<td>Lit. (This Paper)</td>
</tr>
<tr>
<td>( Q_0 )</td>
<td>.118(0)</td>
<td>.10(0)</td>
<td>.119(0)</td>
</tr>
<tr>
<td>( Q_1 )</td>
<td>.554(0)</td>
<td>.57(0)</td>
<td>.642(0)</td>
</tr>
<tr>
<td>( Q_2 )</td>
<td>.154(0)</td>
<td>.12(0)</td>
<td>.191(0)</td>
</tr>
<tr>
<td>( Q_3 )</td>
<td>.222(-1)</td>
<td>.01(0)</td>
<td>.327(-1)</td>
</tr>
<tr>
<td>( Q_4 )</td>
<td>.278(-2)</td>
<td>--</td>
<td>.520(-2)</td>
</tr>
<tr>
<td>( Q_5 )</td>
<td>.341(-3)</td>
<td>--</td>
<td>.838(-3)</td>
</tr>
<tr>
<td>( Q_t )</td>
<td>.851(0)</td>
<td>.80(0)</td>
<td>.991(0)</td>
</tr>
</tbody>
</table>
HELIUM (1s - ION)
EPSIL = .860

<table>
<thead>
<tr>
<th>ENERGY</th>
<th>LOG N = .0969</th>
<th>LOG N = .176</th>
<th>LOG N = .243</th>
</tr>
</thead>
<tbody>
<tr>
<td>Qe</td>
<td>(This Paper)</td>
<td>Lit(1)</td>
<td>(This Paper)</td>
</tr>
<tr>
<td>Q0</td>
<td>.774(-2)</td>
<td>.1(-2)</td>
<td>.159(-1)</td>
</tr>
<tr>
<td>Q1</td>
<td>.391(-1)</td>
<td>.3(-1)</td>
<td>.868(-1)</td>
</tr>
<tr>
<td>Q2</td>
<td>.410(-2)</td>
<td>.1(-1)</td>
<td>.109(-1)</td>
</tr>
<tr>
<td>Q3</td>
<td>.215(-3)</td>
<td>.1(-2)</td>
<td>.817(-3)</td>
</tr>
<tr>
<td>Q4</td>
<td>.883(-5)</td>
<td>--</td>
<td>.548(-4)</td>
</tr>
<tr>
<td>Q5</td>
<td>.336(-6)</td>
<td>--</td>
<td>.362(-5)</td>
</tr>
<tr>
<td>Qt</td>
<td>.512(-1)</td>
<td>.6(-1)</td>
<td>.115(0)</td>
</tr>
<tr>
<td>*Q</td>
<td>(experiment)</td>
<td>.7(-1)</td>
<td>.17(0)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ENERGY</th>
<th>LOG N = 0.301</th>
<th>LOG N = 0.398</th>
<th>LOG N = 0.439</th>
</tr>
</thead>
<tbody>
<tr>
<td>Qe</td>
<td>(This Paper)</td>
<td>(This Paper)</td>
<td>(This Paper)</td>
</tr>
<tr>
<td>Q0</td>
<td>0.262(-1)</td>
<td>0.336(-1)</td>
<td>0.178(0)</td>
</tr>
<tr>
<td>Q1</td>
<td>0.157(0)</td>
<td>0.194(0)</td>
<td>0.205(0)</td>
</tr>
<tr>
<td>Q2</td>
<td>0.239(-1)</td>
<td>0.327(-1)</td>
<td>0.360(-1)</td>
</tr>
<tr>
<td>Q3</td>
<td>0.262(-2)</td>
<td>0.445(-2)</td>
<td>0.526(-2)</td>
</tr>
<tr>
<td>Q4</td>
<td>0.286(-3)</td>
<td>0.625(-3)</td>
<td>0.816(-3)</td>
</tr>
<tr>
<td>Q5</td>
<td>0.318(-4)</td>
<td>0.918(-4)</td>
<td>0.139(-3)</td>
</tr>
<tr>
<td>Qt</td>
<td>0.210(0)</td>
<td>0.266(0)</td>
<td>0.426(0)</td>
</tr>
<tr>
<td>*Q</td>
<td>0.28(0)</td>
<td>0.32(0)</td>
<td>0.36(0)</td>
</tr>
</tbody>
</table>

* Loc. Cit.
LITHIUM

\[ \text{EPSIL} = \]

<table>
<thead>
<tr>
<th>ENERGY</th>
<th>( N = 2.00 )</th>
<th>( N = 2.50 )</th>
<th>( N = 2.75 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \log N = .301 )</td>
<td>( \log N = .398 )</td>
<td>( \log N = .439 )</td>
</tr>
<tr>
<td>( Q_e )</td>
<td>(This Paper)</td>
<td>Lit(1)</td>
<td>(This Paper)</td>
</tr>
<tr>
<td>( Q_0 )</td>
<td>( .250(0) )</td>
<td>( .1(0) )</td>
<td>( .447(0) )</td>
</tr>
<tr>
<td>( Q_1 )</td>
<td>( .822(0) )</td>
<td>( .6(0) )</td>
<td>( .779(0) )</td>
</tr>
<tr>
<td>( Q_2 )</td>
<td>( .226(1) )</td>
<td>( .18(1) )</td>
<td>( .234(1) )</td>
</tr>
<tr>
<td>( Q_3 )</td>
<td>( .913(0) )</td>
<td>( .7(0) )</td>
<td>( .105(1) )</td>
</tr>
<tr>
<td>( Q_4 )</td>
<td>( .196(0) )</td>
<td>( .15(0) )</td>
<td>( .268(0) )</td>
</tr>
<tr>
<td>( Q_5 )</td>
<td>( .334(-1) )</td>
<td>( .5(-1) )</td>
<td>( .576(-1) )</td>
</tr>
<tr>
<td>( Q_t )</td>
<td>( .447(1) )</td>
<td>( .34(1) )</td>
<td>( .494(1) )</td>
</tr>
</tbody>
</table>
### SODIUM

**EPSIL =**

<table>
<thead>
<tr>
<th>ENERGY</th>
<th>LOG N = 2.00</th>
<th>LOG N = 2.50</th>
<th>LOG N = 2.75</th>
</tr>
</thead>
<tbody>
<tr>
<td>Qe</td>
<td>(This Paper)</td>
<td>Lit(2)</td>
<td>(This Paper)</td>
</tr>
<tr>
<td></td>
<td>.415(0)</td>
<td>.5(0)</td>
<td>.543(1)</td>
</tr>
<tr>
<td>Qo</td>
<td>.690(0)</td>
<td>.4(0)</td>
<td>.105(1)</td>
</tr>
<tr>
<td>Q1</td>
<td>.255(1)</td>
<td>.25(1)</td>
<td>.285(1)</td>
</tr>
<tr>
<td>Q2</td>
<td>.117(1)</td>
<td>.11(1)</td>
<td>.146(1)</td>
</tr>
<tr>
<td>Q3</td>
<td>.270(0)</td>
<td>.2(0)</td>
<td>.381(0)</td>
</tr>
<tr>
<td>Q4</td>
<td>.478(-1)</td>
<td>.3(-1)</td>
<td>.822(-1)</td>
</tr>
<tr>
<td>Qt</td>
<td>.514(1)</td>
<td>.05(1)</td>
<td>.113(2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ENERGY</th>
<th>LOG N = 3.01</th>
<th>LOG N = 3.98</th>
<th>LOG N = 4.39</th>
</tr>
</thead>
<tbody>
<tr>
<td>Qo</td>
<td>.319(4)</td>
<td>.5(0)</td>
<td></td>
</tr>
<tr>
<td>Q1</td>
<td>.420(2)</td>
<td>.55(0)</td>
<td></td>
</tr>
<tr>
<td>Q2</td>
<td>.188(2)</td>
<td>.23(1)</td>
<td></td>
</tr>
<tr>
<td>Q3</td>
<td>.788(1)</td>
<td>.12(1)</td>
<td></td>
</tr>
<tr>
<td>Q4</td>
<td>.861(0)</td>
<td>.3(0)</td>
<td></td>
</tr>
<tr>
<td>Q5</td>
<td>.132(0)</td>
<td>.4(-1)</td>
<td></td>
</tr>
<tr>
<td>Qt</td>
<td>.326(4)</td>
<td>.50(1)</td>
<td></td>
</tr>
</tbody>
</table>
POTASSIUM (4s - ION)

\[ \text{EPSIL} = 0.309 \]

<table>
<thead>
<tr>
<th>ENERGY</th>
<th>( N = 2.00 )</th>
<th>( N = 2.50 )</th>
<th>( N = 2.75 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Q_e )</td>
<td>(This Paper)</td>
<td>(This Paper)</td>
<td>(This Paper)</td>
</tr>
<tr>
<td>( Q_0 )</td>
<td>0.113(1)</td>
<td>0.123(1)</td>
<td>0.155(1)</td>
</tr>
<tr>
<td>( Q_1 )</td>
<td>0.704(0)</td>
<td>0.983(0)</td>
<td>0.136(1)</td>
</tr>
<tr>
<td>( Q_2 )</td>
<td>0.322(1)</td>
<td>0.312(1)</td>
<td>0.317(1)</td>
</tr>
<tr>
<td>( Q_3 )</td>
<td>0.235(1)</td>
<td>0.252(1)</td>
<td>0.253(1)</td>
</tr>
<tr>
<td>( Q_4 )</td>
<td>0.687(0)</td>
<td>0.852(0)</td>
<td>0.897(0)</td>
</tr>
<tr>
<td>( Q_5 )</td>
<td>0.140(0)</td>
<td>0.214(0)</td>
<td>0.243(0)</td>
</tr>
<tr>
<td>( Q_t )</td>
<td>0.823(1)</td>
<td>0.892(1)</td>
<td>0.975(1)</td>
</tr>
</tbody>
</table>
RUBIDIUM (5s - ION)

$$\epsilon = 0.291$$

$N = 2.00 \quad N = 2.50$

<table>
<thead>
<tr>
<th>ENERGY</th>
<th>LOG $N = 0.301$</th>
<th>LOG $N = 0.398$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_e$</td>
<td>(This Paper)</td>
<td>(This Paper)</td>
</tr>
<tr>
<td>$Q_0$</td>
<td>0.136(1)</td>
<td>0.893(4)</td>
</tr>
<tr>
<td>$Q_1$</td>
<td>0.100(1)</td>
<td>0.466(1)</td>
</tr>
<tr>
<td>$Q_2$</td>
<td>0.328(1)</td>
<td>0.230(2)</td>
</tr>
<tr>
<td>$Q_3$</td>
<td>0.283(1)</td>
<td>0.447(2)</td>
</tr>
<tr>
<td>$Q_4$</td>
<td>0.902(0)</td>
<td>0.156(2)</td>
</tr>
<tr>
<td>$Q_5$</td>
<td>0.193(0)</td>
<td>0.881(1)</td>
</tr>
<tr>
<td>$Q_t$</td>
<td>0.957(1)</td>
<td>0.903(4)</td>
</tr>
<tr>
<td>ENERGY</td>
<td>LOG $N = 0.301$</td>
<td>(This Paper)</td>
</tr>
<tr>
<td>--------</td>
<td>----------------</td>
<td>--------------</td>
</tr>
<tr>
<td>$Q_0$</td>
<td>0.127(1)</td>
<td></td>
</tr>
<tr>
<td>$Q_1$</td>
<td>0.203(1)</td>
<td></td>
</tr>
<tr>
<td>$Q_2$</td>
<td>0.315(1)</td>
<td></td>
</tr>
<tr>
<td>$Q_3$</td>
<td>0.380(1)</td>
<td></td>
</tr>
<tr>
<td>$Q_4$</td>
<td>0.142(1)</td>
<td></td>
</tr>
<tr>
<td>$Q_5$</td>
<td>0.333(0)</td>
<td></td>
</tr>
<tr>
<td>$Q_t$</td>
<td>0.120(1)</td>
<td></td>
</tr>
</tbody>
</table>
2) Discussion

From earlier discussion recall the following:

The Born-Coulomb approximation used in this calculation uses the coulomb wave final state wave function.

In this calculation the coulomb wave-function is obtained by use of a series that was limited to 30 terms.

As indicated by the tables, the calculation is valid for a certain range of parameters. Beyond the range of parameters the partial cross-sections, and hence the total cross-sections, are invalid. The reason for the limitation to a range of parameters is the computational difficulty in obtaining coulomb wave functions for a wide range of the variables \( k_F, l_F, r \). A review of these computational difficulties was given by Froberg (1955) in Rev. of Mod. Physics 27, 399. He suggested that numerical tables should be generated for an intermediate range of variables. This suggestion led to the tables of coulomb wave functions published by N.B.S. in Abramowitz (1964). This is mentioned to emphasize the difficulties associated with coulomb wave function calculations over large ranges of the variables.

This computational problem is isolated by the use of the subroutine FLNR and satisfactory values of the wave functions are produced for, small values of the arguments \( l_F, r, k_F \). The validity of the calculation in this "small value" range is established by comparison with the literature. The computational problem of the coulomb wave function can be overcome by use of different series expansions to obtain values in other regions of the function.
variables. When the subroutine FLNR is modified in this manner, the program will compute ionization cross-sections in a "general" manner.

Let us examine the nature of the "breakdown" of the calculation. The first "spurious" partial cross-section is for lithium Qo (2.75). For this energy (2.75), the higher partial cross-sections appear to be valid.

The next dramatic change is the sodium Qo (2.50) partial cross-section. All cross-section beyond this appear in error.

As will be indicated further, this problem should be overcome in future research.
VIII. CONCLUSIONS AND FUTURE RESEARCH

The intent of the present research was to provide inexact but reasonable excitation cross-section values for all elements. This has been achieved. The usefulness of these calculations should be to provide order of magnitude cross-sections for all cases to astrophysicists who, in some cases, have been forced to use $\pi a_B^2$ (which can be within four orders of magnitude of the actual cross-sections). By selecting the Alkali (best case) and Inert elements (worst case) as examples of the data available from the calculation, it has been shown that the expected range of validity for other cases using this program is an order of magnitude accuracy.

As mentioned in the introduction precise statements as to the accuracy of the cross-section values are difficult since no "bench mark" seems to exist. However, we would expect that the cross-sections here are quite good (within 10%) in the Born tail (threshold energies greater than 30) and could be used by experimentalists for normalization of their relative data.

For this reason, the possibility of publishing standard high energy cross-section tables for the first several transitions for elements below $Z = 50$ will be pursued.

Furthermore, the use of this technique to compute electron-excitation cross-sections for ions will be investigated. It is clear that since these calculations will involve use of coulomb wave functions for the scattering electron, the problem encountered in the ionization calculation of this research will have to be overcome.
The solution of that problem appears, at this stage, to be the use of an integral expression for the coulomb wave function. This will result in a six-fold integration for the final cross-section and such a numerical calculation would be pursued using Monte-Carlo integration techniques.

The calculation of these cross-sections would be motivated by the active interest of the astrophysicists in investigating the same phenomena (nebulae, aurorae, and solar corona, see Page 1) that motivated the present work. Furthermore, these cross-sections are of interest to people doing stellar modeling. (See Athay (1972).)

Since a set of atomic wave functions for a general calculation is readily available, general calculation of other atomic parameters (e.g. oscillator strengths, transition probabilities) may be attempted, and this may prove useful to the "beam-foil" group at The University of Toledo.
REFERENCES

17. Gottfried, K., 1966, Quantum Mechanics, W. A. Benjamin, Inc., N. Y.
42. Piper, W. W., 1956, Transactions AIEE (I), 75, 152.
46. Roothan, C. C., 1960, Rev. of Mod. Phys. 32, 179.
48. Schiff, L. I., 1968, Quantum Mechanics, McGraw-Hill Book Co., N. Y.
52. Slater, J. C., 1951, Phys. Rev. 81, 385.
   Consistent Fields with Exchange".
55. Stevenson, R., 1965, Multiplet Structure of Atoms and Molecules,
   W. B. Saunders Co., Philadelphia.
   Ltd., Pub. #3200.
APPENDIX I

Notation

$Q = \text{cross-section}$

$\vec{r}_i = \text{position vector of } i\text{th electron}$

$A = \text{set of quantum numbers for total atom}$

$a = \text{set of quantum numbers for a particular orbital}$

$\Phi_A(\vec{r}_L, \vec{r}_L) = \text{total wave function (including spin) for atom with}$

$\text{electrons in a state } A$

$\Psi_A(\vec{r}_L, \vec{r}_L) = \text{total wave function (neglecting spin) for atom with}$

$\text{electrons in a state } A$

$\mathcal{G}_a(\vec{r}_i) = \text{single orbital wave function (including spin) for atom}$

$\text{with } i\text{th electron in an orbital state}$

$\mathcal{G}_a(\vec{r}_i) = \text{single orbital wave function (neglecting spin) for}$

$\text{atom with } i\text{th electron in an orbital state}$

$\vec{r}_o = \text{this is reserved for the incident electron position}$

$\text{vector in the scattering problem}$

$\vec{r}_e = \text{this is reserved for the emitted electron (secondary}$

$\text{electron) position vector in the ionization problem}$

$\varepsilon_{ijk} = \text{Levi-Chivita symbol (see Landau (1957))}$

$\delta_{ij} = \text{Kroneker -delta (see Landau (1957))}$
APPENDIX II

Atomic Units

There are two sets of atomic units in common use. They are simply related and are based in the attempt to make parameters of interest dimensionless. Recall the Schröedinger Equation in cgs units,

\[ \left[-\frac{h^2}{2m} \nabla^2 - \frac{e\, \tilde{e}}{\tilde{r}^2} - E_T \right] \Psi_T = 0 \]  \hspace{1cm} (148)

Let \( a_B = \frac{\hbar^2}{m\epsilon^2} \) and \( \alpha_0 = 2R_D = m\epsilon\sqrt{\hbar^2} \).

Multiply equation (148) by \( \frac{R}{m\epsilon} \).

\[ \left[-\frac{\hbar^2}{2m} \nabla^2 - \left( \frac{\hbar^2}{m\epsilon} \right) \frac{1}{r} - \left( \frac{\hbar^2}{m\epsilon} \right) E_T \right] \Psi_T = 0 \]  \hspace{1cm} (149)

Then may be written

\[ \frac{1}{2} a_B^2 \nabla^2 - \frac{a_B^2 \tilde{e}}{r} - \frac{E_T}{a_B^2} \Psi_T = 0 \]  \hspace{1cm} (150)

Hence, if we measure length in units \( a_B \) and energy in units \( R \) (i.e. twice the Rydberg) the wave equation is

\[ \left[ \frac{1}{2} a_B^2 \nabla^2 - \frac{1}{r} - E_T \right] \Psi = 0 \]  \hspace{1cm} (151)

In these units \( \epsilon = \hbar = m = 1 \) (see Landau pg. 116 (1957)) for reference call these atomic units I (A.U.I.)

Alternatively we might multiply equation (148) by \( 2/R \) and write

the wave equation

\[ a_B^2 \nabla^2 - \left( \frac{a_B^2 \tilde{e}}{r} \right) - \frac{E_T}{2R} \Psi_T = 0 \]  \hspace{1cm} (152)

Then measuring energy in Rydbergs and length in Bohr radii, the wave equation is

\[ \left[ \nabla^2 - \frac{E_T}{2r} \right] \Psi = 0 \]  \hspace{1cm} (153)

these are the atomic units (for reference A.U.II) used by some authors.

Notice in (auI) \( k = \sqrt{2E} \) but in (au II) \( k = \sqrt{E} \).
For all discussions in this paper atomic units I are used. That is

\[
\text{Unit of length } = \frac{\hbar^2}{me^2} = \text{Bohr Radius } = 0.529 \text{ Å}
\]

\[
\text{Unit of energy } = \frac{me^4}{\hbar^2} = 2 \text{ Rydberg } = 27.2 \text{ eV}
\]

Formulae may be obtained by \( e = \hbar = \bar{m} = 1 \).

A convention of referring to units A.U.I as "Hartree Units" and units A.U. II as "Atomic Units" appears to be emerging in recent literature. However, many references to "Hartree Units" as "Atomic Units" already exist.
3-j Symbol Identity

A standard text for discussions of angular momentum in quantum mechanics is the work of Edmonds (1960). The necessary relationship required will use results cited without proof from this work.

Consider

\[ \sum_{m_i m_f} \int d\Omega \ Y_{\ell, m_i}^+ (\Omega) Y_{\lambda, \omega} (\Omega) Y_{\lambda', \omega'} (\Omega) Y_{\lambda, m_f}^+ (\Omega) Y_{\lambda', m_f} (\Omega) Y_{\lambda, m_f} (\Omega) \]

Then the sum of interest may be written

\[ I (\ell, \lambda, \lambda') = \sum_{m_i m_f} (-1)^{m_i + m_f} (\ell, \lambda, \lambda') \]

The 3-j symbol is zero unless \( m_1 + m_2 + m_3 = 0 \). Hence, for the sum

\[ (-1)^{m_1 + m_2} = 1. \]

Consider

\[ J = \sum_{m_i m_f} (\ell, \lambda, \lambda') (m_i, m_f, m_i, m_f) \]
Two symmetry properties of the 3-j symbol from pg. 47 are useful.

Property I: An even permutation of the columns is equivalent to multiplication by $[-1]^{j_1+j_2+j_3}$. 

Property II: 

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}$$  \hspace{1cm} (159)$$

Using Property I: 

$$J = \sum_{m_l, m_f} \left( \begin{pmatrix} l_i & l_f & \lambda \\ m_i & m_f & 0 \end{pmatrix} \right) \left( \begin{pmatrix} l_i & l_f & \lambda \\ -m_i & 0 & 0 \end{pmatrix} \right)$$  \hspace{1cm} (160)$$

$$= \sum_{m_i, m_f} (-1)^{l_i + \lambda' + l_f} \left( \begin{pmatrix} l_i & l_f & \lambda \\ m_i & 0 & 0 \end{pmatrix} \right) \left( \begin{pmatrix} l_i & l_f & \lambda \\ m_i & m_f & 0 \end{pmatrix} \right)$$ 

Using Property II: 

$$J = \sum_{m_l, m_f} (-1)^{l_i + \lambda' + l_f} \left( \begin{pmatrix} l_i & l_f & \lambda \\ m_i & 0 & 0 \end{pmatrix} \right) \left( \begin{pmatrix} l_i & l_f & \lambda' \\ m_i & m_f & 0 \end{pmatrix} \right) (-1)^{l_i + l_f + \lambda'}$$  \hspace{1cm} (161)$$

But pg. 47 of Edmonds gives 

$$\sum_{m_1, m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1' & j_2' & j_3' \\ m_1' & m_2' & m_3' \end{pmatrix} = (2 J_3 + 1)^{-1} \sum_{j_3} \sum_{m_3} \Delta(j_1 j_2 j_3)$$  \hspace{1cm} (162)$$

where $\Delta(j_1 j_2 j_3)$ indicates the triangle rule must be satisfied.

So 

$$J = (2 \lambda + 1)^{-1} \sum_{\lambda' \lambda} \Delta \left( \begin{pmatrix} l_i & l_f & \lambda \\ 0 & 0 & 0 \end{pmatrix} \right)$$  \hspace{1cm} (163)$$

and 

$$I = \frac{(2 l_i + 1)(2 l_f + 1)}{4 m} \left( \begin{pmatrix} l_i & l_f & \lambda \\ 0 & 0 & 0 \end{pmatrix} \right)^2 \sum_{\lambda' \lambda} \Delta \left( \begin{pmatrix} l_i & l_f & \lambda \\ 0 & 0 & 0 \end{pmatrix} \right)$$  \hspace{1cm} (164)$$
APPENDIX IV

Equivalent Bethe Approximation

In the Modified Bethe discussion it is asserted that the first non-zero term of the series

\[
\mathbf{f}(\mu) = \left( -\frac{2}{\mathbf{\kappa}^2} \right) \left\{ \int d\mathbf{r} \, \mathbf{\psi}_f^*(\mathbf{r}) \left[ \sum_{L=0}^\infty \frac{(\mathbf{i} \mathbf{K} \cdot \mathbf{r})^L}{L!} \right] \mathbf{\psi}_l(\mathbf{r}) = \langle f \mid \sum_{L=0}^\infty \frac{(\mathbf{i} \mathbf{K} \cdot \mathbf{r})^L}{L!} \mid i \rangle \right\}
\]

is identical to the first non-zero term in the series

\[
\mathbf{f}'(\mu) = \left( -\frac{2}{\mathbf{\kappa}^2} \right) \int d\mathbf{r}' \exp \left( \mathbf{i} \mathbf{K} \cdot \mathbf{r}' \right) \langle f \mid \sum_{L=0}^\infty \frac{(\mathbf{r}')^L}{L!} \mathbf{P}_L(\mathbf{r} \cdot \mathbf{r}') \mid i \rangle .
\]

Let us prove this assertion by reducing Eq. (165) to Eq. (166).

Recall the addition theorem (Jackson (1962) pg. 63),

\[
\mathbf{P}_L(\mathbf{r} \cdot \mathbf{r}') = \left( \frac{4\pi}{2\mathbf{\kappa}^2+1} \right) \sum_m \mathbf{Y}_{\lambda m} \langle \mathbf{\mu}_r \mid \mathbf{r}_r \rangle \mathbf{Y}_{\lambda' m}^* \langle \mathbf{\mu}'_{r'} \mid \mathbf{r}'_{r'} \rangle .
\]

Applying this identity to Eq. (166) we may write

\[
\mathbf{f}'(\mu) = \left( -\frac{2}{\mathbf{\kappa}^2} \right) \int d\mathbf{r}' \exp \left( \mathbf{i} \mathbf{K} \cdot \mathbf{r}' \right) \langle f \mid \sum_{L=0}^\infty \frac{(\mathbf{r}')^L}{L!} \mathbf{P}_L(\mathbf{r} \cdot \mathbf{r}') \mid i \rangle .
\]

Choose the integration axis such that \( \mathbf{K} \) is along the z-axis and \( \mathbf{K} \cdot \mathbf{r}' = \mathbf{K} \cdot \mathbf{r} \cdot \cos \theta' \) then

\[
\mathbf{f}'(\mu) = \left( -\frac{2}{\mathbf{\kappa}^2} \right) \int d\mathbf{r} \exp \left( \mathbf{i} \mathbf{K} \cdot \mathbf{r} \right) \langle f \mid \sum_{L=0}^\infty \frac{(\mathbf{r})^L}{L!} \mathbf{P}_L(\mathbf{r} \cdot \mathbf{r}) \mathbf{Y}_{\lambda m} \langle \mathbf{\mu}_r \mid \mathbf{\mu}'_{r'} \rangle \mathbf{Y}_{\lambda' m}^* \langle \mathbf{\mu}'_{r'} \mid \mathbf{\mu}_r \rangle \mid i \rangle .
\]

Rewrite the integral over \( \phi \) in Eq. (169) using (Jackson (1962) pg. 65)

\[
\mathbf{Y}_{\lambda m}(\mathbf{\mu}', \mathbf{\mu}) = \exp(\mathbf{i}m\phi') \mathbf{P}_m(\mathbf{\mu}) \left( \frac{(2\mathbf{\kappa}+1)}{4\pi} \left( \frac{l-m}{l+m} \right)! \right)^{1/2} \int_0^{2\pi} d\phi' \mathbf{Y}_{\lambda m}^*(\mathbf{\mu}', \mathbf{\mu}) \mathbf{P}_m(\mathbf{\mu}) \left( \frac{2\pi}{\mathbf{\kappa}} \delta_m \right)
\]

Summing over \( m \), Eq. (14i) can then be written,
\[ f'(\ell) = \left( -\frac{1}{2\pi} \right) (2\pi) \sum_k <f| \frac{4\pi}{2\ell+1} (r)^{\ell} Y_\ell^+ (\ell, \ell) \int_0^\infty \frac{dr'}{r'} P_{2\ell+1} (r') \right> \]

\[ \times \int_{-1}^1 dx P_{2\ell} (x) \exp (iKr'x) \left< \frac{(2\ell+1)}{4\pi} \right| i > \]  

(171)

The integral over \( dx \) may be done by use of the following identity

(Abramowitz (1964) pg. 438)

\[ j_\ell (Kr') = \left[ (-i)^{\ell/2} \right] \int_{-1}^1 \exp (iKr'x) P_{\ell} (x) dx \]  

(172)

where \( j_\ell (r) \) is the spherical Bessel function.

Applying Eq. (172) to Eq. (171) we find

\[ f'(\ell) = \sum_k \left( \frac{4\pi}{2\ell+1} \right) <f| Y_\ell^+ (\ell, \ell) \int_0^\infty \frac{dr'}{(r')^{\ell+1}} (2\ell+1)^{\ell} j_{2\ell} (Kr') \right> \]

(173)

Let \( y = Kr' \), \( dy = Kdr' \) then

\[ f'(\ell) = \left( \frac{2\ell}{k^2} \right) \sum_k \left( \frac{4\pi}{2\ell+1} \right) <f| Y_\ell^+ (\ell, \ell) \int_0^\infty \frac{dy}{y^{\ell+1}} j_{2\ell} (y) \right> \]

From (Abramowitz (1964) pg. 486 we obtain

\[ \int_0^\infty t^\mu J_\ell (t) dt = 2^\mu \Gamma \left( \frac{\mu + \ell + 1}{2} \right) / \Gamma \left( \frac{\mu - \ell + 1}{2} \right) \]  

(174)

For the case \( \mu = -(\ell-\frac{1}{2}) \), \( \nu = \ell+\frac{1}{2} \). This is

\[ \int_0^\infty t^{-(\ell+\frac{1}{2})} J_{\ell+\frac{1}{2}} (t) dt = (2)^{-(\ell+\frac{1}{2})} \frac{\Gamma (\ell + \frac{1}{2})}{\Gamma (\ell + \frac{3}{2})} = \sqrt{\frac{2}{\pi}} \frac{1}{(2\ell+1)!!} \]  

(176)

where (Abramowitz (1964) pg. 256)

\[ \Gamma (\ell + \frac{1}{2}) = (2\ell+1)!! ; \quad \Gamma (\ell + \frac{1}{2}) = 2^\ell \sqrt{\pi} (2\ell+1)!! \]  

(177)

Then since \( j_{2\ell} (x) = \frac{\pi}{2x} J_{2\ell} (x) \), Jackson (1964), Eq. (176) may be used to write,

\[ \int_0^\infty \frac{dt}{t^{\ell+1}} \frac{j_{2\ell} (t)}{t} = \frac{\pi}{2} \int_0^\infty \frac{dt}{t^{\ell+1}} \frac{J_{2\ell} (t)}{t} = \frac{1}{(2\ell-1)!!} \]  

(178)

Applying Eq. (178) to Eq. (174) we write,

\[ f'(\ell) = \left( \frac{2\ell}{k^2} \right) \sum_k <f| \frac{4\pi}{2\ell+1} Y_\ell^+ (\ell, \ell) \frac{(iK)^{\ell}}{(2\ell-1)!!} \right> \]  

(179)
But recall (Jackson (1962) pg. 66)

\[ Y_{\ell \alpha}(\mathbf{r}) = \left( \frac{2\ell+1}{4\pi} \right)^{\frac{1}{2}} P_{\ell}^{\alpha}(\cos \Theta) \]  

then \( f'(\Omega) \) is

\[ f'(\mathbf{r}) = \frac{1}{\kappa z} \sum_{\ell} \langle f | (iKr)^{\ell} P_{\ell}^{\alpha}(\cos \Theta)^{k} | i \rangle \]  

By choosing our axis of quantization along \( \hat{K} \) so that \( \hat{K} \cdot \mathbf{r} = K \cos \Theta \) we may write Eq. (165) as,

\[ f'(\mathbf{r}) = \left( -\frac{2}{Kz} \right) \sum_{\ell} \langle f | \hat{K} Kr \| \ell \rangle (\cos \Theta)^{\ell} \]  

To continue, recall (Abramowitz (1964) pg. 798)

\[ P_{\ell}(\cos \Theta) = \sum_{\varphi=0}^{\ell} a_{\ell} (\cos \Theta)^{\varphi} \] 

Since we are interested in comparing only the first non-zero term in Eq. (181) and Eq. (182) we need only \( a_{\ell} \) in series.

From Magnus and Oberhettinger pg. 66 the generalized Legendre Polynomial \( P_{\ell}^{\mu}(z) \) has the behavior

\[ P_{\ell}^{\mu}(z) = \left( \frac{1}{\pi} \right)^{\frac{1}{2}} \left( \frac{2\ell-1}{2\ell+2} \right)^{\frac{1}{2}} \left( \frac{1}{\rho \Gamma(\ell+2)} \right) \left( \frac{z}{\rho} \right)^{\ell} \left( 1 + O(z^{2}) \right) \] 

Therefore, recalling Eq. (183)

\[ P_{\ell}(z) \rightarrow \left( \frac{2\ell}{\pi} \right)^{\frac{1}{2}} \left( \frac{1}{\Gamma(\ell+1)} \right) \left( \frac{z}{\rho} \right)^{\ell} \left( 1 + O(z^{2}) \right) \] 

Then since \( \Gamma(\ell+1) = \ell! \), Eq. (183) is of the form:

\[ P_{\ell}(\cos \Theta) = \sum_{\varphi=0}^{2\ell-1} a_{\ell} (\cos \Theta)^{\varphi} \] 

Since the matrix elements of all lower powers of \( \cos \Theta \) are zero by assumption, Eq. (181) becomes:

\[ f'(\mathbf{r}) = \frac{1}{\kappa z} \sum_{\ell} \langle f | (iKr)^{\ell} \left( \frac{(2\ell-1)!}{(2\ell)!} \right) (\cos \Theta)^{\ell} | i \rangle \] 

which agrees with Eq. (182) to within a factor (-1). Since the object to be measured is \( Q = \int d\Omega |f(\Omega)|^{2} \), the Eqs. (187) and (182) are equivalent for our purpose.
APPENDIX V

Partial Wave Analysis

The decomposition of the Born cross-section $Q_{\text{born}}$ in terms of partial wave cross-section $Q_{\text{born}}^l$ where $l$ refers to components of the incident wave with angular momentum $\sqrt{l(l+1)}$ proceeds as follows.

The Born scattering amplitude is

$$f_{\text{Born}}(\alpha) = -\frac{i}{2\pi} \int \frac{d^3p'}{p'_0} \exp \left[ i \cdot (\mathbf{k}_0 - \mathbf{k}_F) \cdot \mathbf{r}_o' \right] \mathcal{V}_{t+1}(\mathbf{r}_o')$$

(188)

where $\mathbf{r}_o'$ is the position vector of the incident electron, and where

$$\mathcal{V}_{t+1}(\mathbf{r}_o') = \int \frac{dV}{V} \Psi^*(\mathbf{r}) \frac{4}{|V - \mathbf{r}'_o|} \Psi(\mathbf{r})$$

(189)

Choosing the coordinate system such that $\mathbf{k}_t$ is along the z-axis we write the expansions (Jackson (1962) pg. 567),

$$e^{-i\mathbf{k}_t \cdot \mathbf{r}_o'} = (4\pi)^{l} \sum_{l'=0}^{\infty} (-1)^{l'} j_{l'}(k_0 \mathbf{r}_o') Y_{l'M}^{*} (\Omega_{l'}) Y_{l'm'}(\Omega_{l'})$$

(190)

and

$$e^{i\mathbf{k}_t \cdot \mathbf{r}_o'} = \sum_{l'} (i)^{l'} j_{l'}(k_0 \mathbf{r}_o') \left[ (4\pi)^{l'} (2l'+1) \right] Y_{l'M} (\Omega_{l'})$$

(191)

Applying Eq. (190) and Eq. (191) to Eq. (188) we write

$$f_{\text{Born}}(\alpha) = (-\frac{1}{2\pi}) \int \frac{d^3p'}{p'_0} \mathcal{V}_{t+1}(\mathbf{r}_o') (4\pi)^{l} \sum_{l'=0}^{\infty} (i)^{l'} j_{l'}(k_0 \mathbf{r}_o') \left[ (4\pi)^{l'} (2l'+1) \right]$$

$$\times Y_{l'm'}^{*} (\Omega_{l'}) Y_{l'M}^{*} (\Omega_{l'}) Y_{l'm'}(\Omega_{l'}) j_{l'}(k_0 \mathbf{r}_o')$$

(192)

The wave functions used in the present calculation can be written:

$$\Psi_{l}(\mathbf{r}) = \mathcal{R}_{l}(\mathbf{r}) Y_{l|m} (\Omega_{l}) \quad ; \quad \Psi_{l}^{\dagger}(\mathbf{r}) = \mathcal{R}_{l}^{\dagger}(\mathbf{r}) Y_{l|m'}^{\dagger} (\Omega_{l})$$

(193)

and use can be made of expansion (Jackson (1962) pg. 69),

$$\frac{1}{|\mathbf{r}_o' - \mathbf{r}'|} = 4\pi \sum_{l,m} (l+1)^{-1} \left[ \frac{\mathbf{l}_o^l}{\mathbf{r}_o'} \right] Y_{l'm}^{*} (\Omega_{l'}) Y_{l'm} (\Omega_{l'})$$

(194)

to rewrite Eq. (189) as
\[
V_{t_{ii}} (r_o) = 4\pi \sum_{l,m} (2l+1) \frac{Y_{lm}(\Omega_{r_o})}{2} \int_0^\infty r^2 dr \left[ \frac{1}{r_{r_o}^2} \right] R_f(r) R_i(r)
\]

(195)

\[
\times \int d\Omega_r \ Y_{l,m_i}^+ (\Omega_r) Y_{l,m} (\Omega_r) Y_{l,m_j} (\Omega_r)
\]

Let us define the two integrals in Eq. (195) as

\[
\mathcal{R}_{l,l'}^{\text{Barn}} (r_o) = \int_0^\infty r^2 dr \left[ \frac{1}{r_{r_o}^2} \right] R_f(r) R_i(r)
\]

and

\[
\langle l, m_i | l, m_j | l, m_j \rangle = \int d\Omega_r \ Y_{l,m_i}^+ (\Omega_r) Y_{l,m} (\Omega_r) Y_{l,m_j} (\Omega_r)
\]

(197)

Then applying Eq. (195) to Eq. (192) we may write

\[
f_{\text{Barn}} (\Omega_n) = \left( -\frac{1}{2\pi} \right) \sum_{l,m} (4\pi)^2 (i)^l (j)^l (2l+1)^{-1} \frac{1}{4\pi (2l'+1)} \langle l, m_i | l, m_j | l, m_j \rangle \cdot \int d^2 r \left[ R_{l,l'}^{\text{Barn}} (r_o) \right] \cdot \langle \Omega_r | j_{l', l} (r_o) \rangle
\]

(198)

where our last term is defined in a manner analogous to Eq. (197).

To simplify the algebra that follows, we define the quantities

\[
C (l, l' l'' l''' l''') = \langle i \rangle \delta (-i) \delta (2l + 1) \frac{1}{4\pi (2l' + 1)}
\]

(199)

\[
P (l, l'' l''' l''') = \int_0^\infty r_o^2 dr_o \ \mathcal{R}_{l,l'}^{\text{Barn}} (r_o) \cdot \langle \Omega_r | j_{l', l} (r_o) \rangle \cdot \langle \Omega_r | j_{l, l''} (r_o) \rangle
\]

(200)

and rewrite as,

\[
f_{\text{Barn}} (\Omega_n) = \left( \frac{1}{2\pi} \sum_{l,m_i} C (l, l'' l''' l''') \langle l, m_i \rangle \langle l, m_i \rangle \langle l, m_j \rangle \langle l, m_j \rangle \int d^2 r \left[ R_{l,l'}^{\text{Barn}} (r_o) \right] \cdot \langle \Omega_r | j_{l', l} (r_o) \rangle \cdot \langle \Omega_r | j_{l, l''} (r_o) \rangle
\]

(201)

\[
\cdot \langle \Omega_r | j_{l, l''} (r_o) \rangle \cdot \langle \Omega_r | j_{l, l''' l'''} l''''} (r_o) \rangle \cdot \langle \Omega_r | j_{l, l''' l'''} l''''} (r_o) \rangle
\]

(202)

To obtain the cross-section we require
Since we are interested in transitions $Q(n_\alpha \to n'_\alpha)$ we can average the above over $m_1$ and sum over $m_f$, the result of which we indicate by the prime

$$|f_{\text{Born}}'(\lambda_\alpha)|^2 = \frac{16\pi^2}{2\Gamma_1 + 1} \sum_{L'nm''} \sum_{L''nm'} c(\ell\ell''m') c^*(\ell'\ell''m'') P(\ell\ell'n'i) P(\ell'\ell'n'i')$$

$$\times \langle \ell''m'\ell'nm''|LL'M'\rangle \langle L''m'\ell'nm''|L'm'M'' \rangle \gamma_{L''m''}^+ (\Omega_{K_F}) \gamma_{L'm'} (\Omega_{K_F})$$

Using the results of Appendix III to sum over $m_1 m_f$

$$|f_{\text{Born}}'(\lambda_\alpha)|^2 = \frac{16\pi^2}{2\Gamma_1 + 1} \sum_{L'nm''} \sum_{L''nm'} c(\ell\ell''m') c^*(\ell'\ell''m'') P(\ell\ell'n'i) P(\ell'\ell'n'i')$$

$$\times \langle \ell''m'\ell'nm''|LL'M'\rangle \langle L''m'\ell'nm''|L'm'M'' \rangle \gamma_{L''m''}^+ (\Omega_{K_F}) \gamma_{L'm'} (\Omega_{K_F})$$

Finally after summing over $L$ and $M$, the above can be written

$$|f_{\text{Born}}'(\lambda_\alpha)|^2 = \frac{16\pi^2}{2\Gamma_1 + 1} \sum_{L'nm''} \sum_{L''nm'} c(\ell\ell''m') c^*(\ell'\ell''m'') P(\ell\ell'n'i) P(\ell'\ell'n'i')$$

$$\times P(\ell\ell'n'i) \langle \ell''m'\ell'nm''|LL'M'\rangle \langle L''m'\ell'nm''|L'm'M'' \rangle \gamma_{L''m''}^+ (\Omega_{K_F}) \gamma_{L'm'} (\Omega_{K_F})$$

The cross-section is then:
The sums over \( L'M' \) and \( L' \) can be carried out explicitly to give the results.

\[
Q_{\text{Born}} = (16\pi)(2L_i + 1) \left[ \frac{K_i}{k_x} \right] \sum_{L'M'} \sum_{L''} c(\ell L' \ell' M') c^*(\ell L'' \ell' M'') \mathcal{P}(\ell L' \ell' M'') \mathcal{P}(\ell L'' \ell' M'') \]

\[
\times \int d\Omega_{\ell' M'}(\Omega_{L_i}) \int d\Omega_{\ell'' M''}(\Omega_{L_i}) \delta_{\ell'' M''} \delta_{\ell' M'} \]

\[
= (16\pi)(2L_i + 1) \left[ \frac{K_i}{k_x} \right] \sum_{L'L''} \left| c(\ell L' \ell' M') \right|^2 \left| \mathcal{P}(\ell L' \ell' M'') \right|^2 \left( \begin{array}{c} L_i \ell_i \ell_i' \\ 0 \end{array} \right) \left( \begin{array}{c} L_i \ell_i \ell_i' \\ 0 \end{array} \right) \frac{2L_i + 1}{4\pi}
\]

Recalling the definitions of \( C(\ell L' \ell' M') \) and \( \mathcal{P}(\ell L' \ell' M'') \), \( Q_{\text{Born}} \) can be written.

\[
Q_{\text{Born}} = (+)(2L_i + 1) \left[ \frac{K_i}{k_x} \right] \sum_{L'L''} \frac{4\pi(2L_i + 1)(2L_i + 1)}{(2L_i + 1)^2} \left( \begin{array}{c} L_i \ell_i \ell_i' \\ 0 \end{array} \right) \left( \begin{array}{c} L_i \ell_i \ell_i' \\ 0 \end{array} \right) \left[ \int_0^{\infty} r^2 dr \left( \frac{K_i}{r_{0'}^2 + 1} \right) \mathcal{R}_k(r) \mathcal{R}_l(r') \right] \]

where, as defined above,

\[
\mathcal{R}_{\ell'}(r') = \int_0^{\infty} r^2 dr \left[ \frac{K_i}{r_{0'}^2 + 1} \right] \mathcal{R}_{\ell'}(r) \mathcal{R}_l(r')
\]

Since \( L' \) is defined in Eq. (191) to refer to the incident electron, the partial cross-section corresponding to incident electrons with angular momentum \( \sqrt{2}(\ell' + 1) \) and scattered electrons with all possible values of angular momentum is,
\[ Q_{\text{Bar}} = (16\pi)(2L_f + 1) \left( \frac{\mathbf{k}_f}{\mathbf{k}_t} \right) \sum_{\mathbf{k}} \left( \frac{2L'_t + 1}{2L + 1} \right)^2 \left( \frac{\mathbf{L}_f \cdot \mathbf{L}_t}{\mathbf{L}_t \cdot \mathbf{L}_t} \right)^2 \]

\[ \mathbf{J} \left( \frac{\mathbf{L}_t \cdot \mathbf{L}_f}{\mathbf{L}_t \cdot \mathbf{L}_t} \right)^2 \int_0^\infty dr_0 r_0^2 \mathcal{R}_{\mathbf{k}'}(r_0' r_0') j_{\mathbf{k}'}(\mathbf{k}_t r_0') j_{\mathbf{k}'}(\mathbf{k}_f r_0') \cdot \]

\text{NOTE: The presence of a 3j-symbol in an expression such as}

\[ \sum_{\mathbf{L}} \left( \frac{\mathbf{L}_1 \cdot \mathbf{L}_2 \cdot \mathbf{L}_3}{\mathbf{L}_1 \cdot \mathbf{L}_1 \cdot \mathbf{L}_3} \right) f(\mathbf{L}_1 \cdot \mathbf{L}_3) \] implies the triangle condition and reduces the sum range from \( L_3 = 0, \infty \) to \( L_3 = |L_1 - L_2|, \cdots |L_1 + L_2| \), (Edmonds (1960) pg. 45).
Ochkur Expression of $f_E(n)$

Recall from our discussion in Chapter III, Section 5, the Born-Oppenheimer approximation to the exchange scattering amplitude for a Helium-like target is written

\[
f_e = \frac{1}{(2\pi)^3} \int d\vec{p}_F d\vec{r}_F \Psi_F^\dagger(\vec{r}_F, \vec{r}_0) e^{-i\vec{k}_F \cdot \vec{r}} \left[ \frac{1}{1 - \frac{2}{\vec{r}_0 - \vec{r}_1}} \right] \Psi_x(\vec{r}_1, \vec{r}_0) e^{i\vec{k}_x \cdot \vec{r}}
\]  

(211)

Let us break this up into three terms

\[
f_1 = \frac{1}{(2\pi)^3} \int d\vec{p}_F d\vec{r}_F \Psi_F^\dagger(\vec{r}_F, \vec{r}_0) e^{-i\vec{k}_F \cdot \vec{r}} \left[ \frac{1}{1 - \frac{2}{\vec{r}_0 - \vec{r}_1}} \right] \Psi_x(\vec{r}_1, \vec{r}_0) e^{i\vec{k}_x \cdot \vec{r}}
\]  

(212)

\[
f_2 = \frac{1}{(2\pi)^3} \int d\vec{r}_0 d\vec{r}_F d\vec{r}_1 \Psi_F^\dagger(\vec{r}_F, \vec{r}_0) e^{-i\vec{k}_F \cdot \vec{r}} \left[ \frac{1}{1 - \frac{2}{\vec{r}_0 - \vec{r}_1}} \right] \Psi_x(\vec{r}_1, \vec{r}_0) e^{i\vec{k}_x \cdot \vec{r}}
\]  

(213)

\[
f_3 = \frac{1}{(2\pi)^3} \int d\vec{r}_0 d\vec{r}_F d\vec{r}_1 \Psi_F^\dagger(\vec{r}_F, \vec{r}_0) e^{-i\vec{k}_F \cdot \vec{r}} \left[ -\frac{2}{\vec{r}_0} \right] \Psi_x(\vec{r}_1, \vec{r}_0) e^{i\vec{k}_x \cdot \vec{r}}
\]  

(214)

Consider the first term

\[
f_1 = \frac{1}{(2\pi)^3} \int d\vec{p}_F d\vec{r}_F d\vec{z}_x \Psi_F^\dagger(\vec{r}_F, \vec{z}_x) e^{-i\vec{k}_x \cdot \vec{r}_x} \left[ \frac{1}{1 - \frac{2}{\vec{r}_0 - \vec{r}_1}} \right] \Psi_x(\vec{z}_x, \vec{r}_0) e^{i\vec{k}_x \cdot \vec{r}}
\]  

(215)

\[
= \frac{1}{(2\pi)^3} \int d\vec{r}_0 d\vec{z}_x \Psi_x(\vec{z}_x, \vec{r}_0) \mathcal{I}_F(\vec{z}_x, \vec{r}_0) \exp\left[i\vec{k}_x \cdot (\vec{r}_0 - \vec{r}_1)\right]
\]

where $\vec{k}_x = \vec{k}_F - \vec{k}_I$ and

\[
\mathcal{I}_F(\vec{r}_0, \vec{r}_1) = \int d\vec{r}_x \Psi_F(\vec{r}_x, \vec{r}_0) \exp\left[i\vec{k}_x \cdot (\vec{r}_0 - \vec{r}_1)\right]/\left|\vec{r}_0 - \vec{r}_1\right|
\]  

(216)

Let us evaluate $\mathcal{I}_F$. Introducing the notation $\vec{r}_{01} = \vec{r}_0 - \vec{r}_1$ let us change variables from $\vec{r}_0$ to $\vec{r}_{01}$.
\[ I_F (\vec{r}_1, \vec{r}_1') = \int r_2 \, d\rho_2 \, d(\cos \theta_2) \, d\phi_2 \, \bar{\Psi}_F (\vec{r}_2, \vec{r}_1') e^{iK_4r_1'r_1} \]

\[ = \int r_1 \, d\rho_1 \, d(\cos \theta_1) \, d\phi_1 \, \bar{\Psi}_F (\vec{r}_2, \vec{r}_1, \vec{r}_1') e^{iK_4r_1'r_1} \]

Defining \( X = \cos \theta_1 \)

\[ I_F (\vec{r}_1, \vec{r}_1') = \int r_1 \, d\rho_1 \, d\phi_1 \, \bar{\Phi}_F (\vec{r}_2, \vec{r}_1, \vec{r}_1', X) e^{iK_4r_1'r_1} \]  

where

\[ \bar{\Phi}_F (\vec{r}_2, \vec{r}_1, \vec{r}_1', X) = \int d\phi_1 \, \bar{\Psi}_F (\vec{r}_2, \vec{r}_1 + \vec{r}_1') \]

(The use of \( \phi \) here does not imply the total wave function including spin.) Let us integrate by parts with respect to \( X \) and with respect to \( r_{01} \) and neglect each time terms of higher order of smallness.

We obtain

\[ I_F (\vec{r}_1, \vec{r}_1') = \frac{1}{\sqrt{k}} \int_{\rho_1} \, d\rho_1 \left[ \bar{\Phi}_F (\vec{r}_2, \vec{r}_1, 1) e^{iK_4r_1'r_1} - \bar{\Phi}_F (\vec{r}_2, \vec{r}_1, r_{01}, -1) e^{iK_4r_1'r_1} \right] \]

Noting that

\[ \bar{\Phi}_F (\vec{r}_2, \vec{r}_1, \rho_{01}, X) \xrightarrow{r_{01} \to \infty} 0 \]

we write

\[ I_F (\vec{r}_1, \vec{r}_1') = -k_4^2 \left[ \bar{\Phi}_F (\vec{r}_2, \vec{r}_1, 0, 1) + \bar{\Phi}_F (\vec{r}_2, \vec{r}_1, 0, -1) \right] \]

Then since

\[ \bar{\Phi}_F (\vec{r}_2, \vec{r}_1, 0, \pm 1) = -\frac{\pi}{k_4^2} \bar{\Psi}_F (\vec{r}_2, \vec{r}_1) \]

our result is:

\[ I_F (\vec{r}_1, \vec{r}_1') = \left[ \frac{4\pi}{k_4^2} \right] \bar{\Psi}_F (\vec{r}_2, \vec{r}_1) \]

Ochkur (1964) argues that by a similar calculation it may be shown that

\[ f_2 = O(K_4^{-6}) \]

\[ f_3 = O(K_4^{-6}) \]
Therefore, he claims the exchange amplitude $f_E$, may be approximated

$$f_E \approx \frac{4i}{\kappa_s} \int \frac{d\vec{r}_1}{2\pi^2} \frac{d\vec{r}_2}{2\pi^2} \Psi_I(\vec{r}_1, \vec{r}_2) \mathcal{E}^{\frac{i\vec{r}_1 \cdot \vec{r}_2}{\kappa_s}} \Psi_F^+(\vec{r}_1, \vec{r}_2)$$

(225)

$$= \frac{2}{\kappa_s^2} \int \frac{d\vec{r}_1}{2\pi^2} \frac{d\vec{r}_2}{2\pi^2} \Psi_I(\vec{r}_1, \vec{r}_2) \mathcal{E}^{\frac{i\vec{R} \cdot \vec{R}}{\kappa_s^2}} \Psi_F^+(\vec{r}_1, \vec{r}_2).$$
APPENDIX VII

User Manual

This section describes the details of the administration of the computer programs. The three programs used in this work are:

HFSWF; the Herman-Skillman Hartree-Fock-Slater Wave Function program with the modification discussed earlier.

EXCST; the excitation cross-section program with four options (Born, Bethe, Ochkur, Mod. Bethe) for the approximation to the cross-section.

IONCST; the ionization cross-section program that uses the Born-Coulomb approximation.

For each of these programs a sample of the input data in the form to be entered into the computer is given. Note in the examples, following standard Fortran IV usage, a "blank" data value results in the assigning of the value zero to the variable being read (e.g. Read (IR, 10) X, Y, Z with data 10, , 15 assigns the values x = 10, y = 0, z = 15).

The input data are discussed in the sequence in which they appear on the data cards of the program. For each data card the format statement number as it appears in the program listing is given as follows:

Data Card #N (Format M).

Finally a sample output is given and briefly discussed

1) HFSWF: Hartree-Fock-Slater Wave Function

A) Sample Input
C FORTRAN PARM=NOMAP
PROGRAM HFSWF(INPUT)

* * * * HFSWF * * *
* A FORTRAN PROGRAM TO CALCULATE HARTREE-FOCK-SLATER *
* NUMERICAL WAVE FUNCTIONS AS PUNCHED CARD OUTPUT. *

END
SUBROUTINE SCHEQ (ZEN,A,AMBD,NOFI,MMES,SCF,THRESH)

END

YSIN DD *
TON= 4 CASFS

00   0.9858  0.97892  0.96819  0.95748  0.94688  0.93524  0.92614  0.91604  0.90613
42   0.8756  0.85941  0.84195  0.82516  0.80902  0.79352  0.77862  0.76430  0.75051
19   0.7184  0.68796  0.65536  0.62355  0.59158  0.55949  0.52612  0.49222  0.45786
36   0.5045  0.47648  0.44838  0.42017  0.39204  0.36390  0.33575  0.30758  0.27932
36   0.29967  0.26547  0.24131  0.21714  0.19306  0.16898  0.14489  0.12080  0.09669
22   0.13376  0.12884  0.10906  0.09901  0.08895  0.07887  0.06878  0.05869  0.04859
53   0.05466  0.04911  0.04356  0.03801  0.03246  0.02691  0.02136  0.01580  0.00999
78   0.02778  0.02778  0.02778  0.02778  0.02778  0.02778  0.02778  0.02778  0.02778
78   0.02778  0.02778  0.02778  0.02778  0.02778  0.02778  0.02778  0.02778  0.02778
78   0.02778  0.02778  0.02778  0.02778  0.02778  0.02778  0.02778  0.02778  0.02778
8   0
2-1080.6
2-135.53
6-123.25
2-19.728
6-15.249
10-7.0975
2-1.9456
6-0.9519

1-0.2199
1-0.1049
1-0.0561

EXHIBIT 1
HFSWF SAMPLE INPUT
B) Input Data Values

Data Card #1 (Format 138)

This card contains heading information. Any 72 characters of information may be put in by the user for a title for his output. In the sample input the title chosen was "Krypton - 4 cases".

Data Card #2 (Format 131)

This card contains the program control information. The parameters are: KEY, TOL, THRESH, IPRATT, MAXIT, NOCOPY, KUT, IP, IM, IR, ID, DEFAULT, JE. The usual values of these parameters for the cross-section calculation are denoted by **.

KEY: This determines the nature of the starting potential. The allowed values are:

** 0; The normalized (1) potential on a 110-point mesh is read in and used to construct the 441-point starting potential. (Suggested normalized potentials are found in Table A at the end of this Manual).

1; The starting potential is given in the same format as the unabridged self-consistent potential that is output from the calculation. (i.e. 441 points)

2; The starting potential for Z is obtained by a linear extrapolation of the two unabridged potentials for atoms ZE2 and ZE3 where Z-ZE3 = ZE3-ZE2. Both unabridged potentials must be read into the program.

(Note: The options 1 and 2 for the parameter KEY are included because they might be used if a series of elements were to be calculated. In that case the series would be started for the first element with the option KEY = 0, but the self-consistent potential, all 441 points, might be saved and used as the starting potential for the next element in the series. If this were done the option KEY = 1 would be used for the start of the second element).

TOL: This is the tolerance for self-consistency defined as TOL = \text{MAX}\left[|rV_o f(r)|, |rV_o f(r)|, |rV_o f(r)|\right]. Herman and Skillman (1963) (H.A.S.) note that since tests of TOL = .001, .0001, .00001 yield potentials mutually consistent the first value is suggested.

\footnote{The normalized potential \( U(r) \) is defined. \( U(r) = -rV(r)/2Z \).}
** .001; the value found by trial and error to be preferred by H.A.S.

THRESH: The eigenvalue accuracy criterion defined by

** .00001; the value found by H.A.S. to be consistent with TOL = 001

MESH: The number of points used in the integration mesh for the Schröedinger equation subroutine. (SCHEQ).

** 441: The usual value for the integration mesh.

481: These values are used for the highly excited configuration where orbitals extend out to very large (radial) distances.

521: 

IPRATT: The number of times an improvement scheme due to Pratt (1952) should be used.

** 1; Normal value found by trial and error by H.A.S.

MAXIT: The maximum number of iterations permitted.

** 20: Recommended value.

30: If for some reason (such as a poor choice of starting potential) a large number of interactions is expected to reach self-consistency, assign this value.

NOCOPY: This controls the nature of the output

** 0: The active electron wave functions are the output.

1: The output is the self-consistent potential (441-points) and all radial wave functions.

KUT: The analytic form of the potential is selected as either a potential computed from the wave functions for the entire range of r, or

\[ V(r) = \begin{cases} V_0(r) & r < r_o \\ -2(z - N + 1)/r & r > r_o \end{cases} \]

where \( r_o \) is the value of r for which \( V_0(r) = -2(z - N + 1)/r \).

** 0; The potential is \( V(r) \). (This is a restriction of the Slater assumption to the interior region).

1; The potential is \( V_0(r) \) for all r.
IP, IM, IR, ID: These parameters control the type of device used for input (IR) and output (IP, IM, ID). The allowed devices are:

- 5 = card reader
- 6 = printer
- 7 = card punch
- no = some storage device (unit tape or disk).

IR is the input control
IP is the online output information
IM is the total wave functions and the potential control (see NOCOPY)
ID is the active electron wave function control.

** 6, 6, 5, 7; These are the normal input output devices. That is input is punched cards. Output is printer and punched cards.

DEFOLT: This parameter controls whether or not the normal values (denoted above by **) are to be used.

- 0: Set parameters equal to normal values
- 1: All parameters are read as input.

JE: The number of excited states to be calculated using the self-consistent potential.

** 1: Normal value

N: Used to produce a set of N excited state wave functions.

Data Card #3 (Format 124)

This card contains the atomic potential. Eleven of these cards are used to read in the starting atomic potential RU2(m) in the normal form of a 110-point mesh.

(See "KEY" discussion above.)

RU2(m): m values from 1 to 441 by 4's. The suggested values for RU2 for all atoms are found in Table A.

Data Card #4 (Format 125)

This card contains information about the configuration of the atom.

Z: The atomic number
NCORES: The number of core (i.e. filled) orbitals.

NVALENCE: The number of valence (i.e. unfilled) orbitals.

ION: The Ionicity (i.e. the net charge) on the atom.

(Note: Although the option of calculating wave functions for ions was not used in the present work the HFSWF program will compute such wave functions.)

Data Card #5 (Format 127)

This card contains orbital information. A set of (NCORES + NVALENCE) of these cards are read (see the sample input). The parameters are: NNLZ, WWNL, EE.

NNLZ: The principal and orbital quantum numbers.

(Note: NNLZ = 100n + 10λ + c, where n is the principal quantum number, λ is the angular quantum number and c an integer (0,1,...9) which can be used to distinguish different configurations from one another at the discretion of the user.)

WWNL: The occupation number (i.e. the number of electrons in the orbital).

EE: The starting eigenvalue for the orbital.

Suggested values for NNLZ, WWNL, and EE are given for ground state configuration in Table A.

Data Card #6 (Format 127)

This card is a special use of the data card #4. The value -1 is assigned to the atomic charge parameter Z. The program interprets Z = -1 as signifying the end of the ground state configuration. Control is transferred to the excited state calculation section of the program.

Data Card #7 (Format 127)

This card contains excited state orbital information. This is a series of JE cards (see Data Card 1) containing NNLZ, WWNL, EE for the excited states. The value of E (in Rydbergs) should be obtained from the C. Moore (1950) table or other reference tables.

The positions of the data for these cards may be seen
from the sample input or read from the appropriate format statements in program listing given in Chapter V, Section 1.

C) Sample Output

For the "normal" values of the parameters discussed above, the output from program HFSWF is of two types:

1) The printed output, which gives information about each iteration (see Exhibit 2). The first item is the "title" as discussed above (Data Card #1). The second item is the value of the parameter KEY which indicates the type of starting potential used (as discussed above in Data Card #2).

Next for each iteration the following is printed

\( \text{ITER} = \) "iteration" number

\( Z = \) atomic number

\( \text{DELTA} = \) measure of self-consistency (when \( \text{DELTA} < .001 \) calculation stops)

\( I(\text{DEL}) = \) serial number of mesh point at which self-consistency is poorest

\( X(\text{DEL}) = \) corresponding value of \( X \)

\( I(\text{CUT}) = \) serial number of mesh point closest to \( r_0 \)

\( \text{where } r_0V_o(r_0) = -2(ION+1) \)

\( X(\text{CUT}) = \) corresponding value of \( X \)

\( N \) cards and \( M \) cards denote the number of cards that would be produced by a punching of all wave functions in the configuration.

2) The punched output which is decks of about 90 cards for each wave function.

For each wave function the first card contains \( NLZ, XL, EE, WWNL, KKK \), according to (Format 142).

\( NLZ = 100n + 10\lambda + c; \) (identical to \( NNLZ \) in Data Card #5 above)

\( XL = \) numerical value of \( \lambda \) in floating point form

\( EE = \) energy eigenvalue
WWNL = occupation number

KKK = last mesh point for tabular representation of $P(n, \lambda : r)$

$Z = \text{atomic charge.}$

The KKK values of $P_{n\lambda}(r)$ appear in the next $(KKK-1)/5+1$ cards. There are 5 entries per card on the first $(KKK-1)/5$ cards of the set, and a single entry (the KKKth) on the final line in this set. This cycle is then repeated for each of the remaining orbitals.

The serial numbers 1 to KKK have the following values of the true radial distance $r$ associated with them.

Recall $x = r/\mu$

where $\mu = \frac{1}{2} \left( \frac{Z}{\mu} \right)^{1/3} Z - \frac{1}{3}$

The serial numbers refer to the integration mesh ($x$-mesh) used in the radial wave function integration. It is composed of 11 blocks of 41 points each. Each block has 40 equally spaced intervals.

<table>
<thead>
<tr>
<th>BLOCK NUMBER</th>
<th>INITIAL X</th>
<th>INTERVAL $\Delta X$</th>
<th>FINAL X</th>
<th>LAST POINT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
<td>0.025</td>
<td>0.1</td>
<td>41</td>
</tr>
<tr>
<td>2</td>
<td>0.1</td>
<td>0.005</td>
<td>0.3</td>
<td>81</td>
</tr>
<tr>
<td>3</td>
<td>0.3</td>
<td>0.01</td>
<td>0.7</td>
<td>121</td>
</tr>
<tr>
<td>11</td>
<td>102.3</td>
<td>2.56</td>
<td>204.7</td>
<td>441</td>
</tr>
</tbody>
</table>

(Note: Any wave functions may be used with programs EXCST and IONCST provided they are scaled into this mesh and arranged into the format of the wave functions output from HFSWF. This was done with the analytic wave functions of hydrogen to test the cross-section programs.)
<table>
<thead>
<tr>
<th>Iter</th>
<th>Z</th>
<th>DELTA</th>
<th>I(DEL)</th>
<th>X(DEL)</th>
<th>I(CUT)</th>
<th>X(CUT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>36.</td>
<td>2.0038214E 00</td>
<td>405</td>
<td>112.540</td>
<td>441</td>
<td>204.700</td>
</tr>
<tr>
<td>2</td>
<td>36.</td>
<td>1.0018797E 00</td>
<td>402</td>
<td>104.860</td>
<td>270</td>
<td>10.940</td>
</tr>
<tr>
<td>3</td>
<td>36.</td>
<td>2.7208328E-03</td>
<td>279</td>
<td>12.380</td>
<td>270</td>
<td>10.940</td>
</tr>
<tr>
<td>4</td>
<td>36.</td>
<td>1.3160706E-03</td>
<td>279</td>
<td>12.380</td>
<td>270</td>
<td>10.940</td>
</tr>
<tr>
<td>5</td>
<td>36.</td>
<td>4.0054321E-04</td>
<td>270</td>
<td>10.940</td>
<td>270</td>
<td>10.940</td>
</tr>
</tbody>
</table>

**EXHIBIT 2**

HFSWF Sample Output (Printed Output)
EXHIBIT 3

HFSWF SAMPLE OUTPUT (PUNCHED OUTPUT)
2) EXCST: Excitation Cross-Sections
   a) Sample Input
EXCSCT SAMPLE INPUT

EXHIBIT 4
B) Input Data Values

Data Card #1 (Format 46)

This card contains the program control information. The parameters are: N, NTC, NC, NOTP, AQ.

N: This determines the number of energy values to be read into the program.

-1; If this value is used a standard set of energy values is assumed. (See Data Card #2)

NTC: The type of case is indicated by this parameter.

1; A single case (i.e. A cross-section for a single transition in a single approximation is given say Na (3s-3p) in the Bethe approximation.)

2; A multiple approximation for a fixed transition (i.e. For a specific transition Na(3s-3p) the cross-section is calculated in more than one approximation, say the Born and the Bethe approximations.)

3; A multiple excited state function case. (i.e. For a series of excited states, the cross-section is calculated for a specified approximation for each transition say Na(3s-3p), Born; Na(3s-4p), Bethe.)

NC: The number of cases. This should be in agreement with the value of NTC. (i.e. NTC = 1 NC = 1; if NTC = 2 NC = number of approximations used; if NTC = 3 NC = number of excited state wave functions.

NOTP: The type of output format (See sample outputs at end of this section.)

1; Punched Cards

2; Single List

3; Multiple List

AQ: The atomic element name as it will appear in the output. This is limited to an 8 character length (e.g. potassium = potassium).

Data Card #2 (Format 47)

This is the set of incident energy values. These energies are in threshold units of energy. As indicated above
a value of \( N = -1 \) on Data Card #1 assumes a set of 20 energy values. They are (1.2, 1.35, 1.50, 1.75, 2.00, 2.33, 2.67, 3.0, 3.5, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 12.0, 15.0, 18.0, 21.0, 24.0).

If the \( N = -1 \) is chosen, no Data Cards #2 are included in the deck.

If \( N \neq -1 \), the number of values on this card must equal \( N \).

**Data Card #3 (Format 48)**

This is the first atomic wave function Data Card. It contains information about the ground state wave function the parameters are NLZI, XLI, EEI, WWNL1, KKKI, Z.

**NLZI:** This is the principal and orbital angular momentum quantum number. (e.g. 3s→30)

**XLI:** This is the orbital angular momentum quantum number.

**EEI:** This is the eigenenergy of the orbital.

**WWNL1:** This is the occupation number (i.e. number of electrons) for the orbital.

**KKKI:** This is the number of points in the Herman-Skillman mesh used to give the wave function.

**Z:** This is the atomic number.

**Data Card #4 (Format 49)**

This card contains \( 5 \) of the values of the initial radial wave function. There are \( (KKKI-1)/5+1 \) of these cards for the initial state wave function. Notice that since the radial wave function is the function \( P(nl;r) \) and the boundary condition requires \( P = 0 \) at \( r = 0 \), then the first wave function value is always 0.0.

**PIN(N):** The values of the initial state radial wave function.

**Data Card #5 (Format 48)**

This is the first final state wave function Data Card. The parameters are NLZ2, XLI, EE2, WWNL2, KKK2, Z. This card is of the same form as Data Card #3 and the parameters are described above.
Data Card #6 (Format 49)

This card contains 5 values of the final state radial wave function. These are \((KKK2-1)/5+1\) of these cards for the final state wave function.

PF(N): The values of the final state radial wave function.

N.B. Cards 5 and 6 are repeated for each of the final states for which cross-sections are to be calculated.

Data Card #7 (Format 51)

This is the approximation specification card. The parameters are: IPROX, BQ.

IPROX: The numeric value of the approximation

1; Born Approximation
2; Ochkur Approximation
3; Bethe Approximation
4; Modified Bethe Approximation

BQ: The 8 character abbreviation of the approximation, as it will be printed in the output.

C) Sample Output

There are three possible forms for the output. The form used is selected by a choice of the parameter NOTP as discussed above in Section B. Examples for each form follow.
<table>
<thead>
<tr>
<th>Value</th>
<th>Result</th>
<th>Description</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.200</td>
<td>0.405E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>1.350</td>
<td>0.677E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>1.550</td>
<td>0.82E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>1.750</td>
<td>0.948E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>2.000</td>
<td>0.990E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>2.330</td>
<td>0.101E 03AETHF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>2.670</td>
<td>0.932E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>3.000</td>
<td>0.955E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>3.500</td>
<td>0.997E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>4.000</td>
<td>0.959E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>5.000</td>
<td>0.772E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>5.000</td>
<td>0.699E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>7.000</td>
<td>0.639E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>8.000</td>
<td>0.589E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>10.000</td>
<td>0.511E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>12.000</td>
<td>0.452E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>15.000</td>
<td>0.388E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>18.000</td>
<td>0.341E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>21.000</td>
<td>0.304E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
<tr>
<td>24.000</td>
<td>0.276E 02THF</td>
<td>(11.) SODIUM (30-31) (EPSIL = 0.753E-01)</td>
<td></td>
</tr>
</tbody>
</table>

**EXHIBIT 5**

EXCST SAMPLE OUTPUT (NOTP = 1)
CROSS-SECTIONS ARE IN UNITS OF PLUMMER RADII^2.

INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (EPSIL).

EPSIL IS IN UNITS OF TWICE THE RYDBERG.

<table>
<thead>
<tr>
<th>N</th>
<th>SIG(N)</th>
<th>N</th>
<th>SIG(N)</th>
<th>N</th>
<th>SIG(N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.200</td>
<td>4.043E 01</td>
<td>1.250</td>
<td>6.766E 01</td>
<td>1.500</td>
<td>8.245E 01</td>
</tr>
<tr>
<td>1.750</td>
<td>7.451E 01</td>
<td>2.000</td>
<td>6.905E 01</td>
<td>2.330</td>
<td>9.997E 01</td>
</tr>
<tr>
<td>4.000</td>
<td>8.588E 01</td>
<td>5.000</td>
<td>7.716E 01</td>
<td>6.000</td>
<td>6.991E 01</td>
</tr>
<tr>
<td>7.000</td>
<td>6.392E 01</td>
<td>8.000</td>
<td>5.892E 01</td>
<td>10.000</td>
<td>5.109E 01</td>
</tr>
<tr>
<td>12.000</td>
<td>4.524E 01</td>
<td>15.000</td>
<td>3.877E 01</td>
<td>18.000</td>
<td>3.405E 01</td>
</tr>
<tr>
<td>21.000</td>
<td>3.045E 01</td>
<td>24.000</td>
<td>2.759E 01</td>
<td>0.000</td>
<td>1.484E 01</td>
</tr>
</tbody>
</table>

EXHIBIT 6

EXCST OUTPUT (NOTP = 2)
**Cross-sections are in units of \( \pi r^2 \) (Bohr radius)**.

**Incident energies (N) are in threshold energy units (\( \epsilon \)).**

\( \epsilon \) is in units of twice the Rydberg.

<table>
<thead>
<tr>
<th>N</th>
<th>( \text{SIG}(N) )</th>
<th>( \text{SIG}(N) )</th>
<th>( \text{SIG}(N) )</th>
<th>( \text{SIG}(N) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.200</td>
<td>9.936E-01</td>
<td>8.027E-01</td>
<td>4.048E-01</td>
<td>0.0</td>
</tr>
<tr>
<td>1.350</td>
<td>9.936E-01</td>
<td>9.062E-01</td>
<td>6.766E-01</td>
<td>0.0</td>
</tr>
<tr>
<td>1.500</td>
<td>1.064E-02</td>
<td>9.468E-01</td>
<td>8.245E-01</td>
<td>1.326E-01</td>
</tr>
<tr>
<td>2.000</td>
<td>1.098E-02</td>
<td>9.598E-01</td>
<td>9.05E-01</td>
<td>3.448E-01</td>
</tr>
<tr>
<td>2.670</td>
<td>1.329E-02</td>
<td>9.133E-01</td>
<td>9.824E-01</td>
<td>4.397E-01</td>
</tr>
<tr>
<td>4.000</td>
<td>8.701E-01</td>
<td>9.013E-01</td>
<td>8.598E-01</td>
<td>4.664E-01</td>
</tr>
<tr>
<td>5.000</td>
<td>7.750E-01</td>
<td>7.262E-01</td>
<td>7.716E-01</td>
<td>4.526E-01</td>
</tr>
<tr>
<td>9.000</td>
<td>5.437E-01</td>
<td>5.263E-01</td>
<td>5.470E-01</td>
<td>3.681E-01</td>
</tr>
<tr>
<td>10.000</td>
<td>5.074E-01</td>
<td>4.930E-01</td>
<td>5.109E-01</td>
<td>3.490E-01</td>
</tr>
<tr>
<td>12.000</td>
<td>4.487E-01</td>
<td>4.385E-01</td>
<td>4.524E-01</td>
<td>3.182E-01</td>
</tr>
<tr>
<td>15.000</td>
<td>3.942E-01</td>
<td>3.775E-01</td>
<td>3.877E-01</td>
<td>2.804E-01</td>
</tr>
<tr>
<td>18.000</td>
<td>3.374E-01</td>
<td>3.326E-01</td>
<td>3.405E-01</td>
<td>2.514E-01</td>
</tr>
<tr>
<td>21.000</td>
<td>3.016E-01</td>
<td>2.996E-01</td>
<td>3.045E-01</td>
<td>2.278E-01</td>
</tr>
<tr>
<td>24.000</td>
<td>2.732E-01</td>
<td>2.706E-01</td>
<td>2.759E-01</td>
<td>2.088E-01</td>
</tr>
</tbody>
</table>

**Approximate (NL-NIL) EpSil**

- PORN: 7.531E-02
- OCHKUR: 7.531E-02
- RETHE: 7.531E-02
- VCDARETHE: 7.531E-02

EXHIBIT 7

EXCST SAMPLE OUTPUT (NOTP = 3)
3) IONCST: Ionization Cross-Sections
   a) Sample Input
JOBN, MSGLEVEL=(0,0)

EXEC FORTRAN,PARM='DCU,NUSOURCE'

FORT. SYST DD *

PROGRAM IONCST(INPUT)

A 1
A 2
A 3
A 4
A 5
A 6
A 7
A 8

END

FUNCTION FINR (L,RHO,ETA)

END

GO.SYSIN

HELIUM

A 1
A 2
A 3
A 4
A 5
A 6
A 7
A 8

EXHIBIT 8

SAMPLE INPUT IONCST
b) Input Data Values

Data Card #1 (Format 17)

This is a heading card. The 8 character abbreviation for the element as it will appear in the output.

Data Card #2 (Format 18)

This is the initial (bound) state atomic data card. The parameters are: NLZI, XLI, EEI, WWNLI, KKKI, Z.

NLZI: This is the principal and orbital angular momentum quantum numbers (e.g. 1s-10).

XLI: This is the orbital angular momentum quantum number.

EEI: This is the eigenenergy of the orbital.

WWNLI: The occupation number (i.e. number of electrons) for the orbital.

KKKI: This is the number of points in the H-S mesh used to give the initial state radial wave function.

Z: This is the atomic number.

Data Card #3 (Format 19)

This card contains the 5 of the values of the initial radial wave function. There are (KKKI-1)/5+1 of these cards for the initial state radial wave function.

PIN(N): The values of the initial state radial wave function.

Data Card #4 (Format 21)

This card is the incident energy value (in threshold units) for which the ionization cross-section will be calculated.

c) Sample Output

The output from this program is a table of partial cross-sections $Q_\lambda$ equal the total cross-section $Q$ obtained summing $Q_\lambda$. A sample output follows.
HELIUM$^4$COULBORN

CROSS-SECTIONS ARE IN UNITS OF $\pi(\text{ROHR RADIUS})^2$.
INCIDENT ENERGIES ($N$) ARE IN THRESHOLD ENERGY UNITS ($\epsilonpsilon$).
$\epsilonpsilon$ IS IN UNITS OF TWICE THE RYDBERG.

(\text{AT. NO.} = 1.0) \quad (\text{FPSIL} = 5.000E-01) \quad (\log(N) = 4.393E-01)

<table>
<thead>
<tr>
<th>L</th>
<th>SIG(L)</th>
<th>L</th>
<th>SIG(L)</th>
<th>L</th>
<th>SIG(L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.693E-01</td>
<td>1.000</td>
<td>6.615E-01</td>
<td>2.000</td>
<td>2.020E-01</td>
</tr>
<tr>
<td>3.000</td>
<td>5.678E-02</td>
<td>4.000</td>
<td>6.666E-03</td>
<td>5.000</td>
<td>1.256E-03</td>
</tr>
</tbody>
</table>

N = 2.750 \quad \log(N) = 4.393E-01 \quad \text{SIG(TOTAL)} = 1.078E 00

$\rho_{\text{MAX}} = 2.3229645E 01 \quad \eta_{\text{MAX}} = -9.7186023E-01$
$\rho_{\text{MIN}} = 2.0704012E-04 \quad \eta_{\text{MIN}} = -1.0690453E-01$

EXHIBIT 9

IONCST SAMPLE OUTPUT
Values for the starting potentials for the HFSWF program are given for each element. Also the occupation number and suggested eigenenergies for each orbital are listed.

TABLE A
<table>
<thead>
<tr>
<th>X</th>
<th>U(X)</th>
<th>HF 2</th>
<th>LI 3</th>
<th>BE 4</th>
<th>P 5</th>
<th>C 6</th>
<th>N 7</th>
<th>O 8</th>
<th>F 9</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.01</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.02</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.03</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.04</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.05</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.06</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.07</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.08</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.09</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.10</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>U(x)</td>
<td>X</td>
<td>HE 2</td>
<td>LI 3</td>
<td>RE 4</td>
<td>B 5</td>
<td>C 6</td>
<td>N 7</td>
<td>O 8</td>
<td>F 9</td>
</tr>
<tr>
<td>------</td>
<td>---</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>05.34</td>
<td>0.00000</td>
<td>0.50000</td>
<td>0.33333</td>
<td>0.25000</td>
<td>0.20000</td>
<td>0.16667</td>
<td>0.14286</td>
<td>0.12500</td>
<td>0.11111</td>
</tr>
<tr>
<td>05.66</td>
<td>0.00000</td>
<td>0.50000</td>
<td>0.33333</td>
<td>0.25000</td>
<td>0.20000</td>
<td>0.16667</td>
<td>0.14286</td>
<td>0.12500</td>
<td>0.11111</td>
</tr>
<tr>
<td>05.98</td>
<td>0.00000</td>
<td>0.50000</td>
<td>0.33333</td>
<td>0.25000</td>
<td>0.20000</td>
<td>0.16667</td>
<td>0.14286</td>
<td>0.12500</td>
<td>0.11111</td>
</tr>
<tr>
<td>SHELL (1S) 0</td>
<td>(1S) 2</td>
<td>(1S) 2</td>
<td>(1S) 2</td>
<td>(1S) 2</td>
<td>(1S) 2</td>
<td>(1S) 2</td>
<td>(1S) 2</td>
<td>(1S) 2</td>
<td>(1S) 2</td>
</tr>
<tr>
<td>SHELL (2S) 0</td>
<td>(2S) 0</td>
<td>(2S) 1</td>
<td>(2S) 2</td>
<td>(2S) 2</td>
<td>(2S) 2</td>
<td>(2S) 2</td>
<td>(2S) 2</td>
<td>(2S) 2</td>
<td></td>
</tr>
<tr>
<td>0.</td>
<td>0.4039</td>
<td>0.6012</td>
<td>0.9239</td>
<td>1.2896</td>
<td>1.6599</td>
<td>2.1440</td>
<td>2.6349</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SHELL (2P) 0</td>
<td>(2P) 0</td>
<td>(2P) 0</td>
<td>(2P) 1</td>
<td>(2P) 1</td>
<td>(2P) 1</td>
<td>(2P) 1</td>
<td>(2P) 1</td>
<td>(2P) 1</td>
<td></td>
</tr>
<tr>
<td>0.</td>
<td>0.4089</td>
<td>0.6603</td>
<td>0.8445</td>
<td>1.0409</td>
<td>1.2502</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table Note:**
- U(x) represents the energy levels.
- X indicates the electron configuration.
- HE 2 and LI 3 denote the configurations for helium and lithium, respectively.
- RE 4 through F 9 represent the energy levels for other elements.

**Additional Information:**
- The table provides a detailed breakdown of electron configurations and energy levels, useful for understanding quantum mechanics and atomic physics.
<table>
<thead>
<tr>
<th>U(X)</th>
<th>X</th>
<th>CA 2G</th>
<th>SC 21</th>
<th>TI 22</th>
<th>V 23</th>
<th>CR 24</th>
<th>MN 25</th>
<th>FE 26</th>
<th>CO 27</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.02</td>
<td>0.56</td>
<td>0.59</td>
<td>0.58</td>
<td>0.54</td>
<td>0.56</td>
<td>0.58</td>
<td>0.55</td>
<td>0.56</td>
<td>0.57</td>
</tr>
<tr>
<td>0.04</td>
<td>0.60</td>
<td>0.62</td>
<td>0.60</td>
<td>0.58</td>
<td>0.60</td>
<td>0.62</td>
<td>0.60</td>
<td>0.61</td>
<td>0.62</td>
</tr>
<tr>
<td>0.08</td>
<td>0.64</td>
<td>0.66</td>
<td>0.64</td>
<td>0.63</td>
<td>0.65</td>
<td>0.67</td>
<td>0.65</td>
<td>0.66</td>
<td>0.67</td>
</tr>
<tr>
<td>0.10</td>
<td>0.65</td>
<td>0.67</td>
<td>0.65</td>
<td>0.65</td>
<td>0.66</td>
<td>0.67</td>
<td>0.66</td>
<td>0.68</td>
<td>0.69</td>
</tr>
<tr>
<td>0.12</td>
<td>0.67</td>
<td>0.69</td>
<td>0.68</td>
<td>0.68</td>
<td>0.69</td>
<td>0.70</td>
<td>0.70</td>
<td>0.71</td>
<td>0.72</td>
</tr>
<tr>
<td>0.14</td>
<td>0.69</td>
<td>0.71</td>
<td>0.70</td>
<td>0.70</td>
<td>0.71</td>
<td>0.73</td>
<td>0.72</td>
<td>0.74</td>
<td>0.75</td>
</tr>
<tr>
<td>0.16</td>
<td>0.71</td>
<td>0.73</td>
<td>0.72</td>
<td>0.72</td>
<td>0.73</td>
<td>0.75</td>
<td>0.74</td>
<td>0.76</td>
<td>0.77</td>
</tr>
</tbody>
</table>

Note: The table continues with similar entries for other values of X.
<table>
<thead>
<tr>
<th>U(X) x CS 55</th>
<th>BA 56</th>
<th>LA 57</th>
<th>CE 58</th>
<th>PR 59</th>
<th>NO 60</th>
<th>PM 61</th>
<th>SW 62</th>
<th>EU 63</th>
</tr>
</thead>
<tbody>
<tr>
<td>05.98</td>
<td>0.07627</td>
<td>0.08105</td>
<td>0.08263</td>
<td>0.07766</td>
<td>0.07577</td>
<td>0.07400</td>
<td>0.07225</td>
<td>0.07055</td>
</tr>
<tr>
<td>06.30</td>
<td>0.07142</td>
<td>0.07622</td>
<td>0.07765</td>
<td>0.07279</td>
<td>0.07105</td>
<td>0.06934</td>
<td>0.06766</td>
<td>0.06602</td>
</tr>
<tr>
<td>06.94</td>
<td>0.06326</td>
<td>0.06796</td>
<td>0.06902</td>
<td>0.06464</td>
<td>0.06292</td>
<td>0.06138</td>
<td>0.05981</td>
<td>0.05830</td>
</tr>
<tr>
<td>07.58</td>
<td>0.05656</td>
<td>0.06106</td>
<td>0.06176</td>
<td>0.05786</td>
<td>0.05630</td>
<td>0.05480</td>
<td>0.05334</td>
<td>0.05195</td>
</tr>
<tr>
<td>08.22</td>
<td>0.05053</td>
<td>0.05618</td>
<td>0.05556</td>
<td>0.05211</td>
<td>0.05066</td>
<td>0.04925</td>
<td>0.04791</td>
<td>0.04663</td>
</tr>
<tr>
<td>08.86</td>
<td>0.04613</td>
<td>0.05009</td>
<td>0.05022</td>
<td>0.04718</td>
<td>0.04583</td>
<td>0.04452</td>
<td>0.04328</td>
<td>0.04210</td>
</tr>
<tr>
<td>09.50</td>
<td>0.04186</td>
<td>0.04565</td>
<td>0.04560</td>
<td>0.04291</td>
<td>0.04165</td>
<td>0.04064</td>
<td>0.03930</td>
<td>0.03822</td>
</tr>
<tr>
<td>10.14</td>
<td>0.03837</td>
<td>0.04176</td>
<td>0.04158</td>
<td>0.03919</td>
<td>0.03801</td>
<td>0.03699</td>
<td>0.03585</td>
<td>0.03486</td>
</tr>
<tr>
<td>10.78</td>
<td>0.03250</td>
<td>0.03534</td>
<td>0.03510</td>
<td>0.03264</td>
<td>0.03165</td>
<td>0.03083</td>
<td>0.02986</td>
<td>0.02894</td>
</tr>
<tr>
<td>11.42</td>
<td>0.03239</td>
<td>0.03533</td>
<td>0.03509</td>
<td>0.03311</td>
<td>0.03211</td>
<td>0.03118</td>
<td>0.03029</td>
<td>0.02946</td>
</tr>
<tr>
<td>12.06</td>
<td>0.02958</td>
<td>0.03272</td>
<td>0.03251</td>
<td>0.03067</td>
<td>0.02976</td>
<td>0.02890</td>
<td>0.02809</td>
<td>0.02734</td>
</tr>
<tr>
<td>12.70</td>
<td>0.02766</td>
<td>0.03046</td>
<td>0.03031</td>
<td>0.02859</td>
<td>0.02775</td>
<td>0.02697</td>
<td>0.02624</td>
<td>0.02555</td>
</tr>
<tr>
<td>13.34</td>
<td>0.02391</td>
<td>0.02691</td>
<td>0.02684</td>
<td>0.02534</td>
<td>0.02465</td>
<td>0.02399</td>
<td>0.02338</td>
<td>0.02281</td>
</tr>
<tr>
<td>14.06</td>
<td>0.02101</td>
<td>0.02439</td>
<td>0.02425</td>
<td>0.02304</td>
<td>0.02245</td>
<td>0.02190</td>
<td>0.02137</td>
<td>0.02088</td>
</tr>
<tr>
<td>14.74</td>
<td>0.01848</td>
<td>0.02253</td>
<td>0.02232</td>
<td>0.02136</td>
<td>0.02084</td>
<td>0.02034</td>
<td>0.01987</td>
<td>0.01943</td>
</tr>
<tr>
<td>15.42</td>
<td>0.01818</td>
<td>0.02110</td>
<td>0.02072</td>
<td>0.02002</td>
<td>0.01955</td>
<td>0.01909</td>
<td>0.01866</td>
<td>0.01826</td>
</tr>
<tr>
<td>16.10</td>
<td>0.01818</td>
<td>0.01865</td>
<td>0.01935</td>
<td>0.01888</td>
<td>0.01845</td>
<td>0.01802</td>
<td>0.01762</td>
<td>0.01724</td>
</tr>
<tr>
<td>16.78</td>
<td>0.01818</td>
<td>0.01882</td>
<td>0.01814</td>
<td>0.01787</td>
<td>0.01746</td>
<td>0.01705</td>
<td>0.01667</td>
<td>0.01632</td>
</tr>
<tr>
<td>17.46</td>
<td>0.01818</td>
<td>0.01796</td>
<td>0.01754</td>
<td>0.01724</td>
<td>0.01695</td>
<td>0.01667</td>
<td>0.01639</td>
<td>0.01613</td>
</tr>
<tr>
<td>18.14</td>
<td>0.01818</td>
<td>0.01766</td>
<td>0.01754</td>
<td>0.01724</td>
<td>0.01695</td>
<td>0.01667</td>
<td>0.01639</td>
<td>0.01613</td>
</tr>
<tr>
<td>18.82</td>
<td>0.01818</td>
<td>0.01766</td>
<td>0.01754</td>
<td>0.01724</td>
<td>0.01695</td>
<td>0.01667</td>
<td>0.01639</td>
<td>0.01613</td>
</tr>
</tbody>
</table>

**Notes:**
- The table above lists values for various columns, possibly representing data in a scientific or mathematical context.
- Each row provides a set of numerical values for different categories, with the first column (U(X)) likely indicating some variable or parameter.
| X1  | X2  | X3  | X4  | X5  | X6  | X7  | X8  | X9  | X10 | X11 | X12 | X13 | X14 | X15 | X16 | X17 | X18 | X19 | X20 | X21 | X22 | X23 | X24 | X25 | X26 | X27 | X28 | X29 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

**Note:** The table above represents a section of a larger table or matrix, with each entry denoting a specific value or calculation result. The values are formatted to indicate precision and measurement, typically relevant in scientific or engineering contexts. Each row and column might correspond to different parameters or variables, with the entries showing relationships or outcomes between these variables.
<table>
<thead>
<tr>
<th>U(x)</th>
<th>X</th>
<th>A</th>
<th>9</th>
<th>M</th>
<th>9</th>
<th>C</th>
<th>9</th>
<th>K</th>
<th>9</th>
<th>C</th>
<th>9</th>
<th>F</th>
<th>9</th>
<th>F</th>
<th>9</th>
<th>E</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td>1.00000</td>
<td></td>
</tr>
<tr>
<td>0.01</td>
<td>0.99966</td>
<td>0.99893</td>
<td>0.99872</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td>0.99880</td>
<td></td>
</tr>
<tr>
<td>0.02</td>
<td>0.97988</td>
<td>0.97766</td>
<td>0.97725</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td>0.97758</td>
<td></td>
</tr>
<tr>
<td>0.03</td>
<td>0.96955</td>
<td>0.96640</td>
<td>0.96582</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td>0.96600</td>
<td></td>
</tr>
<tr>
<td>0.04</td>
<td>0.95928</td>
<td>0.95527</td>
<td>0.95455</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td>0.95473</td>
<td></td>
</tr>
<tr>
<td>0.05</td>
<td>0.94903</td>
<td>0.94435</td>
<td>0.94350</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td>0.94368</td>
<td></td>
</tr>
<tr>
<td>0.06</td>
<td>0.93887</td>
<td>0.93365</td>
<td>0.93270</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td>0.93288</td>
<td></td>
</tr>
<tr>
<td>0.07</td>
<td>0.92885</td>
<td>0.92315</td>
<td>0.92215</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
<td>0.92233</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>L(0)</td>
<td>TE6</td>
<td>R6</td>
<td>C9</td>
<td>E09</td>
<td>F100</td>
<td>M500</td>
<td>N900</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>------</td>
<td>-----</td>
<td>----</td>
<td>----</td>
<td>-----</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.06</td>
<td>0.07</td>
<td>0.08</td>
<td>0.09</td>
<td>0.09</td>
<td>0.09</td>
<td>0.09</td>
<td>0.09</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.07</td>
<td>0.08</td>
<td>0.09</td>
<td>0.10</td>
<td>0.10</td>
<td>0.10</td>
<td>0.10</td>
<td>0.10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.08</td>
<td>0.09</td>
<td>0.10</td>
<td>0.11</td>
<td>0.11</td>
<td>0.11</td>
<td>0.11</td>
<td>0.11</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.09</td>
<td>0.10</td>
<td>0.11</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>0.11</td>
<td>0.12</td>
<td>0.13</td>
<td>0.13</td>
<td>0.13</td>
<td>0.13</td>
<td>0.13</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.11</td>
<td>0.12</td>
<td>0.13</td>
<td>0.14</td>
<td>0.14</td>
<td>0.14</td>
<td>0.14</td>
<td>0.14</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.12</td>
<td>0.13</td>
<td>0.14</td>
<td>0.15</td>
<td>0.15</td>
<td>0.15</td>
<td>0.15</td>
<td>0.15</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.13</td>
<td>0.14</td>
<td>0.15</td>
<td>0.16</td>
<td>0.16</td>
<td>0.16</td>
<td>0.16</td>
<td>0.16</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: The table is designed to represent the values corresponding to the given x and y axes, which are not explicitly shown in the image provided.
<table>
<thead>
<tr>
<th>U(X)</th>
<th>X</th>
<th>NI</th>
<th>CE</th>
<th>TB</th>
<th>RK</th>
<th>CF</th>
<th>F</th>
<th>FM100</th>
<th>MV101</th>
<th>ND102</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.14</td>
<td>0.03571</td>
<td>0.04029</td>
<td>0.03322</td>
<td>0.03033</td>
<td>0.02937</td>
<td>0.02874</td>
<td>0.02813</td>
<td>0.02754</td>
<td>0.02698</td>
<td></td>
</tr>
<tr>
<td>10.78</td>
<td>0.03571</td>
<td>0.03691</td>
<td>0.03048</td>
<td>0.02765</td>
<td>0.02634</td>
<td>0.02626</td>
<td>0.02570</td>
<td>0.02516</td>
<td>0.02465</td>
<td></td>
</tr>
<tr>
<td>11.42</td>
<td>0.03571</td>
<td>0.03401</td>
<td>0.02817</td>
<td>0.02520</td>
<td>0.02463</td>
<td>0.02460</td>
<td>0.02358</td>
<td>0.02309</td>
<td>0.02263</td>
<td></td>
</tr>
<tr>
<td>12.06</td>
<td>0.03571</td>
<td>0.03152</td>
<td>0.02622</td>
<td>0.02322</td>
<td>0.02270</td>
<td>0.02221</td>
<td>0.02174</td>
<td>0.02129</td>
<td>0.02086</td>
<td></td>
</tr>
<tr>
<td>12.70</td>
<td>0.03571</td>
<td>0.02940</td>
<td>0.02455</td>
<td>0.02148</td>
<td>0.02010</td>
<td>0.01955</td>
<td>0.02012</td>
<td>0.01971</td>
<td>0.01932</td>
<td></td>
</tr>
<tr>
<td>13.98</td>
<td>0.03571</td>
<td>0.02608</td>
<td>0.02204</td>
<td>0.01863</td>
<td>0.01822</td>
<td>0.01784</td>
<td>0.01748</td>
<td>0.01714</td>
<td>0.01681</td>
<td></td>
</tr>
<tr>
<td>15.26</td>
<td>0.03571</td>
<td>0.02363</td>
<td>0.02013</td>
<td>0.01647</td>
<td>0.01613</td>
<td>0.01582</td>
<td>0.01552</td>
<td>0.01523</td>
<td>0.01497</td>
<td></td>
</tr>
<tr>
<td>16.54</td>
<td>0.03571</td>
<td>0.02174</td>
<td>0.01861</td>
<td>0.01489</td>
<td>0.01461</td>
<td>0.01434</td>
<td>0.01410</td>
<td>0.01386</td>
<td>0.01364</td>
<td></td>
</tr>
<tr>
<td>17.82</td>
<td>0.03571</td>
<td>0.02020</td>
<td>0.01733</td>
<td>0.01373</td>
<td>0.01349</td>
<td>0.01327</td>
<td>0.01306</td>
<td>0.01285</td>
<td>0.01266</td>
<td></td>
</tr>
<tr>
<td>19.10</td>
<td>0.03571</td>
<td>0.01887</td>
<td>0.01620</td>
<td>0.01285</td>
<td>0.01264</td>
<td>0.01245</td>
<td>0.01226</td>
<td>0.01208</td>
<td>0.01191</td>
<td></td>
</tr>
<tr>
<td>20.38</td>
<td>0.03571</td>
<td>0.01769</td>
<td>0.01538</td>
<td>0.01154</td>
<td>0.01136</td>
<td>0.01120</td>
<td>0.01094</td>
<td>0.01074</td>
<td>0.01054</td>
<td></td>
</tr>
<tr>
<td>21.66</td>
<td>0.03571</td>
<td>0.01724</td>
<td>0.01538</td>
<td>0.01060</td>
<td>0.01083</td>
<td>0.01068</td>
<td>0.01053</td>
<td>0.01038</td>
<td>0.01024</td>
<td></td>
</tr>
<tr>
<td>22.94</td>
<td>0.03571</td>
<td>0.01724</td>
<td>0.01538</td>
<td>0.01050</td>
<td>0.01034</td>
<td>0.01020</td>
<td>0.01009</td>
<td>0.01000</td>
<td>0.00990</td>
<td></td>
</tr>
<tr>
<td>24.22</td>
<td>0.03571</td>
<td>0.01724</td>
<td>0.01538</td>
<td>0.01051</td>
<td>0.01031</td>
<td>0.01020</td>
<td>0.01010</td>
<td>0.01000</td>
<td>0.00999</td>
<td></td>
</tr>
<tr>
<td>25.50</td>
<td>0.03571</td>
<td>0.01724</td>
<td>0.01538</td>
<td>0.01050</td>
<td>0.01020</td>
<td>0.01010</td>
<td>0.01000</td>
<td>0.00999</td>
<td>0.00999</td>
<td></td>
</tr>
<tr>
<td>28.66</td>
<td>0.03571</td>
<td>0.01724</td>
<td>0.01538</td>
<td>0.01050</td>
<td>0.01020</td>
<td>0.01010</td>
<td>0.01000</td>
<td>0.00999</td>
<td>0.00990</td>
<td></td>
</tr>
<tr>
<td>30.86</td>
<td>0.03571</td>
<td>0.01724</td>
<td>0.01538</td>
<td>0.01050</td>
<td>0.01020</td>
<td>0.01010</td>
<td>0.01000</td>
<td>0.00999</td>
<td>0.00990</td>
<td></td>
</tr>
<tr>
<td>31.91</td>
<td>0.03571</td>
<td>0.01724</td>
<td>0.01538</td>
<td>0.01050</td>
<td>0.01020</td>
<td>0.01010</td>
<td>0.01000</td>
<td>0.00999</td>
<td>0.00990</td>
<td></td>
</tr>
<tr>
<td>35.74</td>
<td>0.03571</td>
<td>0.01724</td>
<td>0.01538</td>
<td>0.01050</td>
<td>0.01020</td>
<td>0.01010</td>
<td>0.01000</td>
<td>0.00999</td>
<td>0.00990</td>
<td></td>
</tr>
</tbody>
</table>

**Notes:**
- U(X) and X are variables in the table.
- The values for CE, TB, RK, CF, F, FM100, MV101, and ND102 are provided in the table.
- The table contains numerical data for various calculations or measurements.

**Formulas:**
- For each row, there are calculations involving CE, TB, RK, CF, F, FM100, MV101, and ND102.
- The values are rounded to the nearest decimal place.
<table>
<thead>
<tr>
<th>UX</th>
<th>FM100</th>
<th>MV101</th>
<th>NO102</th>
<th>LW103</th>
</tr>
</thead>
<tbody>
<tr>
<td>00.04</td>
<td>0.95255</td>
<td>0.95250</td>
<td>0.95245</td>
<td>0.95241</td>
</tr>
<tr>
<td>00.05</td>
<td>0.94123</td>
<td>0.94117</td>
<td>0.94112</td>
<td>0.94106</td>
</tr>
<tr>
<td>00.06</td>
<td>0.93020</td>
<td>0.93014</td>
<td>0.93008</td>
<td>0.93001</td>
</tr>
<tr>
<td>00.07</td>
<td>0.91946</td>
<td>0.91939</td>
<td>0.91933</td>
<td>0.91926</td>
</tr>
<tr>
<td>00.08</td>
<td>0.90901</td>
<td>0.90894</td>
<td>0.90887</td>
<td>0.90879</td>
</tr>
<tr>
<td>00.09</td>
<td>0.89882</td>
<td>0.89876</td>
<td>0.89868</td>
<td>0.89861</td>
</tr>
<tr>
<td>00.10</td>
<td>0.88892</td>
<td>0.88885</td>
<td>0.88877</td>
<td>0.88870</td>
</tr>
<tr>
<td>00.11</td>
<td>0.86990</td>
<td>0.86982</td>
<td>0.86974</td>
<td>0.86966</td>
</tr>
<tr>
<td>00.12</td>
<td>0.85181</td>
<td>0.85173</td>
<td>0.85164</td>
<td>0.85156</td>
</tr>
<tr>
<td>00.13</td>
<td>0.83452</td>
<td>0.83443</td>
<td>0.83434</td>
<td>0.83425</td>
</tr>
<tr>
<td>00.14</td>
<td>0.81793</td>
<td>0.81783</td>
<td>0.81773</td>
<td>0.81762</td>
</tr>
<tr>
<td>00.15</td>
<td>0.80155</td>
<td>0.80147</td>
<td>0.80138</td>
<td>0.80121</td>
</tr>
<tr>
<td>00.16</td>
<td>0.78653</td>
<td>0.78642</td>
<td>0.78630</td>
<td>0.78617</td>
</tr>
<tr>
<td>00.17</td>
<td>0.77165</td>
<td>0.77152</td>
<td>0.77140</td>
<td>0.77126</td>
</tr>
<tr>
<td>00.18</td>
<td>0.75726</td>
<td>0.75713</td>
<td>0.75695</td>
<td>0.75685</td>
</tr>
<tr>
<td>00.19</td>
<td>0.74335</td>
<td>0.74321</td>
<td>0.74307</td>
<td>0.74291</td>
</tr>
<tr>
<td>00.20</td>
<td>0.72985</td>
<td>0.72974</td>
<td>0.72959</td>
<td>0.72943</td>
</tr>
<tr>
<td>00.21</td>
<td>0.70424</td>
<td>0.70409</td>
<td>0.70392</td>
<td>0.70375</td>
</tr>
<tr>
<td>00.22</td>
<td>0.68016</td>
<td>0.68003</td>
<td>0.67986</td>
<td>0.67968</td>
</tr>
<tr>
<td>00.23</td>
<td>0.65766</td>
<td>0.65743</td>
<td>0.65725</td>
<td>0.65707</td>
</tr>
<tr>
<td>00.24</td>
<td>0.63633</td>
<td>0.63615</td>
<td>0.63597</td>
<td>0.63577</td>
</tr>
<tr>
<td>00.25</td>
<td>0.61624</td>
<td>0.61605</td>
<td>0.61585</td>
<td>0.61564</td>
</tr>
<tr>
<td>00.26</td>
<td>0.59715</td>
<td>0.59699</td>
<td>0.59678</td>
<td>0.59655</td>
</tr>
<tr>
<td>00.27</td>
<td>0.57909</td>
<td>0.57888</td>
<td>0.57865</td>
<td>0.57841</td>
</tr>
<tr>
<td>00.28</td>
<td>0.56187</td>
<td>0.56164</td>
<td>0.56139</td>
<td>0.56114</td>
</tr>
<tr>
<td>00.29</td>
<td>0.54544</td>
<td>0.54519</td>
<td>0.54494</td>
<td>0.54466</td>
</tr>
<tr>
<td>00.30</td>
<td>0.52975</td>
<td>0.52949</td>
<td>0.52922</td>
<td>0.52893</td>
</tr>
<tr>
<td>00.31</td>
<td>0.50035</td>
<td>0.49911</td>
<td>0.49883</td>
<td>0.49851</td>
</tr>
<tr>
<td>00.32</td>
<td>0.47347</td>
<td>0.47318</td>
<td>0.47298</td>
<td>0.47265</td>
</tr>
<tr>
<td>00.33</td>
<td>0.44876</td>
<td>0.44847</td>
<td>0.44816</td>
<td>0.44783</td>
</tr>
<tr>
<td>00.34</td>
<td>0.42606</td>
<td>0.42577</td>
<td>0.42547</td>
<td>0.42514</td>
</tr>
<tr>
<td>00.35</td>
<td>0.40517</td>
<td>0.40489</td>
<td>0.40459</td>
<td>0.40427</td>
</tr>
<tr>
<td>00.36</td>
<td>0.38585</td>
<td>0.38562</td>
<td>0.38531</td>
<td>0.38499</td>
</tr>
<tr>
<td>00.37</td>
<td>0.36804</td>
<td>0.36776</td>
<td>0.36745</td>
<td>0.36712</td>
</tr>
<tr>
<td>00.38</td>
<td>0.35145</td>
<td>0.35117</td>
<td>0.35087</td>
<td>0.35053</td>
</tr>
<tr>
<td>00.39</td>
<td>0.33602</td>
<td>0.33575</td>
<td>0.33544</td>
<td>0.33510</td>
</tr>
<tr>
<td>00.40</td>
<td>0.32166</td>
<td>0.32138</td>
<td>0.32106</td>
<td>0.32072</td>
</tr>
<tr>
<td>00.41</td>
<td>0.29574</td>
<td>0.29544</td>
<td>0.29510</td>
<td>0.29477</td>
</tr>
<tr>
<td>00.42</td>
<td>0.27295</td>
<td>0.27265</td>
<td>0.27225</td>
<td>0.27180</td>
</tr>
<tr>
<td>00.43</td>
<td>0.25280</td>
<td>0.25239</td>
<td>0.25191</td>
<td>0.25138</td>
</tr>
<tr>
<td>00.44</td>
<td>0.23476</td>
<td>0.23426</td>
<td>0.23370</td>
<td>0.23309</td>
</tr>
<tr>
<td>00.45</td>
<td>0.21857</td>
<td>0.21800</td>
<td>0.21737</td>
<td>0.21668</td>
</tr>
<tr>
<td>00.46</td>
<td>0.20404</td>
<td>0.20340</td>
<td>0.20270</td>
<td>0.20194</td>
</tr>
<tr>
<td>00.47</td>
<td>0.19095</td>
<td>0.19023</td>
<td>0.18944</td>
<td>0.18859</td>
</tr>
<tr>
<td>00.48</td>
<td>0.17505</td>
<td>0.17423</td>
<td>0.17335</td>
<td>0.17239</td>
</tr>
<tr>
<td>00.49</td>
<td>0.16914</td>
<td>0.16822</td>
<td>0.16723</td>
<td>0.16617</td>
</tr>
<tr>
<td>00.50</td>
<td>0.15807</td>
<td>0.15705</td>
<td>0.15597</td>
<td>0.15482</td>
</tr>
<tr>
<td>00.51</td>
<td>0.14122</td>
<td>0.13894</td>
<td>0.13770</td>
<td>0.13641</td>
</tr>
<tr>
<td>00.52</td>
<td>0.12472</td>
<td>0.12344</td>
<td>0.12211</td>
<td>0.12074</td>
</tr>
<tr>
<td>00.53</td>
<td>0.11153</td>
<td>0.11019</td>
<td>0.10883</td>
<td>0.10745</td>
</tr>
<tr>
<td>00.54</td>
<td>0.10023</td>
<td>0.09889</td>
<td>0.09757</td>
<td>0.09616</td>
</tr>
<tr>
<td>00.55</td>
<td>0.09053</td>
<td>0.08922</td>
<td>0.08789</td>
<td>0.08656</td>
</tr>
<tr>
<td>00.56</td>
<td>0.08220</td>
<td>0.08092</td>
<td>0.07956</td>
<td>0.07838</td>
</tr>
<tr>
<td>00.57</td>
<td>0.07561</td>
<td>0.07439</td>
<td>0.07305</td>
<td>0.07136</td>
</tr>
<tr>
<td>00.58</td>
<td>0.06890</td>
<td>0.06763</td>
<td>0.06648</td>
<td>0.06533</td>
</tr>
<tr>
<td>00.59</td>
<td>0.06341</td>
<td>0.06230</td>
<td>0.06126</td>
<td>0.05612</td>
</tr>
<tr>
<td>00.60</td>
<td>0.05870</td>
<td>0.05764</td>
<td>0.05660</td>
<td>0.05568</td>
</tr>
<tr>
<td>00.61</td>
<td>0.05092</td>
<td>0.04995</td>
<td>0.04901</td>
<td>0.04810</td>
</tr>
<tr>
<td>U(X)</td>
<td>FM100</td>
<td>MV101</td>
<td>NO102</td>
<td>LW103</td>
</tr>
<tr>
<td>------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>07.58</td>
<td>0.04475</td>
<td>0.04387</td>
<td>0.04303</td>
<td>0.04220</td>
</tr>
<tr>
<td>09.22</td>
<td>0.03974</td>
<td>0.03895</td>
<td>0.03819</td>
<td>0.03745</td>
</tr>
<tr>
<td>08.86</td>
<td>0.03563</td>
<td>0.03488</td>
<td>0.03419</td>
<td>0.03353</td>
</tr>
<tr>
<td>09.50</td>
<td>0.03212</td>
<td>0.03147</td>
<td>0.03084</td>
<td>0.03024</td>
</tr>
<tr>
<td>10.14</td>
<td>0.02916</td>
<td>0.02856</td>
<td>0.02799</td>
<td>0.02745</td>
</tr>
<tr>
<td>10.78</td>
<td>0.02661</td>
<td>0.02607</td>
<td>0.02555</td>
<td>0.02505</td>
</tr>
<tr>
<td>11.42</td>
<td>0.02440</td>
<td>0.02390</td>
<td>0.02343</td>
<td>0.02298</td>
</tr>
<tr>
<td>12.06</td>
<td>0.02248</td>
<td>0.02203</td>
<td>0.02160</td>
<td>0.02119</td>
</tr>
<tr>
<td>12.70</td>
<td>0.02081</td>
<td>0.02040</td>
<td>0.02001</td>
<td>0.01964</td>
</tr>
<tr>
<td>13.26</td>
<td>0.01813</td>
<td>0.01779</td>
<td>0.01746</td>
<td>0.01716</td>
</tr>
<tr>
<td>14.54</td>
<td>0.01464</td>
<td>0.01440</td>
<td>0.01418</td>
<td>0.01397</td>
</tr>
<tr>
<td>16.82</td>
<td>0.01350</td>
<td>0.01329</td>
<td>0.01310</td>
<td>0.01291</td>
</tr>
<tr>
<td>19.10</td>
<td>0.01258</td>
<td>0.01240</td>
<td>0.01222</td>
<td>0.01205</td>
</tr>
<tr>
<td>20.38</td>
<td>0.01161</td>
<td>0.01164</td>
<td>0.01148</td>
<td>0.01132</td>
</tr>
<tr>
<td>21.66</td>
<td>0.01113</td>
<td>0.01097</td>
<td>0.01082</td>
<td>0.01067</td>
</tr>
<tr>
<td>22.94</td>
<td>0.01051</td>
<td>0.01037</td>
<td>0.01022</td>
<td>0.01009</td>
</tr>
<tr>
<td>24.22</td>
<td>0.01000</td>
<td>0.00980</td>
<td>0.00980</td>
<td>0.00971</td>
</tr>
<tr>
<td>SHELL (1S)</td>
<td>2</td>
<td>(1S)</td>
<td>2</td>
<td>(1S)</td>
</tr>
<tr>
<td>SHELL (2S)</td>
<td>2</td>
<td>(2S)</td>
<td>2</td>
<td>(2S)</td>
</tr>
<tr>
<td>SHELL (2P)</td>
<td>6</td>
<td>(2P)</td>
<td>6</td>
<td>(2P)</td>
</tr>
<tr>
<td>SHELL (3S)</td>
<td>2</td>
<td>(3S)</td>
<td>2</td>
<td>(3S)</td>
</tr>
<tr>
<td>SHELL (3P)</td>
<td>6</td>
<td>(3P)</td>
<td>6</td>
<td>(3P)</td>
</tr>
<tr>
<td>SHELL (4S)</td>
<td>2</td>
<td>(4S)</td>
<td>2</td>
<td>(4S)</td>
</tr>
<tr>
<td>SHELL (4P)</td>
<td>6</td>
<td>(4P)</td>
<td>6</td>
<td>(4P)</td>
</tr>
<tr>
<td>SHELL (5S)</td>
<td>2</td>
<td>(5S)</td>
<td>2</td>
<td>(5S)</td>
</tr>
<tr>
<td>SHELL (5P)</td>
<td>6</td>
<td>(5P)</td>
<td>6</td>
<td>(5P)</td>
</tr>
<tr>
<td>SHELL (6S)</td>
<td>2</td>
<td>(6S)</td>
<td>2</td>
<td>(6S)</td>
</tr>
<tr>
<td>SHELL (6P)</td>
<td>6</td>
<td>(6P)</td>
<td>6</td>
<td>(6P)</td>
</tr>
<tr>
<td>SHELL (7S)</td>
<td>2</td>
<td>(7S)</td>
<td>2</td>
<td>(7S)</td>
</tr>
<tr>
<td>SHELL (7P)</td>
<td>6</td>
<td>(7P)</td>
<td>6</td>
<td>(7P)</td>
</tr>
</tbody>
</table>