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A Thesis

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# 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

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# 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.

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# 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:

$$Z(n_i \ell_i m_i) + e \rightarrow Z(n_f \ell_f m_f) + e \quad . \qquad (1)$$

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 Moiseiwitsch 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 Heddle 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:

$$H\Phi_A = E_A\Phi_A \tag{2}$$

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:

$$H = -\frac{1}{2}\sum_{i=1}^{n} \nabla_i^2 - \sum_{i=1}^{n} \frac{Z}{r_i} + \sum_{ij}' \frac{1}{r_{ij}} \quad . \qquad (3)$$

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.

$$\Phi = \phi_a(\vec{r}_i)\cdots\phi_z(\vec{r}_n) \qquad (4)$$

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

$$\sum_{ij}' \frac{1}{r_{ij}} \rightarrow \sum_{i} \left\{ \sum_{j} \int dr_j \frac{|\phi(r_j)|^2}{r_{ij}} \equiv U(r_i) \right\} \qquad (5)$$

The Schröedinger equation for this system is then

$$\sum_{i=1}^{n} \left(-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i} + U(r_i)\right) \prod_k \phi_{a_k}(\vec{r}_k) = E \prod_k \phi_{a_k}(\vec{r}_k) \qquad (6)$$

This equation separates into the set of n-equations

$$\left[-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i} + U(r_i)\right] \phi_{a_i}(\vec{r}_i) = E_i\, \phi_{a_i}(\vec{r}_i) \qquad (7)$$

(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:

$$\left[\frac{d^2}{dr^2} + 2\left(E_{n\ell} + \frac{Z}{r} - U(r)\right) - \frac{\ell(\ell+1)}{r^2}\right] P(N\ell:r) = 0 \quad . \qquad (8)$$

For computational ease in the numerical procedures required by the

Hartree model, this equation is traditionally written:

$$\left\{\frac{d^2}{dr^2} + \frac{2}{r}\left[Y(r) + Y_\circ(n\ell:n\ell:r)\right] - \varepsilon_{n\ell,n\ell} - \frac{\ell(\ell+1)}{r^2}\right\} P(n\ell:r) = 0 \quad (9)$$

where

$$Y(r) = Z - \sum_{n'\ell'} q(n'\ell')\, Y_\circ(n'\ell':n'\ell':r) \quad (10)$$

and where $q(n\ell)$ represents the number of electrons in each shell. $Y_\circ(n'\ell':n'\ell':r)$ is a spherically symmetric charge distribution of radial charge density $|P(n'\ell':r)|^2$. 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.

$$E \leq \int \Psi^+ H \Psi \, d\tau / \int \Psi^+ \Psi \, d\tau \quad . \quad (11)$$

(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 $\Psi = \psi_a(\vec{r}_1)\cdots\psi_z(\vec{r}_n)$ and finding the best solutions of the Schroedinger equation by minimizing $\int \Psi^+ H \Psi \, d\tau / \int \Psi^+ \Psi \, d\tau$ 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, $\Phi_A$, 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

$$\Phi_A = \frac{1}{\sqrt{n!}} \varepsilon_{\alpha\beta\cdots\pi} \, \phi_\alpha(1) \, \phi_\beta(2) \cdots \phi_\pi(n) \tag{12}$$

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

$$\phi(i) = \psi(\vec{r}_i) \, \chi(\sigma_i) \quad . \tag{13}$$

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 analagous to the Hartree equation obtained above. The (H-F) equation is: (See Cyszak (1968).)

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} Y(r) - \varepsilon_{n\ell,n\ell} - \frac{\ell(\ell+1)}{r^2}\right] P(n\ell:r) = -2\int_0^\infty K(n\ell:r,s) \, P(n\ell:s)ds$$
$$+ \sum_{n'\neq n} \varepsilon_{n\ell,n'\ell} \, P(n'\ell:r) \tag{14}$$

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

$$\mathcal{U}_k(r,r') = r_<^{k}/r_>^{k+1} \text{ where } r_{\lessgtr} \text{ refers to } r \text{ or } r'$$

$$K_k(n'\ell';rs) = P(n'\ell':r) \, \mathcal{U}_k(r,s) \, P(n'\ell':s)$$

$$K(n\ell:rs) = \sum_{\substack{n'\ell'\neq n\ell \\ k'}} K_{k'}(n'\ell';rs) + \sum_k \alpha_{k\ell} \, K_k(n\ell:rs) \tag{15}$$

where the $\alpha$'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 $\vec{L}^2$, $\vec{S}^2$ 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 calculation, 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 computers Piper (1956) and Vainshtein (1957) made separate attempts to use the Hartree-Fock model to calculate large numbers of atomic wave functions. In 1963 two authors, Herman and Skillman, produced a calculation of all ground state atomic wave functions for all elements. Other calculations 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:

$$P_i(r) = \sum_j c_{ij} \left[ \frac{(2Z_j)^{2\ell+2A_j+3}}{(2\ell+2A_j+2)!} \right] r^{\ell+A_j+1} e^{-Z_j r} \qquad (16)$$

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 define 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 $\int \Psi^+ H \Psi \, d\tau$ 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 straight forward numerical integration of the Hartree-Fock equation is carried out and the $P(n\ell:r)$ 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,

$$\sum_{n'\neq n} \varepsilon_{n\ell,n'\ell}\, P(n'\ell;r) \quad .$$

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)),

$$V^{\text{exch}}(r) = -6[3/8\pi\,\rho(r)]^{1/3} \quad .$$

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:

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - V(r) - \varepsilon_{n\ell,n\ell}\right] P(n\ell{:}r) = 0 \quad . \qquad (17)$$

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

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

$$\sigma(r) = \sum_{n\ell} q_{n\ell}\,|P(n\ell{:}r)|^2 ; \quad \rho(r) = 4\pi r^2\sigma(r) ; \quad q_{n\ell} = \left[\begin{matrix}\text{occupation}\\ \text{number}\end{matrix}\right] \quad . \qquad (18)$$

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

$$J_{\alpha\gamma}^{\nu} = \int_0^\infty e^{-\lambda z} z^{\nu} F(\alpha,\gamma,kz)\, F(\alpha',\gamma';kz)\, dz \qquad (19)$$

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 $\vec{k}$ 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

$$\psi_c^{-}(\vec{r}) = \frac{1}{4\pi K} \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1)\, e^{-i\delta_\ell} R_{K\ell}(r)\, P_\ell(\hat{k}\cdot\hat{r}) \qquad (20)$$

where $\delta_\ell \equiv \mathrm{ARG}\ \Gamma(\ell+1-i/k)$, $P_\ell$ is the Legendre Polynomial $\hat{i}$ a unit vector and

$$R_{k\ell}(r) = \frac{C_{k\ell}}{(2\ell+1)!}(2kr)e^{-ikr}\,{}_1F_1\left(\frac{i}{k}+\ell+1, 2\ell+2, 2ikr\right) \qquad (21)$$

where

$$C_{k\ell} = \frac{2\sqrt{k}}{(1-\exp(-2\pi/k))}\prod_{s=1}^{\ell}(s^2+1/k^2)^{1/2} \quad \text{Note } \ell=0 \Rightarrow \prod^{\ell}=1 \qquad (22)$$

and where ${}_1F_1(a,b,c)$ is the confluent hypergeometric (i.e. Kummer's) function, (see McGuire (1973)). These wave functions have the asymptotic form

$$\psi_c^-(r) \sim \frac{1}{k^2}\sin\left[kr-\frac{\ell\pi}{2}+\frac{1}{k}\ln(2kr)+\delta_\ell\right] \qquad (23)$$

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

$$e^{-ikr}\,{}_1F_1\left(\frac{i}{k}+\ell+1, 2\ell+2, 2ikr\right) = \sum_{N=\ell+1}^{\infty} A_N^{\ell}(k)(kr)^{N-\ell-1} \qquad (24)$$

where

$$A_{\ell+1}^{\ell}(k) = 1 \;; \quad A_{\ell+2}^{\ell}(k) = -\frac{1}{k}(\ell+1)$$

and

$$(N+\ell)(N-\ell-1)A_N^{\ell}(k) = -(2/k)A_{N-1}^{\ell}(k) - A_{N-2}^{\ell}(k)\,. \qquad (25)$$

This expression is given by Abramowitz (1964). The convergence of this series over the range of $\ell$,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, $Q(n_i\ell_i \rightarrow n_f\ell_f)$, we are interested in calculating may be obtained from the scattering amplitude $f(\theta,\phi)$. The general expression is developed below.

The Schröedinger 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:

$$\left(\left[-\frac{1}{2}\sum_s \nabla_s^2 - \sum_s \frac{Z}{r_s} + \sum_{st}{}' \frac{1}{r_{st}}\right] + \left[-\frac{1}{2}\nabla_o^2 - \frac{Z}{r_o} + \sum_s \frac{1}{r_{os}}\right]\right)\Psi(\vec{r}_o,\vec{r}_1\cdots\vec{r}_Z) = E\,\Psi(\vec{r}_o,\vec{r}_1\cdots\vec{r}_Z) \tag{26}$$

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

$$\left[-\frac{1}{2}\sum_s \nabla_s^2 - \sum_s \frac{Z}{r_s} + \sum_{st}{}' \frac{1}{r_{st}}\right]\Psi_A(\vec{r}_1\cdots\vec{r}_Z) = E_A\,\Psi_A(\vec{r}_1\cdots\vec{r}_Z) \tag{27}$$

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.

$$\Psi(\vec{r}_o,\vec{r}_1\cdots\vec{r}_Z) = \int_P F_P(\vec{r}_o)\,\Psi_P(\vec{r}_1\cdots\vec{r}_Z) \tag{28}$$

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

$$\left[\nabla^2 + k_F^2\right] F_F(\vec{r}_o) = 2\int d\vec{r}_1\cdots d\vec{r}_Z\,\Psi_F(\vec{r}_1\cdots\vec{r}_Z)\,V(\vec{r}_o,\vec{r}_1\cdots\vec{r}_Z)\,\Psi(\vec{r}_o,\vec{r}_1\cdots\vec{r}_Z) \tag{29}$$

where

$$V(\vec{r}_0,\vec{r}_1\cdots\vec{r}_Z)=\sum_{s}\frac{1}{r_{0s}}-\frac{Z}{r_0} \tag{30}$$

and

$k_F^2 = 2(E-E_F)$;

$E$ = total energy of system;

$E_F$ = final energy of atomic target.

Assuming the incoming electron is incident with wave vector $\vec{k}_I$ then our problem requires the asymptotic boundry condition

$$F_F(\vec{r}_0)\backsim \exp\left[i\vec{k}\cdot\vec{r}_0\right]\delta_{FI}+r_0^{-1}\exp\left[ik_F r_0\right]f_F(\theta,\phi) \tag{31}$$

Since our equation for $F_F(\vec{r}_0)$ is of the Helmholtz form with a source term, we may write the solution in terms of a Green's function $G(\vec{r}_0,\vec{r}\,')$

$$\begin{aligned}F_F(\vec{r}_0)=\exp\left[i\vec{k}_I\cdot\vec{r}_0\right]\delta_{FI}+2\int d\vec{r}\,'d\vec{r}_1\cdots d\vec{r}_Z\,\Psi_F(\vec{r}_1\cdots\vec{r}_Z)\\ \times V(\vec{r}\,',\vec{r}_1\cdots\vec{r}_Z)\,G(\vec{r}_0,\vec{r}\,')\,\Psi(\vec{r}_0,\vec{r}_1\cdots\vec{r}_Z).\end{aligned} \tag{32}$$

Here G satisfies the equation

$$\left[\nabla^2+k_F^2\right]G(\vec{r}_0,\vec{r}_1)=\delta(\vec{r}_0-\vec{r}\,') \tag{33}$$

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

$$G(\vec{r}_0,\vec{r}_1)=-\exp\left[ik_F|\vec{r}_0-\vec{r}\,'|\right]/(4\pi|\vec{r}_0-\vec{r}\,'|) \tag{34}$$

Then expanding equation G for large $\vec{r}_0$ and using

$$k_F|\vec{r}_0-\vec{r}\,'|=k_F r_0-\vec{k}_F\cdot\vec{r}\,' \qquad \text{where } \hat{k}_F=\hat{r}_0$$

we can compare the asymptotic expression for Eq. (32) with that given in Eq. (31) to obtain the result

$$f_F(\Theta\phi) = -\left(\frac{2}{4\pi}\right)\int d\vec{r}\, d\vec{r}_1 \ldots d\vec{r}_z \exp[-i\vec{K}_F\cdot\vec{r}]\, \Psi_F^{+}(\vec{r}_1\ldots\vec{r}_z)\, V(\vec{r},\vec{r}_1\ldots\vec{r}_z)\, \Psi(\vec{r},\vec{r}_1\ldots\vec{r}_z) \tag{35}$$

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

$$S(\vec{r},t) = \frac{1}{2i}\left[\Psi^{+}(\vec{r},t)\nabla_r\Psi(\vec{r},t) - \nabla_r\Psi^{+}(\vec{r},t)\Psi(\vec{r},t)\right] \tag{36}$$

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

$$dQ/d\Omega = (K_F/K_I)|f(\Theta\phi)|^2 \tag{37}$$

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

$$Q = (K_F/K_I)\int d\Omega\, |f_F(\Omega)|^2 \tag{38}$$

It can be seen from Eq. (35) that the scattering amplitude involves the total wave function for the incident electron and the atomic target, $\Psi(\vec{r}_o, \vec{r}_1\cdots\vec{r}_2)$. 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.

$$\Psi(\vec{r}_0, \vec{r}_1, \ldots \vec{r}_z) = \exp[i\vec{K}_I \cdot \vec{r}_0]\, \Psi(\vec{r}_1, \ldots \vec{r}_z) \; . \tag{39}$$

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

$$f_{BORN}(d\Omega) = -(1/2\pi)\int d\vec{r}\,' \exp[i(\vec{K}_I - \vec{K}_F)\cdot r'] \, V(\vec{r}\,') \tag{40}$$

where

$$V_{FI}(\vec{r}\,') = \int d\vec{r}_1 \cdots d\vec{r}_z \, \Psi_F^{+}(\vec{r}_1, \ldots \vec{r}_z)\left[-\frac{Z}{r'} + \sum_s \frac{1}{|\vec{r}\,' - \vec{r}_s|}\right] \Psi_I(\vec{r}_1, \ldots \vec{r}_z) \tag{41}$$

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)),

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

where $\vec{K} \equiv \vec{k}_I - \vec{k}_F$, the first Born Scattering amplitude can be rewritten

$$f_{BORN}(\Omega) = -(2/K^2)\, I_{FI} \qquad F \neq I \tag{43}$$

where

$$I_{FI} = \sum_{s=1}^{Z} \int d\vec{r}_1 \ldots d\vec{r}_Z \exp[i\vec{K}\cdot\vec{r}_s] \Psi_F^{+}(\vec{r}_1 \ldots \vec{r}_Z) \Psi_I(\vec{r}_1 \ldots \vec{r}_Z) \quad . \tag{44}$$

A further simplification results from the following argument.

Recall that a Hartree-Fock wave is an antisymmetrized product wave function of the form

$$\Phi_A = (1/\sqrt{Z!})\, \varepsilon_{\alpha\beta\ldots\pi} \phi_\alpha(1)\phi_\beta(2) \ldots \phi_\pi(Z) \quad . \tag{45}$$

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 $\chi(\sigma_1 \cdots \sigma_Z)$)

$$\begin{aligned} &\sum_{s=1}^{Z} \int d\vec{r}_1 \ldots d\vec{r}_Z \Psi_F^{*}(\vec{r}_1 \ldots \vec{r}_Z) \exp[i\vec{K}\cdot\vec{r}_s] \Psi_I(\vec{r}_1 \ldots \vec{r}_Z) \chi_F(\sigma_1 \ldots \sigma_Z) \chi_I(\sigma_1 \ldots \sigma_Z) = \\ &\left(\frac{1}{Z!}\right) \sum_{s=1}^{Z} \varepsilon_{\alpha' \ldots \pi'} \varepsilon_{\alpha \ldots \pi} \int d\vec{r}_1 \ldots d\vec{r}_Z \phi_{\alpha'}^{(f)*}(\vec{r}_1\sigma_1) \ldots \phi_{\pi'}^{(f)*}(\vec{r}_Z\sigma_Z) \exp[i\vec{K}\cdot\vec{r}_s] \\ &\qquad \times \phi_\alpha^{(i)}(\vec{r}_1\sigma_1) \cdots \phi_\pi^{(i)}(\vec{r}_Z\sigma_Z) \end{aligned} \tag{46}$$

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

$$\varepsilon_{\alpha\beta\ldots\pi} \varepsilon_{\alpha\beta\ldots\pi'} = (Z-1)!\,\delta_{\pi\pi'} \tag{47}$$

(where Z is the number of indices). Consider the p^th^ term of the sum over s in Eq. (44)

$$J_p' = [\varepsilon_{\alpha'\ldots\pi'}\varepsilon_{\alpha\ldots\pi}/Z!]\int d\vec{r}_1\ldots d\vec{r}_p\ldots d\vec{r}_Z\,\phi_{\alpha'}^{(f)*}(\vec{r}_1\sigma_1)\cdots\phi_{\gamma'}^{(f)*}(\vec{r}_p\sigma_p)\cdots\phi_{\pi'}^{(f)*}(\vec{r}_Z\sigma_Z)$$

$$\exp[i\vec{K}\cdot\vec{r}_p]\phi_\alpha^{(i)}(\vec{r}_1\sigma_1)\cdots\phi_\gamma^{(i)}(\vec{r}_p\sigma_p)\cdots\phi_\pi^{(i)}(\vec{r}_Z\sigma_Z) = [\varepsilon_{\alpha'\ldots\pi'}\varepsilon_{\alpha\ldots\pi}/Z!] \tag{48}$$

$$\int d\vec{r}_1\phi_{\alpha'}^{(f)*}(1)\phi_\alpha^{(i)}(1)\cdots\int d\vec{r}_p\phi_{\gamma'}^{(f)*}(\vec{r}_p)\exp[i\vec{K}\cdot\vec{r}_p]\phi_\gamma^{(i)}(p)\cdots\int d\vec{r}_Z\phi_{\pi'}^{(f)*}(Z)\phi_\pi^{(i)}(Z)$$

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

$$J_p' = \frac{\varepsilon_{\alpha\ldots\gamma\ldots\pi}\,\varepsilon_{\alpha\ldots\gamma'\ldots\pi}}{Z!}\int d\vec{r}_p\phi_{\gamma'}^{(f)*}(\vec{r}_p\sigma_p)\exp[i\vec{K}\cdot\vec{r}_p]\phi_\gamma^{(i)}(r_p\sigma_p) \tag{49}$$

which gives

$$J_p' = \frac{(Z-1)!}{Z!}\,\delta_{\gamma\gamma'}\int d\vec{r}_p\phi_{\gamma'}^{(f)*}(\vec{r}_p,\sigma_p)\phi_\gamma^{(i)}(\vec{r}_p,\sigma_p)\exp[i\vec{K}\cdot\vec{r}_p] \tag{50}$$

where $\phi_\gamma^i$ and $\phi_{\gamma'}^f$ 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, $\phi(\vec{r}_p,\sigma_p) = \psi(\vec{r}_p)\chi(\sigma_p)$ .) Since $J_p$ is clearly independent of p (after integration over $\vec{r}_p$) the sum in $I_{FI}$ results only in a factor of Z, and the expression for $f_{born}$ reduces to the form,

$$f_{BORN}(\Omega) = -(2/K^2)\int d\vec{r}\,\psi_f^+(\vec{r})\exp[i\vec{K}\cdot\vec{r}]\psi_i(\vec{r}) \tag{51}$$

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

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

$$K^2 = K_I^2 + K_F^2 - 2K_IK_F\cos\Theta\,;\quad K\,dK = K_IK_F\sin\Theta\,d\Theta \tag{52}$$

and the total cross-section can be expressed in the form

$$Q = (K_I/K_F)\int d\Omega\,|f_{BORN}(\Omega)|^2 = (K_I/K_F)(2\pi)\int_0^{\pi}|f(\Theta)|^2\sin\Theta\, d\Theta \tag{53}$$

$$= (2\pi/K_I^2)\int_{K_{min}}^{K_{max}}|f(K)|^2 dK\ ; \quad K_{min}^{max} = K_I \pm K_F$$

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

$$Q[\pi a_B^2] = \int_{K_{min}}^{K_{max}}\left(\frac{2}{K_I^2}\right)|f_{BORN}(K)|^2 K\, dK \tag{54}$$

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

Consider.

$$\sum_{m_i m_f}\frac{|f(K)|^2}{(2\ell_i+1)} = \frac{4}{K^4(2\ell_i+1)}\sum_{m_i m_f}\left|\int d\vec{r}\,\Psi_f^{\dagger}(\vec{r})\exp[i\vec{K}\cdot\vec{r}]\Psi_i(\vec{r})\right|^2 \tag{55}$$

For the integration over $\vec{r}$ choose the z-axis along the $\vec{K}$-direction and recall, (Jackson (1962))

$$\exp[iKr\cos\Theta] = \sum_{\lambda} i^{\lambda}[4\pi(2\lambda+1)]^{1/2} j_{\lambda}(Kr)\, Y_{\lambda 0}(\Omega) \tag{56}$$

Since $\psi_{n\ell m}(\vec{r})$ can be written as $\dfrac{P_{n\ell}(r)Y_{\ell m}(\Omega)}{r}$

we may write

$$\sum_{m_i m_f}\left|\int d\vec{r}\,\Psi_f^{+}(\vec{r})\exp[iKr\cos\Theta]\,\Psi_i(\vec{r})\right|^2=\sum_{m_i m_f}\Big|\sum_{\lambda}[4\pi(2\lambda+1)]^{1/2}$$
$$\times\int dr\,P(f)\,j_\lambda(Kr)\,P(i)\int d\Omega\,Y_{\ell_f m_f}^{+}(\Omega)\,Y_{\lambda 0}(\Omega)\,Y_{\ell_i m_i}(\Omega)\Big|^2=$$
$$\sum_{\lambda\lambda'}(i)^{\lambda}(-i)^{\lambda'}(4\pi)[(2\lambda+1)(2\lambda'+1)]^{1/2}\int dr\,dr'\,\{P(f)\,j_\lambda(Kr)\,P(i) \tag{57}$$
$$\times P'(f)\,j_{\lambda'}(K'r')\,P'(i)\}\sum_{m_i m_f}\int d\Omega\,Y_{\ell_f m_f}^{+}(\Omega)\,Y_{\lambda 0}(\Omega)\,Y_{\ell_i m_i}(\Omega)\int d\Omega'\,Y_{\ell_f m_f}(\Omega')\,Y_{\lambda' 0}(\Omega')\,Y_{\ell_i m_i}(\Omega')$$

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,

$$\sum_{m_i m_f}\left|\int d\vec{r}\,\Psi_f^{+}(\vec{r})\exp[i\vec{K}\cdot\vec{r}]\,\Psi_i(\vec{r})\right|^2=\sum_{\lambda\lambda'}(i)^{\lambda}(-i)^{\lambda'}(4\pi)[(2\lambda+1)(2\lambda'+1)]^{1/2}$$
$$\times\left[\int_0^\infty dr\,P(i)\,j_\lambda(Kr)\,P(f)\int dr'\,P'(i)\,j_{\lambda'}(Kr')\,P'(f)\right]\frac{(2\ell_f+1)(2\ell_i+1)}{4\pi} \tag{58}$$
$$\times\begin{pmatrix}\ell_i & \ell_f & \lambda\\ 0 & 0 & 0\end{pmatrix}^2\delta_{\lambda\lambda'}\,\Delta(\ell_i\ell_f\lambda)=\sum_{\lambda=0}^{\infty}(2\ell_f+1)(2\ell_i+1)(2\lambda+1)\begin{pmatrix}\ell_i & \ell_f & \lambda\\ 0 & 0 & 0\end{pmatrix}^2$$
$$\times\left|\int_0^\infty dr\,P_{n_i\ell_i}(r)\,j_\lambda(Kr)\,P_{n_f\ell_f}(r)\right|^2\Delta(\ell_i\ell_f\lambda)$$

Since the triangle rule, $\Delta(\ell_i\ell_f\lambda)$, requires $\lambda(\text{minimum}) = |\ell_i-\ell_f|$ and $\lambda(\text{maximum}) = \ell_i+\ell_f$, we obtain for the required sum the result

$$\left|f'_{BORN}(K)\right|^2=\sum_{m_i m_f}\left|f_{BORN}(K)\right|^2\Big/(2\ell_i+1)=(4/K^4)\sum_{\lambda=\lambda_{min}}^{\lambda=\lambda_{max}}(2\ell_f+1)(2\lambda+1) \tag{59}$$
$$\times\begin{pmatrix}\ell_i & \ell_f & \lambda\\ 0 & 0 & 0\end{pmatrix}^2\left|\int dr\,P_{n_f\ell_f}(r)\,j_\lambda(Kr)\,P_{n_i\ell_i}(r)\right|^2$$

Finally the expression for the Born-approximation cross-section $Q[n_i\ell_i\rightarrow n_f\ell_f]$ reduces to

$$Q[\pi a_B^2]=(2/K_I^2)\int_{K_I-K_F}^{K_I+K_F}\left|f'_{BORN}(K)\right|^2K\,dK \tag{60}$$

This form of $|f'_{born}(K)|^2$ is used in the Born option of the cross-section program.

### 3. Bethe Approximation

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

$$|f_{BORN}(K)|^2 = \left| -(2/K^2)\int d\vec{r}\,\Psi_f^{+}(\vec{r})\exp[i\vec{K}\cdot\vec{r}]\Psi_i(\vec{r})\right|^2 \tag{61}$$

When the z-axis is chosen in the K-direction for the integration and exp[iKr cosθ] is expanded, the following series is obtained

$$|f_{BORN}(K)|^2 = (4/K^4)\left[K^2|(z)_{if}|^2 + (K^4/4)|(z^2)_{if}|^2 + \cdots\right] \tag{62}$$

where

$$(z^s)_{if} = \int \Psi_f^{+}(\vec{r})(r\cos\Theta)^s\Psi_i(\vec{r})\,d\vec{r} \tag{63}$$

This series converges provided $Ka_B \ll 1$ where $a_B$, the Bohr radius, is the approximate range of the atomic wave functions. For $Ka_B \gg 1$ $|\underset{Born}{f(K)}|^2$ 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 $P_\ell(X)$ has $X^\ell$ as its highest power of X, the next highest being $X^{\ell-2}$, and so on. This may be seen by the power series solution of the Legendre equation, (Jackson (1962)). Recall that

$$Y_{\ell 0}(\Theta,\Phi) = \sqrt{\frac{(2\ell+1)}{4\pi}}\, P_\ell(\cos\Theta) \tag{64}$$

Hence (see Abramowitz (1964))

$$(\cos\Theta)^S = \sum_{t=0}^{S} a_t Y_{t0}(\Omega) \tag{65}$$

Using $\Psi_{n\ell m}(\vec{r}) = P_{n\ell}(r)\, Y_{\ell m}(\Omega)/r$

we may write

$$(z^S)_{if} = \int_0^\infty dr\,(r)^S P_{n_f\ell_f}(r) P_{n_i\ell_i}(r) \sum_{t=0}^{S} a_t \langle \ell_f m_f | t0 | \ell_i m_i \rangle \tag{66}$$

Once again we must average over $m_i$ and sum over $m_f$:

$$\sum_{m_i m_f} |f(K)|^2/(2\ell_i+1) = \left(\frac{4}{K^4}\right)(2\ell_i+1)^{-1} \sum_{m_i m_f} (K)^{2S} \,|(z^S)_{if}|^2$$
$$= \left[\frac{4\,K^{2S}}{[K^4(2\ell_i+1)]}\right] \Big| \int_0^\infty dr\,(r)^S P_{n_f\ell_f}(r) P_{n_i\ell_i}(r) \int_0^\infty dr'(r')^S P_{n_f\ell_f}(r') P_{n_i\ell_i}(r') \tag{67}$$
$$\times \sum_{tt'} a_t a_{t'} \sum_{m_i m_f} \langle \ell_f m_f | t0 | \ell_i m_i \rangle \langle \ell_i m_i | t'0 | \ell_f m_f \rangle \Big| .$$

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

$$|f'_{Bethe}(K)|^2 = \frac{4K^{2S}}{K^4} \left| \int_0^\infty dr\,(r)^S P_{n_i\ell_i}(r) P_{n_f\ell_f}(r) \right|^2$$
$$\times \sum_{t=0}^{S} \frac{a_t^2\,(2\ell_f+1)}{4\pi} \begin{pmatrix} \ell_i & \ell_f & t \\ 0 & 0 & 0 \end{pmatrix}^2 \Delta(\ell_i \ell_f t) \tag{68}$$

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

The cross-section $Q_{bethe}(n_i\ell_i \to n_f\ell_f)$ is:

$$Q_{Bethe} = \left(\frac{2}{K_I^2}\right)\int_{k_I - k_F}^{k_I + k_F} \left| f_{Bethe}(K)\right|^2 K\, dK \quad . \tag{69}$$

Noting that the K-dependence is isolated, we may write

$$Q_{Bethe} = \left(\frac{2}{K_I^2}\right)(4)\int_{K_{min}}^{K_{max}} \frac{(K)^{2S}}{(K)^3}\, dK \left|\int_0^{\infty} dr\,(r)^S \right. \tag{70}$$
$$\left. \times P_{n_i l_i}(r) P_{n_f l_f}(r)\right|^2 \sum_{t=0}^{S}\left(\frac{a_t^2}{4\pi}\right)(2l_f+1)\begin{pmatrix} l_i & l_f & t \\ 0 & 0 & 0\end{pmatrix}^2 \Delta(l_i l_f t) .$$

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

$$P_l(x) = \sum_{t=0}^{l} a_t x^t \quad ; \quad a_t = \frac{(2t)!}{2^t\,(t!)^2} \tag{71}$$

### 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 $\hbar[\ell(\ell+1)]^{\frac{1}{2}}$. For these (components) a limiting value of $Q^{\ell}_{max}$ 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 $Q^{\ell}_{bethe} < \frac{1}{2}Q^{\ell}_{max}$ and to put $Q^{\ell} = \frac{1}{2}Q^{\ell}_{max}$ if $Q^{\ell}_{bethe} \geq \frac{1}{2}Q^{\ell}_{max}$."

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

$$f(\theta) = (2ik)^{-1} \sum_{\ell=0}^{\infty} (2\ell+1)(\exp[2i\delta_\ell]-1) P_\ell(\cos\theta) \quad (72)$$

where $\delta_\ell$ 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 $\delta_\ell=\alpha_\ell+i\beta_\ell$. The elastic, absorption, and total cross-sections may be written in terms of these phase shifts. Introducing $s_\ell=\exp[2i\delta_\ell]$ the expression for the absorption cross-section is:

$$Q_{ABS} = \left(\frac{\pi}{k_I}\right)^2 \sum_{\ell=0}^{\infty} (2\ell+1)(1-|s_\ell|^2) \quad (73)$$

Since $|s_\ell|^2$ cannot be less than zero the partial absorption cross-section $Q^\ell$ has a limiting value expressed by the relation

$$Q^\ell \leq \left[ \left(\frac{\pi}{k_I^2}\right)(2\ell+1) \equiv Q^\ell_{max} \right] \quad (74)$$

(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

$$f_{Born}(\Omega) = -\left(\frac{2}{K^2}\right)\int d\vec{r}\; \psi_f^{\dagger}(\vec{r})\; \exp[i\vec{K}\cdot\vec{r}]\; \psi_i(\vec{r}) \tag{75}$$

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

$$f(\Omega) = -\left(\frac{2}{K^2}\right)\int d\vec{r}\; \psi_f^{\dagger}(\vec{r}) \left(\sum_{\ell} \frac{(i\vec{K}\cdot\vec{r})^{\ell}}{\ell!}\right) \psi_i(\vec{r}) \tag{76}$$

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,

$$f_{Born}(\Omega) = -\left(\frac{1}{2\pi}\right)\int d\vec{r}_0\; \exp[i\vec{K}\cdot\vec{r}_0] \left\{\int d\vec{r}_i\; \frac{\psi_f^{\dagger}(\vec{r}_i)\, \psi_i(\vec{r}_i)}{|\vec{r}_0 - \vec{r}_i|}\right\} \tag{77}$$

The asymptotic form for the potential

$$V(\vec{r}_0, \vec{r}_i) = 1/|\vec{r}_0 - \vec{r}_i|$$

for large $|\vec{r}_0|$ is obtained from the expression

$$\frac{1}{|\vec{r}_0 - \vec{r}_i|} = \sum_{\ell=0}^{\infty} \frac{r_<^{\ell}}{r_>^{\ell+1}}\, P_{\ell}(\cos[\hat{r}_0\cdot\hat{r}_i]);\; r_{\lessgtr} \text{ is } r_0 \text{ or } r_i \tag{78}$$

That is

$$V_{Asymp}(\vec{r}_0, \vec{r}_i) \equiv \lim_{r_0\to\infty} \left(\frac{1}{|\vec{r}_0 - \vec{r}_i|}\right) = \sum_{\ell=0}^{\infty} \frac{r_i^{\ell}}{r_0^{\ell+1}}\, P_{\ell}(\cos[\hat{r}_0\cdot\hat{r}_i]) \tag{79}$$

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

$$f(\Omega) = -\left(\frac{1}{2\pi}\right)\int d\vec{r}_0\, e^{i\vec{K}\cdot\vec{r}_0}\left\{\sum_{\ell=0}^{\infty}\int d\vec{r}_1\, \psi_f^{\dagger}(\vec{r}_1)\, \psi_i(\vec{r}_1)\, \frac{r_1^{\ell}}{r_0^{\ell+1}}\, P_\ell\left(\cos[\hat{r}_0\cdot\hat{r}_1]\right)\right\}. \qquad (80)$$

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:

$$Q_{\text{Born}}^{\ell'} = (18)\,(2\ell_f+1)\,\frac{K_F}{K_I}\sum_{\ell\ell''}\frac{(2\ell'+1)(2\ell''+1)}{(2\ell+1)}\begin{pmatrix}\ell_i & \ell_f & \ell\\ 0 & 0 & 0\end{pmatrix}^2$$
$$\times\begin{pmatrix}\ell & \ell' & \ell''\\ 0 & 0 & 0\end{pmatrix}^2\left|\int_0^{\infty} dr_0\, r_0^2\, \mathcal{R}_\ell^{\text{Born}}(r_0)\, \mathring{j}_{\ell'}(K_I r_0)\, \mathring{j}_{\ell''}(K_F r_0)\right|^2 \qquad (81)$$

where

$$\mathcal{R}_\ell^{\text{Born}}(r_0) = \int_0^{\infty} r_1^2\, dr_1\, \frac{r_<^{\ell}}{r_>^{\ell+1}}\, R_{n_f\ell_f}(r_1)\, R_{n_i\ell_i}(r_1)\;;\quad r_\lessgtr = \left\{\begin{matrix} r_0\\ \text{or}\\ r_1\end{matrix}\right\} \qquad (82)$$

Notice that since the Born expression explicitly contains the term $r_<^{\ell}/r_>^{\ell+1}$, we may apply the "potential statement" of the Bethe approximation and obtain the Bethe partial cross-section $Q_{\text{bethe}}^{\ell}$ by the replacement of $\mathcal{R}_\ell^{\text{Born}}(r_0)$ with $\mathcal{R}_\ell^{\text{Bethe}}(r_0) = \int P(f)\,P(i)\,\frac{r_1^{\ell}}{r_f^{\ell+1}}\, dr_1$ in Eq. (81). Then

$$Q_\ell^{\text{Bethe}} = (18)\,(2\ell_f+1)\,\frac{K_F}{K_I}\sum_{\ell'\ell''}\frac{(2\ell'+1)(2\ell''+1)}{(2\ell+1)}\begin{pmatrix}\ell_f & \ell_i & \ell\\ 0 & 0 & 0\end{pmatrix}^2 \qquad (83)$$
$$\times\begin{pmatrix}\ell' & \ell'' & \ell\\ 0 & 0 & 0\end{pmatrix}^2\left|\int_0^{\infty} dr_0\,(r_0)^2\, \mathcal{R}_\ell^{\text{Bethe}}(r_0)\, \mathring{j}_{\ell'}(K_I r_0)\, \mathring{j}_{\ell''}(K_F r_0)\right|^2.$$

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 $\ell_o$ be a value of $\ell$ such that

$$Q^{\ell}_{Bethe} < \left[\frac{1}{2}\,Q^{\ell}_{max} = \left(\frac{1}{2K_I^2}\right)(2\ell+1)\right] \text{ for } (\ell > \ell_o)$$
$$Q^{\ell}_{Bethe} \geqslant \left[\frac{1}{2}\,Q^{\ell}_{max}\right] \text{ for } (\ell \leq \ell_o) \tag{84}$$

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

$$Q_{MB} \doteq \sum_{\ell=0}^{\ell_o} \frac{1}{2}\,Q^{\ell}_{max} + \sum_{\ell=\ell_o+1}^{\infty} Q^{\ell}_{Bethe} \tag{85}$$

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

$$Q_{Bethe} = \sum_{\ell=0}^{\ell_o} Q^{\ell}_{Bethe} + \sum_{\ell=\ell_o+1}^{\infty} Q^{\ell}_{Bethe} \tag{86}$$

or

$$\sum_{\ell=\ell_o+1}^{\infty} Q^{\ell}_{Bethe} = Q_{Bethe} - \sum_{\ell=0}^{\ell_o} Q^{\ell}_{Bethe} \tag{87}$$

Also notice

$$\sum_{\ell=0}^{\ell_o} \frac{1}{2}\,Q^{\ell}_{max} = \left(\frac{1}{2K_I^2}\right)\sum_{\ell=0}^{\ell_o}(2\ell+1) = \left(\frac{1}{2K_I^2}\right)(\ell_o+1)^2 \tag{88}$$

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

$$Q_{MB} = Q_{Bethe} + \left(\frac{1}{2K_I^2}\right)(\ell_o+1)^2 - \sum_{\ell=0}^{\ell_o} Q^{\ell}_{Bethe} \tag{89}$$

The computer program of the present calculation computes $Q^{\ell}_{bethe}$ 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:

$$Q_{Bethe}^{(optical)} = \left(\frac{8\pi}{3K_I^2}\right)(2l_f+1)\begin{pmatrix} l_f & l_i & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 \ln\left[\frac{K_{max}}{K_{min}}\right] \qquad (90)$$

$$\times \left\{\left|\int_0^\infty dr\,(r)\,P_{n_f l_f}(r)\,P_{n_i l_i}(r)\right|^2 \equiv |\langle r\rangle_{if}|^2\right.$$

$$Q_{Bethe}^{l'(optical)} = (72\pi)(2l_f+1)\begin{pmatrix} l_f & l_i & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 |\langle r\rangle_{if}|^2$$

$$\times\ (2l'+1)\left\{\begin{pmatrix} 1 & l' & l'-1 \\ 0 & 0 & 0 \end{pmatrix}^2 J^2(l'-1) + \begin{pmatrix} 1 & l' & l'+1 \\ 0 & 0 & 0 \end{pmatrix} J^2(l'+1)\right. \qquad (91)$$

where

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

(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

$$\Psi(\vec{r}_0,\vec{r}_1) = \int_P F_P(\vec{r}_0)\,\Psi_P(\vec{r}_1) \tag{93}$$

where $\vec{r}_0$ and $\vec{r}_1$ are the position vectors of the scattered electron and the valence electron respectively. The summation 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 $\Psi(\vec{r}_0,\vec{r}_1)$ when $r_0$ is large and when $r_1$ is large. These asymptotic behaviors are:

$$\Psi(\vec{r}_0,\vec{r}_1) \xrightarrow[r_0 \to \infty]{} \Psi_I(\vec{r}_1) \exp(i\vec{k}_I\cdot\vec{r}_0) + r_0^{-1}\exp(ik_F r_0) f_d(\Omega)\Psi_F(\vec{r}_1) \quad (94)$$

$$\Psi(\vec{r}_0,\vec{r}_1) \xrightarrow[r_1 \to \infty]{} \Psi_F(\vec{r}_0)\left[r_1^{-1}\exp(ik_F r_1) f_E(\Omega)\right] \quad (95)$$

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 $(\Psi(\vec{r}_0,\vec{r}_1) - \Psi(\vec{r}_1,\vec{r}_0)$. Similarly the antisymmetric singlet spin eigenfunction must be multiplied by the symmetric spatial function $(\Psi(\vec{r}_0,\vec{r}_1) + \Psi(\vec{r}_1,\vec{r}_0))$.

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

$$\begin{aligned}\Psi(\vec{r}_0,\vec{r}_1) \pm \Psi(\vec{r}_1,\vec{r}_0) \xrightarrow[r_0 \to \infty]{} & \exp(i\vec{k}_I\cdot\vec{r}_0)\Psi_I(\vec{r}_1) \\ & + r_0^{-1}\exp(ik_F r_0)\left[f_d(\Omega) \pm f_e(\Omega)\right]\Psi_F(\vec{r}_1). \end{aligned} \quad (96)$$

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

$$\frac{dQ}{d\Omega} = \frac{1}{4} \left| f_d(\Omega) + f_e(\Omega) \right|^2 + \frac{3}{4} \left| f_d(\Omega) - f_e(\Omega) \right|^2 \qquad (97)$$

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:

$$\bar{\Psi}(\vec{r}_0,\vec{r}_1) = \int_p \left[ F_p(\vec{r}_0)\, \bar{\Psi}_p(\vec{r}_1) \pm F_p(\vec{r}_1)\, \bar{\Psi}_p(\vec{r}_0) \right] \qquad (98)$$

could be approximated

$$\psi(\vec{r}_0,\vec{r}_1) = \exp(i\vec{K}_I\cdot\vec{r}_0)\, \bar{\Psi}_p(\vec{r}_1) \pm \exp(i\vec{K}_F\cdot\vec{r}_1)\, \bar{\Psi}(\vec{r}_0) \qquad (99)$$

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

$$f_d(\Omega) = -\left(\frac{1}{2\pi}\right) \int d\vec{r}_0 \exp\left(i\,[\vec{K}_I - \vec{K}_F]\cdot\vec{r}_0\right) V_{FI}(\vec{r}_0) \qquad (100)$$

where

$$V_{FI}(\vec{r}_0) = \int d\vec{r}_1\, \Psi_F^{\dagger}(\vec{r}_1)\, \frac{1}{|\vec{r}_0 - \vec{r}_1|}\, \Psi_I(\vec{r}_1) \qquad (101)$$

and the exchange amplitude $f_e$ may be written

$$f_E(\Omega) = \left(\frac{1}{2\pi}\right) \iint d\vec{r}_0\, d\vec{r}_1 \exp(i\vec{K}_I\cdot\vec{r}_1)\, \Psi_I(\vec{r}_0) \times \frac{1}{|\vec{r}_0 - \vec{r}_1|} \exp(-i\vec{K}_F\cdot\vec{r}_0)\, \Psi_F^{\dagger}(\vec{r}_1) . \qquad (102)$$

The extension of the above formulae to the 3 electron case is straight forward 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:

$$f_d = -\left(\frac{1}{2\pi}\right)\int d\vec{r}_0 \exp\left(i\left[\vec{K}_I - \vec{K}_F\right]\cdot\vec{r}_0\right) V_{FI}(\vec{r}_0) \tag{103}$$

$$V_{FI}(\vec{r}_0) = \int d\vec{r}_1\, d\vec{r}_2\, \Psi_F^{\dagger}(\vec{r}_1,\vec{r}_2)\left[\frac{1}{|\vec{r}_0-\vec{r}_1|}+\frac{1}{|\vec{r}_0-\vec{r}_2|}\right]\Psi_I(\vec{r}_1,\vec{r}_2) \tag{104}$$

and

$$f_e = \left(\frac{1}{2\pi}\right)\int d\vec{r}_0\, d\vec{r}_1\, d\vec{r}_2\, \Psi_F^{\dagger}(\vec{r}_2,\vec{r}_0)\exp(-i\vec{K}_F\cdot\vec{r}_1) \times\left[\frac{1}{r_{01}}+\frac{1}{r_{02}}\right]\Psi_I(\vec{r}_1,\vec{r}_2)\exp(i\vec{K}_I\cdot\vec{r}_0)\,. \tag{105}$$

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" descrepancy. 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 descrepancy. 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 analagous manner."

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

$$f_e(\Omega) = \left(\frac{2}{K_I^2}\right)\int d\vec{r}_1\, d\vec{r}_2\, \Psi_F^{\dagger}(\vec{r}_2,\vec{r}_1) \exp(i[\vec{K}_I-\vec{K}_F]\cdot\vec{r}_1)\, \Psi_I(\vec{r}_1,\vec{r}_2) \quad (106)$$

Notice that the "direct" scattering amplitude $f_d$ given in Eq. (103) is the Born scattering amplitude, $f_{born}$, 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:

$$f_e = \frac{K^2}{k_I^2} f_{Born} \quad (107)$$

where $\vec{K} \equiv \vec{K}_I - \vec{K}_F$

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

$$\frac{dQ^{\pm}}{d\Omega} = \left|f_d(\Omega) \pm f_e(\Omega)\right|^2 = \left|\left(1 \pm \frac{K^2}{K_I^2}\right) f_{Born}(\Omega)\right|^2 \quad (108)$$

and use Eq. (97) to write

$$\frac{dQ}{d\Omega} = \left(\frac{1}{4}\right)\frac{dQ^+}{d\Omega} + \left(\frac{3}{4}\right)\frac{dQ^-}{d\Omega} \quad (109)$$

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

$$Q = \frac{k_I}{k_F}\int d\Omega\, \frac{dQ}{d\Omega} = \left(\frac{2\pi}{K_I^2}\right)\int_{K_{min}}^{K_{max}} K\, dK\, \frac{dQ}{dK} \quad (110)$$

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

$$\begin{aligned} Q_{Ochkur} &= \left(\frac{2}{K_I^2}\right)\int_{K_{min}}^{K_{max}} K\,dK \left\{\left(\frac{1}{4}\right)\left(1 + \frac{2K^2}{K_I^2} + \frac{K^4}{K_I^4}\right) + \left(\frac{3}{4}\right)\left(1 - \frac{2K^2}{K_I^2} + \frac{K^4}{K_I^4}\right)\right\} \left|f_{BORN}(K)\right|^2 \\ &= \left(\frac{2}{K_I^2}\right)\int_{K_{min}}^{K_{max}} K\,dK \left(1 - \frac{K^2}{K_I^2} + \frac{K^4}{K_I^4}\right) \left|f_{BORN}(K)\right|^2 . \end{aligned} \tag{112}$$

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

$$Q_{Born} = \left(\frac{2}{K_I^2}\right)\int_{K_I - K_F}^{K_I + K_F} dK \; K \; \left| f'_{Born}(K) \right|^2 \tag{113}$$

where

$$\left| f'_{Born}(K) \right|^2 = \left(\frac{4}{K^4}\right) \sum_{\lambda = l_i - l_f}^{l_i + l_f} (2l_f + 1)(2\lambda + 1) \begin{pmatrix} l_i & l_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \left| \int_0^\infty dr \, P_{n_f l_f}(r) \, j_\lambda(Kr) \, P_{n_i l_i}(r) \right|^2 \tag{114}$$

B) Bethe

$$Q_{Bethe} = \left(\frac{8}{K_I^2}\right) \int_{K_I - K_F}^{K_I + K_F} dK \left(\frac{K^{2S}}{K^3}\right) \left| \int_0^\infty dr \, (r)^3 P_{n_f l_f}(r) \, P_{n_i l_i}(r) \right|^2$$
$$\times \sum_{t = l_i - l_f}^{S} \left(\frac{2l_f + 1}{4\pi}\right) \begin{pmatrix} l_i & l_f & t \\ 0 & 0 & 0 \end{pmatrix}^2 \left(\frac{[2t]!}{2^t [t]!}\right)^2 \tag{115}$$

C) Modified Bethe

$$Q^{(OPTICAL)}_{MOD.\,Bethe} = Q_{Bethe} + \left(\frac{1}{2K_I^2}\right)(l_0 + 1)^2 - \sum_{l=0}^{l_0} Q^{l}_{Bethe} \tag{116}$$

where

$$Q^{l'}_{Bethe}(optical) = (72)\;(2l_f + 1) \begin{pmatrix} l_i & l_f & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 \left| \int_0^\infty dr \, P_{n_f l_f}(r) \right.$$
$$\left. \times [r] P_{n_i l_i}(r) \right|^2 (2l' + 1) \left\{ \begin{pmatrix} 1 & l' & l'-1 \\ 0 & 0 & 0 \end{pmatrix}^2 J^2(l'-1) + \begin{pmatrix} 1 & l' & l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2 J^2(l'+1) \right. . \tag{117}$$

and where

$$J(l' \pm 1) = \int_0^\infty dr' \, j_{l'}(K_I r) \, j_{l' \pm 1}(K_F r) \tag{118}$$

D) Ochkur

$$Q_{Ochkur} = \left(\frac{2}{K_I^2}\right) \int_{K_I - K_F}^{K_I + K_F} K \, dK \left(1 - \frac{K^2}{K_I^2} + \frac{K^4}{K_I^4}\right) \left| f_{Born}(K) \right|^2 . \tag{119}$$

where $f_{born}(K)$ 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:

$Q \rightarrow \mathrm{SIG}$

$K_I \rightarrow \mathrm{XIN}$

$K_F \rightarrow \mathrm{XF}$

$\ell_i \rightarrow \mathrm{L1}$

$\ell_f \rightarrow \mathrm{L2}$

$P_{n_f \ell_f} \rightarrow \mathrm{PF}$

$K \rightarrow X$

$r \rightarrow Y$

$\lambda \rightarrow \mathrm{LAM}$

$J \rightarrow F$

$j_\lambda \rightarrow \mathrm{BJ}$

$\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} \rightarrow \mathrm{TJ(L1, L2, L3)}$

$$\left| \int_0^\infty dr\, P_{n_f \ell_f}(r)\, j_\lambda(Kr)\, P_{n_i \ell_i}(r) \right|^2 \longrightarrow \mathrm{RDINT\ (BJ, LAM, X)}$$

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

$$\frac{1}{K_I} \left| \int_0^\infty \exp(iK_I r) \sin(K_I r)\, U(r)\, dr \right| << 1$$

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

$$Z \sqrt{E_H} << \sqrt{E}$$

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 $E << mc^2$. Hence the region of validity for the Born approximation in eV is

$$(Z)(3.7) << \sqrt{E} << 7.1 \times 10^2, \text{ or } Z << 200$$

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

$$\left[ (K3)^s_{IF} / s! \right] / \left[ (K3)^{s-1}_{IF} / (s-1)! \right] << 1 .$$

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 $\vec{K}_e$. Therefore, an ionization cross-section is excitated 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 $\vec{k}_I$ 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 $k_F$ 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 $\exp(-i\vec{k}_F \cdot \vec{r})$ and the inert-core approximation recall:

$$\frac{dQ}{d\vec{K}_e}[\pi a_0^2] = \left(\frac{2}{K_I^2}\right)\int_{K_I-K_F}^{K_I+K_F} K\,dK\,\left|f_{Born}(\vec{K},\vec{K}_e)\right|^2 \tag{120}$$

where

$$f_{Born}(\vec{K}_e,K) = \left(\frac{2}{K^2}\right)\int d\vec{r}\,\psi_f^{\dagger}(\vec{K}_e,\vec{r})\,\exp(i\vec{K}\cdot\vec{r})\,\psi_i(\vec{r}) \tag{121}$$

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

$$\psi_i(\vec{r}) = R_{n_i \ell_i}(r)\,Y_{\ell_i m_i}(\Omega) \tag{122}$$

$$\psi_f(\vec{K}_e,\vec{r}) = \sum_{\ell_e=0}^{\infty} R_{\ell_e}(K_e,r)\,P_{\ell_e}(\hat{K}_e\cdot\hat{r}) \tag{123}$$

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

$$\exp(iKr\cos\theta) = \sum_{\lambda=0}^{\infty} i^{\lambda}\left[4\pi(2\lambda+1)\right]^{1/2} j_\lambda(Kr)\,Y_{\lambda 0}(\Omega) \tag{124}$$

Using the addition theorem to write

$$\psi_f(\vec{K}_e,\vec{r}) = \sum_{\ell_e,m_e}\left\{\frac{4\pi}{(2\ell_e+1)}R_{\ell_e}(K_e,r)\,Y^{\dagger}_{\ell_e m_e}(\Omega_{K_e})\right\}Y_{\ell_e m_e}(\Omega_r) \tag{125}$$

then Eq. (121) may be expanded as

$$f_{\mathrm{Born}}(\vec{\mathcal{K}}_e, K) = -\left(\frac{2}{K^2}\right)\sum_{l_e m_e \lambda}\left\{\left(\frac{4\pi}{2l_e+1}\right) i^{\lambda}\left[4\pi(2\lambda+1)\right]^{1/2} \equiv C(l_e,\lambda)\right\}$$

$$\times Y_{l_e m_e}(\Omega_{\mathcal{K}_e})\left\{\int d\Omega_r\, Y^{\dagger}_{l_e m_e}(\Omega_r)\, Y_{\lambda 0}(\Omega_i)\, Y_{l_i m_i}(\Omega_r) \equiv \langle l_e m_e|\lambda 0|l_i m_i\rangle\right\} \qquad (126)$$

$$\times\left\{\int_0^{\infty} r^2 dr\, R_{l_e}(\mathcal{K}_e, r)\, j_{\lambda}(Kr)\, R_{n_i l_i}(r) \equiv \mathcal{R}(l_e,\lambda,l_i)\right\}$$

$$= -\left(\frac{2}{K^2}\right)\sum_{l_e m_e \lambda} C(l_e,\lambda)\, Y_{l_e m_e}(\Omega_{\mathcal{K}_e})\,\langle l_e m_e|\lambda 0|l_i m_i\rangle\, \mathcal{R}(l_e,\lambda,l_i)\,.$$

To find the cross-section we require

$$|f_{\mathrm{Born}}(\vec{\mathcal{K}}_e,\vec{K})|^2 = \left(\frac{4}{K^4}\right)\sum_{l_e m_e \lambda}\ \sum_{L_e M_e \Lambda} C(l_e\lambda)\, C^{\dagger}(L_e\Lambda)\, Y_{l_e m_e}(\Omega_{\mathcal{K}_e})\, Y^{\dagger}_{L_e M_e}(\Omega_{\mathcal{K}_e}) \qquad (127)$$

$$\times\langle l_e m_e|\lambda 0|l_i m_i\rangle\langle l_i m_i|\Lambda 0|L_e M_e\rangle\, \mathcal{R}(l_e\lambda l_i)\, \mathcal{R}(L_e\Lambda l_i)\,.$$

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

$$Q^{\mathrm{IONIZATION}}_{\mathrm{Born}} = \int_{\mathrm{all}\ \vec{\mathcal{K}}_e} d\vec{\mathcal{K}}_e\,\frac{dQ}{d\vec{\mathcal{K}}_e} = \int_0^{\mathcal{K}_e^{max}}\mathcal{K}_e^2\, d\mathcal{K}_e\int d\Omega_{\mathcal{K}_e}\,\frac{dQ}{d\vec{\mathcal{K}}_e} \qquad (128)$$

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

$$E_e^{\mathrm{max}} = E_i - E_{\mathrm{ionization}}\,.$$

We may rewrite Eq. (128) as

$$Q^{\mathrm{Ion.}}_{\mathrm{Born}} = \left(\frac{2}{K_I^2}\right)\int_0^{\mathcal{K}_e^{max}}\mathcal{K}_e^2\, d\mathcal{K}_e\int d\Omega_{\mathcal{K}_e}\int_{K_{min}}^{K_{max}} K\, dK\,|f_{\mathrm{Born}}(\vec{\mathcal{K}}_e, K)|^2 \qquad (129)$$

Using Eq. (127) and noting

$$\int d\Omega_{\varkappa_e}\, Y_{\ell_e m_e}(\Omega_{\varkappa_e})\, Y^{\dagger}_{L_e M_e}(\Omega_{\varkappa_e}) = \delta_{\ell_e L_e}\,\delta_{m_e M_e} \tag{130}$$

we can sum over $L_e M_e$ and write

$$\begin{aligned} |f(K,\varkappa_e)|^2 &= \int d\Omega_{\varkappa_e}\, |f(K,\vec{\varkappa}_e)|^2 = \left(\frac{4}{K^4}\right) \sum_{\lambda\Lambda\ell_e m_e} C(\ell_e\lambda)\,C^{\dagger}(\ell_e\Lambda) \\ &\times \langle \ell_e m_e | \lambda 0 | \ell_i m_i\rangle \langle \ell_i m_i | \Lambda 0 | \ell_e m_e\rangle\, \mathcal{R}(\ell_e\lambda\ell_i)\, \mathcal{R}(\ell_e\Lambda\ell_i) \end{aligned} \tag{131}$$

averaging over $m_i$ we write

$$\begin{aligned} |f'(K,\varkappa_e)|^2 &= \sum_{m_i} \frac{|f(K,\varkappa_e)|^2}{(2\ell_i+1)} = \left(\frac{4}{K^4}\right) \sum_{\lambda\Lambda\ell_e} C(\ell_e\lambda)\,C^{\dagger}(\ell_e\Lambda) \\ &\times \mathcal{R}(\ell_e\lambda\ell_i)\, \mathcal{R}(\ell_e\Lambda\ell_i) \sum_{m_i m_e} \langle \ell_e m_e | \lambda 0 | \ell_i m_i\rangle \langle \ell_i m_i | \Lambda 0 | \ell_e m_e\rangle \end{aligned} \tag{132}$$

With Appendix III we can write

$$\begin{aligned} \sum_{m_i m_e} \langle \ell_e m_e | \lambda 0 | \ell_i m_i\rangle \langle \ell_i m_i | \Lambda 0 | \ell_e m_e\rangle &= \frac{(2\ell_e+1)(2\ell_i+1)}{4\pi} \\ &\times \begin{pmatrix} \ell_i & \ell_e & \lambda \\ 0 & 0 & 0 \end{pmatrix} \delta_{\lambda\Lambda}\, \Delta(\ell_i\ell_e\lambda) \end{aligned} \tag{133}$$

summing over Λ in Eq. (132) we write

$$\begin{aligned} |f'(K,\varkappa_e)|^2 &= \left(\frac{4}{K^4}\right) \sum_{\lambda\ell_e} |C(\ell_e,\lambda)|^2 |\mathcal{R}(\ell_i\lambda\ell_e)|^2 \frac{(2\ell_e+1)}{4\pi} \begin{pmatrix} \ell_e & \ell_i & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \\ &= \left(\frac{4}{K^4}\right) \sum_{\lambda\ell_e} \begin{pmatrix} \ell_i & \ell_e & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \left| \int_0^{\infty} dr\, r^2 R_{\ell_e}(\varkappa_e,r)\, j_\lambda(Kr)\, R_{n_i\ell_i}(r) \right|^2 \\ &\times \left\{ \left(\frac{2\ell_e+1}{4\pi}\right) \left(\frac{4\pi}{2\ell_e+1}\right)^2 [4\pi(2\lambda+1)] = (4\pi)^2 \left(\frac{2\lambda+1}{2\ell_e+1}\right) \right\} \end{aligned} \tag{134}$$

In summary, the total ionization cross-section in the Born-Approximation is:

$$Q^{\mathrm{Ion}}_{\mathrm{Born}} = \int_0^{\varkappa_e^{\max}} \varkappa_e^2\, d\varkappa_e\, \frac{dQ}{d\varkappa_e} \tag{135}$$

$$\frac{dQ}{d\varkappa_e} = \left(\frac{2}{K_I^2}\right) \int_{K_I-K_F}^{K_I+K_F} K\,dK\, |f'_{\mathrm{Born}}(K,\varkappa_e)|^2 \tag{136}$$

$$\left|f'_{Born}(K,\kappa_e)\right|^2 = \left(\frac{64\pi^2}{K^4}\right)\sum_{\lambda\, l_e}\begin{pmatrix} l_i & l_e & \lambda \\ 0 & 0 & 0\end{pmatrix}^2 \frac{(2\lambda+1)}{(2l_e+1)}\left|\int_0^\infty r^2 dr\, R_{l_e}\, j_\lambda\, R_{n_i l_i}\right|^2 \qquad (137)$$

where $K_e^{max}$ in atomic units is

$$\kappa_e^{max} = \sqrt{(K_I^2 - 2I)} \qquad I = \text{Ionization Energy}$$

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 $E_e^{max}$ equal to $E_e^{max}/2$. Then

$$\kappa_e^{max'} = \sqrt{2(K_I^2 - 2I)} \qquad (138)$$

### 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.

$$Q_{Born}^{ION} = \int_0^{\kappa_e^{max}} \kappa_e^2\, d\kappa_e\, \frac{dQ}{d\kappa_e} \qquad (139)$$

$$\frac{dQ}{d\kappa_e} = \left(\frac{2}{K_I^2}\right)\int_{K_I-K_F}^{K_I+K_F} K\, dK\, \left|f'_{Born}(K,\kappa_e)\right|^2 \qquad (140)$$

$$\left|f'_{Born}(K,\kappa_e)\right|^2 = \left(\frac{64\pi^2}{K^4}\right)\sum_{\lambda=l_i-l_e}^{l_i+l_e}\begin{pmatrix} l_i & l_e & \lambda \\ 0 & 0 & 0\end{pmatrix}^2 \frac{(2\lambda+1)}{(2l_e+1)} \times \left|\int_0^\infty dr\, P_{l_e}(\kappa_e, r)\, j_\lambda(Kr)\, P_{n_i l_i}(r)\right|^2 \qquad (141)$$

The program listing and discussion is presented in Chapter V, Section 3. Some of the Fortran variable names are:

$K_e \rightarrow$ KAPA

$\ell_e \rightarrow$ L2

$\pi \rightarrow$ PI

$P_{\ell e}(K_e, r) \rightarrow$ 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

```
C     PROGRAM HFSWF(INPUT)
C
C      =========================================================
C      *                                                       *
C      *                * * *     HFSWF     * * *              *
C      *                                                       *
C      * A FORTRAN PROGRAM TO CALCULATE HARTREE-FOCK-SLATER    *
C      *  NUMERICAL WAVE FUNCTIONS AS PUNCHED CARD OUTPUT.     *
C      * ITERATION NUMBER,MEASURE OF SELF-CONSISTENCY AND      *
C      *  ATOMIC NUMBER Z ARE ALWAYS PRINTED ON-LINE.          *
C      *                                                       *
C      * IF KEY=0 NORMALIZED NUMERICAL ATOMIC POTENTIAL IS     *
C      *  READ IN AS 110 VALUES,EVERY 4TH MESH POINT 1 TO 437.*
C      *                                                       *
C      * IF KEY=1 COMPLETE ATOMIC POTENTIAL IS READ IN (437PT)*
C      * IF KEY=2 EXTRAPOLATE STARTING POTENTIAL               *
C      *                                                       *
C      * MAXIT=MAXIMUM NO.OF ITERATIONS(MAXIT=0 IMPLIES 20).   *
C      *                                                       *
C      * IF KUT=0,MODIFIED H-F-S POTENTIAL IS USED IN WV.-EQ.  *
C      * IF KUT=1,UNMODIFIED H-F-S POTENTIAL IS USED IN WV.-EQ*
C      *                                                       *
C      * IF NOCOPY=0,ACTIVE ELECTRN WAVE FUNCTIONS ARE PUNCHED*
C      * IF NOCOPY=1 ALL WV. FNCTS. AND SELF-CONSISTENT        *
C      *  POTENTIAL ARE PRINTED ON-LINE.                       *
C      =========================================================
C
C         ***********************************************
C          *                 PROGRAM AND SUBROUTINES              *
C          *                  ORIGINALLY WRITTEN BY                *
C         *    SHERWOOD SKILLMAN,RCA-LAB,PRINCETON NJ,SPR 1961 *
C        *                       MODIFIED BY                       *
C         *    (1)F.HERMAN,RCA-LAB, PRINCETON NJ,SUMMER 1961    *
C          *   (2)R.KORTUM,LCKHEED RSRCH-LAB,PALO ALTO,SM 1962*
C           *  (3)T.GREENE,UNIV.OF TOLEDO,TOL.OHIO,FALL1971. *
C         ***********************************************
C
      DIMENSION X(521), RSCORE(521), RUINL1(521), RU2(521), RU(521), NNL
     1Z(24), R(521), RSVALE(521), RUFNL1(521), RU3(521), XI(521), WWNL(2
     24), V(521), RSATOM(521), RUINL2(521), XNUM(521), XJ(521), NKKK(24)
     3, EE(24), RUEXCH(521), RUFNL2(521), DENM(521), SNL(10,521), SNLO(5
     421), A(4,5)
      COMMON V,SNLO,R,RSCORE,RSVALE,RU,RUEXCH,XI,XJ,RSATOM,SNL,RUINL1,RU
     1FNL1,RUINL2,RUFNL2,RU2,RU3,NNLZ,WWNL,NKKK,EE,A
      EQUIVALENCE (RSCORE,XNUM), (RSVALE,DENM), (GQ,RSATOM)
      NFILES=0
    1 CONTINUE
C
C     READ HEADING CARD.
C
      READ (5,138)
      WRITE (6,138)
C
C     READ CONTROL CARDS AND INPUT POTENTIALS. CALCULATE TRIAL POTENTIAL
C
      NCARDS=50
      PRINT 132, KEY
      READ (5,131) KEY,TOL,THRESH,MESH,IPRATT,MAXIT,NOCOPY,KUT,IP,IM,IR,
     1ID,DEFOLT,JE
```

```
      IF (DEFOLT) 2,2,3
    2 KEY=0
      TOL=.001
      THRESH=.00001
      MESH=441
      IPRATT=1
      MAXIT=20
      NOCOPY=1
      KUT=0
      IP=6
      IM=6
      IR=5
      IC=7
      JE=1
      GO TO 5
    3 IF (MAXIT) 4,4,5
    4 MAXIT=20
    5 CONTINUE
      NBLOCK=(MESH)/40
C
C     CONSTRUCT X MESH AND R MESH
C
      I=1
      X(I)=0.0
      R(I)=0.0
      DELTAX=0.0025
      DO 7 J=1,NBLOCK
      DO 6 K=1,40
      I=I+1
    6 X(I)=X(I-1)+DELTAX
    7 DELTAX=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
C
C     READ IN ATOMIC POTENTIAL
C
    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
      AZ=Z
      IZ=Z
      NCSPVS=NCORES+NVALES
      C=0.88534138/Z**(1.0/3.0)
      TWOION=ION+ION
      ZZZ=ION+1
      TWOZZZ=ZZZ+ZZZ
      DO 13 I=2,MESH
   13 R(I)=C*X(I)
      READ (IR,127) (NNLZ(I),WWNL(I),EE(I),I=1,NCSPVS)
      WWW=0.0
      DO 14 I=1,NCSPVS
```

```
   14 WWW=WWW+WWNL(I)
      IF (ABS(Z+1.0-WWW-ZZZ)-0.001) 16,15,15
   15 PRINT 126, WWW,ZZZ,Z,NCORES,NVALES,NCSPVS
      CALL EXIT
   16 CONTINUE
      IF (KEY-1) 21,26,17
C
C     CONSTRUCT ATOMIC POTENTIAL
C
   17 IF (ABS(ZE3-ZE2-Z+ZE3)-0.001) 19,19,18
   18 WRITE (IP,139) Z,ZE2,ZE3
      CALL EXIT
   19 DO 20 I=1,441
      RU(I)=RU3(I)+RU3(I)-RU2(I)
   20 CONTINUE
      GO TO 31
   21 TWOZ=Z+Z
      DO 22 I=1,437,4
   22 RU(I)=-RU2(I)*TWOZ
      RU(441)=RU(437)
      RU(445)=RU(437)
      M=9
      DO 25 I=1,437,4
      M=M-1
      IF (M) 23,24,24
   23 RU(I+1)=(22.0*RU(I)+11.0*RU(I+4)-RU(I+8))/32.0
      RU(I+2)=(10.0*RU(I)+15.0*RU(I+4)-RU(I+8))/24.0
      RU(I+3)=(6.0*RU(I)+27.0*RU(I+4)-RU(I+8))/32.0
      M=9
      GO TO 25
   24 RU(I+1)=(21.0*RU(I)+14.0*RU(I+4)-3.0*RU(I+8))/32.0
      RU(I+2)=(3.0*RU(I)+6.0*RU(I+4)-RU(I+8))/8.0
      RU(I+3)=(5.0*RU(I)+30.0*RU(I+4)-3.0*RU(I+8))/32.0
   25 CONTINUE
      GO TO 31
   26 IF (ABS(ZE3-Z)-0.001) 27,27,29
   27 DO 28 I=1,441
      RU(I)=RU3(I)
   28 CONTINUE
      GO TO 31
   29 ZOZ=Z/ZE3
      DO 30 I=1,441
      RU(I)=RU3(I)*ZOZ
   30 CONTINUE
   31 V(1)=-9.9E35
      M=MIN0(441,MESH)
      IF (KUT) 32,37,32
   32 DO 33 I=1,M
   33 V(I)=RU(I)/R(I)
      IF (MESH-M) 34,34,36
   34 DO 35 I=442,MESH
   35 V(I)=-TWOION/R(I)
   36 LIMIT=M
      ICUT=MESH
      IC=MESH
      GO TO 47
   37 CONTINUE
      ICUT=0
      DO 42 I=2,M
```

```
      IF (ICUT) 38,38,40
   38 IF (TWOZZZ+RU(I)) 41,41,39
   39 ICUT=I
   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=442,MESH
   46 V(I)=-TWOZZZ/R(I)
   47 CONTINUE
      DELTA=1000000.
      NITER=0
      NONMON=3
      IPRSW=0
      PRINT 133
C
C     START ITERATION
C
   48 MCARDS=90
      IF (MAXIT-NITER) 49,51,51
   49 CONTINUE
      WRITE (IP,140)
      DO 50 I=1,MESH,5
      WRITE (IP,141) I,X(I),RU3(I),RUINL1(I),RUFNL1(I),RUINL2(I),RUFNL2(
     1I),RU(I)
   50 CONTINUE
      GO TO 11
   51 DO 52 I=1,MESH
      RSCORE(I)=0.0
   52 RSVALE(I)=0.0
C
C     SOLVE SCHROEDINGER EQUATION FOR EACH ORBITAL IN TURN
C     CALCULATE CORE AND VALENCE ELECTRONIC DENSITIES
C
      DO 59 M=1,NCSPVS
      E=EE(M)
      NN=NNLZ(M)/100
      LAM=NNLZ(M)/10-10*NN
      XL=LAM
C
      CALL SCHEQ (Z,E,LAM,NN,KKK,MESH,C,THRESH)
C
      IF (M-NCORES) 53,53,55
   53 DO 54 I=1,KKK
   54 RSCORE(I)=RSCORE(I)+WWNL(M)*SNLO(I)**2
      GO TO 57
   55 DO 56 I=1,KKK
   56 RSVALE(I)=RSVALE(I)+WWNL(M)*SNLO(I)**2
   57 DO 58 I=1,KKK
   58 SNL(M,I)=SNLO(I)
      NKKK(M)=KKK
      MCARDS=MCARDS+2+((KKK-1)/40)*8
   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))/315.82734)**(1.0/3.0)
C
C     CALCULATE ATOMIC COULOMB POTENTIAL
C
      A1=0.0
      ASUM=0.0
      B1=0.0
      BSUM=0.0
      H=0.0025*C
      I=1
      XI(1)=0.0
      XJ(1)=0.0
      DO 62 J=1,NBLOCK
      DO 61 K=1,40
      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
   61 B1=B1+B2
      ASUM=XI(I)
      BSUM=XJ(I)
      A1=A2
      B1=B2
   62 H=H+H
      DO 63 I=1,MESH
      XI(I)=-2.0*Z+2.0*(XI(I)+R(I)*(XJ(MESH)-XJ(I)))
      XJ(I)=XI(I)+RUEXCH(I)
   63 CONTINUE
      DO 64 I=1,MESH
      RUINL1(I)=RUINL2(I)
      RUFNL1(I)=RUFNL2(I)
      RUINL2(I)=RU(I)
   64 RUFNL2(I)=XJ(I)
      NITER=NITER+1
      PDELTA=DELTA
      DELTA=0.0
      DO 66 I=1,LIMIT
      SNLO(I)=RU(I)-XJ(I)
      XI(I)=ABS(SNLO(I))
      IF (XI(I)-DELTA) 66,66,65
   65 DELTA=XI(I)
      IDELTA=I
   66 CONTINUE
      PRINT 128, NITER,Z,DELTA,IDELTA,X(IDELTA),ICUT,X(ICUT)
C
C     TEST SELF-CONSISTENCY OF ATOMIC POTENTIAL.
C
      IF (DELTA-TOL) 106,67,67
C
C     IF SCF CRITERION NOT SATISFIED, CALCULATE NEXT TRIAL POTENTI
C
```

```
   67 IF (IPRSW) 68,68,73
   68 DO 69 I=2,LIMIT
   69 RU(I)=0.5*(RU(I)+XJ(I))
      IF (MESH-LIMIT) 72,72,70
   70 RUZM=XJ(MESH)
      RATIO=(RUZM-RU(LIMIT))/(RUZM-XJ(LIMIT))
      DO 71 I=LIMIT,MESH
   71 RU(I)=RUZM-RATIO*(RUZM-XJ(I))
      LIMIT=MESH
   72 IPRSW=IPRATT
      GO 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 NONMON=NONMON-1
      IF (NONMON) 68,68,76
   76 ALPH=0.5
C
C     PRATT IMPROVEMENT SCHEME
C
      DO 84 I=2,ICUT
      XNUM(I)=RUINL1(I)*RUFNL2(I)-RUINL2(I)*RUFNL1(I)
      DENM(I)=RUFNL2(I)-RUFNL1(I)-RUINL2(I)+RUINL1(I)
      IF (ABS(DENM(I)/RUINL2(I))-0.0001) 77,77,78
   77 CONTINUE
      ALPH=0.5
      GO TO 83
   78 ALPH=(XNUM(I)/DENM(I)-RUFNL2(I))/SNLO(I)
      IF (ALPH) 79,82,80
   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=IPRSW-1
      IF (KUT) 87,85,87
   85 CONTINUE
      IC=ICUT+20
      IC1=ICUT+1
      ADEL=XI(ICUT)/20.
      DO 86 I=IC1,IC
      XI(I)=XI(I-1)-ADEL
   86 XJ(I)=XI(I)
   87 CONTINUE
      XJ(1)=0.5
      XJ(2)=XI(2)
      ASUM=XI(2)+XI(3)+XI(4)+XI(5)
      DO 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
```

```
      DO 90 I=IC1,MESH
      XJ(I)=0.0
   90 RU(I)=RUFNL2(I)
   91 CONTINUE
      DO 92 I=2,IC
   92 RU(I)=RUFNL2(I)+XJ(I)*SNLO(I)
   93 CONTINUE
      IF (KUT) 94,96,94
   94 ICUT=MESH
      LIMIT=MESH
      DO 95 I=2,MESH
      VLAST=V(I)
      V(I)=RU(I)/R(I)
   95 XI(I)=V(I)-VLAST
      GO TO 102
   96 CONTINUE
      ICUT=0
      DO 101 I=2,MESH
      VLAST=V(I)
      IF (ICUT) 97,97,99
   97 IF (TWOZZZ+RU(I)) 100,100,98
   98 ICUT=I
   99 V(I)=-TWOZZZ/R(I)
      GO TO 101
  100 V(I)=RU(I)/R(I)
  101 XI(I)=V(I)-VLAST
  102 CONTINUE
      XI(1)=0.0
C
C     NEXT TRIAL EIGENVALUES PREDICTED BY PERTURBATION THEORY
C
      NCARDS=90
      DO 105 M=1,NCSPVS
      K=(NKKK(M)-1)/40
      H=0.0025*C
      ASUM=0.0
      A1=0.0
      I=1
      DO 104 J=1,K
      DO 103 L=1,40
      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
      GO TO 48
C
C     WHEN NOCOPY=1 ALL RESULTS TRANS FROM INTERN MEMORY TO PRINTE
C
C     WHEN NOCOPY=0 OUTPUT IS LAST ORBITAL WV. FNCT. ONLY
C
  106 CONTINUE
      IF (NOCOPY) 107,114,107
  107 CONTINUE
      PRINT 130, NCARDS,MCARDS
      NC=1
```

```
      WRITE (IM,135) Z,NCORES,NVALES,ION,IZ,NC
      DO 110 I=1,441
      IF (TWOION+RUINL2(I)) 110,110,108
  108 DO 109 M=I,441
  109 RUINL2(M)=-TWOION
      GO TO 111
  110 CONTINUE
  111 CONTINUE
      DO 112 MIN=1,440,5
      MAX=MIN+4
      NC=NC+1
      WRITE (IM,136) (RUINL2(M),M=MIN,MAX),IZ,NC
  112 CONTINUE
      NC=NC+1
      WRITE (IM,137) RUINL2(441),IZ,NC
      DO 114 M=1,NCSPVS
      NLZ=NNLZ(M)
      KKK=NKKK(M)
      XL=NLZ/10-10*(NLZ/100)
      LP=XL+1.0
      NC=NC+1
      WRITE (IM,134) NLZ,XL,EE(M),WWNL(M),KKK,IZ,NC
      K1=KKK-1
      DO 113 MIN=1,K1,5
      NC=NC+1
      MAX=MIN+4
      WRITE (IM,136) (SNL(M,I),I=MIN,MAX),IZ,NC
  113 CONTINUE
      NC=NC+1
      WRITE (IM,137) SNL(M,KKK),IZ,NC
  114 CONTINUE
      IF (KEY-1) 115,116,118
  115 KEY=1
  116 DO 117 I=1,MESH
  117 RU3(I)=RU(I)
      ZE3=Z
      GO TO 11
  118 DO 119 I=1,MESH
      RU2(I)=RU3(I)
  119 RU3(I)=RU(I)
      ZE2=ZE3
      ZE3=Z
      GO TO 11
  120 CONTINUE
C
C     PUNCH GROUND STATE WAVE FUNCTIONS
C
      Z=AZ
      NC=0
      M=NCSPVS
      NLZ=NNLZ(M)
      KKK=NKKK(M)
      XL=NLZ/10-10*(NLZ/100)
      NC=NC+1
      WRITE (ID,142) NLZ,XL,EE(M),WWNL(M),KKK,Z,IZ,NC
      K1=KKK-1
      DO 121 MIN=1,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
C     CALCULATE EXCITED STATE WAVE FUNCTIONS
C
      DO 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)/10-10*NN
      XL=LAM
      CALL SCHEQ (Z,E,LAM,NN,KKK,MESH,C,THRESH)
C
C     PUNCH EXCITED STATE WAVE FUNCTIONS
C
      NC=0
      M=NCSPVS+1
      NLZ=NNLZ(M)
      XL=NLZ/10-10*(NLZ/100)
      NC=NC+1
      WRITE (ID,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 (ID,136) (SNLO(I),I=MIN,MAX),IZ,NC
  122 CONTINUE
      NC=NC+1
      WRITE (ID,137) SNLO(KKK),IZ,NC
  123 CONTINUE
      CALL EXIT
C
  124 FORMAT (F8.5,9F7.5)
  125 FORMAT (F4.0,3I4)
  126 FORMAT (6H WWW= F4.0,6H ZZZ= F4.0,6H    Z= F4.0,10H    NCORES=I4,11H
     1   NVALES= I4,11H   NCSPVS= I4/25H CONTROL CARDS INCORRECT.)
  127 FORMAT (I4,F4.0,F8.4)
  128 FORMAT (I7,F7.0,1PE14.7,0P2(I6,F9.3))
  129 FORMAT (1PE15.7,1P4E14.7)
  130 FORMAT (10H  NCARDS= I4,10H MCARDS=I4)
  131 FORMAT (I4,2F8.6,11I4)
  132 FORMAT (8H  KEY = I4)
  133 FORMAT (6H  ITER,7X,1HZ,4X5HDELTA,7X,30HI(DEL)  X(DEL)  I(CUT)  X(
     1CUT))
  134 FORMAT (I4,1P3E14.7,I4,1PE14.7,8X,1HZ,I3,I4)
  135 FORMAT (F4.0,3I4,56X,1HZ,I3,I4)
  136 FORMAT (1PE15.7,1P4E14.7,1X,1HZ,I3,I4)
  137 FORMAT (1PE15.7,57X,1HZ,I3,I4)
  138 FORMAT (72H
     1                )
  139 FORMAT (27H0STARTING POTENTIALS AND Z=,F4.0,9H IN ERROR,2F4.0)
  140 FORMAT (40H1I,X,RU3,RUINL1,RUFNL1,RUINL2,RUFNL2,RU )
  141 FORMAT (I8,F10.4,1P6E16.7)
  142 FORMAT (I4,1P3E14.7,I4,0PF4.0,18X,1HZ,I3,I4)
```

```
      END
      SUBROUTINE SCHEQ (ZZ,EN,LAMBDA,NOFL,KKK,MESS,SCF,THRESH)
C
C     SUBROUTINE SCHEQ
C     COMPUTE ENERGY EIGENVALUE AND WAVE FUNCTION
C      ORIGINALLY WRITTEN BY SHERWOOD SKILLMAN
C       RCA LABORATORIES, PRINCETON, NEW JERSEY, SPRING 1961
C      MODIFIED BY FRANK HERMAN, SUMMER 1961
C      FURTHER MODIFIED BY RICHARD KORTUM AND PAUL KELLY, LOCKHEED
C      RESEARCH LABORATORIES, PALO ALTO, CALIFORNIA, SUMMER 1962
C
C     POTENTIAL AVAILABLE IN COMMON STORAGE AT START. WAVE FUNCTION,
C       COMPUTED EIGENVALUE, AND KKK LOCAATED IN COMMON STORAGE AT
C       RETURN FROM SCHEQ.
C
C     NOTATION: ATOMIC NUMBER(ZZ=Z); TRIAL EIGENVALUE(EN=E); ORBIT.
C       QUANT. NO.(LAMBDA=XL); PRINC.QUANT NO.(NOFL=N); NO. OF MESH
C       PTS. USED FOR WV. FNCT.(KKK); NO. OF INTEGRATION MESH PTS.
C       (MESS=MESH); SCALE FACTOR(SCF);EIGENVALUE ACCUR. CRIT.(THRESH)
C
      DIMENSION P(5), Q(5), T(5), D(5)
      DIMENSION R(521), RSCORE(521), RUINL1(521), RU2(521), RU(521), NNL
     1Z(24), RSVALE(521), RUFNL1(521), RU3(521), XI(521), WWNL(24), V(52
     21), RSATOM(521), RUINL2(521), XNUM(521), XJ(521), NKKK(24), EE(24)
     3, RUEXCH(521), RUFNL2(521), DENM(521), SNL(10,521), SNLO(521), QQ(
     4521)
      COMMON V,SNLO,R,RSCORE,RSVALE,RU,RUEXCH,XI,XJ,RSATOM,SNL,RUINL1,RU
     1FNL1,RUINL2,RUFNL2,RU2,RU3,NNLZ,WWNL,NKKK,EE
      EQUIVALENCE (RSCORE,XNUM), (RSVALE,DENM), (QQ,RSATOM)
C
C     SET UP CONSTANTS AND INITIALIZE
C
      IR=5
      IP=6
      IM=6
      Z=ZZ
      LAM=LAMBDA
      NN=NOFL
      MESH=MESS
      C=SCF
      MANY=200
      E=EN
      MOREV=0
      LESSV=0
      EMORE=0.0
      ELESS=0.0
      MORE=0
      LESS=0
      CE=0.0
      NPRINT=0
      LAMM=LAM-1
      LAMP=LAM+1
      XLP=LAMP
      NCCR=NN-LAMP
      B=LAM*LAMP
      OC=R(2)
      H=OC
      HSQ=H*H
      B3=(V(3)-V(2))/H-Z/HSQ
```

```
      Y=H+H
      FLPS=4*LAM+6
      SLPT=6*LAM+12
      ELPT=8*LAM+20
      A1=-Z/XLP
      YSQ=Y*Y
      B1=-Z-Z
      AB1=A1*B1
      AB3=A1*B3
C
C     RAISE H AND Y TO LAM+1
C
      HTL=H
      YTL=Y
      IF (LAM) 6,3,1
    1 DO 2 I=1,LAM
      HTL=HTL*H
    2 YTL=YTL*Y
    3 H1=HSQ
      BOHS=B/HSQ
      BOH=B1/H
      BTH=B3*H
      BQ3=BOHS+BOH+BTH
      BQ4=BOHS/4.+BOH/2.+BTH+BTH
      EPL=8+LAM
      FPL=5+LAM
      XIFC=C*.21701389E-4
C
C     START OUTWARD INTEGRATION
C
    4 NPRINT=NPRINT+1
      EPS=E-EG
      EG=E
      IF (MANY-NPRINT) 5,8,8
    5 WRITE (IP,95) NN,LAM,Z
      CALL EXIT
    6 NSTOP=77
    7 WRITE (IP,96) NSTOP
      CALL EXIT
    8 DO 9 I=1,MESH
    9 SNLO(I)=0.0
      IF (NPRINT-1) 6,10,17
   10 CONTINUE
      DO 11 I=4,MESH
      QQ(I)=V(I)+B/(R(I)*R(I))-E
   11 CONTINUE
   12 M=MESH
      DO 14 I=4,MESH
      IF (QQ(M)) 13,14,14
   13 IK=M+1
      GO TO 15
   14 M=M-1
      NSTOP=521
C
C     Q IS EVERYWHERE POSITIVE
C
      GO TO 7
   15 IF (MESH-IK) 16,16,19
   16 EPS=QQ(MESH-40)
```

```
      E=E+EPS
   17 CONTINUE
      DO 18 I=4,MESH
   18 QQ(I)=QQ(I)-EPS
      GO TO 12
   19 CONTINUE
      NCROSS=0
      SIGN=1.0
      H=OC
      Y=H+H
C     B= LAM*(LAM+1)
C     B1= -2.*Z
      B2=3.0*Z/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=(A2*B1+A1*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+A1*B3)/(8*LAM+20)
      P(3)=(1.0+H*(A1+H*(A2+H*(A3+H*A4))))*HTL
C     P(3)=(1.0+A1*H+A2*H**2+A3*H**3+A4*H**4)*H**(XL+1.0)
      P(4)=(1.C+Y*(A1+Y*(A2+Y*(A3+Y*A4))))*YTL
C     P(4)=(1.C+A1*Y+A2*Y**2+A3*Y**3+A4*Y**4)*Y**(XL+1.0)
      Q(3)=BQ3+B2
C     Q(3)=(B+B1*H+B2*H**2+B3*H**3)/H**2
      Q(4)=BQ4+B2
C     Q(4)=(B+B1*Y+B2*Y**2+B3*Y**3)/Y**2
      SNLO(2)=P(3)
      SNLO(3)=P(4)
      I=3
      DX=OC
      H1=H**2
      H2=H1/12.C
      T(3)=P(3)*(1.0-H2*Q(3))
      T(4)=P(4)*(1.0-H2*Q(4))
      D(4)=T(4)-T(3)
      NCOUNT=3
      NINT=2
   20 I=I+1
C
C     IF END OF MESH IS REACHED, MODIFY TRIAL EIGENVALUE
C
      IF (I-MESH) 22,21,21
   21 IF (NDCR-NCROSS) 37,44,44
C
C     RETURN TO BEGINNING OF OUTWARD INTEGRATION IF NECESSARY
C
   22 Q(5)=QQ(I)
      IF (IK-I) 34,34,23
   23 D(5)=D(4)+H1*Q(4)*P(4)
      T(5)=D(5)+T(4)
      IF (1.0-ABS(H2*Q(5))) 21,21,24
   24 P(5)=T(5)/(1.0-H2*Q(5))
      SNLO(I)=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
C
C     COUNT CHANGES IN SIGN
C
      SIGN=-SIGN
   28 NCOUNT=NCOUNT+1
      IF (7-NCOUNT) 6,29,30
   29 NCOUNT=2
   30 NINT=NINT+1
      IF (40-NINT) 6,31,32
   31 DX=DX+DX
      H=DX
      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))
      D(5)=T(5)-T(3)
   32 DO 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) 6,35,23
   35 IF (NINT-4) 23,23,36
C
C     MATCHING RADIUS HAS BEEN REACHED GOING OUT
C
C     IF NOCR NOT EQUAL TO NCROSS, MODIFY TRIAL EIGENVALUE
C
   36 EIGEN=E
      IF (NOCR-NCROSS) 37,52,44
   37 MORE=1
C
C     TOO MANY CROSSINGS, INCREASE ABSF(E)
C
      MOREV=MOREV+1
      IF (MOREV-1) 38,40,39
   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
C
C     TOO FEW CROSSINGS, DECREASE ABSF(E)
C
      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
      GC TO 7
   50 E=0.75*EG
      GC TO 4
   51 E=0.5*(EMORE+ELESS)
      GC TO 4
   52 IF (ABS(SNLO(I-1))-ABS(SNLO(I-2))) 53,56,56
C
C     CHECK TO SEE THAT WAVE IS IN THE DAMPED REGION (ABSOLUTE VALUE
C     DECREASING AND SIGNS ALIKE)
C
   53 IF (P(5)) 54,23,55
   54 IF (SNLO(I-2)) 57,23,23
   55 IF (SNLO(I-2)) 23,23,57
   56 IF (1.0E+25-ABS(P(5))) 44,44,23
C
C     LARGE ABSOLUTE VALUE OF P IN WHAT SHOULD BE THE DAMPED REGION
C     INDICATES TOO FEW PEAKS, DECREASE ABSF(E)
C
C     NOW NDCR = NCROSS AND MATCHING RADIUS LIES IN DAMPED REGION
C
   57 IMATCH=I-2
      XMATCH=R(I-2)
      PPOUT=(T(4)-T(2)-0.5*(P(4)-P(2)))/H
      S2=PPOUT/P(3)
C
C     INTEGRATION IS BY 8 APPLICATIONS OF NEWTON-COTES CLOSED
C     QUADRATURE FOR FIVE INTERVALS ON EACH BLOCK
C
C     XIFC =(5*H(BLOCK 1)/288)/2 ,H(1) =0.0025*SCALE FACTOR
C
      SUM1=0.0
      XIF=XIFC
      I=1
      VALUE=C.C
   58 MM=8
      SUM2=0.C
      XIF=XIF+XIF
   59 Y=VALUE
      VALUE=SNLO(I+5)**2
      SUM2=SUM2+19.0*(VALUE+Y)+75.0*(SNLO(I+4)**2+SNLO(I+1)**2)+50.0*(SN
     1LO(I+2)**2+SNLO(I+3)**2)
      I=I+5
      IF (IMATCH-I) 6,62,6C
   60 MM=MM-1
      IF (MM) 6,61,59
   61 SUM1=SUM2*XIF+SUM1
      GC 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
C
C     FOR N =1, START INWARD INTEGRATION AT(8+LAM)*XMATCH OR X MAX
C
      GO TO 65
   64 XINW=FPL*XMATCH
C
```

```
C     FOR N NOT=1, START AT (5+LAM)*XMATCH OR X MAX (END OF MESH)
C
   65 DO 67 I=41,MESH,40
      IF (XINW-R(I)) 66,66,67
   66 KKK=I
      GO TO 68
   67 CONTINUE
      KKK=MESH
   68 I=KKK
      DX=R(I-1)-R(I)
      H=DX
      XIF=0.17361111E-1*DX
      HSQ=H*H
      HSQ12=HSQ/12.0
      Q(3)=QQ(I)
      P(3)=EXP(-R(I)*SQRT(Q(3)))
      SUM3=P(3)/Q(3)
      I=I-1
      Q(4)=QQ(I)
      P(4)=EXP(-R(I)*SQRT(Q(4)))
      IF (ABS(P(4))-1.0E-35) 69,69,71
   69 KKK=KKK-40
      IF (KKK-IMATCH) 70,70,68
   70 WRITE (IP,97) Z,NN,LAM,KKK
      KKK=KKK+40
      P(4)=1.5E-35
      P(3)=1.0E-35
   71 IF (PMATCH) 72,6,73
   72 P(3)=-P(3)
      P(4)=-P(4)
   73 SNLO(I+1)=P(3)
      SNLO(I)=P(4)
      T(3)=P(3)*(1.0-HSQ12*Q(3))
      T(4)=P(4)*(1.0-HSQ12*Q(4))
      D(4)=T(4)-T(3)
   74 DO 76 M=2,40
      I=I-1
      Q(5)=QQ(I)
      D(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) 6,78,75
   75 SNLO(I)=P(5)
      DO 76 K=1,4
      P(K)=P(K+1)
      T(K)=T(K+1)
      D(K)=D(K+1)
   76 Q(K)=Q(K+1)
      Q(5)=QQ(I-2)
      D(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)=1.09375*P(4)+0.2734375*P(5)-0.546875*P(3)+0.21875*P(2)-0.0390
     1625*P(1)
      I=I-1
      DX=DX/2.0
      Q(5)=QQ(I)
      H=DX
      HSQ=H*H
```

```
      HSQ12=HSQ/12.0
      T(5)=P(5)*(1.0-HSQ12*Q(5))
      T(4)=P(4)*(1.0-HSQ12*Q(4))
      D(5)=T(5)-T(4)
      SNLO(I)=P(5)
      DO 77 L=1,4
      P(L)=P(L+1)
      T(L)=T(L+1)
      D(L)=D(L+1)
   77 Q(L)=Q(L+1)
      GO TO 74
C
C     MATCHING RADIUS HAS BEEN REACHED COMING IN
C
   78 K=KKK
      VALUE=SNLO(K)**2
      GO TO 80
   79 CONTINUE
      SUM3=SUM3+XIF*SUM4
      XIF=XIF*0.5
   80 MM=8
      SUM4=0.0
   81 Y=VALUE
      VALUE=SNLO(K-5)**2
      SUM4=SUM4+19.0*(VALUE+Y)+75.0*(SNLO(K-1)**2+SNLO(K-4)**2)+50.0*(SN
     1LO(K-2)**2+SNLO(K-3)**2)
      K=K-5
      IF (K-IMATCH) 6,83,82
   82 MM=MM-1
      IF (MM) 6,79,81
   83 SUM3=SUM3+XIF*SUM4
      S3=SUM3/P(4)**2
      PPIN=(T(5)-T(3)-0.5*(P(5)-P(3)))/H
      S4=PPIN/P(4)
      DE=(S2-S4)/(S1-S3)
      IF (ABS(DE/E)-THRESH) 86,84,84
   84 E=E+DE
      IF (E) 4,85,85
   85 E=E-DE
      DE=DE/2.0
      GO TO 84
C
C     IMPROVE TRIAL EIGENVALUE BY PERTURBATION THEORY IF NECESSARY
C     CALCULATE THE NORMALIZED WAVE FUNCTIONS
C
   86 POP=PMATCH/P(4)
      DO 87 J=IMATCH,KKK
   87 SNLO(J)=SNLO(J)*POP
      SUM1=0.0
      J=1
      XIF=XIFC
      VALUE=0.0
   88 MM=8
      XIF=XIF+XIF
      SUM2=0.0
   89 Y=VALUE
      VALUE=SNLO(J+5)**2
      SUM2=SUM2+19.0*(VALUE+Y)+75.*(SNLO(J+4)**2+SNLO(J+1)**2)+50.0*(SNL
     1O(J+2)**2+SNLO(J+3)**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=SQRT(SUM1)
      IF (SNLO(3)) 92,6,93
   92 C1=-C1
   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 (5H0STOP,I4,8HIN SCHEQ)
   97 FORMAT (6H0AT Z=,F6.0,6H  NL =,I3,I1,7H KKK =,I5,23H IS LESS THAN
     1 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

$$\left[ \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - V(r) - E_{n\ell} \right] P_{n\ell}(r) = 0 \qquad (142)$$

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

$$x = \frac{r}{\mu} \qquad \text{where} \qquad \mu \equiv \left(\frac{1}{2}\right)\left(\frac{3\pi}{4}\right)^{2/3}\left(\frac{1}{Z}\right)^{1/3}$$

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

$$V(M) = \operatorname{Min}\left[\frac{RU(M)}{R(M)}, \frac{-2Z}{R(M)}\right] \quad \text{or} \quad V(M) = \frac{RU(M)}{R(M)} \qquad (143)$$

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 exceded 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 Schröedinger equation is solved using the constructed potential V(M). By calling SCHEQ the electronic densities for each orbital (RSCORE(M) and RSVALE(M)) and the total electronic density (RSATOM(M) = RSCORE(M) + RSVALE(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

$$\text{DELTA} = \text{MAX} \mid \text{XJ(M)} - \text{RU(M)} \mid \qquad (144)$$

a comparison with the required tolerance for self-consistency, TOL, is made. If DELTA < 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

$$\text{RU(M)} = \frac{\text{RUI(M)} + \text{XJ(M)}}{2} \qquad (145)$$

or by use of the Pratt improvement scheme,

$$\text{RU(M)} = 2\ \text{RUI(M)} + (1 - \alpha)\ \text{XJ(M)} \qquad (146)$$

where $0 \leq \alpha \leq 0.5$ below M = 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,

$$E = E + < M \mid H' \mid M > \quad . \tag{147}$$

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

```
C       PROGRAM EXCSCT(INPUT)
C
C        ==============================================================
C        *                                                            *
C        *                     * * *    EXCSCT    * * *               *
C        *                                                            *
C        * A FORTRAM PROGRAM TO CALCULATE EXCITATION CROSS-           *
C        * SECTIONS FOR THE ELECTRON IMPACT EXCITATION OF ATOMS.      *
C        *                                                            *
C        * ENERGY IS MEASURED IN UNITS OF THRESHOLD ENERGY,EPSIL      *
C        * EPSIL IS MEASURED IN UNITS OF TWICE THE RYDBERG.           *
C        *                                                            *
C        * IPROX=THE APPROXIMATION USED.ALLOWED VALUES ARE:           *
C        *  (1=BORN;2=OCHKUR;3=BETHE;4=MODIFIED BETHE).               *
C        *                                                            *
C        * N.B.*** MODIFIED BETHE (IPROX=4) MAY ONLY BE USED FOR      *
C        *         OPTICALLY ALLOWED TRANSITIONS***                   *
C        ==============================================================
C
C                         **************************
C                        *          PROGRAM           *
C                       *     AND SUBROUTINES BY       *
C                      *          TOM J GREENE          *
C                       *    UNIVERSITY OF TOLEDO      *
C                        *         1970-1973          *
C                         **************************
C
      REAL*8 AQ,BO(4),BQ
      DIMENSION ZN(25), SIG(25), FX(1001), XMSH(1001), SG(8), EPSL(4), N
     1L1(4), NL2(4), SIGM(25,4)
      COMMON PIN(521),PF(521),C,RANS,Y(521),KKK
      EXTERNAL BJ,RN
      DATA N,ZN(1),ZN(2),ZN(3),ZN(4),ZN(5),ZN(6),ZN(7),ZN(8),ZN(9)/20,1.
     120,1.35,1.50,1.75,2.00,2.33,2.67,3.0,3.5/,ZN(10),ZN(11),ZN(12),ZN(
     213),ZN(14),ZN(15),ZN(16),ZN(17),ZN(18),ZN(19),ZN(20)/4.00,5.00,6.0
     30,7.00,8.00,10.00,12.00,15.00,18.00,21.00,24.00/
      NCC=0
      IP=6
      IM=5
      IR=5
C
C     READ CONTRL CARD; N=NO. OF VALUES OF INCIDENT ENERGY;
C
C        NTC=TYPE OF SERIES; NC=NO.OF SERIES;NOTP=OUTPUT OPTION;
C              A=ELEMENT NAME.
C     NTC: 1=SINGLE CASE;2=MULTIPLE APPROX.;3=MULTIPLE WV. FNCT.
C     NOTP:1=PUNCHED CARD;2=SINGLE LIST;3=MULTIPLE LIST;
C
      READ (IM,46) N,NTC,NC,NOTP,AQ
C
C     READ ENERGY RANGE
C     ZN(N)=VALUES OF INCIDENT ENERGY IN THRESHOLD UNITS.
C
      IF (N.NE.-1) GO TO 1
      N=19
      GO TO 2
    1 READ (IR,47) (ZN(I),I=1,N)
    2 CONTINUE
C
```

```
C     READ INPUT WAVE FUNCTIONS
      READ (IR,48) NLZ1,XL1,EE1,WWNL1,KKK1,Z
      K11=KKK1-1
      DO 3 MIN=1,K11,5
      MAX=MIN+4
      READ (IR,49) (PIN(I),I=MIN,MAX)
    3 CONTINUE
      READ (IR,50) PIN(KKK1)
    4 READ (IR,48) NLZ2,XL2,EE2,WWNL2,KKK2,Z
      K21=KKK2-1
      DO 5 MIN=1,K21,5
      MAX=MIN+4
      READ (IR,49) (PF(I),I=MIN,MAX)
    5 CONTINUE
      READ (IR,50) PF(KKK2)
      KKK=AMIN0(KKK1,KKK2)
      C=0.885341381/Z**(.333333333)
      EPSIL=(ABS(EE2-EE1)/2.)
      N1=NLZ1/10
      N2=NLZ2/10
C
C     READ THE APPROXIMATION ,IPROX.
C     IPROX VALUES ARE; 1=BORN; 2=OCHKUR; 3=BETHE; 4=MODIFIED BETHE
    6 READ (IM,51) IPROX,BQ
C
C     TRANSFER TO THE APPROPRIATE APPROXIMATION.
      MWTCH=2
      IF (IPROX.EQ.1.OR.IPROX.EQ.2) MWTCH=1
      GO TO (26,7), MWTCH
C
C      BETHE APPROXIMATION
C
C     FIND ROMO
    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
C     FIND ANGFCT
      ANGFCT=(2.*XL2+1.)*((TJ(XL1,XL2,XLAM)*(2.**XLAM)*(FACT(XLAM)/F
     12.*XLAM)))**2)/(2.*XLAM+1.)
C
C     FIND CUTOFF FOR BETHE
C
      ZW=30.
      WMAX=SQRT(2.*ZW*EPSIL)*(1.+SQRT((ZW-1.)/ZW))
      WMIN=SQRT(2.*ZW*EPSIL)*(1.-SQRT((ZW-1.)/ZW))
      WKIN=2.*ZW*EPSIL
      LAMIN=LAM
      LAMAX=XL2+XL1
C     FIND SBRNW
      WSUM=0.0
      WANS=0.0
      DELW=(WMAX-WMIN)/100.
      W=WMIN-DELW
```

```
      KW=1
      DO 11 IW=1,101
      W=W+DELW
      FW=0.0
      DO 8 I=LAMIN,LAMAX
      WI=I
      CALL RDINT (BJ,I,W)
      FW=(FW+(2.*XL2+1.)*(2.*WI+1.)*((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)
      RDMO=(RANS**2)
      ANGFCT=(2.*XL2+1.)*((TJ(XL1,XL2,XLAM)*(2.**XLAM)*(FACT(XLAM)/FACT(
     12.*XLAM)))**2)/(2.*XLAM+1.)
C
   12 WFF=8.*RDMO*ANGFCT/WKIN
      IF (LAM.EQ.1) GO TO 13
      XLAM2=2.*XLAM-2.
      WKUT=(XLAM2*SGBRN/WFF+WMIN**XLAM2)**(1./XLAM2)
      GO TO 14
   13 WKUT=(EXP(SGBRN/WFF)*WMIN)
   14 CONTINUE
C
C     FIND ENGFCT
      DO 17 I=1,N
      XMAX=WKUT
      XMIN=SQRT(2.*ZN(I)*EPSIL)*(1.-SQRT((ZN(I)-1.)/ZN(I)))
      ZKIN=2.*ZN(I)*EPSIL
      IF (XLAM.EQ.1.) GO TO 15
      XKINT=(XMAX**(2.*XLAM-2.))/(2.*XLAM-2.)-(XMIN**(2.*XLAM-2.))/(2.*X
     1LAM-2.)
      GO TO 16
   15 XKINT=ALOG(XMAX/XMIN)
   16 ENFCT=(8.*XKINT)/ZKIN
C
   17 SIG(I)=RDMO*ANGFCT*ENFCT
      IF (IPROX.EQ.3) GO TO 36
C
C     MODIFIED BETHE CALCULATION
C
      DO 25 I=1,N
      IF (ZN(I).LT.1.5) GO TO 23
      ZKIN=2.*ZN(I)*EPSIL
      SZ=(ZN(I)-1.)/ZN(I)
      STUFF=RDMO*ANGFCT*4./(3.*ZKIN)
      DO 20 LP1=1,8
      LP=LP1-1
      XLP=LP
      IF (LP.EQ.0) GO TO 18
```

```
      ZETA=((XLP+1.)*(F(1,LP,SZ)**2)+XLP*(SZ**2)*(F(2,LP+1,SZ)**2))*(SZ*
     1*(XLP-.5))/(2.*XLP+1.)
      REST=(2.*XLP+1.)*ZETA/(XLP*(XLP+1.))
      GO TO 19
   18 REST=(SZ**1.5)*(F(2,1,SZ)**2)
   19 SG(LP1)=STUFF*REST
C
C     FIND SGMXL
      SGMXL=(2.*XLP+1.)/ZKIN
C
C     FIND L-ZERO
      IF (SG(LP1).LT.(.5*SGMXL)) GO TO 21
   20 CONTINUE
      WRITE (6,52)
   21 CONTINUE
      LO=LP-1
      IF (LP.EQ.0) LO=0
      XLO=LO
C
C     FIND LO-TERM
      TRMLO=((XLO+1.)**2)/(2.*ZKIN)
C
C     FIND SUM-TERM
      TRMSM=0.0
      DO 22 LS=1,LP
   22 TRMSM=TRMSM+SG(LS)
C
C     FIND MOD. BETHE C-SECTION
      GO TO 24
   23 SIG(I)=0.0
      GO TO 25
   24 SIG(I)=SIG(I)+TRMLO-TRMSM
   25 CONTINUE
      GO TO 36
C
C     BORN + OCHKUR
C
   26 CONTINUE
      XMXN=SQRT(2.*ZN(N)*EPSIL)*(1.+SQRT((ZN(N)-1.)/ZN(N)))
      XMNN=SQRT(2.*ZN(N)*EPSIL)*(1.-SQRT((ZN(N)-1.)/ZN(N)))
      DELX=(XMXN-XMNN)/1000.
      X=XMNN-DELX
      DO 28 IX=1,1001
      X=X+DELX
      LAMIN=ABS(XL2-XL1)
      LAMAX=XL2+XL1
      DO 27 I=LAMIN,LAMAX
      XI=I
      FX(IX)=0.0
C
      CALL ROINT (BJ,I,X)
C
      FX(IX)=(FX(IX)+(2.*XL2+1.)*(2.*XI+1.)*((TJ(XL1,XL2,XI)*RANS)**2))/
     1X**3
   27 CONTINUE
      XMSH(IX)=X
   28 CONTINUE
C
C     FIND K-LIMITS AND COMPUTE SIG
```

```
      DO 34 I=1,N
      XMAX=SQRT(2.*ZN(I)*EPSIL)*(1.+SQRT((ZN(I)-1.)/ZN(I)))
      XMIN=SQRT(2.*ZN(I)*EPSIL)*(1.-SQRT((ZN(I)-1.)/ZN(I)))
      ZKIN=2.*ZN(I)*EPSIL
      DO 29 J=LAMIN,LAMAX
      XJ=J
      FXMAX=0.0
      FXMIN=0.0
      CALL RDINT (BJ,J,XMAX)
      FXMAX=(FXMAX+(2.*XL2+1.)*(2.*XJ+1.)*((TJ(XL1,XL2,XJ)*RANS)**2))/XM
     1AX**3
      CALL RDINT (BJ,J,XMIN)
      FXMIN=(FXMIN+(2.*XL2+1.)*(2.*XJ+1.)*((TJ(XL1,XL2,XJ)*RANS)**2))/XM
     1IN**3
   29 CONTINUE
C
C     BEGIN K-INTEGRATION
      XSUM=0.0
      XANS=0.0
      LP=(XMIN-XMNN)/DELX+1.
      LQ=1001.-(XMXN-XMAX)/DELX
C     TEST FOR NO. OF INTG. PTS. EVEN FOR SIMSON'S RULE INTG.
      XLP=LP
      XLQ=LQ
      T1=(LP-LQ)/2
      T2=(XLP-XLQ)/2.
      IF (T1-T2.EQ.0.0) GO TO 30
      LQ=LQ-1
C     FIND CORRECTIN (C1) USING TRAPEZOID INTG. APPROX.
   30 DILX1=XMIN-XMSH(LP)
      C1=(FX(LP)+FXMIN)*DILX1/2.
      X=XMSH(LP)-DELX
      KX=1
      DO 33 IX=LP,LQ
      XIX=IX
      X=X+DELX
      A=(1.-(X**2/ZKIN)+((X**2/ZKIN)**2))
      IF (IPROX.EQ.1.) A=1.0
      DSIG=FX(IX)*A
      KX=-KX
      IF ((IX-LP)*(IX-LQ)*KX) 31,33,32
   31 XSUM=XSUM+2.*DSIG
   32 XSUM=XSUM+DSIG
   33 XSUM=XSUM+DSIG
      XANS=XSUM*DELX/3.
      DILX2=XMAX-X
      C2=(FX(IX)+FXMAX)*DILX2/2.
      XANSC=XANS-C1+C2
   34 SIG(I)=(8.*XANSC)/ZKIN
      GO TO 36
C
C     OUTPUT ROUTINES
C
   35 WRITE (6,53)
      CALL EXIT
   36 IF (NOTP-2) 37,39,41
C
C     NOTP=1;PUNCHED CARDS
   37 NCC=NCC+1
```

```
      DO 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)
      DO 40 I=1,N,3
      WRITE (IP,55)
      WRITE (IP,59)
      WRITE (IP,58) ZN(I),SIG(I),ZN(I+1),SIG(I+1),ZN(I+2),SIG(I+2)
      WRITE (IP,59)
      WRITE (IP,55)
   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
      DO 42 I=1,N
   42 SIGM(I,NCC)=SIG(I)
      EPSL(NCC)=EPSIL
      BO(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)
      DO 43 I=1,N
      WRITE (IP,64) ZN(I),SIGM(I,1),SIGM(I,2),SIGM(I,3),SIGM(I,4)
   43 CONTINUE
      WRITE (IP,69) BO(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
     1(4)
      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,I4,0PF4.0)
   49 FORMAT (1PE15.7,1P4E14.7)
   50 FORMAT (1PE15.7)
   51 FORMAT (I3,A8)
   52 FORMAT (2X,'**ERROR**LP1 HAS EXCEEDED VALUE OF 8 ')
```

```
   53 FORMAT (1X,'***ERROR***MOD. BETHE CAN ONLY BE USED FOR OPTICAL TRA
     1NSITIONS')
   54 FORMAT (1X,F8.3,2X,E10.3,A8,'(',F3.0,')',2X,A8,'(',I2,'-',I2,')','
     1(EPSIL=',E10.3,')')
   55 FORMAT (1X,'*******************************************************
     1*****************************')
   56 FORMAT (1X,3('*',4X,'N',5X,'|',5X,'SIG(N)',4X),'*')
   57 FORMAT (3X,'(AT. NO.=',F4.0,')',13X,'(EPSIL=',1PE10.3,')',10X,'(NL
     1-N''L'':',I2,'-',I2,')')
   58 FORMAT (1X,3('*',0PF8.3,2X,'|',3X,1PE10.3,2X),'*')
   59 FORMAT (1X,3('*',10X,'|',15X),'*')
   60 FORMAT (32X,A8,'-',A8//)
   61 FORMAT (6X,'CROSS-SECTIONS ARE IN UNITS OF PI*(BOHR RADIUS**2).')
   62 FORMAT (6X,'INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (E
     1PSIL).')
   63 FORMAT (6X,'EPSIL IS IN UNITS OF TWICE THE RYDBERG.'/)
   64 FORMAT (2X,F8.3,4(6X,1PE10.3)/)
   65 FORMAT (3X,'EPSIL',2X,4(6X,1PE10.3)//)
   66 FORMAT (32X,A8,15X,'(AT.NO.=',F3.0,')'/)
   67 FORMAT (1X,5X,'N',2X,4(10X,'SIG(N)')/)
   68 FORMAT (3X,'(NL-N''L'')',4(6X,'(',I2,'-',I2,')',3X))
   69 FORMAT (3X,'APPROX.',4(8X,A8))
      END
      SUBROUTINE RDINT (GRND,LAM,X)
C
C     DO INTEGRATION OVER  WAVE FUNCTIONS
C
      COMMON PIN(521),PF(521),C,RANS,Y(521),KKK
      YSUM=0.0
      YANS=0.0
      DELY=0.0025
      Y(1)=0.0
      YMIN=0.0
      YMAX=0.1
      KY=1
      L=1
      JY=41
    1 DO 10 IY=L,JY
      IF (IY-1) 2,4,2
    2 IF (IY-L) 5,3,5
    3 Y(L)=YMIN
      GO TO 6
    4 SMTX=0.0
      GO TO 7
    5 Y(IY)=Y(IY-1)+DELY
    6 CONTINUE
      W=C*Y(IY)*X
      F=GRND(LAM,W)
      SMTX=PF(IY)*F*PIN(IY)
    7 KY=-KY
      IF ((IY-L)*(IY-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
      END
      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.*SW/(W**3)-3.*CW/(W**2)-SW/W
      RETURN
    4 BJ=15.*SW/(W**4)-15.*CW/(W**3)-6.*SW/(W**2)+CW/W
      RETURN
    5 BJ=105.*SW/(W**5)-105.*CW/(W**4)-45.*SW/(W**3)+10.*CW/(W**2)+SW/W
      RETURN
    6 BJ=945.*SW/(W**6)-945.*CW/(W**5)-420.*SW/(W**4)+105.*CW/(W**3)+15.
     1*SW/(W**2)-CW/W
      RETURN
    7 BJ=12285.*SW/(W**7)-12285.*CW/(W**6)-7140.*SW/(W**5)+2140.*CW/(W**
     14)+240.*SW/(W**3)-23.*CW/(W**2)-SW/W
      RETURN
    8 BJ=184275.*SW/(W**8)-184275.*CW/(W**7)-108045.*SW/(W**6)+4095.*CW/
     1W**5+4020.*SW/(W**4)-450.*CW/(W**3)-30.*SW/(W**2)-CW/W
      RETURN
      END
      FUNCTION RN (L,W)
      RN=W**L
      RETURN
      END
      FUNCTION TJ (X1,X2,X3)
C     CALCULATE 3-J SYMBOL
      A=X1+X2-X3
      AF=FACT(A)
      B=X1+X3-X2
      BF=FACT(B)
      C=X2+X3-X1
      CF=FACT(C)
      D=X1+X2+X3+1.
      DF=FACT(D)
      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.
      IF (A.EQ.0.0) A=1.0
      J=A
      DO 1 I=1,J
      B=I
    1 FACT=FACT*B
      RETURN
      END
      FUNCTION F (M,N,Z)
      DIMENSION AL(8,8)
C
      AL(1,1)=-1.
      AL(1,2)=1.
      AL(2,2)=-1.
      AL(1,3)=.5
      AL(2,3)=1.
      AL(3,3)=-1.5
      AL(1,4)=.5
      AL(2,4)=.5
      AL(3,4)=1.5
      AL(4,4)=-2.5
      AL(1,5)=.625
      AL(2,5)=.5
      AL(3,5)=.75
      AL(4,5)=2.5
      AL(5,5)=-4.375
      AL(1,6)=.875
      AL(2,6)=.625
      AL(3,6)=.75
      AL(4,6)=1.25
      AL(5,6)=4.375
      AL(6,6)=-7.875
      AL(1,7)=1.3125
      AL(2,7)=.875
      AL(3,7)=.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.**(XN-1.))
C
      B=.5*ALOG((1.+SQRT(Z))/(1.-SQRT(Z)))
C
C     FIND E,D+C
C
      N1=N+1
      GO TO (1,8), M
C     FIND E
    1 CONTINUE
```

```
      IF (N-1) 2,2,3
    2 E=0.
      GO TO 6
    3 E=0.
      DO 5 IP1=3,N1
      S=0.
      IP1M2=IP1-2
      DO 4 IN1=1,IP1M2
      XIN1=IN1
    4 S=S+(Z**(IN1-1))/(2.*(XIN1-1.)+1.)
    5 E=E+AL(N1-IP1+1,N1)*(Z**(-IP1+2))*S
C     FIND D
    6 D=AL(N1,N1)
C     FIND  C
      C=0.
      DO 7 IP1=1,N1
      XIP1=IP1
    7 C=C+AL(N1-IP1+1,N1)*(Z**(1.5-XIP1))
      GO TO 15
C
C
C     FIND E
    8 CONTINUE
      IF (N-1) 9,10,10
    9 E=0.
      GO TO 13
   10 E=0.
      DO 12 IP1=2,N1
      S=0.
      IP1M1=IP1-1
      DO 11 IN1=1,IP1M1
      XIN1=IN1
   11 S=S+(Z**(IN1-1))/(2.*(XIN1-1.)+1.)
   12 E=E+AL(IP1,N1)*(Z**(-IP1+1))*S
   13 CONTINUE
C     FIND D
      D=0.
C     FIND C
      C=0.
      DO 14 IP1=1,N1
      XIP1=IP1
   14 C=C+AL(IP1,N1)*(Z**(.5-XIP1))
C
C
   15 F=A*(B*C-D-E)
      RETURN
C
      END
```

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 ($N \neq -1$), or the standard values are retained ($N = -1$). The initial and final state wave functions and related data (i.e. eigenenergies, EEI; 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 ($\Delta\ell = 1$), then the radial integral

$$\int_0^\infty dr\; r^2\, R_{n_i\ell_i}(r)^{\ell}\, R_{n_f\ell_f}$$

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 $Q_L < \frac{1}{2} Q_L^{max}$ this value of LP is designated LO. 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 $f_{born}(k)$ is found over the range KMAX(ZN(N)) to KMIN(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 KMAX(ZN(N)) = XMXN and KMIN(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 $\int_{K(LP)}^{K(LQ)} \frac{d\sigma}{dK}\, dK$ is carried out using Simson's rule, and selecting either the Ochkur (A ≠ 1) or Born (A = 1) expression.

The correction terms

$$\int_{K(LP)}^{K(MIN)} \frac{d\sigma}{dK}\, dK \qquad \text{and} \qquad \int_{K(LQ)}^{K\,MAX} \frac{d\sigma}{dK}\, dK \qquad \text{are}$$

found using a trapezoid integration and these correction terms are added to the tabular integration to obtain the cross-section SIG(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 entegral 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

```
C        PROGRAM  IONCST(INPUT)
C
C         ============================================================
C         *                                                          *
C         *                 * * *     IONCST    * * *                *
C         *                                                          *
C         * A FORTRAN PROGRAM TO CALCULATE PARTIAL CROSS-SECTIONS    *
C         *        FOR NEUTRAL ATOMS IONIZED BY INCIDENT ELECTRONS   *
C         * THE CALCULATION USES NUMERICAL WAVE FUNCTIONS FOR THE    *
C         *        ATOM AND THE BORN-COULOMB APPROXIMATION           *
C         *                                                          *
C         ============================================================
C
C                         ***************************
C                        *          PROGRAM          *
C                       *      AND SUBROUTINES BY     *
C                      *          TOM J GREENE         *
C                       *     UNIVERSITY OF TOLEDO    *
C                        *           1973            *
C                         ***************************
C
        REAL*4 KAPA,KAPAMX
        REAL*8 AQ
        DIMENSION ZN(2), SGGL(6), ZL2(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
C
        DO 15 ITG1=1,1
C
C       READ BOUND STATE WAVE FUNCTION
C
        READ (IM,17) AQ
        READ (IR,18) NLZ1,XL1,EE1,WWNL1,KKK1,Z
        K11=KKK1-1
        DO 1 MIN=1,K11,5
        MAX=MIN+4
        READ (IR,19) (PIN(I),I=MIN,MAX)
      1 CONTINUE
        READ (IR,20) PIN(KKK1)
        EPSIL=(ABS(EE1)/2.)
        PI=3.1415927
        C=0.885341381/Z**(.333333333)
        KKK=KKK1
C
C       BUILD Y(I1)
C
        NBLOCK=KKK1/40
        I1=1
        Y(I1)=0.0
        DELTAY=.0025
        DO 3 J1=1,NBLOCK
        DO 2 K1=1,40
```

```
      I1=I1+1
    2 Y(I1)=Y(I1-1)+DELTAY
    3 DELTAY=DELTAY+DELTAY
      PF(1)=0.0
C
C     READ ENERGY IN THRESHOLD UNITSAND FIND XINITIAL
C
      N=1
      DO 15 ITG=1,1
      READ (IR,21) ZN(1)
      XIN=SQRT(2.*EPSIL*ZN(1))
C
      SG=0.0
C     PICK XL2 AND FIND LAMAX1 AND LAMIN1
      DO 14 IXL2P1=1,6
      IXL2=IXL2P1-1
      XL2=IXL2
      LAMIN1=ABS(XL2-XL1+1)
      LAMAX1=XL2+XL1+1
C
C     FIND KAPAMX AND PICK KAPPA
      DSGKAP=0.0
      KAPAMX=SQRT((ZN(1)-1.)*EPSIL)
      SGLSUM=0.0
      DELKAP=KAPAMX/10.
      KAPA=0.0
      KS=1
      DSGL=0.0
      DO 13 IKS=1,11
      KAPA=KAPA+DELKAP
      ETA=-1./KAPA
      ETAMAX=AMAX1(ETAMAX,ETA)
      ETAMIN=AMIN1(ETAMIN,ETA)
C     TABULATE PF(EK,R,ETA,L2)
C
      DO 4 I1=2,KKK1
      R=Y(I1)*C
      RHO=KAPA*R
      RHOMAX=AMAX1(RHOMAX,RHO)
      RHOMIN=AMIN1(RHOMIN,RHO)
      F=FLNR(IXL2,RHO,ETA)
      PF(I1)=FLNR(IXL2,RHO,ETA)*(2.*XL2+1.)/(KAPA*((2.*PI)**1.5))
    4 CONTINUE
      IF (XL1.NE.XL2) GO TO 6
C
C     ORTHOGONALIZE PF+PI (PF'=PF-C*PI )
C
      IJK=0
      XYZ=1.0
      CALL RDINT (RN,IJK,XYZ)
      CNR=RANS
      DO 5 I1=2,KKK
      PF(I1)=PF(I1)-CNR*PIN(I1)
    5 CONTINUE
    6 CONTINUE
C     FIND THE LIMITS ON THE K-INTEGRATICN(200 PTS.)
C
C
      X=0.0
```

```
      XFN=SQRT(-KAPA**2+2.*(ZN(1)-1.)*EPSIL)
      XMIN=XIN-XFN
      XMAX=XIN+XFN
      DELX=(XMAX-XMIN)/20.
      XSUM=0.0
      XANS=0.0
      X=XMIN-DELX
      KX=1
      DO 10 IX=1,21
      X=X+DELX
      FPR=0.0
      FLAM=0.0
      XINTG=0.0
      DO 7 LAM1=LAMIN1,LAMAX1
      LAM=LAM1-1
      XLAM=LAM
      CALL RDINT (BJ,LAM,X)
      XTJ=TJ(XL1,XL2,XLAM)
    7 FLAM=(2.*XLAM+1.)*((XTJ*RANS)**2)/(2.*XL2+1.)+FLAM
      FPR=FLAM
      XINTG=FPR/(X**3)
      KX=-KX
      IF ((IX-1)*(IX-201)*KX) 8,10,9
    8 XSUM=XSUM+2.*XINTG
    9 XSUM=XSUM+XINTG
   10 XSUM=XSUM+XINTG
      XANS=XSUM*DELX/3.
      DSGL=(128.*XANS)*((KAPA*PI/XIN)**2)
      KS=-KS
      IF ((IKS-1)*(IKS-11)*KS) 11,13,12
   11 SGLSUM=SGLSUM+2.*DSGL
   12 SGLSUM=SGLSUM+DSGL
   13 SGLSUM=SGLSUM+DSGL
      SGL=SGLSUM*DELKAP/3.
      ZNLG=ALOG10(ZN(1))
      N1=NLZ1/10
      SGGL(IXL2P1)=SGL
      ZL2(IXL2P1)=XL2
   14 SG=SG+SGL
   15 CONTINUE
C     OUTPUT ROUTINE
      WRITE (IP,22) AQ
      WRITE (IP,27)
      WRITE (IP,28)
      WRITE (IP,29)
      WRITE (IP,26) Z,EPSIL,N1
      WRITE (IP,24)
      WRITE (IP,25)
      DO 16 I=1,6,3
      WRITE (IP,24)
      WRITE (IP,32)
      WRITE (IP,31) ZL2(I),SGGL(I),ZL2(I+1),SGGL(I+1),ZL2(I+2),SGGL(I+2)
      WRITE (IP,32)
   16 CONTINUE
      WRITE (IP,24)
      WRITE (IP,23)
      WRITE (IP,30) ZN(1),ZNLG,SG
      WRITE (IP,23)
      WRITE (IP,24)
```

```
      WRITE (IP,34) RHOMAX,ETAMAX
      WRITE (IP,33) RHOMIN,ETAMIN
      WRITE (IP,24)
      RETURN
C
   17 FORMAT (A8)
   18 FORMAT (I4,1P3E14.7,I4,0PF4.0)
   19 FORMAT (1PE15.7,1P4E14.7)
   20 FORMAT (1PE15.7)
   21 FORMAT (12F6.2)
   22 FORMAT (32X,A8,'**COUL-BORN'//)
   23 FORMAT (1X,'*',80X,'*')
   24 FORMAT (1X,'******************************************************
     1****************************')
   25 FORMAT (1X,3('*',4X,'L',5X,'|',5X,'SIG(L)',4X),'*')
   26 FORMAT (3X,'(AT. NO.=',F4.0,')',13X,'(EPSIL=',1PE10.3,')',10X,'(NL
     1-N''L'':',I2,'-CONTINUUM)')
   27 FORMAT (6X,'CROSS-SECTIONS ARE IN UNITS OF PI*(BOHR RADIUS**2).')
   28 FORMAT (6X,'INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (E
     1PSIL).')
   29 FORMAT (6X,'EPSIL IS IN UNITS OF TWICE THE RYDBERG.'/)
   30 FORMAT (1X,'*',8X,'N=',0PF8.3,8X,'LOG(N)=',1PE10.3,8X,'SIG(TOTAL)=
     1',1PE10.3,16X,'*')
   31 FORMAT (1X,3('*',0PF8.3,2X,'|',3X,1PE10.3,2X),'*')
   32 FORMAT (1X,3('*',10X,'|',15X),'*')
   33 FORMAT (1X,'*','RHO(MIN)=',1PE14.7,34X,'ETA(MIN)=',1PE14.7,'*')
   34 FORMAT (1X,'*','RHO(MAX)=',1PE14.7,34X,'ETA(MAX)=',1PE14.7,'*')
      END
      FUNCTION FLNR (L,RHO,ETA)
      XL=L
      PI=3.14159265
C     FLNR=CLN*(RHO**(L+1))*PHI
C     FIND  CLN=PROD*(2.**L)*(SQRT(2.*PI*ETA))/(FACT(2.*XL+1.)*SQRT(1.-E
C     (2.*PI*ETA))
      A=2.*PI*ETA
      B=2.*XL+1.
      C=ABS(1.-EXP(A))
      FCT=FACT(B)
      PROD=1.0
      IF (L.EQ.0) GO TO 2
      DO 1 I=1,L
      S=I
      PROD=PROD*SQRT(S**2+ETA**2)
    1 CONTINUE
    2 CONTINUE
      CLN=PROD*(2.**L)*SQRT(-A)/(FCT*SQRT(C))
C     FIND  PHI=AKL*(RHO**K-L-1)
      AKM2=1.0
      AKM1=ETA/(XL+1.)
      CSUM=1.0+AKM1*RHO
      TCSUM=0.0
      L3=L+3
      L30=L+30
      DO 3 K=L3,L30
      XK=K
      AK=(2.*ETA*AKM1-AKM2)/((XK+XL)*(XK-XL-1.))
      IF ((RHO**(K-L-1)).LT.(1.E-40).AND.(AK.LT.1.E-20)) GO TO 4
      CSUM=CSUM+AK*(RHO**(K-L-1))
      TCSUM=CSUM
```

```
      AKM2=AKM1
      AKM1=AK
    3 CONTINUE
    4 CONTINUE
      PHI=CSUM
      FLNR=CLN*(RHO**(L+1))*PHI
      RETURN
      END
      SUBROUTINE RDINT (GRND,LAM,X)
C
C     DO INTEGRATION OVER  WAVE FUNCTIONS
C
      COMMON PIN(521),PF(521),C,RANS,Y(521),KKK
      YSUM=0.0
      YANS=0.0
      DELY=0.0025
      Y(1)=0.0
      YMIN=0.0
      YMAX=0.1
      KY=1
      L=1
      JY=41
    1 DO 10 IY=L,JY
      IF (IY-1) 2,4,2
    2 IF (IY-L) 5,3,5
    3 Y(L)=YMIN
      GO TO 6
    4 SMTX=0.0
      GO TO 7
    5 Y(IY)=Y(IY-1)+DELY
    6 CONTINUE
      W=C*Y(IY)*X
      F=GRND(LAM,W)
      SMTX=PF(IY)*F*PIN(IY)
      IP=6
    7 KY=-KY
      IF ((IY-L)*(IY-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
      END
      FUNCTION BJ (L,W)
      IF (W.LT.1.) GO TO 8
      SW=SIN(W)
      CW=COS(W)
      L1=L+1
      GO TO (1,2,3,4,5,6,7), L1
    1 BJ=SW/W
```

```
      RETURN
    2 BJ=SW/(W**2)-CW/W
      RETURN
    3 BJ=3.*SW/(W**3)-3.*CW/(W**2)-SW/W
      RETURN
    4 BJ=15.*SW/(W**4)-15.*CW/(W**3)-6.*SW/(W**2)+CW/W
      RETURN
    5 BJ=105.*SW/(W**5)-105.*CW/(W**4)-45.*SW/(W**3)+10.*CW/(W**2)+SW/W
      RETURN
    6 BJ=945.*SW/(W**6)-945.*CW/(W**5)-420.*SW/(W**4)+105.*CW/(W**3)+15.
     1*SW/(W**2)-CW/W
      RETURN
    7 BJ=10395.*SW/(W**7)-10395.*CW/(W**6)-4725.*SW/(W**5)+1260.*CW/(W**
     14)+210.*SW/(W**3)-21.*CW/(W**2)-SW/W
      RETURN
    8 XL=L
      XN=XL+1.
      A=(W**2)/(2.*(2.*XL+3.))
      B=(W**4)/(8.*(2.*XL+3.)*(2.*XL+5.))
      BJ=((W**XL)*(2.**XN)*FACT(XN)/FACT(2.*XN))*(1.-A+B)
      RETURN
      END
      FUNCTION RN (L,W)
      RN=W**L
      RETURN
      END
      FUNCTION TJ (X1,X2,X3)
C     CALCULATE 3-J SYMBOL
      A=X1+X2-X3
      AF=FACT(A)
      B=X1+X3-X2
      BF=FACT(B)
      C=X2+X3-X1
      CF=FACT(C)
      D=X1+X2+X3+1.
      DF=FACT(D)
      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.
      AA=A
      IF (A.EQ.0.0) AA=1.0
      J=AA
      DO 1 I=1,J
      B=I
    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(I1)) 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. $PF = \{PF - [\int dr(PF)(PIN)]\, PIN\}\, N$.

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.

γ

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 Alkalis 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 EPSIL is in units of twice the Rydberg; and the cross-sections are measured in units of $\pi a_B{}^2$.

---

*Vainshtein, L. A., V. Opykhtin, and L. Presnyakov, 1964a, P. N. Lebedev Institute of Physics Report A-53.

and

Vainshtein, L. A., V. Opykhtin, and L. Presnyakov 1964b, Zh. Eksperim. Teor. Fiz <u>47</u>, 2306 English Transla: Soviet Physics. - JETP <u>18</u>, 1383 (1964) as reprinted in Moiseiwitsch and Smith (1968).

# 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 |

| | | | | | |
|---|---|---|---|---|---|
| Li: | 2s-3p | Born(1), | Born(2), | Bethe, | Ochkur |
| | 2s-4p | Born(1), | Born(2), | Bethe, | Ochkur |
| | 2s-5p | Born(1), | Born(2), | Bethe, | Ochkur |
| | 2s-3s | Born(1), | Born(2), | Bethe, | Ochkur |
| | 2s-4s | Born(1), | Born(2), | Bethe, | Ochkur |
| | 2s-5s | Born(1), | Born(2), | Bethe, | Ochkur |
| | 2s-3d | Born(1), | Born(2), | Bethe, | Ochkur |
| | 2s-4d | Born(1), | Born(2), | Bethe, | Ochkur |
| | 2s-5d | Born(1), | Born(2), | Bethe, | Ochkur |

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 $K_{max}<K_{min}$ 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.

|  | LITHIUM<br>2s-2p<br>EPSIL = 6.79 (-2) |  |  |  |  | SODIUM<br>3s-3p<br>EPSIL = 7.73 (-2) |  |  |  |  |  |
|---|---|---|---|---|---|---|---|---|---|---|---|
| N | BORN(1) | BORN(2) | OCHKUR | BETHE | MODBETHE | BORN(1) | BORN(2) | OCHKUR | BETHE | MODBETHE | EXP* |
| 1.02 | 4.14(1) | 4.07(1) | 3.99(1) | 6.96(0) | 0.0 | 3.07(1) | 3.08(1) | 3.00(1) | 0.0 | 0.0 | 1.75(1) |
| 1.04 | 5.71(1) | 5.62(1) | 5.54(1) | 2.43(1) | 0.0 | 4.26(1) | 4.27(1) | 4.14(1) | 0.0 | 0.0 | 1.81(1) |
| 1.08 | 7.71(1) | 7.58(1) | 7.55(1) | 4.68(1) | 0.0 | 5.78(1) | 5.79(1) | 5.62(1) | 0.0 | 0.0 | 1.94(1) |
| 1.16 | 9.98(1) | 9.81(1) | 9.55(1) | 7.36(1) | 0.0 | 7.56(1) | 7.58(1) | 7.07(1) | 2.50(1) | 0.0 | 2.20(1) |
| 1.32 | 1.20(2) | 1.18(2) | 1.14(2) | 1.00(2) | 0.0 | 9.32(1) | 9.32(1) | 8.45(1) | 5.87(1) | 0.0 | 2.72(1) |
| 1.64 | 1.31(2) | 1.28(2) | 1.19(2) | 1.18(2) | 5.55(1) | 1.04(2) | 1.04(2) | 9.14(1) | 8.56(1) | 1.80(1) | 3.30(1) |
| 2.28 | 1.24(2) | 1.22(2) | 1.10(2) | 1.18(2) | 6.38(1) | 1.02(2) | 1.03(2) | 9.04(1) | 9.56(1) | 3.76(1) | 3.52(1) |
| 3.56 | 1.03(2) | 1.01(2) | 9.17(1) | 9.98(1) | 6.14(1) | 8.84(1) | 8.85(1) | 8.07(1) | 8.66(1) | 4.43(1) | 3.65(1) |
| 6.12 | 7.53(1) | 7.35(1) | 6.92(1) | 7.38(1) | 5.06(1) | 6.66(1) | 6.66(1) | 6.33(1) | 6.67(1) | 4.11(1) | 3.56(1) |
| 11.24 | 5.01(1) | 4.89(1) | 4.74(1) | 4.93(1) | 3.66(1) | 4.54(1) | 4.53(1) | 4.42(1) | 4.57(1) | 3.17(1) | 3.15(1) |
| 21.48 | 3.12(1) | 3.04(1) | 3.00(1) | 3.07(1) | 2.40(1) | 2.87(1) | 2.87(1) | 2.84(1) | 2.90(1) | 2.17(1) | 2.42(1) |
| 41.96 | 1.86(1) | 1.81(1) | 1.80(1) | 1.83(1) | 1.48(1) | 1.73(1) | 1.73(1) | 1.72(1) | 1.75(1) | 1.37(1) | 1.66(1) |

* Linear Interpolation From "Enemark, E. A., and A. Gallagher, (1972) Phys. Rev. A, 6, 192".

| | POTASSIUM<br>4s-4p<br>EPSIL = 5.93 (-2) | | | | | RUBIDIUM<br>5s-5p<br>EPSIL = 5.78 (-2) | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| N | BORN(1) | BORN(2) | OCHKUR | BETHE | MODBETHE | BORN(1) | BORN(2) | OCHKUR | BETHE | MODBETHE |
| 1.02 | 5.47(1) | 5.51(1) | 5.36(1) | 0.0 | 0.0 | 5.85(1) | 5.66(1) | 5.47(1) | 0.0 | 0.0 |
| 1.04 | 7.57(1) | 7.65(1) | 7.39(1) | 0.0 | 0.0 | 8.11(1) | 7.86(1) | 7.54(1) | 0.0 | 0.0 |
| 1.08 | 1.03(2) | 1.04(2) | 1.00(2) | 0.0 | 0.0 | 1.10(2) | 1.07(2) | 1.02(2) | 0.0 | 0.0 |
| 1.16 | 1.35(2) | 1.37(2) | 1.26(2) | 2.77(1) | 0.0 | 1.46(2) | 1.42(2) | 1.29(2) | 1.11(0) | 0.0 |
| 1.32 | 1.66(2) | 1.69(2) | 1.51(2) | 9.58(1) | 0.0 | 1.80(2) | 1.78(2) | 1.55(2) | 8.33(1) | 0.0 |
| 1.64 | 1.87(2) | 1.91(2) | 1.65(2) | 1.52(2) | 8.85(0) | 2.03(2) | 2.04(2) | 1.73(2) | 1.53(2) | 0.0 |
| 2.28 | 1.86(2) | 1.91(2) | 1.67(2) | 1.75(2) | 4.80(1) | 2.02(2) | 2.07(2) | 1.80(2) | 1.86(2) | 3.59(1) |
| 3.56 | 1.59(2) | 1.66(2) | 1.51(2) | 1.62(2) | 6.92(1) | 1.76(2) | 1.82(2) | 1.66(2) | 1.76(2) | 6.59(1) |
| 6.12 | 1.20(2) | 1.26(2) | 1.20(2) | 1.26(2) | 6.86(1) | 1.33(2) | 1.39(2) | 1.33(2) | 1.39(2) | 7.10(1) |
| 11.24 | 8.21(1) | 8.60(1) | 8.41(1) | 8.67(1) | 5.54(1) | 9.13(1) | 9.60(1) | 9.39(1) | 9.67(1) | 5.94(1) |
| 21.48 | 5.20(1) | 5.47(1) | 5.41(1) | 5.52(1) | 3.89(1) | 5.80(1) | 6.13(1) | 6.07(1) | 6.19(1) | 4.25(1) |
| 41.96 | 3.14(1) | 3.31(1) | 3.29(1) | 3.34(1) | 2.51(1) | 3.51(1) | 3.72(1) | 3.71(1) | 3.76(1) | 2.77(1) |

CESIUM

6s-6p

EPSIL = 5.21 (-2)

| N | BORN(1) | BORN(2) | OCHKUR | BETHE | MODBETHE |
|---|---|---|---|---|---|
| 1.02 | 7.50(1) | 7.06(1) | 6.81(1) | 0.0 | 0.0 |
| 1.04 | 1.04(2) | 9.82(1) | 9.38(1) | 0.0 | 0.0 |
| 1.08 | 1.41(2) | 1.35(2) | 1.27(2) | 0.0 | 0.0 |
| 1.16 | 1.86(2) | 1.79(2) | 1.60(2) | 0.0 | 0.0 |
| 1.32 | 2.30(2) | 2.26(2) | 1.95(2) | 8.78(1) | 0.0 |
| 1.64 | 2.60(2) | 2.62(2) | 2.21(2) | 1.88(2) | 0.0 |
| 2.28 | 2.60(2) | 2.69(2) | 2.34(2) | 2.39(2) | 2.63(1) |
| 3.56 | 2.26(2) | 2.39(2) | 2.19(2) | 2.31(2) | 7.27(1) |
| 6.12 | 1.72(2) | 1.85(2) | 1.77(2) | 1.84(2) | 8.56(1) |
| 11.24 | 1.17(2) | 1.28(2) | 1.25(2) | 1.29(2) | 7.45(1) |
| 21.48 | 7.46(1) | 8.21(1) | 8.14(1) | 8.29(1) | 5.46(1) |
| 41.96 | 4.52(1) | 5.00(1) | 4.98(1) | 5.05(1) | 3.61(1) |

## LITHIUM

| | 2s-3p | | | | 2s-4p | | | |
|---|---|---|---|---|---|---|---|---|
| | EPSIL = 1.41 (-1) | | | | EPSIL = 1.66 (-1) | | | |
| N | BORN(1) | BORN(2) | BETHE | OCHKUR | BORN(1) | BORN(2) | BETHE | OCHKUR |
| 1.02 | 9.67(-1) | 9.74(-1) | 2.76(-0) | 9.72(-1) | 2.24(-1) | 2.27(-1) | 3.24(-1) | 2.28(-1) |
| 1.04 | 1.30(0) | 1.32(0) | 2.72(-0) | 1.34(-1) | 3.01(-1) | 3.05(-1) | 3.30(-1) | 3.14(-1) |
| 1.08 | 1.68(0) | 1.70(0) | 2.64(-0) | 1.79(-0) | 3.84(-1) | 3.90(-1) | 3.35(-1) | 4.16(-1) |
| 1.16 | 2.01(0) | 2.03(0) | 2.48(-0) | 2.15(-0) | 4.49(-1) | 4.56(-1) | 3.33(-1) | 4.95(-1) |
| 1.32 | 2.11(0) | 2.15(0) | 2.21(-0) | 2.29(-0) | 4.67(-1) | 4.67(-1) | 3.18(-1) | 5.10(-1) |
| 1.64 | 1.87(0) | 1.92(0) | 1.80(-0) | 1.90(-0) | 3.91(-1) | 4.02(-1) | 2.82(-1) | 4.04(-1) |
| 2.28 | 1.39(0) | 1.43(0) | 1.33(-0) | 1.27(-0) | 2.84(-1) | 2.93(-1) | 2.26(-1) | 2.56(-1) |
| 3.56 | 8.91(-1) | 9.22(-1) | 8.71(-1) | 7.34(-1) | 1.84(-1) | 1.89(-1) | 1.62(-1) | 1.56(-1) |
| 6.12 | 5.20(-1) | 5.37(-1) | 5.19(-1) | 4.66(-1) | 1.13(-1) | 1.13(-1) | 1.05(-1) | 9.76(-2) |
| 11.24 | 2.88(-1) | 2.94(-1) | 2.90(-1) | 2.69(-1) | 6.67(-2) | 6.55(-2) | 6.39(-1) | 5.99(-2) |
| 21.48 | 1.55(-1) | 1.56(-1) | 1.56(-1) | 1.49(-1) | 3.85(-2) | 3.69(-2) | 3.69(-2) | 3.53(-2) |
| 41.96 | 8.23(-2) | 8.16(-1) | 8.19(-2) | 7.95(-2) | 2.19(-2) | 2.05(-2) | 2.07(-2) | 2.00(-2) |

## LITHIUM

| | 2s-5p | | | | 2s-3s | | | |
|---|---|---|---|---|---|---|---|---|
| | EPSIL = 1.78 (-1) | | | | EPSIL = 1.24 (-1) | | | |
| N | BORN(1) | BORN(2) | BETHE | OCHKUR | BORN(1) | BORN(2) | BETHE | OCHKUR |
| 1.02 | 8.95(-2) | 9.07(-2) | 7.90(-2) | 9.12(-2) | 1.21(0) | 1.23(-0) | 1.03(0) | 1.20(-0) |
| 1.04 | 1.20(-1) | 1.21(-1) | 8.43(-2) | 1.26(-1) | 1.66(0) | 1.68(-0) | 1.83(0) | 1.64(-0) |
| 1.08 | 1.52(-1) | 1.54(-1) | 9.03(-2) | 1.66(-1) | 2.21(0) | 2.24(-0) | 2.72(0) | 2.17(-0) |
| 1.16 | 1.76(-1) | 1.79(-1) | 9.58(-2) | 1.97(-1) | 2.79(0) | 2.83(-0) | 3.55(0) | 2.62(-0) |
| 1.32 | 1.77(-1) | 1.82(-1) | 9.81(-2) | 2.00(-1) | 3.25(0) | 3.27(-0) | 4.04(0) | 2.91(-0) |
| 1.64 | 1.50(-1) | 1.55(-1) | 9.35(-2) | 1.56(-1) | 3.33(0) | 3.32(-0) | 3.94(0) | 2.83(-0) |
| 2.28 | 1.09(-1) | 1.12(-1) | 8.00(-2) | 9.78(-2) | 2.90(0) | 2.88(-0) | 3.23(0) | 2.45(-0) |
| 3.56 | 7.21(-2) | 7.32(-2) | 6.09(-2) | 6.02(-2) | 2.12(0) | 2.10(-0) | 2.25(0) | 1.86(-0) |
| 6.12 | 4.54(-2) | 4.51(-2) | 4.15(-2) | 3.89(-2) | 1.34(0) | 1.33(-0) | 1.37(0) | 1.23(-0) |
| 11.24 | 2.78(-2) | 2.69(-2) | 2.62(-2) | 2.47(-2) | 7.68(0) | 7.55(-1) | 7.66(-1) | 7.24(-1) |
| 21.48 | 1.65(-2) | 1.56(-2) | 1.56(-2) | 1.50(-2) | 4.12(0) | 4.05(-1) | 4.06(-1) | 3.96(-1) |
| 41.96 | 9.63)-3) | 8.89(-3) | 8.99(-3) | 8.71(-3) | 2.14(0) | 2.10(-1) | 2.10(-1) | 2.08(-1) |

## LITHIUM

| | 2s-4s | | | | 2s-5s | | | |
|---|---|---|---|---|---|---|---|---|
| | EPSIL = 1.60(-1) | | | | EPSIL = 1.75 (-1) | | | |
| N | BORN(1) | BORN(2) | BETHE | OCHKUR | BORN(1) | BORN(2) | BETHE | OCHKUR |
| 1.02 | 2.13(-1) | 2.17(-1) | 4.43(-1) | 2.11(-1) | 7.81(-2) | 7.89(-2) | 1.83(-1) | 7.65(-2) |
| 1.04 | 2.91(-1) | 2.96(-1) | 5.31(-1) | 2.86(-1) | 1.07(-1) | 1.08(-1) | 2.10(-1) | 1.04(-1) |
| 1.08 | 3.86(-1) | 3.91(-1) | 6.24(-1) | 3.76(-1) | 1.41(-1) | 1.42(-1) | 2.36(-1) | 1.36(-1) |
| 1.16 | 4.84(-1) | 4.88(-1) | 7.00(-1) | 4.47(-1) | 1.76(-1) | 1.76(-1) | 2.59(-1) | 1.60(-1) |
| 1.32 | 5.55(-1) | 5.56(-1) | 7.24(-1) | 4.86(-1) | 2.01(-1) | 2.00(-1) | 2.62(-1) | 1.73(-1) |
| 1.64 | 5.58(-1) | 5.56(-1) | 6.64(-1) | 4.64(-1) | 2.00(-1) | 1.98(-1) | 2.37(-1) | 1.65(-1) |
| 2.28 | 4.76(-1) | 4.71(-1) | 5.25(-1) | 3.96(-1) | 1.60(-1) | 1.67(-1) | 1.85(-1) | 1.40(-1) |
| 3.56 | 3.42(-1) | 3.37(-1) | 3.57(-1) | 2.97(-1) | 1.21(-1) | 1.18(-1) | 1.25(-1) | 1.04(-1) |
| 6.12 | 2.13(-1) | 2.09(-1) | 2.15(-1) | 1.93(-1) | 7.50(-2) | 7.32(-2) | 7.52(-2) | 6.76(-2) |
| 11.24 | 1.20(-1) | 1.18(-1) | 1.19(-1) | 1.13(-1) | 4.23(-2) | 4.12(-2) | 4.17(-2) | 3.94(-2) |
| 21.48 | 6.43(-2) | 6.30(-2) | 6.31(-2) | 6.15(-2) | 2.25(-2) | 2.19(-2) | 2.20(-2) | 2.14(-2) |
| 41.96 | 3.32(-2) | 3.25(-2) | 3.25(-2) | 3.22(-2) | 1.16(-2) | 1.13(-2) | 1.13(-2) | 1.12(-2) |

# LITHIUM

| | 2s-3d | | | | 2s-4d | | | |
|---|---|---|---|---|---|---|---|---|
| | EPSIL = 1.43 (-1) | | | | EPSIL = 1.67 (-1) | | | |
| N | BORN(1) | BORN(2) | BETHE | OCHKUR | BORN(1) | BORN(2) | BETHE | OCHKUR |
| 1.02 | 1.38(0) | 1.31(-0) | 0.0 | 1.26(-0) | 4.09(-1) | 3.91(-1) | 0.0 | 3.79(-1) |
| 1.04 | 1.90(0) | 1.80(-0) | 0.0 | 1.73(-0) | 5.62(-1) | 5.36(-1) | 0.0 | 5.16(-1) |
| 1.08 | 2.56(0) | 2.43(-0) | 0.0 | 2.31(-0) | 7.56(-1) | 7.15(-1) | 0.0 | 6.83(-1) |
| 1.16 | 3.31(0) | 3.13(-0) | 0.0 | 2.83(-0) | 9.53(-1) | 9.07(-1) | 2.60(-1) | 8.25(-1) |
| 1.32 | 3.96(0) | 3.73(-0) | 9.82(-1) | 3.24(-0) | 1.11(0) | 1.06(-0) | 7.26(-1) | 9.22(-1) |
| 1.64 | 4.19(0) | 3.94(-0) | 2.81(-1) | 3.32(-0) | 1.14(0) | 1.08(-0) | 9.54(-1) | 9.10(-1) |
| 2.28 | 3.77(0) | 3.52(-0) | 3.18(-0) | 3.01(-0) | 9.86(-1) | 9.35(-1) | 9.00(-1) | 7.94(-1) |
| 3.56 | 2.82(0) | 2.63(-0) | 2.56(-0) | 2.35(-0) | 7.16(-1) | 6.79(-1) | 6.72(-1) | 6.02(-1) |
| 6.12 | 1.81(0) | 1.69(-0) | 1.67(-0) | 1.58(-0) | 4.50(-1) | 4.26(-1) | 4.25(-1) | 3.96(-1) |
| 11.24 | 1.04(0) | 9.70(-1) | 9.69(-1) | 9.35(-1) | 2.56(-1) | 2.42(-1) | 2.42(-1) | 2.32(-1) |
| 21.48 | 5.62(-1) | 5.23(-1) | 5.23(-1) | 5.13(-1) | 1.37(-1) | 1.30(-1) | 1.30(-1) | 1.26(-1) |
| 41.96 | 2.92(-1) | 2.72(-1) | 2.72(-1) | 2.69(-1) | 7.08(-2) | 6.71(-2) | 6.71(-2) | 6.63(-2) |

# LITHIUM

2s-5d

EPSIL = 1.78 (-1)

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

SODIUM

| | 3s-4p | | | 3s-5p | | | 3s-6p | | |
|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 1.38 (-1) | | | EPSIL = 1.60 (-1) | | | EPSIL = 1.70 (-1) | | |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 1.43(0) | 6.61(-0) | 1.40(-1) | 3.85(-1) | 1.66(-0) | 3.75(-1) | 1.64(-1) | 6.77(-1) | 1.59(-1) |
| 1.04 | 1.95(0) | 6.56(-0) | 1.91(-0) | 5.23(-1) | 1.64(-0) | 5.11(-1) | 2.22(-1) | 6.66(-1) | 2.16(-1) |
| 1.08 | 2.58(0) | 6.42(-0) | 2.53(-0) | 6.83(-1) | 1.59(-0) | 6.68(-1) | 2.89(-1) | 6.44(-1) | 2.82(-1) |
| 1.16 | 3.20(0) | 6.10(-0) | 3.03(-0) | 8.37(-1) | 1.49(-0) | 7.88(-1) | 3.51(-1) | 6.30(-1) | 3.30(-1) |
| 1.32 | 3.63(0) | 5.52(-0) | 3.28(-0) | 9.25(-1) | 1.33(-0) | 8.32(-1) | 3.84(-1) | 5.34(-1) | 3.44(-1) |
| 1.64 | 3.60(0) | 4.60(-0) | 3.06(-0) | 8.90(-1) | 1.09(-0) | 7.46(-1) | 3.65(-1) | 4.35(-1) | 3.04(-1) |
| 2.28 | 3.06(0) | 3.45(-0) | 2.53(-0) | 7.30(-1) | 7.97(-1) | 5.92(-1) | 2.96(-1) | 3.17(-1) | 2.37(-1) |
| 3.56 | 2.22(0) | 2.32(-0) | 1.88(-0) | 5.13(-1) | 5.22(-1) | 4.26(-1) | 2.05(-1) | 2.06(-1) | 1.68(-1) |
| 6.12 | 1.42(0) | 1.42(0) | 1.26(-0) | 3.18(-1) | 3.11(-1) | 2.75(-1) | 1.26(-1) | 1.22(-1) | 1.08(-1) |
| 11.24 | 8.39(-1) | 8.10(-1) | 7.62(-1) | 1.82(-1) | 1.73(-1) | 1.63(-1) | 7.10(-2) | 6.73(-1) | 6.30(-2) |
| 21.48 | 4.68(-1) | 4.45(-1) | 4.32(-1) | 9.91(-2) | 9.30(-2) | 9.00(-2) | 3.83(-2) | 3.58(-2) | 3.47(-2) |
| 41.96 | 2.54(-1) | 2.39(-1) | 2.36(-1) | 5.25(-2) | 4.88(-2) | 4.81(-2) | 2.01(-2) | 1.86(-2) | 1.84(-2) |

SODIUM

|  | 3s-7p |  |  | 3s-4s |  |  | 3s-5s |  |  |
|---|---|---|---|---|---|---|---|---|---|
|  | EPSIL = 1.76 (-1) |  |  | EPSIL = 1.17 (-1) |  |  | EPSIL = 1.51 (-1) |  |  |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 8.65(-2) | 3.47(-1) | 8.38(-2) | 1.27(0) | 6.92(-1) | 1.32(-0) | 2.25(-1) | 4.60(-1) | 2.32(-1) |
| 1.04 | 1.17(-1) | 3.41(-1) | 1.14(-1) | 1.75(0) | 1.70(0) | 1.81(-0) | 3.08(-1) | 5.70(-1) | 3.14(-1) |
| 1.08 | 1.52(-1) | 3.30(-1) | 1.48(-1) | 2.33(0) | 2.83(0) | 2.39(-0) | 4.09(-1) | 6.89(-1) | 4.12(-1) |
| 1.16 | 1.84(-1) | 3.08(-1) | 1.73(-1) | 2.96(0) | 3.89(0) | 2.89(-0) | 5.15(-1) | 7.89(-1) | 4.90(-1) |
| 1.32 | 2.01(-1) | 2.73(-1) | 1.78(-1) | 3.47(0) | 4.57(0) | 3.23(-0) | 5.96(-1) | 8.29(-1) | 5.37(-1) |
| 1.64 | 1.90(-1) | 2.21(-1) | 1.57(-1) | 3.58(0) | 4.54(0) | 3.19(-0) | 6.06(-1) | 7.67(-1) | 5.24(-1) |
| 2.28 | 1.53(-1) | 1.61(-1) | 1.21(-1) | 3.15(0) | 3.76(0) | 2.82(-0) | 5.21(-1) | 6.10(-1) | 4.58(-1) |
| 3.56 | 1.06(-1) | 1.04(-1) | 8.54(-2) | 2.32(0) | 2.63(0) | 2.17(-0) | 3.76(-1) | 4.17(-1) | 3.46(-1) |
| 6.12 | 6.47(-2) | 6.13(-2) | 5.43(-2) | 1.47(0) | 1.61(0) | 1.44(-0) | 2.35(-1) | 2.52(-1) | 2.27(-1) |
| 11.24 | 3.65(-2) | 3.38(-2) | 3.17(-2) | 8.43(-1) | 9.00(-1) | 8.51(-1) | 1.33(-1) | 1.40(-1) | 1.32(-1) |
| 21.48 | 1.96(-2) | 1.79(-2) | 1.73(-2) | 4.53(-1) | 4.78(-1) | 4.66(-1) | 7.11(-2) | 7.40(-2) | 7.21(-2) |
| 41.96 | 1.03(-2) | 9.30(-3) | 9.16(-3) | 2.35(-1) | 2.46(-1) | 2.44(-1) | 3.68(-2) | 3.81(-2) | 3.77(-2) |

## SODIUM

| | 3s-6s | | | 3s-7s | | | 3s-3d | | |
|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 1.66 (-1) | | | EPSIL = 1.73 (-1) | | | EPSIL = 1.33 (-1) | | |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 8.02(-2) | 1.96(-1) | 8.40(-2) | 3.94(-2) | 1.00(-1) | 4.07(-2) | 1.94(0) | 0.0 | 1.80(-0) |
| 1.04 | 1.10(-1) | 2.30(-1) | 1.14(-1) | 5.40(-2) | 1.16(-1) | 5.50(-2) | 2.67(0) | 0.0 | 2.46(-0) |
| 1.08 | 1.46(-1) | 2.65(-1) | 1.48(-1) | 7.16(-2) | 1.31(-1) | 7.17(-2) | 3.60(0) | 0.0 | 3.28(-0) |
| 1.16 | 1.83(-1) | 2.94(-1) | 1.76(-1) | 8.99(-2) | 1.44(-1) | 8.46(-2) | 4.62(0) | 0.0 | 4.02(-0) |
| 1.32 | 2.11(-1) | 3.01(-1) | 1.91(-1) | 1.03(-1) | 1.46(-1) | 9.19(-2) | 5.49(0) | 0.0 | 4.60(-0) |
| 1.64 | 2.14(-1) | 2.73(-1) | 1.86(-1) | 1.04(-1) | 1.32(-1) | 8.93(-2) | 5.76(0) | 4.00(-0) | 4.70(-0) |
| 2.28 | 1.83(-1) | 2.15(-1) | 1.62(-1) | 8.87(-2) | 1.03(-1) | 7.75(-2) | 5.13(0) | 4.50(-0) | 4.25(-0) |
| 3.56 | 1.31(-1) | 1.46(-1) | 1.22(-1) | 6.34(-2) | 6.96(-2) | 5.81(-2) | 3.82(0) | 3.60(-0) | 3.31(-0) |
| 6.12 | 8.17(-2) | 8.79(-2) | 7.92(-2) | 3.94(-2) | 4.18(-2) | 3.77(-2) | 2.44(0) | 2.36(-0) | 2.22(-0) |
| 11.24 | 4.61(-2) | 4.88(-2) | 4.62(-2) | 2.22(-2) | 2.32(-2) | 2.20(-2) | 1.40(0) | 1.36(-0) | 1.31(-0) |
| 21.48 | 2.46(-2) | 2.58(-2) | 2.53(-2) | 1.18(-2) | 1.23(-2) | 1.19(-2) | 7.56(-1) | 7.35(-1) | 7.21(-1) |
| 41.96 | 1.27(-2) | 1.33(-2) | 1.31(-2) | 6.11(-3) | 6.30(-3) | 6.24(-3) | 3.93(-1) | 3.82(-1) | 3.78(-1) |

## SODIUM

| | 3s-4d | | | 3s-5d | | | 3s-6d | | |
|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 1.57 (-1) | | | EPSIL = 1.69 (-1) | | | EPSIL 1.75 (-1) | | |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 5.45(-1) | 0.0 | 5.11(-1) | 2.34(-1) | 0.0 | 2.19(-1) | 1.22(-1) | 0.0 | 1.16(-1) |
| 1.04 | 7.46(-1) | 0.0 | 6.96(-1) | 3.19(-1) | 0.0 | 2.98(-1) | 1.67(-1) | 3.28(-2) | 1.57(-1) |
| 1.08 | 9.92(-1) | 0.0 | 9.16(-1) | 4.22(-1) | 1.53(-1) | 3.92(-1) | 2.20(-1) | 1.26(-1) | 2.06(-1) |
| 1.16 | 1.25(0) | 5.30(-1) | 1.11(-0) | 5.28(-1) | 3.60(-1) | 4.69(-1) | 2.75(-1) | 2.18(-1) | 2.46(-1) |
| 1.32 | 1.44(0) | 1.06(-0) | 1.23(-0) | 6.02(-1) | 5.15(-1) | 5.14(-1) | 3.11(-1) | 2.83(-1) | 2.67(-1) |
| 1.64 | 1.46(0) | 1.30(-0) | 1.20(-0) | 6.00(-1) | 5.62(-1) | 4.94(-1) | 3.07(-1) | 2.96(-1) | 2.54(-1) |
| 2.28 | 1.25(0) | 1.20(-0) | 1.04(-0) | 5.05(-1) | 4.90(-1) | 4.89(-1) | 2.57(-1) | 2.52(-1) | 2.14(-1) |
| 3.56 | 9.01(-1) | 8.77(-1) | 7.82(-1) | 3.59(-1) | 3.52(-1) | 3.11(-1) | 1.81(-1) | 1.79(-1) | 1.57(-1) |
| 6.12 | 5.62(-1) | 5.51(-1) | 5.12(-1) | 2.22(-1) | 2.18(-1) | 2.02(-1) | 1.12(-1) | 1.10(-1) | 1.02(-1) |
| 11.24 | 3.18(-1) | 3.13(-1) | 3.00(-1) | 1.25(-1) | 1.23(-1) | 1.18(-1) | 6.27(-1) | 6.20(-2) | 5.93(-2) |
| 21.48 | 1.70(-1) | 1.67(-1) | 1.63(-1) | 6.65(-2) | 6.56(-2) | 6.40(-2) | 3.33(-2) | 3.30(-2) | 3.22(-2) |
| 41.96 | 8.79(-2) | 8.65(-2) | 8.55(-2) | 3.44(-2) | 3.39(-2) | 3.35(-2) | 1.72(-2) | 1.71(-2) | 1.68(-2) |

SODIUM

3s-7d

EPSIL = 1.79 (-1)

| N | BORN(1) | BETHE | OCHKUR |
|---|---|---|---|
| 1.02 | 7.31(-2) | 0.0 | 6.89(-2) |
| 1.04 | 9.97(-2) | 3.86(-2) | 9.35(-2) |
| 1.08 | 1.31(-1) | 8.92(-2) | 1.23(-1) |
| 1.16 | 1.63(-1) | 1.38(-1) | 1.46(-1) |
| 1.32 | 1.84(-1) | 1.72(-1) | 1.58(-1) |
| 1.64 | 1.81(-1) | 1.75(-1) | 1.49(-1) |
| 2.28 | 1.50(-1) | 1.48(-1) | 1.25(-1) |
| 3.56 | 1.06(-1) | 1.05(-1) | 9.16(-2) |
| 6.12 | 6.48(-2) | 6.42(-2) | 5.91(-2) |
| 11.24 | 3.64(-2) | 3.60(-2) | 3.44(-2) |
| 21.48 | 1.94(-2) | 1.92(-2) | 1.87(-2) |
| 41.96 | 9.97(-3) | 9.88(-3) | 9.76(-3) |

POTASSIUM

| | 4s-5p | | | 4s-6p | | | 4s-7p | | |
|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 1.13 (-1) | | | EPSIL = 1.32 (-1) | | | EPSIL = 1.42 (-1) | | |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 2.24(0) | 1.13(+1) | 2.19(0) | 5.92(-1) | 2.72(0) | 5.78(-1) | 2.51(-1) | 1.09(0) | 2.44(-1) |
| 1.04 | 3.06(0) | 1.12(+1) | 2.98(0) | 8.05(-1) | 2.67(0) | 7.81(-1) | 3.40(-1) | 1.07(0) | 3.30(-1) |
| 1.08 | 4.03(0) | 1.09(+1) | 3.90(0) | 1.06(0) | 2.59(0) | 1.01(0) | 4.44(-1) | 1.04(0) | 4.26(-1) |
| 1.16 | 5.01(0) | 1.03(+1) | 4.63(0) | 1.29(0) | 2.42(0) | 1.18(0) | 5.42(-1) | 9.68(-1) | 4.92(-1) |
| 1.32 | 5.69(0) | 9.20(0) | 5.00(0) | 1.44(0) | 2.14(0) | 1.24(0) | 5.99(-1) | 8.55(-1) | 5.11(-1) |
| 1.64 | 5.57(0) | 7.60(0) | 4.74(0) | 1.40(0) | 1.74(0) | 1.14(0) | 5.76(-1) | 6.92(-1) | 4.62(-1) |
| 2.28 | 4.84(0) | 5.63(0) | 4.02(0) | 1.16(0) | 1.27(0) | 9.30(-1) | 4.70(-1) | 5.01(-1) | 3.72(-1) |
| 3.56 | 3.32(0) | 3.73(0) | 3.02(0) | 8.21(-1) | 8.24(-1) | 6.74(-1) | 3.28(-1) | 3.24(-1) | 2.67(-1) |
| 6.12 | 2.25(0) | 2.25(0) | 2.00(0) | 5.11(-1) | 4.86(-1) | 4.33(-1) | 2.02(-1) | 1.90(-1) | 1.70(-1) |
| 11.24 | 1.32(0) | 1.27(0) | 1.20(0) | 2.92(-1) | 2.70(-1) | 2.53(-1) | 1.14(-1) | 5.01(-1) | 9.82(-2) |
| 21.48 | 7.34(-1) | 6.90(-1) | 6.71(-1) | 1.59(-1) | 1.43(-1) | 1.39(-1) | 6.17(-2) | 3.24(-1) | 5.35(-2) |
| 41.96 | 3.97(-1) | 3.66(-1) | 3.62(-1) | 8.44(-2) | 7.43(-2) | 7.34(-2) | 3.24(-2) | 1.90(-1) | 2.81(-2) |

## POTASSIUM

| | 4s-5s | | | 4s-6s | | | 4s-7s | | |
|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 9.58 (-2) | | | EPSIL = 1.25 (-1) | | | EPSIL = 1.38 (-1) | | |
| N | BORN (1) | BETHE | OCHKUR | BORN (1) | BETHE | OCHKUR | BORN (1) | BETHE | OCHKUR |
| 1.02 | 1.66(0) | 0.0 | 1.91(0) | 2.90(-1) | 5.38(-1) | 3.24(-1) | 1.01(-1) | 2.58(-1) | 1.17(-1) |
| 1.04 | 2.29(0) | 9.14(-1) | 2.60(0) | 4.00(-1) | 7.56(-1) | 4.39(-1) | 1.39(-1) | 3.25(-1) | 1.57(-1) |
| 1.08 | 3.09(0) | 3.22(0) | 3.45(0) | 5.38(-1) | 9.95(-1) | 5.77(-1) | 1.87(-1) | 3.96(-1) | 2.06(-1) |
| 1.16 | 3.96(0) | 5.48(0) | 4.19(0) | 6.93(-1) | 1.21(0) | 6.94(-1) | 2.41(-1) | 4.57(-1) | 2.47(-1) |
| 1.32 | 4.77(0) | 7.08(0) | 4.79(0) | 8.24(-1) | 1.32(0) | 7.89(-1) | 2.88(-1) | 4.82(-1) | 2.81(-1) |
| 1.64 | 5.06(0) | 7.38(0) | 5.00(0) | 8.66(-1) | 1.26(0) | 8.20(-1) | 3.02(-1) | 4.48(-1) | 2.92(-1) |
| 2.28 | 4.38(0) | 6.28(0) | 4.66(0) | 7.53(-1) | 1.01(0) | 7.52(-1) | 2.67(-1) | 3.57(-1) | 2.66(-1) |
| 3.56 | 3.42(0) | 4.46(0) | 3.69(0) | 5.60(-1) | 6.98(-1) | 5.82(-1) | 1.94(-1) | 2.44(-1) | 2.04(-1) |
| 6.12 | 2.19(0) | 2.75(0) | 2.47(0) | 3.53(-1) | 4.24(-1) | 3.83(-1) | 1.22(-1) | 1.48(-1) | 1.34(-1) |
| 11.24 | 1.26(0) | 1.55(0) | 1.47(0) | 2.01(-1) | 2.36(-1) | 2.25(-1) | 6.90(-2) | 8.21(-2) | 7.01(-2) |
| 21.48 | 6.80(-1) | 8.22(0) | 8.04(-1) | 1.08(-1) | 1.25(-1) | 1.22(-1) | 3.59(-2) | 4.34(-2) | 4.25(-2) |
| 41.96 | 3.53(-1) | 4.24(-1) | 4.22(-1) | 5.57(-2) | 6.45(-2) | 6.40(-2) | 1.91(-2) | 2.24(-2) | 2.22(-2) |

## POTASSIUM

| | 4s-3d | | | 4s-4d | | | 4s-5d | | |
|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 9.81 (-2) | | | EPSIL = 1.25 (-1) | | | EPSIL = 1.38 (-1) | | |
| N | BORN (1) | BETHE | OCHKUR | BORN (1) | BETHE | OCHKUR | BORN (1) | BETHE | OCHKUR |
| 1.02 | 7.64(0) | 1.77(+1) | 8.27(0) | 1.36(0) | 0.0 | 5.91(-1) | 4.27(-1) | 0.0 | 5.25(-2) |
| 1.04 | 1.04(1) | 9.86(+1) | 1.14(-1) | 1.84(0) | 0.0 | 8.38(-1) | 5.75(-1) | 0.0 | 8.48(-2) |
| 1.08 | 1.38(1) | 7.84(-1) | 1.53(+1) | 2.39(0) | 1.99(-1) | 1.15(0) | 7.39(-1) | 0.0 | 1.40(-1) |
| 1.16 | 1.74(1) | 8.50(0) | 1.87(+1) | 2.88(0) | 5.12(-1) | 1.46(0) | 8.76(-1) | 0.0 | 2.18(-1) |
| 1.32 | 1.98(1) | 1.59(+1) | 2.10(+1) | 3.11(0) | 7.49(-1) | 1.64(0) | 9.17(-1) | 0.0 | 3.10(-1) |
| 1.64 | 1.97(1) | 1.91(+1) | 1.99(+1) | 2.87(0) | 8.25(-1) | 1.37(0) | 8.12(-1) | 0.0 | 3.22(-1) |
| 2.28 | 1.67(1) | 1.73(+1) | 1.60(+1) | 2.23(0) | 7.22(-1) | 8.45(-1) | 6.07(-1) | 1.52(-1) | 2.47(-1) |
| 3.56 | 1.20(1) | 1.27(+1) | 1.14(+1) | 1.49(0) | 5.20(-1) | 4.65(-1) | 3.93(-1) | 1.68(-1) | 1.70(-1) |
| 6.12 | 7.46(0) | 7.98(0) | 7.31(0) | 8.86(-1) | 3.23(-1) | 2.75(-1) | 2.30(-1) | 1.23(-1) | 1.15(-1) |
| 11.24 | 4.23(0) | 4.52(0) | 4.29(0) | 4.88(-1) | 1.82(-1) | 1.63(-1) | 1.25(-1) | 7.47(-2) | 7.06(-2) |
| 21.48 | 2.26(0) | 2.42(0) | 2.35(0) | 2.57(-1) | 9.70(-2) | 2.08(-2) | 6.65(-1) | 4.12(-2) | 3.98(-2) |
| 41.96 | 1.17(0) | 1.25(0) | 1.23(0) | 1.32(-1) | 5.01(-2) | 4.83(-2) | 3.35(-2) | 2.17(-2) | 2.13(-2) |

# POTASSIUM

4s-6d

EPSIL = 1.44 (-1)

| N | BORN (1) | BETHE | OCHKUR |
|---|---|---|---|
| 1.02 | 2.08(-1) | 0.0 | 8.01(-3) |
| 1.04 | 2.80(-1) | 0.0 | 1.72(-2) |
| 1.08 | 3.59(-1) | 0.0 | 3.76(-2) |
| 1.16 | 4.23(-1) | 0.0 | 7.39(-2) |
| 1.32 | 4.39(-1) | 0.0 | 1.28(-1) |
| 1.64 | 3.86(-1) | 1.18(-2) | 1.56(-1) |
| 2.28 | 2.87(-1) | 1.01(-1) | 1.40(-1) |
| 3.56 | 1.86(-1) | 1.06(-1) | 1.06(-1) |
| 6.12 | 1.08(-1) | 7.65(-2) | 7.28(-2) |
| 11.24 | 5.89(-2) | 4.62(-2) | 4.45(-2) |
| 21.48 | 3.08(-2) | 2.55(-2) | 2.49(-2) |
| 41.96 | 1.58(-2) | 1.34(-2) | 1.32(-2) |

RUBIDIUM

| | 5s-6p | | | 5s-7p | | | 5s-8p | | |
|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 1.08 (-1) | | | EPSIL = 1.27 (-1) | | | EPSIL = 1.36 (-1) | | |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 2.47(0) | 1.32(+1) | 2.36(0) | 6.48(-1) | 3.29(0) | 6.29(-1) | 2.79(-1) | 1.35(0) | 2.68(-1) |
| 1.04 | 3.37(0) | 1.31(+1) | 3.20(0) | 8.84(-1) | 3.25(0) | 8.48(-1) | 3.80(-1) | 1.33(0) | 3.60(-1) |
| 1.08 | 4.47(0) | 1.28(+1) | 4.20(0) | 1.17(0) | 3.15(0) | 1.10(0) | 5.01(-1) | 1.28(0) | 4.65(-1) |
| 1.16 | 5.62(0) | 1.21(+1) | 5.01(0) | 1.46(0) | 2.96(0) | 1.29(0) | 6.23(-1) | 1.20(0) | 5.42(-1) |
| 1.32 | 6.47(0) | 1.10(+1) | 5.51(0) | 1.67(0) | 2.64(0) | 1.39(0) | 7.08(-1) | 1.07(0) | 5.76(-1) |
| 1.64 | 6.68(0) | 9.15(0) | 5.43(0) | 1.68(0) | 2.16(0) | 1.33(0) | 7.06(-1) | 8.70(-1) | 5.46(-1) |
| 2.28 | 5.73(0) | 6.86(0) | 4.81(0) | 1.44(0) | 1.59(0) | 1.14(0) | 6.00(-1) | 6.35(-1) | 4.61(-1) |
| 3.56 | 4.26(0) | 4.60(0) | 3.72(0) | 1.05(0) | 1.04(0) | 8.50(-1) | 4.33(-1) | 4.13(-1) | 3.39(-1) |
| 6.12 | 2.77(0) | 2.81(0) | 2.51(0) | 6.76(-1) | 6.21(-1) | 5.55(-1) | 2.75(-1) | 2.45(-1) | 2.19(-1) |
| 11.24 | 1.65(0) | 1.60(0) | 1.52(0) | 3.98(-1) | 3.47(-1) | 3.28(-1) | 1.50(-1) | 1.36(-1) | 1.28(-1) |
| 21.48 | 9.29(-1) | 8.83(-1) | 8.60(-1) | 2.22(-1) | 1.87(-1) | 1.82(-1) | 8.86(-2) | 7.25(-2) | 7.06(-2) |
| 41.96 | 5.08(-1) | 4.74(-1) | 4.69(-1) | 1.20(-1) | 9.81(-2) | 9.70(-2) | 4.47(-2) | 3.78(-2) | 3.74(-2) |

RUBIDIUM

|  | 5s-6s |  |  | 5s-7s |  |  | 5s-8s |  |  |
|---|---|---|---|---|---|---|---|---|---|
|  | EPSIL = 9.17 (-2) |  |  | EPSIL = 1.20 (-1) |  |  | ESPIL 1.32 (-1) |  |  |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 1.80(-1) | 0.0 | 2.00(0) | 2.78(-1) | 4.80(-1) | 3.35(-1) | 1.06(-1) | 2.54(-1) | 1.20(-1) |
| 1.04 | 2.51(0) | 0.0 | 2.72(0) | 3.85(-1) | 1.48(-1) | 4.54(-1) | 1.47(-1) | 3.36(-1) | 1.62(-1) |
| 1.08 | 3.38(0) | 2.78(0) | 3.62(0) | 5.22(-1) | 1.04(0) | 6.01(-1) | 1.99(-1) | 4.25(-1) | 2.14(-1) |
| 1.16 | 4.38(0) | 5.62(0) | 4.43(0) | 6.81(-1) | 1.31(0) | 7.31(-1) | 2.58(-1) | 5.03(-1) | 2.60(-1) |
| 1.32 | 5.27(0) | 7.71(0) | 5.15(0) | 8.25(-1) | 1.47(0) | 8.50(-1) | 3.12(-1) | 5.40(-1) | 3.03(-1) |
| 1.64 | 5.64(0) | 8.27(0) | 5.52(0) | 8.81(-1) | 1.42(0) | 9.11(-1) | 3.31(-1) | 5.07(-1) | 3.25(-1) |
| 2.28 | 5.10(0) | 7.14(0) | 5.27(0) | 7.88(-1) | 1.15(0) | 8.52(-1) | 2.92(-1) | 4.07(-1) | 3.02(-1) |
| 3.56 | 3.84(0) | 5.10(0) | 4.22(0) | 5.83(-1) | 7.99(-1) | 6.65(-1) | 2.14(-1) | 2.79(-1) | 2.34(-1) |
| 6.12 | 2.47(0) | 3.16(0) | 2.84(0) | 3.69(-1) | 4.86(-1) | 4.40(-1) | 1.35(-1) | 1.69(-1) | 1.54(-1) |
| 11.24 | 1.42(0) | 1.78(0) | 1.69(0) | 2.10(-1) | 2.71(-1) | 2.58(-1) | 7.67(-2) | 9.42(-2) | 8.98(-2) |
| 21.48 | 7.66(-1) | 9.47(-1) | 9.26(-1) | 1.13(-1) | 1.44(-1) | 1.41(-1) | 4.10(-2) | 4.99(-2) | 4.88(-2) |
| 41.96 | 3.98(-1) | 4.89(-1) | 4.86(-1) | 5.85(-2) | 7.42(-2) | 7.36(-2) | 2.12(-2) | 2.57(-2) | 2.55(-2) |

RUBIDIUM

| | 5s-4d | | | 5s-5d | | | 5s-6d | | |
|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 8.82 (-2) | | | EPSIL = 1.17 (-1) | | | EPSIL 1.31 (-1) | | |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 1.04(+1) | 0.0 | 1.15(+1) | 1.24(0) | 0.0 | 8.25(-1) | 3.38(-1) | 0.0 | 1.32(-1) |
| 1.04 | 1.43(+1) | 0.0 | 1.59(+1) | 1.67(0) | 1.43(-1) | 1.16(0) | 4.65(-1) | 0.0 | 1.96(-1) |
| 1.08 | 1.88(+1) | 1.61(0) | 2.13(+1) | 2.15(0) | 4.94(-1) | 1.58(0) | 5.83(-1) | 0.0 | 2.85(-1) |
| 1.16 | 2.35(+1) | 1.35(+1) | 2.61(+1) | 2.58(0) | 8.38(-1) | 1.96(0) | 6.89(-1) | 0.0 | 3.86(-1) |
| 1.32 | 2.66(+1) | 2.28(+1) | 2.92(+1) | 2.71(0) | 1.08(0) | 2.13(0) | 7.11(-1) | 0.0 | 4.63(-1) |
| 1.64 | 2.62(+1)) | 2.65(+1) | 2.74(+1) | 2.42(0) | 1.13(0) | 1.73(0) | 6.18(-1) | 5.08(-2) | 4.08(-1) |
| 2.28 | 2.18(+1) | 2.38(+1) | 2.18(+1) | 1.81(0) | 9.59(-1) | 1.05(0) | 4.62(-1) | 1.84(-1) | 2.74(-1) |
| 3.56 | 1.54(+1) | 1.73(+1) | 1.54(+1) | 1.17(0) | 6.80(-1) | 5.94(-1) | 2.91(-1) | 1.84(-1) | 1.77(-1) |
| 6.12 | 9.52(0) | 1.08(+1) | 9.90(0) | 6.84(-1) | 4.19(-1) | 3.58(-1) | 1.79(-1) | 1.30(-1) | 1.18(-1) |
| 11.24 | 5.36(0) | 6.12(0) | 5.80(0) | 3.72(-1) | 2.36(-1) | 2.11(-1) | 9.29(-2) | 7.82(-2) | 7.26(-2) |
| 21.48 | 2.86(0) | 3.27(0) | 3.17(0) | 1.95(-1) | 1.25(-1) | 1.18(-1) | 4.88(-2) | 4.30(-2) | 4.11(-2) |
| 41.96 | 1.48(0) | 1.69(0) | 1.66(0) | 9.98(-2) | 6.47(-2) | 6.25(-2) | 2.50(-2) | 2.25(-2) | 2.20(-2) |

## RUBIDIUM

5s-7d

EPSIL = 1.38 (-1)

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

CESIUM

|  | 6s-7p |  |  | 6s-8p |  |  | 6s-9p |  |  |
|---|---|---|---|---|---|---|---|---|---|
|  | EPSIL = 9.96 (-2) |  |  | EPSIL = 1.17 (-1) |  |  | EPSIL = 1.26 (-1) |  |  |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 2.88(0) | 1.69(+1) | 2.75(0) | 7.64(-1) | 4.11(0) | 7.23(-1) | 3.26(-1) | 1.67(0) | 3.06(-1) |
| 1.04 | 3.95(0) | 1.68(+1) | 3.72(0) | 1.04(0) | 4.05(0) | 9.73(-1) | 4.44(-1) | 1.64(0) | 4.11(-1) |
| 1.08 | 5.25(0) | 1.63(+1) | 4.88(0) | 1.38(0) | 3.92(0) | 1.26(0) | 5.84(-1) | 1.58(0) | 5.31(-1) |
| 1.16 | 6.66(0) | 1.54(+1) | 5.83(0) | 1.74(0) | 3.67(0) | 1.49(0) | 7.25(-1) | 1.48(0) | 6.21(-1) |
| 1.32 | 7.78(0) | 1.39(+1) | 6.50(0) | 2.00(0) | 3.26(0) | 1.62(0) | 8.20(-1) | 1.31(0) | 6.72(-1) |
| 1.64 | 8.04(0) | 1.15(+1) | 6.56(0) | 2.03(0) | 2.66(0) | 1.60(0) | 8.13(-1) | 1.06(0) | 6.54(-1) |
| 2.28 | 7.12(0) | 8.52(0) | 5.90(0) | 1.75(0) | 1.94(0) | 1.38(0) | 6.84(-1) | 7.70(-1) | 5.60(-1) |
| 3.56 | 5.36(0) | 5.66(0) | 4.56(0) | 1.28(0) | 1.26(0) | 1.03(0) | 4.88(-1) | 4.99(-1) | 4.11(-1) |
| 6.12 | 3.53(0) | 3.42(0) | 3.05(0) | 8.24(-1) | 7.47(-1) | 6.70(-1) | 3.06(-1) | 2.94(-1) | 2.64(-1) |
| 11.24 | 2.12(0) | 1.94(0) | 1.83(0) | 4.84(-1) | 4.15(-1) | 3.92(-1) | 1.76(-1) | 1.62(-1) | 1.53(-1) |
| 21.48 | 1.21(0) | 1.05(0) | 1.03(0) | 2.70(-1) | 2.21(-1) | 2.16(-1) | 9.65(-2) | 8.58(-2) | 8.36(-2) |
| 41.96 | 6.66(-1) | 5.60(-1) | 5.55(-1) | 1.46(-1) | 1.15(-1) | 1.42(-1) | 5.14(-2) | 4.45(-2) | 4.40(-2) |

## CESIUM

| | 6s-7s | | | 6s-8s | | | 6s-9s | | |
|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 8.44 (-2) | | | EPSIL = 1.11 (-1) | | | EPSIL = 1.23 (-1) | | |
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 1.83(0) | 0.0 | 2.17(0) | 2.93(-1) | 3.19(-1) | 3.54(-1) | 1.02(-1) | 2.36(-1) | 1.25(-1) |
| 1.04 | 2.54(0) | 0.0 | 2.96(0) | 4.08(-1) | 6.99(-1) | 4.81(-1) | 1.43(-1) | 3.52(-1) | 1.70(-1) |
| 1.08 | 3.46(0) | 1.56(0) | 3.96(0) | 5.60(-1) | 1.13(0) | 6.44(-1) | 1.98(-1) | 4.79(-1) | 2.28(-1) |
| 1.16 | 4.54(0) | 5.75(0) | 4.92(0) | 7.43(-1) | 1.53(0) | 8.04(-1) | 2.64(-1) | 5.95(-1) | 2.86(-1) |
| 1.32 | 5.57(0) | 8.97(0) | 5.93(0) | 9.21(-1) | 1.78(0) | 9.81(-1) | 3.29(-1) | 6.59(-1) | 3.51(-1) |
| 1.64 | 6.09(0) | 1.01(+1) | 6.67(0) | 1.01(0) | 1.76(0) | 1.10(0) | 3.59(-1) | 6.32(-1) | 3.95(-1) |
| 2.28 | 5.61(0) | 8.97(0) | 6.58(0) | 9.13(-1) | 1.45(0) | 1.07(0) | 3.24(-1) | 5.13(-1) | 3.77(-1) |
| 3.56 | 4.27(0) | 6.50(0) | 5.36(0) | 6.81(-1) | 1.02(0) | 8.44(-1) | 2.40(-1) | 3.55(-1) | 2.96(-1) |
| 6.12 | 2.76(0) | 4.05(0) | 3.65(0) | 4.34(-1) | 6.20(-1) | 5.62(-1) | 1.52(-1) | 2.16(-1) | 1.96(-1) |
| 11.24 | 1.60(0) | 2.29(0) | 2.17(0) | 2.48(-1) | 3.47(-1) | 3.31(-1) | 8.69(-2) | 1.20(-1) | 1.15(-1) |
| 21.48 | 8.62(-1) | 1.22(0) | 1.20(0) | 1.33(-1) | 1.84(-1) | 1.80(-1) | 4.69(-2) | 6.37(-2) | 6.25(-2) |
| 41.96 | 4.49(-1) | 6.31(-1) | 6.28(-1) | 6.92(-2) | 9.50(-2) | 9.44(-2) | 2.41(-2) | 3.28(-2) | 3.26(-2) |

## CESIUM

| | 6s-5d<br>EPSIL = 6.63 (-2) | | | 6s-6d<br>EPSIL = 1.03 (-1) | | | 6s-7d<br>EPSIL = 1.19 (-1) | | |
|---|---|---|---|---|---|---|---|---|---|
| N | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR | BORN(1) | BETHE | OCHKUR |
| 1.02 | 1.62(1) | 1.24(+1) | 1.52(+1) | 3.44(-1) | 0.0 | 1.67(-1) | 2.76(-2) | 0.0 | 1.17(-1) |
| 1.04 | 2.21(1) | 1.93(+1) | 2.13(+1) | 4.78(-1) | 0.0 | 2.80(-1) | 4.83(-2) | 0.0 | 1.76(-1) |
| 1.08 | 2.92(1) | 2.71(+1) | 2.90(+1) | 6.53(-1) | 0.0 | 5.39(-1) | 8.98(-2) | 0.0 | 2.88(-1) |
| 1.16 | 3.64(1) | 3.42(+1) | 3.66(+1) | 8.53(-1) | 0.0 | 1.02(0) | 1.64(-1) | 0.0 | 4.67(-1) |
| 1.32 | 4.09(1) | 3.82(+1) | 4.23(+1) | 1.01(0) | 0.0 | 1.91(0) | 2.67(-1) | 0.0 | 7.71(-1) |
| 1.64 | 3.97(1) | 3.68(+1) | 3.96(+1) | 1.04(0) | 0.0 | 2.88(0) | 3.54(-1) | 5.95(-1) | 1.07(0) |
| 2.28 | 3.22(1) | 3.00(+1) | 2.92(+1) | 9.12(-1) | 2.15(0) | 3.29(0) | 3.70(-1) | 1.10(0) | 1.14(0) |
| 3.56 | 2.22(1) | 2.08(+1) | 1.85(+1) | 6.89(-1) | 2.80(0) | 2.93(0) | 3.08(-1) | 1.00(0) | 9.62(-1) |
| 6.12 | 1.35(1) | 1.27(+1) | 1.13(+1) | 4.55(-1) | 2.14(0) | 2.11(0) | 2.11(-1) | 6.90(-1) | 6.65(-1) |
| 11.24 | 7.52(0) | 7.06(0) | 6.54(0) | 2.68(-1) | 1.32(0) | 1.30(0) | 1.26(-1) | 4.08(-1) | 3.99(-1) |
| 21.48 | 3.98(0) | 3.74(0) | 3.58(0) | 1.47(-1) | 7.35(-1) | 7.27(-1) | 6.93(-2) | 2.23(-1) | 2.20(-1) |
| 41.96 | 2.05(0) | 1.93(0) | 1.88(0) | 7.70(-2) | 3.88(-1) | 3.85(-1) | 3.64(-2) | 1.17(-1) | 1.16(-1) |

# CESIUM

6s-8d

EPSIL = 1.27 (-1)

| N | BORN(1) | BETHE | OCHKUR |
|---|---|---|---|
| 1.02 | 2.18(-2) | 0.0 | 6.56(-2) |
| 1.04 | 3.38(-2) | 0.0 | 9.61(-2) |
| 1.08 | 5.46(-2) | 0.0 | 1.52(-1) |
| 1.16 | 8.74(-2) | 0.0 | 2.37(-1) |
| 1.32 | 1.28(-1) | 0.0 | 3.74(-1) |
| 1.64 | 1.58(-1) | 4.04(-1) | 5.00(-1) |
| 2.28 | 1.57(-1) | 5.39(-1) | 5.20(-1) |
| 3.56 | 1.28(-1) | 4.56(-1) | 4.29(-1) |
| 6.12 | 8.69(-2) | 3.05(-1) | 2.92(-1) |
| 11.24 | 5.17(-2) | 1.78(-1) | 1.74(-1) |
| 21.48 | 2.83(-2) | 9.67(-2) | 9.54(-2) |
| 41.96 | 1.48(-2) | 5.04(-2) | 5.00(-2) |

### 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

| | | |
|---|---|---|
| He: | 1s - 2p | Born, Ochkur, Bethe, Mod. Bethe |
| | 1s - 2s | Born, Ochkur |
| | 1s - 3s | Born, Ochkur |
| Ne: | 2p - 3p | Born, Ochkur, Bethe, Mod. Bethe |
| | 2p - 3p | Born, Ochkur |
| | 2p - 4s | Born, Ochkur |
| Ar: | 3p - 4s | Born, Ochkur, Bethe, Mod. Bethe |
| | 3p - 4p | Born, Ochkur |
| | 3p - 3d | Born, Ochkur |
| Kr: | 4p - 5s | Born, Ochkur, Bethe, Mod. Bethe |
| | 4p - 5p | Born, Ochkur |
| | 4p - 4d | Born, Ochkur |
| Xe: | 5p - 6s | Born, Ochkur, Bethe, Mod. Bethe |
| | 5p - 6p | Born, Ochkur |
| | 5p - 4d | Born, Ochkur |
| RN: | 6p - 7s | Born, Ochkur, Bethe, Mod. Bethe |
| | 6p - 7p | Born, Ochkur |
| | 6p - 6d | Born, Ochkur |

## HELIUM

| | 1s - 2p | | | | | 1s - 2s | | | 1s - 3s | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 7.74(-1) | | | | | EPSIL = 7.38(-1) | | | EPSIL = 8.37(-1) | | |
| N | BORN | OCHKUR | BETHE | MODBETHE | LIT(1) | BORN | OCHKUR | LIT(2) | BORN | OCHKUR | LIT |
| 1.05 | 3.22(-2) | 2.98(-2) | 0.0 | 0.0 | 0.0 | 2.48(-2) | 2.48(-2) | 2.60(-2) | 4.63(-3) | 4.65(-3) | |
| 1.10 | 4.52(-2) | 4.06(-2) | 0.0 | 0.0 | 0.0 | 3.24(-2) | 3.24(-2) | 3.40(-2) | 6.03(-3) | 6.04(-3) | |
| 1.20 | 6.26(-2) | 5.37(-2) | 0.0 | 0.0 | 0.0 | 3.96(-2) | 4.04(-2) | 3.20(-2) | 7.33(-3) | 7.49(-3) | |
| 1.80 | 1.02(-1) | 8.63(-2) | 4.14(-2) | 2.12(-1) | 1.05(-1) | 4.10(-2) | 3.97(-2) | 0.0 | 7.43(-3) | 7.16(-3) | |
| 2.50 | 1.08(-1) | 9.60(-2) | 8.16(-2) | 2.00(-1) | 1.33(-1) | 3.35(-2) | 3.08(-2) | 0.0 | 6.00(-3) | 5.48(-3) | |
| 5.00 | 9.20(-2) | 8.78(-2) | 8.78(-2) | 1.43(-1) | 1.28(-1) | 1.88(-2) | 1.70(-2) | 0.0 | 3.33(-3) | 3.00(-3) | |
| 10.00 | 6.54(-2) | 6.41(-2) | 6.53(-2) | 9.10(-2) | 9.70(-2) | 9.87(-3) | 9.23(-3) | 0.0 | 1.74(-3) | 1.62(-3) | |
| 15.00 | 5.12(-2) | 5.06(-2) | 5.16(-2) | 6.83(-2) | 7.70(-2) | 6.68(-3) | 6.36(-3) | 0.0 | 1.17(-3) | 1.12(-3) | |
| 20.00 | 4.25(-2) | 4.22(-2) | 4.29(-2) | 5.52(-2) | 6.43(-2) | 5.04(-3) | 4.86(-3) | 0.0 | 8.86(-4) | 8.53(-4) | |
| 30.00 | 3.22(-2) | 3.20(-2) | 3.25(-2) | 4.06(-2) | 0.0 | 3.39(-3) | 3.30(-3) | 0.0 | 5.95(-4) | 5.79(-4) | |
| 50.00 | 2.22(-2) | 2.12(-2) | 2.25(-2) | 2.72(-2) | 0.0 | 2.04(-3) | 2.01(-3) | 0.0 | 3.58(-4) | 3.53(-4) | |
| 30.00 | 1.56(-2) | 1.55(-2) | 1.57(-2) | 1.87(-2) | 0.0 | 1.28(-3) | 1.27(-3) | 0.0 | 2.25(-4) | 2.22(-4) | |

(1) Linear Interpolation From "Ochkur, V.I. and V.F. Bratsev, (1965) Opt. Spectry - USSR 19, 274"; Ochkur Approximation

(2) Linear Interpolation From "Marriot, R. in Atomic Collision Processes, M.R.C. McDowell, Ed., Pub. by North-Holland Publ. Co., Amersterdam"; Close-coupling Calculation

## NEON

| | 2p - 3s | | | | | 2p - 3p | | | 3p - 4s | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 6.12(-1) | | | | | EPSIL = 6.83(-1) | | | EPSIL = 7.24(-1) | | |
| N | BORN | OCHKUR | BETHE | MODBETHE | LIT | BORN | OCHKUR | LIT | BORN | OCHKUR | LIT |
| 1.05 | 3.07(-3) | 2.60(-3) | 0.0 | 0.0 | | 1.06(-3) | 9.60(-4) | | 4.16(-4) | 3.45(-4) | |
| 1.10 | 4.74(-3) | 3.87(-3) | 0.0 | 0.0 | | 1.45(-3) | 1.27(-3) | | 6.61(-4) | 5.31(-4) | |
| 1.20 | 7.46(-3) | 5.78(-3) | 0.0 | 0.0 | | 1.91(-3) | 1.57(-3) | | 1.07(-3) | 8.31(-4) | |
| 1.80 | 1.58(-2) | 1.39(-2) | 2.09(-3) | 2.27(-1) | | 2.54(-3) | 2.18(-3) | | 2.34(-3) | 2.10(-3) | |
| 2.50 | 1.83(-2) | 1.70(-2) | 1.22(-2) | 1.73(-1) | | 2.33(-3) | 2.19(-3) | | 2.68(-3) | 2.52(-3) | |
| 5.00 | 1.68(-2) | 1.63(-2) | 1.57(-2) | 9.54(-2) | | 1.48(-3) | 1.48(-3) | | 2.41(-3) | 2.34(-3) | |
| 10.00 | 1.23(-2) | 1.21(-2) | 1.23(-2) | 5.18(-2) | | 8.14(-4) | 8.01(-4) | | 1.74(-3) | 1.71(-3) | |
| 15.00 | 9.77(-3) | 9.67(-3) | 9.83(-3) | 3.61(-2) | | 5.59(-4) | 5.48(-4) | | 1.37(-3) | 1.36(-3) | |
| 20.00 | 8.16(-3) | 8.10(-3) | 8.24(-3) | 2.79(-2) | | 4.25(-4) | 4.17(-4) | | 1.14(-3) | 1.13(-3) | |
| 30.00 | 6.23(-3) | 6.20(-3) | 6.31(-3) | 1.94(-2) | | 2.87(-4) | 2.83(-4) | | 8.67(-4) | 8.63(-4) | |
| 50.00 | 4.33(-3) | 4.32(-3) | 4.39(-3) | 1.22(-2) | | 1.74(-4) | 1.73(-4) | | 5.99(-4) | 5.98(-4) | |
| 80.00 | 3.05(-3) | 3.05(-3) | 3.09(-3) | 7.97(-3) | | 1.10(-4) | 1.09(-4) | | 4.21(-4) | 4.21(-4) | |

ARGON

| | 3p - 4s | | | | | 3p - 4p | | | 3p - 3d | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 4.26(-1) | | | | | EPSIL = 4.82(-1) | | | EPSIL = 5.16(-1) | | |
| N | BORN | OCHKUR | BETHE | MODBETHE | LIT | BORN | OCHKUR | LIT | BORN | OCHKUR | LIT |
| 1.05 | 6.20(-3) | 4.96(-3) | 0.0 | 0.0 | | 1.81(-3) | 1.50(-3) | | 2.66(-3) | 2.68(-3) | |
| 1.10 | 1.07(-2) | 8.46(-3) | 0.0 | 0.0 | | 2.79(-3) | 2.24(-3) | | 3.42(-3) | 3.47(-3) | |
| 1.20 | 1.91(-2) | 1.49(-2) | 0.0 | 0.0 | | 4.30(-3) | 3.41(-3) | | 4.10(-3) | 4.29(-3) | |
| 1.80 | 4.85(-2) | 4.37(-2) | 0.0 | 3.08(-1) | | 7.60(-3) | 7.60(-3) | | 3.91(-3) | 3.96(-3) | |
| 2.50 | 5.89(-2) | 5.49(-2) | 3.16(-2) | 2.58(-1) | | 7.43(-3) | 7.71(-3) | | 3.04(-3) | 2.89(-3) | |
| 5.00 | 5.69(-2) | 5.50(-2) | 5.22(-2) | 1.62(-1) | | 4.90(-3) | 4.79(-3) | | 1.59(-3) | 1.42(-3) | |
| 10.00 | 4.30(-2) | 4.24(-2) | 4.26(-2) | 9.62(-2) | | 2.73(-3) | 2.64(-3) | | 8.01(-4) | 7.34(-4) | |
| 15.00 | 3.45(-2) | 3.42(-2) | 3.47(-2) | 7.00(-2) | | 1.89(-3) | 1.83(-3) | | 5.35(-4) | 5.01(-4) | |
| 20.00 | 2.90(-2) | 2.88(-2) | 2.93(-2) | 5.56(-2) | | 1.44(-3) | 1.41(-3) | | 4.01(-4) | 3.81(-4) | |
| 30.00 | 2.23(-2) | 2.22(-2) | 2.26(-2) | 4.00(-2) | | 9.75(-4) | 9.59(-4) | | 2.67(-4) | 2.58(-4) | |
| 50.00 | 1.56(-2) | 1.55(-2) | 1.58(-2) | 2.62(-2) | | 5.93(-4) | 5.87(-4) | | 1.61(-4) | 1.58(-4) | |
| 80.00 | 1.10(-2) | 1.10(-2) | 1.12(-2) | 1.77(-2) | | 3.74(-4) | 3.71(-4) | | 1.01(-4) | 9.99(-5) | |

## KRYPTON

|  | 4p - 5s |  |  |  |  | 4p - 5p |  |  | 4p - 4d |  |  |
|---|---|---|---|---|---|---|---|---|---|---|---|
|  | EPSIL = 3.66(-1) |  |  |  |  | EPSIL = 4.22(-1) |  |  | EPSIL = 4.48(-1) |  |  |
| N | BORN | OCHKUR | BETHE | MODBETHE | LIT | BORN | OCHKUR | LIT | BORN | OCHKUR | LIT |
| 1.05 | 1.14(-2) | 9.19(-3) | 0.0 | 0.0 |  | 2.04(-3) | 1.64(-3) |  | 6.35(-3) | 6.44(-3) |  |
| 1.10 | 1.95(-2) | 1.54(-2) | 0.0 | 0.0 |  | 3.39(-3) | 2.70(-3) |  | 8.19(-3) | 8.33(-3) |  |
| 1.20 | 3.43(-2) | 2.66(-2) | 0.0 | 0.0 |  | 5.65(-3) | 4.67(-3) |  | 9.77(-3) | 1.03(-2) |  |
| 1.80 | 8.58(-2) | 7.63(-2) | 0.0 | 3.49(-1) |  | 1.10(-2) | 1.16(-2) |  | 9.21(-3) | 9.24(-3) |  |
| 2.50 | 1.04(-1) | 9.57(-2) | 5.66(-2) | 3.15(-1) |  | 1.09(-2) | 1.14(-2) |  | 7.10(-3) | 6.61(-3) |  |
| 5.00 | 1.00(-1) | 9.65(-2) | 9.19(-2) | 2.15(-1) |  | 7.22(-3) | 6.96(-3) |  | 3.69(-3) | 3.25(-3) |  |
| 10.00 | 7.55(-2) | 7.43(-2) | 7.49(-2) | 1.34(-1) |  | 4.05(-3) | 3.90(-3) |  | 1.86(-3) | 1.70(-3) |  |
| 15.00 | 6.05(-2) | 5.99(-2) | 6.08(-2) | 9.98(-2) |  | 2.80(-3) | 2.72(-3) |  | 1.25(-3) | 1.17(-3) |  |
| 20.00 | 5.08(-2) | 5.05(-2) | 5.13(-2) | 8.02(-2) |  | 2.14(-3) | 2.09(-3) |  | 9.48(-4) | 9.02(-4) |  |
| 30.00 | 3.90(-2) | 3.89(-2) | 3.95(-2) | 5.86(-2) |  | 1.45(-3) | 1.43(-3) |  | 6.72(-4) | 6.51(-4) |  |
| 50.00 | 2.73(-2) | 2.72(-2) | 2.77(-2) | 3.90(-2) |  | 8.83(-4) | 8.74(-4) |  | 3.77(-4) | 3.69(-4) |  |
| 80.00 | 1.93(-2) | 1.93(-2) | 1.96(-2) | 2.66(-2) |  | 5.57(-4) | 5.53(-4) |  | 1.47(-3) | 1.46(-3) |  |

XENON

|  | 5p - 6s |  |  |  |  | 5p - 6p |  |  | 5p - 5d |  |  |
|---|---|---|---|---|---|---|---|---|---|---|---|
|  | EPSIL = 3.06(-1) |  |  |  |  | EPSIL = 3.58(-1) |  |  | EPSIL = 3.70(-1) |  |  |
| N | BORN | OCHKUR | BETHE | MODBETHE | LIT | BORN | OCHKUR | LIT | BORN | OCHKUR | LIT |
| 1.05 | 1.26(-2) | 9.86(-3) | 0.0 | 0.0 |  | 2.30(-3) | 1.82(-3) |  | 2.36(-2) | 2.42(-2) |  |
| 1.10 | 2.34(-2) | 1.84(-2) | 0.0 | 0.0 |  | 4.31(-2) | 3.52(-3) |  | 3.03(-2) | 3.14(-2) |  |
| 1.20 | 4.42(-2) | 3.50(-2) | 0.0 | 0.0 |  | 7.94(-3) | 7.13(-3) |  | 3.61(-2) | 3.93(-2) |  |
| 1.80 | 1.21(-1) | 1.09(-1) | 0.0 | 3.85(-1) |  | 1.68(-2) | 1.85(-2) |  | 3.35(-2) | 3.50(-2) |  |
| 2.50 | 1.50(-1) | 1.38(-1) | 7.19(-2) | 3.76(-1) |  | 1.68(-2) | 1.74(-2) |  | 2.56(-2) | 2.42(-2) |  |
| 5.00 | 1.48(-1) | 1.43(-1) | 1.34(-1) | 2.77(-1) |  | 1.13(-2) | 1.07(-2) |  | 1.32(-2) | 1.15(-2) |  |
| 10.00 | 1.13(-1) | 1.11(-1) | 1.12(-1) | 1.80(-1) |  | 6.35(-3) | 6.11(=3) |  | 6.74(-3) | 6.12(-3) |  |
| 15.00 | 9.09(-2) | 9.01(-2) | 9.13(-2) | 1.36(-1) |  | 4.40(-3) | 4.27(-3) |  | 4.63(-3) | 4.33(-3) |  |
| 20.00 | 7.66(-2) | 7.61(-2) | 7.73(-2) | 1.10(-1) |  | 3.36(-3) | 3.29(-3) |  | 3.80(-3) | 3.62(-3) |  |
| 30.00 | 5.90(-2) | 5.88(-2) | 5.98(-2) | 8.13(-2) |  | 2.28(-3) | 2.25(-3) |  | 3.22(-3) | 3.14(-3) |  |
| 50.00 | 4.14(-2) | 4.13(-2) | 4.20(-2) | 5.48(-2) |  | 1.39(-3) | 1.38(-3) |  | 1.18(-3) | 1.15(-3) |  |
| 80.00 | 2.94(-2) | 2.93(-2) | 2.98(-2) | 3.77(-2) |  | 8.77(-4) | 8.72(-4) |  | 3.92(-3) | 3.91(-3) |  |

RADON

| | 6p - 7s | | | | | 6p - 7p | | | 6p - 6d | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | EPSIL = 2.51(-1) | | | | | EPSIL = 3.09(-1) | | | EPSIL = 3.19(-1) | | |
| N | BORN | OCHKUR | BETHE | MODBETHE | LIT | BORN | OCHKUR | LIT | BORN | OCHKUR | LIT |
| 1.05 | 2.56(-2) | 2.04(-2) | 0.0 | 0.0 | | 3.34(-3) | 2.64(-3) | | 4.07(-2) | 4.22(-2) | |
| 1.10 | 4.42(-2) | 3.48(-2) | 0.0 | 0.0 | | 6.12(-3) | 5.00(-3) | | 5.25(-2) | 5.49(-2) | |
| 1.20 | 7.83(-2) | 6.11(-2) | 0.0 | 0.0 | | 1.11(-2) | 9.96(-3) | | 6.24(-2) | 6.91(-2) | |
| 1.80 | 1.96(-1) | 1.75(-1) | 0.0 | 4.98(-1) | | 2.30(-2) | 2.55(-2) | | 5.76(-2) | 6.13(-2) | |
| 2.50 | 2.35(-1) | 2.17(-1) | 1.34(-1) | 5.00(-1) | | 2.27(-2) | 2.37(-2) | | 4.38(-2) | 4.16(-2) | |
| 5.00 | 2.25(-1) | 2.17(-1) | 2.08(-1) | 3.78(-1) | | 1.51(-2) | 1.43(-2) | | 2.27(-2) | 1.97(-2) | |
| 10.00 | 1.69(-1) | 1.67(-1) | 1.68(-1) | 2.48(-1) | | 8.46(-3) | 8.12(-3) | | 1.19(-2) | 1.08(-2) | |
| 15.00 | 1.35(-1) | 1.34(-1) | 1.36(-1) | 1.88(-1) | | 5.85(-3) | 5.67(-3) | | 8.29(-3) | 7.75(-3) | |
| 20.00 | 1.14(-1) | 1.13(-1) | 1.15(-1) | 1.53(-1) | | 4.47(-3) | 4.36(-3) | | 6.43(-3) | 6.11(-3) | |
| 30.00 | 8.72(-2) | 8.69(-2) | 8.84(-2) | 1.13(-1) | | 3.03(-3) | 2.98(-3) | | 4.94(-3) | 4.79(-3) | |
| 50.00 | 6.09(-2) | 6.08(-2) | 6.19(-2) | 7.66(-2) | | 1.84(-3) | 1.83(-3) | | 2.74(-3) | 2.68(-3) | |
| 80.00 | 4.31(-2) | 4.31(-2) | 4.37(-2) | 5.28(-2) | | 1.16(-3) | 1.16(-3) | | 2.25(-3) | 2.23(-3) | |

## 2) Discussion

A comparison of the Born calculations for the Alkalis 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 descrepancy 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:

| E | 1.02 | 1.08 | 1.64 | 2.28 |
|---|---|---|---|---|
| Born(1) | 1.36(0) | 2.39(0) | 3.11(0) | 2.23(0) |
| Born(2) | 5.77(-1) | 1.00(0) | 1.11(0) | 8.31(-1) |

| E | 6.12 | 11.24 | 21.48 | 41.96 |
|---|---|---|---|---|
| Born(1) | 8.86(-1) | 4.88(-1) | 2.57(-1) | 1.32(-1) |
| Born(2) | 3.28(-1) | 1.83(-1) | 9.70(-2) | 5.11(-2) |

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 descrepancy 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 eroneous; 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 Epsil 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

| | |
|---|---|
| Hydrogen | (1s → Continuum) |
| Helium | (1s → Continuum) |
| Lithium | (2s → Continuum) |
| Sodium | (3s → Continuum) |
| Potassium | (4s → Continuum) |
| Rubidium | (5s → Continuum) |
| Cesium | (6s → Continuum) |

The literature (Lit) data are referenced as follows:

Lit$^{(1)}$: Peach, G. (1965) Proc. Phys. Soc. 85, 709
Lit$^{(2)}$: Peach, G. (1966) Proc. Phys. Soc. 87, 375

The data given from these sources is graphically interpolated.

HYDROGEN (1s - ION)

EPSIL = .500

|  | N = 2.00 |  | N = 2.50 |  | N = 2.75 |  |
|---|---|---|---|---|---|---|
| ENERGY | LOG N = .301 |  | LOG N = .398 |  | LOG N = .439 |  |
| Qe | (This Paper) | Lit. | (This Paper) | Lit. | (This Paper) | Lit. |
| Qo | .118(0) | .10(0) | .119(0) | .10(0) | .169(0) | .10(0) |
| Q1 | .554(0) | .57(0) | .642(0) | .61(0) | .661(0) | .63(0) |
| Q2 | .154(0) | .12(0) | .191(0) | .19(0) | .202(0) | .19(0) |
| Q3 | .222(-1) | .01(0) | .327(-1) | .02(0) | .368(-1) | .02(0) |
| Q4 | .278(-2) | -- | .520(-2) | -- | .669(-2) | -- |
| Q5 | .341(-3) | -- | .838(-3) | -- | .126(-2) | -- |
| Qt | .851(0) | .80(0) | .991(0) | .92(0) | .108(1) | .94(0) |

HELIUM (1s - ION)

EPSIL = .860

| | N = 1.25 | | N = 1.50 | | N = 1.75 | |
|---|---|---|---|---|---|---|
| ENERGY | LOG N = .0969 | | LOG N = .176 | | LOG N = .243 | |
| Qe | (This Paper) | Lit(1) | (This Paper) | Lit(1) | (This Paper) | Lit. |
| Qo | .774(-2) | .1(-2) | .159(-1) | .5(-1) | .220(-1) | .6(-1) |
| Q1 | .391(-1) | .3(-1) | .868(-1) | .9(-1) | .127(0) | .13(0) |
| Q2 | .410(-2) | .1(-1) | .109(-1) | .15(-1) | .178(-1) | .19(-1) |
| Q3 | .215(-3) | .1(-2) | .817(-3) | .1(-2) | .167(-2) | .1(-2) |
| Q4 | .883(-5) | -- | .548(-4) | -- | .150(-3) | -- |
| Q5 | .336(-6) | -- | .362(-5) | -- | .135(-4) | -- |
| Qt | .512(-1) | .6(-1) | .115(0) | .2(0) | .168(0) | .2(0) |
| *Q (experiment) | | .7(-1) | | .17(0) | | .27(0) |

* McDaniel, E. W., J. W. Hooper, D. W. Martin, and D. S. Harmer (1961), _Proc. 5th Int. Cont. on Ionization Phenomena in Gases_, Vol (Amersterdam, North-Holland), p. 60

HELIUM (1s - ION)

EPSIL = .860

| ENERGY | N = 2.00<br>LOG N = .301 | | N = 2.50<br>LOG N = .398 | | N = 2.75<br>LOG N = .439 | |
|---|---|---|---|---|---|---|
| Qe | (This Paper) | Lit(1) | (This Paper) | Lit(1) | (This Paper) | Lit(1) |
| Qo | .262(-1) | .1(-1) | .336(-1) | .2(-1) | .178(0) | .21(-1) |
| Q1 | .157(0) | .25(0) | .194(0) | .34(0) | .205(0) | .35(0) |
| Q2 | .239(-1) | .4(-1) | .327(-1) | .5(-1) | .360(-1) | .53(-1) |
| Q3 | .262(-2) | .1(-2) | .445(-2) | .5(-2) | .526(-2) | .5(-2) |
| Q4 | .286(-3) | -- | .625(-3) | -- | .816(-3) | -- |
| Q5 | .318(-4) | -- | .918(-4) | -- | .139(-3) | -- |
| Qt | .210(0) | .3(0) | .266(0) | .4(0) | .426(0) | .43(0) |
| *Q | | .28(0) | | .32(0) | | .36(0) |

* Loc. Cit.

LITHIUM

EPSIL =

| ENERGY | N = 2.00<br>LOG N = .301 | | N = 2.50<br>LOG N = .398 | | N = 2.75<br>LOG N = .439 | |
|---|---|---|---|---|---|---|
| Qe | (This Paper) | Lit(1) | (This Paper) | Lit(1) | (This Paper) | Lit(1) |
| Qo | .250(0) | .1(0) | .447(0) | .15(0) | .160(2) | .16(0) |
| Q1 | .822(0) | .6(0) | .779(0) | .58(0) | .844(0) | .56(0) |
| Q2 | .226(1) | .18(1) | .234(1) | .19(1) | .236(1) | .185(1) |
| Q3 | .913(0) | .7(0) | .105(1) | .9(0) | .107(1) | .9(0) |
| Q4 | .196(0) | .15(0) | .268(0) | .2(0) | .292(0) | .23(0) |
| Q5 | .334(-1) | .5(-1) | .576(-1) | .8(-1) | .688(-1) | .90(-1) |
| Qt | .447(1) | .34(1) | .494(1) | .38(1) | .206(-2) | .38(1) |

SODIUM

EPSIL =

| ENERGY | N = 2.00<br>LOG N = .301 | | N = 2.50<br>LOG N = .398 | | N = 2.75<br>LOG N = .439 | |
|---|---|---|---|---|---|---|
| Qe | (This Paper) | Lit(2) | (This Paper) | Lit(2) | (This Paper) | Lit(2) |
| Qo | .415(0) | .5(0) | .543(1) | .5(0) | .319(4) | .5(0) |
| Q1 | .690(0) | .4(0) | .105(1) | .5(0) | .420(2) | .55(0) |
| Q2 | .255(1) | .25(1) | .285(1) | .25(1) | .188(2) | .23(1) |
| Q3 | .117(1) | .11(1) | .146(1) | .12(1) | .788(1) | .12(1) |
| Q4 | .270(0) | .2(0) | .381(0) | .3(0) | .861(0) | .3(0) |
| Q5 | .478(-1) | .3(-1) | .822(-1) | .4(-1) | .132(0) | .4(-1) |
| Qt | .514(1) | .05(1) | .113(2) | .55(1) | .326(4) | .50(1) |

POTASSIUM (4s - ION)

EPSIL = .309

| ENERGY | N = 2.00<br>LOG N = .301 | N = 2.50<br>LOG N = .398 | N = 2.75<br>LOG N = .439 |
|---|---|---|---|
| Qe | (This Paper) | (This Paper) | (This Paper) |
| Qo | .113(1) | .123(1) | .155(1) |
| Q1 | .704(0) | .983(0) | .136(1) |
| Q2 | .322(1) | .312(1) | .317(1) |
| Q3 | .235(1) | .252(1) | .253(1) |
| Q4 | .687(0) | .852(0) | .897(0) |
| Q5 | .140(0) | .214(0) | .243(0) |
| Qt | .823(1) | .892(1) | .975(1) |

## RUBIDIUM (5s - ION)

EPSIL = .291

| ENERGY | N = 2.00<br>LOG N = .301 | N = 2.50<br>LOG N = .398 |
|---|---|---|
| Qe | (This Paper) | (This Paper) |
| Qo | .136(1) | .893(4) |
| Q1 | .100(1) | .466(1) |
| Q2 | .328(1) | .230(2) |
| Q3 | .283(1) | .447(2) |
| Q4 | .902(0) | .156(2) |
| Q5 | .193(0) | .881(1) |
| Qt | .957(1) | .903(4) |

CESIUM (6s - ION)

EPSIL = 2.62

| | N = 2.00 | N = 2.50 |
|---|---|---|
| ENERGY | LOG N = .301 | LOG N = .398 |
| Qe | (This Paper) | (This Paper) |
| Qo | .127(1) | .907(3) |
| Q1 | .203(1) | .300(1) |
| Q2 | .315(1) | .744(1) |
| Q3 | .380(1) | .833(1) |
| Q4 | .142(1) | .366(1) |
| Q5 | .333(0) | .124(1) |
| Qt | .120(1) | .931(3) |

## 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.

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# APPENDIXES

# APPENDIX I

## Notation

$Q$ = cross-section

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

$A$ = set of quantum numbers for total atom

$a$ = set of quantum numbers for a particular orbital

$\Phi_A(\vec{r}_1 \cdots \vec{r}_Z)$ = total wave function (including spin) for atom with electrons in a state A

$\Psi_A(\vec{r}_1 \cdots \vec{r}_Z)$ = total wave function (neglecting spin) for atom with electrons in a state A

$\phi_a(\vec{r}_j)$ = single orbital wave function (including spin) for atom with $i^{th}$ electron in an orbital state

$\psi_a(\vec{r}_j)$ = single orbital wave function (neglecting spin) for atom with $i^{th}$ electron in an orbital state

$\vec{r}_o$ = this is reserved for the incident electron position vector in the scattering problem

$\vec{r}_e$ = this is reserved for the emitted electron (secondary electron) position vector in the ionization problem

$\epsilon_{ij\cdots k}$ = Levi-Chivita symbol (see Landau (1957))

$\delta_{ij}$ = 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,

$$\left[-(\hbar^2/2m)\nabla^2 - e^2/r - E_T\right]\Psi_T = 0 \quad . \tag{148}$$

Let $a_B = \frac{\hbar^2}{me^2}$ and $\mathcal{R} = 2R_D = me^4/\hbar^2$

Multiply equation (148) by $\hbar^2/me^4$

$$\left[\left(\frac{\hbar^2}{me^4}\right)\left(\frac{\hbar^2}{2m}\right)\nabla^2 - \left(\frac{\hbar^2e^2}{me^4}\right)\frac{1}{r} - \left(\frac{\hbar^2}{me^4}\right)E_T\right]\Psi_T = 0 \tag{149}$$

Then may be written

$$\left[\frac{1}{2}a_B^2\nabla^2 - \frac{a_B}{r} - E/\mathcal{R}\right]\Psi_r = 0 \tag{150}$$

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

$$\left[\frac{1}{2}\nabla^2 - \frac{1}{r} - E_T\right]\Psi = 0 \tag{151}$$

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

Alternatively we might multiply equation (148) by $2/\mathcal{R}$ and write the wave equation

$$\left[a_B^2\nabla^2 - \frac{2a_B}{r} - \frac{E_T}{R_D}\right]\Psi_T = 0 \tag{152}$$

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

$$\left[\nabla^2 - 2/r - E_T\right]\Psi = 0 \tag{153}$$

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

$$\text{Unit of length} = \hbar^2/me^2 = \text{Bohr Radius} = .529\ \text{Å}$$

$$\text{Unit of energy} = me^4/\hbar^2 = 2\ \text{Rydberg} = 27.2\ \text{eV} \quad .$$

Formulae may be obtained by $e = \hbar = m = 1$.

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.

# APPENDIX III

## 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

$$\sum_{m_i m_f} \int d\Omega\, Y^{+}_{\ell_f m_f}(\Omega) Y_{\lambda 0}(\Omega) Y_{\ell_i m_i}(\Omega) \int d\Omega'\, Y_{\ell_f m_f}(\Omega') Y^{+}_{\ell_i m_i}(\Omega') Y_{\lambda' 0}(\Omega') \tag{154}$$

$$\equiv \sum_{m_i m_f} \langle \ell_f m_f | \lambda 0 | \ell_i m_i \rangle \langle \ell_i m_i | \lambda' 0 | \ell_f m_f \rangle = I(\ell_i\, \ell_f\, \lambda \lambda')$$

Edmonds (pg. 63) gives the following integral in terms of the 3-j symbol

$$\int d\Omega\, Y_{\ell_1 m_1}(\Omega) Y_{\ell_2 m_2}(\Omega) Y_{\ell_3 m_3} = \left[\frac{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}{4\pi}\right]^{1/2} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \tag{155}$$

But

$$Y^{+}_{\ell_1 m_1}(\Omega) = (-1)^{m_1} Y_{\ell_1 -m_1} \quad \text{so}$$

$$\langle \ell_f m_f | \lambda 0 | \ell_i m_i \rangle = (-1)^{m_f} \left[\frac{(2\ell_f+1)(2\lambda+1)(2\ell_i+1)}{4\pi}\right]^{1/2} \begin{pmatrix} \ell_f & \lambda & \ell_i \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_f & \lambda & \ell_i \\ -m_f & 0 & m_i \end{pmatrix} \tag{156}$$

then the sum of interest may be written

$$I(\ell_i\, \ell_f\, \lambda \lambda') = \left[\frac{(2\ell_f+1)(2\ell_i+1)}{4\pi} \sqrt{(2\lambda+1)(2\lambda'+1)}\right] \begin{pmatrix} \ell_f & \lambda & \ell_i \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_i & \lambda' & \ell_f \\ 0 & 0 & 0 \end{pmatrix} \tag{157}$$

$$\times \sum_{m_i m_f} (-1)^{m_i + m_f} \begin{pmatrix} \ell_f & \lambda & \ell_i \\ -m_f & 0 & m_i \end{pmatrix} \begin{pmatrix} \ell_i & \lambda' & \ell_f \\ -m_i & 0 & m_f \end{pmatrix} :$$

The 3-j symbol is zero unless $m_1+m_2+m_3 = 0$. Hence, for the sum $(-1)^{m_1+m} = 1$. Consider

$$J = \sum_{m_i m_f} \begin{pmatrix} \ell_f & \lambda & \ell_i \\ -m_f & 0 & m_i \end{pmatrix} \begin{pmatrix} \ell_i & \lambda' & \ell_f \\ -m_i & 0 & m_f \end{pmatrix} \tag{158}$$

Two symmetry properties of the 3-j symbol from pg. 47 are useful.

Property I: An $\begin{bmatrix}\text{even}\\ \text{odd}\end{bmatrix}$ permutation of the columns is equivalent to multiplication by $\left[\begin{matrix}(+1)\\(-1)\end{matrix}^{j_1+j_2+j_3}\right]$.

Property II:

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

Using Property I:

$$\begin{aligned} J &= \sum_{m_i m_f} \begin{pmatrix} \ell_i & \ell_f & \lambda \\ m_i & m_f & 0 \end{pmatrix} \cdot \begin{pmatrix} \ell_i & \lambda' & \ell_f \\ -m_i & 0 & m_f \end{pmatrix} \\ &= \sum_{m_i m_f} (-1)^{\ell_i+\lambda'+\ell_f} \begin{pmatrix} \ell_i & \ell_f & \lambda \\ m_i & -m_f & 0 \end{pmatrix} \begin{pmatrix} \ell_i & \ell_f & \lambda' \\ -m_i & m_f & 0 \end{pmatrix} \end{aligned} \tag{160}$$

Using Property II:

$$\begin{aligned} J &= \sum_{m_i m_f} (-1)^{\ell_i+\lambda'+\ell_f} \begin{pmatrix} \ell_i & \ell_f & \lambda \\ m_i & -m_f & +0 \end{pmatrix} \begin{pmatrix} \ell_i & \ell_f & \lambda' \\ m_i & -m_f & 0 \end{pmatrix} (-1)^{\ell_i+\ell_f+\lambda'} \\ &= \sum_{m_i m_f} \begin{pmatrix} \ell_i & \ell_f & \lambda \\ m_i & -m_f & 0 \end{pmatrix} \begin{pmatrix} \ell_i & \ell_f & \lambda' \\ m_i & -m_f & 0 \end{pmatrix} \end{aligned} \tag{161}$$

But pg. 47 of Edmonds gives

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

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

So

$$J = (2\lambda+1)^{-1} \delta_{\lambda\lambda'} \Delta(\ell_i \ell_f \lambda) \tag{163}$$

and

$$I = \frac{(2\ell_f+1)(2\ell_i+1)}{4\pi} \begin{pmatrix} \ell_i & \ell_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \delta_{\lambda\lambda'} \Delta(\ell_i \ell_f \lambda) \tag{164}$$

# APPENDIX IV

## Equivalent Bethe Approximation

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

$$f(\Omega) = \left(-\frac{2}{K^2}\right)\left\{\int d\vec{r}\, \psi_f^{\dagger}(\vec{r}) \left[\sum_{\ell=0}^{\infty} \frac{(i\vec{K}\cdot\vec{r})^{\ell}}{\ell!}\right]\psi_i(\vec{r}) \equiv \langle f \left|\sum_{\ell} \frac{(i\vec{K}\cdot\vec{r})^{\ell}}{\ell!}\right| i\rangle\right\} \qquad (165)$$

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

$$f'(\Omega) = -\left(\frac{1}{2\pi}\right)\int d\vec{r}\,'\, \exp(i\vec{K}\cdot\vec{r}\,')\, \langle f \,|\sum_{\ell} \frac{(r)^{\ell}}{(r')^{\ell+1}} P_{\ell}(\cos[\hat{r}\cdot\hat{r}'])\,|\, i\rangle\,. \qquad (166)$$

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

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

$$P_{\ell}(\cos[\hat{r}\cdot\hat{r}']) = \left(\frac{4\pi}{2\ell+1}\right)\sum_{m} Y_{\ell m}(\Omega_r)\, Y^{\dagger}_{\ell m}(\Omega_r') \qquad (167)$$

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

$$f'(\Omega) = -\frac{1}{2\pi}\sum_{\ell m}\left(\frac{4\pi}{2\ell+1}\right)\langle f \,|\int d\vec{r}\,'\, Y_{\ell m}(\Omega_r)\, Y^{\dagger}_{\ell m}(\Omega_{r'})\, \frac{(r)^{\ell}}{(r')^{\ell+1}} \times \exp(i\vec{K}\cdot\vec{r}\,')\,|\, i\rangle \qquad (168)$$

Choose the integration axis such that $\vec{K}$ is along the z-axis and $\vec{K}\cdot\vec{r}\,' =$ $Kr'\cos\theta'$ then

$$f'(\Omega) = -\frac{1}{2\pi}\sum_{\ell}\langle f \,|\left(\frac{4\pi}{2\ell+1}\right)(r)^{\ell}\sum_{m} Y_{\ell m}(\Omega_r)\int_0^{\infty}\frac{dr'\,r'^2}{(r')^{\ell+1}} \times\int_{-1}^{+1} d(\cos\theta')\exp(iKr'\cos\theta')\int_0^{2\pi} d\phi'\, Y^{\dagger}_{\ell m}(\theta',\phi')\,|\, i\rangle\,. \qquad (169)$$

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

$$Y_{\ell m}(\Omega') = \exp(im\phi')\, P_{\ell}^{m}(\cos\theta')\left[\frac{(2\ell+1)}{4\pi}\,\frac{(\ell-m)!}{(\ell+m)!}\right]^{1/2}$$

$$\int_0^{2\pi} d\phi'\, Y^{\dagger}_{\ell m}(\theta',\phi') = \left[\frac{(2\ell+1)}{4\pi}\,\frac{(\ell-m)!}{(\ell+m)!}\right]^{1/2} P_{\ell}^{m}(\cos\phi')\,\left[2\pi\,\delta_{m0}\right] \qquad (170)$$

Summing over m, Eq. (169) can then be written,

$$f'(\Omega) = \left(-\frac{1}{2\pi}\right)(2\pi)\sum_{\ell} \langle f|\, \frac{4\pi}{2\ell+1}\, (r)^{\ell}\, Y_{\ell 0}^{+}(\Omega) \int_0^{\infty} \frac{dr'}{(r')^{\ell+2}} \times \int_{-1}^{+1} dx\, P_{\ell}(x)\, \exp(ikr'x) \sqrt{\frac{(2\ell+1)}{4\pi}}\, |i\rangle \tag{171}$$

The integral over dx may be done by use of the following identity (Abramowitz (1964) pg. 438)

$$j_e(Kr') = \left[(-i)^{e}/2\right] \int_{-1}^{+1} \exp(iKr'x)\, P_e(x)\, dx \tag{172}$$

where $j_e(r)$ is the spherical Bessel function.

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

$$f'(\Omega) = \sum_{\ell} \left(\sqrt{\frac{4\pi}{(2\ell+1)}}\right) \langle f|\, Y_{\ell 0}^{+}(\Omega)\, (r)^{\ell} \int_0^{\infty} \frac{dr'}{(r')^{\ell-1}} (2)(i)^{\ell}\, j_{\ell}(Kr')|i\rangle \tag{173}$$

Let y = Kr', dy = Kdr' then

$$f'(\Omega) = \left(\frac{2}{K^2}\right)\sum_{\ell} \sqrt{\frac{4\pi}{2\ell+1}} \langle f|\, Y_{\ell 0}^{+}(\Omega)\, (iKr)^{\ell} \int_0^{\infty} \frac{dy}{y^{\ell-1}}\, j_{\ell}(y)\,|i\rangle \tag{174}$$

From (Abramowitz (1964) pg. 486 we obtain

$$\int_0^{\infty} t^{\mu} J_{\nu}(t)\, dt = \left[2^{\mu}\, \Gamma\left(\frac{\nu+\mu+1}{2}\right)\right] \Big/ \left[\Gamma\left(\frac{\nu-\mu+1}{2}\right)\right] \tag{175}$$

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

$$\int_0^{\infty} t^{-(\ell+1/2)} J_{\ell+1/2}(t)\, dt = (2)^{-(\ell-1/2)}\, \frac{\Gamma(1)}{\Gamma(\ell+1/2)} = \sqrt{\frac{2}{\pi}}\, \frac{1}{(2\ell-1)!!} \tag{176}$$

where (Abramowitz (1964) pg. 256)

$$\Gamma(\ell+1/2) = (2\ell-1)!! \quad ; \quad \Gamma\left(\frac{1}{2}\right) = 2^{-\ell}\sqrt{\pi}\,(2\ell-1)!! \tag{177}$$

Then since $j_{\ell}(x) = \sqrt{\frac{\pi}{2x}}\, J_{\ell+1/2}(x)$, Jackson (1964), Eq. (176) may be used to write,

$$\int_0^{\infty} \frac{dt}{t^{\ell-1}}\, j_{\ell}(t) = \sqrt{\frac{\pi}{2}} \int_0^{\infty} \frac{dt}{\sqrt{t}}\, \frac{J_{\ell+1/2}(t)}{t^{\ell-1}} = \frac{1}{(2\ell-1)!!} \tag{178}$$

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

$$f'(\Omega) = \left(\frac{2}{K^2}\right)\sum_{\ell} \langle f|\, \sqrt{\frac{4\pi}{2\ell+1}}\, Y_{\ell 0}^{+}(\Omega)\, \frac{(iKr)^{\ell}}{(2\ell-1)!!}\, |i\rangle \tag{179}$$

But recall (Jackson (1962) pg. 66)

$$Y_{\ell 0}(\Omega) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta) \qquad (180)$$

then f'(Ω) is

$$f'(\Omega) = \left(\frac{2}{K^2}\right)\sum_{\ell} \langle f|\, \frac{(ikr)^\ell P_\ell(\cos\theta)}{(2\ell-1)!!}\, |i\rangle \qquad (181)$$

By choosing our axis of quantization along $\vec{K}$ so that $\vec{K}\cdot\vec{r} = Kr\cos\theta$ we may write Eq. (165) as,

$$f'(\Omega) = \left(-\frac{2}{K^2}\right)\sum_{\ell} \langle f|\,(ikr)^\ell(\cos\theta)^\ell/\ell!\,|i\rangle \ . \qquad (182)$$

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

$$P_\ell(\cos\theta) = \sum_{S=0}^{\ell} a_s(\cos\theta)^S \qquad (183)$$

Since we are interested in comparing only the first non-zero term in Eq. (181) and Eq. (182) we need only $a_e$ in series.

From Magnus and Oberhettigner pg. 66 the generalized Legendre Polynomial $P_u^\mu(z)$ has the behavior

$$P_\nu^\mu(z) = \left[\frac{2^\nu\,\Gamma(\nu+1/2)}{\sqrt{\pi}\,\Gamma(\nu-\mu+1)}\, z^\nu + O(z^{-\nu-1})\right]\left[1 + O(z^{-\nu})\right] \qquad (184)$$

therefore, recalling Eq. (183)

$$P_\ell(z) \xrightarrow[z\to\infty]{} \left[\frac{2^\ell\,\Gamma(\ell+1/2)}{\sqrt{\pi}\,\Gamma(\ell+1)}\right] z^\ell = \frac{2^\ell(2^{-\ell})\sqrt{\pi}\,(2\ell-1)!!}{\sqrt{\pi}\,\Gamma(\ell+1)}\, z^\ell \qquad (185)$$

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

$$P_\ell(\cos\theta) = \sum_{S=0}^{\ell-1} a_s(\cos\theta)^S + \frac{(2\ell-1)!!\,(\cos\theta)^\ell}{\ell!} \qquad (186)$$

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

$$f'(\Omega) = \frac{2}{K^2}\sum_{\ell} \langle f|\,(ikr)^\ell\left[\frac{(2\ell-1)!!}{(2\ell-1)!!}\right]\frac{(\cos\theta)^\ell}{\ell!}\,|i\rangle \qquad (187)$$

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 $Q_{born}$ in terms of partial wave cross-section $Q^{\ell}_{born}$, where $\ell$ refers to components of the incident wave with angular momentum $\sqrt{\ell(\ell+1)}$ proceeds as follows.

The Born scattering amplitude is

$$f_{Born}(\Omega) = -\frac{1}{2\pi}\int d\vec{r}_o{}' \exp\left[i(\vec{K}_I - \vec{K}_F)\cdot\vec{r}_o{}'\right] V_{fi}(\vec{r}_o{}') \qquad (188)$$

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

$$V_{fi}(\vec{r}_o{}') = \int d\vec{r}\; \psi_f^{\dagger}(\vec{r}) \frac{1}{|\vec{r}-\vec{r}_o{}'|} \psi_i(\vec{r}) \qquad i \neq f \qquad (189)$$

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

$$e^{-i\vec{K}_F\cdot\vec{r}_o{}'} = (4\pi)\sum_{\ell'' m''} (-i)^{\ell''} j_{\ell''}(K_F r_o') Y^{+}_{\ell'' m''}(\Omega_{K_F}) Y_{\ell'' m''}(\Omega_{r_o'}) \qquad (190)$$

and

$$e^{i\vec{K}_I\cdot\vec{r}_o{}'} = \sum_{\ell'} (i)^{\ell'} j_{\ell'}(K_I r_o') \sqrt{4\pi(2\ell'+1)}\; Y_{\ell' 0}(\Omega_{r_o'}) \qquad (191)$$

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

$$f_{Born}(\Omega) = \left(-\frac{1}{2\pi}\right)\int d\vec{r}_o{}' V_{fi}(\vec{r}_o{}') (4\pi)\sum_{\ell'\ell'' m''} (i)^{\ell'}(-i)^{\ell''}\sqrt{4\pi(2\ell'+1)}$$
$$\times Y^{+}_{\ell'' m''}(\Omega_{K_F}) Y_{\ell' 0}(\Omega_{r_o'}) Y_{\ell'' m''}(\Omega_{r_o'}) j_{\ell'}(K_I r_o') j_{\ell''}(K_F r_o') \qquad (192)$$

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

$$\psi_i(\vec{r}) = R_i(r) Y_{\ell_i m_i}(\Omega_r) \quad ; \qquad \psi_f^{+}(\vec{r}) = R_f(r) Y^{\dagger}_{\ell_f m_f}(\Omega_r) \qquad (193)$$

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

$$\frac{1}{|\vec{r}_o{}' - \vec{r}|} = 4\pi\sum_{\ell,m} (2\ell+1)^{-1}\left[\frac{r_<^{\ell}}{r_>^{\ell+1}}\right] Y^{+}_{\ell m}(\Omega_{r_o'}) Y_{\ell m}(\Omega_r) \qquad (194)$$

to rewrite Eq. (189) as

$$V_{fi}(\vec{r}_o') = 4\pi \sum_{\ell m} (2\ell+1)^{-1} Y_{\ell m}^{+}(\Omega_{r_o'}) \int_o^\infty r^2 dr \left[ \frac{r_<^{\ell}}{r_>^{\ell+1}} \right] R_f(r) R_i(r) \tag{195}$$

$$\times \int d\Omega_r \, Y_{\ell_f m_f}^{+}(\Omega_r) \, Y_{\ell m}(\Omega_r) \, Y_{\ell_i m_i}(\Omega_r)$$

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

$$\mathcal{R}_\ell^{Born}(r_o') \equiv \int_o^\infty r^2 dr \left[ \frac{r_<^{\ell}}{r_>^{\ell+1}} \right] R_f(r) \, R_i(r) \tag{196}$$

and

$$\langle \ell_f m_f \,|\, \ell m \,|\, \ell_i m_i \rangle = \int d\Omega_r \, Y_{\ell_f m_f}^{+}(\Omega_r) \, Y_{\ell m}(\Omega_r) \, Y_{\ell_i m_i}(\Omega_r) \tag{197}$$

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

$$f_{Born}(\Omega) = \left(-\frac{1}{2\pi}\right) \sum_{\ell'\ell''m''\ell m} (4\pi)^2 (i)^{\ell'} (-i)^{\ell''} (2\ell+1)^{-1} \sqrt{4\pi(2\ell'+1)}$$

$$\langle \ell_f m_f \,|\, \ell m \,|\, \ell_i m_i \rangle \, Y_{\ell'' m''}^{+}(\Omega_{K_F}) \int r_o'^2 dr_o' \left[ \mathcal{R}_\ell^{Born}(r_o) \, j_{\ell'}(K_I r_o') \right.$$

$$\left. \times \, j_{\ell''}(K_F r_o') \right] \langle \ell m \,|\, \ell' o \,|\, \ell'' m'' \rangle \tag{198}$$

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

To simplify the algebra that follows, we define the quantities

$$C(\ell, \ell', \ell'') \equiv (i)^{\ell'} (-i)^{\ell''} (2\ell+1)^{-1} \sqrt{4\pi(2\ell'+1)} \tag{199}$$

$$P(\ell, \ell' \ell'' i f) \equiv \int_o^\infty r_o'^2 dr_o' \, \mathcal{R}_\ell^{Born}(r_o') \, j_{\ell'}(K_I r_o') \, j_{\ell''}(K_F r_o') \tag{200}$$

and rewrite as,

$$f_{Born}(\Omega) = -(8\pi) \sum_{\substack{\ell'\ell''m'' \\ \ell m}} C(\ell \ell' \ell'') \langle \ell_f m_f \,|\, \ell m \,|\, \ell_i m_i \rangle \tag{201}$$

$$\times \, P(\ell, \ell', \ell'', i, f) \langle \ell m \,|\, \ell' o \,|\, \ell'' m'' \rangle \, Y_{\ell'' m''}^{+}(\Omega_{K_F}) \tag{202}$$

To obtain the cross-section we require

$$\left|f_{Born}(\Omega)\right|^2 = \sum_{\substack{\ell'\ell''m'' \\ \ell m}} \sum_{\substack{L'L''M'' \\ LM}} C(\ell\ell'\ell'')C^{+}(LL'L'') \langle \ell_f m_f | \ell m | \ell_i m_i \rangle \langle \ell_i m_i | LM | \ell_f m_f \rangle$$

$$\times P(\ell\ell'\ell'' if)\, P(LL'L'' if)\, [64\pi^2] \tag{203}$$

$$\times \langle \ell m | \ell' o | \ell'' m'' \rangle \langle L''M'' | L' o | LM \rangle\, Y^{+}_{\ell'' m''}(\Omega_{K_F})\, Y_{L''M''}(\Omega_{K_F}) \, .$$

Since we are interested in transitions Q(nℓ→n'ℓ") we can average the above over $m_i$ and sum over $m_f$ the result of which we indicate by the prime

$$\left|f'_{Born}(\Omega)\right|^2 = \left(\frac{64\pi^2}{2\ell_i+1}\right) \sum_{\substack{\ell'\ell''m'' \\ \ell m}} \sum_{\substack{L'L''M'' \\ LM}} C(\ell\ell'\ell'')\, C^{+}(LL'L'')\, P(\ell\ell'\ell'' if)\, P(LL'L'' if)$$

$$\times \langle \ell m | \ell' o | \ell'' m'' \rangle \langle L''M'' | L' o | LM \rangle$$

$$\times \sum_{m_i m_f} \langle \ell_f m_f | \ell m | \ell_i m_i \rangle \langle \ell_i m_i | LM | \ell_f m_f \rangle \tag{204}$$

$$\times Y^{+}_{\ell'' m''}(\Omega_{K_F})\, Y_{L''M''}(\Omega_{K_F})$$

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

$$\left|f'_{Born}(\Omega)\right|^2 = \left(\frac{64\pi^2}{2\ell_i+1}\right) \sum_{\substack{\ell'\ell''m'' \\ \ell m}} \sum_{\substack{L'L''M'' \\ LM}} C(\ell\ell'\ell'')\, C^{+}(LL'L'')\, P(\ell\ell'\ell'' if)\, P(LL'L'' if)$$

$$\times \langle \ell m | \ell' o | \ell'' m'' \rangle \langle L''M'' | L' o | LM \rangle \tag{205}$$

$$\times Y^{+}_{\ell'' m''}(\Omega_{K_F})\, Y_{L''M''}(\Omega_{K_F})$$

$$\times \frac{(2\ell_f+1)(2\ell_i+1)}{4\pi} \begin{pmatrix} \ell_f & \ell_i & \ell \\ 0 & 0 & 0 \end{pmatrix}^2 \delta_{\ell L}\, \delta_{mM}$$

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

$$\left|f'_{Born}(\Omega)\right|^2 = (16\pi)(2\ell_f+1) \sum_{\substack{\ell'\ell''m'' \\ \ell m}} \sum_{L'L''M''} C(\ell\ell'\ell'')\, C^{+}(\ell, L', L'')\, P(\ell\ell'\ell'' if)$$

$$\times P(\ell L'L'' if)\, \langle \ell m | \ell' o | \ell'' m'' \rangle \langle L''M'' | L' o | \ell m \rangle \tag{206}$$

$$\times \begin{pmatrix} \ell_f & \ell_i & \ell \\ 0 & 0 & 0 \end{pmatrix}^2 Y^{+}_{\ell'' m''}(\Omega_{K_F})\, Y_{L''M''}(\Omega_{K_F})$$

The cross-section is then:

$$
\begin{aligned}
Q_{\text{Born}} &= \left[\frac{K_F}{K_I}\right]\int d\Omega_{K_F}\,\left|f'_{\text{Born}}(\Omega_{K_F})\right|^2 = (16\pi)(2l_f+1)\left[\frac{K_F}{K_I}\right] \\
&\times \sum_{\substack{l'l''m'' \\ lm}}\ \sum_{L'L''M''} C(ll'l'')\,C^{\dagger}(lL'L'')\,P(ll'l'';if)\,P(lL'L'';if) \\
&\times \langle lm|l'0|l''m''\rangle\langle L''M''|L'0|lm\rangle \begin{pmatrix} l_f & l_i & l \\ 0 & 0 & 0 \end{pmatrix}^2 \\
&\times \left[\int d\Omega_{K_F}\, Y^{\dagger}_{l''m''}(\Omega_{K_F})\, Y_{L''M''}(\Omega_{K_F}) = \delta_{l''L''}\,\delta_{m''M''}\right]
\end{aligned}
\tag{207}
$$

The sums over L"M" and L' can be carried out explicitly to give the results

$$
\begin{aligned}
Q_{\text{Born}} &= (16\pi)(2l_f+1)\left[\frac{K_F}{K_I}\right]\sum_{l'l''l}\ \sum_{L'} C(ll'l'')\,C^{\dagger}(lL'l'')\begin{pmatrix} l_f & l_i & l \\ 0 & 0 & 0 \end{pmatrix}^2 \\
&\times P(ll'l'';if)\,P(lL'l'';if)\left[\sum_{mm''}\langle lm|l'0|l''m''\rangle\langle l''m''|L'0|lm\rangle = \frac{(2l+1)(2l''+1)}{4\pi}\,\delta_{L'l'}\begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix}^2\right] \\
&= (16\pi)(2l_f+1)\left[\frac{K_F}{K_I}\right]{\sum_{ll'l''}}'\left|C(ll'l'')\right|^2\left|P(ll'l'';if)\right|^2 \\
&\times \begin{pmatrix} l_f & l_i & l \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix}^2 \frac{(2l+1)(2l''+1)}{4\pi}
\end{aligned}
\tag{208}
$$

Recalling the definitions of $C(ll'l'')$ and $P(ll'l''k_ik_f)$, $Q_{\text{born}}$ can be written

$$
\begin{aligned}
Q_{\text{Born}} &= (4)(2l_f+1)\left[\frac{K_F}{K_I}\right]\sum_{ll'l''}\frac{4\pi(2l'+1)}{(2l+1)^2}(2l+1)(2l''+1) \\
&\times \begin{pmatrix} l_f & l_i & l \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix}^2 \left[\int_0^{\infty} dr_0'\,(r_0')^2\,\mathcal{R}_l^{\text{Born}}(r_0')\, j_{l'}(K_I r_0')\, j_{l''}(K_F r_0')\right]^2
\end{aligned}
\tag{209}
$$

where, as defined above,

$$
\mathcal{R}_l^{\text{Born}}(r_0') \equiv \int_0^{\infty} r^2\,dr\,\left[\frac{r_<^{\,l}}{r_>^{\,l+1}}\right] R_f(r)\,R_i(r)
$$

Since $l'$ is defined in Eq. (191) to refer to the incident electron, the partial cross-section corresponding to incident electrons with angular momentum $\sqrt{l'(l'+1)}$ and scattered electrons with all possible values of angular momentum is,

$$Q^{\ell'}_{Born} = (16\pi)(2\ell_f + 1)\left[\frac{K_F}{K_I}\right]\sum_{\ell\ell''}\frac{(2\ell'+1)(2\ell''+1)}{(2\ell+1)}\begin{pmatrix}\ell_f & \ell_i & \ell\\ 0 & 0 & 0\end{pmatrix}^2$$

$$\times\begin{pmatrix}\ell & \ell' & \ell''\\ 0 & 0 & 0\end{pmatrix}^2\int_0^\infty dr_0'\, r_0'^2\, \mathcal{R}_\ell^{Born}(r_0')\, j_{\ell'}(K_I r_0')\, j_{\ell''}(K_F r_0') \,. \tag{210}$$

NOTE: The presence of a 3j-symbol in an expression such as $\sum_{\ell_3=0}^{\infty}\begin{pmatrix}\ell_1 & \ell_2 & \ell_3\\ 0 & 0 & 0\end{pmatrix} f(\ell_1\ell_2\ell_3)$ implies the triangle condition and reduces the sum range from $\ell_3 = 0,\infty$ to $\ell_3 = |\ell_1-\ell_2|,\cdots|\ell_1+\ell_2|$, (Edmonds (1960) pg. 45).

## APPENDIX VI

### Ochkur Expression of $f_E(\Omega)$

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

$$f_E = \left(\frac{1}{2\pi}\right)\int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \, \Psi_F^{\dagger}(\vec{r}_2,\vec{r}_0)\, e^{-i\vec{K}_F\cdot\vec{r}_1}\left[\frac{1}{|\vec{r}_0-\vec{r}_1|}-\frac{2}{r_0}+\frac{1}{|\vec{r}_0-\vec{r}_2|}\right]\Psi_I(\vec{r}_1,\vec{r}_2)\, e^{i\vec{K}_I\cdot\vec{r}_0} \tag{211}$$

Let us break this up into three terms

$$f_1 = \left(\frac{1}{2\pi}\right)\int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \, \Psi_F^{\dagger}(\vec{r}_2,\vec{r}_0)\, e^{-i\vec{K}_F\cdot\vec{r}_1}\left[\frac{1}{|\vec{r}_0-\vec{r}_1|}\right]\Psi_I(\vec{r}_1,\vec{r}_2)\, e^{i\vec{K}_I\cdot\vec{r}_0} \tag{212}$$

$$f_2 = \left(\frac{1}{2\pi}\right)\int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \, \Psi_F^{\dagger}(\vec{r}_2,\vec{r}_0)\, e^{-i\vec{K}_F\cdot\vec{r}_1}\left[\frac{1}{|\vec{r}_0-\vec{r}_2|}\right]\Psi_I(\vec{r}_1,\vec{r}_2)\, e^{i\vec{K}_I\cdot\vec{r}_0} \tag{213}$$

$$f_3 = \left(\frac{1}{2\pi}\right)\int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \, \Psi_F^{\dagger}(\vec{r}_2,\vec{r}_0)\, e^{-i\vec{K}_F\cdot\vec{r}_1}\left[-\frac{2}{r_0}\right]\Psi_I(\vec{r}_1,\vec{r}_2)\, e^{i\vec{K}_I\cdot\vec{r}_0} \tag{214}$$

Consider the first term

$$\begin{aligned} f_1 &= \left(\frac{1}{2\pi}\right)\int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \, \Psi_F^{\dagger}(\vec{r}_2,\vec{r}_0)\, e^{-i\vec{K}_F\cdot\vec{r}_1}\left[\frac{1}{|\vec{r}_0-\vec{r}_1|}\right]\Psi_I(\vec{r}_1,\vec{r}_2)\, e^{i\vec{K}_I\cdot\vec{r}_0} \\ &= \left(\frac{1}{2\pi}\right)\int d\vec{r}_1 d\vec{r}_2 \, \Psi_I(\vec{r}_1,\vec{r}_2)\, I_F(\vec{r}_1,\vec{r}_2)\, \exp[i\vec{K}\cdot\vec{r}_1] \end{aligned} \tag{215}$$

where $\vec{K} \equiv \vec{k}_I - \vec{k}_F$ and

$$I_F(\vec{r}_1,\vec{r}_2) = \int d\vec{r}_0 \, \Psi_F(\vec{r}_2,\vec{r}_0)\, \frac{\exp[i\vec{K}_I\cdot(\vec{r}_0-\vec{r}_1)]}{|\vec{r}_0-\vec{r}_1|} \tag{216}$$

Let us evaluate $I_F$. Introducing the notation $\vec{r}_{01} = \vec{r}_0 - \vec{r}_1$ let us change variables from $\vec{r}_0$ to $\vec{r}_{01}$

$$I_F(\vec{r}_1,\vec{r}_2) = \int r_0^2\, dr_0\, d(\cos\theta_0)\, d\phi_0\, \bar{\Psi}_F^{\dagger}(\vec{r}_2,\vec{r}_0)\, \frac{e^{i\vec{K}_I\cdot\vec{r}_{01}}}{r_{01}} \tag{217}$$

$$= \int r_{01}\, dr_{01}\, d(\cos\theta_{01})\, d\phi_{01}\, \bar{\Psi}^F(\vec{r}_2, \vec{r}_1 + \vec{r}_{01})\, e^{iK_I r_{01}\cos\theta_{01}}$$

Defining $X = \cos\theta_{01}$

$$I_F(\vec{r}_1,\vec{r}_2) = \int r_{01}\, dr_{01}\, dx\, \Phi_F(\vec{r}_2,\vec{r}_1, r_{01}, x)\, e^{iK_I r_{01} x} \tag{218}$$

where

$$\Phi_F(\vec{r}_2,\vec{r}_1, r_{01}, x) = \int d\phi_{01}\, \bar{\Psi}_F(\vec{r}_2, \vec{r}_1 + \vec{r}_{01}) \tag{219}$$

(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

$$I_F(\vec{r}_1,\vec{r}_2) = \frac{1}{iK_F}\int_0^\infty dr_{01}\left[\Phi_F(\vec{r}_2,\vec{r}_1, r_{01}, 1)e^{iK_F r_{01}} - \Phi_F(\vec{r}_2,\vec{r}_1, r_{01}, -1)e^{-iK_F r_{01}}\right] + \cdots \tag{220}$$

Noting that

$$\Phi_F(\vec{r}_2,\vec{r}_1, r_{01}, x) \xrightarrow[r_{01}\to\infty]{} 0 \tag{221}$$

we write

$$I_F(\vec{r}_1,\vec{r}_2) = -k_I^{2}\left[\Phi_F(\vec{r}_2,\vec{r}_1, 0, 1) + \Phi_F(\vec{r}_2,\vec{r}_1, 0, -1)\right] \tag{222}$$

Then since

$$\Phi_F(\vec{r}_2,\vec{r}_1, 0, \pm 1) = 2\pi\, \bar{\Psi}_F^{\dagger}(\vec{r}_2,\vec{r}_1) \tag{223}$$

our result is:

$$I_F(\vec{r}_1,\vec{r}_2) = \left[\frac{4\pi}{K_I^2}\right] \bar{\Psi}_F(\vec{r}_2,\vec{r}_1) \tag{224}$$

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

$$f_2 = O(K_I^{-6})$$

$$f_3 = O(K_I^{-6})$$

Therefore, he claims the exchange amplitude $f_E$, may be approximated

$$
\begin{aligned}
f_E &\cong \frac{4\pi}{K_I^2}\,\frac{1}{2\pi}\int d\vec{r}_1\, d\vec{r}_2\; \Psi_I(\vec{r}_1,\vec{r}_2)\; e^{i\vec{K}\cdot\vec{r}_1}\,\Psi_F^{\dagger}(\vec{r}_2,\vec{r}_1) \\
&= \frac{2}{K_I^2}\int d\vec{r}_1\, d\vec{r}_2\; \Psi_I(\vec{r}_1,\vec{r}_2)\; e^{i\vec{K}\cdot\vec{r}_1}\,\Psi_F^{\dagger}(\vec{r}_2,\vec{r}_1) \quad .
\end{aligned}
\tag{225}
$$

## 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

```
     JOB ,           ,.,                          ,.MSGLEVEL=(0,0)
C FORTGCLG.PARM=NOMAP
.SYSIN DD *
PROGRAM HFSWF(INPUT)                                                      A  010
                                                                          A  020
 ============================================================             A  030
 *                                                          *             A  040
 *                * * *    HFSWF    * * *                   *             A  050
 *                                                          *             A  060
 * A FORTRAN PROGRAM TO CALCULATE HARTREE-FOCK-SLATER      *             A  070
 *   NUMERICAL WAVE FUNCTIONS AS PUNCHED CARD OUTPUT.      *             A  080
                              .
                              .
                              .
END                                                                       A 531-
SUBROUTINE SCHEQ (ZZ,EN,LAMBDA,NOFL,KKK,MESS,SCF,THRESH)                  B   1
                              .
                              .
                              .
END                                                                       B 430-

YSIN DD *
TON- 4 CASES
.001  0.00001  521   1  20   1   0   6   6   5   7   1   1
00 .98958 .97892 .96819 .95748 .94688 .93642 .92614 .91604 .90613
42 .87756 .85941 .84195 .82516 .80902 .79352 .77862 .76430 .75051
19 .71184 .68796 .66536 .64393 .62355 .60415 .58564 .56796 .55105
86 .50445 .47648 .45070 .42717 .40540 .38525 .36651 .34902 .33266
36 .28967 .26547 .24431 .22577 .20943 .19492 .18195 .17029 .15976
22 .13376 .12024 .10906 .09965 .09154 .08441 .07807 .07238 .06725
53 .05466 .04811 .04268 .03811 .03424 .03092 .02805 .02778 .02778
78 .02778 .02778 .02778 .02778 .02778 .02778 .02778 .02778 .02778
78 .02778 .02778 .02778 .02778 .02778 .02778 .02778 .02778 .02778
78 .02778 .02778 .02778 .02778 .02778 .02778 .02778 .02778 .02778
78 .02778 .02778 .02778 .02778 .02778 .02778 .02778 .02778 .02778
 8   0
 2-1030.6
 2-135.53
 6-123.25
 2-19.728
 6-15.249
10-7.0975
 2-1.9456
 6-0.9519

 1-.2199
 1-.1089
 1-.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, DEFOLT, 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 Ƶ is obtained by a linear extrapolation of the two unabridged potentials for atoms ƵE2 and ƵE3 where Ƶ-ƵE3 = ƵE3-ƵE2. 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 = $\mathrm{MAX}|rV_{\circ}^{f}(r)-rV_{\circ}^{f}(r)|$. 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.

---

(1) 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

$$V(r) = \begin{cases} V_0(r) & r < r_0 \\ -2(Z-N+1)/r & r \geq r_0 \end{cases}$$

where $r_0$ 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, WWML, EE.

NNLZ: The principal and orbital quantum numbers.

(Note: NNLZ = 100n + 10$\lambda$ + c, where n is the principal quantum number, $\lambda$ 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

ITER = "iteration" number

Z = atomic number

DELTA = measure of self-consistency (when DELTA < .001 calculation stops)

I(DEL) = serial number of mesh point at which self-consistency is poorest

X(DEL) = corresponding value of X

I(CUT) = serial number of mesh point closest to $r_\circ$ where $r_\circ V_\circ(r_\circ) = -2(\mathrm{ION}+1)$

X(CUT) = corresponding value of X

N cards and M cards denote the number of cards that would be produced by a punching of <u>All</u> 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 + 10λ + c; (identical to NNLZ in Data Card #5 above)

XL = numerical value of λ in floating point form

EE = energy eigenvalue

WWNL = occupation number

KKK = last mesh point for tabular representation of $P(n,\lambda:r)$

$Z$ = 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 $\mu = \frac{1}{2}\left(\frac{3\pi}{4}\right)^{2/3} Z^{-1/3}$

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.

| BLOCK NUMBER | INITIAL X | INTERVAL ΔX | FINAL X | LAST POINT |
|---|---|---|---|---|
| 1 | 0.0 | .0025 | .1 | 41 |
| 2 | 0.1 | .005 | .3 | 81 |
| 3 | .3 | .01 | .7 | 121 |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| 11 | 102.3 | 2.56 | 204.7 | 441 |

(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.)

```
KRYPTON  4 CASES
KEY = 0
ITER        Z     DELTA       I(DEL)  X(DEL)  I(CUT)  X(CUT)
    1      36.  2.0038214E 00  405    112.540   441   204.700
    2      36.  1.0018797E 00  402    104.860   270    10.940
    3      36.  2.7208328E-03  279     12.380   270    10.940
    4      36.  1.3160706E-03  279     12.380   270    10.940
    5      36.  4.0054321E-04  270     10.940   270    10.940
NCARDS=   578  MCARDS=14
NCARDS=   578  MCARDS=14
```

EXHIBIT 2

HFSWF SAMPLE OUTPUT (PRINTED OUTPUT)

```
410 1.0000000E 00-9.5209509E-01 6.0000000E 00 401 36.                      Z 36   1
 0.0           7.0760769E-05 2.7964660E-04 6.2165153E-04 1.0918884E-03 Z 36   2
 1.6855842E-03 2.3980788E-03 3.2248199E-03 4.1613765E-03 5.2034073E-03 Z 36   3
                              .
                              .
                              .
 5.6951222E-10 4.1242476E-10 2.9837133E-10 2.1548405E-10 1.5512808E-10 Z 36  81
 1.1100898E-10                                                         Z 36  82
500 0.0          -2.1989995E-01 1.0000000E 00 441 36.                      Z 36   1
 0.0           2.5549415E-03 4.9868859E-03 7.2991028E-03 9.4948038E-03 Z 36   2
                              .
                              .
                              .
 7.8121731E-10                                                         Z 36  90
510 1.0000000E 00-1.0889995E-01 1.0000000E 00 441 36.                      Z 36   1
                              .
                              .
                              .
-1.4592098E-07                                                         Z 36  90
420 2.0000000E 00-5.6100000E-02 1.0000000E 00 441 36.                      Z 36   1
                              .
                              .
                              .
-2.9764298E-05-2.4344161E-05-1.9828294E-05-1.6053091E-05-1.2880814E-05 Z 36  89
-1.0194870E-05                                                         Z 36  90
```

EXHIBIT 3

HFSWF SAMPLE OUTPUT (PUNCHED OUTPUT)

## 2) EXCST: Excitation Cross-Sections

### a) Sample Input

```
//          JOB '          ','                        ',MSGLEVEL=(0,0)
// EXEC FORTGCLG,PARM='BCD,NOSOURCE'
//FORT.SYSIN DD *
C     PROGRAM EXCSCT(INPUT)                                           C    1
C                                                                     C    2
C      ============================================================   C    3
C      *                                                          *   C    4
C      *                 * * *   EXCSCT   * * *                   *   C    5
C      *                                                          *   C    6
C      * A FORTRAN PROGRAM TO CALCULATE EXCITATION CROSS-         *   C    7
C      * SECTIONS FOR THE ELECTRON IMPACT EXCITATION OF ATOMS.*       C    8
                              .
                              .
                              .
      END                                                             C 363-
      SUBROUTINE PDINT (GRND,LAM,X)                                   D    1
                              .
                              .
                              .
      END                                                             I   99-
/*
//GO.SYSIN DD *
 12  1  1  1SODIUM
  1.05  1.10  1.20  1.80  2.50  5.00 10.00 15.00 20.00 30.00 50.00 80.00
 300 0.0          -3.7781912E-01 1.0000000E 00 401 11.                Z 11    1
  0.0             3.0446039E-03 6.0226806E-03 8.9350902E-03 1.1782687E-02 Z 11    2
  1.4566310E-02 1.7286804E-02 1.9944981E-02 2.2541702E-02 2.5077760E-02 Z 11    3
                              .
                              .
                              .
  1.7836356E-08 1.3301566E-08 9.9009725E-09 7.3463475E-09 5.4206950E-09 Z 11   81
  3.9600607E-09                                                       Z 11   82
 310 1.0000000E 00-2.2318995E-01 1.0000000E 00 441 11.                Z 11    1
  0.0             4.7134745E-06 1.8751074E-05 4.1959924E-05 7.4188909E-05 Z 11    2
                              .
                              .
                              .
 -3.1195364E-13-1.9791888E-13-1.2539492E-13-7.9215009E-14-4.9704662E-14 Z 11   89
 -3.0670301E-14                                                       Z 11   90
  3BETHE
/*
```

EXHIBIT 4

EXCSCT SAMPLE INPUT

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 = potasium).

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 ≠ -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 NLƵI, XLI, EEI, WWNLI, KKKI, Ƶ.

NLƵI: 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.

WWNLI: 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.

Ƶ: 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 boundry 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 NLƵ2, XL2, EE2, WWNL2, KKK2, Ƶ. 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.

```
   1.200    0.405E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   1.350    0.677E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   1.500    0.825E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   1.750    0.945E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   2.000    0.990E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   2.330    0.100E 03BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   2.670    0.982E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   3.000    0.955E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   3.500    0.907E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   4.000    0.859E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   5.000    0.772E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   6.000    0.699E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   7.000    0.639E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
   8.000    0.589E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
  10.000    0.511E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
  12.000    0.452E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
  15.000    0.388E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
  18.000    0.341E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
  21.000    0.304E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
  24.000    0.276E 02BETHE    (11.)    SODIUM   (30-31)(EPSIL= 0.753E-01)
```

EXHIBIT 5

EXCST SAMPLE OUTPUT (NOTP = 1)

```
                              SODIUM  -BETHE

      CROSS-SECTIONS ARE IN UNITS OF PI*(BOHR RADIUS**2).
      INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (EPSIL).
      EPSIL IS IN UNITS OF TWICE THE RYDBERG.

  (AT. NO.= 11.)                (EPSIL= 7.531E-02)              (NL-N'L':30-31)
*****************************************************************************
*     N     |      SIG(N)     *     N     |      SIG(N)     *     N     |      SIG(N)
*****************************************************************************
*           |                 *           |                 *           |
*   1.200   |    4.048E 01    *   1.350   |    6.766E 01    *   1.500   |    8.245E 01
*           |                 *           |                 *           |
*****************************************************************************
*****************************************************************************
*           |                 *           |                 *           |
*   1.750   |    9.451E 01    *   2.000   |    9.905E 01    *   2.330   |    9.997E 01
*           |                 *           |                 *           |
*****************************************************************************
*****************************************************************************
*           |                 *           |                 *           |
*   2.670   |    9.824E 01    *   3.000   |    9.550E 01    *   3.500   |    9.070E 01
*           |                 *           |                 *           |
*****************************************************************************
*****************************************************************************
*           |                 *           |                 *           |
*   4.000   |    8.588E 01    *   5.000   |    7.716E 01    *   6.000   |    6.991E 01
*           |                 *           |                 *           |
*****************************************************************************
*****************************************************************************
*           |                 *           |                 *           |
*   7.000   |    6.392E 01    *   8.000   |    5.892E 01    *  10.000   |    5.109E 01
*           |                 *           |                 *           |
*****************************************************************************
*****************************************************************************
*           |                 *           |                 *           |
*  12.000   |    4.524E 01    *  15.000   |    3.877E 01    *  18.000   |    3.405E 01
*           |                 *           |                 *           |
*****************************************************************************
*****************************************************************************
*           |                 *           |                 *           |
*  21.000   |    3.045E 01    *  24.000   |    2.759E 01    *   0.000   |    1.484E-78
*           |                 *           |                 *           |
*****************************************************************************
```

EXHIBIT 6

EXCST OUTPUT (NOTP = 2)

```
                                     F  O                    (AT.NO.=11.)
CROSS-SECTIONS ARE IN UNITS OF PI*(BOHR RADIUS**2).
INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (EPSIL).
EPSIL IS IN UNITS OF TWICE THE RYDBERG.

     N              SIG(N)              SIG(N)              SIG(N)              SIG(N)

   1.200          9.534E 01          8.027E 01          4.048E 01          0.0
   1.350          9.984E 01          9.062E 01          6.766E 01          0.0
   1.500          1.064E 02          9.468E 01          8.245E 01          1.326E 01
   1.750          1.101E 02          9.631E 01          9.451E 01          2.607E 01
   2.000          1.098E 02          9.598E 01          9.905E 01          3.448E 01
   2.330          1.069E 02          9.408E 01          9.997E 01          4.110E 01
   2.670          1.029E 02          9.133E 01          9.824E 01          4.397E 01
   3.000          9.871E 01          8.860E 01          9.550E 01          4.557E 01
   3.500          9.261E 01          8.427E 01          9.070E 01          4.661E 01
   4.000          8.701E 01          8.013E 01          8.588E 01          4.664E 01
   5.000          7.750E 01          7.262E 01          7.716E 01          4.526E 01
   6.000          6.989E 01          6.631E 01          6.991E 01          4.317E 01
   9.000          5.437E 01          5.263E 01          5.470E 01          3.681E 01
  10.000          5.074E 01          4.930E 01          5.109E 01          3.499E 01
  12.000          4.487E 01          4.385E 01          4.524E 01          3.182E 01
  15.000          3.942E 01          3.775E 01          3.877E 01          2.804E 01
  18.000          3.374E 01          3.326E 01          3.405E 01          2.511E 01
  21.000          3.016E 01          2.980E 01          3.045E 01          2.278E 01
  24.000          2.732E 01          2.705E 01          2.759E 01          2.088E 01
 APPROX.            BORN              OCHKUR              BETHE             MODBETHE
 (NL-N'L')        (30-31)            (30-31)            (30-31)            (30-31)
 EPSIL           7.531E-02          7.531E-02          7.531E-02          7.531E-02
```

EXHIBIT 7

EXCST SAMPLE OUTPUT (NOTP = 3)

### 3) IONCST: Ionization Cross-Sections

#### a) Sample Input

```
//          JOB '        ','                    ',MSGLEVEL=(0,0)
// EXEC FORTGCLG,PARM='BCD,NOSOURCE'
//FORT.SYSIN DD *
C     PROGRAM  IONCST(INPUT)                                            A   1
C                                                                       A   2
C      ==========================================================      A   3
C      *                                                        *      A   4
C      *                 * * *    IONCST    * * *               *      A   5
C      *                                                        *      A   6
C      * A FORTRAN PROGRAM TO CALCULATE PARTIAL CROSS-SECTIONS  *      A   7
C      *      FOR NEUTRAL ATOMS IONIZED BY INCIDENT ELECTRONS   *      A   8
                              .
                              .
                              .
      END                                                               A 204-
      FUNCTION FINR (L,RHO,ETA)                                         B   1
                              .
                              .
                              .
      END                                                               G  11-
/*
//GO.SYSIN DD *
 HELIUM
 100 0.0           -1.7212696E 00 2.0000000E 00 321  2.                 Z  2   1
  0.0            8.4950104E-03 1.6930431E-02 2.5306545E-02 3.3623707E-02 Z  2   2
  4.1882206E-02 5.0082348E-02 5.8224466E-02 6.6308796E-02 7.4335754E-02 Z  2   3
                              .
                              .
                              .
  6.2946981E-09 4.7294328E-09 3.5502439E-09 2.6611420E-09 1.9896926E-09 Z  2  65
  1.4811201E-09                                                         Z  2  66
 2.75      BORN
/*
```

EXHIBIT 8

SAMPLE INPUT IONCST

b) Input Data Values

<u>Data Card #1</u> (Format 17)

This is a heading card. The 8 character abbreviation for the element as it will appear in the output.

<u>Data Card #2</u> (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.

<u>Data Card #3</u> (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.

<u>Data Card #4</u> (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 equal the total cross-section Q obtained summing Qλ. A sample output follows.

```
                                HELIUM**COUL-BORN

     CROSS-SECTIONS ARE IN UNITS OF PI*(BOHR RADIUS**2).
     INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (EPSIL).
     EPSIL IS IN UNITS OF TWICE THE RYDBERG.

  (AT. NO.=  1.)                (EPSIL= 5.000E-01)              (NL-N'L'=10-CONTINUUM)
*******************************************************************
*    L      |     SIG(L)     *    L     |     SIG(L)     *    L      |     SIG(L)    *
*******************************************************************
*           |                *          |                *           |               *
*   0.0     |   1.693E-01    *  1.000   |   6.615E-01    *  2.000    |   2.020E-01   *
*           |                *          |                *           |               *
*******************************************************************
*           |                *          |                *           |               *
*   3.000   |   3.678E-02    *  4.000   |   6.686E-03    *  5.000    |   1.256E-03   *
*           |                *          |                *           |               *
*******************************************************************
*                                                                                    *
*N=   2.750         LOG(N)= 4.393E-01          SIG(TOTAL)= 1.078E 00                 *
*                                                                                    *
*******************************************************************
*RHO(MAX)= 2.3229645E 01                                      ETA(MAX)=-9.7186023E-01*
*RHO(MIN)= 2.0704012E-04                                      ETA(MIN)=-1.0690455E 01*
*******************************************************************
```

EXHIBIT 9

IONCST SAMPLE OUTPUT

# TABLE A

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.

| U(X) X | | HE 2 | LI 3 | BE 4 | B 5 | C 6 | N 7 | O 8 | F 9 |
|---|---|---|---|---|---|---|---|---|---|
| X | U(X) | U(X) | U(X) | U(X) | U(X) | U(X) | U(X) | U(X) | U(X) |
| 00.00 | 0.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 |
| 00.01 | 0.00000 | 0.99609 | 0.99529 | 0.99480 | 0.99432 | 0.99384 | 0.99337 | 0.99292 | 0.99247 |
| 00.02 | 0.00000 | 0.99205 | 0.99041 | 0.98941 | 0.98845 | 0.98748 | 0.98653 | 0.98562 | 0.98473 |
| 00.03 | 0.00000 | 0.98787 | 0.98539 | 0.98387 | 0.98241 | 0.98095 | 0.97952 | 0.97815 | 0.97681 |
| 00.04 | 0.00000 | 0.98357 | 0.98023 | 0.97819 | 0.97624 | 0.97428 | 0.97238 | 0.97054 | 0.96877 |
| 00.05 | 0.00000 | 0.97916 | 0.97495 | 0.97239 | 0.96995 | 0.96750 | 0.96513 | 0.96284 | 0.96063 |
| 00.06 | 0.00000 | 0.97464 | 0.96957 | 0.96649 | 0.96356 | 0.96064 | 0.95781 | 0.95508 | 0.95244 |
| 00.07 | 0.00000 | 0.97002 | 0.96409 | 0.96051 | 0.95711 | 0.95371 | 0.95043 | 0.94727 | 0.94422 |
| 00.08 | 0.00000 | 0.96531 | 0.95853 | 0.95445 | 0.95059 | 0.94674 | 0.94302 | 0.93944 | 0.93599 |
| 00.09 | 0.00000 | 0.96053 | 0.95290 | 0.94834 | 0.94403 | 0.93974 | 0.93560 | 0.93162 | 0.92778 |
| 00.10 | 0.00000 | 0.95566 | 0.94721 | 0.94218 | 0.93745 | 0.93273 | 0.92818 | 0.92381 | 0.91959 |
| 00.12 | 0.00000 | 0.94574 | 0.93568 | 0.92979 | 0.92424 | 0.91873 | 0.91341 | 0.90830 | 0.90337 |
| 00.14 | 0.00000 | 0.93558 | 0.92402 | 0.91734 | 0.91107 | 0.90483 | 0.89880 | 0.89301 | 0.88742 |
| 00.16 | 0.00000 | 0.92524 | 0.91228 | 0.90492 | 0.89800 | 0.89111 | 0.88443 | 0.87800 | 0.87179 |
| 00.18 | 0.00000 | 0.91477 | 0.90053 | 0.89257 | 0.88509 | 0.87760 | 0.87033 | 0.86332 | 0.85652 |
| 00.20 | 0.00000 | 0.90418 | 0.88880 | 0.88035 | 0.87238 | 0.86436 | 0.85654 | 0.84898 | 0.84163 |
| 00.22 | 0.00000 | 0.89352 | 0.87713 | 0.86828 | 0.85991 | 0.85141 | 0.84308 | 0.83500 | 0.82713 |
| 00.24 | 0.00000 | 0.88282 | 0.86555 | 0.85641 | 0.84769 | 0.83876 | 0.82996 | 0.82139 | 0.81301 |
| 00.26 | 0.00000 | 0.87210 | 0.85410 | 0.84475 | 0.83574 | 0.82642 | 0.81718 | 0.80814 | 0.79926 |
| 00.28 | 0.00000 | 0.86139 | 0.84279 | 0.83332 | 0.82408 | 0.81440 | 0.80474 | 0.79523 | 0.78587 |
| 00.30 | 0.00000 | 0.95071 | 0.83165 | 0.82214 | 0.81271 | 0.80269 | 0.79263 | 0.78266 | 0.77282 |
| 00.34 | 0.00000 | 0.82949 | 0.80992 | 0.80052 | 0.79083 | 0.78020 | 0.76934 | 0.75848 | 0.74769 |
| 00.38 | 0.00000 | 0.80858 | 0.78899 | 0.77994 | 0.77007 | 0.75887 | 0.74722 | 0.73546 | 0.72373 |
| 00.42 | 0.00000 | 0.78807 | 0.76892 | 0.76038 | 0.75038 | 0.73860 | 0.72614 | 0.71349 | 0.70083 |
| 00.46 | 0.00000 | 0.76804 | 0.74972 | 0.74181 | 0.73168 | 0.71929 | 0.70601 | 0.69245 | 0.67890 |
| 00.50 | 0.00000 | 0.74854 | 0.73140 | 0.72417 | 0.71389 | 0.70084 | 0.68671 | 0.67227 | 0.65788 |
| 00.54 | 0.00000 | 0.72961 | 0.71392 | 0.70739 | 0.69690 | 0.68315 | 0.66817 | 0.65289 | 0.63775 |
| 00.58 | 0.00000 | 0.71127 | 0.69727 | 0.69142 | 0.68065 | 0.66616 | 0.65033 | 0.63428 | 0.61848 |
| 00.62 | 0.00000 | 0.69354 | 0.68140 | 0.67617 | 0.66506 | 0.64979 | 0.63316 | 0.61641 | 0.60007 |
| 00.66 | 0.00000 | 0.67642 | 0.66628 | 0.66159 | 0.65005 | 0.63400 | 0.61661 | 0.59929 | 0.58252 |
| 00.70 | 0.00000 | 0.65991 | 0.65195 | 0.64762 | 0.63557 | 0.61874 | 0.60069 | 0.58292 | 0.56583 |
| 00.78 | 0.00000 | 0.62870 | 0.62491 | 0.62124 | 0.60802 | 0.58976 | 0.57073 | 0.55242 | 0.53490 |
| 00.86 | 0.00000 | 0.59981 | 0.60021 | 0.59664 | 0.58213 | 0.56278 | 0.54333 | 0.52485 | 0.50694 |
| 00.94 | 0.00000 | 0.57311 | 0.57740 | 0.57350 | 0.55777 | 0.53786 | 0.51849 | 0.49995 | 0.48145 |
| 01.02 | 0.00000 | 0.54844 | 0.55620 | 0.55160 | 0.53493 | 0.51509 | 0.49609 | 0.47731 | 0.45798 |
| 01.10 | 0.00000 | 0.52566 | 0.53636 | 0.53082 | 0.51367 | 0.49448 | 0.47585 | 0.45652 | 0.43612 |
| 01.18 | 0.00000 | 0.50461 | 0.51766 | 0.51107 | 0.49409 | 0.47596 | 0.45741 | 0.43719 | 0.41561 |
| 01.26 | 0.00000 | 0.50000 | 0.49995 | 0.49238 | 0.47628 | 0.45930 | 0.44042 | 0.41906 | 0.39628 |
| 01.34 | 0.00000 | 0.50000 | 0.48309 | 0.47479 | 0.46026 | 0.44420 | 0.42458 | 0.40194 | 0.37801 |
| 01.42 | 0.00000 | 0.50000 | 0.46699 | 0.45837 | 0.44596 | 0.43038 | 0.40965 | 0.38569 | 0.36073 |
| 01.50 | 0.00000 | 0.50000 | 0.45159 | 0.44323 | 0.43319 | 0.41755 | 0.39549 | 0.37025 | 0.34438 |
| 01.66 | 0.00000 | 0.50000 | 0.42277 | 0.41705 | 0.41136 | 0.39410 | 0.36908 | 0.34156 | 0.31434 |
| 01.82 | 0.00000 | 0.50000 | 0.39654 | 0.39632 | 0.39294 | 0.37273 | 0.34486 | 0.31558 | 0.28759 |
| 01.98 | 0.00000 | 0.50000 | 0.37307 | 0.38021 | 0.37659 | 0.35292 | 0.32259 | 0.29212 | 0.26384 |
| 02.14 | 0.00000 | 0.50000 | 0.35267 | 0.36742 | 0.36151 | 0.33441 | 0.30215 | 0.27098 | 0.24280 |
| 02.30 | 0.00000 | 0.50000 | 0.33560 | 0.35674 | 0.34730 | 0.31711 | 0.28341 | 0.25196 | 0.22416 |
| 02.46 | 0.00000 | 0.50000 | 0.33333 | 0.34727 | 0.33379 | 0.30095 | 0.26628 | 0.23486 | 0.20764 |
| 02.62 | 0.00000 | 0.50000 | 0.33333 | 0.33849 | 0.32089 | 0.28586 | 0.25061 | 0.21948 | 0.19297 |
| 02.78 | 0.00000 | 0.50000 | 0.33333 | 0.33011 | 0.30857 | 0.27180 | 0.23629 | 0.20563 | 0.17990 |
| 02.94 | 0.00000 | 0.50000 | 0.33333 | 0.32198 | 0.29681 | 0.25871 | 0.22319 | 0.19313 | 0.16823 |
| 03.10 | 0.00000 | 0.50000 | 0.33333 | 0.31403 | 0.28559 | 0.24652 | 0.21120 | 0.18182 | 0.15777 |
| 03.42 | 0.00000 | 0.50000 | 0.33333 | 0.29859 | 0.26478 | 0.22462 | 0.19011 | 0.16223 | 0.13984 |
| 03.74 | 0.00000 | 0.50000 | 0.33333 | 0.28379 | 0.24597 | 0.20558 | 0.17224 | 0.14590 | 0.12508 |
| 04.06 | 0.00000 | 0.50000 | 0.33333 | 0.26971 | 0.22902 | 0.18896 | 0.15696 | 0.13214 | 0.11276 |
| 04.38 | 0.00000 | 0.50000 | 0.33333 | 0.25643 | 0.21375 | 0.17441 | 0.14380 | 0.12500 | 0.11111 |
| 04.70 | 0.00000 | 0.50000 | 0.33333 | 0.25000 | 0.20001 | 0.16667 | 0.14286 | 0.12500 | 0.11111 |
| 05.02 | 0.00000 | 0.50000 | 0.33333 | 0.25000 | 0.20000 | 0.16667 | 0.14286 | 0.12500 | 0.11111 |

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U(X) X          HE  2   LI  3   BE  4   B   5   C   6   N   7   O   8   F   9
 05.34 0.00000 0.50000 0.33333 0.25000 0.20000 0.16667 0.14286 0.12500 0.11111
 05.66 0.00000 0.50000 0.33333 0.25000 0.20000 0.16667 0.14286 0.12500 0.11111
 05.98 0.00000 0.50000 0.33333 0.25000 0.20000 0.16667 0.14286 0.12500 0.11111
 SHELL (1S) 0  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  0.      1.721   4.398   8.698   14.373  21.378  29.737  39.456  50.538
 SHELL (2S) 0  (2S) 0  (2S) 1  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  0.      0.      .4039   .6012   0.9239  1.2895  1.6959  2.1440  2.6349
 SHELL (2P) 0  (2P) 0  (2P) 0  (2P) 0  (2P) 1  (2P) 2  (2P) 3  (2P) 4  (2P) 5
 (-E)  0.      0.      0.      0.      0.4898  0.6603  0.8445  1.0409  1.2502
U(X) X NE 10   NA 11   MG 12   AL 13   SI 14   P  15   S  16   CL 17   A  18
   X    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
 00.01 0.99205 0.99186 0.99170 0.99157 0.99144 0.99131 0.99119 0.99106 0.99094
 00.02 0.98387 0.98349 0.98317 0.98291 0.98265 0.98239 0.98213 0.98188 0.98164
 00.03 0.97552 0.97496 0.97448 0.97408 0.97369 0.97330 0.97292 0.97255 0.97218
 00.04 0.96705 0.96630 0.96567 0.96515 0.96463 0.96412 0.96363 0.96314 0.96266
 00.05 0.95850 0.95758 0.95680 0.95616 0.95552 0.95490 0.95429 0.95370 0.95311
 00.06 0.94990 0.94881 0.94790 0.94715 0.94641 0.94568 0.94497 0.94427 0.94359
 00.07 0.94128 0.94003 0.93900 0.93815 0.93731 0.93649 0.93569 0.93490 0.93413
 00.08 0.93266 0.93127 0.93012 0.92919 0.92827 0.92736 0.92648 0.92561 0.92475
 00.09 0.92407 0.92255 0.92130 0.92029 0.91929 0.91831 0.91735 0.91641 0.91549
 00.10 0.91553 0.91388 0.91254 0.91147 0.91041 0.90936 0.90834 0.90733 0.90634
 00.12 0.89862 0.89677 0.89528 0.89411 0.89294 0.89179 0.89066 0.88954 0.88844
 00.14 0.88202 0.88001 0.87841 0.87717 0.87593 0.87470 0.87348 0.87228 0.87109
 00.16 0.86578 0.86364 0.86197 0.86069 0.85940 0.85811 0.85683 0.85556 0.85429
 00.18 0.84994 0.84770 0.84598 0.84468 0.84335 0.84202 0.84069 0.83936 0.83802
 00.20 0.83451 0.83219 0.83043 0.82913 0.82778 0.82642 0.82504 0.82366 0.82227
 00.22 0.81947 0.81709 0.81532 0.81402 0.81266 0.81127 0.80987 0.80844 0.80700
 00.24 0.80484 0.80241 0.80062 0.79934 0.79798 0.79657 0.79514 0.79368 0.79220
 00.26 0.79058 0.78811 0.78632 0.78506 0.78370 0.78229 0.78083 0.77935 0.77785
 00.28 0.77670 0.77419 0.77240 0.77117 0.76982 0.76840 0.76694 0.76545 0.76393
 00.30 0.76316 0.76062 0.75884 0.75764 0.75631 0.75491 0.75345 0.75196 0.75044
 00.34 0.73706 0.73447 0.73274 0.73164 0.73038 0.72904 0.72764 0.72620 0.72473
 00.38 0.71215 0.70956 0.70791 0.70696 0.70584 0.70463 0.70335 0.70203 0.70066
 00.42 0.68835 0.68580 0.68430 0.68357 0.68267 0.68165 0.68056 0.67940 0.67816
 00.46 0.66558 0.66316 0.66187 0.66145 0.66083 0.66007 0.65920 0.65821 0.65710
 00.50 0.64381 0.64160 0.64063 0.64058 0.64028 0.63980 0.63915 0.63832 0.63732
 00.54 0.62303 0.62112 0.62053 0.62091 0.62096 0.62074 0.62028 0.61958 0.61866
 00.58 0.60322 0.60170 0.60155 0.60236 0.60274 0.60276 0.60246 0.60186 0.60097
 00.62 0.58438 0.58331 0.58360 0.58483 0.58551 0.58574 0.58556 0.58502 0.58416
 00.66 0.56648 0.56589 0.56662 0.56823 0.56917 0.56955 0.56947 0.56899 0.56814
 00.70 0.54948 0.54937 0.55050 0.55245 0.55361 0.55413 0.55413 0.55368 0.55285
 00.78 0.51795 0.51868 0.52049 0.52300 0.52452 0.52527 0.52542 0.52506 0.52427
 00.86 0.48923 0.49063 0.49296 0.49595 0.49779 0.49878 0.49910 0.49885 0.49813
 00.94 0.46280 0.46473 0.46750 0.47096 0.47316 0.47442 0.47494 0.47483 0.47416
 01.02 0.43822 0.44063 0.44387 0.44784 0.45043 0.45200 0.45274 0.45276 0.45214
 01.10 0.41523 0.41815 0.42190 0.42643 0.42947 0.43137 0.43233 0.43246 0.43184
 01.18 0.39363 0.39714 0.40148 0.40663 0.41014 0.41237 0.41353 0.41372 0.41304
 01.26 0.37332 0.37752 0.38251 0.38833 0.39232 0.39486 0.39615 0.39634 0.39553
 01.34 0.35422 0.35922 0.36492 0.37142 0.37587 0.37867 0.38004 0.38016 0.37916
 01.42 0.33627 0.34216 0.34861 0.35578 0.36066 0.36366 0.36504 0.36502 0.36377
 01.50 0.31941 0.32627 0.33349 0.34132 0.34657 0.34969 0.35102 0.35080 0.34927
 01.66 0.28880 0.29777 0.30650 0.31549 0.32127 0.32444 0.32546 0.32473 0.32262
 01.82 0.26198 0.27315 0.28323 0.29313 0.29915 0.30210 0.30266 0.30140 0.29887
 01.98 0.23853 0.25186 0.26306 0.27356 0.27955 0.28212 0.28220 0.28058 0.27789
 02.14 0.21805 0.23338 0.24541 0.25623 0.26199 0.26414 0.26389 0.26217 0.25953
 02.30 0.20015 0.21726 0.22983 0.24074 0.24617 0.24799 0.24764 0.24603 0.24348
 02.46 0.18447 0.20310 0.21594 0.22677 0.23189 0.23357 0.23335 0.23190 0.22926
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U(X) X NE 10   NA 11   MG 12   AL 13   SI 14   P  15   S  16   CL 17   A  18
 02.62 0.17068 0.19057 0.20345 0.21412 0.21905 0.22082 0.22083 0.21940 0.21645
 02.78 0.15851 0.17939 0.19215 0.20267 0.20758 0.20961 0.20980 0.20817 0.20468
 02.94 0.14773 0.16933 0.18188 0.19233 0.19743 0.19977 0.19995 0.19790 0.19376
 03.10 0.13812 0.16022 0.17251 0.18305 0.18849 0.19106 0.19102 0.18838 0.18354
 03.42 0.12180 0.14431 0.15626 0.16746 0.17369 0.17617 0.17509 0.17107 0.16493
 03.74 0.10847 0.13086 0.14301 0.15534 0.16187 0.16348 0.16102 0.15567 0.14852
 04.06 0.10000 0.11941 0.13248 0.14583 0.15193 0.15222 0.14837 0.14194 0.13412
 04.38 0.10000 0.10971 0.12425 0.13807 0.14314 0.14200 0.13695 0.12973 0.12152
 04.70 0.10000 0.10162 0.11781 0.13142 0.13516 0.13266 0.12664 0.11889 0.11053
 05.02 0.10000 0.09505 0.11263 0.12547 0.12779 0.12411 0.11736 0.10930 0.10094
 05.34 0.10000 0.09091 0.10829 0.11999 0.12094 0.11628 0.10901 0.10080 0.09255
 05.66 0.10000 0.09091 0.10449 0.11487 0.11457 0.10911 0.10148 0.09324 0.08517
 05.98 0.10000 0.09091 0.10105 0.11003 0.10864 0.10255 0.09470 0.08652 0.07866
 06.30 0.10000 0.09091 0.09784 0.10546 0.10311 0.09655 0.08858 0.08050 0.07289
 06.94 0.10000 0.09091 0.09191 0.09701 0.09317 0.08599 0.07799 0.07023 0.06311
 07.58 0.10000 0.09091 0.08646 0.08941 0.08454 0.07706 0.06921 0.06182 0.05556
 08.22 0.10000 0.09091 0.08333 0.08261 0.07704 0.06947 0.06250 0.05882 0.05556
 08.86 0.10000 0.09091 0.08333 0.07692 0.07143 0.06667 0.06250 0.05882 0.05556
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  62.99   78.05   94.95   113.66  134.04  156.11  179.89  205.36  232.54
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  2.168   4.723   6.552   8.715   11.087  13.684  16.510  19.570  22.865
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  1.471   2.669   4.144   5.947   7.954   10.180  12.628  15.303  18.207
 SHELL (3S) 0  (3S) 1  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  0.      0.3777  0.5051  0.7445  0.9975  1.2588  1.5300  1.8124  2.1068
 SHELL (3P) 0  (3P) 0  (3P) 0  (3P) 1  (3P) 2  (3P) 3  (3P) 4  (3P) 5  (3P) 6
U(X) X K  19   CA 20   SC 21   TI 22   V  23   CR 24   MN 25   FE 26   CO 27
 (-E)  0.      0.      0.      0.3582  0.4802  0.6139  0.7462  0.9067  1.0653
   X    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
 00.01 0.99088 0.99082 0.99073 0.99064 0.99055 0.99043 0.99037 0.99027 0.99018
 00.02 0.98151 0.98140 0.98122 0.98104 0.98086 0.98063 0.98049 0.98030 0.98012
 00.03 0.97200 0.97184 0.97158 0.97131 0.97104 0.97069 0.97049 0.97021 0.96994
 00.04 0.96242 0.96221 0.96187 0.96152 0.96117 0.96071 0.96046 0.96009 0.95974
 00.05 0.95283 0.95258 0.95217 0.95175 0.95132 0.95076 0.95046 0.95002 0.94959
 00.06 0.94327 0.94299 0.94252 0.94203 0.94154 0.94089 0.94055 0.94003 0.93953
 00.07 0.93378 0.93348 0.93296 0.93241 0.93186 0.93112 0.93074 0.93016 0.92960
 00.08 0.92439 0.92408 0.92350 0.92291 0.92230 0.92148 0.92108 0.92043 0.91982
 00.09 0.91511 0.91479 0.91418 0.91354 0.91288 0.91199 0.91156 0.91086 0.91020
 00.10 0.90596 0.90564 0.90499 0.90431 0.90362 0.90265 0.90221 0.90146 0.90075
 00.12 0.88807 0.88777 0.88706 0.88632 0.88555 0.88446 0.88398 0.88314 0.88234
 00.14 0.87074 0.87048 0.86973 0.86894 0.86811 0.86690 0.86640 0.86548 0.86460
 00.16 0.85398 0.85377 0.85299 0.85215 0.85127 0.84994 0.84944 0.84844 0.84748
 00.18 0.83777 0.83761 0.83680 0.83593 0.83500 0.83357 0.83306 0.83199 0.83097
 00.20 0.82207 0.82197 0.82116 0.82025 0.81929 0.81775 0.81725 0.81611 0.81503
 00.22 0.80687 0.80685 0.80602 0.80509 0.80410 0.80247 0.80198 0.80079 0.79966
 00.24 0.79214 0.79220 0.79138 0.79044 0.78943 0.78771 0.78725 0.78601 0.78484
 00.26 0.77788 0.77803 0.77722 0.77628 0.77526 0.77347 0.77304 0.77177 0.77056
 00.28 0.76406 0.76432 0.76353 0.76261 0.76159 0.75974 0.75935 0.75805 0.75681
 00.30 0.75069 0.75107 0.75032 0.74942 0.74841 0.74650 0.74616 0.74483 0.74357
 00.34 0.72525 0.72592 0.72527 0.72444 0.72346 0.72144 0.72121 0.71983 0.71850
 00.38 0.70150 0.70249 0.70196 0.70120 0.70025 0.69811 0.69796 0.69650 0.69510
 00.42 0.67934 0.68064 0.68022 0.67951 0.67857 0.67626 0.67618 0.67462 0.67309
 00.46 0.65860 0.66019 0.65985 0.65916 0.65819 0.65570 0.65565 0.65396 0.65231
 00.50 0.63911 0.64096 0.64066 0.63996 0.63895 0.63625 0.63622 0.63439 0.63259
 00.54 0.62070 0.62280 0.62252 0.62179 0.62071 0.61778 0.61777 0.61579 0.61384
 00.58 0.60326 0.60557 0.60530 0.60453 0.60337 0.60022 0.60022 0.59809 0.59599
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U(X) X K  19   CA 20   SC 21   TI 22   V  23   CR 24   MN 25   FE 26   CO 27
 00.62 0.58667 0.58920 0.58892 0.58811 0.58688 0.58350 0.58350 0.58123 0.57898
 00.66 0.57087 0.57361 0.57333 0.57247 0.57116 0.56755 0.56756 0.56513 0.56273
 00.70 0.55580 0.55875 0.55847 0.55756 0.55617 0.55232 0.55234 0.54976 0.54720
 00.78 0.52767 0.53105 0.53076 0.52975 0.52819 0.52385 0.52386 0.52096 0.51807
 00.86 0.50199 0.50578 0.50546 0.50432 0.50256 0.49771 0.49768 0.49443 0.49120
 00.94 0.47847 0.48265 0.48226 0.48095 0.47894 0.47355 0.47346 0.46985 0.46627
 01.02 0.45685 0.46137 0.46085 0.45933 0.45705 0.45109 0.45092 0.44696 0.44307
 01.10 0.43690 0.44169 0.44100 0.43922 0.43664 0.43013 0.42989 0.42562 0.42145
 01.18 0.41837 0.42337 0.42246 0.42041 0.41754 0.41051 0.41025 0.40571 0.40133
 01.26 0.40109 0.40624 0.40510 0.40279 0.39965 0.39216 0.39192 0.38719 0.38263
 01.34 0.38488 0.39016 0.38880 0.38626 0.38292 0.37502 0.37487 0.36998 0.36528
 01.42 0.36963 0.37504 0.37349 0.37078 0.36730 0.35905 0.35902 0.35399 0.34913
 01.50 0.35526 0.36082 0.35914 0.35633 0.35277 0.34420 0.34429 0.33910 0.33405
 01.66 0.32898 0.33502 0.33327 0.33040 0.32671 0.31744 0.31768 0.31207 0.30657
 01.82 0.30584 0.31261 0.31092 0.30794 0.30399 0.29387 0.29410 0.28796 0.28197
 01.98 0.28571 0.29324 0.29147 0.28819 0.28378 0.27269 0.27282 0.26617 0.25974
 02.14 0.26821 0.27632 0.27423 0.27043 0.26545 0.25341 0.25344 0.24637 0.23963
 02.30 0.25281 0.26122 0.25859 0.25420 0.24865 0.23576 0.23576 0.22839 0.22145
 02.46 0.23897 0.24744 0.24421 0.23923 0.23318 0.21957 0.21963 0.21208 0.20507
 02.62 0.22632 0.23471 0.23088 0.22539 0.21893 0.20476 0.20494 0.19733 0.19034
 02.78 0.21459 0.22286 0.21850 0.21258 0.20583 0.19124 0.19160 0.18401 0.17710
 02.94 0.20366 0.21181 0.20698 0.20074 0.19379 0.17891 0.17948 0.17198 0.16520
 03.10 0.19343 0.20148 0.19629 0.18981 0.18275 0.16768 0.16849 0.16111 0.15451
 03.42 0.17493 0.18287 0.17717 0.17043 0.16332 0.14817 0.14943 0.14240 0.13619
 03.74 0.15880 0.16667 0.16070 0.15391 0.14692 0.13199 0.13361 0.12698 0.12118
 04.06 0.14478 0.15257 0.14648 0.13977 0.13300 0.11848 0.12037 0.11415 0.10877
 04.38 0.13258 0.14022 0.13413 0.12759 0.12110 0.10712 0.10918 0.10338 0.09839
 04.70 0.12193 0.12934 0.12334 0.11703 0.11085 0.09750 0.09968 0.09427 0.08966
 05.02 0.11259 0.11969 0.11386 0.10783 0.10200 0.08929 0.09156 0.08653 0.08226
 05.34 0.10433 0.11110 0.10551 0.09981 0.09434 0.08225 0.08461 0.07993 0.07597
 05.66 0.09698 0.10346 0.09817 0.09283 0.08771 0.07618 0.07865 0.07429 0.07060
 05.98 0.09039 0.09667 0.09174 0.08676 0.08199 0.07094 0.07353 0.06945 0.06601
 06.30 0.08445 0.09067 0.08613 0.08151 0.07705 0.06639 0.06913 0.06528 0.06205
 06.94 0.07425 0.08087 0.07708 0.07305 0.06910 0.05897 0.06199 0.05853 0.05562
 07.58 0.06596 0.07359 0.07034 0.06669 0.06306 0.05327 0.05649 0.05330 0.05061
 08.22 0.05937 0.06822 0.06521 0.06174 0.05829 0.04880 0.05208 0.04909 0.04657
 08.86 0.05431 0.06413 0.06113 0.05772 0.05436 0.04521 0.04841 0.04559 0.04321
 09.50 0.05263 0.06083 0.05771 0.05430 0.05101 0.04226 0.04527 0.04258 0.04032
 10.14 0.05263 0.05798 0.05471 0.05129 0.04805 0.04167 0.04252 0.03995 0.03781
 10.78 0.05263 0.05543 0.05201 0.04858 0.04541 0.04167 0.04008 0.03846 0.03704
 11.42 0.05263 0.05306 0.04953 0.04611 0.04348 0.04167 0.04000 0.03846 0.03704
 12.06 0.05263 0.05085 0.04762 0.04545 0.04348 0.04167 0.04000 0.03846 0.03704
 12.70 0.05263 0.05000 0.04762 0.04545 0.04348 0.04167 0.04000 0.03846 0.03704
 13.98 0.05263 0.05000 0.04762 0.04545 0.04348 0.04167 0.04000 0.03846 0.03704
 15.26 0.05263 0.05000 0.04762 0.04545 0.04348 0.04167 0.04000 0.03846 0.03704
 16.54 0.05263 0.05000 0.04762 0.04545 0.04348 0.04167 0.04000 0.03846 0.03704
 17.82 0.05263 0.05000 0.04762 0.04545 0.04348 0.04167 0.04000 0.03846 0.03704
 SHELL (1S) 2   (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  262.09   293.52  326.29  360.77  396.95  434.45  474.47  515.81  558.89
 SHELL (2S) 2   (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  27.060   31.627  35.973  40.521  45.289  49.823  55.509  60.957  66.648
 SHELL (2P) 6   (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  22.008   26.180  30.130  34.279  38.646  42.779  48.050  53.084  58.358
 SHELL (3S) 2   (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  2.9521   3.8750  4.4308  4.9813  5.5371  5.7114  6.6804  7.2691  7.8785
 SHELL (3P) 6   (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  1.7328   2.4823  2.8831  3.2760  3.6704  3.6910  4.4776  4.8912  5.3200
 SHELL (3D) 0   (3D) 0  (3D) 1  (3D) 2  (3D) 3  (3D) 4  (3D) 5  (3D) 6  (3D) 7
```

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| (-E) | 0. | 0. | 0.5308 | 0.6279 | 0.7183 | 0.4789 | 0.8859 | 0.9625 | 1.0415 |
| SHELL | (4S) 1 | (4S) 2 | (4S) 2 | (4S) 2 | (4S) 2 | (4S) 1 | (4S) 2 | (4S) 2 | (4S) 2 |
| (-E) | 0.3086 | 0.3987 | 0.4309 | 0.4578 | 0.4819 | 0.4312 | 0.5253 | 0.5451 | 0.5647 |
| U(X) X | NI 28 | CU 29 | ZN 30 | GA 31 | GE 32 | AS 33 | SE 34 | BR 35 | KR 36 |
| X | U(X) | U(X) | U(X) | U(X) | U(X) | U(X) | U(X) | U(X) | U(X) |
| 00.00 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 |
| 00.01 | 0.99009 | 0.98997 | 0.98990 | 0.98984 | 0.98979 | 0.98973 | 0.98968 | 0.98963 | 0.98958 |
| 00.02 | 0.97993 | 0.97969 | 0.97956 | 0.97945 | 0.97933 | 0.97923 | 0.97912 | 0.97902 | 0.97892 |
| 00.03 | 0.96966 | 0.96931 | 0.96912 | 0.96895 | 0.96879 | 0.96863 | 0.96848 | 0.96833 | 0.96819 |
| 00.04 | 0.95938 | 0.95892 | 0.95867 | 0.95846 | 0.95825 | 0.95805 | 0.95786 | 0.95767 | 0.95748 |
| 00.05 | 0.94915 | 0.94859 | 0.94829 | 0.94803 | 0.94779 | 0.94755 | 0.94732 | 0.94710 | 0.94688 |
| 00.06 | 0.93903 | 0.93837 | 0.93802 | 0.93773 | 0.93745 | 0.93719 | 0.93693 | 0.93667 | 0.93642 |
| 00.07 | 0.92903 | 0.92828 | 0.92789 | 0.92758 | 0.92727 | 0.92698 | 0.92669 | 0.92641 | 0.92614 |
| 00.08 | 0.91919 | 0.91835 | 0.91793 | 0.91759 | 0.91726 | 0.91695 | 0.91664 | 0.91634 | 0.91604 |
| 00.09 | 0.90951 | 0.90859 | 0.90814 | 0.90778 | 0.90743 | 0.90710 | 0.90677 | 0.90645 | 0.90613 |
| 00.10 | 0.90001 | 0.89901 | 0.89853 | 0.89815 | 0.89778 | 0.89743 | 0.89709 | 0.89675 | 0.89642 |
| 00.12 | 0.88151 | 0.88036 | 0.87983 | 0.87943 | 0.87903 | 0.87865 | 0.87828 | 0.87792 | 0.87756 |
| 00.14 | 0.86367 | 0.86238 | 0.86182 | 0.86139 | 0.86096 | 0.86057 | 0.86018 | 0.85979 | 0.85941 |
| 00.16 | 0.84648 | 0.84504 | 0.84445 | 0.84400 | 0.84356 | 0.84315 | 0.84274 | 0.84235 | 0.84195 |
| 00.18 | 0.82988 | 0.82832 | 0.82769 | 0.82724 | 0.82679 | 0.82638 | 0.82596 | 0.82556 | 0.82516 |
| 00.20 | 0.81388 | 0.81218 | 0.81154 | 0.81108 | 0.81063 | 0.81023 | 0.80981 | 0.80941 | 0.80902 |
| 00.22 | 0.79844 | 0.79663 | 0.79598 | 0.79553 | 0.79509 | 0.79469 | 0.79429 | 0.79390 | 0.79352 |
| 00.24 | 0.78357 | 0.78165 | 0.78099 | 0.78056 | 0.78013 | 0.77975 | 0.77937 | 0.77899 | 0.77862 |
| 00.26 | 0.76925 | 0.76722 | 0.76657 | 0.76615 | 0.76575 | 0.76538 | 0.76502 | 0.76466 | 0.76430 |
| 00.28 | 0.75546 | 0.75333 | 0.75268 | 0.75229 | 0.75190 | 0.75156 | 0.75120 | 0.75085 | 0.75051 |
| 00.30 | 0.74218 | 0.73994 | 0.73930 | 0.73892 | 0.73855 | 0.73822 | 0.73788 | 0.73754 | 0.73719 |
| 00.34 | 0.71702 | 0.71456 | 0.71390 | 0.71355 | 0.71319 | 0.71287 | 0.71253 | 0.71219 | 0.71184 |
| 00.38 | 0.69350 | 0.69077 | 0.69009 | 0.68973 | 0.68936 | 0.68903 | 0.68868 | 0.68833 | 0.68796 |
| 00.42 | 0.67135 | 0.66835 | 0.66761 | 0.66724 | 0.66685 | 0.66650 | 0.66613 | 0.66575 | 0.66536 |
| 00.46 | 0.65040 | 0.64711 | 0.64631 | 0.64591 | 0.64549 | 0.64513 | 0.64473 | 0.64434 | 0.64393 |
| 00.50 | 0.63052 | 0.62693 | 0.62607 | 0.62564 | 0.62520 | 0.62481 | 0.62439 | 0.62398 | 0.62355 |
| 00.54 | 0.61161 | 0.60771 | 0.60679 | 0.60633 | 0.60587 | 0.60546 | 0.60503 | 0.60459 | 0.60415 |
| 00.58 | 0.59359 | 0.58939 | 0.58840 | 0.58792 | 0.58743 | 0.58701 | 0.58656 | 0.58611 | 0.58564 |
| 00.62 | 0.57640 | 0.57189 | 0.57085 | 0.57034 | 0.56983 | 0.56939 | 0.56892 | 0.56845 | 0.56796 |
| 00.66 | 0.55998 | 0.55517 | 0.55406 | 0.55352 | 0.55299 | 0.55253 | 0.55204 | 0.55155 | 0.55105 |
| 00.70 | 0.54427 | 0.53915 | 0.53797 | 0.53742 | 0.53686 | 0.53637 | 0.53587 | 0.53537 | 0.53486 |
| 00.78 | 0.51478 | 0.50905 | 0.50773 | 0.50712 | 0.50652 | 0.50600 | 0.50548 | 0.50497 | 0.50445 |
| 00.86 | 0.48754 | 0.48120 | 0.47976 | 0.47911 | 0.47848 | 0.47797 | 0.47745 | 0.47697 | 0.47648 |
| 00.94 | 0.46226 | 0.45534 | 0.45380 | 0.45315 | 0.45255 | 0.45207 | 0.45161 | 0.45120 | 0.45078 |
| 01.02 | 0.43874 | 0.43128 | 0.42969 | 0.42909 | 0.42856 | 0.42818 | 0.42781 | 0.42749 | 0.42717 |
| 01.10 | 0.41686 | 0.40892 | 0.40733 | 0.40683 | 0.40640 | 0.40612 | 0.40586 | 0.40564 | 0.40540 |
| 01.18 | 0.39653 | 0.38816 | 0.38660 | 0.38621 | 0.38590 | 0.38573 | 0.38556 | 0.38542 | 0.38525 |
| 01.26 | 0.37765 | 0.36888 | 0.36736 | 0.36708 | 0.36687 | 0.36678 | 0.36669 | 0.36662 | 0.36651 |
| 01.34 | 0.36013 | 0.35093 | 0.34944 | 0.34926 | 0.34913 | 0.34911 | 0.34909 | 0.34908 | 0.34902 |
| 01.42 | 0.34379 | 0.33416 | 0.33267 | 0.33257 | 0.33251 | 0.33257 | 0.33261 | 0.33266 | 0.33266 |
| 01.50 | 0.32850 | 0.31841 | 0.31692 | 0.31689 | 0.31691 | 0.31703 | 0.31715 | 0.31728 | 0.31736 |
| 01.66 | 0.30054 | 0.28955 | 0.28805 | 0.28819 | 0.28840 | 0.28872 | 0.28905 | 0.28939 | 0.28967 |
| 01.82 | 0.27547 | 0.26368 | 0.26225 | 0.26265 | 0.26314 | 0.26374 | 0.26434 | 0.26495 | 0.26547 |
| 01.98 | 0.25289 | 0.24044 | 0.23919 | 0.23996 | 0.24081 | 0.24176 | 0.24268 | 0.24356 | 0.24431 |
| 02.14 | 0.23254 | 0.21962 | 0.21864 | 0.21986 | 0.22113 | 0.22245 | 0.22369 | 0.22483 | 0.22577 |
| 02.30 | 0.21427 | 0.20102 | 0.20039 | 0.20211 | 0.20382 | 0.20549 | 0.20702 | 0.20836 | 0.20943 |
| 02.46 | 0.19789 | 0.18445 | 0.18422 | 0.18644 | 0.18857 | 0.19057 | 0.19232 | 0.19380 | 0.19492 |
| 02.62 | 0.18325 | 0.16972 | 0.16990 | 0.17262 | 0.17513 | 0.17739 | 0.17930 | 0.18085 | 0.18195 |
| 02.78 | 0.17015 | 0.15664 | 0.15721 | 0.16039 | 0.16323 | 0.16568 | 0.16769 | 0.16924 | 0.17029 |
| 02.94 | 0.15844 | 0.14501 | 0.14596 | 0.14955 | 0.15265 | 0.15524 | 0.15728 | 0.15879 | 0.15976 |
| 03.10 | 0.14795 | 0.13467 | 0.13595 | 0.13989 | 0.14320 | 0.14586 | 0.14790 | 0.14934 | 0.15022 |
| 03.42 | 0.13008 | 0.11722 | 0.11904 | 0.12354 | 0.12709 | 0.12977 | 0.13171 | 0.13301 | 0.13376 |
| 03.74 | 0.11553 | 0.10322 | 0.10541 | 0.11027 | 0.11390 | 0.11652 | 0.11835 | 0.11956 | 0.12024 |

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U(X) X NI 28   CU 29   ZN 30   GA 31   GE 32   AS 33   SE 34   BR 35   KR 36
 04.06 0.10355 0.09185 0.09427 0.09936 0.10299 0.10553 0.10730 0.10845 0.10906
 04.38 0.09358 0.08251 0.08507 0.09030 0.09390 0.09639 0.09812 0.09920 0.09965
 04.70 0.08521 0.07475 0.07740 0.08272 0.08630 0.08876 0.09042 0.09135 0.09154
 05.02 0.07815 0.06825 0.07095 0.07634 0.07991 0.08232 0.08385 0.08454 0.08441
 05.34 0.07217 0.06276 0.06551 0.07095 0.07449 0.07681 0.07813 0.07852 0.07807
 05.66 0.06707 0.05807 0.06088 0.06636 0.06985 0.07201 0.07308 0.07315 0.07238
 05.98 0.06270 0.05406 0.05692 0.06241 0.06581 0.06776 0.06855 0.06831 0.06725
 06.30 0.05894 0.05058 0.05350 0.05898 0.06224 0.06396 0.06445 0.06392 0.06263
 06.94 0.05282 0.04492 0.04792 0.05328 0.05619 0.05738 0.05732 0.05631 0.05466
 07.58 0.04804 0.04052 0.04355 0.04867 0.05116 0.05185 0.05132 0.04997 0.04811
 08.22 0.04418 0.03703 0.04001 0.04482 0.04687 0.04711 0.04623 0.04465 0.04268
 08.86 0.04095 0.03448 0.03706 0.04151 0.04314 0.04302 0.04187 0.04014 0.03811
 09.50 0.03820 0.03448 0.03454 0.03861 0.03988 0.03945 0.03811 0.03628 0.03424
 10.14 0.03580 0.03448 0.03333 0.03605 0.03699 0.03632 0.03483 0.03294 0.03092
 10.78 0.03571 0.03448 0.03333 0.03376 0.03442 0.03356 0.03196 0.03004 0.02805
 11.42 0.03571 0.03448 0.03333 0.03226 0.03214 0.03111 0.02944 0.02857 0.02778
 12.06 0.03571 0.03448 0.03333 0.03226 0.03125 0.03030 0.02941 0.02857 0.02778
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  603.7   649.7   698.4   749.2   801.8   856.3   912.5   970.7   1030.6
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  72.57   78.15   85.12   92.64   100.51  108.73  117.30  126.24  135.53
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  63.86   69.02   75.55   82.63   90.05   97.82   105.95  114.43  123.25
 SHELL (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  3(S) 2  (3S) 2  (3S) 2
 (-E)  8.500   8.634   9.793   11.238  12.762  14.375  16.074  17.857  19.728
 SHELL (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  5.756   5.709   6.661   7.892   9.197   10.587  12.058  13.611  15.249
 SHELL (3D) 8  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10
 (-E)  1.1151  0.7431  1.2582  2.0400  2.8901  3.8229  4.8340  5.9245  7.0975
 SHELL (4S) 2  (4S) 1  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2
 (-E)  0.5831  0.5091  0.6185  0.8377  1.0571  1.2754  1.4953  1.7185  1.9456
 SHELL (4P) 0  (4P) 0  (4P) 0  (4P) 1  (4P) 2  (4P) 3  (4P) 4  (4P) 5  (4P) 6
 (-E)  0.      0.      0.      0.3619  0.4683  0.5826  0.7015  0.8247  0.9519
U(X) X RB 37   SR 38   YT 39   ZR 40   NB 41   MO 42   TC 43   RU 44   RH 45
  X      U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
 00.01 0.98955 0.98952 0.98948 0.98944 0.98940 0.98936 0.98933 0.98928 0.98924
 00.02 0.97886 0.97880 0.97873 0.97866 0.97857 0.97849 0.97844 0.97834 0.97827
 00.03 0.96810 0.96802 0.96792 0.96781 0.96768 0.96757 0.96749 0.96736 0.96725
 00.04 0.95738 0.95728 0.95715 0.95702 0.95685 0.95672 0.95661 0.95644 0.95630
 00.05 0.94676 0.94665 0.94650 0.94635 0.94615 0.94599 0.94588 0.94567 0.94551
 00.06 0.93629 0.93617 0.93601 0.93584 0.93562 0.93544 0.93531 0.93508 0.93490
 00.07 0.92600 0.92588 0.92570 0.92552 0.92528 0.92509 0.92495 0.92469 0.92450
 00.08 0.91590 0.91578 0.91560 0.91540 0.91514 0.91494 0.91480 0.91452 0.91430
 00.09 0.90600 0.90588 0.90569 0.90549 0.90521 0.90499 0.90485 0.90455 0.90433
 00.10 0.89629 0.89617 0.89598 0.89577 0.89548 0.89525 0.89511 0.89479 0.89455
 00.12 0.87744 0.87734 0.87714 0.87692 0.87660 0.87636 0.87623 0.87587 0.87562
 00.14 0.85931 0.85923 0.85903 0.85882 0.85848 0.85823 0.85811 0.85772 0.85745
 00.16 0.84188 0.84182 0.84164 0.84143 0.84107 0.84083 0.84072 0.84031 0.84004
 00.18 0.82512 0.82510 0.82493 0.82474 0.82437 0.82413 0.82405 0.82362 0.82335
 00.20 0.80902 0.80905 0.80890 0.80872 0.80836 0.80814 0.80808 0.80764 0.80738
 00.22 0.79356 0.79364 0.79352 0.79337 0.79301 0.79280 0.79277 0.79232 0.79206
 00.24 0.77872 0.77884 0.77875 0.77863 0.77827 0.77807 0.77807 0.77760 0.77735
 00.26 0.76444 0.76462 0.76456 0.76445 0.76408 0.76389 0.76392 0.76344 0.76317
 00.28 0.75070 0.75091 0.75087 0.75078 0.75041 0.75022 0.75027 0.74976 0.74949
 00.30 0.73742 0.73768 0.73766 0.73757 0.73719 0.73700 0.73706 0.73653 0.73625
 00.34 0.71214 0.71246 0.71246 0.71238 0.71196 0.71177 0.71186 0.71126 0.71095
 00.38 0.68831 0.68869 0.68870 0.68863 0.68817 0.68797 0.68808 0.68742 0.68709
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U(X) X RB 37   SR 38   YT 39   ZR 40   NB 41   MO 42   TC 43   RU 44   RH 45
 00.42 0.66577 0.66620 0.66623 0.66616 0.66566 0.66545 0.66558 0.66486 0.66451
 00.46 0.64438 0.64487 0.64491 0.64486 0.64432 0.64409 0.64426 0.64348 0.64310
 00.50 0.62406 0.62461 0.62467 0.62462 0.62405 0.62381 0.62401 0.62317 0.62278
 00.54 0.60471 0.60532 0.60540 0.60536 0.60475 0.60451 0.60474 0.60385 0.60345
 00.58 0.58626 0.58693 0.58703 0.58700 0.58637 0.58612 0.58638 0.58545 0.58503
 00.62 0.56864 0.56938 0.56949 0.56948 0.56882 0.56858 0.56888 0.56791 0.56749
 00.66 0.55179 0.55259 0.55273 0.55274 0.55206 0.55183 0.55218 0.55117 0.55076
 00.70 0.53566 0.53652 0.53670 0.53673 0.53604 0.53584 0.53624 0.53522 0.53482
 00.78 0.50540 0.50643 0.50670 0.50681 0.50613 0.50600 0.50654 0.50550 0.50516
 00.86 0.47762 0.47886 0.47926 0.47949 0.47885 0.47881 0.47951 0.47846 0.47818
 00.94 0.45215 0.45362 0.45417 0.45453 0.45394 0.45398 0.45483 0.45377 0.45353
 01.02 0.42877 0.43046 0.43116 0.43164 0.43108 0.43119 0.43218 0.43109 0.43088
 01.10 0.40723 0.40914 0.40997 0.41055 0.41000 0.41018 0.41129 0.41016 0.40998
 01.18 0.38728 0.38939 0.39034 0.39102 0.39048 0.39072 0.39195 0.39079 0.39065
 01.26 0.36874 0.37104 0.37211 0.37288 0.37236 0.37266 0.37403 0.37284 0.37273
 01.34 0.35144 0.35395 0.35514 0.35602 0.35552 0.35590 0.35740 0.35619 0.35611
 01.42 0.33530 0.33802 0.33934 0.34033 0.33987 0.34033 0.34196 0.34072 0.34068
 01.50 0.32022 0.32316 0.32463 0.32574 0.32532 0.32585 0.32761 0.32634 0.32632
 01.66 0.29301 0.29642 0.29819 0.29954 0.29918 0.29984 0.30182 0.30044 0.30041
 01.82 0.26930 0.27318 0.27523 0.27678 0.27642 0.27715 0.27928 0.27771 0.27759
 01.98 0.24862 0.25292 0.25518 0.25687 0.25645 0.25715 0.25937 0.25754 0.25727
 02.14 0.23049 0.23514 0.23755 0.23930 0.23872 0.23935 0.24160 0.23947 0.23904
 02.30 0.21449 0.21942 0.22190 0.22364 0.22287 0.22339 0.22566 0.22324 0.22266
 02.46 0.20026 0.20540 0.20792 0.20962 0.20863 0.20903 0.21135 0.20866 0.20798
 02.62 0.18752 0.19285 0.19536 0.19701 0.19580 0.19613 0.19852 0.19559 0.19482
 02.78 0.17605 0.18155 0.18407 0.18568 0.18428 0.18454 0.18702 0.18384 0.18297
 02.94 0.16570 0.17139 0.17392 0.17551 0.17393 0.17412 0.17667 0.17323 0.17221
 03.10 0.15637 0.16225 0.16480 0.16638 0.16460 0.16471 0.16728 0.16353 0.16232
 03.42 0.14035 0.14665 0.14921 0.15068 0.14844 0.14825 0.15073 0.14629 0.14464
 03.74 0.12729 0.13390 0.13633 0.13754 0.13471 0.13411 0.13639 0.13129 0.12923
 04.06 0.11645 0.12320 0.12535 0.12619 0.12273 0.12171 0.12379 0.11811 0.11574
 04.38 0.10722 0.11396 0.11575 0.11617 0.11213 0.11073 0.11265 0.10655 0.10398
 04.70 0.09918 0.10581 0.10721 0.10724 0.10271 0.10102 0.10282 0.09643 0.09376
 05.02 0.09206 0.09853 0.09957 0.09925 0.09434 0.09242 0.09414 0.08759 0.08488
 05.34 0.08570 0.09199 0.09269 0.09208 0.08688 0.08482 0.08648 0.07987 0.07718
 05.66 0.07998 0.08608 0.08648 0.08563 0.08025 0.07810 0.07971 0.07312 0.07049
 05.98 0.07483 0.08073 0.08086 0.07982 0.07435 0.07215 0.07371 0.06721 0.06466
 06.30 0.07017 0.07585 0.07577 0.07458 0.06908 0.06687 0.06839 0.06202 0.05957
 06.94 0.06211 0.06732 0.06692 0.06557 0.06017 0.05800 0.05946 0.05343 0.05118
 07.58 0.05540 0.06015 0.05957 0.05819 0.05300 0.05094 0.05236 0.04670 0.04464
 08.22 0.04972 0.05408 0.05349 0.05216 0.04720 0.04527 0.04669 0.04134 0.03946
 08.86 0.04487 0.04899 0.04848 0.04726 0.04248 0.04067 0.04213 0.03703 0.03530
 09.50 0.04070 0.04477 0.04440 0.04327 0.03862 0.03692 0.03843 0.03352 0.03192
 10.14 0.03710 0.04132 0.04108 0.04001 0.03543 0.03382 0.03537 0.03063 0.02914
 10.78 0.03402 0.03855 0.03838 0.03732 0.03278 0.03124 0.03282 0.02821 0.02681
 11.42 0.03142 0.03631 0.03614 0.03505 0.03054 0.02906 0.03064 0.02617 0.02486
 12.06 0.02926 0.03449 0.03424 0.03309 0.02863 0.02719 0.02875 0.02443 0.02319
 12.70 0.02750 0.03296 0.03258 0.03138 0.02698 0.02558 0.02708 0.02293 0.02222
 13.98 0.02703 0.03047 0.02978 0.02844 0.02439 0.02381 0.02427 0.02273 0.02222
 15.26 0.02703 0.02840 0.02742 0.02598 0.02439 0.02381 0.02326 0.02273 0.02222
 16.54 0.02703 0.02657 0.02564 0.02500 0.02439 0.02381 0.02326 0.02273 0.02222
 17.82 0.02703 0.02632 0.02564 0.02500 0.02439 0.02381 0.02326 0.02273 0.02222
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  1092.9  1157.2  1223.0  1290.7  1359.9  1431.2  1504.6  1579.2  1656.0
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  145.68  156.27  166.97  177.97  189.03  200.68  212.98  224.97  237.63
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  132.94  143.06  153.29  163.83  174.41  185.58  197.41  208.92  221.09
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U(X) X RB 37    SR 38    YT 39    ZR 40    NB 41    MO 42    TC 43    RU 44    RH 45
 SHELL (3S) 2   (3S) 2   (3S) 2   (3S) 2   (3S) 2   (3S) 2   (3S) 2   (3S) 2   (3S) 2
 (-E)  22.203   24.820   27.285   29.797   32.100   34.711   37.720   40.156   42.990
 SHELL (3P) 6   (3P) 6   (3P) 6   (3P) 6   (3P) 6   (3P) 6   (3P) 6   (3P) 6   (3P) 6
 (-E)  17.487   19.866   22.089   24.358   26.415   28.780   31.539   33.725   36.305
 SHELL (3D)10   (3D)10   (3D)10   (3D)10   (3D)10   (3D)10   (3D)10   (3D)10   (3D)10
 (-E)  8.869    10.777   12.528   14.322   15.901   17.785   20.063   21.761   23.853
 SHELL (4S) 2   (4S) 2   (4S) 2   (4S) 2   (4S) 2   (4S) 2   (4S) 2   (4S) 2   (4S) 2
 (-E)  2.6124   3.3055   3.7821   4.2339   4.4359   4.8484   5.5469   5.6733   6.0877
 SHELL (4P) 6   (4P) 6   (4P) 6   (4P) 6   (4P) 6   (4P) 6   (4P) 6   (4P) 6   (4P) 6
 (-E)  1.4775   2.0351   2.3929   2.7285   2.8271   3.1252   3.6974   3.7207   4.0197
 SHELL (4D) 0   (4D) 0   (4D) 1   (4D) 2   (4D) 4   (4D) 5   (4D) 5   (4D) 7   (4D) 8
 (-E)  0.       0.       0.4088   0.5159   0.4478   0.5261   0.8259   0.6857   0.7663
 SHELL (5S) 1   (5S) 2   (5S) 2   (5S) 2   (5S) 1   (5S) 1   (5S) 2   (5S) 1   (5S) 1
 (-E)  0.2905   0.3682   0.4069   0.4359   0.4019   0.4169   0.4980   0.4424   0.4533
U(X) X PD 46    AG 47    CD 48    IN 49    SN 50    SB 51    TE 52    I  53    XE 54
  X     U(X)     U(X)     U(X)     U(X)     U(X)     U(X)     U(X)     U(X)     U(X)
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
 00.01 0.98920 0.98917 0.98914 0.98911 0.98909 0.98907 0.98904 0.98902 0.98900
 00.02 0.97817 0.97811 0.97806 0.97801 0.97797 0.97792 0.97788 0.97783 0.97779
 00.03 0.96711 0.96703 0.96695 0.96689 0.96682 0.96676 0.96670 0.96664 0.96658
 00.04 0.95613 0.95603 0.95593 0.95586 0.95578 0.95570 0.95563 0.95556 0.95549
 00.05 0.94530 0.94519 0.94508 0.94499 0.94490 0.94482 0.94474 0.94465 0.94457
 00.06 0.93466 0.93454 0.93442 0.93432 0.93423 0.93414 0.93405 0.93397 0.93388
 00.07 0.92423 0.92410 0.92397 0.92388 0.92378 0.92369 0.92360 0.92351 0.92342
 00.08 0.91402 0.91388 0.91375 0.91365 0.91355 0.91346 0.91336 0.91327 0.91319
 00.09 0.90402 0.90387 0.90374 0.90364 0.90354 0.90345 0.90336 0.90327 0.90318
 00.10 0.89423 0.89408 0.89394 0.89385 0.89375 0.89366 0.89357 0.89348 0.89339
 00.12 0.87525 0.87510 0.87496 0.87488 0.87479 0.87470 0.87462 0.87454 0.87446
 00.14 0.85705 0.85691 0.85678 0.85671 0.85663 0.85656 0.85649 0.85643 0.85636
 00.16 0.83961 0.83948 0.83936 0.83931 0.83926 0.83921 0.83916 0.83911 0.83907
 00.18 0.82291 0.82279 0.82270 0.82267 0.82264 0.82262 0.82259 0.82257 0.82254
 00.20 0.80692 0.80682 0.80674 0.80674 0.80674 0.80674 0.80674 0.80674 0.80674
 00.22 0.79158 0.79150 0.79145 0.79147 0.79149 0.79151 0.79153 0.79155 0.79157
 00.24 0.77685 0.77678 0.77674 0.77679 0.77683 0.77687 0.77690 0.77694 0.77697
 00.26 0.76265 0.76259 0.76256 0.76263 0.76269 0.76274 0.76279 0.76284 0.76288
 00.28 0.74894 0.74888 0.74887 0.74895 0.74901 0.74908 0.74914 0.74920 0.74926
 00.30 0.73566 0.73561 0.73560 0.73569 0.73577 0.73585 0.73592 0.73600 0.73606
 00.34 0.71030 0.71026 0.71025 0.71037 0.71047 0.71057 0.71067 0.71076 0.71084
 00.38 0.68637 0.68633 0.68633 0.68648 0.68661 0.68673 0.68685 0.68697 0.68708
 00.42 0.66372 0.66369 0.66371 0.66389 0.66404 0.66419 0.66434 0.66449 0.66462
 00.46 0.64226 0.64224 0.64228 0.64248 0.64267 0.64285 0.64303 0.64321 0.64338
 00.50 0.62187 0.62187 0.62193 0.62217 0.62239 0.62261 0.62282 0.62304 0.62325
 00.54 0.60248 0.60250 0.60258 0.60287 0.60313 0.60339 0.60365 0.60391 0.60416
 00.58 0.58402 0.58406 0.58418 0.58451 0.58483 0.58514 0.58544 0.58576 0.58605
 00.62 0.56643 0.56651 0.56667 0.56706 0.56743 0.56779 0.56816 0.56853 0.56889
 00.66 0.54968 0.54979 0.55000 0.55046 0.55089 0.55132 0.55175 0.55219 0.55261
 00.70 0.53372 0.53388 0.53415 0.53468 0.53518 0.53568 0.53617 0.53667 0.53715
 00.78 0.50402 0.50430 0.50469 0.50537 0.50601 0.50665 0.50727 0.50789 0.50849
 00.86 0.47702 0.47741 0.47791 0.47873 0.47950 0.48025 0.48100 0.48173 0.48243
 00.94 0.45233 0.45282 0.45342 0.45436 0.45525 0.45612 0.45696 0.45779 0.45858
 01.02 0.42963 0.43021 0.43091 0.43196 0.43296 0.43393 0.43488 0.43580 0.43668
 01.10 0.40868 0.40934 0.41013 0.41131 0.41241 0.41349 0.41453 0.41554 0.41650
 01.18 0.38930 0.39004 0.39093 0.39222 0.39343 0.39460 0.39573 0.39682 0.39786
 01.26 0.37133 0.37217 0.37314 0.37454 0.37585 0.37711 0.37831 0.37947 0.38056
 01.34 0.35466 0.35558 0.35663 0.35813 0.35953 0.36086 0.36212 0.36333 0.36446
 01.42 0.33917 0.34016 0.34128 0.34286 0.34432 0.34570 0.34701 0.34825 0.34940
 01.50 0.32474 0.32578 0.32695 0.32859 0.33010 0.33152 0.33285 0.33410 0.33526
 01.66 0.29862 0.29971 0.30092 0.30265 0.30420 0.30565 0.30700 0.30826 0.30942
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U(X) X PD 46   AG 47   CD 48   IN 49   SN 50   SB 51   TE 52   I  53   XE 54
 01.82 0.27553 0.27661 0.27780 0.27956 0.28115 0.28262 0.28399 0.28529 0.28650
 01.98 0.25489 0.25593 0.25711 0.25892 0.26056 0.26210 0.26355 0.26493 0.26623
 02.14 0.23634 0.23737 0.23858 0.24049 0.24223 0.24387 0.24543 0.24690 0.24827
 02.30 0.21968 0.22074 0.22202 0.22405 0.22591 0.22765 0.22927 0.23078 0.23216
 02.46 0.20475 0.20586 0.20720 0.20935 0.21128 0.21305 0.21469 0.21618 0.21753
 02.62 0.19133 0.19248 0.19385 0.19605 0.19800 0.19977 0.20137 0.20281 0.20409
 02.78 0.17920 0.18033 0.18168 0.18389 0.18582 0.18755 0.18910 0.19048 0.19170
 02.94 0.16810 0.16918 0.17047 0.17267 0.17456 0.17625 0.17776 0.17909 0.18026
 03.10 0.15787 0.15886 0.16008 0.16226 0.16414 0.16579 0.16727 0.16857 0.16970
 03.42 0.13948 0.14032 0.14144 0.14364 0.14552 0.14717 0.14864 0.14990 0.15099
 03.74 0.12345 0.12423 0.12532 0.12763 0.12958 0.13129 0.13277 0.13402 0.13506
 04.06 0.10950 0.11031 0.11146 0.11393 0.11600 0.11777 0.11926 0.12047 0.12144
 04.38 0.09741 0.09833 0.09960 0.10225 0.10442 0.10623 0.10771 0.10884 0.10972
 04.70 0.08699 0.08807 0.08945 0.09228 0.09453 0.09635 0.09777 0.09882 0.09959
 05.02 0.07803 0.07927 0.08077 0.08374 0.08604 0.08783 0.08918 0.09014 0.09082
 05.34 0.07032 0.07173 0.07331 0.07640 0.07871 0.08045 0.08173 0.08261 0.08324
 05.66 0.06369 0.06525 0.06690 0.07006 0.07235 0.07404 0.07526 0.07609 0.07669
 05.98 0.05796 0.05965 0.06134 0.06455 0.06682 0.06845 0.06963 0.07043 0.07100
 06.30 0.05301 0.05480 0.05651 0.05975 0.06198 0.06358 0.06473 0.06550 0.06604
 06.94 0.04495 0.04688 0.04861 0.05187 0.05405 0.05559 0.05670 0.05737 0.05775
 07.58 0.03876 0.04077 0.04249 0.04576 0.04790 0.04941 0.05041 0.05091 0.05106
 08.22 0.03392 0.03595 0.03770 0.04097 0.04308 0.04449 0.04533 0.04560 0.04548
 08.86 0.03006 0.03211 0.03389 0.03715 0.03919 0.04046 0.04109 0.04112 0.04077
 09.50 0.02693 0.02898 0.03082 0.03405 0.03598 0.03707 0.03747 0.03728 0.03675
 10.14 0.02434 0.02642 0.02830 0.03147 0.03327 0.03416 0.03434 0.03396 0.03328
 10.78 0.02218 0.02429 0.02620 0.02928 0.03092 0.03161 0.03160 0.03107 0.03028
 11.42 0.02174 0.02251 0.02442 0.02738 0.02886 0.02936 0.02919 0.02853 0.02766
 12.06 0.02174 0.02128 0.02289 0.02571 0.02702 0.02735 0.02703 0.02628 0.02535
 12.70 0.02174 0.02128 0.02155 0.02423 0.02537 0.02555 0.02511 0.02427 0.02331
 13.98 0.02174 0.02128 0.02083 0.02169 0.02253 0.02244 0.02182 0.02087 0.01987
 15.26 0.02174 0.02128 0.02083 0.02041 0.02017 0.01987 0.01923 0.01887 0.01852
 16.54 0.02174 0.02128 0.02083 0.02041 0.02000 0.01961 0.01923 0.01887 0.01852
 17.82 0.02174 0.02128 0.02083 0.02041 0.02000 0.01961 0.01923 0.01887 0.01852
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  1734.3  1815.0  1897.7  1982.5  2069.1  2157.6  2248.0  2340.3  2434.4
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  250.28  263.96  278.08  292.76  307.82  323.27  339.13  335.39  372.05
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  233.26  246.45  260.08  274.27  288.83  303.78  319.14  334.90  351.05
 SHELL (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  45.558  48.886  52.393  56.173  60.068  64.091  68.245  72.529  76.945
 SHELL (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  38.619  41.691  44.940  48.459  52.093  55.853  59.743  63.761  67.910
 SHELL (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10
 (-E)  25.674  28.253  31.005  34.025  37.159  40.417  43.802  47.314  50.955
 SHELL (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2
 (-E)  6.185   6.925   7.745   8.743   9.761   10.812  11.899  13.023  14.184
 SHELL (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6
 (-E)  4.009   4.624   5.313   6.178   7.060   7.973   8.921   9.903   10.923
 SHELL (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10
 (-E)  0.5861  0.9300  1.3439  1.9269  2.5262  3.1564  3.8208  4.5206  5.2570
 SHELL (5S) 0  (5S) 1  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2
 (-E)  0.      0.4724  0.5670  0.7451  0.9192  1.0898  1.2594  1.4296  1.6004
 SHELL (5P) 0  (5P) 0  (5P) 0  (5P) 1  (5P) 2  (5P) 3  (5P) 4  (5P) 5  (5P) 6
 (-E)  0.      0.      0.      0.3452  0.4370  0.5337  0.6328  0.7341  0.8369
U(X) X CS 55   BA 56   LA 57   CE 58   PR 59   ND 60   PM 61   SM 62   EU 63
   X    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
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| U(X) X | CS 55 | BA 56 | LA 57 | CE 58 | PR 59 | ND 60 | PM 61 | SM 62 | EU 63 |
|---|---|---|---|---|---|---|---|---|---|
| 00.01 | 0.98899 | 0.98897 | 0.98896 | 0.98892 | 0.98889 | 0.98886 | 0.98883 | 0.98880 | 0.98877 |
| 00.02 | 0.97777 | 0.97774 | 0.97771 | 0.97764 | 0.97758 | 0.97752 | 0.97747 | 0.97741 | 0.97735 |
| 00.03 | 0.96655 | 0.96652 | 0.96648 | 0.96637 | 0.96629 | 0.96621 | 0.96612 | 0.96604 | 0.96596 |
| 00.04 | 0.95545 | 0.95542 | 0.95537 | 0.95523 | 0.95513 | 0.95503 | 0.95493 | 0.95483 | 0.95472 |
| 00.05 | 0.94454 | 0.94451 | 0.94446 | 0.94429 | 0.94418 | 0.94406 | 0.94394 | 0.94382 | 0.94370 |
| 00.06 | 0.93385 | 0.93383 | 0.93378 | 0.93358 | 0.93345 | 0.93332 | 0.93319 | 0.93305 | 0.93292 |
| 00.07 | 0.92340 | 0.92338 | 0.92333 | 0.92311 | 0.92297 | 0.92283 | 0.92268 | 0.92253 | 0.92238 |
| 00.08 | 0.91317 | 0.91316 | 0.91311 | 0.91288 | 0.91273 | 0.91257 | 0.91242 | 0.91226 | 0.91209 |
| 00.09 | 0.90317 | 0.90317 | 0.90313 | 0.90287 | 0.90271 | 0.90255 | 0.90238 | 0.90221 | 0.90204 |
| 00.10 | 0.89340 | 0.89340 | 0.89337 | 0.89309 | 0.89293 | 0.89276 | 0.89258 | 0.89240 | 0.89222 |
| 00.12 | 0.87449 | 0.87452 | 0.87451 | 0.87420 | 0.87402 | 0.87384 | 0.87365 | 0.87345 | 0.87325 |
| 00.14 | 0.85642 | 0.85649 | 0.85649 | 0.85616 | 0.85597 | 0.85578 | 0.85558 | 0.85538 | 0.85517 |
| 00.16 | 0.83916 | 0.83927 | 0.83930 | 0.83894 | 0.83876 | 0.83856 | 0.83836 | 0.83815 | 0.83792 |
| 00.18 | 0.82268 | 0.82283 | 0.82289 | 0.82250 | 0.82232 | 0.82212 | 0.82191 | 0.82169 | 0.82146 |
| 00.20 | 0.80691 | 0.80709 | 0.80718 | 0.80677 | 0.80658 | 0.80638 | 0.80616 | 0.80593 | 0.80569 |
| 00.22 | 0.79178 | 0.79200 | 0.79211 | 0.79167 | 0.79147 | 0.79126 | 0.79103 | 0.79078 | 0.79052 |
| 00.24 | 0.77721 | 0.77746 | 0.77760 | 0.77712 | 0.77691 | 0.77669 | 0.77644 | 0.77618 | 0.77590 |
| 00.26 | 0.76315 | 0.76343 | 0.76358 | 0.76307 | 0.76285 | 0.76261 | 0.76235 | 0.76206 | 0.76176 |
| 00.28 | 0.74956 | 0.74986 | 0.75003 | 0.74948 | 0.74925 | 0.74899 | 0.74871 | 0.74841 | 0.74809 |
| 00.30 | 0.73638 | 0.73672 | 0.73691 | 0.73632 | 0.73607 | 0.73580 | 0.73550 | 0.73518 | 0.73484 |
| 00.34 | 0.71123 | 0.71162 | 0.71184 | 0.71118 | 0.71090 | 0.71060 | 0.71027 | 0.70991 | 0.70953 |
| 00.38 | 0.68752 | 0.68797 | 0.68824 | 0.68750 | 0.68720 | 0.68687 | 0.68650 | 0.68611 | 0.68569 |
| 00.42 | 0.66513 | 0.66564 | 0.66595 | 0.66514 | 0.66482 | 0.66446 | 0.66407 | 0.66364 | 0.66318 |
| 00.46 | 0.64395 | 0.64453 | 0.64489 | 0.64401 | 0.64366 | 0.64328 | 0.64286 | 0.64240 | 0.64191 |
| 00.50 | 0.62389 | 0.62454 | 0.62496 | 0.62400 | 0.62364 | 0.62325 | 0.62280 | 0.62232 | 0.62180 |
| 00.54 | 0.60488 | 0.60561 | 0.60609 | 0.60507 | 0.60470 | 0.60429 | 0.60383 | 0.60332 | 0.60278 |
| 00.58 | 0.58686 | 0.58768 | 0.58823 | 0.58715 | 0.58677 | 0.58635 | 0.58588 | 0.58535 | 0.58479 |
| 00.62 | 0.56979 | 0.57070 | 0.57132 | 0.57018 | 0.56980 | 0.56937 | 0.56888 | 0.56834 | 0.56775 |
| 00.66 | 0.55360 | 0.55461 | 0.55531 | 0.55410 | 0.55372 | 0.55328 | 0.55277 | 0.55220 | 0.55159 |
| 00.70 | 0.53825 | 0.53935 | 0.54012 | 0.53884 | 0.53845 | 0.53800 | 0.53747 | 0.53687 | 0.53622 |
| 00.78 | 0.50977 | 0.51105 | 0.51195 | 0.51052 | 0.51010 | 0.50960 | 0.50901 | 0.50835 | 0.50762 |
| 00.86 | 0.48387 | 0.48531 | 0.48633 | 0.48474 | 0.48427 | 0.48370 | 0.48304 | 0.48230 | 0.48148 |
| 00.94 | 0.46018 | 0.46178 | 0.46292 | 0.46114 | 0.46061 | 0.45998 | 0.45924 | 0.45841 | 0.45749 |
| 01.02 | 0.43843 | 0.44018 | 0.44142 | 0.43945 | 0.43885 | 0.43815 | 0.43732 | 0.43639 | 0.43537 |
| 01.10 | 0.41840 | 0.42028 | 0.42162 | 0.41945 | 0.41878 | 0.41798 | 0.41706 | 0.41603 | 0.41489 |
| 01.18 | 0.39988 | 0.40189 | 0.40331 | 0.40093 | 0.40017 | 0.39927 | 0.39824 | 0.39709 | 0.39584 |
| 01.26 | 0.38271 | 0.38482 | 0.38630 | 0.38370 | 0.38283 | 0.38183 | 0.38069 | 0.37942 | 0.37804 |
| 01.34 | 0.36670 | 0.36890 | 0.37042 | 0.36759 | 0.36662 | 0.36551 | 0.36425 | 0.36286 | 0.36136 |
| 01.42 | 0.35172 | 0.35399 | 0.35554 | 0.35249 | 0.35142 | 0.35019 | 0.34882 | 0.34732 | 0.34572 |
| 01.50 | 0.33765 | 0.33999 | 0.34158 | 0.33831 | 0.33713 | 0.33581 | 0.33434 | 0.33275 | 0.33106 |
| 01.66 | 0.31196 | 0.31446 | 0.31612 | 0.31246 | 0.31113 | 0.30966 | 0.30804 | 0.30630 | 0.30445 |
| 01.82 | 0.28923 | 0.29193 | 0.29372 | 0.28972 | 0.28827 | 0.28666 | 0.28490 | 0.28301 | 0.28100 |
| 01.98 | 0.26918 | 0.27209 | 0.27401 | 0.26965 | 0.26805 | 0.26629 | 0.26435 | 0.26228 | 0.26009 |
| 02.14 | 0.25141 | 0.25447 | 0.25645 | 0.25171 | 0.24993 | 0.24797 | 0.24584 | 0.24358 | 0.24121 |
| 02.30 | 0.23543 | 0.23859 | 0.24057 | 0.23544 | 0.23347 | 0.23132 | 0.22901 | 0.22659 | 0.22407 |
| 02.46 | 0.22086 | 0.22409 | 0.22606 | 0.22057 | 0.21842 | 0.21611 | 0.21367 | 0.21112 | 0.20850 |
| 02.62 | 0.20749 | 0.21077 | 0.21272 | 0.20693 | 0.20464 | 0.20222 | 0.19968 | 0.19705 | 0.19437 |
| 02.78 | 0.19517 | 0.19852 | 0.20046 | 0.19442 | 0.19204 | 0.18954 | 0.18694 | 0.18427 | 0.18157 |
| 02.94 | 0.18381 | 0.18724 | 0.18918 | 0.18296 | 0.18051 | 0.17797 | 0.17534 | 0.17267 | 0.16997 |
| 03.10 | 0.17335 | 0.17686 | 0.17880 | 0.17245 | 0.16998 | 0.16741 | 0.16479 | 0.16212 | 0.15945 |
| 03.42 | 0.15484 | 0.15852 | 0.16047 | 0.15399 | 0.15151 | 0.14897 | 0.14639 | 0.14380 | 0.14122 |
| 03.74 | 0.13909 | 0.14292 | 0.14485 | 0.13840 | 0.13596 | 0.13349 | 0.13101 | 0.12853 | 0.12607 |
| 04.06 | 0.12563 | 0.12959 | 0.13147 | 0.12515 | 0.12280 | 0.12043 | 0.11807 | 0.11572 | 0.11341 |
| 04.38 | 0.11406 | 0.11815 | 0.11999 | 0.11387 | 0.11163 | 0.10938 | 0.10715 | 0.10494 | 0.10277 |
| 04.70 | 0.10409 | 0.10834 | 0.11016 | 0.10426 | 0.10213 | 0.10001 | 0.09791 | 0.09583 | 0.09380 |
| 05.02 | 0.09551 | 0.09994 | 0.10174 | 0.09605 | 0.09404 | 0.09203 | 0.09004 | 0.08809 | 0.08617 |
| 05.34 | 0.08814 | 0.09273 | 0.09450 | 0.08902 | 0.08709 | 0.08518 | 0.08329 | 0.08143 | 0.07962 |
| 05.66 | 0.08179 | 0.08650 | 0.08820 | 0.08292 | 0.08107 | 0.07923 | 0.07742 | 0.07565 | 0.07392 |

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U(X) X CS 55   BA 56   LA 57   CE 58   PR 59   ND 60   PM 61   SM 62   EU 63
 05.98 0.07627 0.08105 0.08263 0.07796 0.07577 0.07400 0.07225 0.07055 0.06890
 06.30 0.07142 0.07622 0.07765 0.07279 0.07105 0.06934 0.06766 0.06602 0.06444
 06.94 0.06326 0.06796 0.06902 0.06464 0.06299 0.06138 0.05981 0.05830 0.05685
 07.58 0.05656 0.06106 0.06176 0.05786 0.05630 0.05480 0.05334 0.05195 0.05062
 08.22 0.05093 0.05518 0.05556 0.05211 0.05066 0.04925 0.04791 0.04663 0.04541
 08.86 0.04613 0.05009 0.05022 0.04718 0.04583 0.04452 0.04328 0.04210 0.04098
 09.50 0.04198 0.04565 0.04560 0.04291 0.04165 0.04044 0.03930 0.03822 0.03719
 10.14 0.03837 0.04176 0.04158 0.03919 0.03801 0.03690 0.03585 0.03486 0.03392
 10.78 0.03520 0.03834 0.03810 0.03594 0.03485 0.03383 0.03286 0.03195 0.03110
 11.42 0.03239 0.03533 0.03509 0.03311 0.03211 0.03118 0.03029 0.02946 0.02868
 12.06 0.02989 0.03272 0.03251 0.03067 0.02976 0.02890 0.02809 0.02734 0.02663
 12.70 0.02766 0.03046 0.03031 0.02859 0.02775 0.02697 0.02624 0.02555 0.02491
 13.98 0.02391 0.02691 0.02684 0.02534 0.02465 0.02399 0.02338 0.02281 0.02227
 15.26 0.02101 0.02438 0.02429 0.02304 0.02245 0.02190 0.02137 0.02088 0.02042
 16.54 0.01884 0.02253 0.02232 0.02136 0.02084 0.02034 0.01987 0.01943 0.01902
 17.82 0.01818 0.02110 0.02072 0.02002 0.01955 0.01909 0.01866 0.01826 0.01788
 19.10 0.01818 0.01989 0.01935 0.01888 0.01845 0.01802 0.01762 0.01724 0.01688
 20.38 0.01818 0.01882 0.01814 0.01787 0.01746 0.01705 0.01667 0.01632 0.01598
 21.66 0.01818 0.01786 0.01754 0.01724 0.01695 0.01667 0.01639 0.01613 0.01587
 22.94 0.01818 0.01786 0.01754 0.01724 0.01695 0.01667 0.01639 0.01613 0.01587
 24.22 0.01818 0.01786 0.01754 0.01724 0.01695 0.01667 0.01639 0.01613 0.01587
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  2530.9  2629.3  2729.5  2830.2  2933.4  3038.5  3145.3  3254.1  3364.6
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  389.53  407.44  425.55  442.70  460.82  479.28  498.08  517.23  536.72
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  368.03  385.44  403.04  419.70  437.33  455.29  473.60  492.26  511.25
 SHELL (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  81.91   87.03   92.07   95.70   100.12  104.59  109.14  113.76  118.45
 SHELL (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  72.60   77.45   82.23   85.59   89.74   93.95   98.22   102.57  106.98
 SHELL (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10
 (-E)  55.138  59.479  63.743  66.605  70.247  73.944  77.709  81.539  85.438
 SHELL (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2
 (-E)  15.793  17.465  18.970  19.196  20.046  20.894  21.741  22.591  23.444
 SHELL (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6
 (-E)  12.388  13.916  15.378  15.275  16.093  16.804  17.515  18.226  18.939
 SHELL (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10
 (-E)  6.437   7.679   8.751   8.625   9.079   9.528   9.974   10.418  10.862
 SHELL (4F) 0  (4F) 0  (4F) 0  (4F) 2  (4F) 3  (4F) 4  (4F) 5  (4F) 6  (4F) 7
 (-E)  0.      0.      0.      0.7446  0.8102  0.8678  0.9191  0.9642  1.0040
 SHELL (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2
 (-E)  2.1187  2.6393  2.9769  2.8258  2.9108  2.9917  3.0717  3.1491  3.2251
 SHELL (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6
 (-E)  1.2543  1.6800  1.9372  1.7894  1.8372  1.8814  1.9249  1.9660  2.0057
 SHELL (5D) 0  (5D) 0  (5D) 0  (5D) 0  (5D) 0  (5D) 0  (5D) 0  (5D) 0  (5D) 0
 (-E)  0.      0.      0.4552  0.      0.      0.      0.      0.      0.
 SHELL (6S) 1  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2
 (-E)  0.2620  0.3280  0.3577  0.3375  0.3417  0.3455  0.3493  0.3530  0.3565
U(X) X GD 64   TB 65   DY 66   HO 67   ER 68   TM 69   YB 70   LU 71   HF 72
   X    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
 00.01 0.98875 0.98871 0.98868 0.98865 0.98862 0.98858 0.98856 0.98853 0.98851
 00.02 0.97731 0.97723 0.97717 0.97711 0.97705 0.97699 0.97693 0.97689 0.97685
 00.03 0.96591 0.96579 0.96571 0.96562 0.96554 0.96545 0.96536 0.96531 0.96525
 00.04 0.95466 0.95451 0.95441 0.95430 0.95419 0.95408 0.95397 0.95390 0.95384
 00.05 0.94363 0.94345 0.94333 0.94320 0.94308 0.94294 0.94282 0.94274 0.94266
 00.06 0.93284 0.93264 0.93250 0.93236 0.93221 0.93206 0.93192 0.93183 0.93175
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| U(X) X | GD 64 | TB 65 | DY 66 | HO 67 | ER 68 | TM 69 | YB 70 | LU 71 | HF 72 |
|---|---|---|---|---|---|---|---|---|---|
| 00.07 | 0.92230 | 0.92208 | 0.92192 | 0.92176 | 0.92160 | 0.92143 | 0.92128 | 0.92118 | 0.92109 |
| 00.08 | 0.91201 | 0.91176 | 0.91159 | 0.91142 | 0.91124 | 0.91105 | 0.91089 | 0.91079 | 0.91069 |
| 00.09 | 0.90195 | 0.90168 | 0.90150 | 0.90132 | 0.90113 | 0.90092 | 0.90074 | 0.90064 | 0.90054 |
| 00.10 | 0.89213 | 0.89184 | 0.89164 | 0.89145 | 0.89125 | 0.89103 | 0.89084 | 0.89073 | 0.89062 |
| 00.12 | 0.87317 | 0.87284 | 0.87262 | 0.87241 | 0.87218 | 0.87194 | 0.87173 | 0.87162 | 0.87151 |
| 00.14 | 0.85510 | 0.85472 | 0.85450 | 0.85427 | 0.85403 | 0.85376 | 0.85354 | 0.85343 | 0.85332 |
| 00.16 | 0.83787 | 0.83746 | 0.83722 | 0.83698 | 0.83672 | 0.83644 | 0.83620 | 0.83609 | 0.83598 |
| 00.18 | 0.82141 | 0.82097 | 0.82072 | 0.82046 | 0.82018 | 0.81987 | 0.81962 | 0.81950 | 0.81940 |
| 00.20 | 0.80565 | 0.80517 | 0.80489 | 0.80461 | 0.80431 | 0.80398 | 0.80370 | 0.80359 | 0.80347 |
| 00.22 | 0.79048 | 0.78996 | 0.78967 | 0.78937 | 0.78904 | 0.78868 | 0.78838 | 0.78825 | 0.78813 |
| 00.24 | 0.77586 | 0.77530 | 0.77498 | 0.77465 | 0.77430 | 0.77391 | 0.77358 | 0.77345 | 0.77332 |
| 00.26 | 0.76173 | 0.76112 | 0.76077 | 0.76042 | 0.76004 | 0.75962 | 0.75927 | 0.75913 | 0.75899 |
| 00.28 | 0.74805 | 0.74739 | 0.74703 | 0.74665 | 0.74624 | 0.74579 | 0.74541 | 0.74526 | 0.74512 |
| 00.30 | 0.73480 | 0.73410 | 0.73370 | 0.73330 | 0.73287 | 0.73239 | 0.73198 | 0.73182 | 0.73167 |
| 00.34 | 0.70950 | 0.70870 | 0.70826 | 0.70781 | 0.70732 | 0.70678 | 0.70632 | 0.70615 | 0.70599 |
| 00.38 | 0.68567 | 0.68477 | 0.68429 | 0.68379 | 0.68325 | 0.68265 | 0.68214 | 0.68196 | 0.68178 |
| 00.42 | 0.66317 | 0.66219 | 0.66166 | 0.66111 | 0.66052 | 0.65987 | 0.65931 | 0.65912 | 0.65894 |
| 00.46 | 0.64192 | 0.64085 | 0.64027 | 0.63969 | 0.63905 | 0.63834 | 0.63774 | 0.63755 | 0.63737 |
| 00.50 | 0.62183 | 0.62067 | 0.62006 | 0.61944 | 0.61876 | 0.61800 | 0.61736 | 0.61717 | 0.61699 |
| 00.54 | 0.60283 | 0.60159 | 0.60095 | 0.60029 | 0.59957 | 0.59877 | 0.59809 | 0.59790 | 0.59772 |
| 00.58 | 0.58487 | 0.58354 | 0.58287 | 0.58217 | 0.58141 | 0.58056 | 0.57984 | 0.57965 | 0.57947 |
| 00.62 | 0.56786 | 0.56644 | 0.56573 | 0.56500 | 0.56419 | 0.56328 | 0.56252 | 0.56232 | 0.56214 |
| 00.66 | 0.55172 | 0.55021 | 0.54945 | 0.54868 | 0.54782 | 0.54686 | 0.54604 | 0.54584 | 0.54565 |
| 00.70 | 0.53637 | 0.53476 | 0.53396 | 0.53314 | 0.53223 | 0.53120 | 0.53033 | 0.53012 | 0.52993 |
| 00.78 | 0.50779 | 0.50598 | 0.50507 | 0.50414 | 0.50311 | 0.50196 | 0.50097 | 0.50073 | 0.50051 |
| 00.86 | 0.48168 | 0.47964 | 0.47863 | 0.47758 | 0.47643 | 0.47514 | 0.47403 | 0.47376 | 0.47351 |
| 00.94 | 0.45770 | 0.45543 | 0.45430 | 0.45314 | 0.45185 | 0.45043 | 0.44919 | 0.44889 | 0.44861 |
| 01.02 | 0.43559 | 0.43309 | 0.43183 | 0.43054 | 0.42912 | 0.42756 | 0.42619 | 0.42585 | 0.42554 |
| 01.10 | 0.41510 | 0.41236 | 0.41098 | 0.40956 | 0.40800 | 0.40629 | 0.40479 | 0.40442 | 0.40407 |
| 01.18 | 0.39603 | 0.39305 | 0.39154 | 0.38999 | 0.38830 | 0.38645 | 0.38483 | 0.38442 | 0.38405 |
| 01.26 | 0.37821 | 0.37500 | 0.37336 | 0.37169 | 0.36988 | 0.36790 | 0.36616 | 0.36574 | 0.36536 |
| 01.34 | 0.36152 | 0.35809 | 0.35634 | 0.35455 | 0.35263 | 0.35055 | 0.34871 | 0.34828 | 0.34790 |
| 01.42 | 0.34588 | 0.34224 | 0.34039 | 0.33851 | 0.33650 | 0.33432 | 0.33239 | 0.33197 | 0.33160 |
| 01.50 | 0.33122 | 0.32740 | 0.32547 | 0.32350 | 0.32140 | 0.31913 | 0.31713 | 0.31672 | 0.31636 |
| 01.66 | 0.30466 | 0.30048 | 0.29839 | 0.29626 | 0.29399 | 0.29156 | 0.28939 | 0.28899 | 0.28866 |
| 01.82 | 0.28125 | 0.27670 | 0.27443 | 0.27213 | 0.26969 | 0.26708 | 0.26475 | 0.26437 | 0.26405 |
| 01.98 | 0.26033 | 0.25542 | 0.25298 | 0.25051 | 0.24791 | 0.24515 | 0.24269 | 0.24235 | 0.24209 |
| 02.14 | 0.24145 | 0.23621 | 0.23362 | 0.23103 | 0.22831 | 0.22546 | 0.22291 | 0.22265 | 0.22247 |
| 02.30 | 0.22432 | 0.21883 | 0.21614 | 0.21347 | 0.21068 | 0.20778 | 0.20521 | 0.20506 | 0.20501 |
| 02.46 | 0.20880 | 0.20310 | 0.20037 | 0.19766 | 0.19487 | 0.19197 | 0.18940 | 0.18940 | 0.18947 |
| 02.62 | 0.19474 | 0.18891 | 0.18617 | 0.18347 | 0.18069 | 0.17783 | 0.17530 | 0.17545 | 0.17567 |
| 02.78 | 0.18203 | 0.17611 | 0.17339 | 0.17072 | 0.16799 | 0.16519 | 0.16272 | 0.16302 | 0.16337 |
| 02.94 | 0.17052 | 0.16456 | 0.16189 | 0.15927 | 0.15660 | 0.15398 | 0.15148 | 0.15192 | 0.15239 |
| 03.10 | 0.16009 | 0.15413 | 0.15151 | 0.14896 | 0.14637 | 0.14373 | 0.14140 | 0.14197 | 0.14255 |
| 03.42 | 0.14202 | 0.13614 | 0.13366 | 0.13126 | 0.12883 | 0.12638 | 0.12421 | 0.12500 | 0.12573 |
| 03.74 | 0.12699 | 0.12128 | 0.11896 | 0.11672 | 0.11446 | 0.11219 | 0.11018 | 0.11114 | 0.11198 |
| 04.06 | 0.11442 | 0.10892 | 0.10676 | 0.10468 | 0.10258 | 0.10049 | 0.09864 | 0.09972 | 0.10063 |
| 04.38 | 0.10386 | 0.09858 | 0.09657 | 0.09464 | 0.09270 | 0.09077 | 0.08905 | 0.09022 | 0.09117 |
| 04.70 | 0.09494 | 0.08988 | 0.08800 | 0.08621 | 0.08440 | 0.08261 | 0.08101 | 0.08223 | 0.08317 |
| 05.02 | 0.08733 | 0.08249 | 0.08073 | 0.07904 | 0.07736 | 0.07569 | 0.07419 | 0.07542 | 0.07632 |
| 05.34 | 0.08076 | 0.07614 | 0.07447 | 0.07289 | 0.07130 | 0.06974 | 0.06832 | 0.06954 | 0.07038 |
| 05.66 | 0.07500 | 0.07061 | 0.06903 | 0.06753 | 0.06603 | 0.06456 | 0.06323 | 0.06441 | 0.06517 |
| 05.98 | 0.06991 | 0.06575 | 0.06425 | 0.06283 | 0.06141 | 0.06003 | 0.05877 | 0.05989 | 0.06056 |
| 06.30 | 0.06537 | 0.06143 | 0.06001 | 0.05866 | 0.05732 | 0.05601 | 0.05482 | 0.05587 | 0.05645 |
| 06.94 | 0.05758 | 0.05411 | 0.05282 | 0.05160 | 0.05040 | 0.04923 | 0.04816 | 0.04905 | 0.04946 |
| 07.58 | 0.05116 | 0.04812 | 0.04695 | 0.04585 | 0.04476 | 0.04372 | 0.04275 | 0.04349 | 0.04375 |
| 08.22 | 0.04578 | 0.04313 | 0.04207 | 0.04107 | 0.04009 | 0.03915 | 0.03827 | 0.03888 | 0.03903 |
| 08.86 | 0.04123 | 0.03891 | 0.03794 | 0.03704 | 0.03614 | 0.03529 | 0.03450 | 0.03501 | 0.03508 |

```
U(X) X GD 64    TB 65    DY 66    HO 67    ER 68    TM 69    YB 70    LU 71    HF 72
 09.50 0.03736 0.03529 0.03442 0.03359 0.03278 0.03201 0.03129 0.03174 0.03178
 10.14 0.03405 0.03219 0.03139 0.03064 0.02990 0.02921 0.02855 0.02899 0.02901
 10.78 0.03123 0.02952 0.02880 0.02812 0.02745 0.02682 0.02622 0.02667 0.02670
 11.42 0.02885 0.02725 0.02659 0.02597 0.02537 0.02480 0.02426 0.02474 0.02476
 12.06 0.02684 0.02533 0.02473 0.02418 0.02363 0.02311 0.02262 0.02312 0.02313
 12.70 0.02515 0.02373 0.02318 0.02268 0.02218 0.02171 0.02127 0.02177 0.02175
 13.98 0.02251 0.02129 0.02083 0.02040 0.01998 0.01959 0.01921 0.01964 0.01952
 15.26 0.02054 0.01956 0.01916 0.01879 0.01842 0.01808 0.01774 0.01802 0.01778
 16.54 0.01898 0.01825 0.01789 0.01755 0.01722 0.01690 0.01659 0.01669 0.01634
 17.82 0.01767 0.01716 0.01683 0.01652 0.01620 0.01591 0.01562 0.01555 0.01510
 19.10 0.01652 0.01621 0.01590 0.01560 0.01531 0.01504 0.01476 0.01453 0.01402
 20.38 0.01562 0.01538 0.01515 0.01493 0.01471 0.01449 0.01429 0.01408 0.01389
 21.66 0.01562 0.01538 0.01515 0.01493 0.01471 0.01449 0.01429 0.01408 0.01389
 22.94 0.01562 0.01538 0.01515 0.01493 0.01471 0.01449 0.01429 0.01408 0.01389
 24.22 0.01562 0.01538 0.01515 0.01493 0.01471 0.01449 0.01429 0.01408 0.01389
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  3477.7  3591.3  3707.4  3825.4  3945.2  4066.9  4190.3  4316.4  444.3
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  557.23  576.74  597.27  618.14  639.38  661.00  682.89  705.89  729.27
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  531.26  550.29  270.32  590.70  611.44  632.57  653.96  676.45  699.33
 SHELL (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  123.95  128.04  132.96  137.94  143.01  148.19  153.38  159.46  165.68
 SHELL (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  112.21  116.03  120.66  125.36  130.16  135.06  139.96  145.75  151.68
 SHELL (3D) 10 (3D) 10 (3D) 10 (3D) 10 (3D) 10 (3D) 10 (3D) 10 (3D) 10 (3D) 10
 (-E)  90.14   93.44   97.56   101.73  106.00  110.37  114.74  119.99  125.37
 SHELL (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2
 (-E)  24.956  25.165  26.034  26.907  27.797  28.702  29.593  31.211  32.878
 SHELL (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6
 (-E)  20.302  20.377  21.102  21.829  22.572  23.328  24.069  25.530  27.037
 SHELL (4D) 10 (4D) 10 (4D) 10 (4D) 10 (4D) 10 (4D) 10 (4D) 10 (4D) 10 (4D) 10
 (-E)  11.933  11.751  12.196  12.642  13.099  13.565  14.013  15.164  16.355
 SHELL (4F) 7  (4F) 9  (4F) 10 (4F) 11 (4F) 12 (4F) 13 (4F) 14 (4F) 14 (4F) 14
 (-E)  1.5912  1.0702  1.0968  1.1170  1.1418  1.1677  1.1748  1.8092  2.4819
 SHELL (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2
 (-E)  3.5683  3.3743  3.4480  3.5194  3.5937  3.6651  3.7389  4.1225  4.4903
 SHELL (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6
 (-E)  2.2693  2.0819  2.1189  2.1538  2.1908  2.2248  2.2612  2.5588  2.8401
 SHELL (5D) 1  (5D) 0  (5D) 0  (5D) 0  (5D) 0  (5D) 0  (5D) 0  (5D) 1  (5D) 2
 (-E)  0.4363  0.      0.      0.      0.      0.      0.      0.3905  0.4902
 SHELL (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2
 (-E)  0.3878  0.3633  0.3666  0.3697  0.3731  0.3759  0.3794  0.4160  0.4437
U(X) X TA 73    W  74    RE 75    OS 76    IR 77    PT 78    AU 79    HG 80    TL 81
   X      U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
 00.01 0.98849 0.98847 0.98845 0.98843 0.98841 0.98839 0.98837 0.98835 0.98834
 00.02 0.97681 0.97677 0.97673 0.97669 0.97665 0.97661 0.97657 0.97654 0.97652
 00.03 0.96520 0.96514 0.96509 0.96503 0.96498 0.96491 0.96486 0.96482 0.96479
 00.04 0.95377 0.95370 0.95363 0.95357 0.95350 0.95342 0.95336 0.95331 0.95327
 00.05 0.94258 0.94251 0.94243 0.94236 0.94228 0.94219 0.94212 0.94206 0.94202
 00.06 0.93166 0.93158 0.93149 0.93141 0.93133 0.93122 0.93114 0.93109 0.93104
 00.07 0.92100 0.92091 0.92082 0.92073 0.92064 0.92052 0.92044 0.92038 0.92033
 00.08 0.91059 0.91049 0.91040 0.91030 0.91021 0.91008 0.90999 0.90993 0.90989
 00.09 0.90043 0.90033 0.90023 0.90013 0.90003 0.89990 0.89980 0.89974 0.89970
 00.10 0.89052 0.89041 0.89031 0.89021 0.89011 0.88996 0.88986 0.88981 0.88977
 00.12 0.87140 0.87130 0.87119 0.87109 0.87098 0.87082 0.87072 0.87067 0.87064
 00.14 0.85321 0.85310 0.85300 0.85289 0.85279 0.85262 0.85252 0.85247 0.85245
```

| U(X) X | TA 73 | W 74 | RE 75 | CS 76 | IR 77 | PT 78 | AU 79 | HG 80 | TL 81 |
|---|---|---|---|---|---|---|---|---|---|
| 00.16 | 0.83587 | 0.83576 | 0.83566 | 0.83555 | 0.83544 | 0.83527 | 0.83516 | 0.83512 | 0.83511 |
| 00.18 | 0.81928 | 0.81917 | 0.81907 | 0.81895 | 0.81884 | 0.81865 | 0.81854 | 0.81850 | 0.81850 |
| 00.20 | 0.80336 | 0.80324 | 0.80312 | 0.80301 | 0.80289 | 0.80268 | 0.80256 | 0.80253 | 0.80253 |
| 00.22 | 0.78801 | 0.78788 | 0.78776 | 0.78764 | 0.78751 | 0.78728 | 0.78716 | 0.78712 | 0.78712 |
| 00.24 | 0.77319 | 0.77305 | 0.77292 | 0.77279 | 0.77265 | 0.77241 | 0.77227 | 0.77223 | 0.77224 |
| 00.26 | 0.75885 | 0.75871 | 0.75857 | 0.75843 | 0.75828 | 0.75802 | 0.75787 | 0.75784 | 0.75785 |
| 00.28 | 0.74497 | 0.74482 | 0.74467 | 0.74452 | 0.74437 | 0.74409 | 0.74393 | 0.74390 | 0.74391 |
| 00.30 | 0.73151 | 0.73136 | 0.73120 | 0.73105 | 0.73089 | 0.73059 | 0.73043 | 0.73039 | 0.73042 |
| 00.34 | 0.70582 | 0.70565 | 0.70548 | 0.70531 | 0.70514 | 0.70481 | 0.70464 | 0.70461 | 0.70464 |
| 00.38 | 0.68160 | 0.68142 | 0.68125 | 0.68107 | 0.68089 | 0.68054 | 0.68035 | 0.68033 | 0.68039 |
| 00.42 | 0.65875 | 0.65857 | 0.65839 | 0.65821 | 0.65802 | 0.65765 | 0.65746 | 0.65746 | 0.65753 |
| 00.46 | 0.63718 | 0.63700 | 0.63682 | 0.63663 | 0.63645 | 0.63606 | 0.63587 | 0.63589 | 0.63599 |
| 00.50 | 0.61680 | 0.61662 | 0.61645 | 0.61627 | 0.61609 | 0.61568 | 0.61549 | 0.61553 | 0.61566 |
| 00.54 | 0.59754 | 0.59736 | 0.59718 | 0.59701 | 0.59683 | 0.59641 | 0.59622 | 0.59627 | 0.59643 |
| 00.58 | 0.57929 | 0.57911 | 0.57893 | 0.57876 | 0.57858 | 0.57814 | 0.57795 | 0.57801 | 0.57819 |
| 00.62 | 0.56196 | 0.56178 | 0.56160 | 0.56142 | 0.56123 | 0.56077 | 0.56057 | 0.56065 | 0.56085 |
| 00.66 | 0.54546 | 0.54527 | 0.54509 | 0.54490 | 0.54471 | 0.54422 | 0.54401 | 0.54410 | 0.54432 |
| 00.70 | 0.52972 | 0.52952 | 0.52933 | 0.52913 | 0.52893 | 0.52842 | 0.52820 | 0.52830 | 0.52853 |
| 00.78 | 0.50029 | 0.50007 | 0.49985 | 0.49963 | 0.49942 | 0.49885 | 0.49861 | 0.49872 | 0.49898 |
| 00.86 | 0.47326 | 0.47302 | 0.47278 | 0.47254 | 0.47229 | 0.47167 | 0.47141 | 0.47153 | 0.47182 |
| 00.94 | 0.44833 | 0.44806 | 0.44779 | 0.44752 | 0.44726 | 0.44657 | 0.44628 | 0.44642 | 0.44674 |
| 01.02 | 0.42522 | 0.42492 | 0.42463 | 0.42434 | 0.42404 | 0.42330 | 0.42299 | 0.42314 | 0.42349 |
| 01.10 | 0.40373 | 0.40340 | 0.40308 | 0.40277 | 0.40246 | 0.40167 | 0.40135 | 0.40152 | 0.40191 |
| 01.18 | 0.38368 | 0.38334 | 0.38301 | 0.38269 | 0.38238 | 0.38155 | 0.38122 | 0.38144 | 0.38188 |
| 01.26 | 0.36498 | 0.36464 | 0.36431 | 0.36399 | 0.36369 | 0.36283 | 0.36251 | 0.36278 | 0.36328 |
| 01.34 | 0.34753 | 0.34719 | 0.34688 | 0.34658 | 0.34629 | 0.34541 | 0.34510 | 0.34542 | 0.34599 |
| 01.42 | 0.33124 | 0.33092 | 0.33062 | 0.33034 | 0.33006 | 0.32917 | 0.32887 | 0.32923 | 0.32986 |
| 01.50 | 0.31602 | 0.31571 | 0.31543 | 0.31516 | 0.31489 | 0.31397 | 0.31368 | 0.31409 | 0.31478 |
| 01.66 | 0.28833 | 0.28805 | 0.28779 | 0.28754 | 0.28730 | 0.28633 | 0.28606 | 0.28656 | 0.28738 |
| 01.82 | 0.26376 | 0.26350 | 0.26328 | 0.26307 | 0.26287 | 0.26188 | 0.26165 | 0.26227 | 0.26323 |
| 01.98 | 0.24184 | 0.24165 | 0.24150 | 0.24136 | 0.24123 | 0.24024 | 0.24008 | 0.24083 | 0.24195 |
| 02.14 | 0.22232 | 0.22223 | 0.22217 | 0.22212 | 0.22208 | 0.22112 | 0.22103 | 0.22193 | 0.22321 |
| 02.30 | 0.20498 | 0.20500 | 0.20505 | 0.20510 | 0.20516 | 0.20421 | 0.20419 | 0.20521 | 0.20664 |
| 02.46 | 0.18957 | 0.18972 | 0.18988 | 0.19003 | 0.19017 | 0.18921 | 0.18925 | 0.19038 | 0.19193 |
| 02.62 | 0.17589 | 0.17615 | 0.17640 | 0.17663 | 0.17684 | 0.17586 | 0.17592 | 0.17713 | 0.17878 |
| 02.78 | 0.16371 | 0.16406 | 0.16440 | 0.16468 | 0.16492 | 0.16390 | 0.16396 | 0.16524 | 0.16697 |
| 02.94 | 0.15283 | 0.15326 | 0.15364 | 0.15397 | 0.15423 | 0.15313 | 0.15318 | 0.15451 | 0.15631 |
| 03.10 | 0.14307 | 0.14355 | 0.14398 | 0.14432 | 0.14458 | 0.14340 | 0.14343 | 0.14480 | 0.14666 |
| 03.42 | 0.12636 | 0.12692 | 0.12737 | 0.12772 | 0.12795 | 0.12658 | 0.12655 | 0.12800 | 0.12999 |
| 03.74 | 0.11268 | 0.11326 | 0.11371 | 0.11403 | 0.11422 | 0.11264 | 0.11253 | 0.11404 | 0.11613 |
| 04.06 | 0.10135 | 0.10193 | 0.10235 | 0.10261 | 0.10273 | 0.10093 | 0.10072 | 0.10225 | 0.10439 |
| 04.38 | 0.09188 | 0.09242 | 0.09278 | 0.09296 | 0.09297 | 0.09093 | 0.09059 | 0.09210 | 0.09427 |
| 04.70 | 0.08384 | 0.08431 | 0.08458 | 0.08465 | 0.08454 | 0.08226 | 0.08178 | 0.08326 | 0.08544 |
| 05.02 | 0.07693 | 0.07730 | 0.07746 | 0.07741 | 0.07717 | 0.07466 | 0.07406 | 0.07551 | 0.07770 |
| 05.34 | 0.07090 | 0.07117 | 0.07121 | 0.07104 | 0.07068 | 0.06798 | 0.06727 | 0.06869 | 0.07090 |
| 05.66 | 0.06559 | 0.06575 | 0.06568 | 0.06540 | 0.06494 | 0.06208 | 0.06128 | 0.06269 | 0.06491 |
| 05.98 | 0.06088 | 0.06094 | 0.06076 | 0.06038 | 0.05983 | 0.05686 | 0.05600 | 0.05739 | 0.05963 |
| 06.30 | 0.05668 | 0.05664 | 0.05637 | 0.05591 | 0.05529 | 0.05224 | 0.05134 | 0.05272 | 0.05498 |
| 06.94 | 0.04952 | 0.04932 | 0.04892 | 0.04834 | 0.04763 | 0.04451 | 0.04359 | 0.04494 | 0.04720 |
| 07.58 | 0.04368 | 0.04338 | 0.04288 | 0.04224 | 0.04148 | 0.03841 | 0.03749 | 0.03880 | 0.04105 |
| 08.22 | 0.03886 | 0.03849 | 0.03795 | 0.03728 | 0.03651 | 0.03353 | 0.03265 | 0.03391 | 0.03613 |
| 08.86 | 0.03487 | 0.03446 | 0.03389 | 0.03322 | 0.03246 | 0.02960 | 0.02876 | 0.02997 | 0.03215 |
| 09.50 | 0.03154 | 0.03111 | 0.03054 | 0.02987 | 0.02914 | 0.02640 | 0.02561 | 0.02677 | 0.02891 |
| 10.14 | 0.02876 | 0.02833 | 0.02776 | 0.02710 | 0.02639 | 0.02376 | 0.02301 | 0.02415 | 0.02624 |
| 10.78 | 0.02644 | 0.02600 | 0.02543 | 0.02479 | 0.02409 | 0.02156 | 0.02086 | 0.02197 | 0.02403 |
| 11.42 | 0.02449 | 0.02404 | 0.02347 | 0.02284 | 0.02216 | 0.01971 | 0.01904 | 0.02015 | 0.02217 |
| 12.06 | 0.02284 | 0.02238 | 0.02180 | 0.02118 | 0.02053 | 0.01814 | 0.01750 | 0.01860 | 0.02059 |
| 12.70 | 0.02143 | 0.02095 | 0.02037 | 0.01975 | 0.01912 | 0.01680 | 0.01619 | 0.01729 | 0.01924 |

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U(X) X TA 73   W  74   RE 75   OS 76   IR 77   PT 78   AU 79   HG 80   TL 81
 13.98 0.01913 0.01862 0.01803 0.01743 0.01683 0.01462 0.01407 0.01517 0.01701
 15.26 0.01732 0.01677 0.01618 0.01560 0.01504 0.01296 0.01266 0.01353 0.01526
 16.54 0.01582 0.01525 0.01467 0.01412 0.01359 0.01282 0.01266 0.01250 0.01382
 17.82 0.01454 0.01397 0.01340 0.01316 0.01299 0.01282 0.01266 0.01250 0.01262
 19.10 0.01370 0.01351 0.01333 0.01316 0.01299 0.01282 0.01266 0.01250 0.01235
 20.38 0.01370 0.01351 0.01333 0.01316 0.01299 0.01282 0.01266 0.01250 0.01235
 21.66 0.01370 0.01351 0.01333 0.01316 0.01299 0.01282 0.01266 0.01250 0.01235
 22.94 0.01370 0.01351 0.01333 0.01316 0.01299 0.01282 0.01266 0.01250 0.01235
 24.22 0.01370 0.01351 0.01333 0.01316 0.01299 0.01282 0.01266 0.01250 0.01235
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  4574.0  4705.8  4839.4  4974.9  5112.3  5251.3  5392.1  5535.7  5681.5
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  753.08  777.29  801.90  826.92  852.34  877.83  903.98  930.98  958.55
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  722.62  746.32  770.42  794.92  819.83  844.80  870.43  896.92  923.96
 SHELL (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  172.04  178.55  185.20  191.99  198.92  205.65  212.81  220.49  228.47
 SHELL (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  157.75  163.97  170.33  176.82  183.45  189.88  196.75  204.12  211.80
 SHELL (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10
 (-E)  130.89  136.56  142.36  148.29  154.35  160.22  166.52  173.33  180.43
 SHELL (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2
 (-E)  34.597  36.367  38.185  40.048  41.956  43.580  455.57  47.934  50.513
 SHELL (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6
 (-E)  28.594  30.199  31.851  33.547  35.287  36.740  38.546  40.746  43.155
 SHELL (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10
 (-E)  17.593  18.875  20.201  21.568  22.976  24.095  25.565  27.430  29.495
 SHELL (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14
 (-E)  3.199   3.961   4.765   5.610   6.497   7.095   8.044   9.386   10.927
 SHELL (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2
 (-E)  4.8525  5.2126  5.5715  5.9297  6.2892  6.3498  6.6945  7.3714  8.1999
 SHELL (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6
 (-E)  3.1151  3.3875  3.6583  3.9281  4.1986  4.1816  4.4370  5.0123  5.7368
 SHELL (5D) 3  (5D)4   (5D) 5  (5D) 6  (5D) 7  (5D)10  (5D)10  (5D)10  (5D)10
 (-E)  0.5875  0.6841  0.7806  0.8771  0.9745  0.873   0.9200  1.2703  1.7644
 SHELL (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 1  (6S) 1  (6S) 2  (6S) 2
 (-E)  0.4664  0.4858  0.5027  0.5177  0.5311  0.4693  0.4775  0.5653  0.7302
 SHELL (6P) 0  (6P) 0  (6P) 0  (6P) 0  (6P) 0  (6P) 0  (6P) 0  (6P) 0  (6P) 1
 (-E)  0.      0.      0.      0.      0.      0.      0.      0.      0.3393
U(X) X PB 82   BI 83   PO 84   AT 85   RN 86   FR 87   RA 88   AC 89   TH 90
   X      U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
 01.01 0.98832 0.98831 0.98830 0.98829 0.98827 0.98827 0.98826 0.98825 0.98824
 00.02 0.97649 0.97647 0.97644 0.97642 0.97640 0.97639 0.97637 0.97636 0.97634
 00.03 0.96476 0.96473 0.96469 0.96466 0.96463 0.96462 0.96460 0.96458 0.96456
 00.04 0.95324 0.95320 0.95316 0.95313 0.95310 0.95308 0.95306 0.95304 0.95302
 00.05 0.94198 0.94194 0.94190 0.94187 0.94183 0.94181 0.94180 0.94178 0.94176
 00.06 0.93100 0.93096 0.93092 0.93088 0.93084 0.93083 0.93082 0.93080 0.93078
 00.07 0.92029 0.92025 0.92021 0.92017 0.92013 0.92013 0.92012 0.92010 0.92009
 00.08 0.90985 0.90981 0.90977 0.90973 0.90969 0.90969 0.90969 0.90968 0.90966
 00.09 0.89966 0.89962 0.89959 0.89955 0.89952 0.89952 0.89953 0.89952 0.89951
 00.10 0.88973 0.88969 0.88966 0.88963 0.88960 0.88961 0.88962 0.88962 0.88962
 00.12 0.87061 0.87059 0.87056 0.87054 0.87052 0.87055 0.87058 0.87059 0.87060
 00.14 0.85244 0.85242 0.85241 0.85239 0.85238 0.85243 0.85248 0.85251 0.85253
 00.16 0.83510 0.83510 0.83509 0.83508 0.83508 0.83515 0.83522 0.83525 0.83529
 00.18 0.81850 0.81850 0.81850 0.81850 0.81850 0.81858 0.81866 0.81871 0.81875
 00.20 0.80253 0.80253 0.80254 0.80254 0.80255 0.80264 0.80273 0.80279 0.80284
 00.22 0.78713 0.78713 0.78714 0.78715 0.78716 0.78726 0.78737 0.78744 0.78749
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| U(X) X | PB 82 | BI 83 | PO 84 | AT 85 | RN 86 | FR 87 | RA 88 | AC 89 | TH 90 |
|---|---|---|---|---|---|---|---|---|---|
| 00.24 | 0.77225 | 0.77226 | 0.77227 | 0.77228 | 0.77230 | 0.77241 | 0.77254 | 0.77261 | 0.77267 |
| 00.26 | 0.75786 | 0.75787 | 0.78789 | 0.75791 | 0.75793 | 0.75806 | 0.75819 | 0.75827 | 0.75835 |
| 00.28 | 0.74393 | 0.74395 | 0.74397 | 0.74399 | 0.74402 | 0.74416 | 0.74431 | 0.74440 | 0.74449 |
| 00.30 | 0.73044 | 0.73046 | 0.73049 | 0.73052 | 0.73055 | 0.73071 | 0.73087 | 0.73097 | 0.73107 |
| 00.34 | 0.70468 | 0.70472 | 0.70476 | 0.70480 | 0.70485 | 0.70504 | 0.70524 | 0.70536 | 0.70548 |
| 00.38 | 0.68044 | 0.68049 | 0.68055 | 0.68062 | 0.68068 | 0.68091 | 0.68115 | 0.68130 | 0.68145 |
| 00.42 | 0.65761 | 0.65769 | 0.65777 | 0.65786 | 0.65795 | 0.65822 | 0.65849 | 0.65869 | 0.65887 |
| 00.46 | 0.63609 | 0.63620 | 0.63631 | 0.63642 | 0.63654 | 0.63685 | 0.63717 | 0.63740 | 0.63761 |
| 00.50 | 0.61578 | 0.61592 | 0.61605 | 0.61619 | 0.61633 | 0.61669 | 0.61705 | 0.61731 | 0.61756 |
| 00.54 | 0.59658 | 0.59674 | 0.59689 | 0.59706 | 0.59722 | 0.59762 | 0.59802 | 0.59831 | 0.59858 |
| 00.58 | 0.57836 | 0.57854 | 0.57872 | 0.57890 | 0.57908 | 0.57952 | 0.57995 | 0.58027 | 0.58057 |
| 00.62 | 0.56103 | 0.56123 | 0.56143 | 0.56163 | 0.56183 | 0.56230 | 0.56277 | 0.56311 | 0.56344 |
| 00.66 | 0.54452 | 0.54473 | 0.54495 | 0.54516 | 0.54538 | 0.54588 | 0.54638 | 0.54675 | 0.54710 |
| 00.70 | 0.52875 | 0.52898 | 0.52921 | 0.52944 | 0.52967 | 0.53020 | 0.53074 | 0.53113 | 0.53151 |
| 00.78 | 0.49923 | 0.49949 | 0.49974 | 0.50001 | 0.50027 | 0.50086 | 0.50147 | 0.50191 | 0.50233 |
| 00.86 | 0.47209 | 0.47238 | 0.47266 | 0.47295 | 0.47324 | 0.47390 | 0.47457 | 0.47505 | 0.47552 |
| 00.94 | 0.44703 | 0.44735 | 0.44766 | 0.44798 | 0.44830 | 0.44903 | 0.44976 | 0.45030 | 0.45082 |
| 01.02 | 0.42382 | 0.42417 | 0.42452 | 0.42487 | 0.42524 | 0.42604 | 0.42685 | 0.42745 | 0.42803 |
| 01.10 | 0.40229 | 0.40268 | 0.40308 | 0.40348 | 0.40390 | 0.40479 | 0.40568 | 0.40636 | 0.40701 |
| 01.18 | 0.38231 | 0.38276 | 0.38322 | 0.38368 | 0.38416 | 0.38514 | 0.38613 | 0.38688 | 0.38761 |
| 01.26 | 0.36377 | 0.36428 | 0.36480 | 0.36533 | 0.36586 | 0.36694 | 0.36802 | 0.36885 | 0.36965 |
| 01.34 | 0.34654 | 0.34711 | 0.34769 | 0.34828 | 0.34887 | 0.35003 | 0.35120 | 0.35210 | 0.35297 |
| 01.42 | 0.33047 | 0.33110 | 0.33174 | 0.33238 | 0.33303 | 0.33428 | 0.33554 | 0.33651 | 0.33744 |
| 01.50 | 0.31545 | 0.31614 | 0.31683 | 0.31752 | 0.31823 | 0.31957 | 0.32092 | 0.32196 | 0.32296 |
| 01.66 | 0.28817 | 0.28898 | 0.28979 | 0.29061 | 0.29144 | 0.29297 | 0.29450 | 0.29570 | 0.29685 |
| 01.82 | 0.26416 | 0.26511 | 0.26606 | 0.26702 | 0.26798 | 0.26971 | 0.27144 | 0.27279 | 0.27408 |
| 01.98 | 0.24304 | 0.24414 | 0.24524 | 0.24633 | 0.24742 | 0.24934 | 0.25125 | 0.25273 | 0.25415 |
| 02.14 | 0.22445 | 0.22569 | 0.22691 | 0.22813 | 0.22933 | 0.23141 | 0.23347 | 0.23507 | 0.23659 |
| 02.30 | 0.20802 | 0.20937 | 0.21070 | 0.21201 | 0.21330 | 0.21552 | 0.21771 | 0.21940 | 0.22099 |
| 02.46 | 0.19341 | 0.19486 | 0.19627 | 0.19765 | 0.19899 | 0.20133 | 0.20364 | 0.20540 | 0.20706 |
| 02.62 | 0.18035 | 0.18186 | 0.18334 | 0.18478 | 0.18617 | 0.18862 | 0.19103 | 0.19286 | 0.19458 |
| 02.78 | 0.16860 | 0.17018 | 0.17171 | 0.17319 | 0.17463 | 0.17719 | 0.17971 | 0.18161 | 0.18340 |
| 02.94 | 0.15800 | 0.15964 | 0.16122 | 0.16275 | 0.16424 | 0.16691 | 0.16953 | 0.17150 | 0.17333 |
| 03.10 | 0.14842 | 0.15011 | 0.15174 | 0.15333 | 0.15485 | 0.15762 | 0.16034 | 0.16235 | 0.16422 |
| 03.42 | 0.13186 | 0.13364 | 0.13536 | 0.13700 | 0.13857 | 0.14149 | 0.14433 | 0.14638 | 0.14827 |
| 03.74 | 0.11807 | 0.11990 | 0.12164 | 0.12328 | 0.12482 | 0.12783 | 0.13074 | 0.13278 | 0.13462 |
| 04.06 | 0.10635 | 0.10818 | 0.10990 | 0.11149 | 0.11298 | 0.11604 | 0.11898 | 0.12097 | 0.12275 |
| 04.38 | 0.09622 | 0.09803 | 0.09969 | 0.10123 | 0.10264 | 0.10574 | 0.10870 | 0.11065 | 0.11235 |
| 04.70 | 0.08738 | 0.08915 | 0.09077 | 0.09224 | 0.09356 | 0.09670 | 0.09968 | 0.10157 | 0.10320 |
| 05.02 | 0.07963 | 0.08136 | 0.08293 | 0.08432 | 0.08556 | 0.08873 | 0.09172 | 0.09355 | 0.09510 |
| 05.34 | 0.07281 | 0.07451 | 0.07602 | 0.07734 | 0.07848 | 0.08168 | 0.08469 | 0.08645 | 0.08792 |
| 05.66 | 0.06681 | 0.06847 | 0.06991 | 0.07116 | 0.07220 | 0.07542 | 0.07845 | 0.08015 | 0.08155 |
| 05.98 | 0.06152 | 0.06313 | 0.06451 | 0.06566 | 0.06661 | 0.06987 | 0.07293 | 0.07458 | 0.07591 |
| 06.30 | 0.05684 | 0.05839 | 0.05970 | 0.06077 | 0.06163 | 0.06493 | 0.06803 | 0.06964 | 0.07091 |
| 06.94 | 0.04899 | 0.05043 | 0.05159 | 0.05252 | 0.05324 | 0.05666 | 0.05985 | 0.06138 | 0.06255 |
| 07.58 | 0.04275 | 0.04407 | 0.04512 | 0.04594 | 0.04657 | 0.05013 | 0.05338 | 0.05480 | 0.05582 |
| 08.22 | 0.03774 | 0.03896 | 0.03992 | 0.04067 | 0.04123 | 0.04488 | 0.04814 | 0.04940 | 0.05024 |
| 08.86 | 0.03368 | 0.03484 | 0.03573 | 0.03641 | 0.03687 | 0.04057 | 0.04377 | 0.04484 | 0.04548 |
| 09.50 | 0.03038 | 0.03148 | 0.03231 | 0.03289 | 0.03324 | 0.03694 | 0.04003 | 0.04090 | 0.04135 |
| 10.14 | 0.02766 | 0.02870 | 0.02945 | 0.02993 | 0.03016 | 0.03382 | 0.03677 | 0.03746 | 0.03774 |
| 10.78 | 0.02540 | 0.02638 | 0.02703 | 0.02740 | 0.02750 | 0.03111 | 0.03390 | 0.03442 | 0.03456 |
| 11.42 | 0.02350 | 0.02440 | 0.02495 | 0.02520 | 0.02518 | 0.02872 | 0.03135 | 0.03173 | 0.03176 |
| 12.06 | 0.02186 | 0.02268 | 0.02312 | 0.02326 | 0.02315 | 0.02660 | 0.02906 | 0.02933 | 0.02928 |
| 12.70 | 0.02044 | 0.02117 | 0.02151 | 0.02155 | 0.02135 | 0.02471 | 0.02701 | 0.02719 | 0.02708 |
| 13.98 | 0.01808 | 0.01862 | 0.01878 | 0.01865 | 0.01833 | 0.02147 | 0.02350 | 0.02360 | 0.02344 |
| 15.26 | 0.01618 | 0.01655 | 0.01655 | 0.01630 | 0.01588 | 0.01881 | 0.02068 | 0.02078 | 0.02061 |
| 16.54 | 0.01459 | 0.01481 | 0.01469 | 0.01435 | 0.01388 | 0.01659 | 0.01847 | 0.01860 | 0.01842 |
| 17.82 | 0.01325 | 0.01334 | 0.01311 | 0.01271 | 0.01220 | 0.01477 | 0.01677 | 0.01691 | 0.01672 |

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U(X) X PB 82    BI 83   PO 84   AT 85   RN 86   FR 87   RA 88   AC 89   TH 90
 19.10 0.01220 0.01208 0.01190 0.01176 0.01163 0.01329 0.01548 0.01559 0.01535
 20.38 0.01220 0.01205 0.01190 0.01176 0.01163 0.01214 0.01449 0.01451 0.01422
 21.66 0.01220 0.01205 0.01190 0.01176 0.01163 0.01149 0.01368 0.01361 0.01326
 22.94 0.01220 0.01205 0.01190 0.01176 0.01163 0.01149 0.01300 0.01283 0.01242
 24.22 0.01220 0.01205 0.01190 0.01176 0.01163 0.01149 0.01239 0.01213 0.01167
 25.50 0.01220 0.01205 0.01190 0.01176 0.01163 0.01149 0.01184 0.01149 0.01111
 28.06 0.01220 0.01205 0.01190 0.01176 0.01163 0.01149 0.01136 0.01124 0.01111
 30.62 0.01220 0.01205 0.01190 0.01176 0.01163 0.01149 0.01136 0.01124 0.01111
 33.18 0.01220 0.01205 0.01190 0.01176 0.01163 0.01149 0.01136 0.01124 0.01111
 35.74 0.01220 0.01205 0.01190 0.01176 0.01163 0.01149 0.01136 0.01124 0.01111
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  5828.9  5978.1  6129.5  6282.6  6437.8  6595.2  6754.1  6915.0  7077.8
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  986.5   1014.9  1043.7  1073.0  1102.7  1133.1  1164.0  1195.2  1226.8
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  951.4   979.2   1007.5  1036.3  1065.4  1095.4  1125.8  1156.4  1187.5
 SHELL (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  236.59  244.87  253.31  261.91  270.67  279.97  289.43  298.89  308.49
 SHELL (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  219.61  227.59  235.72  244.02  252.48  261.46  270.62  279.77  289.06
 SHELL (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10
 (-E)  187.67  195.07  202.63  210.35  218.22  226.62  235.20  243.77  252.48
 SHELL (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2
 (-E)  53.147  55.847  58.611  61.443  64.342  67.675  71.087  74.394  77.750
 SHELL (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6
 (-E)  45.614  48.137  50.724  53.377  56.097  59.249  62.481  65.607  68.780
 SHELL (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10
 (-E)  31.612  33.790  36.032  38.338  40.708  43.510  46.392  49.165  51.985
 SHELL (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14
 (-E)  12.521  14.175  15.893  17.674  19.520  21.797  24.154  26.402  28.697
 SHELL (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2
 (-E)  9.030   9.874   10.736  11.617  12.517  13.802  15.118  16.281  17.447
 SHELL (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6
 (-E)  6.461   7.198   7.952   8.724   9.515   10.689  11.895  12.946  14.000
 SHELL (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10
 (-E)  2.2588  2.7670  3.2927  3.8377  4.4020  5.3476  6.3248  7.1470  7.9729
 SHELL (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2
 (-E)  0.8889  1.0423  1.1934  1.3435  1.4930  1.9516  2.4019  2.6951  2.9759
 SHELL (6P) 2  (6P) 3  (6P) 4  (6P) 5  (6P) 6  (6P) 6  (6P) 6  (6P) 6  (6P) 6
 (-E)  0.4246  0.5133  0.6035  0.6948  0.7867  1.1573  1.5258  1.7506  1.9652
 SHELL (6D) 0  (6D) 0  (6D) 0  (6D) 0  (6D) 0  (6D) 0  (6D) 0  (6D) 1  (6D) 2
 (-E)  0.      0.      0.      0.      0.      0.      0.      0.4294  0.5158
 SHELL (7S) 0  (7S) 0  (7S) 0  (7S) 0  (7S) 0  (7S) 1  (7S) 2  (7S) 2  (7S) 2
 (-E)  0.      0.      0.      0.      0.      0.2506  0.3119  0.3408  0.3642
U(X) X PA 91    U  92   NP 93   PU 94   AM 95   CM 96   BK 97   CF 98   E  99
   X     U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)    U(X)
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
 00.01 0.98822 0.98821 0.98819 0.98817 0.98816 0.98815 0.98813 0.98812 0.98810
 00.02 0.97630 0.97628 0.97625 0.97621 0.97619 0.97617 0.97614 0.97611 0.97608
 00.03 0.96451 0.96447 0.96444 0.96439 0.96435 0.96433 0.96429 0.96425 0.96421
 00.04 0.95296 0.95292 0.95287 0.95281 0.95276 0.95274 0.95269 0.95264 0.95260
 00.05 0.94169 0.94164 0.94159 0.94152 0.94147 0.94144 0.94139 0.94133 0.94128
 00.06 0.93070 0.93065 0.93060 0.93052 0.93046 0.93043 0.93037 0.93032 0.93026
 00.07 0.92000 0.91995 0.91989 0.91980 0.91974 0.91971 0.91965 0.91959 0.91952
 00.08 0.90957 0.90951 0.90946 0.90936 0.90930 0.90927 0.90921 0.90914 0.90907
 00.09 0.89941 0.89935 0.89929 0.89919 0.89913 0.89910 0.89904 0.89897 0.89890
 00.10 0.88951 0.88946 0.88940 0.88929 0.88923 0.88921 0.88914 0.88907 0.88900
 00.12 0.87049 0.87044 0.87038 0.87026 0.87020 0.87019 0.87012 0.87005 0.86997
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| U(X) X | PA 91 | U 92 | NP 93 | PU 94 | AM 95 | CM 96 | BK 97 | CF 98 | E 99 |
|---|---|---|---|---|---|---|---|---|---|
| 00.14 | 0.85242 | 0.85236 | 0.85231 | 0.85218 | 0.85212 | 0.85211 | 0.85204 | 0.85197 | 0.85189 |
| 00.16 | 0.83516 | 0.83511 | 0.83505 | 0.83491 | 0.83485 | 0.83485 | 0.83477 | 0.83469 | 0.83461 |
| 00.18 | 0.81862 | 0.81856 | 0.81850 | 0.81835 | 0.81827 | 0.81828 | 0.81820 | 0.81811 | 0.81802 |
| 00.20 | 0.80269 | 0.80263 | 0.80257 | 0.80240 | 0.80232 | 0.80233 | 0.80224 | 0.80215 | 0.80205 |
| 00.22 | 0.78734 | 0.78727 | 0.78720 | 0.78702 | 0.78693 | 0.78695 | 0.78685 | 0.78675 | 0.78664 |
| 00.24 | 0.77250 | 0.77244 | 0.77236 | 0.77217 | 0.77208 | 0.77209 | 0.77199 | 0.77188 | 0.77177 |
| 00.26 | 0.75816 | 0.75810 | 0.75802 | 0.75781 | 0.75771 | 0.75773 | 0.75763 | 0.75751 | 0.75739 |
| 00.28 | 0.74429 | 0.74422 | 0.74414 | 0.74392 | 0.74382 | 0.74385 | 0.74373 | 0.74361 | 0.74348 |
| 00.30 | 0.73086 | 0.73079 | 0.73071 | 0.73047 | 0.73037 | 0.73040 | 0.73029 | 0.73016 | 0.73003 |
| 00.34 | 0.70526 | 0.70519 | 0.70510 | 0.70485 | 0.70474 | 0.70479 | 0.70467 | 0.70453 | 0.70439 |
| 00.38 | 0.68122 | 0.68115 | 0.68107 | 0.68079 | 0.68068 | 0.68075 | 0.68063 | 0.68049 | 0.68034 |
| 00.42 | 0.65862 | 0.65856 | 0.65848 | 0.65819 | 0.65808 | 0.65817 | 0.65805 | 0.65791 | 0.65776 |
| 00.46 | 0.63735 | 0.63730 | 0.63723 | 0.63691 | 0.63681 | 0.63692 | 0.63679 | 0.63665 | 0.63650 |
| 00.50 | 0.61728 | 0.61723 | 0.61717 | 0.61683 | 0.61672 | 0.61686 | 0.61672 | 0.61657 | 0.61641 |
| 00.54 | 0.59829 | 0.59824 | 0.59817 | 0.59781 | 0.59770 | 0.59785 | 0.59771 | 0.59755 | 0.59738 |
| 00.58 | 0.58026 | 0.58021 | 0.58014 | 0.57975 | 0.57963 | 0.57980 | 0.57965 | 0.57948 | 0.57929 |
| 00.62 | 0.56310 | 0.56305 | 0.56298 | 0.56256 | 0.56244 | 0.56261 | 0.56245 | 0.56227 | 0.56208 |
| 00.66 | 0.54674 | 0.54669 | 0.54661 | 0.54617 | 0.54604 | 0.54623 | 0.54606 | 0.54587 | 0.54566 |
| 00.70 | 0.53113 | 0.53107 | 0.53099 | 0.53052 | 0.53038 | 0.53058 | 0.53040 | 0.53020 | 0.52998 |
| 00.78 | 0.50190 | 0.50184 | 0.50175 | 0.50122 | 0.50107 | 0.50130 | 0.50111 | 0.50089 | 0.50065 |
| 00.86 | 0.47505 | 0.47499 | 0.47489 | 0.47432 | 0.47416 | 0.47443 | 0.47422 | 0.47399 | 0.47374 |
| 00.94 | 0.45032 | 0.45026 | 0.45017 | 0.44956 | 0.44940 | 0.44971 | 0.44951 | 0.44928 | 0.44903 |
| 01.02 | 0.42751 | 0.42747 | 0.42739 | 0.42676 | 0.42662 | 0.42698 | 0.42678 | 0.42656 | 0.42632 |
| 01.10 | 0.40648 | 0.40647 | 0.40642 | 0.40577 | 0.40564 | 0.40605 | 0.40587 | 0.40566 | 0.40543 |
| 01.18 | 0.38707 | 0.38708 | 0.38705 | 0.38639 | 0.38628 | 0.38674 | 0.38658 | 0.38637 | 0.38615 |
| 01.26 | 0.36910 | 0.36914 | 0.36913 | 0.36844 | 0.36834 | 0.36886 | 0.36870 | 0.36851 | 0.36829 |
| 01.34 | 0.35241 | 0.35247 | 0.35248 | 0.35177 | 0.35169 | 0.35225 | 0.35210 | 0.35192 | 0.35170 |
| 01.42 | 0.33687 | 0.33695 | 0.33698 | 0.33626 | 0.33619 | 0.33680 | 0.33666 | 0.33648 | 0.33627 |
| 01.50 | 0.32238 | 0.32249 | 0.32254 | 0.32180 | 0.32174 | 0.32241 | 0.32228 | 0.32211 | 0.32190 |
| 01.66 | 0.29626 | 0.29642 | 0.29652 | 0.29574 | 0.29572 | 0.29649 | 0.29637 | 0.29621 | 0.29600 |
| 01.82 | 0.27348 | 0.27369 | 0.27383 | 0.27300 | 0.27299 | 0.27383 | 0.27371 | 0.27352 | 0.27328 |
| 01.98 | 0.25352 | 0.25375 | 0.25390 | 0.25299 | 0.25296 | 0.25385 | 0.25369 | 0.25346 | 0.25316 |
| 02.14 | 0.23589 | 0.23612 | 0.23625 | 0.23523 | 0.23516 | 0.23608 | 0.23586 | 0.23556 | 0.23519 |
| 02.30 | 0.22020 | 0.22040 | 0.22049 | 0.21936 | 0.21923 | 0.22017 | 0.21988 | 0.21951 | 0.21908 |
| 02.46 | 0.20616 | 0.20633 | 0.20638 | 0.20511 | 0.20493 | 0.20590 | 0.20555 | 0.20512 | 0.20462 |
| 02.62 | 0.19358 | 0.19371 | 0.19372 | 0.19232 | 0.19209 | 0.19308 | 0.19267 | 0.19217 | 0.19160 |
| 02.78 | 0.18228 | 0.18237 | 0.18233 | 0.18080 | 0.18050 | 0.18150 | 0.18102 | 0.18045 | 0.17979 |
| 02.94 | 0.17209 | 0.17213 | 0.17203 | 0.17035 | 0.16998 | 0.17098 | 0.17041 | 0.16973 | 0.16898 |
| 03.10 | 0.16284 | 0.16281 | 0.16263 | 0.16079 | 0.16033 | 0.16131 | 0.16064 | 0.15987 | 0.15901 |
| 03.42 | 0.14658 | 0.14638 | 0.14601 | 0.14384 | 0.14318 | 0.14410 | 0.14324 | 0.14228 | 0.14124 |
| 03.74 | 0.13261 | 0.13223 | 0.13167 | 0.12920 | 0.12837 | 0.12925 | 0.12823 | 0.12712 | 0.12595 |
| 04.06 | 0.12047 | 0.11992 | 0.11921 | 0.11649 | 0.11553 | 0.11639 | 0.11526 | 0.11407 | 0.11282 |
| 04.38 | 0.10985 | 0.10917 | 0.10834 | 0.10544 | 0.10439 | 0.10525 | 0.10406 | 0.10282 | 0.10154 |
| 04.70 | 0.10053 | 0.09975 | 0.09884 | 0.09582 | 0.09472 | 0.09558 | 0.09437 | 0.09311 | 0.09183 |
| 05.02 | 0.09233 | 0.09148 | 0.09052 | 0.08744 | 0.08632 | 0.08718 | 0.08597 | 0.08473 | 0.08347 |
| 05.34 | 0.08510 | 0.08421 | 0.08321 | 0.08012 | 0.07900 | 0.07987 | 0.07868 | 0.07746 | 0.07624 |
| 05.66 | 0.07872 | 0.07781 | 0.07681 | 0.07373 | 0.07262 | 0.07350 | 0.07234 | 0.07116 | 0.06998 |
| 05.98 | 0.07309 | 0.07217 | 0.07118 | 0.06814 | 0.06705 | 0.06793 | 0.06680 | 0.06567 | 0.06454 |
| 06.30 | 0.06813 | 0.06721 | 0.06623 | 0.06323 | 0.06218 | 0.06305 | 0.06196 | 0.06087 | 0.05978 |
| 06.94 | 0.05984 | 0.05893 | 0.05797 | 0.05509 | 0.05409 | 0.05493 | 0.05391 | 0.05290 | 0.05190 |
| 07.58 | 0.05321 | 0.05231 | 0.05136 | 0.04864 | 0.04769 | 0.04846 | 0.04750 | 0.04656 | 0.04564 |
| 08.22 | 0.04776 | 0.04685 | 0.04593 | 0.04339 | 0.04249 | 0.04316 | 0.04227 | 0.04140 | 0.04056 |
| 08.86 | 0.04316 | 0.04226 | 0.04137 | 0.03903 | 0.03818 | 0.03875 | 0.03792 | 0.03712 | 0.03635 |
| 09.50 | 0.03921 | 0.03834 | 0.03748 | 0.03534 | 0.03455 | 0.03502 | 0.03425 | 0.03351 | 0.03280 |
| 10.14 | 0.03578 | 0.03494 | 0.03412 | 0.03219 | 0.03144 | 0.03182 | 0.03111 | 0.03043 | 0.02978 |
| 10.78 | 0.03278 | 0.03198 | 0.03120 | 0.02945 | 0.02875 | 0.02905 | 0.02840 | 0.02777 | 0.02718 |
| 11.42 | 0.03014 | 0.02937 | 0.02865 | 0.02706 | 0.02641 | 0.02664 | 0.02604 | 0.02546 | 0.02492 |
| 12.06 | 0.02780 | 0.02708 | 0.02640 | 0.02495 | 0.02434 | 0.02454 | 0.02398 | 0.02346 | 0.02296 |

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U(X) X PA 91    U  92    NP 93    PU 94    AM 95    CM 96    BK 97    CF 98    E  99
 12.70 0.02574 0.02506 0.02442 0.02308 0.02252 0.02270 0.02219 0.02170 0.02125
 13.98 0.02230 0.02171 0.02116 0.01999 0.01951 0.01969 0.01927 0.01886 0.01848
 15.26 0.01964 0.01913 0.01867 0.01762 0.01721 0.01743 0.01708 0.01674 0.01643
 16.54 0.01761 0.01718 0.01678 0.01584 0.01550 0.01574 0.01544 0.01516 0.01489
 17.82 0.01605 0.01568 0.01534 0.01454 0.01425 0.01445 0.01419 0.01395 0.01372
 19.10 0.01483 0.01450 0.01421 0.01355 0.01330 0.01342 0.01320 0.01298 0.01278
 20.38 0.01384 0.01354 0.01328 0.01277 0.01255 0.01257 0.01237 0.01217 0.01198
 21.66 0.01299 0.01272 0.01248 0.01211 0.01191 0.01183 0.01164 0.01146 0.01129
 22.94 0.01225 0.01200 0.01178 0.01153 0.01134 0.01118 0.01100 0.01083 0.01067
 24.22 0.01159 0.01136 0.01115 0.01101 0.01083 0.01058 0.01042 0.01026 0.01010
 25.50 0.01099 0.01087 0.01075 0.01064 0.01053 0.01042 0.01031 0.01020 0.01010
 28.06 0.01099 0.01087 0.01075 0.01064 0.01053 0.01042 0.01031 0.01020 0.01010
 30.62 0.01099 0.01087 0.01075 0.01064 0.01053 0.01042 0.01031 0.01020 0.01010
 33.18 0.01099 0.01087 0.01075 0.01064 0.01053 0.01042 0.01031 0.01020 0.01010
 35.74 0.01099 0.01087 0.01075 0.01064 0.01053 0.01042 0.01031 0.01020 0.01010
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  7242.8  7409.2  2577.5  7747.2  7919.2  8093.6  8269.4  8447.2  8626.8
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  1218.1  1249.5  1281.3  1313.1  1345.6  1379.1  1412.4  1446.2  1480.4
 SHELL (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  317.28  326.64  336.10  345.20  354.89  365.21  375.21  385.21  395.39
 SHELL (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  297.53  306.58  315.73  324.52  333.89  343.89  353.52  363.26  373.12
 SHELL (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10
 (-E)  260.35  268.81  277.37  285.56  294.34  303.75  312.77  321.92  331.18
 SHELL (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2
 (-E)  80.22   83.16   86.12   88.63   91.63   95.16   98.23   101.33  104.46
 SHELL (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6
 (-E)  71.064  73.819  76.594  78.918  81.734  85.078  87.960  90.873  93.815
 SHELL (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10
 (-E)  53.910  56.308  58.725  60.689  63.143  66.126  68.644  71.192  73.768
 SHELL (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14
 (-E)  30.088  31.954  33.838  35.265  37.184  39.633  41.613  43.622  45.657
 SHELL (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2
 (-E)  17.767  18.490  19.205  19.467  20.157  21.308  22.002  22.695  23.385
 SHELL (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6
 (-E)  14.224  14.844  15.456  15.623  16.209  17.251  17.842  18.432  19.019
 SHELL (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10
 (-E)  8.019   8.438   8.850   8.838   9.226   10.050  10.443  10.834  11.222
 SHELL (5F) 2  (5F) 2  (5F) 2  (5F) 2  (5F) 2  (5F) 2  (5F) 2  (5F) 2  (5F) 2
 (-E)  1.0672  1.1830  1.2952  1.0727  1.1654  1.6156  1.7179  1.8190  1.9181
 SHELL (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2
 (-E)  2.8808  2.9631  3.0399  2.9033  2.9680  3.2515  3.3164  3.3795  3.4409
 SHELL (6P) 6  (6P) 6  (6P) 6  (6P) 6  (6P) 6  (6P) 6  (6P) 6  (6P) 6  (6P) 6
 (-E)  1.8678  1.9181  1.9639  1.8311  1.8674  2.0876  2.1241  2.1595  2.1934
 SHELL (6D) 1  (6D) 1  (6D) 1  (6D) 0  (6D) 0  (6D) 1  (6D) 1  (6D) 1  (6D) 1
 (-E)  0.4449  0.4494  0.4516  0.      0.      0.4540  0.4526  0.4512  0.4490
 SHELL (7S) 2  (7S) 2  (7S) 2  (7S) 2  (7S) 2  (7S) 2  (7S) 2  (7S) 2  (7S) 2
 (-E)  0.3492  0.3530  0.3564  0.3357  0.3387  0.3661  0.3690  0.3720  0.3749
U(X) X NI 28    CE 58    TB 65    BK 97    CF 98    E  99    FM100    MV101    NO102
 00.00 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
 00.01 0.99006 0.98893 0.98872 0.98813 0.98811 0.98810 0.98808 0.98807 0.98805
 00.02 0.97988 0.97766 0.97725 0.97613 0.97610 0.97607 0.97604 0.97602 0.97599
 00.03 0.96959 0.96640 0.96582 0.96427 0.96424 0.96420 0.96416 0.96412 0.96408
 00.04 0.95928 0.95527 0.95455 0.95267 0.95263 0.95258 0.95253 0.95248 0.95244
 00.05 0.94903 0.94435 0.94350 0.94136 0.94131 0.94126 0.94120 0.94115 0.94109
 00.06 0.93887 0.93365 0.93270 0.93035 0.93029 0.93023 0.93017 0.93011 0.93005
 00.07 0.92885 0.92319 0.92215 0.91962 0.91955 0.91949 0.91943 0.91936 0.91929
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| U(X) X | NI 28 | CE 58 | TB 65 | BK 97 | CF 98 | E 99 | FM100 | MV101 | NO1022 |
|---|---|---|---|---|---|---|---|---|---|
| 00.08 | 0.91899 | 0.91297 | 0.91184 | 0.90917 | 0.90910 | 0.90904 | 0.90897 | 0.90890 | 0.90883 |
| 00.09 | 0.90928 | 0.90298 | 0.90177 | 0.89899 | 0.89893 | 0.89886 | 0.89878 | 0.89871 | 0.89864 |
| 00.10 | 0.89975 | 0.89321 | 0.89194 | 0.88909 | 0.88902 | 0.88895 | 0.88888 | 0.88880 | 0.88872 |
| 00.12 | 0.88120 | 0.87434 | 0.87296 | 0.87006 | 0.86999 | 0.86992 | 0.86984 | 0.86976 | 0.86968 |
| 00.14 | 0.86331 | 0.85632 | 0.85487 | 0.85197 | 0.85190 | 0.85182 | 0.85174 | 0.85166 | 0.85157 |
| 00.16 | 0.84606 | 0.83913 | 0.83763 | 0.83470 | 0.83462 | 0.83453 | 0.83444 | 0.83435 | 0.83426 |
| 00.18 | 0.82942 | 0.82272 | 0.82116 | 0.81811 | 0.81802 | 0.81793 | 0.81784 | 0.81774 | 0.81763 |
| 00.20 | 0.81336 | 0.80701 | 0.80538 | 0.80215 | 0.80205 | 0.80195 | 0.80185 | 0.80174 | 0.80162 |
| 00.22 | 0.79787 | 0.79193 | 0.79020 | 0.78675 | 0.78664 | 0.78653 | 0.78642 | 0.78630 | 0.78618 |
| 00.24 | 0.78294 | 0.77741 | 0.77555 | 0.77187 | 0.77176 | 0.77165 | 0.77153 | 0.77140 | 0.77127 |
| 00.26 | 0.76856 | 0.76338 | 0.76140 | 0.75750 | 0.75738 | 0.75726 | 0.75713 | 0.75700 | 0.75686 |
| 00.28 | 0.75472 | 0.74982 | 0.74770 | 0.74359 | 0.74347 | 0.74334 | 0.74321 | 0.74307 | 0.74292 |
| 00.30 | 0.74138 | 0.73668 | 0.73442 | 0.73014 | 0.73001 | 0.72988 | 0.72973 | 0.72959 | 0.72943 |
| 00.34 | 0.71611 | 0.71159 | 0.70908 | 0.70449 | 0.70436 | 0.70422 | 0.70407 | 0.70391 | 0.70374 |
| 00.38 | 0.69246 | 0.68797 | 0.68520 | 0.68043 | 0.68029 | 0.68015 | 0.67999 | 0.67982 | 0.67965 |
| 00.42 | 0.67020 | 0.66567 | 0.66266 | 0.65783 | 0.65769 | 0.65754 | 0.65738 | 0.65721 | 0.65703 |
| 00.46 | 0.64913 | 0.64458 | 0.64137 | 0.63655 | 0.63641 | 0.63625 | 0.63608 | 0.63590 | 0.63571 |
| 00.50 | 0.62912 | 0.62464 | 0.62124 | 0.61646 | 0.61631 | 0.61615 | 0.61597 | 0.61578 | 0.61557 |
| 00.54 | 0.61009 | 0.60576 | 0.60222 | 0.59743 | 0.59727 | 0.59709 | 0.59690 | 0.59670 | 0.59648 |
| 00.58 | 0.59194 | 0.58790 | 0.58422 | 0.57934 | 0.57917 | 0.57898 | 0.57878 | 0.57854 | 0.57833 |
| 00.62 | 0.57463 | 0.57100 | 0.56718 | 0.56213 | 0.56194 | 0.56174 | 0.56153 | 0.56130 | 0.56105 |
| 00.66 | 0.55809 | 0.55498 | 0.55100 | 0.54571 | 0.54551 | 0.54530 | 0.54508 | 0.54483 | 0.54457 |
| 00.70 | 0.54226 | 0.53979 | 0.53561 | 0.53003 | 0.52983 | 0.52960 | 0.52936 | 0.52910 | 0.52883 |
| 00.78 | 0.51252 | 0.51160 | 0.50694 | 0.50069 | 0.50047 | 0.50023 | 0.49996 | 0.49968 | 0.49939 |
| 00.86 | 0.48505 | 0.48595 | 0.48072 | 0.47376 | 0.47353 | 0.47327 | 0.47300 | 0.47271 | 0.47240 |
| 00.94 | 0.45953 | 0.46248 | 0.45662 | 0.44901 | 0.44877 | 0.44852 | 0.44824 | 0.44795 | 0.44764 |
| 01.02 | 0.43578 | 0.44093 | 0.43439 | 0.42624 | 0.42602 | 0.42577 | 0.42550 | 0.42521 | 0.42490 |
| 01.10 | 0.41366 | 0.42106 | 0.41377 | 0.40529 | 0.40508 | 0.40484 | 0.40458 | 0.40429 | 0.40398 |
| 01.18 | 0.39310 | 0.40267 | 0.39457 | 0.38596 | 0.38575 | 0.38552 | 0.38526 | 0.38497 | 0.38466 |
| 01.26 | 0.37400 | 0.38556 | 0.37663 | 0.36804 | 0.36784 | 0.36761 | 0.36736 | 0.36707 | 0.36676 |
| 01.34 | 0.35624 | 0.36959 | 0.35982 | 0.35141 | 0.35121 | 0.35099 | 0.35073 | 0.35045 | 0.35013 |
| 01.42 | 0.33968 | 0.35460 | 0.34407 | 0.33593 | 0.33574 | 0.33552 | 0.33526 | 0.33498 | 0.33466 |
| 01.50 | 0.32416 | 0.34053 | 0.32933 | 0.32151 | 0.32133 | 0.32111 | 0.32086 | 0.32057 | 0.32025 |
| 01.66 | 0.29576 | 0.31492 | 0.30261 | 0.29552 | 0.29535 | 0.29513 | 0.29486 | 0.29456 | 0.29421 |
| 01.82 | 0.27028 | 0.29240 | 0.27902 | 0.27278 | 0.27258 | 0.27233 | 0.27203 | 0.27168 | 0.27127 |
| 01.98 | 0.24731 | 0.27254 | 0.25792 | 0.25268 | 0.25244 | 0.25213 | 0.25176 | 0.25134 | 0.25085 |
| 02.14 | 0.22662 | 0.25480 | 0.23888 | 0.23477 | 0.23446 | 0.23408 | 0.23363 | 0.23312 | 0.23255 |
| 02.30 | 0.20803 | 0.23872 | 0.22164 | 0.21871 | 0.21833 | 0.21788 | 0.21736 | 0.21678 | 0.21614 |
| 02.46 | 0.19138 | 0.22401 | 0.20604 | 0.20430 | 0.20385 | 0.20334 | 0.20275 | 0.20209 | 0.20138 |
| 02.62 | 0.17649 | 0.21051 | 0.19196 | 0.19133 | 0.19082 | 0.19023 | 0.18957 | 0.18883 | 0.18803 |
| 02.78 | 0.16321 | 0.19812 | 0.17925 | 0.17960 | 0.17901 | 0.17834 | 0.17759 | 0.17676 | 0.17585 |
| 02.94 | 0.15135 | 0.18676 | 0.16777 | 0.16890 | 0.16822 | 0.16745 | 0.16660 | 0.16566 | 0.16466 |
| 03.10 | 0.14076 | 0.17632 | 0.15739 | 0.15907 | 0.15828 | 0.15741 | 0.15645 | 0.15542 | 0.15432 |
| 03.42 | 0.12281 | 0.15794 | 0.13945 | 0.14152 | 0.14055 | 0.13950 | 0.13837 | 0.13717 | 0.13592 |
| 03.74 | 0.10832 | 0.14233 | 0.12457 | 0.12639 | 0.12528 | 0.12410 | 0.12285 | 0.12155 | 0.12021 |
| 04.06 | 0.09651 | 0.12901 | 0.11216 | 0.11334 | 0.11214 | 0.11088 | 0.10957 | 0.10823 | 0.10686 |
| 04.38 | 0.08677 | 0.11763 | 0.10175 | 0.10207 | 0.10082 | 0.09954 | 0.09822 | 0.09687 | 0.09550 |
| 04.70 | 0.07866 | 0.10791 | 0.09297 | 0.09234 | 0.09109 | 0.08980 | 0.08849 | 0.08717 | 0.08584 |
| 05.02 | 0.07185 | 0.09960 | 0.08548 | 0.08393 | 0.08269 | 0.08143 | 0.08015 | 0.07887 | 0.07760 |
| 05.34 | 0.06607 | 0.09245 | 0.07900 | 0.07665 | 0.07543 | 0.07421 | 0.07298 | 0.07176 | 0.07054 |
| 05.66 | 0.06115 | 0.08621 | 0.07334 | 0.07032 | 0.06915 | 0.06797 | 0.06680 | 0.06563 | 0.06447 |
| 05.98 | 0.05692 | 0.08069 | 0.06833 | 0.06482 | 0.06369 | 0.06256 | 0.06144 | 0.06033 | 0.05923 |
| 06.30 | 0.05327 | 0.07575 | 0.06386 | 0.06002 | 0.05893 | 0.05785 | 0.05678 | 0.05573 | 0.05469 |
| 06.94 | 0.04731 | 0.06721 | 0.05621 | 0.05207 | 0.05107 | 0.05008 | 0.04911 | 0.04816 | 0.04723 |
| 07.58 | 0.04269 | 0.06005 | 0.04992 | 0.04580 | 0.04488 | 0.04397 | 0.04309 | 0.04223 | 0.04140 |
| 08.22 | 0.03902 | 0.05395 | 0.04466 | 0.04073 | 0.03988 | 0.03905 | 0.03825 | 0.03747 | 0.03672 |
| 08.86 | 0.03606 | 0.04872 | 0.04022 | 0.03654 | 0.03576 | 0.03501 | 0.03427 | 0.03357 | 0.03289 |
| 09.50 | 0.03571 | 0.04420 | 0.03644 | 0.03303 | 0.03231 | 0.03162 | 0.03095 | 0.03031 | 0.02970 |

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U(X) X NI 28   CE 58   TB 65   BK 97   CF 98   E  99   FM100   MV101   ND102
 10.14 0.03571 0.04029 0.03322 0.03003 0.02937 0.02874 0.02813 0.02754 0.02698
 10.78 0.03571 0.03691 0.03048 0.02745 0.02684 0.02626 0.02570 0.02516 0.02465
 11.42 0.03571 0.03401 0.02817 0.02520 0.02463 0.02410 0.02358 0.02309 0.02263
 12.06 0.03571 0.03152 0.02622 0.02322 0.02270 0.02221 0.02174 0.02129 0.02086
 12.70 0.03571 0.02940 0.02459 0.02148 0.02100 0.02055 0.02012 0.01971 0.01932
 13.98 0.03571 0.02608 0.02204 0.01863 0.01822 0.01784 0.01748 0.01714 0.01681
 15.26 0.03571 0.02363 0.02013 0.01647 0.01613 0.01582 0.01552 0.01523 0.01497
 16.54 0.03571 0.02174 0.01861 0.01489 0.01461 0.01434 0.01410 0.01386 0.01364
 17.82 0.03571 0.02020 0.01733 0.01373 0.01349 0.01327 0.01306 0.01285 0.01266
 19.10 0.03571 0.01887 0.01620 0.01285 0.01264 0.01245 0.01226 0.01208 0.01191
 20.38 0.03571 0.01769 0.01538 0.01214 0.01195 0.01178 0.01161 0.01144 0.01129
 21.66 0.03571 0.01724 0.01538 0.01154 0.01136 0.01120 0.01104 0.01089 0.01074
 22.94 0.03571 0.01724 0.01538 0.01100 0.01083 0.01068 0.01053 0.01038 0.01024
 24.22 0.03571 0.01724 0.01538 0.01050 0.01034 0.01020 0.01005 0.00992 0.00980
 25.50 0.03571 0.01724 0.01538 0.01031 0.01020 0.01010 0.01000 0.00990 0.00980
 28.06 0.03571 0.01724 0.01538 0.01031 0.01020 0.01010 0.01000 0.00990 0.00980
 30.62 0.03571 0.01724 0.01538 0.01031 0.01020 0.01010 0.01000 0.00990 0.00980
 33.18 0.03571 0.01724 0.01538 0.01031 0.01020 0.01010 0.01000 0.00990 0.00980
 35.74 0.03571 0.01724 0.01538 0.01031 0.01020 0.01010 0.01000 0.00990 0.00980
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  603.2   2830.8  3591.9  8268.9  8446.7  8626.4  8807.9  8991.3  9176.6
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  72.0    443.3   577.4   1455.0  1489.3  1523.9  1559.0  1594.4  1630.3
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  63.3    420.3   550.9   1411.9  1445.7  1479.8  1514.4  1549.3  1584.6
 SHELL (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  8.02    96.43   128.79  374.62  384.67  394.83  405.12  415.53  426.06
 SHELL (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  5.29    86.32   116.77  352.99  362.72  372.57  382.53  392.62  402.84
 SHELL (3D) 9  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10  (3D)10
 (-E)  0.69    67.32   94.18   312.25  321.38  330.62  339.99  349.48  359.08
 SHELL (4S) 1  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2  (4S) 2
 (-E)  0.49    19.82   25.82   97.72   100.80  103.92  107.07  110.25  113.46
 SHELL (4P) 0  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6  (4P) 6
 (-E)  0.      16.00   21.03   87.44   90.34   93.27   96.23   99.22   102.24
 SHELL (4D) 0  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10  (4D)10
 (-E)  0.      9.215   12.384  68.127  70.661  73.223  75.815  78.437  81.089
 SHELL (4F) 0  (4F) 1  (4F) 8  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14  (4F)14
 (-E)  0.      1.236   1.630   41.093  43.087  45.108  47.157  49.234  51.340
 SHELL (5S) 0  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2  (5S) 2
 (-E)  0.      3.067   3.647   21.523  22.202  22.879  23.555  24.231  24.906
 SHELL (5P) 0  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6  (5P) 6
 (-E)  0.      1.990   2.311   17.370  17.946  18.520  19.093  19.665  20.237
 SHELL (5D) 0  (5D) 1  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10  (5D)10
 (-E)  0.      0.455   0.430   9.989   10.367  10.742  11.116  11.489  11.860
 SHELL (5F) 0  (5F) 0  (5F) 0  (5F) 9  (5F)10  (5F)11  (5F)12  (5F)13  (5F)14
 (-E)  0.      0.      0.      1.3438  1.4304  1.5154  1.5990  1.6808  1.7616
 SHELL (6S) 0  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2  (6S) 2
 (-E)  0.      0.3623  0.3918  3.0885  3.1454  3.2006  3.2541  3.3062  3.3570
 SHELL (6P) 0  (6P) 0  (6P) 0  (6P) 6  (6P) 6  (6P) 6  (6P) 6  (6P) 6  (6P) 6
 (-E)  0.      0.      0.      1.9327  1.9628  1.9914  2.0188  2.0449  2.0700
 SHELL (7S) 0  (7S) 0  (7S) 0  (7S) 2  (7S) 2  (7S) 2  (7S) 2  (7S) 2  (7S) 2
 (-E)  0.      0.      0.      0.3438  0.3462  0.3486  0.3509  0.3531  0.3552
U(X) X FM100   MV101   NO102   LW103
 00.00 1.00000 1.00000 1.00000 1.00000
 00.01 0.98809 0.98807 0.98806 0.98804
 00.02 0.97605 0.97603 0.97600 0.97597
 00.03 0.96417 0.96413 0.96409 0.96405
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U(X) X FM100   MV101   NO102   LW103
 00.04 0.95255 0.95250 0.95245 0.95241
 00.05 0.94123 0.94117 0.94112 0.94106
 00.06 0.93020 0.93014 0.93008 0.93001
 00.07 0.91946 0.91939 0.91933 0.91926
 00.08 0.90901 0.90894 0.90887 0.90879
 00.09 0.89883 0.89876 0.89868 0.89861
 00.10 0.88892 0.88885 0.88877 0.88870
 00.12 0.86990 0.86982 0.86974 0.86966
 00.14 0.85181 0.85173 0.85164 0.85156
 00.16 0.83452 0.83443 0.83434 0.83425
 00.18 0.81793 0.81783 0.81773 0.81762
 00.20 0.80195 0.80184 0.80173 0.80161
 00.22 0.78653 0.78642 0.78630 0.78617
 00.24 0.77165 0.77152 0.77139 0.77126
 00.26 0.75726 0.75713 0.75699 0.75685
 00.28 0.74335 0.74321 0.74307 0.74291
 00.30 0.72989 0.72974 0.72959 0.72943
 00.34 0.70424 0.70409 0.70392 0.70375
 00.38 0.68019 0.68003 0.67986 0.67968
 00.42 0.65760 0.65743 0.65725 0.65707
 00.46 0.63633 0.63615 0.63597 0.63577
 00.50 0.61624 0.61605 0.61585 0.61564
 00.54 0.59719 0.59699 0.59678 0.59655
 00.58 0.57909 0.57888 0.57865 0.57841
 00.62 0.56187 0.56164 0.56139 0.56114
 00.66 0.54544 0.54519 0.54494 0.54466
 00.70 0.52975 0.52949 0.52922 0.52893
 00.78 0.50039 0.50011 0.49982 0.49951
 00.86 0.47347 0.47318 0.47288 0.47255
 00.94 0.44876 0.44847 0.44816 0.44783
 01.02 0.42606 0.42577 0.42547 0.42514
 01.10 0.40517 0.40489 0.40459 0.40427
 01.18 0.38589 0.38562 0.38531 0.38499
 01.26 0.36804 0.36776 0.36745 0.36712
 01.34 0.35145 0.35117 0.35087 0.35053
 01.42 0.33602 0.33575 0.33544 0.33510
 01.50 0.32166 0.32138 0.32106 0.32072
 01.66 0.29574 0.29544 0.29510 0.29472
 01.82 0.27299 0.27265 0.27225 0.27180
 01.98 0.25280 0.25239 0.25191 0.25138
 02.14 0.23476 0.23426 0.23370 0.23309
 02.30 0.21857 0.21800 0.21737 0.21668
 02.46 0.20404 0.20340 0.20270 0.20194
 02.62 0.19095 0.19023 0.18944 0.18859
 02.78 0.17905 0.17823 0.17735 0.17639
 02.94 0.16814 0.16722 0.16623 0.16517
 03.10 0.15807 0.15705 0.15597 0.15482
 03.42 0.14012 0.13894 0.13770 0.13641
 03.74 0.12472 0.12344 0.12211 0.12074
 04.06 0.11153 0.11019 0.10883 0.10745
 04.38 0.10023 0.09889 0.09753 0.09616
 04.70 0.09053 0.08922 0.08789 0.08656
 05.02 0.08220 0.08092 0.07965 0.07838
 05.34 0.07501 0.07379 0.07257 0.07136
 05.66 0.06880 0.06763 0.06648 0.06533
 05.98 0.06341 0.06230 0.06120 0.06012
 06.30 0.05870 0.05764 0.05660 0.05558
 06.94 0.05092 0.04995 0.04901 0.04810
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U(X) X FM100   MV101   NO102   LW103
 07.58 0.04475 0.04387 0.04303 0.04220
 08.22 0.03974 0.03895 0.03819 0.03745
 08.86 0.03560 0.03488 0.03419 0.03353
 09.50 0.03212 0.03147 0.03084 0.03024
 10.14 0.02916 0.02856 0.02799 0.02745
 10.78 0.02661 0.02607 0.02555 0.02505
 11.42 0.02440 0.02390 0.02343 0.02298
 12.06 0.02248 0.02203 0.02160 0.02119
 12.70 0.02081 0.02040 0.02001 0.01964
 13.98 0.01813 0.01779 0.01746 0.01716
 15.26 0.01613 0.01585 0.01558 0.01533
 16.54 0.01464 0.01440 0.01418 0.01397
 17.82 0.01350 0.01329 0.01310 0.01291
 19.10 0.01258 0.01240 0.01222 0.01205
 20.38 0.01181 0.01164 0.01148 0.01132
 21.66 0.01113 0.01097 0.01082 0.01067
 22.94 0.01051 0.01037 0.01022 0.01009
 24.22 0.01000 0.00990 0.00980 0.00971
 SHELL (1S) 2  (1S) 2  (1S) 2  (1S) 2
 (-E)  8808.4  8991.8  9177.1  9364.3
 SHELL (2S) 2  (2S) 2  (2S) 2  (2S) 2
 (-E)  1559.5  15.950  1630.9  1667.1
 SHELL (2P) 6  (2P) 6  (2P) 6  (2P) 6
 (-E)  1514.9  1549.8  1585.2  1620.9
 SHELL (3S) 2  (3S) 2  (3S) 2  (3S) 2
 (-E)  405.69  416.11  426.66  437.33
 SHELL (3P) 6  (3P) 6  (3P) 6  (3P) 6
 (-E)  383.10  393.21  403.43  413.78
 SHELL (3D)10  (3D)10  (3D)10  (3D)10
 (-E)  340.56  350.06  359.68  369.41
 SHELL (4S) 2  (4S) 2  (4S) 2  (4S) 2
 (-E)  107.63  110.82  114.05  117.31
 SHELL (4P) 6  (4P) 6  (4P) 6  (4P) 6
 (-E)  96.79   99.79   102.83  105.90
 SHELL (4D)10  (4D)10  (4D)10  (4D)10
 (-E)  76.374  79.010  81.676  84.373
 SHELL (4F)14  (4F)14  (4F)14  (4F)14
 (-E)  47.720  49.811  51.931  54.080
 SHELL (5S) 2  (5S) 2  (5S) 2  (5S) 2
 (-E)  24.074  24.763  25.452  26.141
 SHELL (5P) 6  (5P) 6  (5P) 6  (5P) 6
 (-E)  19.605  20.190  20.775  21.360
 SHELL (5D)10  (5D)10  (5D)10  (5D)10
 (-E)  11.609  11.995  12.380  12.765
 SHELL (5F)11  (5F)12  (5F)13  (5F)14
 (-E)  2.0159  2.1122  2.2073  2.3011
 SHELL (6S) 2  (6S) 2  (6S) 2  (6S) 2
 (-E)  3.5008  3.5593  3.6167  3.6731
 SHELL (6P) 6  (6P) 6  (6P) 6  (6P) 6
 (-E)  2.2262  2.2578  2.2885  2.3183
 SHELL (6D) 1  (6D) 1  (6D) 1  (6D) 1
 (-E)  0.4463  0.4432  0.4397  0.4358
 SHELL (7S) 2  (7S) 2  (7S) 2  (7S) 2
 (-E)  0.3777  0.3805  0.3832  0.3859
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