NOTICE

PORTIONS OF THIS REPORT ARE ILLEGIBLE. It has been reproduced from the best available copy to permit the broadest possible availability.

UCRL-13994

CALCULATING RAYLEIGH SCATTERING AMPLITUDES FROM 100 ev - 10 Mev

MASTER

J. C. Parker, G.W. Reynaud,
D. J. Botto, R. H. Pratt

May 1, 1979

P. O. 9776403

NOTICE
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness or usefulness of any information, product or process disclosed, or represents that its use would not infringe privately owned rights.

DEPARTMENT OF PHYSICS
UNIVERSITY OF PITTSBURGH
PITTSBURGH, PENNSYLVANIA 152 9

NOTICE

PORTIONS OF THIS REPORT ARE ILLEGIBLE. It has been reproduced from the best available copy to permit the broadest possible availability.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED ²⁶

Section I

Contents

Section I

1. The General Problem	1
2. Approximations Used	12
3. Range of Physical Variables	15
4. Philosophy of Code Design	16

Section II

5. RSCF--Relativistic Self Consistent Field Program	20
A. I/O Summary for RSCF	20
B. LWF.F4 I/O	24
6. ENT5	25
A. To Use ENT	25
B. I/O Summary for ENT5	26
C. Subroutines	31
1. Subroutines I/O	31
2. ORB5 (Subroutine Package)	32
3. INT5 (Subroutine Package)	39
7. SRKLL	44
8. MFSTR1	45
A. I/O of MFSTR1	45
B. To Use MFSTR1	45
9. TARK5	47
References	52
Index	54
Tables and Figures	57

1. The General Problem.

This document attempts to explain how the reader can calculate the contribution to elastic photon-atom scattering due to Rayleigh scattering (the scattering off bound electrons) in the photon energy range $100 \text{ eV} \leq W \leq 10 \text{ MeV}$. All intermediate calculations are described, including the calculation of the potential, bound state wave function, matrix elements and final cross sections.

Since elastic scattering is a coherent process, the total elastic scattering cross section is the squared sum of the Rayleigh amplitude and all other elastic amplitudes (including nuclear Thomson scattering, nuclear resonance scattering and Delbruck scattering). Well below 1 MeV it is generally reasonable to consider the bound electron contribution as dominant and to compare cross sections determined solely from the Rayleigh amplitude with experiment.

For this calculation of Rayleigh amplitudes, the atom is pictured as consisting of an infinitely massive structureless point of charge Ze and N bound electrons. The electrons move in a common central self-consistent potential derived from the Coulomb field of the nucleus screened by all the electrons. The total Rayleigh amplitude is then expressed as the sum of amplitudes due to scattering of a photon off of each electron independently.

Each electron is described by a wave function which is the solution of the Dirac equation in the common central potential, thus taking into account the dynamical effects of spin and special relativity. Higher order QED

effects on wave functions such as the Lamb shift are not considered. The central field approximation, neglecting electron-electron correlations and approximating exchange, by a local exchange potential, simplifies the calculation of the wave functions. In this approximation all the electrons move in a single, relativistic central potential determined by the mutual interactions of all the electrons and the nucleus. This approach to obtaining a potential and atomic wave functions is called the Dirac-Hartree-Fock-Slater (DHFS) method. The potential and wave functions are determined in a "self-consistent" manner. A trial potential is assumed, and the wave functions calculated for the electrons. The charge density resulting from the wave functions is used to determine a new potential and the process is repeated until the wave functions and potential are unchanged between iterations to within a specified tolerance.

In obtaining such a self-consistent description of an atom one must choose a local exchange term which is an approximation to the nonlocal term in the full Hartree-Fock coupled differential equations. The local approximation most extensively used in the calculations performed with this code is the Kohn-Sham exchange term which is $2/3$ of the term originally proposed by Slater. Since the potential each atomic electron sees at large distances is that due to the nucleus of charge Z screened by $N-1$ electrons, the atomic potential obtained as described above is also commonly modified by forcing it to fall off as $(Z-N+1)/r$ for large distances (Latter tail, Z is the atomic number and N is the number of electrons.) For details on

computing the potential and wave functions see section 5 below.

Two integer quantum numbers, n and K , uniquely characterize the electron wavefunction, where n (≥ 1) is the principal quantum number and K ($-\infty \leq K \leq \infty$, $K \neq 0$) is the angular momentum and parity quantum number of the wavefunction ($K = \mp (j+1/2)$ as $j = l + 1/2$, where j is the total angular momentum and l is the orbital angular momentum.)

From the Pauli principle, each subshell can contain at most $2j+1$ electrons. In the ground state of the atom, the inner subshells of all atoms are filled first (small n and $|K|$). With increasing atomic number subshells of increasing n and K are filled. For the outer subshells, though, correlation and exchange effects which are neglected in the DHFS method are increasingly important. The occupation numbers are not uniquely determined within this model (see ref. 7 for occupation numbers determined from photoeffect). In the energy range considered (above 0.1 keV and below 10 MeV) the inner shells dominate the Rayleigh amplitude, except at very low energies and forward angles, again justifying the use of the DHFS model. For convenience the order for the filling of the inner subshells in this model is given in table I. (This table is useful in forming input files for the programs and showing the correspondence of the notation with others.)

In a relativistic, single particle, central potential model the wave functions are of the general form

$$|nKm\rangle = \psi_{nKm}(z) = \begin{pmatrix} (G_K(r)/r) \Omega_{Km}(\hat{r}) \\ (iF_K(r)/r) \Omega_{-Km}(\hat{r}) \end{pmatrix}$$

where $G_K(r)$ and $F_K(r)$ are the radial wave functions. In these functions $i = \sqrt{-1}$, n is the principal quantum number, K is the angular momentum and parity quantum number of the wave function and is given by $K = \tilde{\tau}(j + 1/2)$ as $j = l \pm 1/2$, where j is the total angular momentum of the wave function and l is the orbital angular momentum. The functions $\Omega_{Km}(\hat{r})$ are known functions of the angles with m being the component of j along the Z axis of the coordinate system.

In the single particle model, the photon-electron scattering is described, in lowest order, as a second order quantum electrodynamical (QED) process in the photon-electron interaction. The matrix element is characterized by the following two Furry diagrams, labelled (a) and (e):

Diagram (a) depicts the process in which the photon is first absorbed, while diagram (e) represents the process in which the photon is first emitted. The electron is seen as absorbing (emitting) a photon, with energy W , propagating in a manner determined by the Green's function (electron propagator), and then emitting (absorbing) a photon and returning to its

initial state.

The Rayleigh amplitudes are calculated¹ using an "exact" partial wave expansion for each subshell, as developed by G. E. Brown et al.² and W. R. Johnson and F. D. Peacock³ to obtain dominant subshell amplitudes. (For high subshells often a modified form factor may be used, see Section 2 below.)

The relativistic second order S-matrix is the sum of the two diagrams; i.e.,

$$S_{fi} = S_{fi}^a + S_{fi}^e$$

corresponding to diagrams (a) and (e) respectively. The electron propagator (Green's function), which is represented by the connection between the vertices in the diagrams, may be expanded in terms of a generalized sum over all states. This results in the following expressions for the S-matrices:

$$S_{fi}^a = \frac{-4\pi^2 ie^2}{(k_i k_f)^{1/2}} \delta(E_i + k_i - E_f - k_f) S_n \left\{ \frac{\langle f | A_f | n \rangle \langle n | A_i | i \rangle}{E_i - E_n - k_i} \right\}$$

and

$$S_{fi}^{(e)} = \frac{-4\pi^2 ie^2}{(k_i k_f)^{1/2}} \delta(E_i + k_i - E_f - k_f) S_n \left\{ \frac{\langle f | A_i | n \rangle \langle n | A_f | i \rangle}{E_i - E_n + k_f} \right\},$$

where A is the photon operator $(\vec{a} \cdot \vec{\epsilon} e^{i\vec{K} \cdot \vec{r}})$ and S_n denotes the generalized sum over states.^{1,7}

The total S -matrix may now be written as

$$S_{fi} = \frac{-4\pi^2 i e^2}{(k_i k_f)^{1/2}} \delta(E_i + k_i - E_f - k_f) M_{fi}$$

where

$$M_{fi} = S_n \left(\frac{\langle f | A_f | n \rangle \langle n | A_i | i \rangle}{E_i - E_n - k_i} + \frac{\langle f | A_i | n \rangle \langle n | A_f | i \rangle}{E_i - E_n + k_f} \right).$$

The photon operator A can be expanded in a multipole series

$$A = \sum_{J, M, \lambda} C_{JM}^{\lambda}(k) A_{JM}^{\lambda}$$

where J, M are the photon multipole angular momentum indices (total, projection) and $\lambda (=0, 1)$ characterizes the parity of that multipole; i.e., whether it is a magnetic or an electric multipole.

When this expansion is inserted into the matrix element one obtains

$$M_{fi} = \sum_{J\lambda} \sum_{J'\lambda'} C_{JM}^{\lambda}(k_i) C_{J'M'}^{\lambda'}(k_f) M_{J\lambda, J'\lambda'}$$

where

$$M_{J\lambda, J'\lambda'} = S_n \left(\frac{\langle g | A_{J'+M'}^{\lambda'}(f) | n \rangle \langle n | A_{JM}^{\lambda}(g) \rangle}{E_g + W - E_n} + \frac{\langle g | A_{JM}^{\lambda}(i) | n \rangle \langle n | A_{J'+M'}^{\lambda'}(f) | g \rangle}{E_g - W - E_n} \right).$$

Here the expression has been specialized to the Rayleigh case by setting $|i\rangle = |f\rangle = |g\rangle = |nK_m\rangle$, and $k_i = k_f = W$. These expressions contain one electron's contribution.

This matrix element involves a 6-dimensional integral. Therefore, before its numerical evaluation is attempted further reductions are made. By defining "perturbed orbitals"

$$|nK_{m+}\rangle = \sum_n \frac{|q\rangle \langle q| A_{JM} |nK_m\rangle}{E_{nK} + W - E_q}$$

and

$$|nK_{m-}\rangle = \sum_n \frac{|q\rangle \langle q| A_{JM} |nK_m\rangle}{E_{nK} - W - E_q}$$

the matrix element may be written as

$$\begin{aligned} M_{JM\lambda, J'M'\lambda'} &= \langle nK_m | A_{J'M'}^{\lambda'}(f) | nK_{m+} \rangle \\ &+ \langle nK_m | A_{J'M'}^{\lambda'}(f) | nK_{m-} \rangle. \end{aligned}$$

The perturbed orbitals $|nK_{m+}\rangle$ and $|nK_{m-}\rangle$ represent the result of absorption

and emission, respectively, of a photon (energy W , quantum numbers J, M, λ) by the initial bound electron. By applying the Dirac equation it is found that they satisfy the following inhomogeneous Dirac equations:

$$(E_{nK} + W - H)|nKm\rangle = A_{JM}^{\lambda}|nKm\rangle$$

and

$$\langle nKm| (E_{nK} - W - H) = \langle nKm| A_{JM}^{\lambda},$$

where H is the Dirac Hamiltonian. For the case of a central atomic potential, these perturbed orbitals can be expanded in a spherical basis with the angular dependence described by known functions (analogous to the expansion for the photon operator). For example $|nKm\rangle$ can be expanded as

$$|nKm\rangle = \sum_{K_1 M_1} \begin{pmatrix} (S_{K_1}(r)/r) & \Omega_{K_1 M_1}(\hat{r}) \\ (iT_{K_1}(r)/r) & \Omega_{-K_1 M_1}(\hat{r}) \end{pmatrix}$$

A large reduction in complexity now occurs because of the triangle conditions on the various angular functions, which have well known analytic integrals. Furthermore, the radial functions do not in fact depend on ν . After all the angular dependence has been removed analytically, there remains an inhomogeneous radial Dirac equation for each of the K_1 -th

radial components in the expansion of the perturbed orbital. These are evaluated numerically.

The method chosen for this work was suggested by Brown and Schaefer⁴ and is similar to the method of variation of parameters.⁵ In this method the solution is expressed as a linear combination of linearly independent solutions of the corresponding homogeneous Dirac equation with the proviso that the coefficients depend upon position; for example for $S_{K_1}(r)$

$$S_{K_1}(r) = C_A(r)f(r) + C_B(r)g(r).$$

The coefficients are determined by integrating over the product of the homogeneous solution and the radial part of the driving term of the inhomogeneous Dirac equation. Because the angular integrals in the matrix element, $M_{JM\lambda, J'M'\lambda'}$, are evaluated in terms of known functions (Legendre polynomials of $x = \cos \Theta$, to be precise), the problem has been reduced to the calculation of radial matrix elements, called here R-integrals, for each value of λ, J, K_1 allowed by triangular conditions, and for $\pm W$ (absorption first/emission first). These R-integrals are defined as

$$R_{JK_1}^{\lambda}(\pm W) = \int_0^{\infty} [S_{K_1}^{\lambda}(\pm W) k_{K_1}^{\lambda} + T_{K_1}^{\lambda}(\pm W) l_{K_1}^{\lambda}] dr;$$

$k_{K_1}^\lambda$ and $\ell_{K_1}^\lambda$ are products of the radial components of the bound state wave functions and the spherical Bessel functions from the multipole expansion of the photon operator.

The spin-angle coefficients obtained analytically enter into the amplitudes when the sum on K_1 is performed. The result of this sum is called an X-amplitude and is defined as

$$X_J^\lambda(W) = \sum_{K_1} F_{\lambda}^I \{ R_{JK_1}^\lambda(W) + R_{JK_1}^\lambda(-W) \}$$

where

$$F_{\lambda}^I = \begin{cases} \frac{(K+K_1)^2 (2j_1 + 1)(2j + 1) \Lambda_{KJK_1}}{J(J+1)}, & \text{for } \lambda=0 \\ (j+1)(2j_1 + 1)(2j + 1) \Lambda_{KJK_1}, & \text{for } \lambda=1 \end{cases}$$

with Λ_{KJK_1} being the spin-angle term defined as

$$(2j_1 + 1) \Lambda_{KJK_1} = \begin{cases} c^2(jj_1; 0) & \text{for } K+J+K_1 \text{ even} \\ 0 & \text{for } K+J+K_1 \text{ odd,} \end{cases}$$

with the C 's being the coupling coefficients.

If the Rayleigh amplitude is decomposed into components corresponding to photon polarization parallel and perpendicular to the plane of scattering, ($A_{||}^R$ and $A_{\perp}^R$ respectively) then, in terms of the X -amplitudes we can write these components as

$$A_{||}^R(\omega,) = - \sum_{J=1}^{\infty} (F^{II}(\theta) X_J^I(\omega) + F^{III}(\theta) X_J^0(\omega))$$

and

$$A_{\perp}^R(\omega,) = - \sum_{J=1}^{\infty} (F^{III}(\theta) X_J^I(\omega) + F^{II}(\theta) X_J^0(\omega))$$

with F^{II} and F^{III} known functions of the angle of scattering, θ .

For elastic scattering the differential cross section for unpolarized photons where the final photon polarization is not measured is

$$\frac{d\sigma}{d\Omega} \text{ unpol} = \frac{k_e^2}{2} (|A_{||}^R|^2 + |A_{\perp}^R|^2)$$

where r_e is the classical electron radius.

The differential elastic scattering amplitudes $A_{||}, A_{\perp}$ include the sum of all elastic processes:

$$A_{||} = A_{||}^R + A'_{||},$$

and

$$A_{\perp} = A_{\perp}^R + A'_{\perp}$$

where $A_{||}^R / A_{\perp}^R$ are the Rayleigh amplitudes and $A'_{||} / A'_{\perp}$ are the sums of all other elastic amplitudes.

2. Approximations Used

Aside from the obvious approximation of neglecting higher order QED effects, the most fundamental approximation is the use of the central potential, independent electron model. This means that the basic interaction is considered to be an interaction between a photon and an electron in a potential. Many body effects (electron-electron correlations and core relaxation) are neglected. It can be argued that in the energy range considered these effects should be small.¹ The approximation should be better for higher photon energies and larger atomic numbers. The inner shell structure becomes less dependent on the outer electrons for heavy atoms (the inner shell wavefunctions become more hydrogenic), and higher

energies enhance the relative contributions of the inner parts of the atom.

Distinct from these physical approximations is the use of a modified form factor approximation to estimate the contributions of outer subshells for the total atom amplitudes at higher photon energies. This is desirable for higher Z and W due to the computer time required to calculate the "exact" subshell amplitudes. (For photon energies above 25 times the K-shell's binding energy this is an excellent (1-2%) approximation for all shells.) As is typical with the use of multipole and partial wave series expansions, higher incident energies require calculation of more terms of the series for convergence. Thus, except in light elements, it is advantageous to not calculate all subshells exactly, but to use the modified form factor predictions whenever possible. Fortunately with increasing photon energies, higher subshell contributions become relatively smaller except at forward angles and a form factor estimate of them becomes more reliable. The use of a simple approximate method for higher shells is warranted.¹ Recent calculations allow us to put some rough limits on the validity of the modified form factor (see table V).

Taking advantage of these results, the final program which tabulates differential Rayleigh scattering amplitudes may optionally use a modified form factor approximation (MFF) to estimate the contributions of some (or all) shells.

The modified form factor is defined as

$$g(q) = 4\pi \int \rho(r) \frac{\sin q r}{qr} \frac{1}{1-\epsilon-V(r)} r^2 dr$$

where q is the momentum transfer in units of $m_e c$ and is related to the momentum transfer in inverse angstroms by $Q(\text{\AA}^{-1}) = 20.61q(m_e c)$. A lengthy discussion of this approximation has been given by Kissel.¹

Use of the modified form factor approximation is entirely user dependent. The user can calculate partial wave results for as many inner subshells as is deemed appropriate. These calculations are performed with the ENT5 and SHELL programs.

For the rest of the subshells, the user may use the program MFSTR1 to calculate the modified form factors. The results are combined in the program TABX5 which tabulates differential Rayleigh scattering amplitudes and cross sections as a function of angle and momentum transfer. Detailed descriptions of these programs will be found below (sections 5-8).

It is suggested that the MFF be used only for those subshells whose binding energy is a small fraction of the photon energy (see Table VI). For a photon energy close to that corresponding to a radiative transition to a lower bound level it is also necessary to calculate the corresponding shell's amplitude exactly. Also the MFF is never used for the K-shell (except for extremely high energies) since for large momentum transfers ($q \leq 10 \text{\AA}^{-1}$) the "exact" K-shell amplitudes are required for use with the MFF to estimate higher shells. The K-shell modified forms factors are required as well, not for calculating the K-shell amplitude, but for scaling the higher shell modified form factor predictions when $q > 10 \text{\AA}^{-1}$.

3. Range of Physical Variables

The programs have been designed to work for all atoms with $1 \leq Z \leq 137$, and all incident photon energies above 0.1 kev and below 10 Mev (except at a bound bound transition energy). The code will reject any energy or atomic number not in these ranges. The reason for the upper limit on Z is that the Dirac theory for a point nucleus fails for $Z\alpha > 1$, where α is the fine structure constant equal to approximately $1/137$. The lower limit on the photon energy is due to the neglect of exchange and correlation effects in the DHFS model. Exchange and correlation effects would have to be considered below 0.1 kev. Furthermore the photon energy should be high enough so that inner electrons of heavy (high Z) atoms dominate the Rayleigh amplitudes. The upper end of the photon energy range is restricted because above 10 Mev the implicit assumption of a infinitely massive, structureless point nucleus becomes questionable. Fortunately at these very high energies the Rayleigh amplitudes at other than forward angles become insignificant relative to the total elastic amplitude.

Within the 100 ev to 10 Mev photon energy range, there is the further restriction, caused by the neglect of the finite atomic level widths, that the photon energy must not be too near a bound-bound transition energy. A resonance occurs at photon energies equal to a bound-bound transition energy, $W \sim |E_i - E_f|$ where E_i and E_f refer to two bound state energies in the self-consistent potential. For photon energies below the photoeffect K-edge, this condition should be checked using the energies for

the bound state orbitals calculated by the RSCF program. The Rayleigh scattering code should be valid for energies farther than 1 eV from a resonance.

The validity of the calculated results for neutral, ground state atoms within the variable ranges defined above has been extensively checked. However, the same cannot be said for the cases of ions and excited atoms where extensive calculations have not yet been performed.

There are several other input variables which are limited by definition. The principle quantum number must be a non-negative integer ($n \geq 1$). The bound state angular momentum and parity quantum number, K , cannot be zero, and is restricted by the program to be a small integer ($|K| \leq 10$). The program performs internal checks on these values. Consistency of data files (such as bound state wave function checked against the potential) used in the calculations with these parameters is also internally checked. An inconsistency will generate an error message and the execution will be terminated. JMAX, the maximum number of photon multipoles that may be calculated, is limited to 300 by the code.

4. Philosophy of Code Design

The code is designed to operate in a modular fashion, each module of calculation being as much as possible independent of the others. This modular design led to easy and efficient debugging and modifications.

Each cycle of the main program ENT5 is devoted to the calculation of

one R-integral of a given set of indices J, LAMBDA, KB, IORD. This structure allows the program to be stopped and restarted readily, requiring the storage of only the resultant R-integral of each cycle.

During one cycle of ENT5 modules are called separately that calculate the outward and inward solutions of the homogeneous Dirac equation corresponding to the inhomogeneous Dirac equation, coefficients of these solutions $a(r)$ and $b(r)$ (for constructing the perturbed orbital), and finally the R-integral. (See section 6 below for more details.)

The code is designed to allow a strong sense of confidence in the results since each module checks its input and uniquely identifies its output. The programs are filled with internal consistency checks which protect against blunders. All input to both the main program and subroutines is checked to be sure that it is physically reasonable, and agrees with the data the programs may have from other sources (for example, data in COMMON).

The calculations performed in the code have been done with a view towards using "matched" numerical methods. The calculations performed (integration of a differential equation and numerical quadrature) all deal with numerically evaluated input data, versus analytically known quantities. Because of this, the methods used could not be of too high an order, since the errors introduced would depend on higher derivatives of the numerical data which are not always accurately given by such numerical data. The output to some modules becomes the input of others and so the numerical

methods used in two such related modules are matched in order to avoid the loss of accuracy or introduction of new errors

Furthermore, the methods use variable step-sizes in the integration of the differential equations, and in the evaluation of integrals. Variable step-sizes avoid wasted computer time. The greatest time is spent in the regions of calculation requiring the greatest accuracy. The step-sizes are varied in accordance with explicit error estimates made at each step of the calculation.

To keep track of the reliability of the final results (as far as the numerical errors are concerned) error estimates are made and accumulated at each step of the calculation. This requires the consideration of propagation error and truncation error. The former is due to errors in the input data leading to further errors in subsequent results. The latter is due to the use of the particular numerical method at each step.

The close monitoring of errors allows one to state that within the range of the physical model, the numerical methods give results accurate to the user's requested tolerance. Results better than 1% are obtained if the program's default values are used.¹

Section II

Descriptions of the Codes

5. RSCF--Relativistic Self Consistent Field Program.

This code produces the self-consistent potential and wave-functions for an atom or ion by the method of Liberman et al.,⁶ to which we refer the reader for a discussion of the SCF method. The options available are determined by CARD4 and include: Slater exchange or Kohn-Sham exchange (2/3 the Slater term), with or without the Latter tail ($r V(r) \rightarrow (Z-N+1) \text{ as } r \rightarrow \infty$), and the Rosen-Lindgren potential. The Kohn-Sham exchange with Latter tail has been used most extensively and has proven satisfactory in the keV region.¹

A. I/O Summary for RSCF(see figs. 2,11).

Device 5 Input:

CARD1: Comment Line, 80 ASCII characters in FORMAT(8A10) The first 5 characters are duplicated in columns 73-80 of the output for identification.

CARD2: ZN, XION, RNUC in FORMAT(8G)

ZN = atomic number

XION = Ionic charge

RNUC = Radius of the Nucleus

See Table II for a definition of these variables.

CARD3: RN, H, PHI, EPS, DEL, DELRVR in FORMAT(8G).

RN = the maximum radial position of the output in Bohr radii.

RN = 0.0 defaults to RN = 60.0.

H = A multiple of 8 used to determine the step-size. H = 0.0 defaults to H = 32.0.

PHI = potential averaging factor (V(NEXT iteration) = V(FORMER iteration) + PHI*V(as computed from this iteration)).

PHI = 0.0 defaults to PHI = 0.3.

EPS = practical infinity for the potential in Bohr radii.

EPS = 0.0 defaults to EPS = 75.0.

DEL = Accuracy requirement for the eigenvalues. DEL = 0.0 defaults to DEL = 5.0×10^{-6} .

DELRVR = Accuracy requirement for convergence. DELRVR = 0.0 defaults to DELRVR = 1.0×10^{-4} .

CARD4: KPOT, XALPH, XLATTR, XNNN, FEX in FORMAT(8G)

KPOT = 1 -> New Potential specified by XALPH, XLATTR, XNNN

KPOT = 2 -> Kohn-Sham potential with no Latter tail.

KPOT = 3 -> Slater potential with no Latter tail.

KPOT = 4 -> Rosen-Lindgren Potential.

XALPH = Exchange coefficient (1 for Slater exchange, 2/3 for

Kohn-Sham).

XLATTR = 0 -> No Latter tail.

XLATTR = 1 -> Use the Latter tail.

XNNN = 1 for KPOT = 1, 2, or 3 (this is the default if XNNN = 0.)

XNNN = must be specified for the Rosen-Lindoren Potential.

It is an input number for the exchange term, see Ref. 3.)

FEX is a control parameter for free electron exchange potential and binding energy calculations.

FEX = 1 -> Energy dependent free-electron exchange.

FEX = 2 -> Approximate Hartree-Fock energies.

FEX = 3 -> Energies by difference from the total energy.

CARD5: J, NC1, N, NPRINT, NDEBUG in FORMAT (8G)

J = the number of electron orbitals.

NC1 = the maximum number of cycles before the results are dumped and execution ends. NC1 = 0 defaults to NC1 = 30.

N = the number of points in the radial mesh. N = 0 defaults to N = 421.

NDEBUG = 1 -> Increase the number of printed diagnostics.

NDEBUG = 0 -> Minimum number of diagnostics.

CARD6: For each orbital (I = 1,J),

XN(I), XL(I), XJ(I), XE(I), XZ(I), BCOND in FORMAT (8G).

XN(I) = The orbital's principle quantum number.

XL(I) = Its orbital angular momentum.

XJ(I) = Its total angular momentum.

XE(I) = Its estimated binding energy in Rydbergs (1Ry = 13.6 eV), XE(I) 0.0.

XZ(I) = Its occupation number ($2 \times XJ(I) + 1$) for full orbitals. For partially filled orbitals, we suggest the occupation numbers deduced from photoionization.⁵

BCOND = 0.0 (BCOND = 1.0 should give Wiener-Seitz boundary conditions. This option has never been tried with these codes.)

Device 6 output: Line printer output containing

- (a) the input data verbatim
- (b) error estimates for integrations, etc.
- (c) energy eigenvalues in keV
- (d) a table of radii
- (d) the charge density
- (e) a list of potential screening factors, and
- (f) a copy of the device 7 output.

Device 7 output: (See Fig. 12)

Lines 1-90 contain the relativistic potential. After line 90

come the wavefunctions. The potential and wavefunctions are "packed" on this data file. The Program LWF separates the wave functions from the rest.

B. LWF.F4 I/O

LWF.F4 reads the device 8 output of RSCF, and the user supplied input from device 5 which specifies the desired wavefunction, and outputs this wavefunction in a form suitable for later use by ENT5 and MFSTR1. The user supplied input is

Line 1. IZ = atomic number

Line 2. N, K where N = principle quantum number, and K = quantum number combining the total angular momentum and the parity. $K = \mp(j+1/2)$ as $j = l \pm 1/2$.

Line 3. FNAME = a 10 character ASCII string containing the DEC-10 filename and extension into which the resulting bound state will be written, in FORMAT(A10).

LWF is an interactive program. All of the numbers are read in FORMAT(SG).

6. ENT5

ENT5 is the central program in the calculation of the Rayleigh scattering amplitudes (flowchart Fig. 4). The subroutines of ENT5 calculate the perturbed orbitals and the R-integrals, which are combined in ENT5 to form X-amplitudes. (These quantities are defined in Section 1 and derived in Ref. 1.) As described in Section 4, the calculation is done in a modular fashion, each complete cycle of these modules evaluates one R-integral of indices J, KB, LAMBDA, IORE. After each R-integral is calculated, the run time is checked against TSTOP. If it is greater than TSTOP calculation ceases and the pertinent data (R-integrals, X-amplitudes) are dumped onto intermediate storage files (Devices 7, 8, 9). The program is requeued and the calculation restarted. This process continues until the multipole series has converged or the maximum number of photon multipoles has been exceeded. The principal results are output into the files associated with device 7 (R-integrals) and device 9 (X-amplitudes). All the other storage files generated during the execution of ENT5 may be deleted upon convergence of the series.

A. TO USE ENT.

(Filenames used here are for convenience of discussion.)

(1) Have available the following files on disk: Lnn.POT (contains atomic potential data, nn is atomic number), subshell bound state data file (from LWF), ENT5S.SAV (core image of the loaded object codes of ENT5, with

the subroutine packages ORB5 and INT5 and required utility subroutines).

(2) Create the following files on disk: 2 blank files (called here C.STR and K.STR) which will be used as intermediate storage during the calculation; a main input file (E.CDR).

B. I/O Summary for ENT5

Device 5 input:

The initial control parameters are placed on this device when the calculation is started. Fig. 13 shows the initial file for C⁺⁴. Initially, there are only 8-lines. They contain the following information (see Table III, "Global Variables of ENT5").

Line 1. RUN, TSTOP in FORMAT (A6,F10.3)

Line 2. N, KA in FORMAT (4I5)

Line 3. IZ in FORMAT (4I5)

Line 4. WIN, IUNITS in FORMAT (1PD15.7, I5)

Line 5. JMAX, JINC in FORMAT (4I5). Note JINC is absent in the figure, JINC will be read as 0 and assigned a default value; JINC = 1.

Line 6. ERRORB, ERRINT in FORMAT (1P5D15.7)

Line 7. RMAX1, RMAX2, RMAX3, TOLER1, TOLER2, TOLER3 in
FORMAT(1P3D12.4,3D10.2)

Line 8. XMAX, XOLER in FORMAT (1PD12.4, D10.3)

ENT5 contains default values for the data in lines 6-8, see

Table III.

When a calculation is restarted, line 9 of this file contains the principle restart control parameters J, KB, LAMBDA, and IORD of the last calculated R-integral. A list of X-amplitudes already calculated and, below each X-amplitude, the absolute error in that amplitude appear from line 10 to the end of the file.

ENT5 reads in the above variables whether this is a new calculation or a restart. They are defined in Table III, "Global Variables of ENT".

For a restarted calculation the device 5 input data is identical to the device 9 output of the previous calculation. In order to restart a calculation, this device 9 output must be transferred to device 5 as input to the new calculation.

Device 4 input:

Input on device 4 (K.STR) is used to indicate to ENT5 which solutions to the Dirac equation have already been calculated and stored. Initially it is an empty file. After a run of ENT, a list of filenames of solutions that have been calculated is output on device 8. This should be used as input on device 4 on the next run of ENT. New solutions calculated on this next run will be added to the list and output on device 8.

K.STR contains a list of the filenames used to store the inward and outward solutions of the homogeneous Dirac equation calculated by subroutine ELM. The purpose of this list is to keep

track of which solutions have already been computed. Of the four indices characterizing an R-integral these solutions are identified by IORD and KB only. A solution characterized by IORD and KB may be required for several R-integrals which differ in J and LAMBDA.

An example of K-STR is shown in Fig. 16. Each entry is stored in ASCII array SLIST(I).

Device 12 input:

The bound state wave function is input on device 12 throughout the calculation.

Device 6 output:

If the computation is not proceeding normally error messages appear here. Most of them will be self explanatory. Some, though, will return with a statement IFLAG=N. The values of IFLAG are given in Table IV.

The normal Device 6 output signals control through ENT5. When the multipole series has converged, ENT5 lists all pertinent data and makes a line printer plot of the differential cross section as a function of angle. A sample of the final device 6 output is given in Fig. 17. (But notice that the total elastic cross section represents the analytic integration over angles of the sum of squared amplitudes resulting from the current calculation only. In general the Rayleigh amplitude is not the

only important elastic amplitude. Total cross sections cannot be calculated separately for individual elastic processes.)

Device 7 output:

This (C.STR) is a sequential output of the R-integrals (the partial contributions to the X-amplitudes), and the CPU time required for the calculation of each R-integral. This output is never used again by the current program series, but this output would prove necessary if separate total pair production cross sections are desired. Also, it is useful to indicate important contributions to the X-amplitudes as a function of J, KB, etc.

Device 8 output:

As described previously, onto device 8 (K.STR) is output the list of filenames containing solutions to the Dirac equation which have been calculated by ENT5 and stored. This output is then used as device 4 input when ENT is restarted. Once the multipole series has converged, K.STR may be deleted.

Device 9 output:

Onto device 9 is output a copy of the main control parameters which were input on device 5 at the start of the calculation, the indices (J, KB, LAMBDA, IORD) of the last calculated R-integral, and a list of previously calculated X-amplitudes with their maximum absolute errors. This output data will become the device 5 input data(E.CDR) for a restart of the calculation.

Devices 10, 11, 13, and 14 provide intermediate internal storage, and may be deleted after convergence of the multipole series. Device 10 contains the outward solution (the solution regular at the origin) of the homogeneous Dirac equation. See the sections on ELM and SPRUCE below. Device 11 contains the inward solution (the solution regular at infinity) of the homogeneous solution. See the sections on SUMAC and SPRUCE below. Device 13 contains the values as a function of r of coefficient B (COEFB). See the section on WILLOW below. Device 14 contains the values of the coefficient A (COEFA). See the section on GINKGO below.

COMMON BLOCKS:

Data passed from MAIN (ENT5) to subroutines in both INT5 and ORB5 subroutine packages.

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, VX

/BIRCH/ L, KAPPA, DRAP, AJ, L, LP, GAMMA, PHASE, AMP, ISCALE.

R3STOP, R5STOP

/CONST/PI, ALPHA, RY, CON, ELOG

Data passed from ENT5 to INT5 subroutine package.

/POPLAR/EA, NA, KA, ANORMA, GAMA

/ERRCHK/WRTE, WRPE, ORTE, GRPE, ATERR, ATERRI, APERRR, APERRI

C. Subroutines

The major subroutines of ENT5 are contained in two subroutine packages: ORB5 and INT5. The subroutines in ORB5 produce two linearly independent solutions to the homogeneous Dirac equation. The subroutines in INT5 complete the calculation of the perturbed orbitals and perform the radial integration to determine the R-integral.

1. Subroutines I/O

The readable output from these subroutines identifies itself on the Device 6 output shown in Fig. 17. It consists of diagnostics in the case of errors and lines signaling the call of the given subroutine.

"RMAX = ... RASY = ... TOLER = ..." indicates that ENT has successfully completed input checks and has begun a calculation of an R-integral.

"START OUTWARD SOLUTION... RMAX = ..." signals a call to ELM.

"TIME CHECK..." signals a RETURN to ENT from a subroutine.

"START INWARD SOLUTION... RMAX = ..." signals a call to SUMAC.

"CALCULATE (COEPB)..." signals a call to WILLOW.

"CALCULATE (COEFA)..." signals a call to GINKGO.

"CALCULATE R-INTEGRAL..." signals a call to ALDER.

The following signal flow-through ALDER:

"START DEVICE 10 INPUT: (G0, F0)"

"START DEVICE 11 INPUT: (G1, F1)"

"START DEVICE 13 INPUT: (COEFB)"

"START DEVICE 14 INPUT: (COEFA)".

"CON:..." signals return to ENT.

The dump is performed next (see Section 3 above).

2. ORB5 (Subroutine Package)

These subroutines generate the two linearly independent solutions to the homogeneous Dirac equation.

ELM (RMAX, ERR, ISOL, ERRASY) called by ENT5 (flowchart Fig 5)

ELM controls the calculation of the solution to the homogeneous Dirac equation which is regular at the origin (the so-called outward solution).

The solution is in the form of a vector with two radial components ($G_0(r)$,

$F_0(r)$). To take advantage of the known behavior at the origin

$f(r) \sim r^Y$, ELM initially solves for $(S_G(r), T_0(r)) = (G_0(r),$

$F_0(r))/r^Y$. This is continued to RMAX, or the first zero of $S(r)$,

whichever comes first. Then ELM solves for (G_0, F_0) out to $R = RMAX$.

RMAX -> see Table III.

ERR -> Absolute error tolerance passed to SPRUCE. ERR controls integration step size.

ISOL -> indicates type of solution to be calculated (see Table III).

ERRASY -> Error tolerance in determining asymptotic expansions of the

outward solutions for this RMAX.

COMMON BLOCKS:

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, JX

/BIRCH/E, KAPPA, DKAP, AJ, L, LP, GAMMA, PHASE, AMP, ISCALE, R3STOP.

R5STOP

/CONST/PI, ALPHA, RY, CON, ELOG

Data passed between ELM and its subroutines

/OAK/ EP, FM, G1, G2, H

/PALM/ N, N1, N2, N3, N4, N5

/PINE/ P, ANU, B, C

/LATE/ ARRASY, CRR1, CRR2

ORIGIN (S, SP, T, TP) called by ELM

ORIGIN determines the values of (S_0, T_0) and their derivatives at the origin by means of a power series expansion of the solution. It assumes that the atomic potential can be expanded as

$$V(r) = (-Z \alpha/r)(1 + V_1 \lambda r + V_2 (\lambda r)^2 + V_3 (\lambda r)^3 + \dots).$$

No Input.

Output (S_0, T_0) and $d/dr(S_0, T_0)$ at the origin.

COMMON BLOCKS

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, VX

/BIRCH/E, KAPPA, DKAP, AJ, L, LP, GAMMA, PHASE, AMP, ISCALE,

R3STOP, R5STOP

ASPEN (S, SP, T, TP) called by ELM

This subroutine determines the values of (S_0, T_0) and their derivatives at three more points near the origin. It uses a method similar to one suggested by W. R. Johnson (Notre Dame) and uses interpolation formulas with the differential equations to give simultaneous algebraic equations in the unknowns.

INPUT (S_0, T_0) and $d/dr(S_0, T_0)$ at the origin.

OUTPUT (S_0, T_0) and $d/dr(S_0, T_0)$ at three points near the origin.

COMMON BLOCKS:

Data passed from ELM to ASPEN

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, VX

/BIRCH/E, KAPPA, DKAP, AJ, L, LP, GAMMA, PHASE, AMP, ISCALE.

R3STOP, R5STOP

/OAK/ EP, EN, G1, G2, H

SUMAC (RMAX, ERR, ISOL, ERRASY) called by ENT5 (flowchart Fig. 6)

SUMAC controls the calculation of the solution to the homogeneous Dirac equation which is regular at infinity (the inward solution). The solution is effected by integrating the homogeneous Dirac equation inward from RMAX to the origin R3STOP to find the solutions (G_1, F_1) . Then the program changes variables and solves for $(U_1, V_1) = r^Y (G_1, F_1)$ to R5STOP (very near the origin) taking advantage of the known behavior of the solution $G(r) \sim 1/r^Y$ near the origin.

RMAX -> see Table III.

ERR -> Absolute error tolerance passed to SPRUCE. ERR controls integration step size.

ISOL -> indicates type of solution to be calculated (see Table III).

ERRASY -> Error tolerance in determining asymptotic expansions of the outward solutions for this RMAX.

R3STOP and R5STOP are determined during the calculation of the solution regular at the origin (Subroutine ELM).

R3STOP = position at which outward solution in ELM changes from (S_0, T_0) to (G_0, F_0) .

R5STOP = position to stop (U_1, V_1) integration which is within one step-size of the origin.

COMMON BLOCKS:

Data passed by MAIN to SUMAC

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, VX

/BIRCH/E, KAPPA, DKAP, AJ, L, LP, GAMA, PHASE, AMP, ISCALE,

R3STOP, R5STOP

/CONST/PI, ALPHA, RY, CON, ELOG

Data passed from SUMAC to its subroutines

/OAK/ EP, EM

/PALM/ N, N1, N2, N3, N4, N5

/PINE/ P, ANU, B, C

/LATE/ ARRASY, CRR1, CRR2

/ASH/ NSKI

TAIL (G, GP, F, FP, RMAX, ISOL) called by SUMAC

TAIL provides starting values for inward integration controlled by SUMAC of the homogeneous Dirac equation. It uses asymptotic expansions determined during the calculation of the outward solution to find these values. First, though, it checks that RMAX is indeed in the asymptotic region.

The input variables are described in Table II.

COMMON BLOCKS:

Data passed by MAIN to SUMAC and then to TAIL.

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, VX

/BIRCH/E, KAPPA, DKAP, AJ, L, LP, GAMA, PHASE, AMP, ISCALE,

RJSTOP, R5STOP

/CONST/PI, ALPHA, RY, CON, ELOC

Data passed from SUMAC to TAIL

/OAK/ EP, EM

/PINE/ P, ANU, B, C

/ASH/ NSKI

The output is (G_1, F_1) and $d/dr(G_1, F_1)$ at 4 points in the asymptotic region.

SPRUCE (S, SP, T, TP, RMIN, RMAX, IROUTE, ERR, ISOL) called by ELM and SUMAC

SPRUCE does the actual integration of the radial homogeneous Dirac equation. It outputs the wave functions directly onto device 10 for the outward solution and onto device 11 for the inward solution. Much of the code is devoted to scaling of the data to prevent underflow and overflow by multiplying or dividing the solutions by powers of 10 whenever the solutions become too small or large and keeping track of these powers in a separate integer variable.

A predictor-modifier-corrector method of integration is used.⁹ The step-size is automatically halved or doubled according to the relation of

the truncation error estimate with the tolerances ERR1, ERR2, ERR3.

If ERROR < ERR1 step-size doubled.

If ERROR > ERR2 step-size halved.

If ERROR > ERR3 FATAL ERROR, execution stops.

Four initial points of the solution and its derivatives are required to start the integration. These are stored in arrays S, SP, T, TP.

INPUT: S, SP, T, TP arrays with starting values in them.

IRROUTE = 1 -> Outward integration R^Y , out

= 2 -> Inward R^Y , in

= 3 -> Inward integration R^{-Y} , in

= 4 -> Outward integration R^Y , continuum case

= 5 -> Inward integration R^{-Y} , out.

COMMON BLOCKS:

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, VX

/BIRCH/E, HAPPA, DKAP, AJ, L, LP, GAMA, PHASE, AMP, ISCALE.

R3STOP, R5STOP

/CONST/PI, ALPHA, RY, CON, ELOG

Data passed from SUMAC to its subroutines

/PALM/ N, N1, N2, N3, N4, N5

/PINE/ P, ANU, B, C

/LATE/ ARRASY, CRR1, CRR2

/ASH/ NSKI

3. INT5 (Subroutine Package)

The subroutines in this package generate the final particular solution to the inhomogeneous Dirac equation. WILLOW generates the coefficient(COEFB) of the homogeneous solution which is regular at the origin. GINKGO generates the coefficient(COEFA) of the homogeneous solution which is regular at infinity. ALDER constructs the final particular solution and computes the R-integral.

WILLOW (W, J, LAMBDA, IORD, ERR, ISOL) called by ENT (flowchart Fig. 8)

WILLOW evaluates the integral over outward solution (G_0, F_0) of the homogeneous Dirac equation multiplied by the driving term of the corresponding inhomogeneous Dirac equation. This forms the coefficient of the inward solution COEFB(r) used in forming the particular solution to the inhomogeneous Dirac equation. The integration method used is a three point closed type Newton-Cotes quadrature (see Ralston and Wilf⁹, p.24). This method has been chosen to match the integration method used to evaluate (G_0, F_0) in that the truncation errors of both methods are the same. The step-size is automatically halved or doubled according to the relation between the truncation error estimate and the error tolerances TOLER1, and

TOLER2.

COEFB(r) is output in order of increasing r.

The input variables are described in Table III. "Global Variables of ENT".

The outward solution is input from device 10, and the bound state wavefunction from device 12.

Output.

COEFB(r) is written onto device 13.

COMMON BLOCKS:

Data passed from MAIN (ENT5) to WILLOW

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, VX

/BIRCH/ E, KAPPA, EKAP, AJ, L, LP, GAMMA, PHASE, AMP, ISCALE.

R3STOP, R5STOP

/CONST/PI, ALPHA, RY, CON, ELOG

/POPLAR/LA, NA, KA, ANORMA, GAMA

/ERRCHK/WRTE, WRPE, ORTE, CRPE, ATERR,ATERRI, APERRR, APERRI

Data passed from WILLOW to its subroutines.

/ACORN/ R, B, F, LP, GAM, IREC, AM, EM, ICYCLE, IRECA, TOTAL.

ITOTAL, STEBJ, TBIAS, IBIAS, EBCOND

/BEECH/ RO, GO, FO, MP, GAMO, IRECO, B, C, PHASE, ANU, P, L, NSKO.

ARRO

/HOLLY/ RI, GI, FI, NP, GAMI, IRECI, CAMPI, FAMP, PHASEI, ANUI,

API, LI, NSKI, ARRI

GINKGO (W, J, LAMBDA, IORD, ERR, ISOL) called by ENT5 (flowchart Fig. 9)

GINKGO evaluates the integral over the inward solution to the homogeneous Dirac equation multiplied by the driving term of the corresponding inhomogeneous Dirac equation. This term COEFA(r) is used as the coefficient of the outward solution in forming the particular solution to the inhomogeneous equation. GINKGO uses the same integration method as WILLOW and is quite similar in most respects. The integral is performed from infinity to the origin. Thus, the data from the bound state file is read sequentially backwards starting from the end of the file.

For the definitions of the input variables in the calling string see Table III. The bound state wave function is read in on device 12, and the inward solution, that generated by SLMAC, is read on device 11.

The output consists of the values of COEFA(r) in order of decreasing r, and is placed on device 14.

COMMON BLOCKS:

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, VX

/BIRCH/ E, KAPPA, DKAP, AJ, L, LP, GAMMA, PHASE, AMP, ISCALE.

R3STOP, R5STOP

/CONST/PI, ALPHA, RY, CON, ELOG

/POPLAR/EA, NA, KA, ANORMA, GAMA

/ERRCHK/WRITE, WRPE, ORTE, GRPE, ATERR,ATERRI, APERRR, APERRI

/ACORN/ R, B, F, LP, GAI, IREC, AM, BM, ICYCLE, IRECA, TOTAL.

ITOTAL, STEBJ, TBIAS, IBIAS, EBCOND

/BEECH/ RO, GO, FO, MP, GAMO, IRECO, B, C, PHASE, ANU, P, L, NSKO.

ARRO

/HOLLY/ RI, GI, FI, NP, GAMI, IRECI, GAMPI, FAMPI, PHASEI, ANUI.

API, LI, NSKI, ARRI

ALDER (RINTR, RINTI, IRINT, W, J, LAMBDA, IORD, ERR, ISOL) called by ENT5

(flowchart Fig. 10)

ALDER constructs the required solution of the inhomogeneous Dirac equation (perturbed orbital), incorporating the appropriate boundary conditions, and performs the radial integral over the solution to determine the R-integrals. The integration method is the same as that used in WILLOW and GINKGO.

The input variables, W, J, LAMBDA, IORD, ERR, are defined in Table III ("Global Variables of ENT").

From device 10 is read the outward solution in order of increasing R.

11

inward solution in order of decreasing R.

- 12 bound state in order of increasing R.
- 13 COEFB(r); increasing R.
- 14 COEFA(r); decreasing R.

COMMON BLOCKS:

/MAPLE/Z, IZ, A

/WALNUT/IPOT, AS, ALAMB, SZ, ISZ, VX

/BIRCH/ E, KAPPA, DKAP, AJ, L, LP, GAMMA, PHASE, AMP, ISCALE,

R3STOP, R5STOP

/CONST/PI, ALPHA, RY, CON, ELOG

/POPLAR/EA, NA, KA, ANORMA, GAMA

/ERRCHK/WRTE, WRPE, ORTE, GRPE, ATERR, ATERRI, APERRR, APERRI

/ACORN/ R, B, F, LP, GAM, IREC, AM, BM, ICYCLE, IRECA, TOTAL,

ITOTAL, STEBJ, TBIAS, IBIAS, EBCOND

/BEECH/ RO, CO, FO, MP, GAMO, IRECO, B, C, PHASE, ANU, P, L, NSKO.

ARRO

/HOLLY/ RI, CI, FI, NP, GAMI, IRECI, GAMPI, FAMPI, PHASEI, ANUI.

API, LI, NSKI, ARRI

7. SHELL

After the multipole series has converged in ENT5, the final device 7 output (C.STR) is appended to the final device 9 output (E.CDR). This combined file becomes the device 5 input for SHELL. SHELL takes this data and writes it into a permanent subshell data file which provides the X-amplitudes in a form suitable for use by subsequent codes. Such a code is TABX5 which adds the amplitudes due to several subshells, estimates higher shells using modified form factors and also adds the nuclear Thomson amplitudes. If ENT5 is run with a photon multipole series increment JINC other than 1, then SHELL will interpolate the missing X-amplitudes from the list of X-amplitudes it is given. Care should be exercised when using this feature of the calculation since it has not been fully investigated.

TO USE SHELL (see fig. 18)

Append the final device 7 output (C.STR) of ENT5 to the final device 9 output of ENT5 to form device 5 input to SHELL. The device 6 output of SHELL contains calculation diagnostics while the device 7 output of SHELL is the data referred to as the permanent subshell data file. In the past, the

naming convention for the file containing the permanent subshell data has been of the form "RUN".RAY where RUN is the ASCII literal used to identify the calculation and was in the main parameter input to ENT5 (see section 6 above).

8. MFSTR1 (see fig. 21,22)

MFSTR1 generates the modified form factor $q(q)$ for a given atomic subshell and outputs it as a function of the momentum transfer q . The form factor q is defined in section 2 above.

A. I/O of MFSTR1

The device 5 Input consists of the file name of the bound state wave function for which the calculation is to be performed and the name of the file into which the calculated form factors are to be placed.

The potential L??POT (where ?? is the atomic number) required for $q(q)$ must already be on disk. MFSTR1 reads this potential data from disk.

B. TO USE MFSTR1

To use MFSTR1 have available on disk the necessary bound state wave function file and the corresponding atomic potential file. Device 5 input will consist of pairs of ASCII filenames, each on a separate line. The first filename is the name of the file containing the bound state wave function data. The second filename is the name of the file into which MFSTR1 is to write the modified form factors. MFSTR1 will STOP when it encounters a blank input for the first filename of the pair. Therefore, modified form factors for an indefinite number of different shells may be computed in a single execution of MFSTR1 by providing the necessary input pairs of ASCII information.

An example of device 5 input for the calculation of the modified form factor for the K-shell of carbon would be:

```
CK.HKL  
CKMF.HKL  
blank card
```

Filenames are ASCII strings left justified, in FORMAT(A10).

The bound state wave function data file named in the first record (CK.HKL) is input on device 12. The potential data (L6.HKL) must be

available on disk. This will be input by MFSTR1 on device 1. (MFSTR1 opens the bound state wave function data file and reads the value of the atomic number, in this case 6, and computes the required potential filename.)

Diagnostics of the calculation are output during the course of the calculation onto device 6.

9. TABX5 (see fig. 23,24,25)

TABX5 is the program which produces the final Rayleigh amplitude and differential cross section tabulation. It is output as a function of scattering angle and of momentum transfer. It contains contributions from as many subshells as the user desires (all for the whole atom). The input consists of the files containing the 'exact' inner subshell contributions and the MFSTR output containing the modified form factors for higher shells. These are added coherently and the sum is squared to give the differential cross sections.

The input variable, QMAX, requires explanation. Since the modified form factor is basically the Fourier transform of the charge density there is a value of q , the momentum transfer, beyond which the modified form

factor decreases monotonically to zero despite any structure it has for low q . QMAX is a subshell dependent quantity determining the momentum transfer where the contribution becomes insignificant. The program will ignore this subshell for $q > \text{QMAX}$. It has been customary to set QMAX=100 for all S subshells (K, L_I, M_I , etc.) since these have the most penetrating wavefunctions. In these units ($\hbar = m_e = c = 1$), 100 ($=2061 \text{ \AA}^{-1}$) is a rather large momentum transfer and so contributions are included for almost all q 's. For the other shells there is a default in TABX5. Setting QMAX = -N (N the principle quantum number) forces TABX to set QMAX to a default which depends on the structure of the wavefunctions (which in turn affects the functional form of the modified form factors). The default is $\text{QMAX} = 206.1 * Z / N^2$.

The other variables are straightforward.

A. I/O Summary for TABX5

Device 5 input:

CARD1. For each shell for which the contributions have been computed exactly

FNAME, ELNUM in FORMAT(A10,G).

FNAME is the name of the subshell data file.

ELNUM is the occupation number of the subshell. It is any real positive number $\leq 2j+1$.

CARD2. BLANK

CARD3. FNMK, ELECK in FORMAT (A10,G)

FNMK is the name of modified form factors file for the K-shell. If the modified form factor is used for any outer shell, the K-shell's modified form factor must be input, because for $q > 10A^{-1}$ the ratio of the higher subshell's modified form factors to the K-shell modified form factors is used instead of the higher subshell's modified form factors directly.

ELECK is the occupation number of the K-shell.

CARD4. For each higher shell to be approximated with the modified form factors a card with

FNMO, ELEC, QMAX in FORMAT(A10,3G).

FNMO is a 10 ASCII character name of the file containing the modified form factors for this subshell.

ELEC is the occupation number

QMAX is the maximum momentum transfer.

CARD5. A BLANK CARD.

Note: If all shells are computed exactly then no cards of types 3 and 4 appear. The deck is then just cards of type 1, two blank cards and the following two cards.

CARD6. COM1,COM2 in FORMAT (2A10)

These form a 20 ASCII character comment which is used to label the tabulation.

CARD7. INC,AT in FORMAT (I,F)

INC is the angular increment (integer number of degrees).

INC=0 defaults to INC=15. We have been using INC=5.

AT is the atomic weight of the atom. If it is not zero then the nuclear Thomson amplitudes for a nucleus of the prescribed AT.

The data files named in the CDR file are read from Device 10.

Device 6 output:

Device 6 contains diagnostics and error messages if any, and a list of the CDR input.

Device 8 output:

The device 8 output is the final tabulation. See fig. 25.

References

1. L. D. Kissel "Rayleigh Scattering, Elastic Photon Scattering by Bound Electrons" (Thesis). (This work contains a detailed derivation of the formulas of Section 1, a full description of the numerical techniques employed in ENT5, SHELL and TABXS, and a detailed comparison of numerical results of these codes with other work both theoretical and experimental for neutral atoms with $W > 1 \text{ keV.}$); L. D. Kissel and R. H. Pratt, Phys. Rev. Lett. 40, 287 (1978); L. D. Kissel and R. H. Pratt, to be published.
2. G. E. Brown, R. E. Peierls, J. B. Woodward, Proc. Roy. Soc. A227, 51 (1954).
3. W. R. Johnson and F. D. Feilock, Phys. Rev. 168, 22 (1968).
4. G. E. Brown and G. W. Schaefer, Proc. Roy. Soc. A233, 527 (1956).
5. William E. Boyce, Richard C. DiPrima "Elementary Differential Equations" (Wiley & Sons), p. 119.
6. D. Liberman, J. T. Waber and D. T. Cromer, Phys. Rev. 137, A27 (1965).
7. James H. Scofield "Theoretical Photoionization Cross Sections from 1 to

1500 keV" UCRL-51326 (available from the National Technical Information Center, NBS)

8. W. Franz, Z. Physik 95, 652 (1935); W. Franz, Z. Physik 98, 314 (1935).
9. A. Ralston and H. S. Wilf "Mathematical Methods for Digital Computers" vol. 1, (Wiley), New York, 1960.

INDEX

Accuracy	39
ALDER	49, 57, 60
Angular dependence	8, 25
Angular increment	68
Angular momentum	3-4, 6, 20, 22, 30
ASPEN	52
Bound state	46, 61
Central potential	3, 20
Charge	41
Charge density	2, 29
Code design	16, 35
COEFA	57
COEFB	57
Coherent	1, 19
Control parameters	45, 47
Core relaxation	12, 31
Correlation	3, 12, 30-31
Cross section	1, 14, 19, 33, 46, 65
Dirac equation	8-9, 24-25, 45, 49
Dirac-Hartree-Fock-Slater	2, 29
Elastic cross section	46
Elastic photon-atom scattering	1, 19
Electron propagator	5, 21
ELM	48-51, 55
Energy range	1, 19
ENTS	14, 16-17, 33, 35, 42-50, 53, 58-59, 62
Exchange	2-3, 29-30, 38

GINKGO	48-49, 57, 59, 60
Homogeneous Dirac equation	9, 25, 49
Inhomogeneous Dirac equation	8, 24
Input variables	16, 35
INT5	44, 48-49, 57
Integration method	55, 57
Inward solution	53, 60
Kohn-Sham exchange	2, 30, 38
Lamb shift	2, 29
Latter tail	2, 30, 38
LWF	42
Matrix element (see also R-integral)	6-7, 22-24
Method of integration (see integration method)	
MFSTR1	14, 33, 42, 63
Modified form factor	13-14, 31-32, 63
Modular design	16, 35
Momentum transfer	14, 32
Multipole expansion	10, 26
Multipole series	43, 47
Naming convention	63
Newton-Cotes quadrature	57
Nuclear Thomson amplitudes	62, 69

Occupation numbers 3, 30, 41
 ORB5 44, 48-50
 ORIGIN 51
 Outward solution 50, 54, 57, 60

 Partial wave expansion 5, 20
 Permanent subshell data file 62
 Perturbed orbitals 7-8, 23-24, 43
 Photon multipole 6, 10, 22, 26, 43, 47
 Photon operator 6, 22
 Photon polarization 11, 27
 Potential 1-3, 29-30, 39-42
 Predictor-modifier-corrector 55

 R-integral 9, 17, 26, 35, 43, 46-47, 49, 57
 Radial matrix elements 9, 26
 Radial wave functions. 4, 20
 Rayleigh scattering amplitudes . . . 1, 3, 5, 11-20, 27-29, 32-34, 43, 65
 Rosen-Lindgren potential. 38
 RSCF 16, 34

Table I. Filling of Inner Subshells

Subshell name	Spectroscopic notation	n	κ	j	l	#electrons in a filled shell
K	1s _{1/2}	1	-1	1/2	0	2
L _I	2s _{1/2}	2	-1	1/2	0	2
L _{II}	2p _{1/2}	2	1	1/2	1	2
L _{III}	2p _{3/2}	2	-2	3/2	1	4
M _I	3s _{1/2}	3	-1	1/2	0	2
M _{II}	3p _{1/2}	3	1	1/2	1	2
M _{III}	3p _{3/2}	3	-2	3/2	1	4
M _{IV}	3d _{3/2}	3	2	3/2	2	4
M _V	3d _{5/2}	3	-3	5/2	2	6

TABLE II. Global Variables in RSCF

A	Major component of wave function. Temporary storage.
AAME	Problem name.
A0, B0	Temporary storage.
B	Minor component of wave function. Temporary storage.
BCOND	Gives Wigner-Seitz boundary conditions if set to 1.
BINDEN	Electron binding energies.
CONVRG	Set equal to 1.0 when convergence criterion is met.
DA, DB	Temporary storage.
DENS, Y	Temporary storage.
DEL	Accuracy criterion for eigenvalues.
DELRVR	Accuracy criterion for convergence.
EE2, EY	Exchange energy.
EPS	Parameter used to determine the practical infinity of each orbital.
ET3	Total energy.
EV, ED	E-E potential energy.
EV3, ER	Integral of $\rho\phi(R)=V(R)$
EV4, EZ	E-N potential energy.
FEX	Control parameter for free electron exchange potential and Binding energy calculations.
FN, FL, FJ, E	Current values of XN, XL, XJ, XE.
H	Interval of the logarithmic mesh. read as the reciprocal.
J	Number of shells.
KPOT	The Kohn-Sham and new potential functions may be specified By setting KPOT=2 and KPOT=3 for Slater exchange. Kpot=4 for Rosen-Linderen potential.
N	Number of points in radial mesh.
NC1	Maximum number of cycles before dump.
NDEBUG	If nonzero additional printing is done to aid in debugging.
NPRINT	If set to 1 gives a printout of the orbital functions.
PHI	Averaging factor.
PV	Pressure. Temporary storage.

PVT	Total pressure.
Q	Integral of charge density.
R1	Sphere radius for newpot.
RAD	Table of radii.
RH	Radial charge density.
RHNLJ	Temporary storage.
RN	Maximum radius.
RNUC	Radius of nucleus in Bohr radii.
SUMMA	Sum of eigenvalues.
VO	Constant term in potential near origin.
VR	$R*V(R)$
VRX	Free electron exchange potential correction. Temporary storage.
XALPHA	Slater exchange coefficient.
XE	Eigenvalue.
XION	Ionicity.
XJ	Total angular momentum of orbital.
XK00P	Set to +1.0 or -1.0 when computing binding energies.
XL	Orbital angular momentum of major component.
XLATTR	Coulomb tail parameter.
XN	Radial quantum number.
XZ	Number of electrons in shell.
Z, ZN	Atomic number.

TABLE III. Global Variables of ENT5

AJ	same as J (dble)
AJA	total ang. mom. qu. no. of bound state
AJB	total ang. mom. qu. no. of perturbed orbital
ALAMB	LAMBDA, parameter used by some potentials
AMP	amplitude of asymptotic wave functions
AMUL	coefficient of R-integrals in sum over perturbed orbitals to form X-amplitude
APEI	ALDER propagation error (Im)
APER	ALDER propagation error (Re)
ANORMA	bound state normalization
ATEI	ALDER truncation error (Im)
ATER	ALDER truncation error (Re)
AS	screening multiplier. In some cases, $ALAMB = AS * 1.13 * Z^{1/3} * ALPHA$
EA	bound state total energy
EB	perturbed orbital total energy
ERR?	absolute error tolerance used for controlling step-sizes of integration schemes (ERR is usually in the range 10^{-4} through 10^{-10}) (ERRORB used in calculation of perturbed orbitals, ERRINT used for radial integrals)
FNAMEI	contains 10 character ASCII string for name of disk file containing inward homogeneous solution
FNAMEO	contains 10 character ASCII string for name of disk file containing outward homogeneous solution
GAMA	value of gamma for bound state; $GAMA = \sqrt{KA^{**2} - A^{**2}}$
GRPE	GINCKO relative propagation error
GRTE	GINCKO relative truncation error
IORD	variable identifying order of photon absorption-emission

process (1=> absorption first;-1=> emission first)

IPOT contains code for type of potential being used.

IRINT exponent of R-integrals (RINTR,RINTI)

ISOL flag indicating type of state for perturbed orbitals

ISOL = 1 => bound state, $-1 < EB < 1$

= 2 => positive energy continuum state, $1 < EB$

= 3 => negative energy continuum state, $EB < -1$

ISZ same as SZ (int)

IUNITS switch specifying units of 'WIN' energy input

IUNITS = 0 => 'WIN' in $m_e c^2$ (511 kev)

= 1 => 'WIN' in kev

= 2 => 'WIN' in Rydbergs (13.6 ev)

IZ same as Z (int)

J total ang. mom. qu. no. of photon

JINC increment of photon multipole series

JMAX maximum j of photon angular momentum sum, program may stop before JMAX is reached if sum convergence tolerance is satisfied (see XMAX, XOLER)

KA kappa qu. no. of bound state

KB kappa qu. no. of perturbed orbital

LAMBDA indicator of photon multipolarity:

LAMBDA = 0 => magnetic multipole

= 1 => electric multipole

LA orbital ang. mom. qu. no. of bound state (L)

LB orbital ang. mom. qu. no. of perturbed orbital (L)

LPA orbital ang. mom. qu. no. of bound state (L')

LPB orbital ang. mom. qu. no. of perturbed orbital (L')

NA principle qu. no. of bound state

NAME? contains various ASCII character strings used to form 'FNAMEI' and 'FNAMEO'

PHASE value of phase shift

POTID real, 10 element array containing ASCII string of
 characters identifying potential being used

RASY minimum radial position to which explicit numerical
 solutions are to be found. This value is derived
 from user supplied tolerance, TOLER?

RINTI imaginary part of R-integral

RINTR real part of R-integral

RMAX radial position to which explicit numerical
 solutions to the homogeneous equations will
 be calculated. Maximum of (RASY,RMAX?)

RMAX1 user supplied minimum radial position to which explicit
 numerical solutions to the homogeneous equations are
 to be found for ISOL=1

RMAX2 same as RMAX1 for ISOL=2

RMAX3 same as RMAX1 for ISOL=3

RUN input string of 6 ASCII characters used to form
 filename of disk files containing the homogeneous
 solutions

SLIST array containing the names of the outward
 homogeneous solutions calculated already

SZ asymptotic charge of potential, ionic charge

TOLER1 tolerance used to calculate RASY for ISOL=1
 TOLER1 equals the value of $1/(P \cdot RASY)$

TOLER2 tolerance used to calculate RASY for ISOL=2
 TOLER2 equals value of ratio of the potential
 to the kinetic energy at RASY

TOLER3 same as TOLER2 but for ISOL=3

TSTOP program stops when CPU time used in minutes
 exceeds this input parameter

W photon total energy (frequency)

VX 10 element array containing the potential expansion

coefficients

WIN	incident photon energy input (in units given by 'IUNITS')
WRTE	WILLOW relative truncation error
WRPE	WILLOW relative propagation error
XAMPI	imaginary part of X-amplitude
XAMPR	real part of X-amplitude
XEI	X-amplitude error (Im)
XER	X-amplitude error (Re)
XMAX	value used to test convergence of photon multipole series

When the ratio of the real part of the electric X-amplitude to XMAX becomes less than the value of XOLER, the program terminates. If XMAX=0.0 on input, then the ratio of XAMPR(J,1) is compared to XAMPR(1,1). If this ratio is less than XOLER, the program terminates

XOLER	convergence criteria for multipole series. If XOLER 0.0 on input, default value of 10^{-5} is assigned
Z	atomic number

Table IV. IFLAG

(a) During Initial Input Parameter check

IFLAG	Error
1	$IZ \leq 0$
2	$IZ > 137$
10	$IUNITS < 0$
20	$IUNITS > 2$
100	$JMAX \leq 0$
200	$JMAX > 300$
400	$JINC > 50$
2000	$ERRORB \geq 10^{-4}$
10000	$WIN < 0.0$
200000	$ERRINT > 10^{-4}$

(b) During Data Consistency Checks

(The data are checked for consistency at the beginning of every major subroutine)

IFLAG	Error
1	Data is being read from the wrong device.
20	Atomic number inconsistency.
300	Asymptotic charge of the potentials do not match
4 000	Angular momentum and parity quantum numbers (Kappa) do not match.
50 000	Energies are inconsistent
600 000	The data being input was created with a different type of potential.
7 000 000	Potential screening error
80 000 000	Inconsistency in Lambda.

In the event that more than one of the above errors occur IFLAG will be returned as the sum of the appropriate error flags. For example, 80600301 would signify an inconsistency in Lambda, an inconsistency in the type of potential being used, an inconsistency in the asymptotic charge of the potential, and that the data was found on the wrong device.

Table v. validity of the modified form factor

energy (relative to K -binding)	error in the ψ_{rel}	
	for L -shell amplitudes	for total atom
$2 E_K$	2%	10%
$5 E_K$	0.1%	5%
$10 E_K$	0.0%	3%
$25 E_K$	0.0%	1.5%
$100 E_K$	0.0%	0.1%

FLOW CHART SYMBOLS

FLOW OF CONTROL

TRANSFER OF DATA

PROCESS, PROCEDURE, OR
PROGRAM EXECUTION

HIGH SPEED ON LINE STORAGE
(DISC, ETC.)

DECISION

CONNECTORS

HARD COPY OUTPUT
(LINE PRINTER, ETC.)

INPUT / OUTPUT

Figures

1. Order of the Calculation
2. Data Transfer for Calculating Relativistic SCF Potential and Wave Functions
3. I/O used by ENT5
4. ENT5 flowchart
5. ELM flowchart
6. SUMAC flowchart
7. SPRUCE flowchart
8. WILLOW flowchart
9. GINKGO flowchart
10. ALDER flowchart
11. Input of RSCF for He-like Carbon
12. Output of RSCF for He-like Carbon: potential and wavefunction
13. Initial E.CDR file for neutral Carbon's K-shell at 0.23 kev.
14. Final " " " " " " " " " "
15. Final C.STR file " " " " " " " "
16. Final K.STR file
17. Device 6 output of the last few modules of ENT5
18. I/O for SHELL
19. Device 6 output of SHELL
20. Device 8 output of SHELL
21. I/O of MFSTR1
22. Output of MFSTR1: MFF's for Carbon's K-shell.
23. I/O of TABX5
24. Flowchart of TABX5
25. Final tabulation

ORDER OF THE CALCULATION

DATA TRANSFER FOR CALCULATING RELATIVISTIC SCF POTENTIAL AND WAVE FUNCTION

a. RSCF

b. SEPARATING THE WAVE FUNCTIONS FROM THE POTENTIAL

I/O USED BY ENT5

FLOW CHART OF ENT

FLOW CHART OF ENT

cont.

FLOW CHART OF ENT

cont.

FLOW CHART OF ELM

FLOW CHART OF ELM

cont.

FLOW CHART OF SUMAC

FLOW CHART OF SPRUCE

FLOW CHART OF SPRUCE

cont.

FLOW CHART OF WILLOW

FLOW CHART OF GINKGO

cont.

FLOW CHART OF ALDER

FLOW CHART OF ALDER

cont.

[illegible]

[illegible]

[illegible]

13. Initial E.CDR file for neutral Carbon's K-shell at 0.23 kev.

CH22 10.00

0

1 -1

2.30000000-01 1

10

0.00000000 0.00000000

0.00000+00 0.00000+00 0.00000+00 0.0000 0.0000 0.0000

0.00000+00 0.0000

14. Final E.CDR for neutral Carbon's K-shell at 0.23 kev

CH22 10.000 TIME:01:09 DATE:15-Sep-78 VER 4B 4/13/77

6

1 -1

2.30000000-01 1

3

1.00000000-06 1.00000000-08

0.00000+00 0.00000+00 0.00000+00 1.000-02 1.000-03 1.000-03

0.00000+00 1.000-05

3 4 0 -1

1 1.29101082070+00 0.00000000000+00 -8.52293317590-05 0.00000000000+00

2.20450-05 0.00000+00 5.32310-09 0.00000+00

2 1.91362417920-05 0.00000000000+00 1.61374669540-08 0.00000000000+00

4.21990-10 0.00000+00 1.82420-13 0.00000+00

3 5.5925164840-10 0.00000000000+00 2.28812119560-13 0.00000000000+00

1.21130-14 0.00000+00 2.73690-13 0.00000+00

15. Final C.DR for neutral Carbon's K-shell at 0.23 kev

1 -1 0 1	0.00017824	0.00000000	26.61	1.60-11	0.00+00	4.80-09	0.00+00
1 -1 0 -1	-0.00012144	0.00000000	27.84	9.80-12	0.00+00	2.20-09	0.00+00
1 1 1 1	-0.06373910	0.00000000	24.70	1.50-08	0.00+00	1.10-05	0.00+00
1 1 1 -1	0.52141119	0.00000000	26.43	1.40-08	0.00+00	6.20-06	0.00+00
1 -2 1 1	-1.45912993	0.00000000	25.52	1.50-07	0.00+00	1.70-05	0.00+00
1 -2 1 -1	-0.28955298	0.00000000	27.94	1.20-08	0.00+00	3.30-06	0.00+00
1 2 0 1	0.00001421	0.00000000	28.93	9.20-13	0.00+00	2.50-10	0.00+00
1 2 0 -1	0.00001422	0.00000000	30.18	2.00-12	0.00+00	2.20-10	0.00+00
2 -2 0 1	-0.00000002	0.00000000	19.11	1.30-15	0.00+00	1.80-13	0.00+00
2 -2 0 -1	-0.00000000	0.00000000	24.26	6.80-17	0.00+00	2.10-14	0.00+00
2 2 1 1	0.00000461	0.00000000	18.43	8.80-13	0.00+00	9.00-11	0.00+00
2 2 1 -1	0.00001844	0.00000000	22.81	8.80-13	0.00+00	2.00-10	0.00+00
2 3 1 1	-0.00003146	0.00000000	30.55	1.90-12	0.00+00	3.40-10	0.00+00
2 -3 1 -1	-0.00001072	0.00000000	33.60	7.50-13	0.00+00	1.10-10	0.00+00
2 3 0 1	0.00000000	0.00000000	33.62	5.10-17	0.00+00	1.20-14	0.00+00
2 3 0 -1	0.00000000	0.00000000	37.79	2.90-17	0.00+00	9.80-15	0.00+00
3 -3 0 1	-0.00000000	0.00000000	19.19	9.50-20	0.00+00	2.60-18	0.00+00
3 -3 0 -1	-0.00000000	0.00000000	24.19	2.50-21	0.00+00	6.20-19	0.00+00
3 3 1 1	0.00000000	0.00000000	19.71	3.40-17	0.00+00	2.80-15	0.00+00
3 3 1 -1	0.00000000	0.00000000	23.04	2.40-17	0.00+00	6.50-15	0.00+00
3 -4 1 1	-0.00000000	0.00000000	30.85	1.50-15	0.00+00	9.10-15	0.00+00
3 -4 1 -1	-0.00000000	0.00000000	35.73	5.10-17	0.00+00	3.70-15	0.00+00
3 4 0 1	0.00000000	0.00000000	33.33	2.70-21	0.00+00	3.90-19	0.00+00
3 4 0 -1	0.00000000	0.00000000	40.17	2.00-21	0.00+00	3.00-19	0.00+00

16. Final K.STR file

CKZ2 .C 1
CKZ2 .Y 1
CKZ2 .A 1
CKZ2 .M 1
CKZ2 .C 2
CKZ2 .Y 2
CKZ2 .A 2
CKZ2 .M 2
CKZ2 .C 3
CKZ2 .Y 3
CKZ2 .A 3
CKZ2 .M 3
CKZ2 .C 4
CKZ2 .Y 4
CKZ2 .A 4
CKZ2 .M 4

SHELL I/O

17. Device 6 output of the last few modules of ENT5

PROGRAM ENT5 (RAYLEIGH SCATTERING AMPLITUDES VERSION 20:30, 13-DEC-77)

PCB DATE 15-SEP-78 TIME 22:47

BEGIN DEVICE 5 PARAMETER INPUT:

END OF DEVICE 5 INPUT, INPUT PARAMETERS FOLLOW:

RUN=CL122 TSTOP= 10.0

IZ= 6

NA= 2 KA= -1

WIN= 2.0000000D-01 IUNITS= 1

JMAX= 15 J12C= 1

ERRORN= 1.000-06 PRINT= 1.000-08

RMAX1= 0.00000+00 RMAX2= 0.00000+00 RMAX3= 0.00000+00 TOLERR1= 1.000-02 TOLERR2= 1.000-03 TOLERR3= 1.000-03

XMAX= 0.00000+00 XOLERR= 1.000-05

PHOTON ENERGY IN K*CM**2, W= 5.4794081D-04

INITIALIZING POTENTIAL PACKAGE (SUBROUTINE AWAKE)

SELF-CONSISTANT POTENTIAL PACKAGE

SEARCHING FOR DISK POTENTIAL DATA FILE L 1.POT

CHNL SCF FOR NEUTRAL CARRON (C,Z=6), KORN-SHAN, L

DISK POTENTIAL FILE FOUND

SELF-CONSISTANT POTENTIAL (Z= 6, SZ= 1, IPOT=11)

INITIALIZE DEVICE 12 AND CHECK (DS) PAPA:

IZ= 6 NA= 2 KA= -1 EA= 9.996760D-01 ANORMA= 3.204331D-03

ISZ= 1 IPOT= 11 GAMA= 9.990410D-01 AJA= 0.5 EA= 0 LPA= 1

TIME CHECK: TIME=22:57: 29.6 ABS. CPU TIME (SEC) = 1.0916

RESTARTING AN OLD CALCULATION:

LAST CONTRIBUTION CALCULATED FROM: J= 3 KB= -4 LAMDA= 1 IORD= -1

AMUL= 1.5230095D+00

ITERATION PARAMETERS: J= 3 KB= 4 LAMDA= 0 IORD= 1
FILE NAMES, OUT=CL122 LA 4 IZ=CL122 LB 4 EB= 1.000516D+00 ISOL= 7
OMAX= 1.4163D+04 OMAXV= 1.4163D+04 TOLERR= 1.000-03
START OUTWARD SOLUTION (VERSION 10:30, 13-APR-77) RMAX= 1.4163D+01

ERROR ESTIMATE, ERRNR= 1.6E-03, AT POSITION W= 1.1102D+04 EXCEEDS FATAL ERROR TOLERANCE, ENR= 1.0-04
ERROR OCCURRED ON CYCLE 737 IN SUBROUTINE SPRUCE FOR KAPPA= 1.
PARAMETER DATA:

S(N)= 1.6173064D+09 S'(N-1)= 1.1336220D+09 S'(N-2)= 2.2467112D+09 S'(N-3)= 1.1267700D+09
S'(N)= -1.2760660D+09 S'(N-1)= -1.2755307D+09 S'(N-2)= -1.2739515D+09 S'(N-3)= -1.2713376D+09
T(N)= -6.3786933D+08 T'(N-1)= -6.3740417D+08 T'(N-2)= -6.3681632D+08 T'(N-3)= -6.3630000D+08
T'(N)= -2.2380579D+05 T'(N-1)= -2.1408057D+05 S'(N-2)= -1.1036000D+06 T'(N-1)= -1.1010550D+06
PC1= 2.6471403D+02 PC2= 1.4090626D+01 VTHP= -6.3003374D+07
C1= 2.0005163D+00 C12= -1.5083071D-04 C13= -3.1625762D-04 C22= -3.5003307D-04
C1= -1.1433389D+09 C2= -6.3740542D+08 C1= -1.1433389D+09 C2= -6.3740542D+08
AM1= -1.1433389D+09 AM2= -6.3740542D+08 AM1= -1.1433389D+09 AM2= -6.3740542D+08
RECALCULATING ERRORS:

OLD ANSERP= 2.65E+02
 OLD RELEPR= 1.64E-13
 NEW RELEPR= 7.73E-08
 NEW ERRPR= 7.73E-00

TIME CHECK: TIME=22:57: 57.6 AMS. CPU TIME (SEC) = 20.0115 CPU TIME SINCE LAST CALL (SEC) = 18.9197
 START INWARD SOLUTION (VERSION 15:30, 16-MAR-77) RHAX= 1.43610E+01
 TIME CHECK: TIME=22:58: 25.0 AMS. CPU TIME (SEC) = 40.4163 CPU TIME SINCE LAST CALL (SEC) = 11.6047
 CALCULATE (COEFF) (VERSION 16:30, 04-MAR-77)
 (COEFF) ERROR INDICATORS: WRTE= 1.00E-04 GRPE= 6.04E-03
 TIME CHECK: TIME=22:59: 40.9 AMS. CPU TIME (SEC) = 51.5224 CPU TIME SINCE LAST CALL (SEC) = 11.1061
 CALCULATE (COEFA) (VERSION 16:30, 2-FEB-78)
 (COEFA) ERROR INDICATORS: GRTE= 1.67E-05 GRPE= 1.10E-07
 TIME CHECK: TIME=22:59: 10.1 AMS. CPU TIME (SEC) = 67.0171 CPU TIME SINCE LAST CALL (SEC) = 15.4247
 CALCULATE R-INTEGRAL (VERSION 20:34, 7-FEB-78)
 START DEVICE 12 INPUT: (RS)
 START DEVICE 10 INPUT: (GD,FD)
 START DEVICE 11 INPUT: (GI,FI)
 START DEVICE 13 INPUT: (COEPR)
 START DEVICE 14 INPUT: (COEFA)
 DISK FILES INITIALIZED
 TIME CHECK: TIME=22:59: 59.4 AMS. CPU TIME (SEC) = 89.0663 CPU TIME SINCE LAST CALL (SEC) = 22.0492
 CONT: RE(X)= 0.00000000 IM(X)=-0.00000000 RE(RE,IM)= 3.63E-16 1.21E-16 PE(RE,IM)= 4.93E-14 0.00E-15 1.15 MIN

DUMP OF X-AMPLITUDES FOLLOWS:

J	RE(X(J,1))	IM(X(J,1))	RE(X(J,0))	IM(X(J,0))
1	-1.34072195	0.11064968	-0.00382987	0.00000000
2	-0.00211635	0.00001853	-0.00000537	0.00000000
3	-0.00000309	0.00000000	-0.00000001	0.00000000

ITERATION PARAMETERS: J= 3 KB= 4 LAMDA= 0 TORD= -1
 FILE NAMES: OUT=CL122.LW 4 IN=CL122.LX 4 EN= 9.9941974E-01 ISOL= 1
 RHAX= 2.9359E+03 RASY= 2.9359E+03 TOLN= 1.00E-02
 START OUTWARD SOLUTION (VERSION 10:30, 13-APR-77) RHAX= 2.9359E+03
 TIME CHECK: TIME=23:00: 07.5 AMS. CPU TIME (SEC) = 91.0018 CPU TIME SINCE LAST CALL (SEC) = 4.9155
 START INWARD SOLUTION (VERSION 15:30, 16-MAR-77) RHAX= 2.9366E+03
 TIME CHECK: TIME=23:00: 16.0 AMS. CPU TIME (SEC) = 100.1056 CPU TIME SINCE LAST CALL (SEC) = 8.4037
 CALCULATE (COEFF) (VERSION 16:30, 04-MAR-77)
 (COEFF) ERROR INDICATORS: WRTE= 5.70E-08 GRPE= 1.12E-05
 TIME CHECK: TIME=23:00: 33.6 AMS. CPU TIME (SEC) = 111.2068 CPU TIME SINCE LAST CALL (SEC) = 12.0913
 CALCULATE (COEFA) (VERSION 16:30, 2-FEB-78)
 (COEFA) ERROR INDICATORS: GRTE= 5.33E-09 GRPE= 2.03E-05
 TIME CHECK: TIME=23:00: 55.8 AMS. CPU TIME (SEC) = 127.0972 CPU TIME SINCE LAST CALL (SEC) = 15.8904
 CALCULATE R-INTEGRAL (VERSION 20:34, 7-FEB-78)
 START DEVICE 12 INPUT: (RS)
 START DEVICE 10 INPUT: (GD,FD)
 START DEVICE 11 INPUT: (GI,FI)
 START DEVICE 13 INPUT: (COEPR)
 START DEVICE 14 INPUT: (COEFA)
 DISK FILES INITIALIZED
 TIME CHECK: TIME=23:01: 11.9 AMS. CPU TIME (SEC) = 146.2147 CPU TIME SINCE LAST CALL (SEC) = 19.1176
 CONT: RE(X)= 0.00000000 IM(X)= 0.00000000 RE(RE,IM)= 1.26E-16 3.00E-16 PE(RE,IM)= 1.13E-14 0.00E-15 0.00 MIN

DUMP OF X-AMPLITUDES FOLLOWS:

J	RE(X(J,1))	IM(X(J,1))	RE(X(J,0))	IM(X(J,0))				
1	-1.34872195	0.11064464	-0.00382987	0.00000000	.00001170	.00000533	.00000006	.00000001
2	-0.00231635	0.00001853	-0.00000537	0.00000000	.00000004	.00000001	0.00000000	0.00000000
3	-0.00000369	0.00000000	-0.00000001	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000

PHOTON MULTIPOLE SERIES HAS CONVERGED TO INPUT CRITERIA FOR:

J= 3
 XMAX= 0.00000+00
 XOLEN= 1.000-05

PROGRAM SHELL (RAYLEIGH SCATTERING CROSS SECTIONS VERSION 10:00, 13-MAY-77) RUN DATE 15-Sep-78 TIME 09:01

```

JMAX= 1
ERRHHH= 1.0000-06 ERRINT= 1.0000-08
HMAX1= 0.00000+00 HMAX2= 0.00000+00 HMAX3= 0.00000+00 TOLER1= 1.0000-02 TOLER2= 1.0000-03 TOLER3= 1.0000-03
HMAX= 0.00000+00 KULR= 1.0000-05

```

LAST CONTRIBUTION CALCULATED FOR: J= 3 KB= 4 LAMBDA= 0 IORD= -1

```

JMAX= 3
ERROR= 1.000-02 CRRINT= 1.000-04
HMAX1= 0.00000+00 HMAX2= 0.00000+00 HMAX3= 0.00000+00 TOLER1= 1.000-02 TOLER2= 1.000-03 TOLER3= 1.000-03
XMAX= 0.000000+00 XOLER= 1.000-05

```

$$12 = 6, HA = 1, KA = -1$$

J	HE(X(J,1))	IM(X(J,1))	HE(X(J,0))	IM(X(J,0))
1	1.29101082	0.00000000	-0.00008523	0.00000000
2	0.00001914	0.00000000	0.00000000	0.00000000
3	0.00000000	0.00000000	0.00000000	0.00000000

20. Device & Output of SELL: Permanent Subsnell Data file

*** PROGRAM CONTROL PARAMETERS:

LN22 10.0001LN:01:09 DATE:15-Sep-76 VER 43 4/13/77

0

1 -1

2.30000000-u1 1

3

1.00000000-u0 1.00000000-u0

0.00000000 0.00000000 0.00000000 1.000-u2 1.000-u3 1.000-u3

0.00000000 1.000-u5

*** A-AmPLITUDES:

1 1.29101082070+00 0.00000000000000 -6.52293317590-u5 0.00000000000000

2.20430-u5 0.00000000000000 5.32310-u9 0.00000000000000

2 1.91502417920-u5 0.00000000000000 1.61374669540-u8 0.00000000000000

4.21590-u10 0.00000000000000 1.62420-u13 0.00000000000000

3 5.59251648430-u10 0.00000000000000 2.26612119600-u13 0.00000000000000

1.21150-u14 0.00000000000000 2.73650-u16 0.00000000000000

*** INDIVIDUAL CONTRIBUTIONS TO A-AmPLITUDES:

1 -1 0 1 0.00017024 0.00000000 26.61 1.60-11 0.00+00 4.80-u9 0.00+00

1 -1 0 -1 -0.00012144 0.00000000 27.84 9.00-12 0.00+00 2.20-u9 0.00+00

1 1 1 1 -0.00373910 0.00000000 24.70 1.50-08 0.00+00 1.10-u5 0.00+00

1 1 1 -1 0.52141119 0.00000000 26.48 1.40-08 0.00+00 6.20-u6 0.00+00

1 -2 1 1 -1.45912993 0.00000000 25.52 1.50-u7 0.00+00 1.70-u5 0.00+00

1 -2 1 -1 -0.20953256 0.00000000 27.94 1.20-06 0.00+00 3.50-u6 0.00+00

1 2 0 1 0.00001421 0.00000000 28.93 9.20-13 0.00+00 2.50-u10 0.00+00

1 2 0 -1 0.00001422 0.00000000 30.18 2.00-12 0.00+00 2.20-u10 0.00+00

2 -2 0 1 -0.00000000 0.00000000 19.11 1.50-15 0.00+00 1.60-13 0.00+00

2 -2 0 -1 -0.00000000 0.00000000 24.26 6.80-17 0.00+00 2.10-14 0.00+00

2 2 1 1 0.00000461 0.00000000 18.48 8.80-13 0.00+00 9.00-11 0.00+00

2 2 1 -1 0.00001844 0.00000000 22.61 8.80-13 0.00+00 2.00-10 0.00+00

2 -3 1 1 -0.00003146 0.00000000 30.55 1.90-12 0.00+00 3.40-10 0.00+00

2 -3 1 -1 -0.00001072 0.00000000 35.00 7.50-15 0.00+00 1.10-10 0.00+00

2 3 0 1 0.00000000 0.00000000 33.62 5.10-17 0.00+00 1.20-14 0.00+00

2 3 0 -1 0.00000000 0.00000000 37.79 2.90-17 0.00+00 9.80-15 0.00+00

3 -3 0 1 -0.00000000 0.00000000 19.19 9.50-20 0.00+00 2.80-18 0.00+00

3 -3 0 -1 -0.00000000 0.00000000 24.19 2.50-21 0.00+00 6.20-19 0.00+00

3 3 1 1 0.00000000 0.00000000 19.71 3.40-17 0.00+00 2.80-15 0.00+00

3 3 1 -1 0.00000000 0.00000000 25.64 2.40-17 0.00+00 6.50-15 0.00+00

3 -4 1 1 -0.00000000 0.00000000 36.85 1.50-16 0.00+00 9.10-15 0.00+00

3 -4 1 -1 -0.00000000 0.00000000 35.73 5.10-17 0.00+00 3.70-15 0.00+00

3 4 0 1 0.00000000 0.00000000 33.53 2.70-21 0.00+00 5.90-19 0.00+00

3 4 0 -1 0.00000000 0.00000000 40.17 2.00-21 0.00+00 3.00-19 0.00+00

3 4 0 -1

I/O FOR MFSTR1

22. Aff of neural Caron's K-shell; R, Aff(R), Error

0	1	1	-1	y.994654y48y524640-01	1.7157083238111150-02	9.9904101608016050-01
11	1.00000000000000000000	1.4983989391256720-02	-1	5.00000000000000000000	-01	0
0.00000000000000000000	9.99236370-01	3.80512240-04				
1.00000000000000000000	9.99161970-01	3.80466610-04				
1.25000000000000000000	9.99120120-01	3.80441250-04				
1.50000000000000000000	9.99080980-01	3.80410030-04				
2.00000000000000000000	9.98930830-01	3.80330580-04				
2.50000000000000000000	9.98771520-01	3.80228490-04				
3.00000000000000000000	9.98587100-01	3.80103020-04				
3.50000000000000000000	9.98325000-01	3.79956030-04				
4.00000000000000000000	9.98047060-01	3.79780990-04				
5.00000000000000000000	9.97379050-01	3.79380090-04				
6.00000000000000000000	9.96503570-01	3.78885710-04				
7.00000000000000000000	9.95601190-01	3.78303000-04				
8.00000000000000000000	9.94492500-01	3.77633090-04				
9.00000000000000000000	9.93236520-01	3.76879040-04				
1.00000000000000000000	9.91839890-01	3.76040050-04				
1.25000000000000000000	9.87717500-01	3.73587740-04				
1.50000000000000000000	9.82715840-01	3.70649120-04				
2.00000000000000000000	9.70104180-01	3.63450010-04				
2.50000000000000000000	9.54390280-01	3.54747600-04				
3.00000000000000000000	9.35089580-01	3.44878470-04				
3.50000000000000000000	9.14270180-01	3.34101650-04				
4.00000000000000000000	8.90542700-01	3.22973780-04				
5.00000000000000000000	8.37340990-01	3.00070080-04				
6.00000000000000000000	7.78946440-01	2.77716350-04				
7.00000000000000000000	7.17094290-01	2.56533810-04				
8.00000000000000000000	6.56003420-01	2.36962600-04				
9.00000000000000000000	5.95309600-01	2.19310440-04				
1.00000000000000000000	5.37777120-01	2.03439730-04				
1.25000000000000000000	4.89847900-01	1.89419840-04				
1.50000000000000000000	3.67951770-01	1.40690170-04				
2.00000000000000000000	1.73261100-01	9.70800510-05				
2.50000000000000000000	9.99830520-02	7.27145850-05				
3.00000000000000000000	5.99543850-02	7.11205150-05				
3.50000000000000000000	3.75024820-02	4.91164270-05				
4.00000000000000000000	2.43350420-02	4.05773410-05				
5.00000000000000000000	1.13163600-02	3.17157830-05				
6.00000000000000000000	5.83134290-03	2.85477500-05				
7.00000000000000000000	3.25235520-03	2.10209830-05				
8.00000000000000000000	1.97200350-03	1.59687270-05				
9.00000000000000000000	1.24610040-03	1.47886940-05				
1.00000000000000000000	8.10983810-04	1.30175530-05				
1.25000000000000000000	3.28040150-04	9.64809390-06				
1.50000000000000000000	1.55394220-04	6.78977070-06				
2.00000000000000000000	4.44410790-05	5.20061150-06				
2.50000000000000000000	1.56380040-05	2.90177070-06				
3.00000000000000000000	7.97915470-06	2.80776060-06				
3.50000000000000000000	2.43540810-06	1.95112400-06				
4.00000000000000000000	7.78108960-07	1.81507650-06				
5.00000000000000000000	1.18362130-07	1.07674620-06				
6.00000000000000000000	-4.80409050-07	6.40377890-07				
7.00000000000000000000	-5.22500120-07	7.05610760-07				
8.00000000000000000000	-4.40376480-07	6.67960650-07				
9.00000000000000000000	-3.17393140-07	4.94021330-07				
1.00000000000000000000	-4.23094670-07	3.78316110-07				
1.25000000000000000000	1.47571280-08	2.78471510-07				
1.50000000000000000000	-1.49900540-07	2.52573610-07				
2.00000000000000000000	-1.41805070-07	1.36051940-07				
2.50000000000000000000	-3.41347290-08	9.90708660-08				
3.00000000000000000000	-2.95100440-08	9.18914070-08				
3.50000000000000000000	-1.74375960-08	7.09642220-08				
4.00000000000000000000	-4.80324540-08	4.97746370-08				
5.00000000000000000000	2.32805330-09	3.79299610-08				
6.00000000000000000000	-4.91954300-09	3.54745580-08				
7.00000000000000000000	-4.32852030-09	2.91971780-08				
8.00000000000000000000	8.23908290-09	2.25930800-08				
9.00000000000000000000	5.04048320-09	2.13007170-08				
-1.00000000000000000000	-1.00000000000000000000	-1.00000000000000000000				

I/O FOR TABX5

FLOW CHART OF TABX5

FLOW CHART OF TABX5

cont.

FLOW CHART OF TABX5

cont.

NUMERICAL Differential Rayleigh Scattering Amplitudes
- (in classical electron radii)

25. Final tabulation

C, K ONLY (HKL)
Atomic Number, Z = 6
Photon Energy, ω = 0.23 keV

0- (degrees)	q (1/A)	A 11	A 1-	1 2 2 -(A +A) 2 11 1-	CS(mb)
0.0	0.000(-0)	(1.93644, 0.00000)	(1.93644, 0.00000)	3.74979	297.76202
5.0	0.092(-4)	(1.92907, 0.00000)	(1.93644, 0.00000)	3.73554	296.63100
10.0	1.617(-3)	(1.90701, 0.00000)	(1.93644, 0.00000)	3.69325	293.27228
15.0	2.421(-3)	(1.87044, 0.00000)	(1.93644, 0.00000)	3.62418	287.78795
20.0	3.221(-3)	(1.81964, 0.00000)	(1.93644, 0.00000)	3.53044	280.34468
25.0	4.015(-3)	(1.75498, 0.00000)	(1.93644, 0.00000)	3.41489	271.16868
30.0	4.801(-3)	(1.67697, 0.00000)	(1.93645, 0.00000)	3.28102	260.53880
35.0	5.578(-3)	(1.58619, 0.00000)	(1.93645, 0.00000)	3.13292	248.77810
40.0	6.345(-3)	(1.48334, 0.00000)	(1.93645, 0.00000)	2.97507	236.24399
45.0	7.099(-3)	(1.36920, 0.00000)	(1.93646, 0.00000)	2.81229	223.31736
50.0	7.840(-3)	(1.24463, 0.00000)	(1.93646, 0.00000)	2.64950	210.39107
55.0	8.566(-3)	(1.11060, 0.00000)	(1.93647, 0.00000)	2.49167	197.85793
60.0	9.275(-3)	(0.96811, 0.00000)	(1.93648, 0.00000)	2.34359	186.09881
65.0	9.967(-3)	(0.81825, 0.00000)	(1.93648, 0.00000)	2.20975	175.47107
70.0	1.064(-2)	(0.66216, 0.00000)	(1.93649, 0.00000)	2.09422	166.29766
75.0	1.129(-2)	(0.50104, 0.00000)	(1.93650, 0.00000)	2.00053	158.85734
80.0	1.192(-2)	(0.33610, 0.00000)	(1.93650, 0.00000)	1.93150	153.37624
85.0	1.253(-2)	(0.16860, 0.00000)	(1.93651, 0.00000)	1.88925	150.02090
90.0	1.312(-2)	(-0.00018, 0.00000)	(1.93652, 0.00000)	1.87505	148.89330
95.0	1.368(-2)	(-0.16895, 0.00000)	(1.93652, 0.00000)	1.88933	150.02773
100.0	1.421(-2)	(-0.33645, 0.00000)	(1.93653, 0.00000)	1.93167	153.38974
105.0	1.472(-2)	(-0.50138, 0.00000)	(1.93654, 0.00000)	2.00078	158.87719
110.0	1.520(-2)	(-0.66249, 0.00000)	(1.93654, 0.00000)	2.09455	166.32337
115.0	1.565(-2)	(-0.81857, 0.00000)	(1.93655, 0.00000)	2.21014	175.50208
120.0	1.607(-2)	(-0.96841, 0.00000)	(1.93656, 0.00000)	2.34403	186.13445
125.0	1.645(-2)	(-1.11088, 0.00000)	(1.93656, 0.00000)	2.49217	197.89748
130.0	1.681(-2)	(-1.24490, 0.00000)	(1.93657, 0.00000)	2.65004	210.43380
135.0	1.714(-2)	(-1.36945, 0.00000)	(1.93657, 0.00000)	2.81286	223.36257
140.0	1.743(-2)	(-1.48358, 0.00000)	(1.93658, 0.00000)	2.97567	236.29100
145.0	1.769(-2)	(-1.58641, 0.00000)	(1.93658, 0.00000)	3.13353	248.82634
150.0	1.792(-2)	(-1.67718, 0.00000)	(1.93659, 0.00000)	3.28164	260.58779
155.0	1.811(-2)	(-1.75518, 0.00000)	(1.93659, 0.00000)	3.41551	271.21804
160.0	1.827(-2)	(-1.81982, 0.00000)	(1.93659, 0.00000)	3.53107	280.39416
165.0	1.839(-2)	(-1.87062, 0.00000)	(1.93659, 0.00000)	3.62480	287.83738
170.0	1.848(-2)	(-1.90718, 0.00000)	(1.93660, 0.00000)	3.69387	293.32151
175.0	1.853(-2)	(-1.92923, 0.00000)	(1.93660, 0.00000)	3.73616	296.68024
180.0	1.855(-2)	(-1.93660, 0.00000)	(1.93660, 0.00000)	3.75041	297.81123