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Free-Free Absorption Coefficient of the Negative Hydrogen Ion.

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Free-Free Absorption Coefficient
of the Negative Hydrogen Ion

A Dissertation

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Abstract

The dipole adiabatic exchange wave functions of polarized orbital theory have been employed to obtain the $S \leftrightarrow P$ and $P \leftrightarrow D$ contributions to the free-free absorption coefficient of H^- in the dipole length and dipole velocity formulations. The length and velocity results have been found to be in good agreement, 3% or less at the longer wavelengths where free-free absorption dominates bound-free absorption. These results were found to be in good agreement with other recent calculations and with solar observations. The effects of atomic distortion were found to be small at longer wavelengths (1% for length formulation and 6% for velocity formulation) making inclusion thereof relatively unimportant for astrophysical applications. Asymptotic matrix elements which are convergent over all space reproduce the full results to within 10%.

1 INTRODUCTION

In 1931 Pannekoek¹ discussed the importance of the free-free absorption of light by electrons in the presence of neutral hydrogen atoms for determining the infra-red opacities of the cooler late spectral type stars. The process is described by the reaction

Free electrons cannot absorb photons without a spectator particle (in this case the hydrogen atom) being present to conserve energy and momentum. At photon energies below .75 eV where detachment of an electron from H^- is energetically impossible, free-free absorption should dominate. The fundamental role of this relatively simple process produced immediate and numerous interest which has continued into recent years.

So far as theoretical interest is concerned, the central problem is the determination of the matrix element involved in the expression for the monochromatic absorption coefficient $k_\lambda(T)$ derived in Chapter II where T is the temperature of the stellar atmosphere. The matrix element is given by $\langle f | D_z | i \rangle$ where i and f denote initial and final states, respectively, and D_z is $Z_1 + Z_2$ in the length formulation, $-ih(\frac{\partial}{\partial Z_1} + \frac{\partial}{\partial Z_2})$ in the velocity formulation, and $(Z_1/r_1^3 + Z_2/r_2^3)$ in the acceleration formulation which has not been used in the present calculations.

The present calculation makes use of the dipole adiabatic

exchange approximation (AED) of polarized orbital theory (detailed in Chapter IV) to obtain the continuum state of the external electron. The essential feature is the explicit inclusion of the effects of atomic distortion on the external electron through use of the dipole component of a long range polarization potential which is asymptotically $-\alpha/r^4$ where α is the dipole polarizability of the hydrogen atom. AED includes all of the long range dipole polarizability. In addition the effect of including the distortion of the atomic wave function in the determination of the matrix element is studied here. The two particle wave function is written as

$$\Psi_{\vec{k}}^S(1,2) = \frac{1}{\sqrt{2}} \left[\psi(1;2) \phi_{\vec{k}}^S(2) + (-1)^S \psi(2;1) \phi_{\vec{k}}^S(1) \right]$$

where $\phi_{\vec{k}}^S$ is the single particle state for an electron of momentum $\hbar\vec{k}$ corresponding to total spin S , and $\psi(1;2)$ is the atomic state of electron 1 perturbed by electron 2.

$$\psi(1;2) = u_0(1) + \chi(1;2)$$

where u_0 is the $1s$ state of hydrogen and χ is the first order perturbation thereto. The present calculations include only the dominant long range (dipole) component of χ . The calculations have also been repeated neglecting χ in order to investigate the importance of its inclusion.

This dissertation is arranged as follows: In Chapter II the absorption coefficient is derived. Other calculations are described in Chapter III. The AED wave functions are detailed in Chapter IV.

The matrix element is described in Chapter V. Chapter VI relates the matrix elements employed here to those of many body perturbation theory (MBPT). The results are presented in Chapter VII.

11. The Absorption Coefficient

The free-free absorption coefficient $k_\lambda(T)$ is defined as the averaged absorption cross section per unit incident electron pressure per hydrogen atom. The average is over all photon parameters other than the wavelength λ and over incident electron momenta. At the low electron densities occurring in stellar matter, the electrons may be assumed to be an ideal gas obeying Fermi-Dirac statistics. For sufficiently low densities the wave functions of the electrons overlap very little, and the electrons become essentially distinguishable. As a result the Boltzmann distribution may be used. This is assumed to be the case here.

The rate of transition from a wave vector $\vec{k}_i$ into a state of wave number k_f within the differential solid angle $d\hat{k}_f$ is a function of several parameters.

$$dw_{i \rightarrow f} = f(\vec{k}_f, \vec{k}_i, \vec{k}_\omega, \vec{\epsilon}) d\hat{k}_f \quad (2-1)$$

where $\vec{k}_\omega$ is the wave vector of the photon, $\vec{k}_i$ is the initial electron wave vector, $\vec{k}_f$ is the final electron wave vector, and $\vec{\epsilon}$ is the direction of polarization of the photon ($\vec{\epsilon} \perp \vec{k}_\omega$). $dw_{i \rightarrow f}$ is given by the expression

$$dw_{i \rightarrow f} = \frac{2\pi}{\hbar} |\langle f | \mathcal{U} | i \rangle|^2 \rho_f d\hat{k}_f \quad (2-2)$$

where i and f denote initial and final states, respectively, ρ_f is the density of final states, and $\mathcal{U}$ is the dipole interaction of the electromagnetic field and the electrons.

$$u = \frac{e}{c} \vec{A} \cdot (\vec{v}_1 + \vec{v}_2) \quad (2-3)$$

where $\vec{A}$ is the amplitude of the electromagnetic vector potential. u has been obtained from semi-classical radiation theory as described in Chapter 10 of Schiff.² The initial and final states are assumed normalized to a Dirac delta function in $\vec{k}$ -space which implies that the density of final states is $mk_f/\hbar^2$. It follows that the transition rate is

$$dw_{i \rightarrow f} = \frac{2\pi m k_f e^2}{\hbar^3 c^2} A^2 \left| \langle f | \vec{E} \cdot (\vec{v}_1 + \vec{v}_2) | i \rangle \right|^2 d\hat{k}_f \quad (2-4)$$

The differential cross section is obtained by dividing (2-4) by the incident photon flux, $I/\hbar\omega$, where I is the photon intensity and ω is the frequency of the photon field. I is obtained by taking the time average of the Poynting vector (Powell and Crasemann,³ p. 418) with the result $I = \omega^2 A^2 / 2\pi c$. The differential cross section $d\sigma_{i \rightarrow f}$ is then given as

$$d\sigma_{i \rightarrow f} = \frac{4\pi^2 m k_f \alpha}{\omega} \left| \langle f | \vec{E} \cdot (\vec{v}_1 + \vec{v}_2) | i \rangle \right|^2 d\hat{k}_f \quad (2-5)$$

where $\alpha = e^2/\hbar c$ is the fine structure constant.

The average over $\vec{k}_i$ is accomplished by assuming a Boltzmann distribution at temperature T ; consequently, the fraction $M(\vec{k}_i)$ of particles with wave vector between $\vec{k}_i$ and $\vec{k}_i + d\vec{k}_i$ satisfies

$$M(\vec{k}_i) \propto e^{-\hbar^2 k_i^2 / 2mk_b T}$$

$$\int d^3k_i M(\vec{k}_i) = 1$$

It follows that the average over initial wave vectors may be accomplished by

$$d\bar{\sigma}_{i \rightarrow f} = \frac{(2\pi)^2 \alpha}{\omega \pi^{1/2} (k_b T)^{3/2}} \int_0^\infty d(k_i^2) k_i k_f e^{-\hbar^2 k_i^2 / 2m k_b T} \\ \cdot \frac{1}{4\pi} \int d\hat{k}_i \left| \langle f | \vec{E} \cdot (\vec{v}_i + \vec{v}_e) | i \rangle \right|^2 d\hat{k}_f \quad (2-6)$$

where k_b is Boltzmann's constant.

The total absorption cross section, including average over the photon parameters, at temperature T is then given as

$$\sigma_w(T) = \frac{(2\pi)^2 \alpha}{\omega \pi^{1/2} (k_b T)^{3/2}} \int_0^\infty d(k_i^2) k_i k_f e^{-\hbar^2 k_i^2 / 2m k_b T} \\ \cdot \frac{1}{4\pi} \int d\hat{k}_i \int d\hat{k}_f \overline{\frac{1}{4\pi} \int d\hat{k}_w \left| \langle f | \vec{E} \cdot (\vec{v}_i + \vec{v}_e) | i \rangle \right|^2} \quad (2-7)$$

where the raised bar over the matrix element denotes the average over the independent directions of $\vec{E}$. The absorption coefficient $k_\lambda(T)$ as stated before is the absorption cross section of (2-7) per unit incident electron pressure P_e ; P_e may be determined from the ideal gas law

$$P_e = N_e k_b T$$

where N_e is the number of electrons per unit volume. Since the normalization of the incident state is to a Dirac delta function, it follows that $\langle i | i \rangle = \delta(\vec{0}) = \lim_{V \rightarrow \infty} V / (2\pi)^3$ which implies that $N_e = (2\pi)^{-3}$. Thus

$$k_\lambda(T) = \frac{(2\pi)^5 \alpha a_0^5}{\Delta k^2 \pi^{1/2} (k_b)^{3/2} (k_b k_{j.s.} T)^{3/2}} \int_0^\infty d(k_i^2) k_i k_f e^{-k_i^2 / k_b T} \\ \cdot \frac{1}{4\pi} \int d\hat{k}_i \int d\hat{k}_f \left| \langle f | v_{iz} + v_{ez} | i \rangle \right|^2 \text{ cm}^4 \text{ dyne}^{-1} \quad (2-8)$$

where all quantities other than the Bohr radius a_0 (in cm) and

$(k_b)_{c.g.s.}$ have been expressed in atomic units ($\hbar = 1$, $m = 1/2$, $e^2 = 2$), where the average over photon parameters has been done as described in Appendix A, and $\Delta k^2 = k_f^2 - k_i^2 = \omega$. Formula (2-8) constitutes the dipole velocity matrix element without allowance for spin.

In Appendix B it is shown that the length formula may be obtained from (2-8) by replacing the operator by $Z_1 + Z_2$ and moving Δk^2 to the numerator. Furthermore, spin can be allowed for by employing the usual $1/4:3/4$ sum rule since the Hamiltonian used here contains no spin dependent interactions. Since the effective opacity of a stellar atmosphere is observed, the effects of stimulated emission must be removed. This is accomplished (Ambartsumyan⁴) through multiplication by the factor $(1 - e^{-\Delta k^2/k_b T})$. Finally an expression for the absorption coefficient in the length ($j = 1$) and velocity ($j = 2$) formulations is obtained.

$$\begin{aligned}
 k_{\lambda}^{(j)}(T) = & \frac{(2\pi)^5 \alpha a_0^5 (1 - e^{-\Delta k^2/k_b T}) (\Delta k^2)^{3-2j}}{\pi^{1/2} k_b^{3/2} (k_b)_{c.g.s.} T^{5/2}} \\
 & \cdot \int_0^{\infty} d(k_i^2) k_i k_f e^{-k_i^2/k_b T} \\
 & \cdot \frac{1}{4\pi} \int d\hat{k}_i \int d\hat{k}_f \sum_{s=0}^L \frac{2s+1}{4} \left| \langle f | \left(\frac{d}{dt} \right)^{j-1} (z_1 + z_2) | i \rangle_s \right|^2
 \end{aligned}
 \tag{2-9}$$

In equation (2-9) $\lambda = \frac{911.267}{\Delta k^2}$.

III. Review of Previous Calculations

The earliest calculation of $k_\lambda(T)$ was that of Menzel and Pekeris⁵ (1935) in which the matrix elements of Nedelsky⁶ were employed. Nedelsky replaced the potential interactions felt by the external electron by e^2/a_0 for $r_2 < a_0$ (r_2 is the coordinate of the external electron) and 0 for $r_2 > a_0$ where a_0 is the Bohr radius. He used the acceleration operator to represent the photon interaction. Wheeler and Wildt⁷ sought to improve these results in 1942. They employed instead of the acceleration operator the Hartree acceleration operator given by $-e^2/m \left[\frac{1}{r_2^2} + \frac{2}{a_0} \left(\frac{1}{a_0} + \frac{1}{r_2} \right) \right] e^{-2r_2/a_0}$ where m is the electronic mass. The Hartree acceleration operator is consistent with use of the static potential to represent the interaction of the electron with the hydrogen atom; however, Wheeler and Wildt used plane waves for the external electron. Their results were near those of Menzel and Pekeris, but both were considerably smaller than observations obtained from the solar limb darkening measurements of Chalonge and Kourganoff⁸ in 1946. This led Chalonge and Kourganoff to postulate the existence of an unknown absorber.

Later that year Chandrasekhar and Breen⁹ performed a consistent calculation using the Hartree acceleration operator with Hartree waves for the external electron. Their results, although larger than the observed opacity, indicated that an unknown absorber was not necessary. Their method did not allow either for exchange or

for distortion of the atom and thereby failed to recognize the two electron nature of the problem.

In 1960 Ohmura and Ohmura¹⁰ devised an approximate formula involving only the S-wave phase shifts for the elastic scattering of electrons from hydrogen. They used the asymptotic form of the S wave (Chapter IV) together with the P-wave part of a plane wave and considered only $S \rightarrow P$ transitions. When the length operator was employed together with Hartree wave phase shifts, the results of Chandrasekhar and Breen were closely reproduced at long wavelengths. In 1961 Ohmura and Ohmura¹¹ improved their calculations by allowing for exchange effects through use of the $1/4:3/4$ sum rule together with spin dependent phase shifts originally obtained from Bransden, et. al.¹² They obtained a 40% reduction of Chandrasekhar and Breen's results which appears to be lower than observation. The asymptotic procedures must be regarded with considerable caution, as described in Chapter VII.

In 1962 Romanov¹³ used the Hulthén variational method neglecting atomic distortion to obtain results which agreed closely with Chandrasekhar and Breen.

The first direct allowance for exchange was made by John¹⁴ in 1964, who employed the static exchange approximation with the length operator to obtain the contribution of $S \leftrightarrow P$ transitions. The static exchange approximation does not allow for atomic distortion but does include exchange effects. A reduction of 30 to 40% from Chandrasekhar and Breen was found, but the results remain above those of Ohmura and Ohmura. In the same year Ohmura¹⁵ reduced the

results of Ohmura and Ohmura even more by using the phase shifts of Schwartz¹⁶ which are generally conceded to be the most accurate available.

Later in 1964 Geltman¹⁷ performed the first calculation to directly allow for exchange and distortion effects. Geltman employed the Hulthen-Kohn (Geltman¹⁸) variational principle to determine the variational parameters in the following function:

$$\begin{aligned} \Psi_t^{\pm}(l, k, \vec{r}_1, \vec{r}_2) = & \left(\frac{k}{\pi}\right)^{1/2} \left(\frac{2l+1}{4\pi}\right)^{1/2} \frac{1}{\sqrt{1+a_t^2}} P_l(\cos \theta_{12}) \\ & \cdot \left[\phi(\vec{r}_1) \left[j_l(kr_2) - a_t (1 - e^{-kr_2})^{2l+1} n_l(kr_2) \right] \right. \\ & + \left(\frac{4\pi}{2l+1} \right)^{1/2} \left\{ P_0(\cos \theta_{12}) r_2 e^{-\gamma_0 r_2} \left[C_1 R_{10}(r_1) \right. \right. \\ & + C_2 R_{20}(r_1) + C_3 R_{30}(r_1) \left. \right] + P_1(\cos \theta_{12}) r_2^2 e^{-\gamma_1 r_2} \\ & \cdot \left[C_4 R_{21}(r_1) + C_5 R_{31}(r_1) \right] \\ & \left. + C_6 P_2(\cos \theta_{12}) r_2^3 e^{-\gamma_2 r_2} R_{32}(r_1) \right\} \left. \right] \pm (\vec{r}_1 \leftrightarrow \vec{r}_2) \end{aligned}$$

where $\phi(\vec{r}_1)$ is the unperturbed hydrogen 1s state, the R_{nl} are the unnormalized radial hydrogen functions, and a_t , the γ_i , and the C_i are the variational parameters to be determined. The trial function contains monopole, dipole, and quadrupole distortion and may be considered a restricted form of the 1s-2s-2p-3s-3p-3d close coupling approximation in which only certain parameters rather than the functions describing the external electron are determined. Only 75% of the dipole polarizability can be obtained when the 2p and 3p

states are included (Doughty¹⁹). The phase shifts of Geltman are obtained from the parameter a ($\delta = \tan^{-1} a$) defined by

$$a = a_t - L_t/k$$

$$L_t = \int \Psi_t^\pm (H-E) \Psi_t^\pm d\tau_1 d\tau_2$$

However Geltman used some ad hoc procedures to improve upon the parameter a . He used various methods to obtain better phase shifts and hence a better value of the parameter a . The variational parameters were then changed so as to obtain the improved a . The 1S phase shifts of Schwartz¹⁶ were used for most of Geltman's tabulated energies, and the 3S phase shift of Schwartz was used for the lowest tabulated energy. O'Halley, Spruch, and Rosenberg²⁰ showed that the low energy behavior of the P and D phase shifts depends only upon the polarizability α of the hydrogen atom.

$$\tan \delta_l = \frac{\pi k^2 \alpha}{(2l+3)(2l+1)(2l-1)} + O(k^{2l+1})$$

This relation was used to obtain improved values of a at the two lowest tabulated energies. The results obtained by Geltman appear in excellent agreement with the observations of Chalonge and Kourganoff, but the improved phase shifts may not be available for use in similar problems. It is desirable to develop self-contained formalisms which may be applied with some degree of confidence in related phenomena.

Doughty and Fraser²¹ in 1966 employed the close coupling or eigenfunction expansion method to obtain the absorption coefficient. In this method the two particle state is represented as an expansion in the exact hydrogen eigenstates with the expansion coefficients

being scattering states for the external electron. The method yields a set of coupled integro-differential equations for the scattering states. Doughty and Fraser used the 1s-2s expansion for most of their calculations but also included some 1s-2s-2p calculations. Their results are in close agreement with those of Geltman but tend to be slightly higher at very long wavelengths. Their method suffers from failure to include all of the dipole polarization. The 1s-2s expansion gives no dipole polarization while the 1s-2s-2p expansion gives only 66%.

John²² devised a simplified formula for the absorption coefficient which involves only the scattering phase shifts. The asymptotic functions as described in Chapter IV were approximated as follows

$$kr \left[\cos \delta_l j_l(kr) - \sin \delta_l n_l(kr) \right] \rightarrow \sin \left(kr - \frac{l\pi}{2} + \delta_l \right)$$

This transformation is accomplished by employing the asymptotic forms of the spherical Bessel functions j_l and n_l . The resulting matrix elements contain integrands which are convergent at the origin for all transitions. This is not true of the forms used by Ohmura and Ohmura. John is able to reproduce more elaborate calculations to within 10%. For example when he used his static exchange phases his earlier calculation (1964) is reproduced to within 10% at long wavelengths. The surprising success of such a procedure must be considered purely accidental in light of the gross approximations involved. The simplicity and accidental accuracy of this procedure allow one, however, to give some justification to neglecting transitions higher than $P \leftrightarrow D$. John found that $D \leftrightarrow F$

transitions contributed less than the $S \leftrightarrow P$ transitions by four orders of magnitude.

The wave functions used in the present calculation are described in detail in the following Chapter.

IV. Adiabatic Exchange Wave Functions

A. Formal Theory.

The wave functions required are those describing the motion of a free electron in the field of a hydrogen atom. The Schrödinger equation is

$$(H - E) \Psi_{\vec{k}}^S(1;2) = 0$$

$$\text{where } H = -\nabla_1^2 - \nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_{12}} \quad (4-1)$$

$$E = -1 + k^2$$

All quantities are expressed in atomic units.

The polarized orbital approximation^{23,24} assumes the function $\Psi_{\vec{k}}^S(1,2)$ to be of the form

$$\Psi_{\vec{k}}^S(1,2) = \frac{1}{\sqrt{2}} \left[\psi(1;2) \phi_{\vec{k}}^S(2) + (-1)^S \psi(2;1) \phi_{\vec{k}}^S(1) \right] \quad (4-2)$$

$\phi_{\vec{k}}^S$ is a free state function of momentum $\vec{k}$ corresponding to a total spin S , and $\psi(1;2)$ is the atomic state of electron 1 distorted due to the presence of electron 2.

$$\psi(1;2) = u_0(1) + \chi(1;2)$$

where u_0 is the 1s hydrogen state, and $\chi(1;2)$ is the induced

distortion. χ may be determined analytically from first order perturbation theory, i.e., any partial wave component may be determined analytically.^{25,26} No exchange effects are included in the calculation of χ ; the perturbation by the external electron is regarded only as an external potential which depends parameterically upon the position of the scattering electron. Once χ has been determined an equation for the function ϕ_k^S may be obtained by requiring that variation of $\langle H-E \rangle$ be zero. The resulting equation is known as the polarized orbital equation.

$$\int \psi^*(1;2) [H-E] \Psi_{\vec{k}}^S(1,2) d\gamma_i = 0 \quad (4-3)$$

The adiabatic exchange approximation results when all velocity dependent terms and all exchange polarization terms are dropped from (4-3). The former approximation may be accomplished by replacing $\psi^*(1;2)$ by $u_0^*(1)$. The adiabatic exchange equation is

$$\begin{aligned} & \left[-\nabla_{\vec{R}}^2 - \frac{2}{R} + V_c(R) + V_p(R) - k^2 \right] \phi_{\vec{k}}^S(\vec{R}) \\ &= (-1)^{S+1} \left[-(1+k^2) \int u_0(\vec{r}) \phi_{\vec{k}}^S(\vec{r}) d^3r \right. \\ & \quad \left. + \int u_0(\vec{r}) \frac{2}{|\vec{r}-\vec{R}|} \phi_{\vec{k}}^S(\vec{r}) d^3r \right] u_0(\vec{R}) \end{aligned} \quad (4-4)$$

where V_c and V_p are the usual coulomb and polarization potentials, respectively.

$$V_c(\vec{R}) = \int u_o(\vec{r}) \frac{2}{|\vec{r}-\vec{R}|} u_o(\vec{r}) d^3r \quad (4-5)$$

$$V_p(\vec{R}) = \int u_o(\vec{r}) \frac{2}{|\vec{r}-\vec{R}|} \chi(\vec{r}; \vec{R}) d^3r$$

As discussed by Callaway, LaBahn, Pu, and Duxler,²⁴ the monopole component of the polarization potential is nearly cancelled by a nonadiabatic correction (the distortion potential of Callaway, et. al.). Consequently only the dipole component of the polarization potential has been retained in (4-4).

Only the dipole component of χ is retained in constructing the two particle wave functions $\Psi_{\frac{S}{k}}(1,2)$. As will be seen, neglect of the monopole component does not affect the direct terms in the matrix element to first order in χ . There is some evidence from photoionization calculations in lithium that including the monopole component of χ in the exchange terms leads to incorrect results.²⁷

B. Reduction for Computation.

Partial wave expansions are used to obtain the s, p and d wave scattering states $\phi_{\frac{S}{k}}$. The initial state must behave asymptotically as a plane wave plus an outgoing spherical wave whereas the final state must behave as a plane wave plus an ingoing spherical wave.²⁸

$$\phi_{\vec{k}(\hat{r})}^S(\vec{R}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l i^l e^{\pm i \delta_l^S(k(\hat{r}))} Y_l^{*m}(\hat{k}(\hat{r})) Y_l^m(\hat{R}) \cdot \frac{F_l^S(k(\hat{r}); R)}{R} \quad (4-6)$$

$$u_0(\vec{R}) = U_{1s}(R) Y_0^0(\hat{R}) \quad (4-7)$$

In (4-6) F_l^S has the asymptotic form

$$F_l^S(k; R) \underset{R \rightarrow \infty}{\approx} \sqrt{\frac{2}{\pi}} R \left[\cos \delta_l^S(k) j_l(kR) - \sin \delta_l^S(k) n_l(kR) \right] \quad (4-8)$$

where $\delta_l^S(k)$ is the elastic scattering phase shift for the l th partial wave corresponding to total spin S . When (4-6) and (4-7) are used in (4-4), a radial scattering equation is obtained.

$$\begin{aligned} & \left[-\frac{d^2}{dR^2} + \frac{l(l+1)}{R^2} - 2e^{-2R} \left(1 + \frac{1}{R}\right) + V_p(R) - k^2 \right] F_l^S(k; R) \\ &= (-1)^{S+1} \left\{ -(1+k^2) R^{l+1} A_l \delta_{l,0} \right. \\ & \quad + \frac{2}{2l+1} \left[\frac{1}{R^2} \int_0^R U_{1s}(r) r^{l+1} F_l^S(k; r) dr \right. \\ & \quad \left. - R^{l+1} \int_0^R U_{1s}(r) r^{-2} F_l^S(k; r) dr \right. \\ & \quad \left. + R^{l+1} B_l \right\} U_{1s}(R) \end{aligned} \quad (4-9)$$

where
$$A_\ell = \int_0^\infty U_{1s}(r) r^{\ell+1} F_\ell^s(k; r) dr$$

$$B_\ell = \int_0^\infty U_{1s}(r) r^{-\ell} F_\ell^s(k; r) dr \quad (4-10)$$

$$V_p(R) = -\frac{9}{2R^4} \left[1 - \frac{e^{-2R}}{3} (1 + 2R + 6R^2 + \frac{20}{3}R^3 + \frac{4}{3}R^4) - \frac{2e^{-4R}}{3} (1 + R)^4 \right]$$

Equation (4-9) was solved non-iteratively employing an outward Numerov²⁹ integration. The wave functions and phase shifts at a regular grid of k^2 values were permanently stored on magnetic tape for later use in calculating the absorption coefficient.

A comparison of the AED phase shifts with those obtained from other approximations is given in figures 1-6. The curves labeled T are obtained from the dipole adiabatic exchange calculations of Temkin and Lamkin²³ in which a different polarization potential was used. Temkin and Lamkin's potential differs from the present one in that the perturbation is neglected when the external electron is inside the atomic electron. As might be expected AED and T differ by relatively small amounts. The curves labeled TLS are obtained from the polarized orbital approximation originated by Temkin and Lamkin²³ and modified by Sloan.³⁰ The polarized orbital approximation of Temkin and Lamkin differs from their dipole adiabatic exchange method through inclusion of certain perturbed exchange terms. Sloan's modification consists of including differentiation of the step function that must be used in cutting off the

perturbation; it affects only the p-wave phase shifts of Temkin and Lamkin's polarized orbital method. The curves labeled EP are obtained from the work of Callaway, et. al.²⁴ in which a repulsive potential (the distortion potential) is added to the complete polarization potential to account for certain velocity dependent effects. The curves labeled VAR are obtained from the variational calculations of Schwartz¹⁶ and Armstead.³¹ The VAR results (unavailable for d-wave and higher) are thought to be the best available. Finally the curves labeled G and CC are obtained from the calculations of Geltman¹⁷ and Doughty and Fraser's²¹ 1s-2s-2p close-coupling calculation. G and CC are adequately described in Chapter III.

As can be seen from figures 1 and 2, there is relatively little difference in the s-wave phase shifts of the various calculations. AED gives quite good phase shifts. It is the best simple approximation available for s waves. For the p-waves the AED results are higher than VAR which is again higher than CC and G. The relative differences between AED and VAR and between VAR and G (also VAR and CC) are of the same order of magnitude but different sign. It is seen that EP gives very good p-waves and can probably be used as an "exact" reference for all higher partial waves at low energies. Assuming this to be so, it is seen that the distinction between AED and G and CC for d-waves has roughly the same characteristics as for p-waves.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6

V. The Matrix Elements

A. Formal Development.

The dipole matrix element occurring in (2-9) may be written as

$$\begin{aligned} \langle f | D_{\mathbf{z}}^{(j)} | i \rangle_S &= \langle \psi(1;2) \phi_{\mathbf{k}_f}^S(2) | D_{\mathbf{z}_1}^{(j)} + D_{\mathbf{z}_2}^{(j)} | \psi(1;2) \phi_{\mathbf{k}_i}^S(2) \rangle \\ &\quad + (-1)^S \langle \psi(1;2) \phi_{\mathbf{k}_f}^S(2) | D_{\mathbf{z}_1}^{(j)} + D_{\mathbf{z}_2}^{(j)} | \psi(2;1) \phi_{\mathbf{k}_i}^S(1) \rangle \end{aligned} \quad (5-1)$$

where $D_Z^{(j)} = (\frac{d}{dt})^{j-1} (Z_1 + Z_2)$, and $D_{Z_1}^{(j)}$ and $D_{Z_2}^{(j)}$ have similar meanings. The first of the two terms on the right hand side of (5-1) is the direct term. When $D_{Z_2}^{(j)}$ is the operator in the direct term, the perturbed orbital may be removed by noting that $\psi(1;2)$ is normalized in coordinate 1 for all values of coordinate 2. Thus

$$\begin{aligned} \langle \psi(1;2) \phi_{\mathbf{k}_f}^S(2) | D_{\mathbf{z}_2}^{(j)} | \psi(1;2) \phi_{\mathbf{k}_i}^S(2) \rangle \\ = \langle \phi_{\mathbf{k}_f}^S(2) | D_{\mathbf{z}_2}^{(j)} | \phi_{\mathbf{k}_i}^S(2) \rangle \end{aligned} \quad (5-2)$$

For the velocity case ($j=2$) (5-2) is the only non-vanishing contribution. Since $D_{Z_1}^{(j)}$ involves ∇_1 ,

$$\begin{aligned} & \langle \psi(1;2) \phi_{\vec{k}_f}^S(2) | \nabla_1 | \psi(1;2) \phi_{\vec{k}_i}^S(2) \rangle \\ &= \langle \phi_{\vec{k}_f}^S(2) | \frac{1}{2} \nabla_1 | |\psi(1;2)|^2 \phi_{\vec{k}_i}^S(2) \rangle \\ &= 0 \end{aligned}$$

The length contribution from $D_{Z_1}^{(1)}$ does not vanish, however, and constitutes the only direct term in either formulation which contains the perturbation χ .

As stated earlier, neglect of the monopole component of χ does not affect the direct terms to first order in χ . This is obviously true for the velocity element since χ does not appear in (5-2). All first order terms in χ in the $D_{Z_1}^{(1)}$ contribution to the length matrix element are of odd parity when an even multipole of χ is used, and as a result integration over angles gives zero.

The second term on the right hand side of (5-1) is the exchange term. Note that by interchanging the dummy coordinate labels and using the hermitian property of the operators involved allows the $D_{Z_2}^{(j)}$ contribution to be obtained directly from the $D_{Z_1}^{(j)}$ contribution.

B. Reduction for Computation.

For use in the matrix elements χ is expanded in partial waves retaining only the dipole component as discussed in Chapter V.

$$\chi(\vec{r}; \vec{R}) = \frac{4\pi}{3} \sum_{M=-1}^1 \frac{w(r; R)}{r} Y_1^{*M}(\hat{r}) Y_1^M(\hat{R}) \quad (5-3)$$

where

$$w(r; R) = \begin{cases} \frac{1}{\sqrt{4\pi} R^2} \left[\frac{3(R+1)^2}{4} e^{-2R} \left(\frac{e^{2r}-1}{r^2} - \frac{2}{r} - 2 \right) - \left(\frac{r^2}{2} + r \right) \right] r U_{1s}(r); & r < R \\ \frac{1}{\sqrt{4\pi}} \left\{ \frac{3}{4R^2} [1 - R^2 - e^{-2R} (R+1)^2] \cdot \left[\frac{1}{r^2} + \frac{2}{r} + 2 \right] + \frac{R}{2} \left[\frac{1}{r^2} + \frac{2}{r} \right] \right\} r U_{1s}(r); & r > R \end{cases} \quad (5-4)$$

Through use of the partial wave expansions as detailed in equations (4-6), (4-7), and (5-3), the angular and radial integrations are separated. The resulting angular integrals are easily evaluated, since they consist of products of spherical harmonics, and give rise to the following factors which multiply the radial integrals:

$$S \rightarrow P: -\frac{i}{\sqrt{3}} e^{i[\delta_0^S(k_i) + \delta_1^S(k_f)]} Y_1^0(\hat{k}_f) Y_0^{*0}(\hat{k}_i)$$

$$P \rightarrow S: \frac{i}{\sqrt{3}} e^{i[\delta_1^S(k_i) + \delta_0^S(k_f)]} Y_0^0(\hat{k}_f) Y_1^{*0}(\hat{k}_i)$$

$$P \rightarrow D: -\frac{i}{\sqrt{5}} e^{i[\delta_1^S(k_i) + \delta_2^S(k_f)]} \cdot \left[\frac{2}{\sqrt{3}} Y_2^0(\hat{k}_f) Y_1^{*0}(\hat{k}_i) \right. \\ \left. + Y_2^{-1}(\hat{k}_f) Y_1^{*-1}(\hat{k}_i) + Y_2^1(\hat{k}_f) Y_2^{*1}(\hat{k}_i) \right]$$

$$D \rightarrow P: \frac{i}{\sqrt{5}} e^{i[\delta_2^S(k_i) + \delta_1^S(k_f)]} \cdot \left[\frac{2}{\sqrt{3}} Y_1^0(\hat{k}_f) Y_2^{*0}(\hat{k}_i) \right. \\ \left. + Y_1^{*-1}(\hat{k}_f) Y_2^{*-1}(\hat{k}_i) + Y_1^1(\hat{k}_f) Y_2^{*1}(\hat{k}_i) \right]$$

(5-5)

The factors in (5-4) multiply all terms of the corresponding transitions irregardless of whether they are direct or exchange terms.

From (5-2) the direct radial integrals common to both formulations are of the form

$$\int dR F_{\lambda_f}^S(k_f; R) d_R^{(ij)}(l_f l_i) F_{\lambda_i}^S(k_i; R) \quad (5-6)$$

where l_i and l_f take the values 0, 1, or 2 but differ by 1 ($l_f = l_i \pm 1$) and where

$$d_R^{(1)}(l_f l_i) = R \quad (5-7)$$

$$d_R^{(2)}(l_f l_i) = \frac{d}{dR} - \frac{1}{R} \left[l_f \delta_{l_i, l_f-1} - (l_f+1) \delta_{l_i, l_f+1} \right]$$

The radial integrals occurring in (5-6) are calculated numerically employing the six point formula out to $24.6 a_0$. Since the integrand oscillates, the contribution from $24.6 a_0$ out to infinity may not be negligible. The asymptotic forms of F_ℓ^S , equation (4-8), are employed to obtain this contribution analytically. It was found to be convenient to first calculate the asymptotic contribution to the velocity element. Recursion relations for the spherical Bessel functions can be used to obtain this contribution in terms of the integrals

$$\int_M^\infty R^2 f_\ell(k_f R) f'_\ell(k_i R) dR \quad (5-8)$$

where f_ℓ and f'_ℓ represent either j_ℓ or n_ℓ . The spherical Bessel equation can be used to obtain the integral (5-8) provided that the usual procedure is employed to make the integral absolutely convergent. The convergence procedure is equivalent to choosing wave packets for the scattering states. The resulting corrections are

$$\begin{aligned}
S \rightarrow P: \frac{2i}{\pi \Delta k^2 k_f} \left\{ \frac{\Delta k^2}{k_i k_f M} \left[\cos(\delta_1^S(k_f) - \delta_0^S(k_i) + k_- M) \right. \right. \\
\left. \left. - \cos(\delta_1^S(k_f) + \delta_0^S(k_i) + k_+ M) \right] \right. \\
\left. - k_- \sin(\delta_1^S(k_f) + \delta_0^S(k_i) + k_+ M) \right. \\
\left. - k_+ \sin(\delta_1^S(k_f) - \delta_0^S(k_i) + k_- M) \right\}
\end{aligned}$$

$$\begin{aligned}
P \rightarrow S: \frac{-2i}{\pi \Delta k^2 k_f} \left\{ k_- \sin(\delta_0^S(k_f) + \delta_1^S(k_i) + k_+ M) \right. \\
\left. - k_+ \sin(\delta_0^S(k_f) - \delta_1^S(k_i) + k_- M) \right\}
\end{aligned}$$

$$\begin{aligned}
P \rightarrow D: \frac{2i}{\pi k_f} \left\{ \left[\frac{1}{k_+} - \frac{3k_+}{k_i^2 k_f^2 M^2} \right] \sin(\delta_2^S(k_f) + \delta_1^S(k_i) + k_+ M) \right. \\
\left. - \left[\frac{1}{k_-} - \frac{3k_-}{k_i^2 k_f^2 M^2} \right] \sin(\delta_2^S(k_f) - \delta_1^S(k_i) + k_- M) \right. \\
\left. + \frac{3}{k_i k_f M} \left[1 - \frac{1}{k_i k_f M^2} \right] \cos(\delta_2^S(k_f) + \delta_1^S(k_i) + k_+ M) \right. \\
\left. + \frac{3}{k_i k_f M} \left[1 + \frac{1}{k_i k_f M^2} \right] \cos(\delta_2^S(k_f) - \delta_1^S(k_i) + k_- M) \right\}
\end{aligned}$$

$$\begin{aligned}
D \rightarrow P: \frac{-2i}{\pi \Delta k^2 k_f} \left\{ \frac{\Delta k^2}{k_i k_f M} \left[\cos(\delta_1^S(k_f) - \delta_2^S(k_i) + k_- M) \right. \right. \\
\left. \left. - \cos(\delta_1^S(k_f) + \delta_2^S(k_i) + k_+ M) \right] \right. \\
\left. - k_- \sin(\delta_1^S(k_f) + \delta_2^S(k_i) + k_+ M) \right. \\
\left. - k_+ \sin(\delta_1^S(k_f) - \delta_2^S(k_i) + k_- M) \right\} \quad (5-9)
\end{aligned}$$

where $k_+ = k_f + k_i$ and $k_- = k_f - k_i$

In appendix B, it is shown that the length matrix element can be obtained from the velocity matrix element simply by multiplying by $-i/\omega$ (in atomic units $\omega = \Delta k^2$). Since the asymptotic forms are the exact solutions in the asymptotic region, one might think that the same relation holds between the length and velocity correction formulas. This is not the case, however, since the relation $\dot{\vec{r}} = [\vec{r}, H]$ holds for matrix elements, i.e., integrations are assumed over all space. In the correction formula the integration leaves out a sphere of radius M about the origin. A non-vanishing surface integral term results. This procedure was used to obtain the length corrections below.

$$\begin{aligned}
S \rightarrow P: \frac{1}{\pi k_f k_i} \bigg\{ & \frac{k_+ + k_f}{k_f k_+^2} \sin(\delta_1^S(k_f) + \delta_0^S(k_i) + k_+ M) \\
& - \frac{k_- + k_f}{k_f k_-^2} \sin(\delta_1^S(k_f) - \delta_0^S(k_i) + k_- M) \\
& - \frac{M}{k_+} \cos(\delta_1^S(k_f) + \delta_0^S(k_i) + k_+ M) \\
& + \frac{M}{k_-} \cos(\delta_1^S(k_f) - \delta_0^S(k_i) + k_- M) \bigg\}
\end{aligned}$$

$$\begin{aligned}
P \rightarrow S: \frac{1}{\pi k_f k_i} \bigg\{ & \frac{k_+ + k_i}{k_i k_+^2} \sin(\delta_0^S(k_f) + \delta_1^S(k_i) + k_+ M) \\
& + \frac{k_i - k_-}{k_i k_-^2} \sin(\delta_0^S(k_f) - \delta_1^S(k_i) + k_- M) \\
& - \frac{M}{k_+} \cos(\delta_0^S(k_f) + \delta_1^S(k_i) + k_+ M) \\
& - \frac{M}{k_-} \cos(\delta_0^S(k_f) - \delta_1^S(k_i) + k_- M) \bigg\}
\end{aligned}$$

$$\begin{aligned}
P \rightarrow D: & \frac{1}{\pi k_f k_i} \left\{ \frac{-5k_f k_i - 3k_i^2 - k_f^2}{k_i k_f k_+^2} \sin(\delta_2^S(k_f) + \delta_1^S(k_i) + k_+ M) \right. \\
& + \frac{-5k_f k_i + 3k_i^2 + k_f^2}{k_i k_f k_-^2} \sin(\delta_2^S(k_f) - \delta_1^S(k_i) + k_- M) \\
& + \left[\frac{M}{k_+} - \frac{3}{k_f^2 k_i M} \right] \cos(\delta_2^S(k_f) + \delta_1^S(k_i) + k_+ M) \\
& \left. + \left[\frac{M}{k_-} + \frac{3}{k_f^2 k_i M} \right] \cos(\delta_2^S(k_f) - \delta_1^S(k_i) + k_- M) \right\}
\end{aligned}$$

$$\begin{aligned}
D \rightarrow P: & \frac{1}{\pi k_f k_i} \left\{ \frac{-5k_f k_i - k_i^2 - 3k_f^2}{k_f k_i k_+^2} \sin(\delta_1^S(k_f) + \delta_2^S(k_i) + k_+ M) \right. \\
& + \frac{5k_f k_i - k_i^2 - 3k_f^2}{k_f k_i k_-^2} \sin(\delta_1^S(k_f) - \delta_2^S(k_i) + k_- M) \\
& + \left[\frac{M}{k_+} - \frac{3}{k_f k_i^2 M} \right] \cos(\delta_1^S(k_f) + \delta_2^S(k_i) + k_+ M) \\
& \left. + \left[-\frac{M}{k_-} + \frac{3}{k_f k_i^2 M} \right] \cos(\delta_1^S(k_f) - \delta_2^S(k_i) + k_- M) \right\}
\end{aligned}$$

From (5-9) it is observed that the velocity asymptotic forms diverge as $M \rightarrow 0$ for all transitions except $P \rightarrow S$. From (5-10) it follows that all diverge in the length case except $S \rightarrow P$ and $P \rightarrow S$.

The remaining contribution to the direct term in the length formulation is obtained by using $D_{Z_1}^{(1)}$ in the direct term of (5-1). There are two non-vanishing contributions which are first order in χ ; one involves a perturbed final state and the other a perturbed initial state. The two contributions are easily shown to be identical, and the resulting radial integrals including the factor of 2 are

$$\frac{4\pi^{1/2}}{3} \iint dr dR U_{1s}(r) F_{\ell_f}^S(k_f; R) d_r^{(1)}(\ell_f \ell_i) w(r; R) F_{\ell_i}^S(k_i; R) \quad (5-11)$$

where ℓ_i and ℓ_f are 0, 1, or 2 but differ by 1 ($\ell_f = \ell_i \pm 1$).

The exchange term of (5-1) consists of two terms (from $D_{Z_1}^{(j)}$ and $D_{Z_2}^{(j)}$) which are zero order in χ and two terms which are first order in χ . The zero order terms in χ can yield only $S \leftrightarrow P$ transitions.

The radial integral for the $P \rightarrow S$ transition is

$$\int dR R F_0^S(k_f; R) U_{1s}(R) \cdot \int dr r F_1^S(k_i; r) r^{2-j} U_{1s}(r) \quad (5-12)$$

The $S \rightarrow P$ transition is obtained from (5-12) simply by $(-1)^{j-1}[i \leftrightarrow f]$. In obtaining the total matrix element the interchange of initial and final states must also be made in the $P \rightarrow S$ member of (5-5). The two terms which are first order in χ contain all four transitions. The radial integrals for the $P \rightarrow S$ and $P \rightarrow D$ transitions are

$$\begin{aligned} & \iint dr dR \left[U_{1s}(R) F_{\ell_f}^S(k_f; r) d_r^{(j)}(\ell_f 1) w(r; R) \right. \\ & \quad F_i^S(k_i; R) + w(r; R) F_{\ell_f}^S(k_f; R) \\ & \quad \left. d_R^{(j)}(\ell_f 1) U_{1s}(R) F_i^S(k_i; r) \right] \end{aligned} \quad (5-13)$$

where $\ell_f = 0$ or 2 . The $S \rightarrow P$ and $D \rightarrow P$ transitions are obtained from the $P \rightarrow S$ and $P \rightarrow D$ transitions, respectively, of (5-13) by the procedure discussed in connection with (5-12).

The double integrals appearing in (5-11) and (5-13) were evaluated numerically using a combination of Simpson and six point formulas. Integration over the atomic coordinate r was done with Simpson's rule to yield a function of R at every other grid point. The remaining integration over R was then done with the six point formula over the enlarged grid. Numerical derivatives were calculated by means of the five point interpolation procedure.

The resulting matrix elements were then squared and substituted into (2-9) to obtain the absorption coefficient for various wavelengths and temperatures. Integration over k_i^2 once again employed

the six point formula.

Various analytical tests were used to check the accuracy of the computer programs. The direct terms were tested by using trigonometric functions in place of the continuum functions, the resulting integrals having an analytic form. The numerical and analytic results agreed to at least six figures. Since a numerical computation of V_p involves integration over atomic coordinates, the basic idea of the double integral procedure could be so tested. The numerical V_p agreed to four figures with the analytic one for very small values of R and to six figures for larger R .

VI. Comparison with Many Body Perturbation Theory

It is interesting to compare the present procedure for calculating the matrix element using the polarized orbital method with the diagrammatic methods of many body perturbation theory (MBPT). MBPT has already been applied to scattering³² and photoionization problems³³.

MBPT yields four diagrams which correspond to first order corrections in the electron-electron interaction. These four diagrams are shown in Fig. 7. The dashed lines as usual correspond to the electron-electron interaction $V(i,j)=2/r_{ij}$, wavy lines correspond to the dipole photon interaction, and solid lines correspond to particles when the arrow is up and holes when the arrow is down. 7(a) represents the direct term with a final state correction and 7(b) is the corresponding exchange term. 7(c) and 7(d) are the similar terms with an initial state correction. The direct diagrams can be related to polarized orbital theory, and the procedure for so doing is illustrated for 7(a).

In accord with the usual rules, the matrix element obtained from 7(a) is

(a)

(b)

(c)

(d)

Fig. 7

$$\begin{aligned}
T(a) = \sum_{n,l} \int d\tau_1 u_{nl}^*(1) D_{\vec{z}_1}^{(j)} u_0(1) \iint d\tau_2 d\tau_3 u_0^*(2) \phi_{\vec{k}_f}^{*S}(3) \\
\cdot \frac{V(2,3) u_{nl}(2) \phi_{\vec{k}_i}^S(3)}{\epsilon_{15} - \epsilon_{nl}}
\end{aligned} \quad (6-1)$$

The sum includes continuum states. But from polarized orbital theory, the perturbation $\chi(1;3)$ is given by

$$\chi^*(1;3) = \sum_{nl \neq 15} \frac{u_{nl}^*(1)}{\epsilon_{15} - \epsilon_{nl}} \int d\tau_2 u_0^*(2) V(2,3) u_{nl}(2) \quad (6-2)$$

Using (6-2) in (6-1) then gives

$$\begin{aligned}
T(a) &= \iint d\tau_2 d\tau_1 \chi^*(1;3) \phi_{\vec{k}_f}^{*S}(3) D_{\vec{z}_1}^{(j)} u_0(1) \phi_{\vec{k}_i}^S(3) \\
&= \langle \chi(1;2) \phi_{\vec{k}_f}^S(2) | D_{\vec{z}_1}^{(j)} | u_0(1) \phi_{\vec{k}_i}^S(2) \rangle
\end{aligned} \quad (6-3)$$

But (6-3) is one of the terms included in (5-1). From (6-1) it is seen that $l=1$ due to the appearance of the dipole operator.

It has not been possible to directly relate the exchange diagrams to the exchange matrix elements obtained in Chapter V. This seems to be a usual occurrence for calculations in polarized orbital theory and has been observed in similar calculations.²⁷

Callaway³⁴ has shown that second order corrections included here through use of the polarization potential in (2.5) can be

accounted for by MBPT. They arise from diagrams shown in Fig. 8.

These are not the only second order terms; however they are probably the most important.

Fig. 8

VII. Results and Conclusions

The total absorption coefficient due to $S \leftrightarrow P$ and $P \leftrightarrow D$ transitions for various temperatures (the parameter $\theta = 5040/T$) and wavelengths is given for both dipole length and dipole velocity formulations in Table I. It is seen that the agreement between length and velocity forms is extremely good in the long wavelength region where free-free absorption dominates bound-free absorption. As the wavelength decreases, the difference between length and velocity generally increases reaching a maximum of about 5.5%. This can be contrasted with the results of Doughty and Fraser²¹ where the difference reaches about 10%. Also the present length results are larger than those using the velocity operator whereas the velocity results of Doughty and Fraser are larger than those with the length operator. For both length and velocity, however, the present values are generally lower than those of Doughty and Fraser. Geltman¹⁷ has not given velocity results so that a comparison with his length results cannot be made, and John²² used a simplified approximation in which length and velocity are identical. The ratio of length to velocity results for this calculation is shown in Fig. 9. The ratio is plotted against wavelength at the solar temperature.

In the important long wavelength region ($0 < \Delta k^2 \leq .06$) the present results are generally lower than those of Doughty and Fraser

Table 1. Total free-free absorption coefficient in unit of $10^{-26} \text{ cm}^4 \text{ dyne}^{-1}$. The number in parentheses is the power of 10 by which the corresponding table entry should be multiplied.

ΔK^2	$\lambda (\text{\AA})$	$\theta = 0.5$		$\theta = 0.6$		$\theta = .7$		$\theta = .8$	
		LEN	VEL	LEN	VEL	LEN	VEL	LEN	VEL
.01	91130	2.75(1)	2.75(1)	3.29(1)	3.29(1)	3.80(1)	3.79(1)	4.28(1)	4.28(1)
.02	45560	6.92	6.90	8.27	8.25	9.56	9.53	1.08(1)	1.07(1)
.03	30380	3.10	3.08	3.71	3.69	4.29	4.26	4.84	4.80
.04	22780	1.77	1.74	2.11	2.09	2.44	2.41	2.75	2.72
.05	18230	1.14	1.12	1.36	1.35	1.58	1.55	1.78	1.75
.06	15190	7.98(-1)	7.85(-1)	9.58(-1)	9.41(-1)	1.11	1.09	1.25	1.23
.07	13020	5.92(-1)	5.81(-1)	7.11(-1)	6.96(-1)	8.24(-1)	8.05(-1)	9.31(-1)	9.08(-1)
.08	11390	4.58(-1)	4.48(-1)	5.50(-1)	5.36(-1)	6.37(-1)	6.20(-1)	7.21(-1)	7.00(-1)
.09	10130	3.65(-1)	3.56(-1)	4.39(-1)	4.26(-1)	5.09(-1)	4.93(-1)	5.75(-1)	5.57(-1)
.10	9113	2.98(-1)	2.90(-1)	3.59(-1)	3.47(-1)	4.16(-1)	4.02(-1)	4.70(-1)	4.54(-1)
.12	7594	2.10(-1)	2.03(-1)	2.53(-1)	2.44(-1)	2.93(-1)	2.82(-1)	3.32(-1)	3.19(-1)
.14	6509	1.56(-1)	1.50(-1)	1.88(-1)	1.81(-1)	2.18(-1)	2.09(-1)	2.47(-1)	2.37(-1)
.16	5695	1.21(-1)	1.16(-1)	1.45(-1)	1.39(-1)	1.69(-1)	1.61(-1)	1.92(-1)	1.83(-1)
.18	5063	9.59(-2)	9.20(-2)	1.16(-1)	1.11(-1)	1.35(-1)	1.29(-1)	1.53(-1)	1.46(-1)
.20	4556	7.80(-2)	7.48(-2)	9.41(-2)	9.00(-2)	1.10(-1)	1.05(-1)	1.25(-1)	1.19(-1)
.30	3038	3.44(-2)	3.34(-2)	4.18(-2)	4.05(-2)	4.91(-2)	4.76(-2)	5.65(-2)	5.47(-2)

Δk^2	$\lambda (\text{\AA})$	$\theta = .9$		$\theta = 1.0$		$\theta = 1.1$		$\theta = 1.2$	
		LEN	VEL	LEN	VEL	LEN	VEL	LEN	VEL
.01	91130	4.75(1)	4.74(1)	5.19(1)	5.19(1)	5.62(1)	5.62(1)	6.04(1)	6.03(1)
.02	45560	1.19(1)	1.19(1)	1.31(1)	1.30(1)	1.42(1)	1.41(1)	1.52(1)	1.51(1)
.03	30380	5.37	5.32	5.87	5.82	6.36	6.30	6.83	6.77
.04	22780	3.05	3.02	3.34	3.30	3.62	3.57	3.89	3.83
.05	18230	1.98	1.94	2.17	2.13	2.34	2.30	2.52	2.47
.06	15190	1.39	1.36	1.52	1.49	1.65	1.61	1.77	1.73
.07	13020	1.03	1.01	1.13	1.10	1.23	1.19	1.32	1.29
.08	11390	8.00(-1)	7.76(-1)	8.76(-1)	8.49(-1)	9.49(-1)	9.20(-1)	1.02	9.87(-1)
.09	10130	6.39(-1)	6.18(-1)	7.00(-1)	6.76(-1)	7.58(-1)	7.33(-1)	8.15(-1)	7.87(-1)
.10	9113	5.22(-1)	5.04(-1)	5.73(-1)	5.52(-1)	6.21(-1)	5.98(-1)	6.68(-1)	6.43(-1)
.12	7594	3.69(-1)	3.55(-1)	4.06(-1)	3.89(-1)	4.41(-1)	4.23(-1)	4.75(-1)	4.55(-1)
.14	6509	2.76(-1)	2.64(-1)	3.03(-1)	2.90(-1)	3.31(-1)	3.16(-1)	3.57(-1)	3.41(-1)
.16	5695	2.14(-1)	2.04(-1)	2.36(-1)	2.25(-1)	2.58(-1)	2.46(-1)	2.80(-1)	2.66(-1)
.18	5063	1.72(-1)	1.63(-1)	1.90(-1)	1.80(-1)	2.08(-1)	1.97(-1)	2.25(-1)	2.14(-1)
.20	4556	1.40(-1)	1.34(-1)	1.56(-1)	1.48(-1)	1.71(-1)	1.62(-1)	1.86(-1)	1.76(-1)
.30	3038	6.39(-2)	6.19(-2)	7.13(-2)	6.91(-2)	7.87(-2)	7.63(-2)	8.62(-2)	8.35(-2)

k ²	o (A)	θ = 1.3		θ = 1.4		θ = 1.5		θ = 1.6	
		LEN	VEL	LEN	VEL	LEN	VEL	LEN	VEL
.01	91130	6.45(1)	6.44(1)	6.84(1)	6.83(1)	7.23(1)	7.22(1)	7.60(1)	7.59(1)
.02	45560	1.62(1)	1.61(1)	1.72(1)	1.71(1)	1.82(1)	1.81(1)	1.91(1)	1.90(1)
.03	30380	7.28	7.21	7.72	7.64	8.14	8.06	8.55	8.46
.04	22780	4.14	4.08	4.39	4.32	4.63	4.56	4.86	4.78
.05	18230	2.68	2.63	2.84	2.78	3.00	2.9	3.15	3.08
.06	15190	1.89	1.83	2.00	1.95	2.11	2.05	2.21	2.16
.07	13020	1.40	1.36	1.49	1.44	1.57	1.52	1.65	1.60
.08	11390	1.09	1.05	1.15	1.12	1.22	1.18	1.28	1.24
.09	10130	8.71(-1)	8.40(-1)	9.25(-1)	8.92(-1)	9.77(-1)	9.42(-1)	1.03	9.92(-1)
.10	9113	7.15(-1)	6.88(-1)	7.60(-1)	7.31(-1)	8.04(-1)	7.73(-1)	8.47(-1)	8.14(-1)
.12	7594	5.09(-1)	4.88(-1)	5.43(-1)	5.20(-1)	5.76(-1)	5.51(-1)	6.08(-1)	5.82(-1)
.14	6509	3.84(-1)	3.66(-1)	4.10(-1)	3.91(-1)	4.36(-1)	4.16(-1)	4.62(-1)	4.42(-1)
.16	5695	3.01(-1)	2.86(-1)	3.22(-1)	3.06(-1)	3.43(-1)	3.26(-1)	3.64(-1)	3.46(-1)
.18	5063	2.43(-1)	2.31(-1)	2.61(-1)	2.48(-1)	2.78(-1)	2.64(-1)	2.96(-1)	2.81(-1)
.20	4556	2.01(-1)	1.91(-1)	2.16(-1)	2.05(-1)	2.31(-1)	2.19(-1)	2.45(-1)	2.33(-1)
.30	3038	9.36(-2)	9.08(-2)	1.01(-1)	9.80(-2)	1.08(-1)	1.05(-1)	1.16(-1)	1.12(-1)

λ^2	θ ($^\circ$)	$\theta = 1.7$		$\theta = 1.8$		$\theta = 1.9$		$\theta = 2.0$	
		LEN	VEL	LEN	VEL	LEN	VEL	LEN	VEL
.01	91130	7.97(1)	7.95(1)	8.32(1)	8.31(1)	8.62(1)	8.60(1)	8.91(1)	8.90(1)
.02	45560	2.00(1)	1.99(1)	2.09(1)	2.07(1)	2.17(1)	2.16(1)	2.23(1)	2.24(1)
.03	30380	8.95	8.85	9.33	9.23	9.71	9.59	10.01(1)	9.95
.04	22780	5.08	5.00	5.30	5.21	5.51	5.41	5.71	5.61
.05	18230	3.29	3.22	3.43	3.36	3.57	3.49	3.71	3.61
.06	15190	2.32	2.26	2.42	2.35	2.51	2.44	2.61	2.54
.07	13020	1.73	1.67	1.80	1.75	1.89	1.82	1.95	1.89
.08	11390	1.34	1.30	1.40	1.36	1.46	1.41	1.52	1.47
.09	10130	1.08	1.04	1.13	1.09	1.19	1.13	1.23	1.18
.10	9113	8.90(-1)	8.55(-1)	9.32(-1)	8.95(-1)	9.73(-1)	9.35(-1)	1.01	9.74(-1)
.12	7594	6.40(-1)	6.12(-1)	6.72(-1)	6.43(-1)	7.03(-1)	6.73(-1)	7.34(-1)	7.02(-1)
.14	6509	4.87(-1)	4.64(-1)	5.12(-1)	4.88(-1)	5.37(-1)	5.12(-1)	5.62(-1)	5.35(-1)
.16	5695	3.85(-1)	3.66(-1)	4.06(-1)	3.85(-1)	4.26(-1)	4.05(-1)	4.46(-1)	4.24(-1)
.18	5063	3.13(-1)	2.97(-1)	3.30(-1)	3.13(-1)	3.47(-1)	3.29(-1)	3.64(-1)	3.45(-1)
.20	4556	2.60(-1)	2.46(-1)	2.75(-1)	2.60(-1)	2.89(-1)	2.74(-1)	3.03(-1)	2.87(-1)
.30	3038	1.23(-1)	1.20(-1)	1.30(-1)	1.27(-1)	1.39(-1)	1.34(-1)	1.45(-1)	1.41(-1)

Fig. 9

and Geltman¹⁷ although they are somewhat higher at very long wavelengths. In all of these cases, however, the agreement is fairly close, reaching a maximum difference in the region $.01 \leq \Delta k^2 \leq .06$ of roughly 20% for the velocity results of Doughty and Fraser. The comparison is considerably better when the length results are used. The smaller values observed here seem to be in line with the reduced values in going from the 1s-2s to the 1s-2s-2p approximation of Doughty and Fraser. Geltman's results tend to lie somewhat between those of Doughty and Fraser and the present ones. For short wavelengths the difference between these results and those of Doughty and Fraser jumps up to about 40%. The length results of the present calculation are given in Fig. 10 at the solar temperature. The ratio of Geltman's results to the present length results (G) and of Doughty and Fraser's length results to the present length results (DF) are given in Fig. 11 at the solar temperature. The present results agree more closely with those of John²²; however, this must be considered accidental in light of the rather gross approximation employed by John. The differences between the present results and those of Geltman and Doughty and Fraser appear to be consistent with the values of the scattering phase shifts obtained in Chapter IV.

In Table 2 the contributions from various spins and transitions for a rather typical wavelength (9113Å) are separated. The 1/4:3/4 sum rule has already been included so that the triplet contribution is weighted three times more heavily than the singlet. It is observed that the singlet contribution from higher transitions is

Fig. 10

Fig. 11

Table 2. Contributions to absorption coefficient for various spins and transitions at $\Delta k^2 = .10$ ($\lambda = 9113 \text{ \AA}$). Units are $10^{-26} \text{ cm}^4 \cdot \text{dyne}^{-1}$. $\theta = \frac{5040}{T}$.

θ	S	$L_i \cdot L_f$	AED		1s-2s-2p(Ref. 21)	
			LEN	VEL	LEN	VEL
.5	0	S*P	.0844	.0872	.0874	.0916
	0	P*S	.0156	.0143	.0147	.0131
	1	S*P	.1384	.1240	.1349	.1428
	1	P*S	.0418	.0440	.0431	.0443
	Subtotal		.2802	.2695	.2802	.2918
	0	P*D	.0000	.0000	.0002	.0005
	0	D*P	.0000	.0000	.0001	.0000
	1	P*D	.0126	.0157	.0068	.0054
	1	D*P	.0055	.0046	.0028	.0036
	Subtotal		.0181	.0203	.0094	.0095
	Total		.2983	.2898	.2900	.3013
1.0	0	S*P	.2247	.2315	.2408	.2566
	0	P*S	.0243	.0224	.0230	.0188
	1	S*P	.2620	.2307	.2565	.2823
	1	P*S	.0473	.0498	.0507	.0510
	Subtotal		.5583	.5344	.5709	.6108
	0	P*D	.0000	.0000	.0002	.0005
	0	D*P	.0000	.0000	.0000	.0000
	1	P*D	.0105	.0143	.0054	.0032
	1	D*P	.0038	.0031	.0018	.0027
	Subtotal		.0143	.0174	.0074	.0065
	Total		.5726	.5518	.5783	.6172
2.0	0	S*P	.4883	.5029	.5544	.5979
	0	P*S	.0297	.0274	.0280	.0218
	1	S*P	.4424	.3847	.4464	.5086
	1	P*S	.0439	.0462	.0486	.0525
	Subtotal		1.0043	.9612	1.0773	1.1802
	0	P*D	.0000	.0000	.0001	.0004
	0	D*P	.0000	.0000	.0000	.0000
	1	P*D	.0073	.0111	.0035	.0014
	1	D*P	.0020	.0016	.0010	.0015
	Subtotal		.0093	.0127	.0046	.0033
	Total		1.0136	.9739	1.0819	1.1835

virtually non-existent. The cause for such a drastic difference between singlet and triplet $P \leftrightarrow D$ contributions has been investigated to some extent and has been found to be mirrored by the phase shifts; i.e., the asymptotic contribution shows the same behavior. From Table 2 the $P \leftrightarrow D$ transitions are seen to contribute approximately 6% to the absorption coefficient at $\theta = .5$ with a considerable reduction as θ increases. The $P \leftrightarrow D$ contribution increases slowly with wavelength reaching approximately 10%.

Some authors have employed asymptotic forms, e.g., Ohmura and Ohmura,^{10,11,15} over all space to obtain the matrix elements. Ohmura and Ohmura use the asymptotic form (4-8) for the S wave and the P wave part of a plane wave ($\delta_1 = 0$ in (4-8)) for the P wave to obtain the $S \rightarrow P$ contribution of the matrix element. They consider only $S \rightarrow P$ transitions. As pointed out by Geltman,¹⁷ care must be taken not to apply such methods beyond their range of validity. The integrands are convergent at the origin only for $S \rightarrow P$ and $P \rightarrow S$ transitions in the length formulation and only for $P \rightarrow S$ transitions in the velocity form. The possibility of cutting off the divergent integrals at some small value of r , say r_0 , has been investigated; however, the integrals oscillate very rapidly with r_0 making the determination of r_0 extremely unreliable. Those transitions which are convergent, on the other hand, are capable of reproducing the "exact" results to within 10%.

One of the purposes of this work was to assess the importance of explicitly including atomic distortion. At a rather typical wavelength of $9113 \text{ \AA}$ k_λ was calculated with all terms including the

perturbation χ deleted. The AED scattering functions Φ_k^S and corresponding phases $\delta_\ell^S(k)$ were still used. The velocity results were most affected being reduced by about 6% while the length results were reduced only very slightly (on the order of 1%). For the longer wavelengths the results were even closer to the "exact" ones while the differences became larger at the shorter wavelengths (12.5% for velocity and 5% for length). Recalling from Section II B that the length matrix element contained χ in both direct and exchange terms whereas the velocity matrix element contained χ only in the exchange terms, it is reasonable to expect that the various terms containing χ tend to subtract out in the length form. Furthermore, the length form emphasizes the contribution from the wave function at large radial distances whereas the velocity form emphasizes the behavior at smaller radial distances. Thus neglect of χ is expected to affect velocity results more than length results. It is concluded that the resulting simplification in the matrix elements and the small error incurred at long wavelengths makes inclusion of χ unnecessary for astrophysical calculations. It is recommended that the length formulation be used in such a calculation due to the expected lesser effect in neglecting χ in the length formulation (this lesser effect indeed being observed).

Finally an attempt has been made to relate the present results along with those of Geltman¹⁷ and Doughty and Fraser²¹ to observation. The observations cited are those of Chalonge and Kourganoff⁸; they observed the optical depth τ_λ of the sun as a function of temperature. τ_λ is defined as (Aller³⁵)

$$\tau_{\lambda} = \int_0^x k'_{\lambda} \rho dx$$

where ρ is the density of the stellar material in g.cm^{-3} , k'_{λ} is the absorption coefficient per gram, and x is the linear depth in the medium. The variation of τ_{λ} with temperature is given by Chalonge and Kourganoff as

$$\frac{d\tau_{\lambda}}{dT} = -k_{\lambda} \rho \frac{dx}{dT} \quad (7-1)$$

Chalonge and Kourganoff have calculated $d\tau_{\lambda}$ at $16550 \text{ \AA}$ and 6500°K from their observations of τ_{λ} ; the result is 0.22. Using the present value of k_{λ} in equation (7-1) together with the variation of density and temperature with depth as given by Chalonge and Kourganoff gives the value of $d\tau_{\lambda}$ as 0.20. The results of Doughty and Fraser give 0.21 while the results of Geltman give 0.22. All three of the calculations are in good agreement with observation, and the experimental accuracy is probably not such as to be able to distinguish one from the other.

It is of some interest to compare the present results with the static exchange (SE) results of Doughty and Fraser²¹ and John.¹⁴ This comparison gives one some insight into the importance of polarization effects compared to exchange effects. At a fixed wavelength of $9113\text{\AA}$ the static exchange results are lower than the AED results by 2% to 7%, the closer agreement occurring at lower temperatures. For a fixed temperature of 6300°K , the difference

varies from about 2% at the longest tabulated wavelength to about 3% at the shorter tabulated wavelengths. The figures quoted are for the length results. The velocity results (only a limited comparison with Doughty and Fraser can be made here) are generally in worse agreement by an additional 2%.

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Appendix A

Average Over Photon Parameters

In equation (2-7) there occurs the expression

$$\frac{1}{4\pi} \int d\hat{k}_\omega \overline{|\langle f | \vec{\epsilon} \cdot (\vec{v}_1 + \vec{v}_2) | i \rangle|^2} \quad (\text{A-1})$$

where the raised bar indicates an average over the independent directions of $\vec{\epsilon}$. If a vector $\vec{Q}$ is defined by

$$\vec{Q} = \langle f | \vec{v}_1 + \vec{v}_2 | i \rangle \quad (\text{A-2})$$

then the integrand of (A-1) becomes

$$\overline{|\vec{\epsilon} \cdot \vec{Q}|^2} = \frac{1}{2} (|\vec{\epsilon}_1 \cdot \vec{Q}|^2 + |\vec{\epsilon}_2 \cdot \vec{Q}|^2)$$

where $\vec{\epsilon}_1$ and $\vec{\epsilon}_2$ are the two independent directions of $\vec{\epsilon}$, i.e., $(\vec{\epsilon}_1, \vec{\epsilon}_2, \hat{k}_\omega)$ form a unit triad of vectors. Thus,

$$\overline{|\vec{\epsilon} \cdot \vec{Q}|^2} = \frac{1}{2} (|\vec{Q}|^2 - |\hat{k}_\omega \cdot \vec{Q}|^2)$$

$\vec{Q}$ is now taken as the Z-axis of the coordinate system with k_ω as the radius vector. Then

$$\overline{|\vec{\epsilon} \cdot \vec{Q}|^2} = \frac{|\vec{Q}|^2}{2} (1 - \cos^2 \theta)$$

The integration in (A-1) is then straightforward with the result

$$\begin{aligned} \frac{1}{4\pi} \int d\hat{k}_\omega \overline{|\langle f | \vec{\epsilon} \cdot (\vec{v}_1 + \vec{v}_2) | i \rangle|^2} \\ = \frac{|\langle f | \vec{v}_1 + \vec{v}_2 | i \rangle|^2}{3} \end{aligned} \quad (\text{A-3})$$

(A-3) may be further simplified. Due to the spherical symmetry in the problem, all components of $\vec{v}_1 + \vec{v}_2$ give the same contribution so that the right hand side of (A-3) becomes

$$|\langle f | v_{1z} + v_{2z} | i \rangle|^2$$

Appendix B

Relation Between Length and Velocity Matrix Elements

The velocity matrix element of (2-9) is

$$\langle f | v_{1z} + v_{2z} | i \rangle \equiv \sigma_v \quad (\text{B-1})$$

From quantum mechanics it is known that for systems with a time independent Hamiltonian

$$v_{1z} = \dot{z}_1 = \frac{1}{i\hbar} [z_1, H] \quad (\text{B-2})$$

where H is the full hamiltonian for the system. For the free-free absorption of light by H^- , H has been given in equation (4-1).

Substitution of (B-2) into (B-1) then gives

$$\begin{aligned} \sigma_v &= \frac{1}{i\hbar} \langle f | (z_1 + z_2) H - H (z_1 + z_2) | i \rangle \\ &= \frac{1}{i\hbar} \langle f | (z_1 + z_2) H | i \rangle - \frac{1}{i\hbar} \langle f | H (z_1 + z_2) | i \rangle \\ &= \frac{E_i}{i\hbar} \langle f | z_1 + z_2 | i \rangle - \frac{1}{i\hbar} \langle f | H (z_1 + z_2) | i \rangle \end{aligned} \quad (\text{B-3})$$

But H is an hermitian operator so that

$$\begin{aligned}\langle f | H(z_1 + z_2) | i \rangle &= \langle k | H | f \rangle^* \\ &= E_f \langle f | H | k \rangle\end{aligned}$$

where $|k\rangle = (z_1 + z_2) |i\rangle$. Thus (B-3) becomes

$$\begin{aligned}\sigma_V &= -\frac{E_f - E_i}{i\hbar} \langle f | z_1 + z_2 | i \rangle \\ &\equiv -\frac{E_f - E_i}{i\hbar} \sigma_L\end{aligned}\tag{B-4}$$

In atomic units (B-4) becomes

$$\sigma_V = -\frac{\omega}{i} \sigma_L$$

It is emphasized that the result (B-4) obtains when H is the exact hamiltonian. (B-4) does not follow when approximate hamiltonians like Hartree-Fock or polarized orbital are used. As a result, length and velocity results will not agree exactly. The degree to which they do agree then gives an indication of the validity of the approximate wave functions used.

Chang and McDowell³³ have explicitly evaluated the difference between length and velocity matrix elements in the Hartree-Fock approximation for photoionization of lithium. An extension of their results to the present system gives

$$\sigma_L^{HF} = \frac{1}{i\omega} \left[\sigma_V^{HF} + \frac{1}{3} I_1 - I_2 \right] \quad (B-5)$$

where

$$I_1 = \int dr_2 r_2 U_{1s}(r_2) F_{\ell_f}^S(k_f; r_2) \\ \cdot \left[\frac{1}{r_2^2} \int_0^{r_2} dr_1 r_1^3 U_{1s}(r_1) F_{\ell_i}^S(k_i; r_1) \right. \\ \left. + r_2 \int_{r_2}^{\infty} dr_1 U_{1s}(r_1) F_{\ell_i}^S(k_i; r_1) \right]$$

(B-6)

$$I_2 = \int_0^{\infty} dr_2 r_2 U_{1s}(r_2) F_{\ell_f}^S(k_f; r_2) \\ \cdot \left[\frac{1}{r_2} \int_0^{r_2} dr_1 U_{1s}(r_1) F_{\ell_i}^S(k_i; r_1) r_1^2 \right. \\ \left. + \int_{r_2}^{\infty} dr_1 r_1 U_{1s}(r_1) F_{\ell_i}^S(k_i; r_1) \right]$$

Appendix C

Tables of Phase Shifts

In tables 3, 4, 5 the s, p, and d phase shifts are given as obtained from various approximations. These approximations are adequately described in Chapter IV.

Table 3 S-Wave
Singlet

<u>k</u>	<u>SE</u>	<u>AED</u>	<u>I</u>	<u>TLS</u>	<u>EP</u>	<u>G</u>	<u>CC</u>	<u>VAR</u>
.1	2.40	2.54	2.52	2.58	2.44	2.44	2.54	2.55
.3	1.51	1.67	1.65	1.75	1.54	1.54	1.61	1.70
.5	1.03	1.17	1.16	1.25	1.04	1.04	1.08	1.20
.75	.694	.828	.815	.908	.689	.915	.810	.
1.00	.543	.677	.666	.758	.526			

Triplet

.1	2.91	2.95	2.95	2.95	2.95	2.94	2.94	2.94
.3	2.46	2.53	2.53	2.52	2.53	2.50	2.50	2.50
.5	2.07	2.15	2.15	2.13	2.15	2.10	2.10	2.10
.75	1.68	1.77	1.76	1.75	1.77	1.72	1.72	
1.00	1.39	1.49	1.48	1.46	1.49			

Table 4. P-Wave
Singlet

<u>k</u>	<u>SE</u>	<u>AED</u>	<u>T</u>	<u>TLS</u>	<u>EP</u>	<u>G</u>	<u>CC</u>	<u>VAR</u>
.1	-.0012	.0070	.0069	.0067	.0063	.0040	.0039	.0070
.3	-.0240	.0263	.0237	.0211	.0160	.0020	.0043	.0170
.5	-.0703	.0222	.0136	.0064	-.0068	-.0281	-.0281	-.0007
.75	-.1126	.0166	-.0005	-.0106	-.0404	-.0570	-.0570	
1.00	-.1058	.0418	.0190	.0136	-.0424			

Triplet

.1	.0022	.0184	.0181	.0094	.0102	.0100	.0078	.0114
.3	.0511	.1283	.1220	.1151	.1047	.0880	.0905	.1063
.5	.1694	.3317	.3113	.2868	.2607	.2120	.2364	.2699
.75	.3037	.4960	.4670	.4230	.3871	.3520	.3800	
1.00	.3579	.5304	.5033	.4521	.4119			

Table 5. D-Wave
Singlet

<u>k</u>	<u>SE</u>	<u>AED</u>	<u>I</u>	<u>TLS</u>	<u>EP</u>	<u>G</u>	<u>CC</u>
.1	-.0000	.0013	.0013		.0013	.0010	.0008
.3	-.0005	.0114	.0112	.0113	.0105	.0052	.0074
.5	-.0039	.0263	.0252	.0266	.0215	.0150	.0207
.75	-.0123	.0430	.0388	.0456	.0290	.0238	.0490
1.00	-.0175	.0578	.0494	.0627	.0316		

Triplet

.1	.0000	.0013	.0013		.0013	.0010	.0008
.3	.0008	.0128	.0127	.0118	.0119	.0086	.0085
.5	.0070	.0384	.0372	.0350	.0334	.0240	.0239
.75	.0274	.0873	.0825	.0746	.0713	.0500	.0499
1.00	.0555	.1375	.1278	.1120	.1074		

Appendix D

Listing of Computer Programs

In this appendix, a complete listing of the computer programs used in the calculations is given. The calculations were performed on an IBM 360 Model 65 Computer. The main programs listed are SCATH which generated the AED scattering functions, DIPLN which calculated the absorption coefficient in the dipole length formulation, and DIPVEL which calculated the absorption coefficient in the dipole velocity formulation.

```

C**** SCATH PARAMETERIZED WITH XK2
C**** MAIN PROGRAM FOR ELECTRON-HYDROGEN SCATTERING
      IMPLICIT REAL*8(A-H,O-Z),INTEGER*2(I-M)
      INTEGER*2 POL
      DIMENSION DX(51),VP(300),V(300),P(300),U(300),W(300),G(300),VC(300)
      COMMON R(300),XK,D1,D2,D3,ISPIN,L,M1,M2,M3/BLOCK2/ANDRM
C**** D1,D2,D3 ARE THE STEP SIZES WITH M1,M2,M3 THE LAST POINT OF EACH
C      INTERVAL
C      POL 0 FOR STATIC-EXCHANGE.
      READ(5,100) D1,D2,D3,M1,M2,M3,POL
      100 FORMAT(3D5.0,4I5)
      PI = 3.141592653589793
C**** V0-V4 ARE SERIES EXPANSION COEFFICIENTS FOR POLARIZATION POTENTIAL
      V0 = 0.00
      V1 = 0.00
      V2 = -400/300
      V3 = 9600/3500
      V4 = -4100/1500
C**** ARRAYS STORED ON TAPE AT CONST. INTERVAL
C      A IS DUMMY VARIABLE USED TO READ FOR DESIRED STEP SIZE.
C      R IS RADIUS, V IS TOTAL POTENTIAL, & P IS UNPERTURBED HYDROGEN
C      ORBITAL.
      READ(11) (R(I),I=1,11),(A,A,A,A,R(I),I=12,51),(A,A,A,A,A,A,A,A,A,R
      1(I),I=52,200)
      READ(11) (V(I),I=1,11),(A,A,A,A,V(I),I=12,51),(A,A,A,A,A,A,A,A,A,V
      1(I),I=52,200)
      READ(11) (P(I),I=1,11),(A,A,A,A,P(I),I=12,51),(A,A,A,A,A,A,A,A,A,P
      1(I),I=52,200)
      R1 = R(M3-2)
      R2 = R(M3)
      IF(POL.NE.0) GO TO 1000
      DO 4 N=1,M3
      4 V(N) = V(N)-VP(N)
      V2 = 0.00
      V3 = 0.00
      V4 = 0.00
      1000 CALL SKIP(11,2,0)
C**** MPRINT NON-ZERO TO PRINT WAVEFUNCTIONS.
C      MTAPE NON-ZERO TO WRITE THE TAPE.
      1 READ(5,101) ISPIN,MPRINT,MTAPE,LASTS,KMAX
      101 FORMAT(5I5)
      PM = 1-2*ISPIN
      NK = 0
      2 NK = NK+1
      XK2 = NK*10-2
      XK = DSORT(XK2)
      DO 90 L1=1,3
      L = L1-1
C**** DX ARRAY USED TO RETURN STARTING VALUES FOR NUMEROV DIFF. EQ.
C      SOLUTION.
      CALL STARTV0,V1,V2,V3,V4,0.,DX1
      FL1 = L*L1
      DO 5 N=3,M3
      VP(N) = FL1/(R(N)*R(N))+V(N)-XK2
      5 G(N) = 0.00
      CALL NONITVP,G,P,DX,U1
C**** DX ARRAY ALSO USED TO RETURN INFINITE INTEGRALS AND VALUES FOR
C      PHASE SHIFT CALCULATION.
      U1 = DX(41)

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      U2 = DX(5)
      EIU = DX(1)
      EIU = DX(2)
      CALL START(V0,V1,V2,V3,V4,1.,DX)
      DO 6 N=2,M3
6      G(N) = -(R(N)**L)*P(N)
      CALL NMNT(VP,G,P,DX,W)
      W1 = DX(4)
      W2 = DX(5)
      EIW = DX(1)
      EIW = DX(2)
C**** THE TWO SOLUTIONS ARE JOINED NOW
      E = -(1+KK2)
      IF(L.EQ.0) GO TO 8
      C = -PM*EIU/(1+PM*EIW)
      GO TO 9
      8 C = -PM*(E*FIU/2+EIU)/(1+PM*(E*FIW/2+EIW))
      9 DO 10 N=1,M3
10     U(N) = U(N)+C*W(N)
      U1 = U1+C*W1
      U2 = U2+C*W2
      ETA = PHASE(R1,R2,U1,U2)
      IF(U(2).GE.0D0) GO TO 7
      ANORM = -ANORM
      IF(ETA) 15,7,16
15     ETA = ETA+PI
      GO TO 7
16     ETA = ETA-PI
      7 DO 50 N=1,M3
50     U(N) = ANORM*U(N)
      IF(MTAPE.EQ.0) GO TO 11
      WRITE(11) ISPIN,L,XX2,ETA,(U(I),I=1,M3)
11     WRITE(6,200) ISPIN,L,XX2,ETA,ANORM
200    FORMAT(1H0,'ISPIN = ',I1,5X,'L = ',I1,5X,'XX2 = ',OPF4.2,5X,'ETA = ',
1      ' ',1P014.7,5X,'ANORM = ',1P014.7)
      IF(MPRINT.EQ.0) GO TO 90
      WRITE(6,201)
201    FORMAT(1H0,4(2X,'R',14X,'U',13X),/)
      WRITE(6,202) (R(N),U(N),N=1,M3)
202    FORMAT(14(OPF6.2,5X,1P015,8,5X))
      90 CONTINUE
C**** LOOP FOR ANGULAR MOMENTUM NOW ENDFD
      IF(NK.LT.KMAX) GO TO 2
      IF(LASTS.EQ.0) GO TO 1
      IF(MTAPE.NE.0) END FILE 11
      REWIND 11
C**** TEST FIRST TAPE RECORD.
      CALL SKIP(11,2,0)
      READ(11) ISPIN,L,XX2,ETA,(U(N),N=1,200)
      WRITE(6,299) XX2
      REWIND 11
299    FORMAT(1H0,'XX2 AS READ FROM TAPE = ',OPF4.2)
      STOP
      END
SUBROUTINE SKIP(ITAPE,IFILE,IREC)
C**** ITAPE IS LOGICAL UNIT NO. OF DESIRED TAPE UNIT.
C      IFILE IS NO. OF FILES SKIPPED.
C      IREC IS NO. OF RECORDS SKIPPED WITHIN FILE TO BE READ.
      CALL ERRSET(1217,256,-1,1,1,1)
      I = 0

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      IF(IFILE.EQ.0) GO TO 1
2    READ(1TAPE,END=3)
      GO TO 2
3    I = I+1
      IF(I.LT.IFILE) GO TO 2
1    IF(IREC.EQ.0) RETURN
      DO 10 I1=1,IREC
10   READ(1TAPE)
      RETURN
      END
      SUBROUTINE START(V0,V1,V2,V3,V4,A1,DX)
      IMPLICIT REAL*8(A-H,O-Z),INTEGER*2(I-N)
      DIMENSION DX(5),A(9)
      REAL*4 A1
C**** A1 IS A PARAMETER (0. OR 1.) WHICH DISTINGUISHES THE TWO SOLUTIONS
C**** DX IS A 5-DIMENSIONAL ARRAY WHICH RETURNS X,DDX,X2 STARTERS
      COMMON R(300),XK,D1,D2,D3,ISPIN,L,M1,M2,M3
      PM = 1-2*ISPIN
      L1 = L+1
      XK2 = XK*XK
      F1 = -2.*XK2-V0
      F2 = V2-1.333333333333333D0-PM*4D-1
      F3 = V2-1.333333333333333D0-PM*2.857142857142857D-1
      GO TO (1,2,3), L1
1    CONTINUE
      A(1) = 1D0
      A(2) = -1D0
      A(3) = (2D0-F1-2D0*A1)/6D0
      A(4) = (-2D0*A(3)+F1+2D0*A1+V1)/12D0
      A(5) = (-1.333333333333333D0+V2-PM*1.333333333333333D0-V1-F1*A(3)-
12D0*A(4)-1D0*A1)/2D1
      A(6) = ((1.+PM)*2.666666666666667D0+A1*3.333333333333333D0-1+V3-V2+
1V1*A(3)-F1*A(4)-2D0*A(5))/3D1
      A(7) = (-2.133333333333333D0-PM*2.6D0-8.333333333333333D0-2*A1+V4-V
13+F2*A(3)+V1*A(4)-F1*A(5)-2D0*A(6))/42D0
      DX(4) = -2D0
      GO TO 20
2    CONTINUE
      A(2) = 1D0
      A(3) = -5D-1
      A(4) = (-F1+1D0-2D0*A1)/101
      A(5) = (-1D0-5D-1*V0+5D-1*XK2+V1+2D0*A1-2D0*A(4))/18D0
      A(6) = (-1.333333333333333D0-PM*8D-1+V2-5D-1*V1-1D0*A1-F1*A(4)-2D0
1*A(5))/28D0
      A(7) = (2D0+PM*1.466666666666667D0+0.333333333333333D0*A1+V3-5D-1
1*V2+V1*A(4)-F1*A(5)-2D0*A(6))/4D1
      A(8) = (2.133333333333333D0-PM*1.352380952380952D0-8.333333333333
133D0-2*A1+V4-5D-1*V3+F3*A(4)+V1*A(5)-F1*A(6)-2D0*A(7))/54D0
      DX(4) = 2D0
      GO TO 20
3    CONTINUE
      A(3) = 1D0
      A(4) = -1D0/3D0
      A(5) = (2.666666666666667D0+V0-2D0*A1-XK2)/14D0
      A(6) = (-6.666666666666667D0-1*V0*A(4)-A(4)*XK2+V1+2D0*A1-2D0*A(5))
1/24D0
      A(7) = (-1.333333333333333D0-PM*5.714285714285714D0-1-A1+A(4)*V1+V2
1-F1*A(5)-2D0*A(6))/36D0
      A(8) = (1.777777777777778D0+PM*1.015873015873016D0-A(4)*A1+A(4)*V2
1+V3+V1*A(5)-F1*A(6)-2D0*A(7))/9D1

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      A(9) = (-1.2444444444444444D0-PM*9.253439153439153D-1-0.3333333333
13333D-7*A1+A(4)*V3+V4+(-1.333333333333333D0-PM*2.22222222222222D-
21+V7)*A(5)+V1*A(6)-F1*A(7)-2D0*A(8))/66D0
      GO TO 20
20 CONTINUE
      LL = L1+A
      S = 0D0
      S1 = 0D0
      S2 = 0D0
      D12 = D1/2D0
      D1L = D1**L
      D12L = D12**L
      DO 21 N=1,7
      M = LL-N+1
      S = (S+A(M))*D1
      S1 = (S1+A(M))*D12
      K = M+L
      A(M) = K*(K-1)*A(M)
      S2 = (S2+A(M))*D1
21 CONTINUE
      S = S*D1L
      S1 = S1*D12L
      S2 = S2*D1**L-2)
      DX(2) = S
      DX(3) = S1
      DX(5) = S2
      DX(1) = 0D0
      IF(L.GE.2) DX(4) = 0D0
      RETURN
      END
      SUBROUTINE MNMT(F,G,P,DX,X)
C**** SOLVES FOR. X''+FX+G, WHERE G INCLUDES EXCHANGE INTEGRALS.
      IMPLICIT REAL*8(A-H,O-Z),INTEGER*2(I-N)
      COMMON RI(300),KK,D1,D2,D3,ISPIN,L,M1,M2,M3
      DIMENSION X(300),P(300),F(300),G(300),E(14),DX(5)
      XN1 = DX(1)
      XN0 = DX(2)
      X2N = DX(3)
      DDXN1 = DX(4)
      DDXN0 = DX(5)
      X(1) = XN1
      X(2) = XN0
      PM = 1-2*ISPIN
      F2L = 2*L+1
      7 = 4D0/3D0
      D1L = D1*D1**L-1)
      DL2 = D1**L+2)
C**** E1 ARRAY STORES OVERLAPPING SIMPSON EXCHANGE INTEGRALS.
      E1(1) = 2.*Z*D1L*P(2)*XN0/F2L
      F1(3) = D1**L+1)*E1(1)
      E1(2) = D1L*P(2)*XN0/F2L+Z*2.**L*D1L*2.*DEXP(-D1/2D0)*X2N/F2L
      F1(4) = D1*2*P(2)*XN0/F2L+Z*DL2*2.*DEXP(-D1/2D0)*X2N/(2.**L+1)*F2L
1)
      ORSO = D1*D1/12D0
      DR = D1/3D0
      I = 1
      II = 2
      MI = -1
      NN = MI
      NS = 0

```

```

MM = M1 - INT(D2/D1-.5)
DO 20 N=3,M3
RR = R(N)
RRL = RR*(-L)
RR1 = RR*(L+1)
RR2 = RR*(2*L+1)
IF (N,NF,MM) GO TO 1
XNSAVE = XNO
DOXNIS = DOXNO
IF (N,GT,M1) GO TO 2
MM = M2 - INT(D3/D2-.5)
GO TO 1
2 MM = M3-1
1 GN = G(N)+PM*(RRL*E1(I+2)-RR1*E1(I))*P(N)
C**** NUMEROUS SOLUTION FOLLOWS.
XN = (2D0*XNO-XN1+DRSQ*(1D1*DOXNO+DOXN1+GN))/(1D0-DRSQ*F(N))
XIN1 = XN
IF (N,NE,NN) GO TO 3
D = D2
IF (NN,EQ,M2) D = D3
TT = DR*2.*P(N)*XN*RRL/F2L
TEMP1 = E1(I)+TT
TEMP2 = E1(I+2)+RR2*TT
EIT = D*P(N)*XN*RRL/F2L
E1(I) = TEMP1+EIT
F1(I+2) = TEMP2+RR2*EIT
F1(I) = TEMP1+2D0*EIT/3D0
E1(I+2) = TEMP2+RR2*2D0*EIT/3D0
XNO = XNSAVE
DOXNO = DOXNIS
IF (N,EQ,M2) GO TO 4
DRSQ = D2*D2/12D0
DR = D2/3D0
NS = NN
NN = M2
GO TO 5
4 DRSQ = D3*D3/12D0
DR = D3/3D0
NS = NN
NN = M3+1
GO TO 5
3 EIT = 4D0*DR*P(N)*RRL*XN/F2L
EID = RR2*E1I
E1(I) = F1(I)+EIT
E1(I+2) = E1(I+2)+EID
IF (N,NE,NS+1) GO TO 6
E1(I) = E1(I)-EIT/2D0+D*P(N)*RRL*XN/F2L
E1(I+2) = E1(I+2)-EID/2D0+D*P(N)*RR1*XN/F2L
6 E1(I) = E1(I)+EIT+EID
F1(I+2) = E1(I+2)+EID+EID
5 XN1 = XNO
XNO = XN
DOXN1 = DOXNO
DOXNO = F(N)*XNO+GN
M1 = -M1
I = I+M1
I1 = 3-I
20 CONTINUE
DX(4) = XNSAVE
DX(5) = XN

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```

      DX(1) = F(111)
      DX(2) = F(111+2)
      RETURN
      END
      DOUBLE PRECISION FUNCTION PHASE(R1,R2,V1,V2)
C**** CALCULATES PHASES BY THE TWO PT. TANGENT METHOD.
      IMPLICIT REAL*8(A-H,O-Z),INTEGER*2(I-N)
      COMMON R1(30),AK,D1,D2,D3,ISPIN,L,M1,M2,M3/BLOCK2/ANORM
      IF(L.EQ.0.AND.AK.EQ.0.0D0) GO TO 2
      IF(AK.EQ.0.0D0) GO TO 10
      RK1 = AK*R1
      RK2 = AK*R2
      Y1 = SBESN(RK1,L)*RK1
      Y2 = SBESN(RK2,L)*RK2
      RK1 = SBESJ(RK1,L)*RK1
      RK2 = SBESJ(RK2,L)*RK2
      D = Y1*RK2-RK1*Y2
      Z1 = V2*RK1-RK2*V1
      Z2 = V2*Y1-V1*Y2
      PI = 3.141592653589793
      ANORM = DSQRT(2/(PI*(Z1**2+Z2**2)))*DABS(D)/AK
      IF(D.GT.0.0D0) GO TO 3
      Z1 = -Z1
      Z2 = -Z2
      3 PHASE = DATAN2(Z1,Z2)
      6 RETURN
      2 PHASE = (V1*R2-V2*R1)/(V1-V2)
      ANORM = 1
      RETURN
      10 PHASE = 0
      ANORM = 1
      RETURN
      END
      DOUBLE PRECISION FUNCTION SBESJ(X,L)
C**** REGULAR SPHERICAL BESSEL FUNCTION.
      IMPLICIT REAL*8(A-H,O-Z),INTEGER*2(I-N)
      IF (L.GE.2) GO TO 10
      20 CONTINUE
      XJ1 = DSIN(X)/X
      SBESJ = (XJ1-DCOS(X))/X
      IF (L-1) 1,2,3
      1 SBESJ = XJ1
      2 RETURN
      3 XN = 100
      DO 4 N=2,L
      XN = XN+200
      XJ0 = XJ1
      XJ1 = SBESJ
      4 SBESJ = XN*XJ1/X-XJ0
      RETURN
      10 CONTINUE
      AL = L
      XN = X*X
      A = 50.*XN
      IF (L.GT.10) GO TO 50
      IF (A.GT.6.*AL+21.) GO TO 20
      L21 = 2*L+1
      IF (L.GE.10) GO TO 30
      NF = 1
      DO 11 N=1,L21,2

```

```

11 NF = NF*N
   XF = NF
40 CONTINUE
   A1 = 4.*AL+6.
   A2 = 8.*AL+20.
   SRESJ = (X**L)*(110+XN*(XN/A2-100/A1)/XF
   RETURN
50 CONTINUE
   IF (A.GT.50.*AL+200.) GO TO 20
   L21 = 2*L+1
10 CONTINUE
   XF = 1.
   DO 31 N=1,L21,2
31 XF = XF*N
   GO TO 40
END
DOUBLE PRECISION FUNCTION SBESN(X,L1)
C**** IRREGULAR SPHERICAL BESSEL FUNCTION.
IMPLICIT REAL*8(A-H,O-Z),INTEGER*2(I-NI)
XN1 = -DCOS(X)/X
SBESN = (XN1-DSIN(X))/X
IF (L-1) 1,2,3
1 SBESN = XN1
2 RETURN
3 XN = 100
DO 4 N=2,L
   XN = XN+200
   XN0 = XN1
   XN1 = SBESN
4 SBESN = XN*XN1/X-XN0
RETURN
END
C**** DIPVEL MAIN PROGRAM FOR DIPOLE-VELOCITY CALCULATION
IMPLICIT REAL*8(A-H,O-Z)
INTEGER*2 NOT
REAL*8 KI,KF,INI(3,200),MATRIX(2,4,61),KISQ,KFSQ
DIMENSION FINI(3,200),DIR(4),EX(6),XM(10),EI(3),EF(3),P(200),ABMAT(
1A1),CM1(2,3),CM2(2,3),CM3(3),CM4(3),BARF(6),CRUD(6),OD(3),ID(3)
COMMON RI(200),DUM(200),DUM1(200),DR(3),IN(3)/BLOCK2/DS(3),B(4,200)
1,DR(4,200),S(4,200),INE(3),INS(3)
ABSORB(DKSO,THETA) = (1-DEXP(-DKSO*THETA*31.326322))* (DSORT(THETA)
1)**5*X**4.2154732/DKSO
C**** X REPRESENTS THE INTEGRATION INVOLVED
C**** A ALLIMS READING AT DESIRED STEP SIZE.
READ(1) (R(I),I=1,11),(A,A,A,A,R(I),I=12,51),(A,A,A,A,A,A,A,A,A,R
1(I),I=52,200)
CALL SKIP(11,0,1)
READ(11) (P(I),I=1,11),(A,A,A,A,P(I),I=12,51),(A,A,A,A,A,A,A,A,A,P
1(I),I=52,200)
CALL SKIP(11,1,0)
PI = 3.141592653589793
DO 1 N=1,4
C**** B ARRAYS ARE ATOMIC PARTS OF PERTURBED ORBITAL.
C     S ARRAYS ARE SCATTERED PARTS OF PERTURBED ORBITAL.
C     DB ARRAYS ARE DERIVATIVES OF B ARRAYS.
BIN,1) = 0
1 SIN,1) = 0
DB(2,1) = 2
DB(3,1) = 0
DB(4,1) = 0

```

```

NN 10 N=2,280
RR = R(N)
XX = DEXP(2*RR)
R(1,N) = P(N)*((XX-1)/RR-2*(1+RR))
R(2,N) = -(RR*RR/2+RR)*RR*P(N)
R(3,N) = (1/RR+2*(1+RR))*P(N)
R(4,N) = 1/RR+2)*P(N)
S(1,N) = (3*(RR+1)**2/XX)/(8*DSORT(P)*RR*RR)
S(2,N) = 1/(7*DSORT(P))*RR*RR)
S(3,N) = 3*(1-RR*RR-1/XX*(RR+1)**2)/(8*DSORT(P)*RR*RR)
S(4,N) = RR/(4*DSORT(P))
DR(1,N) = P(N)*((XX+3)/(RR*RR)-2*(XX-1)/RR**3+2*(1+1/RR))
DR(2,N) = P(N)*(-RR*RR+2)/2
DR(3,N) = -P(N)*(2/RR**3+3/(RR*RR)+2*(1+1/RR))
17 DR(4,N) = -P(N)*(2/RR**3+3/(RR*RR)+2/RR)
C**** FOLLOWING I ARRAYS ARE END PTS. OF INTERVALS FOR VARIOUS
C INTEGRATIONS WHILE D ARRAYS ARE CORRESPONDING STEP SIZES.
I(1) = 11
I(2) = 51
I(3) = 276
DI(1) = 10-2
DI(2) = 50-2
DI(3) = 10-1
INE(1) = I(1)
INE(2) = I(2)
INE(3) = 271
DS(1) = 20-2
DS(2) = 10-1
DS(3) = 20-1
INS(1) = 6
INS(2) = 26
INS(3) = 136
DD(1) = 10-2
DD(2) = 10-2
DD(3) = 10-2
ID(1) = 61
ID(2) = 61
ID(3) = 61
C**** CM ARRAYS ARE RESULTS OF ANGULAR INTEGRALS.
DR(1,1) = 400/3
CM1(1,1) = 1/(P(12))
CM1(1,2) = -CM1(1,1)*2
CM1(1,3) = 2*DSORT(P)/3*CM1(1,2)
CM1(2,1) = 100/27
CM1(2,2) = CM1(1,1)
CM1(2,3) = CM1(1,1)*4*DSORT(P)/3
CM2(1,1) = CM1(1,1)
CM2(1,2) = -CM1(1,2)
CM2(1,3) = -CM1(1,3)
CM2(2,1) = CM1(2,1)
CM2(2,2) = CM1(2,2)
CM2(2,3) = CM1(2,3)
CM3(1) = 1/(P(6))
CM3(2) = CM3(1)*4*DSORT(P)/3
CM3(3) = 200/27
CM4(1) = CM3(1)
CM4(2) = -CM3(2)
CM4(3) = CM3(3)
C**** MATRIX IS MATRIX ELEMENT SEPARATED INTO VARIOUS SPIN & TRANSITION
C COMPONENTS.

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      DO 77 I=1,2
      DO 77 J=1,4
      77 MATRIX(I,J,1) = 0
      300 CONTINUE
C**** ABMAT IS TOTAL MATRIX ELEMENT.
      DO 7 N=1,61
      7 ABMAT(N) = 0
C**** NDK*.01 IS ENERGY DIFFERENCE OF INITIAL AND FINAL STATES.
C      IT 1 FOR S-P ONLY, 2 FOR P-D ONLY, 3 FOR ALL TRANSITIONS.
C      ISEP NON-ZERO IF CONTRIBUTION FROM VARIOUS SPINS AND TRANSITIONS
C      ARE TO BE DISPLAYED.
      READ(5,100) NDK,IT,ISEP,NPRINT,LAST
      100 FORMAT(5I5)
      NREC = 3*NDK
      OKSQ = NDK*10-2
      MIN = 1
      MMIN = 1
      MAX = 3
      MMAX = 3
      IF(IT.NE.1) GO TO 3
      MAX = 2
      MMAX = 1
      3 IF(IT.NE.2) GO TO 4
      MIN = 2
      MMIN = 3
      4 ISPIN = 0
      5 PM = 1-2*ISPIN
      FIS = 2*ISPIN+1
      2 NK = 1
C**** POSITION FINAL TAPE FOR PROPER ENERGY DIFFERENCE.
      CALL SKIP(12,0,NREC)
C**** READ WAVEFUNCTIONS,KSQ,PHASES
      9 DO 6 L1=1,3
      6 READ(11) NOT,NOT,KISQ,EI(L1),(INI(L1,J),J=1,280)
      NK = NK+1
      DO 8 L1=1,3
      8 READ(12) NOT,NOT,KFSQ,EF(L1),(FIN(L1,J),J=1,280)
      998 KI = DSQRT(KISQ)
      KF = DSQRT(KFSQ)
C**** CALCULATE DIRECT MATRIX ELEMENT.
      CALL DIRDV(INI,FIN,3,MAX,MIN,DIR)
C**** ADD ASYMPTOTIC CONTRIBUTION.
      CALL DDVCDIR(DIR,EI,EF,KI,KF,24,600,IT)
C**** CALCULATE EXCHANGE MATRIX ELEMENTS.
      CALL EXCHDV(INI,FIN,3,P,IT,EX)
      XM(1) = DIR(1)
      XM(2) = EX(1)
      XM(3) = EX(2)
      XM(4) = DIR(2)
      XM(5) = EX(3)
      XM(6) = EX(4)
      XM(7) = DIR(3)
      XM(8) = EX(5)
      XM(9) = DIR(4)
      XM(10) = EX(6)
C**** CALCULATE ABSOLUTE SQUARE OF MATRIX ELEMENT INCLUDING ANGULAR
C      INTEGRAL CONTRIBUTION.
      IF(IT.EQ.2) GO TO 11
      SUM = 0
      DO 12 I=1,2

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      ON 12 J=1,3
      IF(I.GT.J) GO TO 12
      SGN = 1.
      IF(I.EQ.1.AND.(J.EQ.2.OR.J.EQ.3)) SGN = PM
      SUM = SUM+XM(I)*XM(J)*CM1(I,J)*SGN
12  CONTINUE
      SUM = SUM+XM(3)*XM(3)*CM1(2,1)
      IF(ISEP.EQ.1) GO TO 13
      ABMAT(NK) = ABMAT(NK)+FIS*SUM*K*KF
      GO TO 14
13  MATRIX(ISPIN+1,1,NK) = FIS*SUM*K*KF
14  SUM = 0
      ON 15 I=4,5
      ON 15 J=4,6
      IF(I.GT.J) GO TO 15
      SGN = 1.
      IF(I.EQ.4.AND.(J.EQ.5.OR.J.EQ.6)) SGN = PM
      K = I-3
      KK = J-3
      SUM = SUM+XM(I)*XM(J)*CM2(K,KK)*SGN
15  CONTINUE
      SUM = SUM+XM(6)*XM(6)*CM2(2,1)
      IF(ISEP.EQ.1) GO TO 16
      ABMAT(NK) = ABMAT(NK)+FIS*SUM*K*KF
      GO TO 17
16  MATRIX(ISPIN+1,2,NK) = FIS*SUM*K*KF
17  IF(I.EQ.1) GO TO 18
18  SUM = 0
      ON 19 J=7,9
      K = J-6
      SGN = 1.
      IF(J.NE.7) SGN = PM
19  SUM = SUM+XM(7)*XM(J)*CM3(K)*SGN
      SUM = SUM+XM(8)*XM(8)*CM3(3)
      IF(ISEP.EQ.1) GO TO 21
      ABMAT(NK) = ABMAT(NK)+FIS*SUM*K*KF
      GO TO 22
21  MATRIX(ISPIN+1,3,NK) = FIS*SUM*K*KF
22  SUM = 0
      ON 99 J=9,10
      K = J-8
      SGN = 1
      IF(J.NE.9) SGN = PM
99  SUM = SUM+XM(9)*XM(J)*CM4(K)*SGN
      SUM = SUM+XM(10)*XM(10)*CM4(3)
      IF(ISEP.EQ.1) GO TO 23
      ABMAT(NK) = ABMAT(NK)+FIS*SUM*K*KF
      GO TO 18
23  MATRIX(ISPIN+1,4,NK) = FIS*SUM*K*KF
18  IF(NK.GE.61) GO TO 24
      GO TO 9
24  IF(ISPIN.EQ.1) GO TO 25
      ISPIN = ISPIN+1
      CALL SKIP(11,0,120)
      NNREC = 120-NNREC
      CALL SKIP(12,0,NNREC)
      GO TO 9
25  GO TO (26,27,28),NPRINT
27  WRITE(6,200)
200  FORMAT(1H1)

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      WRITE(6,201) DKSQ,(ABMAT(1),ABMAT(1+31),I=1,31)
201  FORMAT(61X,7MDKSO = ,F3.2,/,/,63X,5HABMAT,/,/(1P20D0.8))
      GO TO 26
20  DO 20 I=1,2
      WRITE(6,200)
      ISPIN = I-1
      WRITE(6,202) DKSQ,ISPIN
202  FORMAT (55X,7MDKSO = ,F3.2,3X,8HISPIN = ,I1,/,/,11X,3HS-P,17X,3HP-S
1,17X,3HP-D,17X,3HD-P)
      WRITE(6,203) (MATRIX(I,1,J),MATRIX(I,2,J),MATRIX(I,3,J),MATRIX(I,4
1,J),J=1,61)
203  FORMAT(1P40D0.8)
20  CONTINUE
26  IF(1SEP.EQ.1) GO TO 31
      WRITE(6,200)
      WRITE(6,204) DKSQ
204  FORMAT (61X,7MDKSO = ,OPF3.2,/,/,1X,5HTHETA,6X,14HAB COEFFICIENT)
C**** CALCULATE ABSORPTION COEFFICIENT.
      DO 30 N=5,20
      THETA = N*10-1
      DO 98 K=1,61
      A = K-1
      KISQ = A*10-2
      DUM(K) = DEXP(-KISQ*THETA*31.326322)
      X = SF(ABMAT,DUM,DD,10)
      COEFF = ABSORB(DKSO,THETA)
      WRITE(6,205) THETA,COEFF
205  FORMAT (3X,OPF3.1,1PD20.8)
      30  CONTINUE
      GO TO 29
31  WRITE(6,200)
      DO 40 I=1,2
      DO 41 K=1,61
      DUM1(K) = MATRIX(I,1,K)
      ABMAT(K) = MATRIX(I,2,K)
      BARF(K) = MATRIX(I,3,K)
      CRUD(K) = MATRIX(I,4,K)
      ISPIN = I-1
      WRITE(6,206) DKSQ,ISPIN
206  FORMAT (1H0,55X,7MDKSO = ,OPF3.2,3X,8HISPIN = ,I1,/,/,1X,5HTHETA,11
1X,3HS-P,17X,3HP-S,17X,3HP-D,17X,3HD-P)
      DO 40 N=5,20
      THETA = N*10-1
      DO 42 K=1,61
      A = K-1
      KISQ = A*10-2
      DUM(K) = DEXP(-KISQ*THETA*31.326322)
      X = SF(DUM,DUM1,DD,10)
      COEFF1 = ABSORB(DKSO,THETA)
      X = SF(DUM,ABMAT,DD,10)
      COEFF2 = ABSORB(DKSO,THETA)
      X = SF(DUM,BARF,DD,10)
      COEFF3 = ABSORB(DKSO,THETA)
      X = SF(DUM,CRUD,DD,10)
      COEFF4 = ABSORB(DKSO,THETA)
      WRITE(6,207) THETA,COEFF1,COEFF2,COEFF3,COEFF4
207  FORMAT(3X,OPF3.1,1P40D0.8)
      40  CONTINUE
29  REWIND 11
      REWIND 12

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      IF (LAST.NE.0) STOP
      CALL SKIP(11,1,0)
      GO TO 300
      END
      SUBROUTINE DIRDV(INI,FIN,MAX,LMAX,LMIN,DIR)
C**** MAX IS VARIABLE DIMENSION.
C      DIR RETURNS MATRIX ELEMENTS FOR VARIOUS TRANSITIONS.
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON R(280),DUM(280),DUM1(280),DR(3),IN(3)
      DIMENSION FIN(MAX,280),DIR(4),DU(280)
      REAL*8 INT(MAX,280)
C**** IF ONLY S-P AND P-S IS DESIRED LMAX=2. OTHERWISE LMAX=3.
C**** LMIN=2 FOR CASE OF P-D AND D-P ONLY.
      M3 = IN(3)
      DO 10 L1=LMIN,LMAX
      DO 2 J=1,M3
      2 DUM(J) = INT(L1,J)
      CALL DERIV(DUM,IN,DR,3,DU)
      IF (L1.EQ.1) GO TO 1
      IF (L1.EQ.LMIN) GO TO 9
      DO 3 J=2,M3
      3 DUM(J) = (L1-1)*INT(L1,J)/R(J)
      DUM(1) = 0
C**** DUM(1) IS NOT ACTUALLY 0, BUT ENTIRE INTEGRAND IS 0 AT ORIGIN.
      DO 4 J=1,M3
      4 DUM1(J) = FIN(L1-1,J)
      DIR(2*L1-2) = SF(DUM1,DU,DR,IN)+SF(DUM1,DUM,DR,IN)
      IF (L1.EQ.LMAX) GO TO 10
      9 DO 6 J=2,M3
      6 DUM(J) = -L1*INT(L1,J)/R(J)
      DUM(1) = 0
      GO TO 5
      1 CONTINUE
      DO 7 J=2,M3
      7 DUM(J) = -INT(L1,J)/R(J)
      DUM(1) = 0
      5 DO 8 J=1,M3
      8 DUM1(J) = FIN(L1+1,J)
      DIR(2*L1-1) = SF(DUM1,DU,DR,IN)+SF(DUM1,DUM,DR,IN)
      10 CONTINUE
      RETURN
      END
      SUBROUTINE DERIV(Y,IN,DR,LAST,DY)
C**** Y IS FUNCTION TO BE DIFFERENTIATED.
C      IN IS ARRAY OF INTERVAL END POINTS.
C      DR IS ARRAY OF INTERVAL STEP SIZES.
C      LAST IS NUMBER OF INTERVALS.
C      DY IS DERIVATIVE ARRAY.
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Y(300),DY(300),X(5),IN(3),DR(3)
      MAX = IN(LAST)
      I = 1
      OI = DR(1)*12
      ORI = DR(1)
      IN1 = IN(1)
      DY(1) = (-25*Y(1)+48*Y(2)-36*Y(3)+16*Y(4)-3*Y(5))/OI
      DY(2) = (-3*Y(1)-10*Y(2)+18*Y(3)-6*Y(4)+Y(5))/OI
      X(2) = Y(1)
      X(3) = Y(2)
      X(4) = Y(3)

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      X(5) = Y(4)
      DO 3 N=3,MAX
      DV = (Y(N)-Y(N-1))/DR1
      IF (N+1-INI) 90,30,90
40 CONTINUE
      DO 2 I=1,4
      2 X(11) = X(11+1)
70 X(5) = Y(N+2)
      DY(N) = ((X(11)-X(5))+8*(X(4)-X(2)))/D1
      GO TO 1
80 DY(N) = (3*X(11)-16*X(2)+36*X(3)-48*X(4)+25*X(5))/D1
      IF (N.EQ.MAX) GO TO 3
      I = I+1
      DR1 = DR(I)
      IN1 = IN(I)
      D1 = DR(I)*12
      MM = N-IDINT(DR(I)/DR(I-1)+.5)
      X(2) = Y(MM)
      X(3) = Y(N)
      X(4) = Y(N+1)
      X(5) = Y(N+2)
      GO TO 1
30 DY(N) = (-X(11)+6*X(2)-19*X(3)+10*X(4)+3*X(5))/D1
      1 CONTINUE
      IF(DABS((DY(N)-DV)/DV).LT.1D0) GO TO 3
      DV = (DV+(Y(N+1)-Y(N))/DR(I)/2
      IF(DABS((DY(N)-DV)/DV).LT.1D0) GO TO 3
      DY(N) = DV
      3 CONTINUE
      RETURN
      END
      DOUBLE PRECISION FUNCTION SF(X,Y,DX,INI)
C**** CALCULATES INTEGRAL OF X*Y.
C      DX AND IN CONTAIN STEP SIZES AND END POINTS.
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION X(300),Y(300),F(6),DX(3),IN(3)
      DS = 0D0
      DR= DX(1)*1.736111111111111D-2
      F(6) = 0D0
      MAX3 = IN(3)
      DO 1 N=6,MAX3,5
      IF(N.EQ.IN(1)+5) DR = DX(2)*1.736111111111111D-2
      IF(N.EQ.IN(2)+5) DR = DX(3)*1.736111111111111D-2
      DO 2 K=1,5
      M = N-K+1
      2 F(K) = X(M)*Y(M)
      S = DR*(19*(F(1)+F(6))+75*(F(2)+F(5))+50*(F(3)+F(4)))
      DS = S+DS
      1 F(6) = F(1)
      SF = DS
      RETURN
      END
      SUBROUTINE DDVCON(X,EI,EF,KI,KF,RO,IT)
C**** X IS MATRIX ELEMENT ARRAY TO BE CORRECTED.
C      EI AND EF ARE INITIAL AND FINAL PHASES.
C      KI AND KF INITIAL AND FINAL WAVE NUMBERS.
C      RO IS MAX VALUE IN NUMERICAL INTEGRATION.
      IMPLICIT REAL*8(A-H,O-Z)
C**** CORRECTION OF DIRECT DIPOLE-VELOCITY MATRIX ELEMENTS FOR
C      ASYMPTOTIC BEHAVIOR

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C**** R0 IS MAX R-VALUE IN NUMERICAL INTEGRATION
REAL*8 K1,KF,KFSQ,KISQ
DIMENSION X(4),F(3),EF(3)
DK = KF-K1
SK = KF+K1
KFSQ = KF*KF
KISQ = K1*K1
DKSQ = KFSQ-KISQ
C = 100/13.141592653589793*DKSQ*KF
IF(ITY.FQ.2) GO TO 1
X(1) = X(1)-C*(DKSQ*(DCOS(EF(2)-EI(1)+DK*R0)-DCOS(EF(2)+EI(1)+SK*R0)))/(K1*KF*R0)-DK*DSIN(EF(2)+EI(1)+SK*R0)-SK*DSIN(EF(2)-EI(1)+DK*R0))
X(2) = X(2)+C*(DK*DSIN(EF(1)+EI(2)+SK*R0)-SK*DSIN(EF(1)-EI(2)+DK*R0))
IF(ITY.EQ.1) GO TO 2
1 A = 1/(K1*KF*R0*R0)
B = 3*(KFSQ*KF-KISQ*K1)/(KFSQ*KISQ*R0*R0)
D = 3*(DKSQ*R0*A
X(3) = X(3)- C*(DKSQ*((1/SK-3*SK*A/(K1*KF))*DSIN(EF(3)+EI(2)+SK*R0)-(1/(DK-3*DK*A/(K1*KF))*DSIN(EF(3)-EI(2)+DK*R0)+3*R0*A*(1-A)*DCOS(EF(3)+EI(2)+SK*R0)+3*R0*A*(1+A)*DCOS(EF(3)-EI(2)+DK*R0))
X(4) = X(4)+ C*(DKSQ*(DCOS(EF(2)-EI(3)+DK*R0)-DCOS(EF(2)+EI(3)+SK*R0)))/(K1*KF*R0)-DK*DSIN(EF(2)+EI(3)+SK*R0)-SK*DSIN(EF(2)-EI(3)+DK*R0))
2 RETURN
END
SUBROUTINE EXCHOV(INI,FIN,MAX,P,IT,EX)
C**** MAX IS VARIABLE DIMENSION.
C P IS UNPERTURBED HYDROGEN ORBITAL.
C EX RETURNS EXCHANGE MATRIX ELEMENTS.
IMPLICIT REAL*8(A-H,O-Z)
C**** IT (1,2,3) FOR S-P ONLY, P-D ONLY, OR BOTH, RESPECTIVELY
REAL*8 IN(MAX,280)
DIMENSION FIN(MAX,280),FX(6),X(280),Y(280),Z(280),P(280),AI(136),
1AIR(136),AID(136),M(280)
COMMON R(280),DUM(280),DUM1(280),DR(3),IN(3)/BLOCK2/DS(3),B(4,280)
1,OB(4,280),SI(4,280),INE(3),INS(3)
IF (IT,FQ.2) GO TO 1
DO 50 LI=1,2
J= 3-LI
DO 2 N=1,280
Z(N) = R(N)*P(N)
Y(N) = IN(LI,N)
2 X(N) = FIN(J,N)
EX(2*LI-1) = SF(Z,Y,DR,IN)*SF(Z,X,DR,IN)
IF (LI,FQ.1) GO TO 3
DO 4 N=1,280
Y(N) = FIN(J,N)
4 X(N) = IN(LI,N)
3 CONTINUE
C**** CALCULATION OF DOUBLE INTEGRALS
CALL RAINT(X,0,AI)
CALL RAINT(Y,1,AID)
DO 5 N=2,280
5 W(N) = Y(N)/R(N)
W(1) = 0
CALL RAINT(W,0,AIR)
DO 6 N=1,136
6 = 2*N-1

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      A1(N) = -A1(N)*P(M)*Y(M)+YAIR(N)+A1D(N))*X(M)*P(M)
      AIR(N) = R(N)
      EX(2*L1) = SF(A1,AIR,DS,INS)
50  CONTINUE
      IF (IT.FO.1) RETURN
      1 CONTINUE
      DO 90 L1=2,3
      J = 5-L1
      IF (L1.FO.3) GO TO 7
      DO 8 N=1,280
      X(N) = INT(L1,N)
      R Y(N) = FIN(J,N)
      GO TO 9
      7. CONTINUE
      DO 11 N=1,280
      X(N) = FIN(J,N)
11  Y(N) = INT(L1,N)
      9 CONTINUE
      CALL RINT(X,0,A1)
      CALL RINT(Y,1,A1D)
      DO 12 N=2,280
12  W(N) = -2*Y(N)/R(N)
      W(1) = 0
      CALL PAINT(W,0,AIR)
      DO 14 N=1,136
      M = 2*N-1
      A1(N) = -A1(N)*P(M)*Y(M)+(AIR(N)+A1D(N))*X(M)*P(M)
14  AIR(N) = R(N)
      EX(L1+3) = SF(A1,AIR,DS,INS)
90  CONTINUE
      RETURN
      END
      SUBROUTINE RINT(X,NOW,Z)
C**** CALCULATES INTEGRAL OVER ATOMIC COORDINATES.
C      X IS ARRAY FOR FUNCTION OF ATOMIC COORDINATE WHICH MULTIPLIES
C      PERTURBED ORBITAL.
C      Z RETURNS FUNCTION OF SCATTERING COORDINATE.
      IMPLICIT REAL*8(A-H,O-Z)
C**** X IS MULTIPLIER ARRAY FOR BOUND FUNCTION
C**** NOW 0,1 FOR R,DR, RESPECTIVELY
      DIMENSION X(280),Z(136)
      COMMON R(280),DUM(280),DUM1(280),DR(3),IN(3)/BLOCK2/DS(3),R(4,280)
      I,DR(4,280),S(4,280),INE(3),INS(3)
      DO 6 N=1,136
      Z(N) = 0
      DO 50 J=1,3,2
      IF(NOW.EQ.1) GO TO 1
      DO 2 N=1,280
      DUM(N) = X(N)*R(J,N)
      2 DUM1(N) = X(N)*R(J+1,N)
      GO TO 3
      1 DO 4 N=1,280
      DUM(N) = X(N)*DR(J,N)
      4 DUM1(N) = X(N)*DR(J+1,N)
      3 CONTINUE
      IF (J.EQ.3) GO TO 7
C**** SIMPSON INTEGRATION FROM 0-R
      D = DR(1)/300
      SUM = 0
      SUM1 = 0

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DO 10 N=2,136
M = 2*N-1
IF(M.EQ.1)NF(1)+2) D = DR(2)/3
IF(M.EQ.1)NE(2)+2) D = DR(3)/3
SUM = SUM+D*(DUM(M)+DUM(M-2)+4*DUM(M-1))
SUM1 = SUM1+D*(DUM1(M)+DUM1(M-2)+4*DUM1(M-1))
10 Z(N) = SUM*S(J,M)+SUM1*S(J+1,M)
GO TO 50
C**** SIMPSON INTEGRATION FROM R-INFINITY
7 SUM = 0
SUM1 = 0
DO 20 N=2,136
M = 273-2*N
IF(M.EQ.1)NE(2)-2) D = DR(2)/3
IF(M.EQ.1)NE(1)-2) D = DR(1)/3
SUM = SUM+D*(DUM(M)+DUM(M+2)+4*DUM(M+1))
SUM1 = SUM1+D*(DUM1(M)+DUM1(M+2)+4*DUM1(M+1))
MM = 137-M
20 Z(MM) = Z(MM)+S(J,M)*SUM+S(J+1,M)*SUM1
50 CONTINUE
RETURN
END
C**** DIPLN. MAIN PROGRAM FOR DIPOLE-LENGTH CALCULATION
IMPLICIT REAL*8(A-M,N-Z)
INTEGER*2 NOT
REAL*8 KI,KF,INI(3,280),MATRIX(2,4,61),KISO,KFSO
DIMENSION FIN(3,280),DIR(8),EX(6),XM(14),EI(3),EF(3),P(280),ABMAT(
161),CM1(10),CM2(6),BARF(61),CRUD(61),OD(3),ID(3)
COMMON R(280),DUM(280),DUM1(280),DR(3),IN(3)/BLOCK2/OS(3),B(4,280)
1,DB(4,280),S(4,280),INE(3),INS(3)
ABSORB(DKSO,THETA) = (1-DEXP(-DKSO*THETA*31.326322))*((DSQRT(THETA)
1)**5*X**4.2154732*DKSO
C**** X REPRESENTS THE INTEGRATION INVOLVED
C**** A ALLOWS READING AT DESIRED STEP SIZE.
READ(11) (R(I),I=1,11),(A,A,A,A,R(I),I=12,51),(A,A,A,A,A,A,A,A,A,R
1(I),I=52,280)
CALL SKIP(11,0,1)
READ(11) (P(I),I=1,11),(A,A,A,A,P(I),I=12,51),(A,A,A,A,A,A,A,A,A,P
1(I),I=52,280)
CALL SKIP(11,1,0)
PI = 3.141592653589793
DO 1 N=1,4
C**** B ARRAYS ARE ATOMIC PARTS OF PERTURBED ORBITAL.
C S ARRAYS ARE SCATTERED PARTS OF PERTURBED ORBITAL.
C DB ARRAYS ARE DERIVATIVES OF B ARRAYS.
B(N,1) = 0
1 S(N,1) = 0
DB(1,1) = 800/3
DR(2,1) = 2
DR(3,1) = 0
DR(4,1) = 0
DO 10 N=2,280
RR = R(N)
XX = DEXP(2*RR)
B(1,N) = P(N)*((XX-1)/RR-2*(1+RR))
B(2,N) = -(RR*RR/2+RR)*RR*P(N)
B(3,N) = (1/RR+2*(1+RR))*P(N)
B(4,N) = (1/RR+2)*P(N)
S(1,N) = (3*(RR+1)**2/XX)/(8*DSQRT(P)*RR*RR)
S(2,N) = 1/(2*DSQRT(P)*RR*RR)

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      S(3,N) = 3*(1-RR*RR-1/XX*(RR+1)**2)/(8*DSQRT(P1)*RR*RR)
      S(4,N) = RR/(4*DSQRT(P1))
      DB(1,N) = P(N)*((XX+3)/(RR*RR)-2*(XX-1)/RR**3+2*(1+1/RR))
      DB(2,N) = P(N)*(-RR*RR+2)/2
      DB(3,N) = -P(N)*(2/RR**3+3/(RR*RR)+2*(1+1/RR))
10   DB(4,N) = -P(N)*(2/RR**3+3/(RR*RR)+2/RR)
C**** FOLLOWING 1 ARRAYS ARE END PTS. OF INTERVALS FOR VARIOUS
C      INTEGRATIONS WHILE D ARRAYS ARE CORRESPONDING STEP SIZES.
      IN(1) = 11
      IN(2) = 51
      IN(3) = 276
      DR(1) = 1D-2
      DR(2) = 5D-2
      DR(3) = 1D-1
      INE(1) = IN(1)
      INE(2) = IN(2)
      INE(3) = 271
      DS(1) = 2D-2
      DS(2) = 1D-1
      DS(3) = 2D-1
      INS(1) = 6
      INS(2) = 26
      INS(3) = 136
      DD(1) = 1D-2
      DD(2) = 1D-2
      DD(3) = 1D-2
      ID(1) = 61
      ID(2) = 61
      ID(3) = 61
C**** CM ARRAYS ARE RESULTS OF ANGULAR INTEGRALS.
      CM1(1) = 1/(P1*12)
      CM1(2) = 8*CM1(1)*DSQRT(P1)/3
      CM1(3) = 2*CM1(1)
      CM1(4) = 2*DSQRT(P1)*CM1(1)/3
      CM1(5) = 16*P1*CM1(1)/9
      CM1(6) = CM1(2)
      CM1(7) = CM1(5)
      CM1(8) = CM1(1)
      CM1(9) = CM1(4)
      CM1(10) = CM1(5)/4
      CM2(1) = 1/(P1*6)
      CM2(2) = 8*DSQRT(P1)*CM2(1)/3
      CM2(3) = CM2(2)/2
      CM2(4) = 8D0/27
      CM2(5) = CM2(4)
      CM2(6) = CM2(5)/4
C**** MATRIX IS MATRIX ELEMENT SEPARATED INTO VARIOUS SPIN & TRANSITION
C      COMPONENTS.
      DO 77 I=1,2
      DO 77 J=1,4
      77 MATRIX(I,J,1) = 0
      300 CONTINUE
C**** ABMAT IS TOTAL MATRIX ELEMENT.
      DO 7 N=1,61
      7 ABMAT(N) = 0
C**** NOK*.01 IS ENERGY DIFFERENCE OF INITIAL AND FINAL STATES.
C      IT 1 FOR S-P ONLY, 2 FOR P-D ONLY, 3 FOR ALL TRANSITIONS.
C      ISEP NON-ZERO IF CONTRIBUTION FROM VARIOUS SPINS AND TRANSITIONS
C      ARE TO BE DISPLAYED.
      READ(5,100) NOK,IT,ISEP,NPRINT,LAST

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100 FORMAT(5I5)
NREC = 3*NDK
DKSQ = NDK*10-2
MIN = 1
MMIN = 1
MAX = 3
MMAX = 3
IF(IT.NE.1) GO TO 3
MAX = 2
MMAX = 1
3 IF(IT.NE.2) GO TO 4
MIN = 2
MMIN = 3
4 ISPIN = 0
5 PM = 1-2*ISPIN
FIS = (2*ISPIN+1)/4.
2 NK = 1
C**** POSITION FINAL TAPE FOR PROPER ENERGY DIFFERENCE.
CALL SKIP(12,0,NREC)
C**** READ WAVEFUNCTIONS,KSQ,PHASES
9 DO 6 L1=1,3
6 READ(11) NOT,NOT,KISQ,EI(L1),(INI(L1,J),J=1,280)
NK = NK+1
DO 8 L1=1,3
8 READ(12) NOT,NOT,KFSQ,EF(L1),(FIN(L1,J),J=1,280)
998 KI = DSORT(KISQ)
KF = DSORT(KFSQ)
C**** CALCULATE DIRECT MATRIX ELEMENT.
CALL DIRDL(INI,FIN,3,MAX,MIN,P,KI,KF,EI,EF,DIR)
C**** CALCULATE EXCHANGE MATRIX ELEMENTS.
CALL EXCHOL(INI,FIN,3,P,IT,EX)
XM(1) = DIR(1)
XM(2) = DIR(5)
XM(3) = EX(1)
XM(4) = EX(2)
XM(5) = DIR(2)
XM(6) = DIR(6)
XM(7) = EX(3)
XM(8) = EX(4)
XM(9) = DIR(3)
XM(10) = DIR(7)
XM(11) = EX(5)
XM(12) = DIR(4)
XM(13) = DIR(8)
XM(14) = EX(6)
C**** CALCULATE ABSOLUTE SQUARE OF MATRIX ELEMENT INCLUDING ANGULAR
C INTEGRAL CONTRIBUTION.
IF(IT.EQ.2) GO TO 11
SUM = 0
NELEM = 0
DO 12 I=1,3
DO 12 J=1,4
IF(I.GT.J) GO TO 12
NELEM = NELEM+1
SGN = 1
IF(I.LE.2.AND.J.GE.3) SGN = PM
SUM = SUM+XM(I)*XM(J)*CM1(NELEM)*SGN
12 CONTINUE
SUM = SUM+XM(4)*XM(4)*CM1(10)
IF(ISEP.EQ.1) GO TO 13

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      ABMAT(NK) = ABMAT(NK)+FIS*SUM*KI*KF
      GO TO 14
13  MATRIX(ISPIN+1,1,NK) = FIS*SUM*KI*KF
14  SUM = 0
      NELEM = 0
      DO 15 I=5,7
      DO 15 J=5,8
      IF(I.GT.J) GO TO 15
      NELEM = NELEM+1
      SGN = 1
      IF(I.LE.6.AND.J.GE.7) SGN = PM
      SUM = SUM+XM(I)*XM(J)*CM1(NELEM)*SGN
15  CONTINUE
      SUM = SUM+XM(8)*XM(9)*CM1(10)
      IF(ISEP.EQ.1) GO TO 16
      ABMAT(NK) = ABMAT(NK)+FIS*SUM*KI*KF
      GO TO 17
16  MATRIX(ISPIN+1,2,NK) = FIS*SUM*KI*KF
17  IF(IY.EQ.1) GO TO 18
18  SUM = 0
      NELEM = 0
      DO 19 I=9,10
      DO 19 J=9,11
      IF(I.GT.J) GO TO 19
      NELEM = NELEM+1
      SGN = 1
      IF(J.EQ.11) SGN = PM
      SUM = SUM+XM(I)*XM(J)*CM2(NELEM)*SGN
19  CONTINUE
      SUM = SUM+XM(11)*XM(11)*CM2(6)
      IF(ISEP.EQ.1) GO TO 21
      ABMAT(NK) = ABMAT(NK)+FIS*SUM*KI*KF
      GO TO 22
21  MATRIX(ISPIN+1,3,NK) = FIS*SUM*KI*KF
22  SUM = 0
      NELEM = 0
      DO 99 I=12,13
      DO 99 J=12,14
      IF(I.GT.J) GO TO 99
      NELEM = NELEM+1
      SGN = 1
      IF(J.EQ.14) SGN = PM
      SUM = SUM+XM(I)*XM(J)*CM2(NELEM)*SGN
99  CONTINUE
      SUM = SUM+XM(14)*XM(14)*CM2(6)
      IF(ISEP.EQ.1) GO TO 23
      ABMAT(NK) = ABMAT(NK)+FIS*SUM*KI*KF
      GO TO 18
23  MATRIX(ISPIN+1,4,NK) = FIS*SUM*KI*KF
18  IF(NK.GE.6) GO TO 24
      GO TO 9
24  IF(ISPIN.EQ.1) GO TO 25
      ISPIN = ISPIN+1
      CALL SKIP(11,0,120)
      NNREC= 120-NREC
      CALL SKIP(12,0,NNREC)
      GO TO 5
25  GO TO (26,27,28),NPRINT
27  WRITE(6,200)
200 FORMAT(1H1)

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      WRITE(6,201) DKSO,(ARMAT(I),ARMAT(I+31),I=1,31)
201  FORMAT(61X,7HDKSO = ,F3.2,/,63X,5HARMAT,/,/(1P2D20.8))
      GO TO 26
28  DO 20 I=1,2
      WRITE(6,200)
      ISPIN = I-1
      WRITE(6,202) DKSO,ISPIN
202  FORMAT (55X,7HDKSO = ,F3.2,3X,8HISPIN = ,I1,/,11X,3HS-P,17X,3HP-S
1,17X,3HP-D,17X,3HD-P)
      WRITE(6,203) (MATRIX(I,1,J),MATRIX(I,2,J),MATRIX(I,3,J),MATRIX(I,4
1,J),J=1,61)
203  FORMAT(1P4D20.8)
20  CONTINUE
26  IF(ISEP.EQ.1) GO TO 31
      WRITE(6,200)
      WRITE(6,204) DKSO
C**** CALCULATE ABSORPTION COEFFICIENT.
204  FORMAT (61X,7HDKSO = ,OPF3.2,/,1X,5HTHETA,6X,14HAB COEFFICIENT)
      DO 30 N=5,20
      THETA = N*10-1
      DO 98 K=1,61
      A = K-1
      KISO = A*10-2
98  DUM(K) = DEXP(-KISO*THETA*31.326322)
      X = SF(ARMAT,DUM,DD,10)
      COEFF = ABSORB(DKSO,THETA)
      WRITE(6,205) THETA,COEFF
205  FORMAT (3X,OPF3.1,1P020.8)
30  CONTINUE
      GO TO 29
31  WRITE(6,200)
      DO 40 I=1,2
      DO 41 K=1,61
      DUM1(K) = MATRIX(I,1,K)
      ARMAT(K) = MATRIX(I,2,K)
      BARF(K) = MATRIX(I,3,K)
41  CRUD(K) = MATRIX(I,4,K)
      ISPIN = I-1
      WRITE(6,206) DKSO,ISPIN
206  FORMAT (1H0,55X,7HDKSO = ,OPF3.2,3X,8HISPIN = ,I1,/,1X,5HTHETA,11
1X,3HS-P,17X,3HP-S,17X,3HP-D,17X,3HD-P)
      DO 40 N=5,20
      THETA = N*10-1
      DO 42 K=1,61
      A = K-1
      KISO = A*10-2
42  DUM(K) = DEXP(-KISO*THETA*31.326322)
      X = SF(DUM,DUM,DD,10)
      COEFF1 = ABSORB(DKSO,THETA)
      X = SF(DUM,ARMAT,DD,10)
      COEFF2 = ABSORB(DKSO,THETA)
      X = SF(DUM,BARF,DD,10)
      COEFF3 = ABSORB(DKSO,THETA)
      X = SF(DUM,CRUD,DD,10)
      COEFF4 = ABSORB(DKSO,THETA)
      WRITE(6,207) THETA,COEFF1,COEFF2,COEFF3,COEFF4
207  FORMAT(3X,OPF3.1,1P4D20.8)
40  CONTINUE
29  REWIND 11
      REWIND 12

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      IF (LAST.NE.0) STOP
      CALL SKIP(11,1,0)
      GO TO 300
      END
      SUBROUTINE DIRDL(INI,FIN,MAX,LMAX,LMIN,P,KI,KF,EI,EF,DIR)
C**** MAX IS VARIABLE DIMENSION.
C      DIR RETURNS MATRIX ELEMENTS FOR VARIOUS TRANSITIONS.
C**** X IS MATRIX ELEMENT ARRAY TO BE CORRECTED.
C      P IS UNPERTURBED HYDROGEN ORBITAL.
      IMPLICIT REAL*8(A-H,O-Z)
C**** CALCULATION OF DIRECT TERMS IN LENGTH FORMULATION
      COMMON R(280),DIM(280),DIM1(280),DR(3),IN(3)/BLOCK2/DS(3),B(4,280)
      1,DR(4,280),S(4,280),INE(3),IJS(3)
      DIMENSION FIN(MAX,280),DIR(8),TEMP(4),X(280),Y(280),P(280),Z(280),
      1A(136),Q(136),EI(3),EF(3)
      REAL*8 INI(MAX,280),KI,KF
C**** IF ONLY S-P AND P-S IS DESIRED LMAX=2. OTHERWISE LMAX=3.
C**** LMIN=2 FOR CASE OF P-D AND D-P ONLY.
      M3 = IN(3)
      DO 10 L1=LMIN,LMAX
      DO 1 N=1,M3
      1 X(N) = R(N)*INI(L1,N)
      IF(L1.EQ.LMIN) GO TO 3
      DO 4 N=1,M3
      4 Y(N) = FIN(L1-1,N)
      TEMP(2*L1-2) = SF(X,Y,DR,IN)
      IF(L1.EQ.LMAX) GO TO 10
      DO 5 N=1,M3
      5 Y(N) = FIN(L1+1,N)
      TEMP(2*L1-1) = SF(X,Y,DR,IN)
      10 CONTINUE
      CALL DOLCOR(TEMP,EI,EF,KI,KF,2.4601,3)
      DO 2 N=1,4
      2 DIR(N) = TEMP(N)
C**** CALCULATION OF DOUBLE INTEGRAL CONTRIBUTIONS
      DO 9 N=1,280
      9 Z(N) = R(N)*P(N)*R(N)
      CALL RAINT(Z,0,A)
      DO 20 L1=LMIN,LMAX
      DO 6 N=1,136
      M = 2*N-1
      6 X(N) = INI(L1,M)
      IF(L1.EQ.LMIN) GO TO 7
      DO 8 N=1,136
      M = 2*N-1
      Y(N) = FIN(L1-1,M)
      8 Q(N) = A(N)*X(N)
      DIR(2*L1+2) = SF(Q,Y,DS,INS)
      IF(L1.EQ.LMAX) GO TO 20
      DO 12 N=1,136
      M = 2*N-1
      Y(N) = FIN(L1+1,M)
      12 Q(N) = A(N)*X(N)
      DIR(2*L1+3) = SF(Q,Y,DS,INS)
      20 CONTINUE
      RETURN
      END
      SUBROUTINE DOLCOR(X,EI,EF,KI,KF,RO,IT)
C      EI AND EF ARE INITIAL AND FINAL PHASES.
C      KI AND KF INITIAL AND FINAL WAVE NUMBERS.

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C      RO IS MAX VALUE IN NUMERICAL INTEGRATION.
      IMPLICIT REAL*8(A-H,O-Z)
C**** CORRECTION OF DIRECT DIPOLE-LENGTH MATRIX ELEMENTS FOR
C      ASYMPTOTIC BEHAVIOR
C**** RO IS MAX R-VALUE IN NUMERICAL INTEGRATION
      REAL*8 KI,KF,KISO,KFSO
      DIMENSION X(1),EI(1),FF(1)
      KISO = KI*KI
      KFSO = KF*KF
      SK = KI+KF
      SK2 = SK*SK
      DK = KF-KI
      DK2 = DK*DK
      C = 100/(3.141592653589793*KF*KI)
      IF(17.EQ.2) GO TO 1
      X(1) = X(1)+C*((SK+KF)/(KF*SK2)*DSIN(EF(2)+EI(1)+SK*RO)-(DK+KF)/(K
1F*DK2)*DSIN(EF(2)-EI(1)+DK*RO)-RO/SK*DCOS(EF(2)+EI(1)+SK*RO)+RO/DK
2*DCOS(EF(2)-EI(1)+DK*RO))
      X(2) = X(2)+C*((SK+KI)/(KI*SK2)*DSIN(EF(1)+EI(2)+SK*RO)+(KI-DK)/(K
11*DK2)*DSIN(EF(1)-EI(2)+DK*RO)-RO/SK*DCOS(EF(1)+EI(2)+SK*RO)-RO/DK
2*DCOS(EF(1)-EI(2)+DK*RO))
      IF(17.EQ.1) GO TO 2
1 CONTINUE
      X(3) = X(3)+ C*((-5*KF*KI-3*KISO-KFSO)/(KF*KI*SK2)*DSIN(EF(3)+F(
12)+SK*RO)+(-5*KF*KI+3*KISO+KFSO)/(KF*KI*DK2)*DSIN(EF(3)-EI(2)+DK*
20)+(RO/SK-3/(KFSO*KI*RO))*DCOS(EF(3)+EI(2)+SK*RO)+(RO/DK+3/(KFSO*K
31*RO))*DCOS(EF(3)-EI(2)+DK*RO))
      X(4) = X(4)+ C*((-5*KF*KI-KISO-3*KFSO)/(KF*KI*SK2)*DSIN(EF(2)+EI(
13)+SK*RO)+(5*KF*KI-KISO-3*KFSO)/(KF*KI*DK2)*DSIN(EF(2)-EI(3)+DK*
21)+(RO/SK-3/(KF*KISO*RO))*DCOS(EF(2)+EI(3)+SK*RO)+(RO/DK+3/(KF*KIS
30*RO))*DCOS(EF(2)-EI(3)+DK*RO))
2 RETURN
      END
      SUBROUTINE EXCHOL(INI,FIN,MAX,P,17,EX)
C**** MAX IS VARIABLE DIMENSION.
C      P IS UNPERTURBED HYDROGEN ORBITAL.
C      EX RETURNS EXCHANGE MATRIX ELEMENTS.
      IMPLICIT REAL*8(A-H,O-Z)
C**** CALCULATION OF EXCHANGE TERMS IN LENGTH FORMULATION
C**** IT (1,2,3) FOR S-P ONLY, P-D ONLY, OR BOTH, RESPECTIVELY
      REAL*8 INI(MAX,280)
      DIMENSION FIN(MAX,280),EX(6),X(280),Y(280),Z(280),P(280),A(136),A
1(2(136),W(280)
      COMMON R(280),DUM(280),DUM1(280),DR(3),IN(3)/BLOCK2/DS(3),B(4,280)
1,DR(4,280),S(4,280),INE(3),INS(3)
      IF(17.EQ.2) GO TO 1
      DO 50 L1=1,2
      J = 3-L1
      IF(L1.EQ.2) GO TO 3
      DO 2 N=1,280
      X(N) = R(N)*INI(L1,N)
      Y(N) = R(N)*FIN(J,N)
      Z(N) = R(N)*P(N)
2 W(N) = FIN(J,N)
      GO TO 4
3 DO 5 N=1,280
      X(N) = R(N)*FIN(J,N)
      Y(N) = R(N)*INI(L1,N)
5 W(N) = INI(L1,N)
4 EX(2*L1-1) = SF(X,P,DR,IN)*SF(Y,Z,DR,IN)

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C***** CALCULATION OF DOUBLE INTEGRALS
CALL RAIN1(X,0,A1)
CALL RAIN1(W,0,A12)
DO 6 N=1,136
  M = 2*N-1
  A1(N) = Y(M)*A1(N)+R(M)*X(M)*A12(N)
  A12(N) = P(M)
  EX(2*N+1) = SF(A1,A12,DS,INS)
50 CONTINUE
  IF(17.EQ.1) RETURN
  1 CONTINUE
  DO 90 L1=2,3
    J = 5-L1
    IF(L1.EQ.3) GO TO 7
    DO 8 N=1,280
      Y(N) = R(N)*IN1(L1,N)
      X(N) = R(N)*FIN(J,N)
      8 W(N) = IN1(L1,N)
    GO TO 9
    7 DO 11 N=1,280
      Y(N) = R(N)*FIN(J,N)
      X(N) = R(N)*IN1(L1,N)
      11 W(N) = FIN(J,N)
    9 CONTINUE
    CALL RAIN1(X,0,A1)
    CALL RAIN1(W,0,A12)
    DO 12 N=1,136
      M = 2*N-1
      A1(N) = Y(M)*A1(N)+R(M)*X(M)*A12(N)
      12 A12(N) = P(M)
      EX(L1+3) = SF(A1,A12,DS,INS)
    90 CONTINUE
  RETURN
END

SUBROUTINE RAIN1(X,NM,Z)
  IMPLICIT REAL*8(A-H,O-Z)
  C***** X IS MULTIPLIER ARRAY FOR BOUND FUNCTION
  C***** NM C.I FOR B,DM, RESPECTIVELY
  DIMENSION X(280),Z(136)
  COMMON R(280),DUM(280),DUM1(280),DR(3),INS(3),B(4,280)
  1,DR(4,280),S(4,280),INE(3),INS(3)
  DO 6 N=1,136
    6 Z(N) = 0
    DO 50 J=1,3,2
      IF(NM.EQ.1) GO TO 1
      DO 2 N=1,280
        DUM(N) = X(N)+B(J,N)
        2 DUM1(N) = X(N)+B(J+1,N)
      GO TO 3
      1 DO 4 N=1,280
        DUM(N) = X(N)+DR(J,N)
        4 DUM1(N) = X(N)+DR(J+1,N)
      3 CONTINUE
      IF (J.EQ.3) GO TO 7
    50 SIMPSON INTEGRATION FROM 0-R
    D = DR(1)/300
    SUM = 0
    SUM1 = 0
    DO 10 N=2,136
      M = 2*N-1

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      IF(M.EQ.INF(1)+2) D = DR(2)/3
      IF(M.EQ.INF(2)+2) D = DR(3)/3
      SUM = SUM+D*(DUM(M)+DUM(M-2)+4*DUM(M-1))
      SUM1 = SUM1+D*(DUM1(M)+DUM1(M-2)+4*DUM1(M-1))
10  Z(M) = SUM*S(J,M)+SUM1*S(J+1,M)
      GO TO 50
C**** SIMPSON INTEGRATION FROM R-INFINITY
7  SUM = 0
   SUM1 = 0
   DO 20 N=2,136
      M = 273-2*N
      IF(M.EQ.INF(2)-2) D = DR(2)/3
      IF(M.EQ.INF(1)-2) D = DR(1)/3
      SUM = SUM+D*(DUM(M)+DUM(M+2)+4*DUM(M+1))
      SUM1 = SUM1+D*(DUM1(M)+DUM1(M+2)+4*DUM1(M+1))
      MM = 137-M
20  Z(MM) = Z(MM)+S(J,M)*SUM+S(J+1,M)*SUM1
90  CONTINUE
      RETURN
      END

```

Vita

Jerry Lee Stilley was born in Albany, Louisiana on October 9, 1941. He grew up in Baton Rouge, Louisiana and attended elementary and secondary schools there receiving his high school diploma from Istrouma Senior High in 1959. He entered Louisiana State University in September, 1959 and received his B.S. in physics in June, 1963. He entered the graduate school of Louisiana State University in September, 1963 and is presently a candidate for the degree of Doctor of Philosophy in the Department of Physics and Astronomy.

EXAMINATION AND THESIS REPORT

Candidate: Jerry Lee Stilley

Major Field: Physics

Title of Thesis: Free-Free Absorption Coefficient of the Negative Hydrogen Ion.

Approved:

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

R. W. Labahn

Date of Examination:

September 12, 1969