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Argonne National Laboratory

NEARREX, A COMPUTER CODE FOR NUCLEAR REACTION CALCULATIONS

by

P. A. Moldauer, C. A. Engelbrecht,
and G. J. Duffy

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NUCLEAR REACTION CALCULATIONS

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I. INTRODUCTION

NEARREX is a FORTRAN program for computing energy averages of integrated compound nucleus scattering, capture, and fission cross sections. This program was developed gradually over several years as an experimental code which was used in part to test theoretical ideas and numerical methods,⁽¹⁾ and in part to conduct a continuing program of neutron-cross-section calculations for purposes of reactor design and research.⁽²⁾ Early parts of the program were coded for the GEORGE computer with the help of Miss M. Fisherkeller of the Applied Mathematics Division. Later developments were carried out in IBM-704 FORTRAN, and most recently the code has been adapted for compilation on the CDC-3600 computer. While the program still bears some marks of its long history of modifications, adaptations, and enlargements, it is now sufficiently compact and unified to make it generally available for cross-section computation.

II. THEORY

The reaction cross section, σ_{ab} , which measures the total number of counts per unit time in the final state b produced by a unit flux incident in the initial state a , can be expanded in the partial waves α of a and β of b , as follows:

$$\sigma_{ab} = \sum_{\alpha\beta} g_{\alpha} \sigma_{\alpha\beta}. \quad (1)$$

Here, g_{α} is the usual statistical factor, $(2J_{\alpha} + 1)/[(2I_a + 1)(2i_a + 1)]$, where J_{α} is the total angular momentum of channel α , and I_a and i_a are the spins of the fragments of state a . The partial-wave cross sections $\sigma_{\alpha\beta}$ are given in terms of the quantum mechanical transition matrix elements $\mathcal{T}_{\alpha\beta}$ by

$$\sigma_{\alpha\beta} = \pi \lambda_a^2 |\mathcal{T}_{\alpha\beta}|^2. \quad (2)$$

The transition matrix elements are assumed to consist of a part $\mathcal{T}_{\alpha\beta}^{\text{direct}}$ arising from direct reaction processes, which we regard here as energy-independent, and a part $\mathcal{T}_{\alpha\beta}^{\text{compound}}$, which is assumed to vary

rapidly with energy. This energy variation can be expressed by a resonance expansion of $\mathcal{T}_{\alpha\beta}^{\text{compound}}$ which involves as parameters the resonance energies and widths E_μ and Γ_μ and the complex resonance channel amplitudes $g_{\mu\alpha}$.⁽³⁾ Correspondingly, $\sigma_{\alpha\beta}$ can be separated into an energy-independent part, $\sigma_{\alpha\beta}^{(0)}$, arising from the energy average of the transition matrix, and a fluctuating part, $\sigma_{\alpha\beta}^{(1)}(E)$, arising from the deviation of $\mathcal{T}_{\alpha\beta}$ from its average. The purpose of this report is to discuss a code for calculating the energy average of $\sigma^{(1)}$, which is generally called the fluctuation cross section (or more loosely, the average compound nucleus cross section),

$$\sigma_{ab}^{\text{fl.}} = \sum_{\alpha\beta} \sigma_{\alpha\beta}^{\text{fl.}} \quad (3a)$$

$$\sigma_{\alpha\beta}^{\text{fl.}} = \overline{\sigma_{\alpha\beta}^{(1)}(E)}, \quad (3b)$$

where the bar denotes an energy average.

We also make the assumption that the energy averages of the off-diagonal elements of $\mathcal{T}_{\alpha\beta}^{\text{compound}}$ vanish, which is thought to be true to a good approximation for low-energy nuclear reactions. Then it can be shown that the fluctuation cross section can be written in the following form:⁽³⁾

$$\sigma_{\alpha\beta}^{\text{fl.}} = \pi \lambda_a^2 \left\{ \left\langle \frac{\Theta_{\mu\alpha} \Theta_{\mu\beta}}{\Theta_\mu} \right\rangle - \frac{1}{4} \delta_{\alpha\beta} Q_\alpha \langle \Theta_{\mu\alpha} \rangle^2 \right\}, \quad (4)$$

where the $\Theta_{\mu\alpha}$ are certain resonance parameters associated with channels α and resonances μ , and

$$\Theta_\mu = \sum_{\alpha} \Theta_{\mu\alpha}, \quad (5)$$

the sum being over all competing open channels. The brackets, $\langle \rangle$, denote an average over resonance indices μ . The parameter Q_α depends on the details of the statistical properties of the E_μ , Γ_μ , and $g_{\mu\alpha}$. It has a maximum value of 2 in the limiting case of isolated resonances ($\langle \Gamma_\mu \rangle \ll D$), where D is the mean spacing of the E_μ . In the limit of infinitely many overlapping resonances ($\Gamma \gg D$), the value of Q_α goes to zero.

In the limiting case of isolated resonances, it can be shown that

$$\Theta_{\mu\alpha} \rightarrow 2\pi \Gamma_{\mu\alpha}/D \quad \Gamma \ll D, \quad (6)$$

where $\Gamma_{\mu\alpha}$ is the usual partial width and

$$\Gamma_\mu = \sum_{\alpha} \Gamma_{\mu\alpha}, \quad (7)$$

so that one obtains the Lane and Lynn formula,⁽⁴⁾

$$\sigma_{\alpha\beta}^{\text{fl.}} \rightarrow \frac{2\pi^2 \lambda_\alpha^2}{D} \left\langle \frac{\Gamma_{\mu\alpha} \Gamma_{\mu\beta}}{\Gamma_\mu} \right\rangle \quad \Gamma \ll D. \quad (8)$$

In more general circumstances, the resonance average of $\langle \Theta_{\mu\alpha} \rangle$ can be related to the average compound nucleus formation cross section for the partial wave α , which is denoted by

$$\langle \sigma_\alpha^{\text{comp.}} \rangle = \pi \lambda_a^2 T_\alpha^{\text{comp.}}. \quad (9)$$

In the case of a channel for which an optical model is defined, the compound-nucleus transmission coefficient, $T_\alpha^{\text{comp.}}$, defined by Eq. (9), equals the optical-model transmission coefficient T_α , less any portion of the transmitted flux which induces direct reaction processes.⁽⁵⁾ That is,

$$T_\alpha^{\text{comp.}} = T_\alpha - \sum_{\beta \neq \alpha} \sigma_{\alpha\beta}^{(0)} / (\pi \lambda_a^2). \quad (10)$$

In general, for low-energy nuclear reactions, where direct processes are unimportant, one may assume that

$$T_\alpha^{\text{comp.}} \sim T_\alpha. \quad (11)$$

The relation between $\langle \Theta_{\mu\alpha} \rangle$ and $T_\alpha^{\text{comp.}}$ under the above assumptions is given by^(3,5)

$$\langle \Theta_{\mu\alpha} \rangle = T_\alpha^{\text{comp.}} + \frac{1}{Q_\alpha} \left[1 - \sqrt{1 - Q_\alpha T_\alpha^{\text{comp.}}} \right]^2, \quad (12)$$

where the choice of the positive sign of the square root gives the correct limit when $\Gamma \ll D$. This relationship between $\langle \Theta_{\mu\alpha} \rangle$ and $T_\alpha^{\text{comp.}}$ is plotted in Fig. 1 for various values of Q_α . It is clear that

$$\langle \Theta_{\mu\alpha} \rangle \rightarrow T_\alpha^{\text{comp.}} \quad (13)$$

when either

$$T_\alpha^{\text{comp.}} \rightarrow 0,$$

or

$$Q_\alpha \rightarrow 0.$$

The latter condition is expected to be valid when $\Gamma \gg D$. If one also assumes that in that limit Θ_μ is not correlated with the values of either $\Theta_{\mu\alpha}$ or $\Theta_{\mu\beta}$ (many-channel limit), one obtains from Eq. (4) the Wolfenstein, Hauser-Feshbach formula,⁽⁶⁾

$$\sigma_{\alpha\beta}^{\text{fl.}} \rightarrow \pi \lambda_a^2 \frac{T_{\alpha}^{\text{comp.}} T_{\beta}^{\text{comp.}}}{\sum_{\gamma} T_{\gamma}^{\text{comp.}}}, \quad (14)$$

when both $\Gamma \gg D$, and the number of competing channels is very large.

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Fig. 1. Dependence of $\langle \Theta_{\mu\alpha} \rangle$ upon $T_{\alpha}^{\text{comp.}}$ for Selected Values of Q_{α} .

For two types of exit channels of interest, no useful optical model exists. This is true of fission, in part because no experiments can be made in which fission is the entrance channel, and thus empirical determination of optical model parameters is not possible. Parenthetically, the same objection holds for nucleon channels which leave the residual nucleus in an excited state; in these cases, it will generally be assumed that the appropriate optical model is the same as that for the ground-state transition.

The second type of exit channel requiring further discussion is radiative capture. Here an analog of the optical model exists for gamma-ray transitions with energies near the giant resonance. However, for most capture processes of interest, the gamma-ray spectrum lies well below giant-resonance energies and is thought to be influenced very little by collective nuclear effects. For both fission and capture, the transmission coefficients are quite small, so that the relation (13) may be used, and when in addition Γ/D is not too large, the relation (6) is expected to be a good approximation. When

neutron-induced capture and neutron-induced fission of fissile isotopes are considered, the thresholds of the gamma-ray and fission channels are well below the neutron threshold, so that one may expect the gamma-ray and fission transmission coefficients observed at low neutron energies to be applicable over a neutron energy range of perhaps several hundred keV. At least that hypothesis may serve as a starting point for calculations. At very low energies, the values of these transmission coefficients may be deduced by means of Eqs. (6) and (13) from the partial radiative and fission widths, and the resonance level spacings may be determined by resonance

analysis. Additional problems arise because such resonance analyses ordinarily yield information only about the decay of states produced by the absorption of s-wave neutrons. We do not discuss the problem of fission further, but will deal in more detail with the gamma-ray channels.

In view of the above discussion, we use Eqs. (6) and (13) to write, for the average resonance parameter describing gamma-ray emission through compound states of total angular momentum J and parity Π and total excitation energy U of the compound system,

$$\langle \Theta_{\mu\gamma}(J, \Pi, U) \rangle \sim 2\pi \langle \Gamma_{\mu\gamma}(J, \Pi, U) \rangle \rho(J, \Pi, U), \quad (15)$$

where $\rho = D^{-1}$ is the density of resonance levels J, Π at excitation energy U . If we assume that the energy dependence of the average radiation width is given by the Weisskopf formula for dipole radiation,⁽⁷⁾

$$\langle \Gamma_{\gamma}(U) \rangle = C_1 \int_0^U (\rho(U - \epsilon)/\rho(U)) \epsilon^3 d\epsilon, \quad (16)$$

where C_1 is a constant, and if we assume the energy dependence of the level density to be given by⁽⁸⁾

$$\rho(U) = C_2 \exp\left(\frac{2\pi^2 U}{3\delta}\right)^{1/2}, \quad (17)$$

where C_2 and δ are constants, the latter being of the order of the spacing of single particle state levels, then the energy dependence of $\langle \Theta_{\mu\gamma} \rangle$ is found to be proportional to the following function⁽⁹⁾ of U and δ :

$$\psi(U, \delta) = e^x [x^4 - 10x^3 + 45x^2 - 105x + 105], \quad (18)$$

where

$$x \equiv \left(\frac{2\pi^2 U}{3\delta}\right)^{1/2}. \quad (19)$$

The angular momentum dependence of the level density is expected to have the functional form⁽⁸⁾

$$F(J) = \exp(-J^2/2\sigma^2) - \exp(-(J+1)^2/2\sigma^2), \quad (20)$$

where σ is a constant parameter which depends on the nuclear mass number and details of the nuclear structure.

We may now write

$$\langle \Theta_{\mu\gamma}(J, \Pi, E) \rangle = 2\pi \left(\frac{\Gamma_\gamma}{D} \right)_0 \frac{F(J, \sigma) \psi(U_0 + E, \delta) Z(\Pi)}{\left[F\left(I_0 - \frac{1}{2}, \sigma\right) + F\left(I_0 + \frac{1}{2}, \sigma\right) \right] \psi(U_0, \delta)}, \quad (21)$$

with

$$F\left(-\frac{1}{2}, \sigma\right) \equiv 0.$$

This formula is particularly adapted to radiative neutron capture. $(\Gamma_\gamma/D)_0$ is the measured ratio of the average radiation width to resonance level spacing for low-energy s-wave neutrons corresponding to radiative transitions from the compound system at the neutron binding energy U_0 . The neutron energy is denoted by E , and the spin of the target nucleus is I_0 . The function $Z(\Pi)$ allows for an arbitrary parity dependence of $\langle \Theta_{\mu\gamma} \rangle$. The same formula can also be applied to proton-capture reactions.

The calculation of capture cross sections at several hundred keV or more above the neutron threshold requires additional discussion. If in Eq. (4) the "channel" β is chosen to represent the gamma-ray emission alternative, then, what is calculated is the average gamma-ray production cross section, $\langle \sigma_{\alpha\gamma} \rangle$, which may, however, include events in which the emission of the gamma ray, or of several gamma rays, is followed by the emission of a neutron. On the other hand, the radiative capture cross section, $\langle \sigma_{\alpha, \text{capt}} \rangle$, as measured and as used in applications, refers exclusively to those events in which only gamma rays are emitted by the compound system (disregarding, of course, long life-time alpha or beta decays). To compute the capture cross section, it is therefore necessary to multiply the gamma-ray production cross section of Eq. (4) by the probability $B_{J,\Pi}(U)$ that the gamma-ray cascade, once initiated, is not interrupted by the emission of a neutron. At any stage of the cascade, the relative probability of further gamma-ray to neutron emission is given by the ratio of average gamma-ray width, $\langle \Gamma_\gamma \rangle$, to the average total neutron width, $\langle \Gamma_n \rangle$. Now $\langle \Gamma_\gamma \rangle$ is small and slowly varying with energy, while $\langle \Gamma_n \rangle$ increases fairly rapidly with energy above the neutron threshold. In fact, ordinarily $\langle \Gamma_n \rangle$ will become very large compared to $\langle \Gamma_\gamma \rangle$ within a relatively small neutron energy interval. It turns out to be a reasonable approximation, therefore, to compute $B_{J,\Pi}(U)$ under the assumption that if the first gamma ray leaves the compound system in a state J, Π , with energy U above a certain compound excitation energy $U_{J\Pi} = U_0 + E_{J\Pi}$, then a neutron is emitted, while a compound state J, Π with an energy U which is less than $U_{J,\Pi}$ is de-excited by a gamma-ray cascade. The energy $E_{J\Pi}$ is of the order of the energy at which $\langle \Gamma_n \rangle = \langle \Gamma_\gamma \rangle$ for the particular angular momentum J and parity Π . When $\langle \Gamma_n \rangle$ is computed for this purpose, it may be necessary to take into account neutron emission to excited states. It is, however, usually sufficient to consider only the compound state produced by the first gamma ray.

Under the above assumptions, and for electric dipole radiation having the properties assumed in Eqs. (16-20), one finds⁽⁹⁾ that

$$B_{J\Pi}(E) = \frac{\sum' F(J') M_{J,\Pi}(E, J')}{\sum' F(J')}, \quad (22)$$

where the sum $\sum'$ is carried over all nonnegative

$J' = J - 1, J, \text{ or } J + 1$, but $J' \neq 0$ if $J = 0$, and

$$\begin{aligned} M_{J,\Pi}(E, J') = \frac{x^2 x'^5 e^{x'}}{48\psi(U, \delta)} & \left\{ \left[1 - \left(\frac{x'}{x} \right)^2 \right]^3 \right. \\ & - \frac{1}{x'} \left[1 - \left(\frac{x'}{x} \right)^2 \right]^2 \left[1 - 7 \left(\frac{x'}{x} \right)^2 \right] \\ & - \frac{6}{x^2} \left[1 - \left(\frac{x'}{x} \right)^2 \right] \left[3 - 7 \left(\frac{x'}{x} \right)^2 \right] \\ & + \frac{6}{x' x^2} \left[3 - 30 \left(\frac{x'}{x} \right)^2 + 35 \left(\frac{x'}{x} \right)^4 \right] \\ & + \frac{120}{x^4} \left[3 - 7 \left(\frac{x'}{x} \right)^2 \right] - \frac{360}{x' x^4} \left[1 - 7 \left(\frac{x'}{x} \right)^2 \right] \\ & \left. - \frac{5040}{x^6} + \frac{5040}{x' x^6} \right\}, \quad (23) \end{aligned}$$

when

$$E_{J', -\Pi} < E;$$

and

$$M_{J,\Pi}(E, J') = 1, \quad \text{when} \quad E_{J', -\Pi} > E;$$

and

$$x' = x (U_0 + E_{J', -\Pi}). \quad (24)$$

So far we have discussed only the calculation of $\langle \Theta_{\mu\alpha} \rangle$ for various types of channels. The evaluation of the first term on the right-hand side of Eq. (4) requires also a knowledge of the distributions and correlations of the fluctuations of the $\Theta_{\mu\alpha}$ about their averages. The determination of these properties is in general quite involved.⁽¹⁰⁾ We discuss here only

the result when the $\Theta_{\mu\alpha}$ for different channel indices α are entirely uncorrelated and if the distributions of each of the $\Theta_{\mu\alpha}$ can be represented by a χ^2 distribution with ν_α degrees of freedom.⁽¹¹⁾ Then we have

$$\left\langle \frac{\Theta_{\mu\alpha_1} \Theta_{\mu\alpha_2}}{\sum_i \Theta_{\mu\alpha_i}} \right\rangle = \frac{\langle \Theta_{\mu\alpha_1} \rangle \langle \Theta_{\mu\alpha_2} \rangle}{\sum_i \langle \Theta_{\mu\alpha_i} \rangle} S_{\alpha_1\alpha_2}, \quad (25)$$

where the so-called fluctuation correction factor $S_{\alpha_1\alpha_2}$ is given by⁽¹²⁾

$$S_{\alpha_1\alpha_2} = \int_0^\infty dt \frac{1 + 2\delta_{\alpha_1\alpha_2}}{f_1 f_2 \prod_i (f_i)^{\nu_{\alpha_i}/2}}, \quad (26)$$

where the product in the denominator is taken over all competing channels α_i , including α_1 and α_2 , and

$$f_j = 1 + \frac{\langle \Theta_{\mu\alpha_j} \rangle}{\sum_i \langle \Theta_{\mu\alpha_i} \rangle} \frac{2t}{\nu_{\alpha_j}}. \quad (27)$$

It is customary to lump all gamma-ray channels together and to assume that the corresponding distribution of the lumped $\Theta_{\mu\gamma}$ is very narrow or that ν_γ is very large. In the limit of infinite ν_γ , one has

$$f_\gamma^{\nu_\gamma/2} \approx f_\gamma^{1+\nu_\gamma/2} \rightarrow \exp \left[- \frac{\langle \Theta_{\mu\gamma} \rangle}{\sum_i \langle \Theta_{\mu\alpha_i} \rangle} t \right]. \quad (28)$$

III. GENERAL DESCRIPTION OF THE PROGRAM

The NEARREX program computes neutron-induced average fluctuation (or compound nucleus) cross sections according to the formulas presented in the preceding section. Provision is made for the computation of compound elastic and inelastic neutron cross sections, radiative capture and fission cross sections, as well as other processes, such as proton emission. The program can also be easily used for the computation of proton-induced average cross sections.

At each incident neutron energy E , a neutron partial wave channel α is specified by its orbital angular-momentum quantum number, ℓ , by the total neutron angular momentum, $j = \ell \pm 1/2$, by the total angular momentum, J , and by the residual state of the target nucleus. These residual states can be any one of the ground or excited states of the target nucleus, for which excitation energies, spins, and parities must be specified. The $\langle \Theta_{\mu\alpha} \rangle$ for each of these neutron channels is computed by means of Eq. (12), and for this purpose the compound transmission coefficients, T_{α}^{comp} , are specified in the input. The latter will usually be obtained from an optical model calculation. The input format for the elastic and inelastic T_{α}^{comp} , is the same as the format of the punched-out transmission coefficients that can be obtained from the ABACUS 2 optical model code. However, the number of transmission coefficients punched out by ABACUS 2 will usually not coincide with the number required in the input of NEARREX. The statistical parameter, Q_{α} , in Eq. (12) must be specified to have the same value for all channels in this program. For this reason, it is in general only safe to specify values lying within the limits $1 \geq Q \geq 0$ (see Fig. 1). This should be no undue restriction since in most cases of interest in heavy nuclei, Q_{α} is fairly small. Each neutron partial wave, $\Theta_{\mu\alpha}$, is assumed to be distributed according to the χ^2 distribution with one degree of freedom (Porter-Thomas).⁽¹¹⁾

The $\langle \Theta_{\mu\gamma} \rangle$ for the radiation channels are computed by means of Eqs. (15-21), with the average radiation width to level spacing for compound states populated by s-wave neutrons of zero energy specified as

$$A_{\gamma}^{(0)} = (F_{\gamma}/D)_0. \quad (29)$$

The parameter σ can be given the values 2, 4, 6, 8, or 10. Setting $\sigma = 0$ or 12 results in $F \equiv 1$, or $F \equiv 2J + 1$, respectively. The lumped $\Theta_{\mu\gamma}$ for each J, Π are assumed to be independent of μ ; that is, ν_{γ} is allowed to go to infinity [see Eq. (28)].

For the fission channels, the $\langle \Theta_{\mu f} \rangle$ for each J, Π must be specified as a linear function of the incident neutron energy E as follows:

$$\langle \Theta_{\mu f(J, \Pi)}(E) \rangle = 2\pi[A_f^{(0)}(J, \Pi) + EA_f^{(1)}(J, \Pi)]. \quad (30)$$

The distribution of each of the $\Theta_{\mu f(J, \Pi)}$ can be specified to follow a χ^2 distribution with an arbitrary ν_f degrees of freedom.

In addition, provision is made for "h" channels which have the same input specification as the fission channels and which may be used for such decay modes as a second fission mode, proton emission, alpha particle emission, etc.

The integral (26) is evaluated in the following manner. The correction factor $S_{\alpha_1 \alpha_2}$ is transformed into

$$S_{\alpha_1 \alpha_2} = (1 + 2\delta_{\alpha_1 \alpha_2}) \frac{\langle \Theta_{\mu} \rangle}{\langle \Theta_{\mu} \gamma(J, \Pi) \rangle} \int_0^{\infty} \frac{e^{-t} dt}{g_1 g_2 \prod_i (g_i)^{\nu_{\alpha_i}/2}}, \quad (31)$$

where

$$g_j = 1 + \frac{\langle \Theta_{\mu \alpha_j} \rangle}{\langle \Theta_{\mu} \gamma(J, \Pi) \rangle} \frac{2t}{\nu_{\alpha_j}}, \quad (32)$$

where the product is over all open channels except the radiation channels. The integral (31) is then changed into an integral over the finite interval (0,1) by the transformation

$$Z = \text{Erf}(\sqrt{t}) \quad (33)$$

and then evaluated by means of the m-point Chebyshev-Gauss quadrature formula,⁽¹³⁾

$$\int_0^1 \frac{f(Z) dZ}{\sqrt{Z(1-Z)}} \sim \frac{\pi}{m} \sum_{r=1}^m f(Z_r), \quad (34)$$

where

$$Z_r = \cos^2\left(\frac{2r-1}{2m} \frac{\pi}{2}\right). \quad (35)$$

For standard operation, m is set equal to 12, and in certain circumstances when $S_{\alpha_1 \alpha_2}$ is close to unity and the quadrature converges poorly, the fluctuation correction factor is set equal to unity.

IV. SPECIFICATION OF INPUT AND OUTPUT

The cards on which the input data should be punched will now be listed. For each card, the information to be punched in the various columns is described, together with an indication of the input format to be used. The letter I denotes integer format and indicates that the quantity under consideration should be written without decimal points and in the extreme right of the specified field. If, for example, a 2 is punched in column 10 of card 2.1, then NMAX would be read in as 20. The floating-point format, Fm.n, on the other hand, indicates that the quantity should include a decimal point and can then be written anywhere in the specified field of length m. If the decimal point is omitted, it will be automatically supplied at a position such that the n right-hand columns of the field appear to the right of the decimal point. Thus, a 1 and a 2 in columns 24 and 25 of card 2.1 will lead to a value of 1.2 for PHP. The format A on card 1.1 indicates the use of any letters (capitals), numbers, or any of the special IBM characters. In the listing which follows, all energies are assumed to be given in MeV, while in the output all cross sections are in barns.

CARD 1.1

Cols. 4-75 (A) TITLE to be written at head of output.

CARD 2.1

Col. 5	(I)	IAG = 1 indicates (n, γ) cross sections desired, = 0 indicates (n, γ) not desired;
Col. 7	(I)	IAF = 1 indicates (n, f) cross sections desired, = 0 indicates (n, f) not desired;
Col. 9	(I)	IAH = 1 indicates (n, h) cross sections desired, = 0 indicates (n, h) not desired;
Cols. 10-11	(I)	NMAX = number of excited levels of target nucleus (≤ 25);
Col. 13	(I)	LMAX = maximum ℓ -value used for transmission coefficients (≤ 8);
Col. 15	(I)	KC = 1 indicates $S_{\alpha\beta}$ of Eq. (26) must be calculated, = 0 indicates all $S_{\alpha\beta J}$ set equal to unity;

Col. 17	(I)	ITPT = 1 indicates cross sections for partial waves (ℓ, j) desired, = 0 indicates only total cross sections desired;
Col. 19	(I)	NE = number of incident neutron energies for which calculations are desired (≤ 35);
Cols. 20-32	(F13.8)	Q = value of Q in Eqs. (4) and (12);
Col. 34	(I)	MN = 0 means $m = 12$ in Eq. (34), = 1 means value of m must be specified in cols. 35-36;
Cols. 35-36	(I)	NINT = value of m used if MN = 1.
<u>CARDS 3.N</u> [N = 0 (target ground state), 1, 2, ..., NMAX]		
Cols. 3-10	(F8.6)	W(N) = excitation energy of level N; for ground state $W(0) = 0.0$;
Cols. 41-50	(F10.6)	HI(N) = spin of level N;
Cols. 51-60	(F10.6)	PI(N) = parity of level N (+1.0 or -1.0).
<u>CARD 4.1</u> (only required when IAG = 1)		
Cols. 1-12	(F12.8)	AGSUP ϕ = $A_{\gamma}^{(0)}$ of Eq. (29);
Col. 14	(I)	MJ = 1 indicates value of σ in Eq. (20) must be read from card 4.1, = 0 indicates $\sigma = 6$;
Col. 16	(I)	ME = 2 indicates that the neutron binding energy U_0 and δ of Eq. (17) must be read from card 4.1, = 1 indicates $U_0 = 8.0$, $\delta = 0.12$, = 0 indicates $\psi = 1$ (see Eq. 18);
Col. 17	(I)	MB = 1 indicates $B_{J\pi}$ is calculated as given in Eq. (22), (σ_{capt} calculated); requires cards 4.2, etc., indicated below, = 0 indicates $B_{J\pi}$ is set equal to unity (σ_{γ} calculated); Cards 4.2, etc., not required;
Col. 18	(I)	MP = 1 indicates $Z(+)$ and $Z(-)$ of Eq. (21) must be read from card 4.1, = 0 indicates $Z_{\text{PLS}} = Z_{\text{MIN}} = 1.0$;

Cols. 19-24 (F6.2) SIGMA = σ of Eq. (20); values of 0, 2, 4, 6, 8, 10, and 12 are permitted; if MJ = 0, the content of this field is ignored;

Cols. 25-34 (F10.5) U = neutron binding energy U_0 of Eq. (21) (ignored if ME = 0 or 1);

Cols. 35-44 (F10.5) DELTA = δ of Eq. (17) (ignored if ME = 0 or 1);

Cols. 45-54 (F10.5) ZPLS = Z(+) (ignored if MP = 0);

Cols. 55-64 (F10.5) ZMIN = Z(-) (ignored if MP = 0);

CARD 4.2 etc. (required only if MB = 1) [see Eqs. (22-24)]

Cols. 1-12 (F12.6) PE(JPI) = E_{J+} , J = 0 or 1/2;

Cols. 13-24 (F12.6) PE(JPI) = E_{J+} , J = 1 or 3/2;

Cols. 25-36 (F12.6) PE(JPI) = E_{J+} , J = 2 or 5/2;

Cols. 37-48 (F12.6) PE(JPI) = E_{J+} , J = 3 or 7/2;

Cols. 49-60 (F12.6) PE(JPI) = E_{J+} , J = 4 or 9/2.

CARD 4.3

Cols. 1-12 (F12.6) J = 5 or 11/2, etc., up to $J_{\max} = HI(0) + LMAX + 3/2$, followed by a similar set of cards listing $EM(JPI) = E_{J-}$ for the negative parity states.

CARD 5.0 (only required when IAF = 1)

Cols. 1-12 (F12.8) FNU = ν_f of Eqs. (26) and (27).

CARDS 5.N [only when IAF = 1; here N = J_1 to $J_{\max}$; see Eq. (30)]

Cols. 1-12 (F12.8) APF(N) = $A_f^{(0)}(J,+)$ of Eq. (30);

Cols. 13-24 (F12.8) AMF(N) = $A_f^{(0)}(J,-)$ of Eq. (30);

Cols. 25-36 (F12.8) BPF(N) = $A_f^{(1)}(J,+)$ of Eq. (30);

Cols. 37-48 (F12.8) BMF(N) = $A_f^{(1)}(J,-)$ of Eq. (30).

CARD 6.0 (only required when IAH = 1)

Cols. 1-12 (F12.8) HNU = ν_h .

CARDS 6.N (similar to cards 5.N, except with h instead of f)

CARD 7.0

Cols. 1-12 (F12.8) E = first incident neutron energy.

CARDS 7.N

Cols. 1-12
 Cols. 13-24
 Cols. 25-36
 Cols. 37-48
 Cols. 49-60
 Cols. 61-72

(F12.8)

$T(N,L,J)$ = compound nucleus transmission coefficients. $J = L - 1/2$ to $L + 1/2$. $L = 0$ to LMAX. $N = 0$ (target ground state) to NMAX. Start new card for each level N . Cards corresponding to levels for which the level energy $W(N)$ is higher than the neutron energy, E , should not be omitted. Instead, the T 's can be left blank or set equal to zero.

CARD 8.0

Cols. 1-12 (F12.8) E = second incident neutron energy.

CARDS 8.N (similar to 7.N for second energy)

CARDS N.M (similar to 7.M and 8.M for successive E values)

To clarify the order of the transmission coefficients, consider an example with LMAX = 2 and with a ground state (level 0) and one excited state (level 1). Then two cards are required (at each neutron energy).

CARD 7.1

Cols. 1-12 T for level 0 with $\ell = 0, j = 1/2$;
 Cols. 13-24 T for level 0 with $\ell = 1, j = 1/2$;
 Cols. 25-36 T for level 0 with $\ell = 1, j = 3/2$;
 Cols. 37-48 T for level 0 with $\ell = 2, j = 3/2$;
 Cols. 49-60 T for level 0 with $\ell = 2, j = 5/2$.

CARD 7.2

Cols. 1-12 T for level 1 with $\ell = 0, j = 1/2$; etc.

The output will not be described in such detail since an illustrative example is presented in the next section. The first page of output contains the title, the value of KC, and the energy levels with spins and parities. If IAG = 1, the output also contains the input parameters of card 4.1; and if IAF = 1, it contains the input data of cards 5.0 and 5.N. On succeeding pages, the transmission coefficients for each energy are given; and, if IPT = 1, the partial cross sections for specific values of ℓ and j of the incident neutrons are printed on separate lines in the order $(\ell, j) = (0, 1/2), (1, 1/2), (1, 3/2), (2, 3/2)$, etc. For the elastic and inelastic scattering cross sections, the separate contributions of different (ℓ', j') outgoing partial waves

are printed in different columns in the same order. A final page presents the total cross sections for scattering to all levels of the target nucleus, as well as cross sections for capture, fission, and other processes.

V. NOTE ON THE PROGRAMMING OF NEARREX

This program was written originally for the IBM 704 using the Fortran II language. Changing "IF ACCUMULATOR OVERFLOW" statements (704 Fortran II) to "IF EXPONENT FAULT" statements made the program compatible with the CDC 3600 (or 1604) Fortran 63 language. By reversing these statement changes and by making the two other changes mentioned in the comments at the beginning of the Appendix, one can again make this program compatible with 704/7090/7094 Fortran II.

Furthermore, by altering Input/Output statements, one can also run the program on either the 7030 (Stretch) or 7094 using Fortran IV.

The 704 will compile this program in about 48 minutes using Fortran II. The 3600 will use about 2 minutes in compiling this with Fortran 63.

For the monitor system on the Argonne IBM-704 computer, the input is on magnetic tape No. 7 and the output is on tape No. 6. For use with other monitor systems, one must employ the necessary EQUIP cards.

Computing time on the IBM-704 was found to be approximately $0.04 \text{ NE}(\text{NMAX} + 1)(2\text{LMAX} + 1)$ minutes.

VI. SAMPLE CALCULATION

For illustration, the input and output of an actual NEARREX calculation of the scattering, capture, and fission cross sections of 400-keV neutrons bombarding U^{234} will now be presented. This calculation is intended as an illustration only, and any resemblance to actual U^{234} is entirely fortuitous.

The following page contains the input information used. This is followed by two pages of output.

704 INPUT DATA FORM I

COST CODE _____

PROGRAM										PROBLEM										ORIGINATOR										DATE										PAGE										OF																																							
1										2										3										4										5										6										7										8																			
1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7	8	9	0																				
SPECIMEN CALCULATION FOR U ²³⁵																																																												C, A, R, D, 1, 1																													
1, 1, 2, 3, 1, 1, 1										1, 5																																																		C, A, R, D, 2, 1																													
0, 0																				0, 0										+ 1, 0																														C, A, R, D, 3, 0																													
0, 0, 4, 5																				2, 0										+ 1, 0																														C, A, R, D, 3, 1																													
0, 1, 5, 0																				4, 0										+ 1, 0																														C, A, R, D, 3, 2																													
0, 0, 0, 2										1, 2, 4, 0										4, 6										0, 0, 7																														C, A, R, D, 4, 1																													
2, 0																																																												C, A, R, D, 5, 0																													
0, 0, 0, 7										0, 0, 1, 3																																																		C, A, R, D, 5, 1																													
0, 0, 0, 4										0, 0, 1, 6																																																		C, A, R, D, 5, 2																													
0, 0, 0, 2																																																												C, A, R, D, 5, 3																													
0, 0																																																												C, A, R, D, 5, 4																													
0, 4																																																												C, A, R, D, 7, 0																													
0, 2, 2, 0										0, 3, 9, 1										0, 5, 0, 3										0, 0, 3, 1										0, 0, 1, 8										0, 0, 0, 6										C, A, R, D, 7, 1																													
0, 0, 1, 0																																																												C, A, R, D, 7, 2																													
0, 2, 1, 1										0, 3, 5, 2										0, 4, 5, 7										0, 0, 2, 5										0, 0, 1, 4																				C, A, R, D, 7, 3																													
0, 0																																																												C, A, R, D, 7, 4																													
0, 1, 8, 7										0, 2, 4, 9										0, 3, 3, 2										0, 0, 1, 3										0, 0, 0, 7																				C, A, R, D, 7, 5																													
0, 0																																																												C, A, R, D, 7, 6																													
1										2										3										4										5										6										7										8																			

NEARREX

SEPT 1964

SPECIMEN CALCULATION FOR U234

CAR

ENERGY LEVELS

KC = 1

0.000000	0.000000	1.000000
0.045000	2.000000	1.000000
0.150000	4.000000	1.000000

A(GAMMA) = 0.002000000

SIGMA	U	DELTA	ZPLS	ZMIN
4.00000000	4.60000000	0.07000000	1.00000000	1.00000000

NU(F) = 2.0000

J	PAFO	AMFO	PAF1	AMF1
0.50000000	0.00700000	0.01300000	-0.00000000	-0.00000000
1.50000000	0.00400000	0.01600000	-0.00000000	-0.00000000
2.50000000	0.00200000	0.00000000	-0.00000000	-0.00000000
3.50000000	0.00000000	0.00000000	-0.00000000	-0.00000000

ENERGY = 0.40000000

Q = 1.50000

TRANSMISSION COEFFICIENTS

0.22000000	0.39100000	0.50300000	0.03100000	0.01800000	0.00600000	0.01000000
0.21100000	0.35200000	0.45700000	0.02500000	0.01400000	-0.00000000	0.00000000
0.18700000	0.24900000	0.33200000	0.01300000	0.00700000	-0.00000000	0.00000000

CROSS SECTIONS FOR CAPTURE FISSION OTHER

0.00	0.50	0.028281	0.030225	0.000000
1.00	0.50	0.022476	0.045302	0.000000
1.00	1.50	0.069723	0.097815	0.000000
2.00	1.50	0.021078	0.007260	0.000000
2.00	2.50	0.024279	0.003390	0.000000
3.00	2.50	0.003183	0.000000	0.000000
3.00	3.50	0.007969	0.000000	0.000000

CROSS SECTIONS FOR SCATTERING

EXCITED LEVEL NUMBER		0		W(N) = 0.000000		SIGMA(N,E) = 1.45312432			
0.00	0.50	0.2736998	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
1.00	0.50	0.0000000	0.3737287	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
1.00	1.50	0.0000000	0.0000000	0.7689385	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
2.00	1.50	0.0000000	0.0000000	0.0000000	0.0234333	0.0000000	0.0000000	0.0000000	0.0000000
2.00	2.50	0.0000000	0.0000000	0.0000000	0.0000000	0.0130329	0.0000000	0.0000000	0.0000000
3.00	2.50	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000528	0.0000000	0.0000000
3.00	3.50	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0002383	0.0000000
EXCITED LEVEL NUMBER		1		W(N) = 0.045000		SIGMA(N,E) = 1.06025000			
0.00	0.50	0.0000000	0.0000000	0.0000000	0.0171124	0.0100222	0.0000000	0.0000000	0.0000000
1.00	0.50	0.0000000	0.0000000	0.1967931	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
1.00	1.50	0.0000000	0.3080226	0.3980327	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
2.00	1.50	0.0363662	0.0000000	0.0000000	0.0068036	0.0040294	0.0000000	0.0000000	0.0000000
2.00	2.50	0.0323573	0.0000000	0.0000000	0.0060955	0.0036124	0.0000000	0.0000000	0.0000000
3.00	2.50	0.0000000	0.0080054	0.0099314	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
3.00	3.50	0.0000000	0.0000000	0.0230527	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
EXCITED LEVEL NUMBER		2		W(N) = 0.150000		SIGMA(N,E) = 0.04691735			
0.00	0.50	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
1.00	0.50	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
1.00	1.50	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
2.00	1.50	0.0000000	0.0000000	0.0000000	0.0000000	0.0021003	0.0000000	0.0000000	0.0000000
2.00	2.50	0.0000000	0.0000000	0.0000000	0.0033734	0.0018836	0.0000000	0.0000000	0.0000000
3.00	2.50	0.0000000	0.0000000	0.0076281	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
3.00	3.50	0.0000000	0.0141535	0.0177684	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000

SCATTERING CROSS SECTIONS

ENERGY	ELASTIC	LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4	LEVEL 5	LEVEL 6	LEVEL 7	LEVEL 8
0.4000000	1.4531243	1.0602500	0.0469173						
ENERGY	CAPTURE	FISSION	OTHER						
0.4000000	0.1769895	0.1839913	0.0000000						

APPENDIX

NEARREX Symbolic Listing

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PROGRAM NEARREFX

NEARREX, A COMPUTER CODE FOR NUCLEAR REACTION CALCULATIONS

1184/RE257 BY C.A. ENGELBRECHT, P. MOLDAUER, G. DUFFY.
THIS IS THE 3600 VERSION (FORTRAN 63 COMPATIBLE) OF NEARREX WHICH
WILL RUN ON 704 FORTRAN II WITH A FEW MINOR MODIFICATIONS.
TO RUN THIS CODE ON A 704 OR 7090/94, MAKE THE FOLLOWING CHANGES-
(1) CHANGE THE INITIALIZE TEMPORARY STORAGE SECTION BY REPLACING
ALL MULTIPLE EQUALITIES WITH A SUITABLE SUBSTITUTE.
(2) CHANGE ALL IF EXPONENT FAULT STATEMENTS TO IF ACCUMULATOR
OVERFLOW STATEMENTS.
(3) THE 2 STATEMENTS FOLLOWING STATEMENT 9500 SET UP AN ERROR
TERMINATION JUMPED TO FROM 20 DIFFERENT LOCATIONS IN THE CODE.
CHANGE THIS SUBROUTINE, CALLED Q8QERROR, TO SUIT YOUR SYSTEM.
THIS VERSION INCLUDES CORRECTIONS TO AUGUST, 1964.

```

DIMENSION W(26),HI(26),PI(26),PE(20),EM(20),PAFO(19),
X AMFC(19),PAF1(19),AMF1(19),PAHO(19),AMHO(19),
X PAH1(19),A(26,17),C(30),XK(30),FINT(13,7),EN(26),
X FHAH(14,7),P(26,17),GO(26,17),G1(26,17),
X ENSIG(26,17,17),BGP(19),AFPLUS(19), BBB(17),
X AFMIN(19),AHPLUS(19),AHMIN(19),AGPLUS(19),
X AGMIN(19),BGM(19),ATEMP(26,17),AMH1(19),
X ATEMP(26,17),GSIG(17),FSIG(17),HSIG(17),
X GSIGN(35),FSIGN(35),RECORD(12),GFUNG(30),
X GSIGN(35),ENISGN(35,26),ESUBP(35),ENSIGE(26)

```

COMPUTE TABLE OF J-COEFFICIENTS

```

3331 DO3331N=1,7
      FFALE(1,N)=0.0
      DO3332N=1,13
        K=N+1
        FINT(N,1)=1.0
3332 FFALE(K,1)=1.0
        SS=2.0
        DO3334N=2,6
          DO3333J=1,13
            AHEL=FLCATF(J-1)
            AHAL=AHEL+0.5
            K=J+1
            CSS=0.5/(SS*SS)
            FINT(J,N)=EXPF(-CSS*AHAL*AHAL)-EXPF(-CSS*(AHAL+1.0))
            X*(AHAL+1.0))
3333 FFALE(K,N)=EXPF(-CSS*AHAL*AHAL)-EXPF(-CSS*(AHAL
            X+1.0)*(AHAL+1.0))
3334 SS=SS+2.0
        FINT(1,7)=1.0
        FFALE(2,7)=1.0
        DO3335J=1,12
          K=J+1
          L=K+1
          FINT(K,7)=FINT(J,7)+2.0
3335 FFALE(L,7)=FFALE(K,7)+1.0

```

INITIALIZE TEMPORARY STORAGE.

301 AE = AFPHI = AGSUPO = AHAL = AHEL = AMTOT = ANAWTA = ANAWTM =
CANAWTP = AN = AOFN = ASBFE = ASUBH = ATEMP = AWTA = AWT =
CAXA = AYA = CSS = DBPROC = DELTA = EJPI = E = EYE =

```

CFINAWT= FKN   = FLN   = FNINT = FNU   = FSIGE = FTEMP1= FTEMP2=
CFTEMP3= GELTA = GSIGE = HNU   = HSIGE = PATOT = PHIUE = PHIU  =
CPHPHP = PHPH  = PIEK  = PIEN  = PIE   = PROD11= PROD12= PROD21=
CPROD22= PSIBAR= SIGMA = SS    = SUMINM= SUMINP= SUMINV= SUMK   =
CSUMOTM= SUMOTP= SUMUPM= SUMUPP= TEMP1  = TEMP2  = TEMP3  = TEMP4  =
CTEMP5  = TEMPAG= TEMPAH= TEMPAO= TEMPA  = TEMPBG= TEMPPA= TEMPJ  =
CTEMPM  = TEMPNE= TEMPNH= TEMPP  = TEMP  = TEMPT  = TEMPX  = U    =
CVEK    = VEL   = VI    = VJ    = VKN   = VK    = VLN   = VL    =
CWCFFN  = XK1   = ZMIN  = ZPLS  = 0.0

DO 9010 I=1,26
  W(I)=HI(I)=PI(I)=EN(I)=ENSIGE(I)=0.0
DO 9010 J=1,17
  A(I,J)=P(I,J)=QO(I,J)=Q1(I,J)=ATEMPP(I,J)=ATEMPM(I,J)=0.0
DO 9010 K=1,17
9010 ENSIG(I,J,K)=0.0
DO 9011 I=1,19
9011 PAFO(I)=AMFO(I)=PAF1(I)=AMF1(I)=PAHO(I)=AMHO(I)=PAH1(I)=BGP(I)=
CAFPLUS(I)=AFMIN(I)=AHPLUS(I)=AHMIN(I)=AGPLUS(I)=AGMIN(I)=BGM(I)=
CAMH1(I)=PE(I)=EM(I)=0.0
PE(20)=EM(20)=0.0
DO 9012 I=1,30
9012 G(I)=XK(I)=GFUNG(I)=0.0
DO 9013 I=1,17
9013 BBB(I)=GSIG(I)=FSIG(I)=HSIG(I)=0.0
DO 9014 I=1,35
  GSIGN(I)=FSIGN(I)=HSIGN(I)=ESUBP(I)=0.0
DO 9014 J=1,26
9014 ENSIGN(I,J)=0.0
C ZERO OUT FIXED POINT TEMPORARIES.
  IAFGH = IAF   = IAG   = IAH   = IAN   = IBG   = IEJPI = INAWT =
  CINO  = IPHI  = ISIGMA= ITPT  = JPI   = J    = JUPPER= KC    =
  CKKK  = K     = LMAX12= LMAX  = L     = MB    = ME    = MJ    =
  CMN    = MP   = M     = NCAE  = NE    = NIE   = NINT  = NLKN  =
  CNLK   = NMAX1= NMAX   = NN    = NOJ1  = NOJ   = N     = O
C READ INPUT
C
  READ INPUT TAPE 7,3001,KKK,(RECORD(I),I=1,12)
302 WRITEOUTPUTTAPE6,3002
  WRITEOUTPUTTAPE6,8006
  WRITEOUTPUTTAPE6,8027,(RECORD(I),I=1,12)
  READINPUTTAPE7,3003,IAG,IAF,IAH,NMAX,LMAX,NCAE,KC,
  XITPT,NE,Q,MN,NINT
  IEJPI=KC
  IF(MN-1)3701,3702,3702
3701 NINT=12
3702 CONTINUE
  LMAX12=2*LMAX+1
  NMAX1=NMAX+1
  WRITEOUTPUTTAPE6,8006
  WRITEOUTPUTTAPE6,8006
  WRITEOUTPUTTAPE6,3004 ,KC
  WRITEOUTPUTTAPE6,8006
  DO304N=1,NMAX1
  READINPUTTAPE7,27,W(N),HI(N),PI(N)
304 WRITEOUTPUTTAPE6,27,W(N),HI(N),PI(N)
  WRITEOUTPUTTAPE6,8006
  SS=HI(1)+0.75
305 IF(SS-1.0)306,307,307
306 INAWT=1
  AWT=0.5

```



```

307 GOTO310
SS=SS-0.5
IF(SS-1.0)308,309,309
308 INAWT=0
AWT=0.0
GOTO310
309 SS=SS-0.5
GOTO305
310 TEMP=FLOATF(LMAX+1)
TEMP=TEMP+HI(1)
IF(INAWT-1)311,312,312
311 TEMP=TEMP+0.5
312 TEMP=TEMP+0.25
NOJ=XINTF(TEMP)
NOJ1=NOJ+1
IF(IAF-1)313,314,314
313 AGSUPO=0.00005
GOTO315
314 READINPUTTAPE7,3101,AGSUPO,MJ,ME,MB,MP,SIGMA,U,DELTA,ZPLS,ZMIN
IF(MJ-1)3141,3142,3142
3141 SIGMA=6.0
ISIGMA=4
GOTO3143
3142 ISIGMA=XINTF(0.5*SIGMA+1.25)
3143 IF(ME-1)3144,3145,3146
3144 IPHI=0
GOTO3147
3145 U=8.0
DELTA=0.12
IPHI=1
GOTO3147
3146 IPHI=1
3147 IF(MP-1)3148,3148,3149
3148 ZPLS=1.0
ZMIN=1.0
3149 WRITEOUTPUTTAPE6,3005,AGSUPO
WRITEOUTPUTTAPE6,8006
WRITE OUTPUT TAPE 6,3102
WRITEOUTPUTTAPE6,26,SIGMA,U,DELTA,ZPLS,ZMIN
IF(MB-1)3150,105,105
3150 IBG=0
GOTO315
105 READINPUTTAPE7,25,(PE(JPI),JPI=1,NOJ1)
WRITE OUTPUT TAPE 6,8006
WRITE OUTPUT TAPE 6,8011
WRITE OUTPUT TAPE 6,8008,(PE(JPI),JPI=1,NOJ1)
READINPUTTAPE7,25,(EM(JPI),JPI=1,NOJ1)
WRITE OUTPUT TAPE 6,8006
WRITE OUTPUT TAPE 6,8012
WRITE OUTPUT TAPE 6,8008,(EM(JPI),JPI=1,NOJ1)
IBG=1
315 IF(IAF-1)318,316,316
316 READINPUTTAPE7,26,FNU
WRITEOUTPUTTAPE6,3006,FNU
AWTA=AWT
WRITEOUTPUTTAPE6,3007
DO317N=1,NOJ
READINPUTTAPE7,26,PAFO(N),AMFO(N),PAF1(N),AMF1(N)
WRITEOUTPUTTAPE6,26 ,AWTA,PAFO(N),AMFO(N),PAF1(N),AMF1(N)
317 AWTA=AWTA+1.0

```

```

318 IF(IAH-1)321,319,319
319 READINPUTTAPE7,26,HNU
WRITEOUTPUTTAPE6,8006
WRITEOUTPUTTAPE6,3009,HNU
AWTA=AWT
WRITEOUTPUTTAPE6,3010
DO320N=1,NOJ
READINPUTTAPE7,26,PAHO(N),AMHO(N),PAH1(N),AMH1(N)
WRITEOUTPUTTAPE6,26 ,AWTA,PAHO(N),AMHO(N),PAH1(N),AMH1(N)
320 AWTA=AWTA+1.0
321 CONTINUE

```

C
C
C

CALCULATE G(K) ETC.

```

1801 FNINT=FLOATF(NINT)
DO 1807 K=1,NINT
TEMP=FLOATF(K)
TEMP1=3.141592654*(2.0*TEMP-1.0)/(2.0*FNINT)
G(K)=SINF(TEMP1)
TEMP=COSF(TEMP1)
1807 XK(K)=0.5*(1.0+TEMP)
FINAWT=2.045/(2.0*HI(1)+1.0)
IF(IPHI-1) 1902,1809,1901
1901 IERR=1701
GO TO 9500
1902 PHIU=1.0
GO TO 1813
1809 TEMP=0.0
CALL PHI (DELTA,TEMP,U,PHIU)
1813 IF(INAWT-1)1825,1814,1814
1814 INO=XINTF(HI(1)+1.25)
TEMP1=FHALE(INO,ISIGMA)
INO=INO+1
TEMP1=TEMP1+FHALE(INO,ISIGMA)
GO TO 1835
1825 INO=XINTF(HI(1)+0.75)
TEMP1=FINT(INO,ISIGMA)
INO=INO+1
TEMP1=TEMP1+FINT(INO,ISIGMA)
1835 AFPHI=AGSUPO/(TEMP1*PHIU)
TEMP=0.5+HI(1)
IF (INAWT-1) 1865,1855,1850
1850 IERR=3472
GO TO 9500
1855 TEMP=TEMP+0.5
GO TO 1870
1865 TEMP=TEMP+1.0
1870 TEMP=TEMP+0.25
JUPPER=XINTF(TEMP)
JUPPER=JUPPER+LMAX
WRITEOUTPUTTAPE6,1370

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TRANSMISSION COEFFICIENT INPUT

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3186 NIE=0
186 NIE=NIE+1
322 READ INPUT TAPE 7,26,E
323 PHPH=Q
327 WRITEOUTPUTTAPE6,3011,E
WRITEOUTPUTTAPE6,3012,PPH

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```

WRITEOUTPUTTAPE6,8006
WRITEOUTPUTTAPE6,3913
WRITEOUTPUTTAPE6,8006
328 DO329NLK=1,NMAX1
READINPUTTAPE7,26,(A(NLK,NN),NN=1,LMAX12)
329 WRITEOUTPUTTAPE6,3914,(A(NLK,NN),NN=1,LMAX12)
DO330NN=1,LMAX12
SS=A(1,NN)
IF (PHPH) 9003,9002,9003
9002 TEMP1=SS
BBB(NN)=0.0
GO TO 330
9003 TEMP=SQRTF(1.0-PHPH*SS)
TEMP1=SS+(1.0-TEMP)*(1.0-TEMP)/PHPH
BBB(NN)=0.1591549*(SS-TEMP1)
330 A(1,NN)=0.1591549*TEMP1
IF(NMAX1-1)333,333,331
331 DO332NLK=2,NMAX1
DO332NN=1,LMAX12
SS=A(NLK,NN)
IF (PHPH) 9001,9000,9001
9000 TEMP1=SS
GO TO 332
9001 TEMP=SQRTF(1.0-PHPH*SS)
TEMP1=SS+(1.0-TEMP)*(1.0-TEMP)/PHPH
332 A(NLK,NN)=0.1591549*TEMP1
333 IAN=2
204 IF (IPHI-1) 2041,2043,2040
2040 IERR=2040
GO TO 9500
2041 PHIUE=1.0
GO TO 205
2043 CALL PHI (DELTA,E,U,PHIUE)
205 CONTINUE
C
C
C      AG(E,J,P) ETC.
400 DO 423 JPI=1,JUPPER
IF (INAWT-1) 405,403,402
402 IERR=402
GO TO 9500
403 TEMP=FHALE(JPI+1,ISIGMA)
GO TO 406
405 TEMP=FINT(JPI,ISIGMA)
406 TEMP1=AFPHI*TEMP*PHIUE
AGPLUS(JPI)=TEMP1*ZPLS
AGMIN(JPI)=TEMP1*ZMIN
IF (IAF-1) 414,411,410
410 IERR=410
GO TO 9500
411 AFPLUS(JPI)=PAFO(JPI)+PAF1(JPI)*E
AFMIN(JPI)=AMFO(JPI)+AMF1(JPI)*E
GO TO 416
414 AFPLUS(JPI)=0.0
AFMIN(JPI)=0.0
416 IF (IAH-1) 421,418,417
417 IERR=417
GO TO 9500
418 AHPLUS(JPI)=PAHO(JPI)+PAH1(JPI)*E
AHMIN(JPI)=AMHO(JPI)+AMH1(JPI)*E

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GO TO 423
421 AHPLUS(JPI)=0.0
    AHMIN(JPI)=0.0
423 CONTINUE

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                BG(E,J,P)
500 IF (IBG-1) 502,506,501
501 IERR=501
    GO TO 9500
502 DO 504 JPI=1,JUPPER
    BGP(JPI)=1.0
504 BGM(JPI)=1.0
    GO TO 800
506 DO 730 JPI=1,JUPPER
    IF (INAWT-1) 700,512,511
511 IERR=511
    GO TO 9500
512 IF (JPI-1) 513,550,515
513 IERR=513
    GO TO 9500
515 FTEMP1=FHALE(JPI,ISIGMA)
    FTEMP2=FHALE(JPI+1,ISIGMA)
    FTEMP3=FHALE(JPI+2,ISIGMA)
    SUMINV=FTEMP1+FTEMP3+FTEMP2
525 EJPI=EM(JPI-1)
    IF (EJPI-E) 529,527,527
527 SUMUPP=FTEMP1
    GO TO 532
529 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
    TEMP=PSIBAR/PHIUE
    SUMUPP=FTEMP1*TEMP
532 EJPI=EM(JPI)
    IF (EJPI-E) 536,534,534
534 SUMUPP=SUMUPP+FTEMP2
    GO TO 539
536 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
    TEMP=PSIBAR/PHIUE
    SUMUPP=FTEMP2*TEMP+SUMUPP
539 EJPI=EM(JPI+1)
    IF (EJPI-E) 543,541,541
541 SUMUPP=FTEMP3+SUMUPP
    GO TO 546
543 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
    TEMP=PSIBAR/PHIUE
    SUMUPP=FTEMP3*TEMP+SUMUPP
546 BGP(JPI)=SUMUPP/SUMINV
    EJPI=PE(JPI-1)
    IF (EJPI-E) 629,627,627
627 SUMUPM=FTEMP1
    GO TO 632
629 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
    TEMP=PSIBAR/PHIUE
    SUMUPM=FTEMP1*TEMP
632 EJPI=PE(JPI)
    IF (EJPI-E) 636,634,634
634 SUMUPM=SUMUPM+FTEMP2
    GO TO 639
636 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
    TEMP=PSIBAR/PHIUE

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```

SUMUPM=FTEMP2*TEMP+SUMUPM
639 EJPI=PE(JPI+1)
IF (EJPI-E) 643,641,641
641 SUMUPM=FTEMP3+SUMUPM
GO TO 646
643 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
TEMP=PSIBAR/PHIUE
SUMUPM=FTEMP3*TEMP+SUMUPM
646 BGM(JPI)=SUMUPM/SUMINV
GO TO 730
550 FTEMP1=FHALE(2,ISIGMA)
FTEMP2=FHALE(3,ISIGMA)
SUMINV=FTEMP1+FTEMP2
EJPI=EM(1)
IF (EJPI-E) 564,562,562
562 SUMUPP=FTEMP1
GO TO 567
564 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
TEMP=PSIBAR/PHIUE
SUMUPP=FTEMP1*TEMP
567 EJPI=EM(2)
IF (EJPI-E) 571,569,569
569 SUMUPP=SUMUPP+FTEMP2
GO TO 574
571 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
TEMP=PSIBAR/PHIUE
SUMUPP=FTEMP2*TEMP+SUMUPP
574 BGP(1)=SUMUPP/SUMINV
EJPI=PE(1)
IF (EJPI-E) 664,662,662
662 SUMUPM=FTEMP1
GO TO 667
664 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
TEMP=PSIBAR/PHIUE
SUMUPM=FTEMP1*TEMP
667 EJPI=PE(2)
IF (EJPI-E) 671,669,669
669 SUMUPM=SUMUPM+FTEMP2
GO TO 674
671 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
TEMP=PSIBAR/PHIUE
SUMUPM=FTEMP2*TEMP+SUMUPM
674 BGM(1)=SUMUPM/SUMINV
GO TO 730
700 IF (JPI-1) 701,702,725
701 IERR=701
GO TO 9500
702 EJPI=EM(2)
IF (EJPI-E) 705,704,704
704 BGP(1)=1.0
GO TO 712
705 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
706 BGP(1)=PSIBAR/PHIUE
712 EJPI=PE(2)
713 IF (EJPI-E) 715,714,714
714 BGM(1)=1.0
7141 GO TO 730
715 CALL PSI (E,U,EJPI,DELTA,PSIBAR)
BGM(1)=PSIBAR/PHIUE
GO TO 730

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```

725 FTEMP1=FINT(JPI-1,ISIGMA)
    FTEMP2=FINT(JPI,ISIGMA)
    FTEMP3=FINT(JPI+1,ISIGMA)
    SUMINV=FTEMP1+FTEMP2+FTEMP3
    GO TO 525

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730 CONTINUE

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SUMS OVER L AND K

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800 DO 1285 NN=1,LMAX12
    GSIG(NN)=0.0
    FSIG(NN)=0.0
    HSIG(NN)=0.0
    DO 810 NLK=1,NMAX1
    DO 810 NLKN=1,LMAX12
810  ENSIG(NLK,NN,NLKN)=0.0
    CALL ELKAY (NN,VLN,VKN)
    DO 1261 JPI=1,JUPPER
    IF (INAWT-1) 860,857,856
856  IERR=756
    GO TO 9500
857  VJ=FLOATF(JPI)
    VJ=VJ-0.5
    GO TO 870
860  VJ=FLOATF(JPI-1)
870  PATOT=AGPLUS(JPI)+AFPLUS(JPI)+AHPLUS(JPI)
    AMTOT=ACMIN(JPI)+AFMIN(JPI)+AHMIN(JPI)
    SUMINP=0.0
    SUMINM=0.0
    DO 923 LKN=1,NMAX1
    SUMOTP=0.0
    SUMOTM=0.0
    DO 921 N=1,LMAX12
    CALL ELKAY (N,VL,VK)
    VI=HI(LKN)
    PIEN=PI(LKN)
    WOFN=W(LKN)
    PIE=1.0
    CALL ANEJLK (VJ,VK,VL,VI,PIE,PIEN,E,WOFN,
    IF (AOFN-1.0) 911,908,907
907  IERR=707
    GO TO 9500
908  ATEMPPP(LKN,N)=A(LKN,N)
    ATEMPM(LKN,N)=0.0
    GO TO 920
911  ATEMPPP(LKN,N)=0.0
    PIE=-1.0
    CALL ANEJLK (VJ,VK,VL,VI,PIE,PIEN,E,WOFN,AOFN)
    IF (AOFN-1.0) 918,916,915
915  IERR=715
    GO TO 9500
916  ATEMPM(LKN,N)=A(LKN,N)
    GO TO 920
918  ATEMPM(LKN,N)=0.0
920  SUMOTP=SUMOTP+ATEMPPP(LKN,N)
921  SUMOTM=SUMOTM+ATEMPM(LKN,N)
    SUMINP=SUMOTP+SUMINP
923  SUMINM=SUMOTM+SUMINM
    PATOT=PATOT+SUMINP
    AMTOT=AMTOT+SUMINM

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AOFN)


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951 IF (ATEMPP(1,NN)-0.0) 953,951,955
952 IF (ATEMPM(1,NN)-0.0) 953,952,960
953 IERR=753
   GO TO 9500
955 TEMPPO=ATEMPP(1,NN)
   PIE=1.0
   TEMPAG=AGPLUS(JPI)
   TEMPBG=BGP(JPI)
   TEMPFA=AFPLUS(JPI)
   TEMPAH=AHPLUS(JPI)
   TEMPAP=PATOT
   GO TO 964
960 TEMPPO=ATEMPM(1,NN)
   PIE=-1.0
   TEMPAG=AGMIN(JPI)
   TEMPBG=BGM(JPI)
   TEMPFA=AFMIN(JPI)
   TEMPAH=AHMIN(JPI)
   TEMPAP=AMTOT
964 TEMPJ=2.0*VJ+1.0
   IF (IEJPI-1) 967,1020,1020
967 ANAWTA=TEMPPO/TEMPA
   GSIG(NN)=GSIG(NN)+ANAWTA*TEMPAG*TEMPBG*TEMPJ
   FSIG(NN)=FSIG(NN)+ANAWTA*TEMPFA*TEMPJ
   HSIG(NN)=HSIG(NN)+ANAWTA*TEMPAH*TEMPJ
   TEMPP=ATEMPP(1,NN)/PATOT
   TEMPM=ATEMPM(1,NN)/AMTOT
   DO 1010 NLK=1,NMAX1
   DO 1010 NLKN=1,LMAX12
   CALL ELKAY (NLKN,VL,VK)
   VI=HI(NLK)
   PIEN=PI(NLK)
   WOFN=W(NLK)
   PIEK=1.0
   CALL ANEJLK (VJ,VK,VL,VI,PIEK,PIEN,E,WOFN,ACFN)
   IF (ACFN-1.0) 1004,1002,1001
1001 IERR=1001
   GO TO 9500
1002 ATEMP=A(NLK,NLKN)
   ENSIG(NLK,NN,NLKN)=ENSIG(NLK,NN,NLKN)+ATEMP*
X      TEMPP*TEMPJ
   GO TO 1010
1004 PIEK=-1.0
   CALL ANEJLK (VJ,VK,VL,VI,PIEK,PIEN,E,WOFN,ACFN)
   IF (ACFN-1.0) 1010,1008,1007
1007 IERR=1007
   GO TO 9500
1008 ATEMP=A(NLK,NLKN)
   ENSIG(NLK,NN,NLKN)=ENSIG(NLK,NN,NLKN)+ATEMP*
X      TEMPM*TEMPJ
1010 CONTINUE
1011 GO TO 1261
C
C      CALCULATE INTEGRAND CASE 1
C
1020 IF (PIE+1.0) 1100,1061,1021
1021 DO 1049 K=1,NINT
1022 XK1=XK(K)
1023 TEMP1=AGPLUS(JPI)*(1.0-XK1)/(PATOT*XK1)

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1024 IF (TEMP1-85.0) 5027,1025,1025
1025 TEMP1=0.123456E38
1026 GO TO 1028
5027 TEMP3=ACPLUS(JPI)/PATOT
5028 IF (TEMP3-0.0001) 5029,5029,5031
5029 TEMP1=1.0
5030 GO TO 5527
5031 TEMP1=EXPF(TEMP1)
5032 GO TO 5527
5527 TEMP4=ATEMPP(1,NN)/PATOT
5528 IF (TEMP4-0.0001) 5529,1027,1027
5529 TEMP1=XK1*XK1*TEMP1
5530 GO TO 1028
1027 TEMP1=XK1*XK1*TEMP1*(1.0+2.0*ATEMPP(1,NN)*
X (1.0-XK1)/(PATOT*XK1))
1028 PROD11=1.0
1029 DO 1047 N=1,LMAX12
1030 PROD21=1.0
1031 CALL ELKAY(N,VEL,VEK)
1032 DO 1046 LK=1,NMAX1
1033 VI=HI(LK)
1034 PIEN=PI(LK)
1035 WOFN=W(LK)
1036 PIEK=1.0
1037 CALL ANEJLK (VJ,VEK,VEL,VI,PIEK,PIEN,E,WOFN,AOFN)
1038 IF (AOFN-1.0) 1040,1042,1039
1039 IERR=1037
GO TO 9500
1040 ANAWTP=0.0
1041 GO TO 1045
1042 ANAWTP=A(LK,N)
1045 CALL PROCD (ANAWTP,PATOT,XK1,DBPROD)
IF EXPONENT FAULT 1044,1044
1044 PROD21=PROD21*DBPROD
4044 IF EXPONENT FAULT 4045,1046
4045 PROD21=0.123456E38
1046 CONTINUE
PROD11=PROD21*PROD11
4047 IF EXPONENT FAULT 4048,1047
4048 PROD11=0.123456E38
1047 CONTINUE
AE=PATOT
TEMPX=(1.0-XK1)/XK1
TEMP5=2.0/AE
ASUBFE=AFPLUS(JPI)
ASUBH=AHPLUS(JPI)
IF (ASUBFE-1.0E-25) 4026,4026,4126
4126 TEMP=ASUBFE/AE
IF (TEMP-0.0001) 4026,4028,4028
4026 TEMPNE=1.0
GO TO 4029
4028 TEMPNE=(1.0+TEMP5*(ASUBFE/FNU)*TEMPX)**(FNU/2.0)
4029 IF (ASUBH-1.0E-25) 4032,4032,4130
4130 TEMP=ASUBH/AE
IF (TEMP-0.0001) 4032,4030,4030
4030 TEMPNH=(1.0+TEMP5*(ASUBH/HNU)*TEMPX)**(HNU/2.0)
GO TO 4033
4032 TEMPNH=1.0
4033 GFUNG(K)=PROD11*TEMP1*TEMPNE*TEMPNH
IF EXPONENT FAULT 4034,1049

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4034 GFUNG(K)=0.123456E38
1049 CONTINUE
1050 GO TO 1101

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C
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CALCULATE INTEGRAND CASE 2

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1061 DO 1089 K=1,NINT
1062 XK1=XK(K)
1063 TEMP2=AGMIN(JPI)*(1.0-XK1)/(AMTOT*XK1)
1064 IF (TEMP2-85.0) 5067,1065,1065
1065 TEMP2=0.123456E38
1066 GO TO 1068
5067 TEMP3=AGMIN(JPI)/AMTOT
5068 IF (TEMP3-0.0001) 5069,5069,5071
5069 TEMP2=1.0
5070 GO TO 5567
5071 TEMP2=EXP(-TEMP2)
5072 GO TO 5567
5567 TEMP4=ATEMPM(1,NN)/AMTOT
5568 IF (TEMP4-0.0001) 5569,1067,1067
5569 TEMP2=XK1*XK1*TEMP2
5570 GO TO 1068
1067 TEMP2=XK1*XK1*TEMP2*(1.0+2.0*ATEMPM(1,NN)*
X      (1.0-XK1)/(AMTOT*XK1))
1068 PROD12=1.0
1069 DO 1087 N=1,LMAX12
1070 PROD22=1.0
1071 CALL ELKAY(N,VEL,VEK)
1072 DO 1086 LK=1,NMAX1
1073 VI=HI(LK)
1074 PIEN=PI(LK)
1075 WOFN=W(LK)
1076 PIEK=-1.0
1077 CALL ANEJLK(VJ,VEK,VEL,VI,PIEK,PIEN,E,WOFN,
X      ACFN)
1078 IF (ACFN-1.0) 1080,1082,1079
1079 IERR=1077
      GO TO 9500
1080 ANAWTM=0.0
1081 GO TO 1085
1082 ANAWTM=A(LK,N)
1085 CALL PROC (ANAWTM,AMTOT,XK1,DBPROD)
      IF EXPONENT FAULT 1084,1084
1084 PROD22=PROD22*DBPROD
4084 IF EXPONENT FAULT 4085,1086
4085 PROD22=0.123456E38
1086 CONTINUE
      PROD12=PROD22*PROD12
4087 IF EXPONENT FAULT 4088,1087
4088 PROD12=0.123456E38
1087 CONTINUE
      AE=AMTOT
      TEMPX=(1.0-XK1)/XK1
      TEMPS=2.0/AE
      ASUBFE=AFMIN(JPI)
      ASUBH=AHMIN(JPI)
      IF (ASUBFE-1.0E-25) 4526,4526,4626
4626 TEMP=ASUBFE/AE
      IF (TEMP-0.0001) 4526,4528,4528
4526 TEMPNE=1.0

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GO TO 4529
4528 TEMPNE=(1.0+TEMP5*(ASUBFE/FNU)*TEMPX)**(FNU/2.0)
4529 IF (ASUBH-1.0E-25) 4532,4532,4630
4630 TEMP=ASUBH/AE
      IF (TEMP-0.0001) 4532,4530,4530
4530 TEMPNH=(1.0+TEMP5*(ASUBH/HNU)*TEMPX)**(HNU/2.0)
      GO TO 4533
4532 TEMPNH=1.0
4533 GFUNG(K)=PROD12*TEMP2*TEMPNE*TEMPNH
      IF EXPONENT FAULT 4534,1089
4534 GFUNG(K)=0.123456E38
1089 CONTINUE
1090 GO TO 1101

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C
C
C SIGMA CAPTURE

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1100 IERR=1100
      GO TO 9500
1101 IF (IEJPI-1) 1109,1107,1111
1107 TEMP=TEMPAO*TEMPAG/(TEMPA*TEMPA)
1108 IF (TEMP-0.0001) 1109,1109,1111
1109 EYE=1.0
1110 GO TO 1115
1111 SUMK=0.0
5112 DO 5116 K=1,NINT
5115 SUMK=SUMK+G(K)/GFUNG(K)
5116 CONTINUE
1114 EYE=3.141592654*SUMK/(2.0*FNINT)
1115 GSIG(NN)=GSIG(NN)+TEMPAO*TEMPJ*EYE*TEMPAG
      X           *TEMPBG/TEMPA

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C
C
C SIGMA FISSION

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1118 IF (IEJPI-1) 1122,1120,1124
1120 TEMP=TEMPAO*TEMPFA/(TEMPA*TEMPA)
1121 IF (TEMP-0.0001) 1122,1122,1124
1122 EYE=1.0
1123 GO TO 1130
1124 TEMP=2.0*TEMPFA/(FNU*TEMPA)
1125 SUMK=0.0
5126 DO 5131 K=1,NINT
6129 TEMP5=TEMPFA/TEMPA
6130 IF (TEMP5-0.0001) 6131,5129,5129
6131 TEMPT=1.0
6132 GO TO 5130
5129 TEMPT=1.0+(1.0-XK(K))*TEMP/XK(K)
5130 SUMK=SUMK+(G(K)/GFUNG(K))/TEMPT
5131 CONTINUE
1129 EYE=3.141592654*SUMK/(2.0*FNINT)
1130 FSIG(NN)=FSIG(NN)+TEMPAO*TEMPJ*EYE*TEMPFA/           TEMPA

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C
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C SIGMA H

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1135 IF (IEJPI-1) 1142,1140,1144
1140 TEMP=TEMPAO*TEMPAH/(TEMPA*TEMPA)
1141 IF (TEMP-0.0001) 1142,1142,1144
1142 EYE=1.0
1143 GO TO 1150
1144 TEMP=2.0*TEMPAH/(HNU*TEMPA)
1145 SUMK=0.0

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```

5146 DO 5151 K=1,NINT
6149 TEMP5=TEMPAH/TEMPA
6150 IF (TEMP5-0.0001) 6151,5149,5149
6151 TEMPT=1.0
6152 GO TO 5150
5149 TEMPT=1.0+(1.0-XK(K))*TEMP/XK(K)
5150 SUMK=SUMK+(G(K)/GFUNG(K))/TEMPT
5151 CONTINUE
1149 EYE=3.141592654*SUMK/(2.0*FNINT)
1150 HSIG(NN)=HSIG(NN)+TEMPAO*TEMPJ*EYE*TEMPAH/      TEMPA
C
C      SIGMA SCATTERING
C
1200 DO 1260 NLK=1,NMAX1
1205 DO 1260 NLKN=1,LMAX12
1210 CALL ELKAY (NLKN,VEL,VEK)
1220 VI=HI(NLK)
1221 PIEN=PI(NLK)
1222 WOFN=W(NLK)
1223 CALL ANEJLK (VJ,VEK,VEL,VI,PIE,PIEN,E,WOFN,
X      AOFN)
1224 IF (AOFN-1.0) 1226,1228,1225
1225 IERR=1225
GO TO 9500
1226 AN=0.0
1227 GO TO 1260
1228 AN=A(NLK,NLKN)
1251 IF (KC-1) 1231,1229,1241
1229 TEMP=TEMPAO*AN/(TEMPA*TEMPA)
1230 IF (TEMP-0.0001) 1231,1231,1241
1231 EYE=1.0
1232 GO TO 1255
1241 IF (NLK-1) 1246,1242,1246
1242 IF (VLN-VEL) 1246,1243,1246
1243 IF (VKN-VEK) 1246,1244,1246
1244 GELTA=3.0
1245 GO TO 1247
1246 GELTA=1.0
1247 TEMP=2.0*AN/TEMPA
1250 SUMK=0.0
5251 DO 5256 K=1,NINT
6254 TEMP5=AN/TEMPA
6255 IF (TEMP5-0.0001) 6256,5254,5254
6256 TEMPT=1.0
6257 GO TO 5255
5254 TEMPT=1.0+TEMP*(1.0-XK(K))/XK(K)
5255 SUMK=SUMK+(G(K)*GELTA/GFUNG(K))/TEMPT
5256 CONTINUE
1254 EYE=3.141592654*SUMK/(2.0*FNINT)
1255 ENSIG(NLK,NN,NLKN)=ENSIG(NLK,NN,NLKN)+TEMPJ*
X      TEMPAO*AN*EYE/TEMPA
1260 CONTINUE
1261 CONTINUE
1270 TEMP=FINAWT/E
1271 GSIG(NN)=TEMP*GSIG(NN)
1272 FSIG(NN)=TEMP*FSIG(NN)
1273 HSIG(NN)=TEMP*HSIG(NN)
1280 DO 1282 NLK=1,NMAX1
1281 DO 1282 NLKN=1,LMAX12
1282 ENSIG(NLK,NN,NLKN)=TEMP*ENSIG(NLK,NN,NLKN)

```

```

      IF(KKK-7)334,334,3341
3341 GOTO1285
      334 ENSIG(1,NN,NN)=ENSIG(1,NN,NN)+TEMP*BBB(NN)*TEMPJ
1285 CONTINUE

```

C
C
C

SUM OVER INCIDENT CHANNELS

```

1300 GSIZE=0.0
1301 FSIGE=0.0
1302 HSIGE=0.0
1305 DO 1308 NN=1,LMAX12
1306 GSIZE=GSIGE+GSIG(NN)
1307 FSIGE=FSIGE+FSIG(NN)
1308 HSIGE=HSIGE+HSIG(NN)
1310 DO 1314 NLK=1,NMAX1
1311 ENSIGE(NLK)=0.0
1312 DO 1314 NN=1,LMAX12
1313 DO 1314 NLKN=1,LMAX12
1314 ENSIGE(NLK)=ENSIGE(NLK)+ENSIG(NLK,NN,NLKN)

```

C
C
C

WRITE OUTPUT MATRIX

```

335 CONTINUE
336 IF(ITPT-1)337,338,338
337 WRITEOUTPUTTAPE6,1370
      GOTO1427
338 IF(IAG-1)339,342,342
339 IF(IAF-1)340,342,342
340 IF(IAH-1)341,342,342
341 IAFGH=0
      GOTO3431
342 WRITEOUTPUTTAPE6,8006
      WRITEOUTPUTTAPE6,3013
      IAFGH=2
      WRITEOUTPUTTAPE6,8006
      DO343NN=1,LMAX12
      CALLELKAY(NN,FLN,FKN)
343 WRITEOUTPUTTAPE6,3014,FLN,FKN,GSIG(NN),FSIG(NN),HSIG(NN)
3431 WRITEOUTPUTTAPE6,8006
      WRITEOUTPUTTAPE6,3015
      DO346NLK=1,NMAX1
      M=NLK-1
      IF(E-W(NLK))346,346,344
344 CONTINUE
      WRITEOUTPUTTAPE6,3016,M,W(NLK),ENSIGE(NLK)
      WRITEOUTPUTTAPE6,8006
      DO345NN=1,LMAX12
      CALLELKAY(NN,FLN,FKN)
      WRITEOUTPUTTAPE6,3017,FLN,FKN,(ENSIG(NLK,NN,NLKN),
      XNLKN=1,LMAX12)
345 CONTINUE
346 CONTINUE
347 CONTINUE

```

C
C
C

WRITE OUTPUT SUMMARY

```

1427 GSIGN(NIE)=GSIGE
1428 FSIGN(NIE)=FSIGE
1429 HSIGN(NIE)=HSIGE
1430 DO 1431 NLK=1,NMAX1

```



```

1431 ENSIGN(NIE,NLK)=ENSIGE(NLK)
1432 ESUBP(NIE)=E
      WRITEOUTPUTTAPE6,1370
3432 IF(NIE-NE)186,348,348
348 CONTINUE
349 WRITEOUTPUTTAPE6,3018
      WRITEOUTPUTTAPE6,3019
      WRITEOUTPUTTAPE6,8006
      DO350NIE=1,NE
350 WRITEOUTPUTTAPE6,3020,ESUBP(NIE),(ENSGN(NIE,NLK),NLK=1,NMAX1)
      IF(IAFGH-1)351,352,352
351 GOTO1501
352 WRITEOUTPUTTAPE6,8006
      WRITEOUTPUTTAPE6,3022
      WRITEOUTPUTTAPE6,8006
353 DO354NIE=1,NE
354 WRITEOUTPUTTAPE6,3020,ESUBP(NIE),GSGN(NIE),FSIGN(NIE),HSIGN(NIE)
355 GOTO1501
1501 GOTO301

```

C
C
C

FORMAT STATEMENTS

```

25 FORMAT (6E12.6)
26 FORMAT (6F12.8)
27 FORMAT (2X,F8.6,30X,2F10.6)
1370 FORMAT(1H1)
3001 FORMAT(I3,12A6)
3002 FORMAT(116H1
      XNEARREX SEPT 1964 MOLDAUER-ENGELBRECHT-DUFFY)
3003 FORMAT(I5,4I2,2I1,2I2,F13.8,2I2)
3004 FORMAT(44H ENERGY LEVELS KC = 12)
3005 FORMAT(13HOA(GAMMA) = F15.9)
3006 FORMAT(10HONU(F) = F8.4)
3007 FORMAT(58HO J PAFO AMFO PAF1 AM
      1F1)
3009 FORMAT(10HONU(H) = F8.4)
3010 FORMAT(58HO J PAHO AMHO PAH1 AM
      1H1)
3011 FORMAT(11HOENERGY = F20.8)
3012 FORMAT(51H
3013 FORMAT(54HOCROSS SECTIONS FOR CAPTURE FISSION Q = F8.5)
3014 FORMAT(1H F13.2,F5.2,3F13.6) OTHER)
3015 FORMAT(30HOCROSS SECTIONS FOR SCATTERING)
3016 FORMAT(23HOEXCITED LEVEL NUMBER 13,14H W(N) = F10.6,20H
      X SIGMA(N,E) = F14.8)
3017 FORMAT(1H 2F5.2,5H 9F11.7/(16H 9F11.7))
3018 FORMAT(26H SCATTERING CROSS SECTIONS)
3019 FORMAT(108HO ENERGY ELASTIC LEVEL 1 LEVEL 2 LEVEL 3
      X LEVEL 4 LEVEL 5 LEVEL 6 LEVEL 7 LEVEL 8)
3020 FORMAT(1H 10F11.7)
3021 FORMAT(21HOOTHER CROSS SECTIONS)
3022 FORMAT(41HO ENERGY CAPTURE FISSION OTHER)
3101 FORMAT(F12.8,2I2,2I1,F6.2,4F10.5)
3102 FORMAT(55HO SIGMA U DELTA ZPLS ZMIN)
3913 FORMAT(26H TRANSMISSION COEFFICIENTS)
3914 FORMAT(1H 9F12.8)
8006 FORMAT(1HO)
8008 FORMAT(8E15.6)
8011 FORMAT(31HOE SUB J AND PI FOR PI POSITIVE)
8012 FORMAT(31HOE SUB J AND PI FOR PI NEGATIVE)

```

```

8027 FORMAT(12A6)
9105 FORMAT(1X,18H***** ERR = ,I4)
C
9500 WRITE OUTPUT TAPE 6,9105,IERR
      MESS=7HO HELL.
      CALL Q8QERROR(0,MESS)
      END
      SUBROUTINE ELKAY(NN,FLN,FKN)
1       TEMP=FLOATF(NN)
5       TEMP1=TEMP/2.0
10      TEMP2=(TEMP-1.0)/2.0
15      ITEMP=XMODF(NN,2)
20      IF (ITEMP-1) 45,30,25
25      IERR=25
      GO TO 9500
30      FLN=TEMP2
35      FKN=TEMP1
40      GO TO 55
45      FLN=TEMP1
50      FKN=TEMP2
55      RETURN
9500 WRITE OUTPUT TAPE 6,9105,IERR
      MESS=7HO HELL.
      CALL Q8QERROR(0,MESS)
9105 FORMAT(1X,18H***** ERR = ,I4)
      END
      SUBROUTINE PHI(DELTA,E,U,PHIUE)
5       TEMP=6.57975*(U+E)/DELTA
10      TEMPR=SQRTF(TEMP)
15      XINV=1.0/TEMPR
20      POLY4=1.0+XINV*(XINV*(45.0-105.0*XINV*(1.0-
25      TEMP1=TEMP*TEMP
30      TEMP2=EXPF(TEMPR)
35      PHIUE=TEMP1*TEMP2*POLY4
40      RETURN
      END
      SUBROUTINE PSI (E,U,EJPI,DELTA,PSIBAR)
C
5       X=SQRTF(6.57975*(U+E)/DELTA)
10      XJPI=SQRTF(6.57975*(U+EJPI)/DELTA)
15      TEMP1=XJPI/X
17      TEMP1=TEMP1*TEMP1
20      TEMP2=1.0-TEMP1
25      TEMP3=TEMP2*TEMP2
30      TEMP4=TEMP3*TEMP2
35      TEMP5=X*X
40      TEMP6=TEMP5*TEMP5
45      TEMP7=TEMP5*TEMP6
50      TEMP17=7.0*TEMP1
55      TEMP37=3.0-TEMP17
60      TEMP17=1.0-TEMP17
65      TEMP=TEMP4-TEMP3*TEMP17/XJPI-6.0
      X      *TEMP2*TEMP37/TEMP5+6.0*(3.0-
      X      TEMP1*(30.0-35.0*TEMP1))/(XJPI*
      X      TEMP5)
70      TEMPE=120.0*(TEMP37-3.0*TEMP17/XJPI)/
      X      TEMP6-5040.0*(1.0-1.0/XJPI)/TEMP7
75      TEMP8=EXPF(XJPI)
80      PSIBAR=TEMP8*(TEMP+TEMPE)*(TEMP5*
      X      XJPI**5.0)/48.0

```

```

85 RETURN
END
SUBROUTINE ANEJLK (VJ,VK,VL,VI,PIE,PIEN,
X      E,WOFN,AOFN)
5  IF (E-WOFN) 10,15,15
10  AOFN=0.0
11  GO TO 55
15  TEMP=ABSF(VJ-VI)
20  IF (TEMP-VK) 25,25,10
25  IF (VK-VJ-VI) 30,30,10
30  TEMP=ABSF(PIEN-PIE)
31  IF (TEMP-0.25) 35,32,45
32  IERR=32
   GO TO 9500
35  ITEMP=XINTF(VL+0.25)
36  ITEMP=XMODF(ITEMP,2)
37  IF (ITEMP-1) 38,10,40
38  AOFN=1.0
39  GO TO 55
40  IERR=40
   GO TO 9500
45  TEMP=ABSF(PIEN+PIE)
46  IF (TEMP-0.25) 50,32,47
47  IERR=47
   GO TO 9500
50  ITEMP=XINTF(VL+0.25)
51  ITEMP=XMODF(ITEMP,2)
52  IF (ITEMP-1) 10,38,40
55  RETURN
9500 WRITE OUTPUT TAPE 6,9105,IERR
      MESS=7HC HELL.
      CALL Q8QERROR(0,MESS)
9105 FORMAT(1X,18H***** ERR = ,I4)
END
SUBROUTINE PELK(FPELK,EN,VLN,VKN,ALPHA,BETA,LN1)
5  TEMP=(ALPHA-BETA*(VKN*(VKN+1.0)-VLN*(VLN+1.0)-0.75))
10  Y=EN*TEMP*TEMP
11  YINV=1.0/Y
15  GO TO (20,25,30,35,40,45,50,55,60),LN1
20  ALNY=1.0
21  GO TO 70
25  ALNY=1.0+YINV
26  GO TO 70
30  ALNY=1.0+YINV*(3.0+9.0*YINV)
31  GO TO 70
35  ALNY=1.0+YINV*(6.0+YINV*(45.0+225.0*YINV))
36  GO TO 70
40  ALNY=1.0+YINV*(10.0+YINV*(135.0+YINV*(1575.0+
X      11025.0*YINV)))
41  GO TO 70
45  ALNY=1.0+YINV*(15.0+YINV*(315.0+YINV*(6300.0+
X      YINV*(99225.0+893025.0*YINV))))
46  GO TO 70
50  ALNY=1.0+YINV*(21.0+YINV*(630.0+YINV*(18900.0+
X      YINV*(496125.0+YINV*(9823275.0+
X      10805603.0E1*YINV))))
51  GO TO 70
55  ALNY=1.0+YINV*(28.0+YINV*(1134.0+YINV*(47250.0+
X      YINV*(1819125.0+YINV*(58939650.0+YINV*
X      (14047283.0E2+18261468.0E3*YINV))))))

```

```

56 GO TO 70
60 ALNY=1.0+YINV*(36.0+YINV*(1890.0+YINV*(103950.0+
X   YINV*(5457375.0+YINV*(25540515.0E1+
X   YINV*(98330983.0E2+YINV*(27392202.0E4+
X   41088304.0E5*YINV))))))
70 TEMPR=SQRTF(Y)
75 FPELK=TEMPR/ALNY
80 RETURN
END
SUBROUTINE PRGD (ASUBN,AE,XK1,DBPROD)
11 IF (ASUBN-1.0E-25) 14,14,112
112 TEMP=ASUBN/AE
113 IF (TEMP-0.0001) 14,5,5
5   TEMPX=(1.0-XK1)/XK1
10  TEMPA=2.0/AE
12  DBPROD=SQRTF(1.0+TEMPA*ASUBN*TEMPX)
13  GO TO 40
14  DBPROD=1.0
40  RETURN
END

```

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