

**SIOB: A FORTRAN Code for Least-Squares
Shape Fitting Several Neutron Transmission
Measurements Using the Breit-Wigner
Multilevel Formula**

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SIOB:* A FORTRAN CODE FOR LEAST-SQUARES SHAPE FITTING
SEVERAL NEUTRON TRANSMISSION MEASUREMENTS USING
THE BREIT-WIGNER MULTILEVEL FORMULA

G. de Saussure, D. K. Olsen, R. B. Perez

*("...seven in one blow...", R. L. Macklin)

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ABSTRACT

The FORTRAN-IV code SIOB was developed to least-square fit the shape of neutron transmission curves. Any number of measurements on a common energy scale for different sample thicknesses can be simultaneously fitted. The computed transmission curves can be broadened with either a Gaussian or a rectangular resolution function or both, with the resolution width a function of energy. The total cross section is expressed as a sum of single-level or multilevel Breit-Wigner terms and Doppler broadened using the fast interpolation routine QUICKW. The number of data points, resonance levels and variables which can be handled simultaneously is only limited by the overall dimensions of two arrays in the program and by the stability of the matrix inversion. In a test problem seven transmissions each with 3750 data points were simultaneously fitted using 74 resonances and 110 variable parameters. The problem took 47 min. of CPU time on an IBM-91, for 3 iterations.

I. INTRODUCTION

In order to improve the accuracy of the ^{238}U resonance parameters up to a few keV, Olsen *et al.* have recently completed two series of neutron-transmission measurements, using flight paths of 40 m and 150 m successively. In both series of measurements the transmissions were obtained through several ^{238}U sample thicknesses.¹

Several existing computer codes were examined²⁻⁵ but none was found entirely suitable for the simultaneous analysis of transmissions on the same energy scale through several thicknesses. The code described herein was primarily designed for this analysis, but it was also successfully applied to the analysis of transmission data through samples composed of medium and lightweight nuclei.⁶

In Section II of this memo we give an outline of the structure of the code, which may be helpful in understanding the other sections of this report and the program. Section III discusses the expression for the theoretical transmission and shows how it is resolution broadened. In Section IV we define several expressions for the total cross-section and outline how these are Doppler broadened. Section V briefly discusses the least-square-fit algorithm and Section VI indicates the relations between two critical array dimensions in the program and the size of the fitting problem. In Section VII we explain the operation of flags by which the user indicates which parameters should be held fixed or varied by the program.

In the Appendices we give a list of the input parameters and their functions, the input and output of a sample problem, and a complete FORTRAN listing of the program.

II. BRIEF DESCRIPTION OF THE PROGRAM

The subroutines and functions used with their arguments are listed in Table I. An outline of the program is given below:

1. The main program reads all input data. A list of these data and their function is given in Appendix I. Some of the input parameters are fixed and specify the problem, other input parameters are initial guesses for parameters which can be varied, and the last input parameters are flags which have a one to one correspondence to the parameters which can be varied. These flags specify which parameters are held fixed (flag is zero) and which parameters are varied (flag is one or two).
2. After reading the input, the main program calls the subroutine PHINEQ. In this subroutine the resolution-broadened theoretical transmissions are computed and compared with the experimental transmissions to obtain the initial χ^2 called PHIOLD. In addition the normal equations for the changes in the variable parameters are constructed before control is returned to the main program.
3. The main program then calls subroutine MVP. In this subroutine the normal equations are solved through a matrix inversion in the subroutine SLV. The variable parameters are altered through addition of the proper components of the solution vector. The

TABLE I. LIST OF SUBROUTINES AND FUNCTIONS USED BY SIOB1. Subprograms called by MAIN

SUBROUTINE PHINEQ(JV)
SUBROUTINE MVP

2. Subprograms called by PHINEQ

FUNCTION RES(E, JRES)
FUNCTION BGR(E, NT)
FUNCTION WEIGHT(NT, IE)
FUNCTION SIG(E, JV)

3. Subprograms called by MVP

SUBROUTINE SLV(NV2)
SUBROUTINE PHINEQ(JV)
FUNCTION PEN(LJ, RHO)

4. Subprograms called by SIG

FUNCTION PHI2(LJ, RHO)
FUNCTION DPH(LJ, RHO)
FUNCTION SHF(LJ, RHO)
FUNCTION DSHF(LJ, RHO)
FUNCTION PEN(LJ, RHO)
FUNCTION FNS(VE, E, N)
SUBROUTINE SVS(AX, YI, REW, AIMW)

5. Subprograms called by SVS

SUBROUTINE W(REZ, AIMI, REW, AIMW)
SUBROUTINE QUICKW(AX, Y, REW, AIMW)

changes in the variable parameters are printed at each iteration. A new value of χ^2 called PHI is then computed and control returned to the main program.

4. The new value of χ^2 is compared to the previous value determined in step 2. If χ^2 has significantly decreased and if the number of iterations has not exceeded a preset number of iterations IT2, the number-of-iterations counter is incremented and the program proceeds again with step 2; otherwise, the program is terminated.

III. CALCULATED RESOLUTION BROADENED TRANSMISSION

The number NT2 of experimental transmission curves are fitted simultaneously. The trial calculated transmissions are:

$$T_{NT}(E) = (1 - \epsilon_{NT}) \cdot \int e^{-\tau_{NT}\sigma(E', \lambda_1, \lambda_2, \dots)} P(E, E') dE' + \beta_{NT} \cdot BGR(E, NT)$$

$NT = 1, 2, \dots, NT2$ (1)

where the ϵ_{NT} , τ_{NT} and β_{NT} are variable parameters which can be searched. The Doppler-broadened cross-section $\sigma(E', \lambda_1, \lambda_2, \dots)$ is a function of other variable parameters λ_i , which will be discussed in the next section. The τ_{NT} 's are the sample thicknesses, in atoms per barn, corresponding to the transmission curves $T_{NT}(E)$. If the experimental transmissions are properly normalized and if the backgrounds are properly subtracted, the values of the ϵ_{NT} and β_{NT} should vanish; however because there are experimental uncertainties associated with the normalization and with the background subtraction, it may be desirable to consider the ϵ_{NT} and β_{NT} as variables to be searched. An energy dependent background shape may be coded for each thickness, as desired, in the function $BGR(E, NT)$.

The resolution function is taken to be of the form:

$$P(E, E') = Ae^{-\left[\frac{E-E'}{R(E)}\right]^2} \quad (2)$$

where A is a normalization constant such that

$$\int P(E, E') dE' = 1 \quad (3)$$

and where the resolution width $R(E)$ may either be coded as desired in the function $RES(E, JRES)$ or, if $JRES = 0$, is taken as:

$$R(E) = [BE2 \cdot E^2 + CE3 \cdot E^3]^{1/2} \quad (4)$$

where $BE2$ and $CE3$ are fixed input parameters. Expression (4) is appropriate for time-of-flight measurement;⁷⁻¹¹ in this case:

$$BE2 = \frac{2}{3} \left(\frac{\delta L}{L} \right)^2 \text{ and } CE3 = \frac{2}{3} \left(\frac{\delta t}{\mu L} \right)^2 \quad (5)$$

where L is the flight-path length, δL is the total uncertainty in flight-path due to the finite thicknesses of the source and of the detector and to the "equivalent length" of the moderation spread; δt is the total uncertainty in timing and the constant $\mu = 72.3 \text{ eV}^{1/2} \mu\text{s}/\text{m}$. The factors $2/3$ in (5) arise from the conversion of an assumed rectangular uncertainty to an equivalent Gaussian uncertainty. For more details on resolution functions, the references should be consulted.

The convolution of Eq. (1) is approximated by the Gauss-Hermite technique:

$$\int y(x) e^{-x^2} dx \approx \sum_{NG=1}^{NG2} A_{NG} \cdot y(x_{NG}) \quad (6)$$

The values of the coefficients A_{NG} and of the roots of the Hermite polynomials x_{NG} were taken from the paper of Salzer, Zucker and Capuano.¹² $NG2$ is an input parameter which can be selected as any odd integer between 1 and 19. The precision of the approximation increases as $NG2$ increases, but so does the run time of the program. Values of $NG2$ between 5 and 9 have been found adequate for most cases. If $NG2 = 1$ the calculated transmissions are not resolution broadened.

When the experimental transmission is measured over successive rectangular time-of-flight channels of nearly equal energy widths, the resolution broadening due to the finite width of the time-of-flight channels can efficiently be represented by fitting a parabola to the compared transmissions at the energies corresponding to the center of the channels $i-1$, i , and $i+1$, and integrating that parabola over the width of the i th channel. This procedure leads to the relation:

$$T_i^* = \frac{1}{24}(T_{i-1} + 22T_i + T_{i+1}) \quad (7)$$

where T_i^* is the time-of-flight-broadened transmission in channel i , and T_i is the unbroadened transmission at the energy corresponding to the center of channel i . A "switch" $JPLY = 1$ allows the program to combine the rectangular broadening given by Eq. (7) with the Gaussian broadening given by Eq. (6).

IV. TOTAL CROSS-SECTION EXPRESSIONS

The Doppler broadened total cross-section and its derivatives with respect to the variable parameters are computed in the function *SIG*.

The basic formulae utilized are the single-level¹³ and multi-level¹⁴ Breit-Wigner formulae as defined in ENDF/B procedures.¹⁵ These formulae and their parametrization are discussed below:

A. The Single-Level-Breit-Wigner Formula

The expression for the total cross section is given by

$$\sigma_{nt}(E) = \sum_{\ell} \sigma_{nt}^{\ell}(E), \quad (8)$$

where

$$\begin{aligned} \sigma_{nt}^{\ell}(E) &= (2\ell + 1) \frac{4\pi}{k^2} \sin^2 \phi \ell \\ &+ \frac{\pi}{k^2} \sum_J g_J \sum_r \frac{\Gamma_{nr} [\Gamma_r \cos 2\phi \ell - 2(E - E_r) \sin 2\phi \ell]}{(E - E_r)^2 + \frac{1}{4} \Gamma_r^2} \end{aligned} \quad (9)$$

and where g_J is the usual spin statistical factor given by

$$g_J = \frac{2J+1}{2 \cdot (2I+1)} \quad (10)$$

The quantity I is the spin of the target nucleus and J is the spin of the resonance state. The energy dependence of the neutron width is given by:

$$\Gamma_{nr}(E) = \frac{\Gamma_{nr} (1/E_r)}{P_{\ell} (1/E_r)} \cdot P_{\ell}(E) \quad (11)$$

where E_r is the resonance level energy. The total width is given by:

$$\Gamma_r(E) = \Gamma_{nr}(E) + \Gamma_{ar} \quad (12)$$

where Γ_{ar} is the reaction width. The shifted resonance energy is given

by:

$$E'_r = E_r + \frac{S_\ell(1E_r) - S_\ell(E)}{2P_\ell(1E_r)} : \Gamma_{nr}(1E_r) \quad (13)$$

The shift factors $S_\ell(ka)$, penetration factors $P_\ell(ka)$ and phase shifts $\phi_\ell(ka)$ are given in Table II for the angular momentum values $\ell = 0, 1, 2$ and 3. The quantity k is the neutron wave number, a the channel radius and \hat{a} the effective scattering radius.

B. The Multilevel-Breit-Wigner Formula

The multilevel-Breit-Wigner expression for the cross section is the same as the single-level expression except that the level-level interference term is added; that is,

$$\begin{aligned} [\sigma_{nt}^\ell(E)]_{ML} &= [\sigma_{nt}^\ell(E)]_{SL} \\ &+ \frac{\pi}{k^2} \sum_J g_J \sum_r \sum_{s \neq r} \frac{\Gamma_{nr}\Gamma_{ns} [(E-E'_r)(E-E'_s) + 1/4\Gamma_r\Gamma_s]}{[(E-E'_r)^2 + \frac{1}{4}\Gamma_r^2] \cdot [(E-E'_s)^2 + \frac{1}{4}\Gamma_s^2]} \end{aligned} \quad (14)$$

where $[\sigma_{nt}^\ell(E)]_{SL}$ represents the cross section given in Eq. (9). The level-level interference term in Eq. (14) can be recast in a form more suitable for Doppler broadening; that is,

$$[\sigma_{nt}^\ell(E)]_{ML} = [\sigma_{nt}^\ell(E)]_{SL} + \frac{\pi}{k^2} P_\ell(E) \sum_J g_J \sum_r \frac{\Gamma_{nr} [\Gamma_r G_r - 2(E-E'_r)B_r]}{(E-E'_r)^2 + \frac{1}{4}\Gamma_r^2} \quad (15)$$

where

$$G_r = \sum_{s \neq r} \Gamma_{ns}^o \frac{g_{rs}}{g_{rs}^2 + h_{rs}^2}, \quad (16)$$

TABLE II. SHIFT FACTORS, PENETRATION FACTORS AND PHASE SHIFTS FOR ANGULAR MOMENTA $\lambda = 0, 1, 2$ and 3

Angular Momentum λ	Shift-factor $S_\lambda(\rho)$	Penetration Factor $P_\lambda(\rho)$	Phase Shift $\phi_\lambda(\rho)$
0	0	ρ	$\rho - \tan^{-1} \rho$
1	$-\frac{1}{1 + \rho^2}$	$\frac{\rho^3}{1 + \rho^2}$	$\rho - \tan^{-1} \left(\frac{3\rho}{3 - \rho^2} \right)$
2	$-\frac{18 + 3\rho^2}{9 + 3\rho^2 + \rho^4}$	$\frac{\rho^5}{9 + 3\rho^2 + \rho^4}$	$\rho - \tan^{-1} \left[\frac{\rho(\rho - 15)}{6\rho^2 - 15} \right]$
3	$-\frac{675 + 90\rho^2 + 6\rho^4}{225 + 45\rho^2 + 6\rho^4 + \rho^6}$	$\frac{\rho^7}{225 + 45\rho^2 + 6\rho^4 + \rho^6}$	$\rho - \tan^{-1} \left[\frac{\rho(\rho - 15)}{6\rho^2 - 15} \right]$

For definitions, see text below Eq. (13).

$$H_r = \sum_{s \neq r} \Gamma_{ns}^{\circ} \frac{d_{rs}}{g_{rs}^2 + h_{rs}^2}, \quad (17)$$

$$\Gamma_{ns}^{\circ} = \frac{\Gamma_{ns}(1Es1)}{P_{\ell}(1Es1)}, \quad (18)$$

$$g_{rs} = \frac{1}{2} (\Gamma_r + \Gamma_s) \text{ and } d_{rs} = E'_r - E'_s. \quad (19)$$

Through the penetration and shift factors of Eqs. (11) and (13), the terms g_{rs} and d_{rs} , and hence also G_r and H_r have a weak energy dependence; however, since the level-level interference is important only in the vicinity of a resonance level, the program evaluates G_r and H_r at the resonance energy E_r and neglects their energy dependence. This is a very good approximation which results in a considerable saving in computer time since G_r and H_r need not be recomputed at each energy.

C. Truncation Effects

The sums over levels in Eqs. (9), (15), (16), and (17) extend over all levels of a given J-sequence. However, since the transmission is computed over a finite energy interval, only those levels within the interval and a few important levels near the boundaries of the interval are explicitly retained. The contribution of the other levels to the cross section may be approximated using a picket-fence model of uniformly spaced levels with average resonance parameters.^{16,17} Using this model the contribution of the levels that are not retained in the sums in Eqs. (9), (15), (16) and (17) are estimated to be $F_1 \sin 2\phi\ell + F_2(\Gamma) \cos 2\phi\ell$, $\frac{1}{2} [F_1^2 + F_2(\Gamma)^2]$, $F_2(\Gamma + \Gamma_r)$ and F_1 respectively, where

$$F_1 = S \cdot P_{\ell}(E) \cdot \ln \left(\frac{EH - E + \epsilon D}{E - EL + \epsilon D} \right) \quad (20)$$

$$F_2(\Gamma) = S \cdot P_\ell(E) \cdot \frac{EH - EL + D}{\left(\frac{EH - E + \frac{1}{2}D}{2}\right)\left(E - EL + \frac{1}{2}D\right)} \cdot \frac{\Gamma}{2} \quad (21)$$

$$\Gamma = \Gamma_\alpha + \langle \Gamma_n^\circ \rangle P_\ell(E) \quad (22)$$

where $\langle \Gamma_n^\circ \rangle$ is the average value of the reduced neutron width, Γ_α is the average reaction width, D the average level spacing and S the strength function. The quantities EH and EL are the energies of the highest and lowest levels explicitly included in the sums, and $\varepsilon = (1 - e)^{-1} \approx .582$. The approximations have been discussed in some detail in Ref. 17.

D. The Total Cross-Section Trial Function.

The total cross-section trial function used by the program is represented by:

$$\sigma = \sum_{NS=1}^{NS2} n_{NS} \cdot \frac{2\pi}{k_{NS}^2} \sum_{J=1}^{J2(NS)} \left[(2\ell+1) \cdot 2 \sin^2 \phi \ell \cdot F_J + g_J P_J \right] \quad (23)$$

$$+ \sum_{N=1}^{NAUX} \gamma_N \cdot f(E, N)$$

where $NS2$ nuclear species NS contribute to the cross section and the parameters n_{NS} allows the program to search for the isotopic concentrations of the species NS . The quantity k_{NS} represents the neutron wave number in the center-of-mass system for a collision with the species NS . For each species there are $J2(NS)$ level sequences for which an angular momentum ℓ and a spin statistical factor g_J are specified. The resonance term P_J will be discussed later. By setting $F_J = 0$ the user may make the contribution of a given sequence to the potential scattering vanish. The last sum in Eq. (23) describes an optional arbitrary function of energy with $NAUX$ parameters which can be searched. The functions $f(E, N)$

may be programmed as desired, and can be used to represent the contributions to the cross-section from far away levels, from isotopes not explicitly included in the first sum, or other sources.

The resonance term P_J vanishes if the number of levels $NR2(J)$ for the given J -sequence is zero; otherwise,

$$P_J = \sum_{NR=1}^{NR2} \Gamma_{nNR} \left[GR_{NR} U_{NR} - HR_{NR} V_{NR} \right] + F_2(\Gamma) \cos(2\phi_\ell) + F_1 \sin(2\phi_\ell) \quad (24)$$

where:

$$GR_{NR} = \cos(2\phi_\ell) + \left[\sum_{S \neq NR} \Gamma_{ns}^o \frac{g_{NRS}}{g_{NRS}^2 + d_{NRS}^2} + F_2(\Gamma + \Gamma_r) \right], \quad (25)$$

$$HR_{NR} = \sin(2\phi_\ell) + \left[\sum_{S \neq NR} \Gamma_{ns}^o \frac{d_{NRS}}{g_{NRS}^2 + d_{NRS}^2} + F_1 \right], \quad (26)$$

$$U_{NR} = \frac{\frac{1}{2} \Gamma_{NR}}{(E'_{NR} - E)^2 + (\frac{1}{2} \Gamma_{NR})^2}, \quad (27)$$

$$V_{NR} = \frac{E'_{NR} - E}{(E'_{NR} - E)^2 + (\frac{1}{2} \Gamma_{NR})^2}. \quad (28)$$

The bracketed terms in Eqs. (25) and (26) are included only when the multi-level formula is used. The terms Γ_{NR} , E'_{NR} , g_{NRS} and d_{NRS} have been defined previously by Eqs. 12, 13, and 19, respectively. In Eqs. 24, 25 and 26, the phase shift ϕ_ℓ is a function of $k_{NS} \cdot \hat{a}_{NS}$ and is given in Table II for different values of the angular momentum ℓ ; \hat{a}_{NS} is the effective scattering radius for the nuclear species NS .

The cross-section parameters which can be searched by the program are the isotopic concentrations n_{NS} and effective scattering radius $\hat{\alpha}_{NS}$ for each nuclear species, the resonance energies E_{NR} , neutron widths Γ_{nNR} and reaction widths Γ_{aNR} of each level and the parameters γ_N of Eq. (23). Expressions (27) and (28) are used to compute the unbroadened cross-section. The Doppler broadening of those expressions is discussed in the next subsection.

E. Doppler Broadening.

The only rapidly varying functions of energy in the expression for the total cross section are the line-shape functions U_{NR} and V_{NR} of Eqs. 27 and 28; hence, the Doppler broadened cross section is obtained by replacing the functions U_{NR} and V_{NR} by their Doppler broadened expressions¹⁸ U_{NR}^* and V_{NR}^* defined by

$$U_{NR}^*(E) = \frac{\Delta}{\sqrt{\pi}} \int U_{NR}(E') e^{-\left(\frac{E-E'}{\Delta}\right)^2} dE' , \quad (29)$$

and

$$V_{NR}^*(E) = \frac{\Delta}{\sqrt{\pi}} \int V_{NR}(E') e^{-\left(\frac{E-E'}{\Delta}\right)^2} dE' . \quad (30)$$

where Δ is the Doppler width. Expressions (29) and (30) are computed by the fast interpolation routine QUICKW developed at Argonne National Laboratory.¹⁹

V. LEAST-SQUARE-FIT ALGORITHM

The best values of the n variable parameters p_1, p_2, \dots, p_n are

obtained by minimizing

$$\phi = \sum_{ij} w_{ij} \left[T_{ij}^{(e)} - T_{ij}(E_i, N_j, p_1, \dots, p_n) \right]^2 \quad (31)$$

with respect to the p_k 's, with perhaps constraints on some of the p_k 's; for example, resonance widths may not become negative. Equation (31) is a double sum where $T_{ij}^{(e)}$ is the measured transmission and T_{ij} the computed transmission at energy E_i for the sample thickness N_j . The quantity w_{ij} is the weight of the measured transmission and, in general, is the inverse square of the statistical uncertainty.

Usually the computed transmissions are not linear functions of the variable parameter p_k ; hence, the minimization problem must be solved by an iterative technique. The program uses a variation of the Gauss-Newton-Marquardt technique²⁰ which has been found efficient and is outlined below. For a justification of the efficiency of the technique, references 20 and 21 should be consulted.

The minimization problem is linearized by expanding the computed transmissions in a Taylor series around guessed or previously iterated values of the parameters $p_k^{(o)}$. Keeping only the first term in the expansion gives

$$\langle \phi \rangle = \sum_{ij} w_{ij} \left[T_{ij}^{(e)} - T_{ij}\left(p_k^{(o)}\right) - \sum_k \frac{\delta T}{\delta p_k} \delta p_k \right]^2 . \quad (32)$$

The linearized expression $\langle \phi \rangle$ is minimized by the solution of a system of linear equations which may be represented in matrix form as

$$M\vec{d} = \vec{v} \quad (33)$$

where $d_k = p_k - p_k^{(0)}$ is a component of the correction vector \vec{d}

$$M_{kp} = \sum_{ij} w_{ij} \cdot \frac{\delta T_{ij}}{\delta p_k} \cdot \frac{\delta T_{ij}}{\delta p_p} \quad (34)$$

and

$$v_k = \sum_{ij} w_{ij} \left[T_{ij}^{(e)} - T_{ij}^{(0)} \right] \frac{\delta T_{ij}}{\delta p_k} \quad (35)$$

Equation (33) is solved by inversion of the matrix M :

$$\vec{d} = M^{-1} \vec{V} \quad (36)$$

The initial values of the variable parameters p_k are changed to the new values

$$p_k^{(1)} = p_k^{(0)} + \eta d_k \quad (37)$$

where η is gauged to insure that none of the parameters which are defined positive will become negative. If for one or several positive-defined parameters p_r we have

$$d_r \leq -p_r^{(0)} \quad (38)$$

then

$$\eta = -0.9 \left[\frac{p_r^{(0)}}{d_r} \right]_{\min} \quad (39)$$

where the bracketed term is the value of $(p_r^{(0)}/d_r)$ for which η is the smallest among the set of positive-defined parameters for which condition (38) holds. If condition (38) never holds for the positive-defined parameters, then η is unity.

There is no guarantee that the value of ϕ computed with the new values $p_k^{(1)}$ will be smaller than the value of ϕ computed with the old values $p_k^{(0)}$ since the minimization was derived for the linearized $\langle\phi\rangle$ of Eq. 37.

The algorithm used to minimize ϕ operates as follows: if $\phi[\vec{p}^{(1)}]$ is smaller or equal to $\phi[\vec{p}^{(0)}]$ then the old values $p_k^{(0)}$ of the parameters are replaced by their new estimates $p_k^{(1)}$ and a new iteration is initiated, unless the maximum number of allowed iterations has been reached. If $\phi[\vec{p}^{(1)}]$ is larger than $\phi[\vec{p}^{(0)}]$, Eq. (33) is replaced by:

$$(M + 2^n b I) \vec{d} = \vec{V} \quad (40)$$

where I is the identity matrix ($I_{k\ell} = \delta_{k\ell}$) and b is a constant defined by

$$b = 0.033 \frac{(\vec{V} M \vec{V})}{(\vec{V} \vec{V})} . \quad (41)$$

The value of n in Eq. (40) is incremented by unit steps from zero to ten, until a value of \vec{d} is found by solving Eq. (40) such that

$$\phi(\vec{p}^{(0)} + n\vec{d}) \leq \phi(\vec{p}_0) . \quad (42)$$

If inequality (42) cannot be satisfied for $n \leq 10$, the search is terminated.

The normal matrix M of Eq. (33) is symmetric and positive definite. To save computer space and time it is stored and used in triangular form. The matrix inversion is done by the Cholesky method which is particularly well-suited for this kind of problem.²²⁻²⁴ The normal vector \vec{V} and normal matrix M are stored in COMMON/VAR/, the inversion and the multiplication of Eq. (36) are performed in the subroutine SLV.

VI. DIMENSIONS OF THE PROGRAM

The number of data points, resonance levels, and variables which can be handled simultaneously is only limited by two critical dimensions which are set in the main part of the program and by the stability of the matrix inversion. In a test problem seven transmissions, each with 3750 data points were simultaneously fitted using 74 resonance levels and 110 variable parameters.

The critical dimensions which control the maximum size of the problem are the dimensions of blank COMMON and of the labeled COMMON/VAR/. These dimensions are referred to as $IG2P$ and $KG2P$ and their values should be inserted in a DATA statement in the main program as shown in the FORTRAN listing in Appendix D. The program will then verify that the critical dimensions are sufficiently large for the problem to be solved before going into the least square search routine. If the dimensions are not sufficiently large, a message is printed and the program stops. The values required for $IG2P$ and $KG2P$ are determined by the following inequalities:

$$IG2P \geq NDAT(3 \cdot NT2 + 1) + 2(3 \cdot NT2 + 3 \cdot NRT + 2NS2 + NAUX + NLS) \quad (43)$$

$$KG2P \geq \frac{NV2}{2} (NV2 + 19) + (1 + NV2)NT2 \quad (44)$$

where $NDAT$ is the number of energy points at which transmissions for $NT2$ sample sizes are given, NRT is the total number of resonance levels, $NS2$ the total number of nuclear species, $NAUX$ the total number of auxiliary parameters (the γ_N 's of Eq. 23), NLS the total number of levels which are treated by the Breit-Wigner-multilevel formula, and $NV2$ is the total number of variable parameters with a positive flag as described in the next section.

VII. VARIABLE PARAMETERS AND FLAGS

The variable parameters whose value can be searched on by the program are:

- (1) the normalizations ϵ_{NT} , thicknesses τ_{NT} and background parameters β_{NT} defined in Eq. (1) and Section III;
- (2) the isotopic concentrations n_{NS} and effective scattering radii \hat{a}_{NS} discussed under Eq. (23) in Section IV D;
- (3) the resonance energies E_{NR} , neutron widths at resonance $\Gamma_{nNR}(E_{NR})$, and reaction widths $\Gamma_{\alpha NR}$ discussed in Section IV A;
- (4) and the cross-section background parameters γ_n defined in the last term of Eq. (23).

A flag is read for each variable parameter which allows the user to control how the variable parameter will be treated; the value of the flags should be set to 0, 1, or 2. Parameters with flags equal to 0 will be treated as constant and their values will not be searched by the program. For parameters with flags equal to 1, an optimum real value will be searched. If the flag is equal to 2 an optimum positive value will be searched. Hence it is advisable to assign a flag equal to 2 to those variable parameters which are defined positives.

It is important to note that varying simultaneously some combinations of parameters may result in an indeterminate problem; in such cases the normal matrix will have a zero determinant, cannot be inverted, and an error message will be printed. For example, if only one sample thickness and only one nuclear species are used, the product $\tau_{NT} n_{NS}$ determines the areal density and only one of the two parameters τ_{NT} or n_{NS} can be varied.

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APPENDIX I. INPUT DATA AND THEIR FUNCTIONS

Various versions of the program SIØB have been in use, which differ mostly by the input format. This appendix discusses the input data required by the version whose FORTRAN is listed in Appendix II.

The input data may be divided into four groups:

- A. Fixed points input switches and floating point input constants which control the operation of the program, as will be explained below.
- B. Transmission data.
- C. Initial guesses.
- D. Flags.

The structure and format of the input data cards is listed immediately below. After this listing the function of these input data will be discussed.

Structure and Format of Input CardsA. Fixed point switches and floating point constants.

1st card: Format (9A8) Legend
2nd card: Format (15I4) *NT2, IT2, NGS, NAUX, JERR, JCAL, JRES,*
 JPAR, LPAR, LMAT, MPAR, LPIT, LDAT, JPLY,
 JKEV

3rd card: Format (6F11.3) *BE2, CE3, EH, EL, RATIØ, DTMIN*

B. Transmission data.

4. Format Card: Format (9A8) *FMDAT*

5. Data Cards: Format (FMDAT), read in 4.

$E, T, \delta T, T_2, \delta T_2 \dots, T_{NT_2}, \delta T_{NT_2}$

6. Terminate transmission data with a blank card.

C. Initial guesses.

I. Transmission Parameters

7. Start with a blank card

8. Sample thicknesses: Format (8F10.5) $\tau_1, \tau_2, \dots, \tau_{NT_2}$

9. Normalisations: Format (8F10.5) $\epsilon_1, \epsilon_2, \dots, \epsilon_{NT_2}$

10. Backgrounds: Format (8F10.5) $\beta_1, \beta_2, \dots, \beta_{NT_2}$

II. Resonance Parameters

8. Format-card: Format (9A8) *FMPAR*

9. Nuclear Species: Format (4E11.3) *FRS, AHAT, AWRI, TEMP*

10. J-Sequence: Format (2I11,5E11.3) *LJ, INT, GSJ, FR, STRF, GNA,*
GAV

11. Level Parameters: Format (*FMPAR*), read in 8

E_0, Γ_n, Γ_j

12. Terminate each J sequence with a blank card.

13. Terminate each Nuclear Species with a blank card.

14. Terminate Resonance Parameters with a blank card.

III. Auxiliary Parameters

15. Auxiliary parameters: Format (7E11.3) $\gamma_1, \dots, \gamma_{NAUX}$

D. Flags

16. Start with a blank card.

17. Flags for thicknesses: Format (4OF2.0) $F_{\tau_1}, \dots, F_{\tau_{NT_2}}$

18. Flags for Normalizations: Format (4OF2.0) $F\epsilon_1, \dots, F\epsilon_{NT_2}$
19. Flags for Backgrounds: Format (4OF2.0) $F\beta_1, \dots, F\beta_{N^2}$
20. Flags of Nuclear Species: Format (2F2.0) $FFRS, FAHAT$
21. Flags of Level Parameters: Format (3F2.0) $FE_0, F\Gamma_n, F\Gamma_\gamma$
22. Terminate each J sequence with a blank card.
23. Terminate resonance parameters with a blank card.
24. Flags for auxiliary parameters: Format (4OF2.0) $F\gamma_1, \dots, F\gamma_{NAUX}$

Functions of Input Data

Legend	This legend is printed at the head of the output print-out
NT_2	Number of transmission samples
IT_2	Maximum number of iterations
NGS	Number of terms in Gauss-Hermite convolution (see Eq. 6 of Section III)
$NAUX$	Number of auxiliary parameters (the γ_n 's of Eq. 23 of Section IV D)
$JERR=0$	For usual options
$JCAL=0$	For usual options
$JRES=0$	The resolution function is computed by Eq. 4 of Section III
$JRES \neq 0$	The resolution function must be coded in the function $RES(E, JRES)$
$JPAR=0$	Level parameters are read in order $E_0, \Gamma_n, \Gamma_\gamma$
$JPAR=1$	Level parameters are read in order $E_0, \Gamma_\gamma, \Gamma_n$
$LPAR=0$	The initial guesses are printed before the iteration loop

<i>LPAR=2</i>	The initial guesses are printed before the iteration loop and the final values after the loop.
<i>LPAR=-1</i>	The initial guesses and final values are not printed.
<i>LMAT<0</i>	The parameter-covariance matrix is not printed
<i>LMAT>0</i>	The parameter-covariance matrix is printed
<i>MPAR<0</i>	The final values of the parameters are punched
<i>MPAR>0</i>	The final values of the parameters are not punched
<i>LPLT<0</i>	No plot-punched cards generated
<i>LPLT>0</i>	Final plot-punched cards generated
<i>LPLT>0</i>	Plot-punched cards generated at each iteration (These punched cards are used with a local utility program to generate plots)
<i>LDAT<0</i>	Calculated and measured transmissions not printed
<i>LDAT>0</i>	Final calc. and meas. transmissions printed
<i>LDAT>1</i>	Calc. and meas. transmissions printed at each iteration
<i>JPLY#0</i>	Transmissions are channel-broadened by Eq. 7 Section III
<i>JPLY=0</i>	Channel broadening is not done
<i>JKEV=0</i>	All energy inputs are in eV
<i>JKEV#0</i>	All energy inputs are in keV
<i>BE2</i> and <i>CE3</i>	Parameters used in computing the resolution width of <i>JRES=0</i> ; see Eq. 4 of Section III
<i>EH, EL</i>	Parameters used in computing the contribution of a picket-fence of levels, see Eq. 20 and 21 of Section IV D
<i>RATIØ</i>	Convergence parameters: the iteration loop is terminated if $\chi^2_{\text{new}} > \text{RATIØ} * \chi^2_{\text{old}}$

<i>DTMIN</i>	A parameter used in function <i>WEIGHT(NT,JE)</i> to define a minimum error on the transmission data
<i>FMDAT</i>	Input format of transmission data
<i>E,T₁,ΔT₁,T₂,ΔT₂,...</i>	Energy, transmission through first sample, error, transmission through second sample, error...
$\tau_i, i=1, NT2$	Sample thickness, see Eq. 1, Section III
$\varepsilon_i, i=1, NT2$	Normalizations, see Eq. 1, Section III
$\beta_i, i=1, NT2$	Backgrounds, see Eq. 1, Section III
<i>FMPAR</i>	Input format of level parameters $E_0, \Gamma_n, \Gamma_\gamma$
<i>FRS</i>	Isotopic concentration of nuclear species (denoted η_{NS} in Eq. 23 Section IV D)
<i>AHAT</i>	Effective scattering radius of a nuclear species (denoted \hat{a}_{NS} in Section IV D)
<i>AWRI</i>	Ratio of the mass of the isotope to that of a neutron
<i>TEMP</i>	Effective temperature for Doppler broadening
<i>LJ</i>	Orbital angular momentum ℓ of a given sequence
<i>INT=0</i>	The J-sequence is treated by the single level formula
<i>INT=1</i>	The J-sequence is treated by the multilevel formula
<i>GSF</i>	Spin statistical factor of a J-sequence
<i>FR</i>	Factor multiplying the potential scattering contribution of the J-sequence (Represented as $F\gamma$ in Eq. 23, Section IV D)
<i>STRF, GNA, GAV</i>	Parameters used in computing the contribution of a picket fence of levels, represented by $S, \langle \Gamma_n^\circ \rangle$ and Γ_α in Eq. 20, 21 and 22 of Section IV C. If STRF=0, the picket-fence contribution is ignored.

E_0 , Γ_n , Γ_γ	Level parameters: resonance energy, neutron width at resonance, capture width. Given in eV if JKEV=0, otherwise in keV
$\gamma_1, \dots, \gamma_{NAUX}$	Auxiliary parameters defined in Eq. 23 Section IV D.
Flags	All the parameters τ_i , ϵ_i , β_i , are <i>FRS</i> , <i>AHAT</i> , E_0 , Γ_n , Γ_γ and γ_i are associated with "flags" which are read in the same order as the parameters. The flag determines how the parameter is to be treated:
Flag=0	The parameter is not varied
Flag=1	The value of the parameter is adjusted to minimize χ^2
Flag=2	The value of the parameter is adjusted to minimize χ^2 but kept positive

(more detail on the operation of the flags are given in Section VII)

APPENDIX II. FORTRAN LISTING OF SIØB PROGRAM AND SUBPROGRAMS

```

**FTN=L,G,E,Y.
REAL * 8 C
REAL * 8 FM(9),LEGEND(9),FMAPB(9),FMDAT(9),FMPAR(9),FMFLG(9)
DIMENSION C(1)
COMMON F(2000)
COMMON/VAR/G(700)
DATA IG2P,KG2P/2000,700/
COMMON/IAD/IF1,IPT2,IPN1,IPN2,IPB1,IPB2,IPS1,IP2,IF1,IFT2,IFN1,
1IFN2,IFR1,IFR2,IFE1,IF2,IG1,IG2
COMMON/KAD/LM1,LS1,NV1,MM1,MS1,KV1,KG1,KG2
COMMON/NAD/NVT,AVV,NVB,NVP,NV2,NT2
COMMON/INDX/JERR,JCAL,JRES,JPAR,LMAT,MPAR,LPLT,LCAT,JPLY,JKEV
COMMON/IEN/IE1,IE2,IE3,IEC1,IGS,NGT
COMMON/LEV/JFLAG,NS2,NAUX,JL(10),NRL(10,10),MOM(10,10),INL(10,10)
COMMON/FLT/BE2,CE3,EH,EL,PHI,DOFINV,DTMIN
COMMON/FLD/AK0(10),CC(10),RAD(10),DELTA(10)
COMMON/FL2/GSPIN(10,10),FRL(10,10),STRFL(10,10),GNAL(10,10),GAVL(10,10)
10,10
EQUIVALENCE(C(1),G(1))
DATA IT1,ITO,ITF,ITC/E,6,7,B/
DATA FMAPB/8H(8F10.5),8*8H
DATA FMDAT/8H(F10.5,1,8H4F5.3) ,7*8H
DATA FMPAR/8H(E11.5,2,8F2X,2E11.,8H5) ,6*8H
DATA FMFLG/8H(4CF2.0),8*8H
DATA NGSP,NAUXP,AKP,B4/1,1,.002196771,.00034465/
DATA ROP,R1P,AWRIF/.123,.08,236.01/
DATA PI/3.141593/
DATA RATIO/.999/
DATA IPLOT/C/
DATA AKPCVT,B4CVT/31.62278,0.0010/
DATA IRTN/C/
1 READ(ITI,101) (LEGEND(I),I=1,9),IT
WRITE(ITO,101)(LEGEND(I),I=1,9)
IF(IT.NE.0) GO TO 1
C READ FIXED POINT INPUT
READ(ITI,102)NT2,IT2,NGS,NAUX,JERR,JCAL,JRES,JPAR,LFAR,LMAT,MPAR,
1LPLT,LCAT,JPLY,JKEV
C READ FLOATING POINT INPUT
READ(ITI,103)BE2,CE3,EH,EL,RATIO,DTMIN
IF(JKEV.NE.0) AKP=AKP*AKPCVT
IF(JKEV.NE.0) B4=E4*B4CVT
IF(NT2.EQ.0) NT2=7
IE1=1
IE3=NT2+1
IF(JERR.EQ.0) IE3=IE3+NT2
IF(JCAL.EQ.0) IE3=IE3+NT2
IE=IE1-IE3
IEC1=IE1+IE3-NT2
IF(IT2.EQ.0) IT2=10
IF(RATIO.EQ.0.0) RATIO=0.9990
IF(DTMIN.EQ.0.0) DTMIN=0.00010
IF(NGS.EQ.0) NGS=NGSP
NGT=(NGS+1)/2
IGS=(NGT*(NGT-1))/2
IF(NAUX.EQ.0) NAUX=NAUXP
IF(LPAR.GE.0) WRITE(ITO,222)NT2,IT2,NGS,NAUX,JERR,JCAL,JRES,JPAR
1,LPAR,LMAT,MPAR,LPLT,LCAT,JPLY,JKEV
C IF(LPAR.GE.0) WRITE(ITO,223)BE2,CE3,EH,EL,RATIO,DTMIN
READ FORMAT FOR TRANSMISSION DATA
READ(ITI,101)(FM(I),I=1,9)
IF(ICCPARE(FM(1),8F      ,8).EQ.0) GO TO 5
DO 3 I=1,9
3 FMDAT(I)=FM(I)
C READ TRANSMISSION DATA
5 IE=IE+IE3
IF(JERR.EQ.0) READ(ITI,FMDAT)F(IE),(F(IE+NT),F(IE+NT2+NT),NT=1,N
IT2)
IF(JERR.NE.0) READ(ITI,FMDAT)F(IE),(F(IE+NT),NT=1,NT2)
IF(F(IE).NE.0) GO TO 5
IE2=IE-IE3
NDAT=((IE-IE1)*NT2)/IE3
IP1=IE
IP0=IP1-1
IE=IE+NT2
C READ FORMAT FOR THICKNESSES
READ(ITI,101)(FM(I),I=1,9)
IF(ICCPARE(FM(1),8F      ,8).EQ.0) GO TO 9
DO 7 I=1,9
7 FMAPB(I)=FM(I)
C READ SAMPLE THICKNESSES IN ATOMS PER EARTH (APB)
9 IPT2=IE-1
READ(ITI,FMAPB)(F(IP),IP=IP1,IPT2)
C READ TRANSMISSION-NORMALISATION ERRORS
IPN1=IPT2+1
IPN2=IPT2+NT2
READ(ITI,FMAPB)(F(IP),IP=IPN1,IPN2)

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C      READ TRANSMISSION BACKGROUNDS
IPB1=IPN2+1
IPB2=IPN2+NT2
READ(ITI,FMAPB)(F(IF),IP=IPB1,IPB2)
IE=IPB2+1
C      READ FORMAT FOR RESONANCE-PARAMETERS
READ(ITI,101)(FM(I),I=1,9)
IF(ICCPARE(FM(1),8F      ,8).EQ.0) GO TO 13
DO 11 I=1,9
11 FMPAR(I)=FM(I)
C      READ INITIAL GUESSES
13 IPS1=IE
NLS=0
NS2=0
14 NS2=NS2+1
READ(ITI,104)FRS,AHAT,AWRI,TEMP,DEL,RN,AK
IF(FRS.EQ.0.) GO TO 19
JL(NS2)=0
F(IE)=FRS
F(IE+1)=AHAT
IE=IE+2
IF(AWRI.EQ.0.) AWRI=AWRIP
IF(TEMP.NE.0.) DEL=SQRT(B4*TEMP/AWRI)
DELTA(NS2)=DEL
IF(RN.EQ.0.) RN=RCP*(AWRI**.333)+R1P
RAD(NS2)=RN
IF(AK.EQ.0.) AK=AKP*AWRI/(1.+AWRI)
AK0(NS2)=AK
CO(NS2)=PI/(AK*AK)
AKRN=AK*RN
15 READ(ITI,106)LJ,INT,GSJ,FR,STRF,GNA,GAV
IF(GSJ.EQ.0.) GO TO 14
J=JL(NS2)+1
JL(NS2)=J
MOM(NS2,J)=LJ
GSPIN(NS2,J)=GSJ
INL(NS2,J)=INT
STRFL(NS2,J)=STRF
GNAL(NS2,J)=GNA
GAVL(NS2,J)=GAV
FRL(NS2,J)=FR
NRL(NS2,J)=0
16 IF(JPAR.EQ.0) READ(ITI,FMPAR)E0,GN,GG
IF(JPAR.EQ.1) READ(ITI,FMPAR)E0,GG,GN
IF(E0.EQ.0.) GO TO 15
NRL(NS2,J)=NRL(NS2,J)+1
IF(INT.NE.0) NLS=NLS+1
F(IE)=E0
F(IE+1)=GG
F(IE+2)=GN/PEN(LJ,AKRN*SQRT(ABS(E0)))
IE=IE+3
GO TO 16
19 NS2=NS2-1
C      READ AUXILIARY PARAMETERS
IP2=IE+NAUX-1
READ(ITI,104)(F(IF),IP=IE,IP2)
C      READ FORMAT FCR FLAGS
READ(ITI,101)(FM(I),I=1,9)
IF(ICCPARE(FM(1),8F      ,8).EQ.0) GO TO 23
DO 21 I=1,9
21 FMFLG(I)=FM(I)
C      READ FLAGS TO VARY THICKNESSES
23 IF1=IP2+1
IFT2=IP2+NT2
READ(ITI,FMFLG)(F(IF),IF=IF1,IFT2)
C      READ FLAGS TO VARY NORMALISATIONS
IFN1=IFT2+1
IFN2=IFT2+NT2
READ(ITI,FMFLG)(F(IF),IF=IFN1,IFN2)
C      READ FLAGS TO VARY BACKGROUNDS
IFB1=IFN2+1
IFB2=IFN2+NT2
READ(ITI,FMFLG)(F(IF),IF=IFB1,IFB2)
IFS1=IFB2+1
IF=IFE2
C      READ FLAGS TO VARY PARAMETERS
DO 27 NS=1,NS2
READ(ITI,FMFLG)F(IF+1),F(IF+2)
IF=IF+2
JL2=JL(NS)
DO 27 J=1,JL2
NR2=NRL(NS,J)
IF(NR2.EQ.0) GO TO 26
DO 25 NR=1,NR2
READ(ITI,FMFLG)(F(IF+N),N=1,3)

```

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25 IF=IF+3
26 CONTINUE
27 READ(ITI,FMFLC)
  READ(ITI,FMFLG)
  IF2=IF+Naux
  IF=IF+1
  READ(ITI,FMFLC)(F(I),I=IF,IF2)
C   SET EH AND EL IF EH=0.
  IF(EH,EQ.0.) EH=F(IPS1+2)
  IF(EH,EQ.0.) EH=F(IP2-Naux-2)
C   IG1,IG2 SPACE FOR STORING INTERFERENCE
C   PARAMETERS USED IN SIG.
  IG1=IF2+1
  IG2=IF2+NLS+NLS
C   COMPUTE THE NUMBER OF VARIABLES NV2
  NVT=0
  NVN=0
  NVB=0
  DO 29 NT=1,NT2
  IF(F(IP2+NT),NE.0.) NVT=NVT+1
  IF(F(IF2+NT),NE.0.) NVN=NVN+1
  IF(F(IFN2+NT),NE.0.) NVB=NVB+1
29 CONTINUE
  NVP=0
  DO 31 IF=IF$1,IF2
  IF(F(IF),NE.0.) NVP=NVP+1
31 CONTINUE
  NV2=NVT+NVN+NVB+NVP
C   NUMBER OF DEGREES OF FREEDOM (FOR CHISQ)
  DOF=NCAT-NV2
  DOFINV=1./DOF
  LM1=NV2+1
  NM=(NV2*(NV2+1))/2
  LS1=LM1+NM
  MV1=LS1+NV2
  MM1=MV1+NV2
  MS1=MM1+NM
  MS2=MS1+NV2-1
  KV1=MS2+MS2+1
  KG1=KV1+NV2
  KG2=KG1+(1+NV2)*NT2-1
C   CHECK COMMON ARRAYS FOR SIZE
  NERR=0
  IF(IG2.GT.IG2P) NERR=NERR+1
  IF(KG2.GT.KG2P) NERR=NERR+1
  IF(NERR,EQ.0) GO TO 33
  WRITE(ITO,201)IG2,IG2P,KG2,KG2P
  CALL ERROR
33 CONTINUE
  WRITE(ITO,217)NCAT,IG2,KG2
  WRITE(ITO,216)EL,EH
  IF(LPAR,GE.0) WRITE(ITO,225)
C   PRINT RESONANCE PARAMETERS
34 IF(LPAR,LT.0) GO TO 40
  IE=IPSI
  DO 37 NS=1,NS2
  AK=AKC(NS)
  RN=RAC(NS)
  DEL=DELTA(NS)
  JL2=JL(NS)
  WRITE(ITO,231)NS,AK,RN,DOP,JL2,F(IE),F(IE+1)
  IE=IE+2
  AKRN=AK*RN
  DO 37 J=1,JL2
  LJ=MOM(NS,J)
  INT=INL(NS,J)
  CSJ=GSPIN(NS,J)
  FR=FRL(NS,J)
  STRF=STRFL(NS,J)
  GNA=GNAL(NS,J)
  GAV=GAVL(NS,J)
  NR2=NRL(NS,J)
  WRITE(ITO,232)LJ,INT,GSJ,FR,STRF,GNA,GAV,NR2
  IF(NR2,EQ.0) GO TO 37
  WRITE(ITO,236)
  DO 35 NR=1,NR2
  EC=F(IE)
  GG=F(IE+1)
  GN=F(IE+2)*PEN(LJ,AKRN*SQRT(ABS(E0)))
  IE=IE+3
35 WRITE(ITO,235)E0,GG,GN
  WRITE(ITO,237)
37 CONTINUE
40 CONTINUE
C   IF(IRTN,EG.1) GO TO 70
  ITERATION LOOP
  DO 45 IT=1,IT2
  LM=LM1
  DO 41 LA=1,NV2
  D(LA)=0.
  DO 41 LB=LA,NV2
  D(LM)=0.

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```

41 LM=LM+1
JFLAG=0
PHI=0.
JV=0
CALL FHINEQ(JV)
PHIOLC=PHI
C PUNCH CARDS FOR PCP10 PLOTS
IF(LPLT.LT.1) GO TO 43
IPLOT=IPLOT+1
NE2=1+(IE2-IE1)/IE3
DO 42 NT=1,NT2
ISN=10*IPLOT+NT
WRITE(ITP,301)ISN,NE2
NTT=NT+NT2
NTN=NTT+NT2
DO 42 IE=IE1,IE2,IE3
WRITE(ITP,301)F(IE),F(IE+NT),F(IE+NTT),F(IE+NTN)
42 CONTINUE
43 CONTINUE
C PRINT TRANSMISSIONS
IF(LCAT.LE.1) GO TO 46
WRITE(ITO,204)
DO 44 IE=IE1,IE2,IE3
IEA=IE+NT2
IEB=IEA+NT2
WRITE(ITO,205)F(IE),(F(IEB+NT),F(IE+NT),F(IEA+NT),F(IP0+NT),NT=1,NT2)
44 CONTINUE
46 CONTINUE
WRITE(ITO,206)IT
CALL MVP
IF(PHI1.GT.RATIO*PHICLD) GO TO 47
45 CONTINUE
GO TO 49
47 WRITE(ITO,202)
JFLAG=0
CALL FHINEQ(-1)
C PUNCH CARDS FOR PCP10 PLOTS
49 IF(LPLT.LT.0) GO TO 55
IPLOT=IPLOT+1
NE2=1+(IE2-IE1)/IE3
DO 51 NT=1,NT2
ISN=10*IPLOT+NT
WRITE(ITP,301)ISN,NE2
NTT=NT+NT2
NTN=NTT+NT2
DO 51 IE=IE1,IE2,IE3
WRITE(ITP,301)F(IE),F(IE+NT),F(IE+NTT),F(IE+NTN)
51 CONTINUE
C PRINT TRANSMISSIONS
55 IF(LCAT.LE.0) GO TO 59
WRITE(ITO,204)
DO 57 IE=IE1,IE2,IE3
IEA=IE+NT2
IEB=IEA+NT2
WRITE(ITO,205)F(IE),(F(IEB+NT),F(IE+NT),F(IEA+NT),F(IP0+NT),NT=1,NT2)
57 CONTINUE
59 CONTINUE
C PUNCH FINAL PARAMETRES
IF(MPAR.LE.0) GO TO 69
WRITE(ITC,101)(FMAPE(I),I=1,9)
WRITE(ITC,FMAFB)(F(IP),IP=IP1,IP2)
WRITE(ITC,FMAFB)(F(IP),IP=IPN1,IPN2)
WRITE(ITC,FMAFB)(F(IP),IP=IPB1,IPB2)
WRITE(ITC,101)(FMFAR(I),I=1,9)
IE=IPS1
DO 63 NS=1,NS2
FRS=F(IE)
AHAT=F(IE+1)
IE=IE+2
DEL=DELTA(NS)
RN=RAD(NS)
AK=AKC(NS)
AKRN=AK*RN
AWRI=C.
TEMP=C.
WRITE(ITC,104)FRS,AHAT,AWRI,TEMP,DEL,RN,AK
JL2=JL(NS)

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DO 62 J=1,JL2
INT=INL(NS,J)
GSJ=GSPIN(NS,J)
FR=FRL(NS,J)
STRF=STRFL(NS,J)
GAV=GAVL(NS,J)
WRITE(ITC,1;E)J,INT,GSJ,FR,STRF,GAV
NR2=NRL(NS,J)
IF(NR2.EQ.0) GO TO 62
DO 61 NR=1,NR2
EO=F(IE)
GG=F(IE+1)
GN=F(IE+2)*PEN(J,AKRN*SGRT(ABS(E0)))
IE=IE+3
IF(JPAR.EQ.0) WRITE(ITC,FMPAR)E0,GN,GG
IF(JPAR.EQ.1) WRITE(ITC,FMPAR)E0,GG,GN
61 WRITE(ITC,101)
62 WRITE(ITC,101)
63 WRITE(ITC,101)
WRITE(ITC,104)(F(IP),IP=IE,IP2)
69 CONTINUE
IF(LPAR.NE.2) GO TO 71
WRITE(ITC,235)
IRTN=1
GO TO 34
70 IRTN=C
71 CONTINUE
READ(ITI,102)IGCTC
IF(IGCTC.EQ.0)CALL EXIT
IF(IGCTC.EQ.1)CALL ERRCR
IF(IGCTC.EQ.2)GC TO 1
101 FORMAT(9A8,I8)
102 FORMAT(20I4)
103 FORMAT(7G11.3)
104 FORMAT(7G11.3)
105 FORMAT(2G11.3,5I11)
106 FORMAT(2I11,5G11.3)
201 FORMAT(1H1,'CCMNCH TOO SMALL',4I20)
202 FORMAT(1H0,'STOP ITERATIONS BECAUSE CONVERGENCE IS TOC SLOW')
203 FORMAT(1H ,08X,7(1X,F10.7,SH APB ))
204 FORMAT(1H1,9X,'ENERGY',11X,'CALCULATION' 4X,'EXPERIMENT'.
1'8X,'ERROR',EX,'ATCNS PER EARN',//)
205 FORMAT(1H ,G20.5,3F15.4,G20.5/(2IX,3F15.4,G20.5))
206 FORMAT(1H0,'J-STATE=',I2,'L-VALUE=',I2,'NUMBER OF LEVELS=',I3,'FG=
1',G11.3,'AK=',G11.3,/ )
207 FORMAT(1H ,3G20.5)
208 FORMAT(1H1,'ITERATION NUMBER',I3)
212 FORMAT(1H ,7G15.5)
216 FORMAT(1H0,'TRUNCATION LIMITS',2G15.5)
217 FORMAT(1H0,'NLMEER CF TRANSMISSION VALUES'18,//' MAXIMUM ADDRESS 0
1F F-ARRAY',I9,//' MAXIMUM ADDRESS OF G-ARRAY',I9)
222 FORMAT(1H0,'FIXED PCINT INPUTS ',20I4)
223 FORMAT(1H , 'FLCATING FOINT INPUTS ',7G11.3)
225 FORMAT(1H0,'//////,15X,'INPUT RESONANCE PARAMETERS',///)
231 FORMAT(1H0,2X,'NUCLEAR SPECIES ',I3.5X,
1'REDUCED MCMENLNM='G12.5,5X,
2'NUCLEAR RADIUS='G12.5,/
38X,'CCFPPLER WIDTH='G12.5,5X,
4'NUMBER OF ANGULAR MEMENTA='I3./,
58X,'FRACTIOAL ABUNDANCE='F7.4,5X
6'EFFECTIVE RADIUS='F7.4,/)
233 FORMAT(1H0,4X,'ANGLULAR MOMENTUM='I2.5X,
1'INTERFERENCE PARAMETER='I2.5X,
2'SPIN STATISTICAL FACTOR='F6.3,5X,
3'POTENTIAL SCATTERING FRACTION='F6.3./,
410X,'STRENGTF-FUNCTION='G12.5,5X,
5'AVERAGE NEUTRCH-WIDTH='G12.5,5X,
6'AVERAGE CAPTURE-WICHT='G12.5,/,10X,
7'NUMBER OF LEVELS='I4)
236 FORMAT(1H0,15X,'RESCNANCE ENERGY',5X,'CAPTURE-WIDTH',5X,'NEUTRON-W
1IDTH',//)
235 FORMAT(14X,3G18.5)
237 FORMAT(1H0)
239 FORMAT(1H1,'FINAL RESCNANCE PARAMETRES',///)
301 FORMAT(2CA4)
END

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C      SUBROUTINE PHINEQ(JV)
C      REQUIRES RES(E,JRES),SIG(E,JV),BGR(E,NT),WEIGHT(NT,IE)
C      REAL * 8 D
C      DIMENSION C(1),X(45)
C      COMMON F(1)
C      COMMON/VAR/G(1)
C      COMMON/IAD/IP1,IP2,IPN1,IPN2,IPB1,IPB2,IPS1,IP2,IF1,IFT2,IFN1,
1IFN2,IFB1,IFB2,IFS1,IF2,IG1,IG2
C      COMMON/KAC/LM1,LS1,MV1,MM1,MS1,MS2,KV1,KG1,KG2
C      COMMON/NAD/NVT,NVN,NVB,NVP,NV2,NT2
C      COMMON/INDX/JERF,JCAL,JRES,JPAR,LPAR,LMAT,MPAR,LPLT,LDAT,JPLY,JKEV
C      COMMON/IEN/IE1,IE2,IE3,IEC1,IGS,NGT
C      COMMON/FLT/BE2,CE2,EH,EL,PHI,DOFINV,DTMIN
C      EQUIVALENCE(C(1),G(1))
C      DATA A/ 1.0GG0E 0.6.6667E-01,1.6667E-01,5.3333E-01,2.2208E-01,
2 1.1257E-C2,4.5714E-01,2.4012E-01,3.0757E-02,5.4827E-04,
3 4.0635E-C1,2.4410E-01,4.9916E-02,2.7891E-03,2.2345E-05,
4 3.6941E-C1,2.4224E-01,6.6139E-02,6.7203E-03,1.9576E-04,
5 8.1218E-07,3.4C99E-01,2.3787E-01,7.9169E-02,1.1771E-02,
6 6.8124E-C4,1.1527E-05,5.2.7226E-08,3.1826E-01,2.3246E-01,
7 8.9418E-C2,1.7366E-02,1.5674E-03,5.6421E-05,5.9754E-07,
8 8.5896E-1C,2.9954E-01,2.2671E-01,9.7406E-02,2.3087E-02,
9 2.8889E-C3,1.6849E-04,4.0127E-06,2.6808E-08,2.5843E-11,
A 2.8377E-01,2.2094E-01,0.1.0360E-01,2.8667E-02,4.5072E-03,
B 3.7850E-04,1.5351E-05,5.2.5322E-07,1.2204E-09,7.4828E-13/
C      DATA X/ 1.224744E0,0.95857251,2.02018261,0.81628788,1.67355156,
2 2.6519E133,0.72355098,1.46855259,2.26658058,3.19099331,
3 0.6568C9E3,1.32655716,2.02594757,2.78328991,3.66847134,
4 0.6057E391,1.22005463,1.85310841,2.51973629,3.24660873,
5 4.10132839,0.56506962,1.13611603,1.71999264,2.32573223,
6 2.9671E595,3.66994953,4.49999142,0.53163302,1.06764889,
7 1.61292362,2.17350292,2.75776291,3.37893200,4.06194687,
8 4.871344E7,0.50352019,1.01036835,1.52417088,2.04923153,
9 2.591134C7,3.15784931,3.76218700,4.42853260,5.22027206/
C      LOOP OVER ENERGIES
IPO=IF1-1
IEC=IEC1-1
DO 69 IE=IE1,IE2,IE3
E=F(IE)
IF(JRES.EQ.0) R=E*SQRT(BE2+CE3*E)
IF(JRES.NE.0) R=RES(E,JRES)
C      LOOP OVER GAUSS INTEGRATION INTERVALS
ENG=E
IG=IGS
JG=IGS-NGT
DO 59 NG=1,NGT
ANG=A(IG+NG)
IF(NG.EQ.1) GC TO 53
DE=R*X(JG+NG)
51 ENG=E+DE
53 CS=SIC(ENG,JV)
C      LOOP OVER TRANSMISSION-SAMPLES
K=KG1
DO 57 NT=1,NT2
APN=F(IPO+NT)
TR=ANG*EXP(-APN*CS)
TN=(1.+F(IP2+NT))*TR
IF(NG.EQ.1) G(K)=F(IPN2+NT)*BGR(E,NT)
G(K)=G(K)+TN
C      LOOP OVER DERIVATIVES
IF(JV.LT.0) GC TO 57
KNV=K+1
NTC=1
DO 54 IF=IF1,IFT2
IF(F(IF).EQ.0.) GO TO 54
IF(NTC.NE.NT.OR.NG.EQ.1) G(KNV)=0.
IF(NTC.EQ.NT) G(KNV)=G(KNV)-CS*TN
KNV=KNV+1
54 NTC=NTC+1
NTC=1
DO 55 IF=IFN1,IFN2
IF(F(IF).EQ.0.) GO TO 55
IF(NTC.NE.NT.OR.NG.EQ.1) G(KNV)=0.
IF(NTC.EQ.NT) G(KNV)=G(KNV)+TR
KNV=KNV+1
55 NTC=NTC+1
KV=KV1
KNV=KNV+NVE
DO 56 NV=1,NVP
IF(NG.EQ.1) G(KNV)=0.
G(KNV)=G(KNV)-AFN*TN*G(KV)
KNV=KNV+1

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56 KV=KV+1
57 K=K+NV2+1
IF(NG.EQ.1.OR.DE.LT.0.) GO TO 59
DE=-DE
GO TO 51
59 CONTINUE
C LOOP OVER TRANSMISSION SAMPLES
K=KG1
DO 65 NT=1,NT2
C STORE COMPUTED TRANSMISSIONS IF NEEDED
IF(JCAL.EQ.0) F(IEC+NT)=G(K)
C CONTRIBUTIONS TO PHI AND NORMAL EQUATIONS
W=WEIGHT(NT,IE)
CTN=F(IE+NT)-G(K)
DTNW=CTN*W
PHI=PHI+DTN*DTNW
IF(JV.LT.0) GC TO 65
C DERIVATIVES OF TRANSMISSION-BACKGROUNDS
K1=K+NVT+NVN+1
NTC=1
DO 61 IF=IFB1,IFB2
IF(F(IF).EQ.0) GC TO 61
G(K1)=0.
IF(NTC.EQ.NT) G(K1)=BGR(E,NT)
K1=K1+1
61 NTC=NTC+1
C NORMAL EQUATIONS
L=L+1
DO 63 NA=1,NV2
GKNA=G(K+NA)
D(NA)=D(NA)+DTNW*CKNA
DO 63 NB=NA,NV2
D(L)=D(L)+W*GKNA*G(K+NB)
63 L=L+1
65 K=K+NV2+1
69 IEC=IEC+IE3
IF(JPLY.EQ.0) RETURN
C CORRECTION FOR CHANNEL WIDTHS
PHI=0.0
IE9=IE1+IE3+IE3
IEC=IEC1-1
DO 71 IE=IE1,IE2,IE3
DO 70 NT=1,NT2
IT=IEC+NT
IF(IE.LE.IE9.OR.IE.EQ.IE2) GO TO 70
F(IT)=G.C416E7*(F(IT+IE3)+F(IT-IE3)+22.0*F(IT))
70 PHI=PHI+WEIGHT(NT,IE)*(F(IE+NT)-F(IT))**2
71 IEC=IEC+IE3
RETURN
END

FUNCTION RES(E,JRES)
RES=0.
RETURN
END

FUNCTION BGR(E,NT)
BGR=1.
RETURN
END

FUNCTION WEIGHT(NT,IE)
COMMON/NAC/NVT,NVN,NVE,NVP,NV2,NT2
COMMON/FLT/BE2,CE2,EH,EL,PHI,DOFINV,DTMIN
COMMON/INDX/JERR,JRES,JPAR,LPAR,LMAT,MPAR,LPLT,LDAT,JPLY,JKEV
DT=F(IE+NT+NT2)
IF(DT.GE.DTMIN) GO TO 10
DT =DTMIN
F(IE+NT+NT2)=DTMIN
10 WEIGHT=1.0/(DT*DT)
RETURN
END

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SUBROUTINE MVP
C  REQUIRES SLV(NV2)
C  MVP DOES A P-SEARCH IF NEEDED
C  SAVE CLD CHISQUARE
REAL * 8 D
DIMENSION D(1)
COMMON F(1)
COMMON/VAR/G(1)
COMMON/IAD/IP1,IPT2,IPN1,IPN2,IPB1,IPB2,IPS1,IP2,IF1,IFT2,IFN1,
1 IFN2,IFB1,IFB2,IFS1,IF2,IG1,IG2
COMMON/KAD/LM1,LS1,MV1,MM1,MS1,MS2,KV1,KG1,KG2
COMMON/NAD/NVT,NVN,NVB,NVP,NV2,NT2
COMMON/INDX/JERR,JCAL,JRES,JPAR,LPAR,LMAT,MPAR,LPLT,LCAT,JPLY,JKEV
COMMON/IEN/IE1,IE2,IE3,IEC1,IGS,NGT
COMMON/LEV/JFLAG,NS2,NAUX,JL(10),NRL(10,10),MOM(10,10),INL(10,10)
COMMON/FLT/BE2,CE2,EH,EL,PHI,DOFINV,DTMIN
COMMON/FLD/AKO(10),CO(10),RAD(10),DELTA(10)
COMMON/FL2/GSPIN(10,1C),GAVL(10,10),STRFL(10,10),FRL(10,10)
EQUIVALENCE(C(1),G(1))
DATA ITI,ITO/E,/
DATA EPP,NPSMAX/.C33.1/
CHIOLD=DOFINV*PHI
NPS=0
C  SAVE NORMAL MATRIX AT MM1
LM=LM1
MM=MM1
DO 11 LA=1,NV2
DO 11 LB=LA,NV2
D(MM)=D(LM)
MM=MM+1
11 LM=LM+1
C  SOLVE NORMAL EQUATIONS
19 CALL SLV(NV2)
C  GAUGE ETA, IF NPS=0 SAVE ORIGINAL PARAMETERS
ETA=1.
IF=IFI
LS=LS1
MV=MV1
DO 25 IP=IP1,IP2
IF(F(IF).EQ.0) GO TO 25
IF(NPS.EQ.0) C(MV)=F(IP)
IF(F(IF).EG.1.) GO TO 23
IF(D(MV)+ETA*D(LS).LE.0.) ETA=-.9*D(MV)/D(LS)
23 MV=MV+1
LS=LS+1
25 IF=IF+1
C  MODIFY VARIABLE PARAMETERS
IF=IFI
LS=LS1
MV=MV1
DO 27 IP=IP1,IP2
IF(F(IF).EG.0.) GO TO 27
F(IP)=D(MV)+ETA*D(LS)
MV=MV+1
LS=LS+1
27 IF=IF+1
C  GET NEW VALUE OF CHI-SQUARE
JFLAG=0
PHI=0.
JV=-1
CALL FHINEQ(JV)
CHISQ=DOFINV*PHI
C  IF NPS=0 STORE ERRORS IN D
IF(NPS.GT.0) GO TO 31
LM=LM1
MS=MS1
DO 29 LA=1,NV2
DO 29 LB=LA,NV2
IF(LA.EQ.LB.OR.LMAT.GT.0) D(LM)=CHISQ*D(LM)
IF(LA.NE.LB) GO TO 29
D(MS)=CSQRT(C(LM))
MS=MS+1
29 LM=LM+1
C  IF LMAT.GT.0 PRINT COVARIANCE-MATRIX
LM2=LS1-1
IF(LMAT.GT.0) WRITE(ITO,204)(D(LM),LM=LM1,LM2)
31 IF(CHISQ.GT.CHIOLD) GO TO 51
WRITE(ITO,201)
WRITE(ITO,202)NFS,ETA,CHIOLD,CHISQ
C  PRINT SAMPLE THICKNESSES
WRITE(ITO,221)
WRITE(ITO,203)
IF=IFI
MS=MS1
MV=MV1
DO 33 IP=IP1,IPT2
IF(F(IF).EQ.0.) GO TO 32
WRITE(ITO,204)D(MV),F(IP),D(MS)
MV=MV+1
MS=MS+1
GO TO 33

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32 WRITE(ITO,204)F(IF)
C 33 IF=IF+1
PRINT NORMALISATION-ERRORS
WRITE(ITO,22E)
WRITE(ITO,203)
DO 82 IP=IPN1,IPN2
IF(F(IF).EQ.0.) GO TO 81
WRITE(ITO,204)D(MV),F(IP),D(MS)
MV=MV+1
MS=MS+1
GO TO 82
81 WRITE(ITO,204)F(IF)
82 IF=IF+1
C PRINT TRANSMISSION BACKGROUNDS
WRITE(ITO,222)
WRITE(ITO,203)
DO 35 IP=IPB1,IPB2
IF(F(IF).EQ.0.) GO TO 34
WRITE(ITO,204)D(MV),F(IP),D(MS)
MV=MV+1
MS=MS+1
GO TO 35
34 WRITE(ITO,204)F(IP)
35 IF=IF+1
C PRINT RESONANCE PARAMETERS
WRITE(ITO,230)
IP=IPB2
DO 46 NS=1,NS2
AK=AKC(NS)
RN=RAD(NS)
AKRN=AK*RN
JL2=JL(NS)
WRITE(ITO,231)NS,JL2
WRITE(ITO,224)
WRITE(ITO,203)
IF(F(IF).EQ.0.) GO TO 36
WRITE(ITO,204)D(MV),F(IP+1),D(MS)
MV=MV+1
MS=MS+1
GO TO 37
36 WRITE(ITO,204)F(IF+1)
37 IF=IF+1
IF(F(IF).EQ.0.) GO TO 38
WRITE(ITO,204)D(MV),F(IP+2),D(MS)
MV=MV+1
MS=MS+1
GO TO 39
38 WRITE(ITO,204)F(IF+2)
39 IF=IF+1
IP=IP+2
DO 46 J=1,JL2
LJ=NCR(NS,J)
NR2=NRL(NS,J)
WRITE(ITO,232)LJ,NR2
IF(NR2.EQ.0.) GO TO 46
WRITE(ITO,225)
WRITE(ITO,203)
WRITE(ITO,227)
DO 43 NR=1,NR2
FLAG=F(IF)+F(IF+1)+F(IF+2)
IF(FLAG.NE.0.) WRITE(ITO,211)
DO 43 M=1,3
IP=IP+1
IF(FLAG.EQ.0.) GO TO 43
T1=F(IP)
IF(M.EQ.1) PENR=PEN(LJ,AKRN+SQRT(AES(T1)))
IF(M.EQ.3) T1=T1*PENR
IF(F(IF).EQ.0.) GO TO 42
T2=D(MV)
T3=D(MS)
MV=MV+1
MS=MS+1
IF(M.NE.3) GO TO 41
T2=T2*PENR
T3=T3*PENR
41 WRITE(ITO,204)T2,T1,T3
GO TO 43
42 WRITE(ITO,204)T1

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43 IF=IF+1
46 CONTINUE
C AUXILIARY PARAMETERS
WRITE(ITO,226)
WRITE(ITO,203)
DO 45 N=1,NAX
IP=IP+1
IF(F(IF).EQ.0.) GO TO 44
WRITE(ITO,204)D(MV),F(IP),D(MS)
MV=MV+1
MS=MS+1
GO TO 45
44 WRITE(ITO,204)F(IF)
45 IF=IF+1
RETURN
C PROCEED WITH P-SEARCH
51 NPS=NPS+1
IF(NPS.GT.NPSMAX) GO TO 71
IF(NPS.GT.1) GO TO 61
C COMPUTE PSC
GMG=C.
MM0=MM1-1
GG=0.
DO 55 LA=1,NV2
SUM=0.
NM=MM0+LA
J=NV2-1
DO 54 LB=1,NV2
SUM=SUM+D(LB)*D(NM)
IF(LB.GE.LA) GO TO 53
NM=NM+J
J=J-1
GO TO 54
53 NM=NM+1
54 CONTINUE
GMG=GMG+SUM*D(LA)
55 GG=GG+D(LA)*D(LA)
PSC=EPP*GMG/GG
C ADD PSC TO DIAGONAL ELEMENTS OF NORMAL MATRIX
C AND RESTORE IN D(LM1)
61 LM=LM1
MM=MM1
DO 63 LA=1,NV2
DO 63 LB=LA,NV2
D(LM)=D(MM)
IF(LA.EQ.LE) D(LM)=D(LM)+PSC
LM=LM+1
63 MM=MM+1
PSC=PSC+PSC
GO TO 19
71 WRITE(ITO,205)
C RESTORE OLD PARAMETERS AND CHIOLD
CHISQ=CHICLD
IF=IFI
MV=MV1
DO 75 IP=IP1,IP2 GO TO 75
    F(IP)=D(MV)
    MV=MV+1
75 IF=IF+1
GO TO 31
201 FORMAT(1H0,8X,'NPS',17X,'ETA',15X,'CHIOLD',14X,
1'CHINEW',// )
202 FORMAT(1H ,110,6X,3G20.5// )
203 FORMAT(1H0,9X,'CLC VALUE',11X,'NEW VALUE',14X,
1'ERROR',// )
204 FORMAT(1H ,6G20.5)
205 FORMAT(1H , 'CAN DC NO GOOD. SORRY')
211 FORMAT(1H )
221 FORMAT(1H0,5X,'SAMPLE-THICKNESSES')
222 FORMAT(1H0,5X,'TRANSMISSION-BACKGROUNDS')
224 FORMAT(1H0,5X,'FRACTICAL ABUNDANCE AND RADIUS')
225 FORMAT(1H0,5X,'RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH')
226 FORMAT(1H0,/////////15X,'AUXILIARY PARAMETERS',///)
227 FORMAT(1H0,7X,(ONLY VARIED LEVELS ARE LISTED))
228 FORMAT(1H0,5X,'NORMALISATION-ERRORS')
230 FORMAT(1H0,/////////15X,'RESONANCE PARAMETERS',///)
231 FORMAT(1H0,/////,1X,'NUCLEAR SPECIES =',I3,5X,
4'NUMBER OF ANGULAR MOMENTA =',I3)
232 FORMAT(1H0,///2X,'ANGULAR MOMENTUM =',I2,5X,
7'NUMBER OF LEVELS =',I4)
END

```

```

SUBROUTINE SLV(N)
IMPLICIT REAL * 8 (A-H,O-Y)
COMMON/VAR/F(1)
REAL * 8 F
IF(N-1) 1,2,3
1 WRITE(6,101)
101 FORMAT (1HC,'NEGATIVE ARGUMENT IN SLV')
RETURN
2 F(2)=1./F(2)
F(3)=F(2)*F(1)
RETURN
3 K=N+1
DO 10 M=1,N
M1=M-1
DO 10 L=M,N
A=0.
IF(M1.LE.0) GO TO 6
KL=N+L
KM=N+N
DO 5 LM=1,M1
A=A+F(KL)*F(KM)
J=N-L
KL=KL+J
5 KM=KM+J
6 T=F(K)-A
IF(L.GT.M) GO TO 5
IF(T.GT.0.) GO TO 7
WRITE(6,102) T
102 FORMAT (1HO,'FAILURE IN SLV T=',G20.5)
7 D=DSQRT(T)
F(K)=D
GO TO 10
9 F(K)=T/D
10 K=K+1
K=N+1
F(K)=1./F(K)
DO 12 L=2,N
K=K+L-L+2
T=1./F(K)
F(K)=T
L1=L-1
KL=N+L
KM=N
DO 12 M=1,L1
LK=KL
A=0.
DO 11 LM=M,L1
I1=KM+LM
A=A-F(KL)*F(I1)
11 KL=KL+N-LM
F(LK)=A*T
J=N-P
KL=LK+J
12 KM=KM+J
K=N+1
DO 14 M=1,N
KL=K
DO 14 L=M,N
KM=K
A=0.
I1=N-L+1
DO 13 LM=1,I1
A=A+F(KL)*F(KM)
KL=KL+1
13 KM=KM+1
F(K)=A
14 K=K+1
DO 16 L=1,N
A=0.
IJ=N+L
JI=0
J=N-1
DO 17 M=1,N
JI=JI+1
A=A+F(IJ)*F(JI)
IF(M.GE.L) GO TO 16
IJ=IJ+J
J=J-1
GO TO 17
16 IJ=IJ+1
17 CONTINUE
F(K)=A
18 K=K+1
RETURN
END

```

```

FUNCTION SIG(E,JV)
C REQUIRES SVS(ZED,ETA,U0,V0) AND FNS(VE,N)
C FOR JV.GE.0 COMPUTES DERIVATIVES
C FOR JFLAG=0 RECOMMUTES INTERFERENCE TERMS
COMMON F(1)
COMMON/VAR/G(1)
COMMON/IAC/IP1,IP2,IPN1,IPN2,IPB1,IPB2,IPS1,IP2,IF1,IFT2,IFN1,
1IFN2,IFB1,IFB2,IFS1,IF2,IG1,IG2
COMMON/KAC/LM1,LS1,MV1,MM1,MS1,KV1,KG1,KG2
COMMON/NAD/NVT,AVN,NVE,NVP,NV2,NT2
COMMON/INOX/JERF,JCAL,JRES,JPAR,LPAR,LMAT,MPAR,LPLT,LCAT,JPLY,JKEV
COMMON/LEV/JFLAG,NS2,NAUX,JL(10),NRFL(10,10),MOM(10,10),INL(10,10)
COMMON/FLT/BE2,CE2,EH,EL,PHI,DOFINV,DTMIN
COMMON/FLD/AKO(10),CO(10),RAD(10),DELTA(10)
COMMON/FL2/GSPIN(10,10),FRL(10,10),STRFL(10,10),GNAL(10,10),GAVL(10,10)
10,10)
DATA SQPI,PI4/1.772454,12.5664/
DATA EPSI/1.E-6/
IF(JFLAG.NE.0) GO TO 21
C COMPUTATION OF LEVEL-LEVEL-INTERFERENCES
C ( IF JFLAG=0)
JFLAG=1
IP=IPS1
K=IG1
DO 20 NS=1,NS2
IP=IP+2
JL2=JL(NS)
AKRNS=AKO(NS)*RAD(NS)
DO 20 J=1,JL2
NR2=NRFL(NS,J)
IF(NR2.EQ.0) GO TO 20
INT=INL(NS,J)
IF(INT.EQ.0) GO TO 13
LJ=MCM(NS,J)
IP0=IP
13 DO 19 NR=1,NR2
IF(INT.EQ.0) GO TO 19
ER=F(IP)
GAR=F(IP+1)
GNR=F(IP+2)
VER=SQRT(AES(ER))
RHOR=AKRNS*VER
PENR=FEN(LJ,RHOR)
SHFR=SHF(LJ,RHCR)
F(K)=0.
F(K+1)=0.
GR=GNR*PENR
14 IPS=IPS
DO 17 MS=1,NR2
IF(MS.EQ.NR) GO TO 17
ES=F(IP)
GNS=F(IP+2)
RHOS=AKRNS*SQRT(AES(ES))
GS=GNS*PENR
DL=ER-ES-(SHF(LJ,RHCS)-SHFR)*GNS
GH=.5*(GAR+F(IP+1)+GR+GS)
TEMP=GNS/(CL+DL+GH*GH)
F(K)=F(K)+TEMP*GH
F(K+1)=F(K+1)+TEMP*DL
17 IPS=IPS+3
K=K+2
19 IP=IP+3
20 CONTINUE
21 CONTINUE
C MAIN PART OF CROSS-SECTION
IP=IPS1
K=IG1
VE=SQRT(E)
SIG=0.
IF(JV.LT.0) GO TO 25
IF=IFS1
KV=KV1
C SUM OVER NUCLEAR SPECIES
25 DO 59 NS=1,NS2
FRS=F(IP)
AHAT=F(IP+1)
IP=IP+2
CNS=2.*CO(NS)/E
AKONS=AKO(NS)
AKNS=AKONS*VE
RADNS=RAD(NS)
AKRNS=AKONS*RADNS
RHO=AKNS*RADNS
RHOHAT=AKNS*AHAT
CFNS=CNS*FRS
JL2=JL(NS)
DEL=DELTA(NS)
IF(DEL.EQ.0.) GO TO 27
DE=1./ (DEL*VE)
SQPI=SQPI*DE

```

```

27 SIGS=C.
  IF(JV.LT.0) GO TO 33
  KVR=0
  KVN=0
  IF(F(IF).EQ.0.) GO TO 29
  KVN=KV
  KV=KV+1
29 IF(F(IF+1).EQ.0.) GO TO 31
  KVR=KV
  GKvj=0.
  KV=KV+1
31 IF=IF+2
  SUM CVEH ANGULAR-MOMENTA
33 DO 49 J=1,JL2
  LJ=MCM(NS,J)
  GSJ=GSPIN(NS,J)
  INT=INL(NS,J)
  NR2=NR1(NS,J)
  PHIL2=PHI2(LJ,RFC+AT)
  SIN2=SIN(PHIL2)
  COS2=COS(PHIL2)

  PENL=FEN(LJ,RFC)
  SHFL=SHF(LJ,RFC)
  CFG=CFNS*GSJ
  FR=FRL(NS,J)
  SIGJ=C.
  IF(FR.EQ.0.) GO TO 34
  ALJ=2*LJ+1
  CCOS=1.-COS2
  IF(COS2.GT..999) CCOS=2.*((SIN(.5*PHIL2)**2))
  SIGJ=ALJ*CCOS*FR
34 CONTINUE
  IF(KVR.NE.0) GKVR=C.
  PICKET-FENCE EXTENSIONS
  STRF=STRFL(NS,J)
  IF(STRF.EQ.0.) GO TO 35
  GAV=GAVL(NS,J)
  GNA=GNAL(NS,J)
  GTA=GAV+GNA*PENL
  DBAR=GNA/STRF
  TEMP=STRF*PENL
  PFS=TEMP*.5*GTA*FNS(DEAR,E,2)
  PFA=-TEMP*FNS(DEAR,E,1)
  FENCE=PFS*COS2-PFA*SIN2
  IF(INT.NE.0) FENCE=FENCE+.5*(PFS*PFS+PFA*PFA)
  SIGJ=SIGJ+GSJ*FENCE
35 CONTINUE
  IF(NR2.EQ.0) GO TO 48
  CONTRIBUTION OF RESONANCES
  DO 47 NR=1,NR2
  ER=F(IP)
  GAR=F(IP+1)
  GNR=F(IP+2)
  IP=IP+3
  GN=GNR*PENL
  RHR=AKRNS*SQRT(ABS(ER))
  SHIFT=SHF(LJ,RHR)-SHFL
  EP=SHIFT*GNR+ER
  GR=COS2
  HR=SIN2
  GH=.5*(GAR+GN)
  DL=EP-E
  IF(INT.EQ.0) GO TO 36
  GR=GR+F(K)*PENL
  HR=HR+F(K+1)*PENL
  K=K+2
  IF(STRF.EQ.0.) GO TO 36
  PFT=PFS+TEMP*GH*FNS(DEAR,E,2)
  GR=GR+PFT
  HR=HR-PFA
36 CONTINUE
  IF(JV.GE.0) FLAG=F(IF)+F(IF+1)+F(IF+2)
  IF(DEL.NE.0.) GO TO 37
  DENINV=1./(GR*GH+DL*DL)
  U=GH*DENINV
  V=DL*DENINV
  IF(FLAG.EQ.0.) GO TO 39
  DP1=-(U+U)*V

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```

DP2=(L+V)*(U-V)
GO TO 39
37 ETA=G+DE
ZED=CL*DE
CALL SVS(ZED,ETA,LO,VO)
U=SQP IDE*UC
V=SQP IDE*VO
IF(FLAG.EQ.0.) GO TO 39
DP1=(CE+DE)*(ETA+V-ZED+U)
DP2=(CE+DE)*(CE-ZED*V-ETA*U)
IF(ABS(ETA*V-ZED*U).LT.EPSI) DP1=-(U+U)*V
IF(ABS(DE-ZED*V-ETA*U).LT.EPSI) DP2=(U+V)*(U-V)
39 UV=GR*U-HR*V
SIGJ=SIGJ+GSJ*UV*GN
C CALCULATION OF DERIVATIVES
IF(JV.LT.0) GC TO 47
C W.R.T. EFFECTIVE RADIAL AHAT
IF(KVR.NE.0) GKVR=GKVR-GN*(V*COS2+U*SIN2)
IF(FLAG.EQ.0.) GO TO 45
C W.R.T. RESONANCE ENERGY ER
IF(F(IF).EQ.C.) GC TO 41
G(KV)=CFG*GN*(GR*DF1-HR*DP2)*(1.+GNR*DSHF(LJ,RHR)*.5*RHR/ER)
KV=KV+1
C W.R.T. CAPTURE WIDTH GAR
41 IF(F(IF+1).EQ.0.) GO TO 43
G(KV)=-.5*CFG*GN*(GR*DP2+HR*DP1)
KV=KV+1
C W.R.T. REDUCED NEUTRON WIDTH GNR
43 IF(F(IF+2).EQ.0.) GC TO 45
UN=DP1*SHIFT-.5*DF2*PENL
VN=.5*DP1*PENL+CP2*SHIFT
G(KV)=CFG*(PENL*UV+GN*(GR*UN-HR*VN))
KV=KV+1
45 IF=IF+3
47 CONTINUE
48 CONTINUE
IF(JV.LT.0) GC TO 49
IF(KVR.NE.0) GKvj=GKvj+(ALJ*SIN2*FR+GSJ*GKVR)*DPH(LJ,RHOHAT)
49 SIG=SIG+SIGJ
IF(JV.LT.C) GC TO 55
IF(KVR.NE.0) G(KV)=(CFNS+CFNS)*AKNS*GKvj
IF(KVN.NE.C) G(KVN)=SIGS*CNS
59 SIG=SIG+SIGS*CFNS
C CONTRIBUTION OF AUXILIARY PARAMETRES
DO 69 N=1,MAXX
SIG=SIG+F(IP)*FNS(VE,E,N)
IF(JV.LT.0) GC TO 69
C DERIVATIVES W.R.T. AUXILIARY PARAMETRES
IF(F(IF).EQ.C.) GC TO 67
G(KV)=FNS(VE,E,N)
KV=KV+1
67 IF=IF+1
69 IP=IP+1
RETURN
END

FUNCTION PHI2(LJ,RHC)
PHI2=RHC+RHO
IF(LJ.EQ.C) RETURN
IF(LJ.NE.1) GC TO 1
PHI2=PHI2-2.*ATAN(RHC)
RETURN
1 IF(LJ.NE.2) GC TO 2
PHI2=2.*((RHO-ATAN(3.*RHO/(3.-RHO*RHO)))
RETURN
2 IF(LJ.NE.3) CALL ERROR
RHOSQ=RHO*RHO
PHI2=2.*((RHO-ATAN(RHO*(RHOSQ-15.)/(6.*RHOSQ-15.))))
RETURN
END

FUNCTION DPH(LJ,RHC)
IF(LJ.NE.0) GC TO 1
DPH=1.
RETURN
1 RHOSQ=RHO*RHO
IF(LJ.NE.1) GC TO 2
DPH=RHC*SQ/(1.+RHOSQ)
RETURN
2 IF(LJ.NE.2) GC TO 3
DPH=9.*RHOSQ/(9.+RHC*SQ*(3.+RHOSQ))
RETURN
3 IF(LJ.NE.3) CALL ERROR
RHO4=RHO*RHOSQ
DPH=(RHO4+RHC4)*(RHOSQ+2.)/
1(225.+45.*RHC*SQ+RHO4*(6.+RHOSQ))
RETURN
END

```

```

FUNCTION SHF(LJ,RHO)
IF(LJ.NE.0) GO TO 1
SHF=0.
RETURN
1 RHOSQ=RHO*RHC
IF(LJ.NE.1) GO TO 2
SHF=-.5/(1.+RHOSQ)
RETURN
2 IF(LJ.NE.2) GO TO 3
SHF=-(9.+1.5*RHCSC)/(9.+RHOSQ*(3.+RHOSQ))
RETURN
3 IF(LJ.NE.3) CALL ERROR
RHO4=RHOSG*RHOSQ
SHF=-(337.5+45.*RHOSQ+3.*RHO4)/(225.+45.*RHOSQ+6.*RHO4
1+RHO4*RHOSG)
RETURN
END

FUNCTION DSHF(LJ,RHC)
IF(LJ.NE.0) GO TO 1
DSHF=0.
RETURN
1 RHOSC=RHO*RHC
IF(LJ.NE.1) GO TO 2
DSHF=RHO/((1.+RHCSC)**2)
RETURN
2 IF(LJ.NE.2) GO TO 3
TEMP=9.+RHCSC*(3.+RHOSQ)
DSHF=3.*RHC*(TEMP+5.*RHOSQ)/(TEMP*TEMP)
RETURN
3 IF(LJ.NE.3) CALL ERROR
RHO4=RHOSG*RHOSC
RHO6=RHO4*RHCSC
TEMP=225.+45.*RHOSQ+6.*RHO4+RHO6
DSHF=1687.5+900.*RHCSC+382.5*RHO4+RHO6*(30.+RHOSQ)
DSHF=6.*RHC*DSHF/(TEMP*TEMP)
RETURN
END

FUNCTION PEN(LJ,RHC)
PEN=RHO
IF(LJ.EQ.0) RETURN
RHOSQ=RHC*RHC
IF(LJ.NE.1) GO TO 1
PEN=PEN*RHOSQ/(1.+RHCSC)
RETURN
1 RHO4=RHCSC*RHOSQ
IF(LJ.NE.2) GO TO 2
PEN=RHC*RHC4/(9.+3.*RHOSQ+RHO4)
RETURN
2 IF(LJ.NE.3) CALL ERROR
RHO6=RHO4*RHOSQ
PEN=RHC*RHC6/(225.+45.*RHOSQ+6.*RHO4+RHO6)
RETURN
END

FUNCTION FNS(VE,E,N)
COMMON/FLT/B2,CE3,EH,EL,PHI,DOFINV,DTMIN
DATA EPS/.582/
FNS=0.
GO TO (21,22,23,24,25,26,27,28,29)N
21 FNS=ALOG((EH-E+EPS*VE)/(E-EL+EPS*VE))
RETURN
22 FNS=(E-EL+VE)/((E-E+.5*VE)*(E-EL+.5*VE))
RETURN
23 FNS=1.
RETURN
24 FNS=E
RETURN
25 FNS=VE
RETURN
26 FNS=1./VE
RETURN
27 CONTINUE
28 CONTINUE
29 CONTINUE
END

```

```

SUBROUTINE SVS(AX,Y1,REW,AIMW)
COMMNCN/TRTI/TR(62,62),TI(62,62),KI
DATA K/0/
IF(K.EQ.1) GO TO 3
K=1
KI=1
X=-.1
DO 2 I=1,62
Y=-.1
DO 1 J=1,62
CALL W(X,Y,TR(I,J),TI(I,J))
1 Y=Y+.1
2 X=X+.1
3 CONTINUE
CALL GUICKW (AX,Y1,REW,AIMW)
RETURN
END

SUBROUTINE NEW(REZ,AIM1,REW,AIMW)
REW=0.
AIMW=0.
AIMZ=ABS (AIM1)
IF(REZ)27,20C1,27
2001 IF(AIM1)27,20C2,27
2002 REW=1.
RETURN
27 R2=REZ*REZ
AI2=AIMZ*AIMZ
ABREZ=ABS (REZ)
IF(ABREZ+1.2E+0)102,102,100
100 IF(ABREZ+1.1*AIMZ-6.6)117,117,116
101 IF(AEREZ+1.43333*AIMZ-4.3)119,119,118
1C2 IF(AEREZ+1.863636*AIMZ-4.1)111,111,104
1C3 IF(AIMZ-1.5)110,120,120
104 IF(AIMZ-1.4)115,115,1C1
1C5 IF(ABREZ+1.07317*AIMZ-4.4)119,119,118
106 IF(AEREZ-2.7)127,128,128
1C7 IF(AEREZ-3.1)106,106,108
1C8 IF(ABREZ-3.4)125,130,130
109 IF(R2+1.18*AI2-5.76)1C3,1C7,107
110 IF(R2+1.7227*AI2-4.41)125,126,126
111 IF(R2+1.71*AI2-2.69)113,119,119
112 IF(R2+1.69*AI2-1.69)123,124,124
113 IF(R2+2.0408*AI2-1.0)114,112,112
114 IF(R2+1.5625*AI2-.25)121,122,122
115 IF(ABREZ+1.43333*AIMZ-4.3)120,120,105
116 NMAX=1
GO TO 15
117 NMAX=2
GO TO 15
118 NMAX=3
GO TO 15
119 NMAX=4
GO TO 15
120 NMAX=6
GO TO 15
121 NMAX=2
GO TO 20
122 NMAX=3
GO TO 20
123 NMAX=4
GO TO 20
124 NMAX=5
GO TO 20
125 NMAX=6
GO TO 20
126 NMAX=7
GO TO 20
127 NMAX=8
GO TO 20
128 NMAX=9
GO TO 20
129 NMAX=10
GO TO 20

```

```

130 NMAX=11
21 KW=2
AIMZ=AIM1
GO TC 200
15 KW=1
IF(AIM1)2000,15C,150
2000 KW=2
AIMZ=AIM1
GO TC 200
C WA IS OBTAINED FROM ASYMTOTIC SERIES
150 RV=2.* (R2-AI2)
AK=4.*REZ*AIMZ
EL=AK
H=0.
B=0.
A=0.
TEMPM=0.
TEMEL=0.
G=1.
C=-1.1283792*AIMZ
D=1.1283792*REZ
AM=RV-1.
AAK=1.
K=0
11 AJTEMF=2.*AAK
TEMP4=(1.-AJTEMF)*AJTEMP
AJP=RV-(4.*AAK+1.)
GO TC 40
41 AAK=AAK+1.
K=K+1
PR=REW
PI=AIMW
12 AMAGN=TEMPN**2+TEMEL**2
REW=(TEMPC*TEMPN+TEMPD*TEMEL)/AMAGN
AIMW=(TEMPN*TEMPD-TEMEL*TEMPC)/AMAGN
IF(ABS (REW-PR)-1.E-6)665,11,11
665 IF(ABS (AIMW-PI)-1.E-6)665,11,11
65 RETURN
C WT IS OBTAINED FROM TAYLOR SERIES
200 TEMP1=R2+AI2
TEMP2=2.*TEMP1*TEMP1
AJ=-(R2-AI2)/TEMP2
AK=2.*REZ*AIMZ/TEMP2
C=0.
B=0.
AJSIG=0.
D=C.
JSIG=C
G=0.
H=0.
EL=0.
A=1.
AM=1.
SIGP=1.5
EXPON=EXP (TEMP2*AJ)
EXPC=EXPON*CCS (TEMP2*AK)
EXPS=-EXPCN*SIN (TEMP2*AK)
SIG2P=2.*SIGP
4 AJ4SIG=4.*AJSIG
AJ4SM1=AJ4SIG-1.
TEMP3=1. / (AJ4SM1*(AJ4SIG+3.))
TT4=SIG2P*(2.*AJ4SIG-1.)
TEMP4=TT4/(AJ4SM1*(AJ4SIG+1.)*(AJ4SIG-3.)*AJ4SM1)
AJP=AJ+TEMP3
GO TC 40
42 AJSIG=AJSIG+1.
JSIG=JSIG+1
6 TEMP7=(AM*AM+EL*EL)*1.7724539
REF=(AIMZ*(C*AM+D*EL)-REZ*(AM*D-C*EL))/1
TEMP7/TEMP1
AIMF=(AIMZ*(AM*C-C*EL)+REZ*(C*AM +D*EL))/TEMP7/TEMP1
PR=REW
PI=AIMW
REW=EXPC-REF
AIMW=EXPS-AIMF
IF(ABS (REW-PR)-1.E-6)664,7,7
664 IF(ABS (AIMW-PI)-1.E-6)664,7,7
64 RETURN
7 SIG2P=2.*AJSIG
GO TC 4
40 TEMPC=AJP*C+TEMP4*A-AK*D
TEMPD=AJP*D+TEMP4*B+AK*C
TEMEL=AJP*EL+TEMP4*I+AK*AM
TEMPM=AJP*AM+TEMP4*G-AK*EL
A=C
B=D
G=AM
H=EL
C=TEMPC
D=TEMPD
AM=TEMPM
EL=TEMEL
IF(AES (TEMPM)+ABS (TEMEL)-1.0E15)49,43,43

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```

43 C=1.0E-15*C
D=1.0E-15*D
AM=1.0E-15*AM
EL=1.0E-15*EL
TEMPC=1.0E-15*TEMPC
TEMPD=1.0E-15*TEMFD
TEMPM=1.0E-15*TEMFM
TEMEL=1.0E-15*TEMEL
GO TO 5C
49 IF(ABS(TEPM)-ABS(TEMEL)-1.0E-15)44,44,50
44 C=1.0E15*C
C=1.0E15*D
AM=1.0E15*AM
EL=1.0E15*EL
TEMPC=1.0E15*TEMPC
TEMPD=1.0E15*TEMFD
TEMPM=1.0E15*TEMFM
TEMEL=1.0E15*TEMEL
50 GO TO(41,42,12345),KW
12345 RETURN
END

```

```

SUBROUTINE QUICKW (AX,Y ,REW,AIMW)
COMM CN/TR TI/TR(62,62),TI(62,62),KI
AKI=SIGN(1.,AX)
X=ABS(AX)
TEST=X*X+Y*Y
IF(TEST.LT.36.)GO TO 10
IF(TEST.LT.144.)GO TO 2
IF(TEST.LT.10000.)GO TO 3
A1=1./(1.7724539*TEST)
REW=Y*A1
IF(KI.GT.0)AIMW=X*A1*AKI
RETURN
10 II=X*10.
JJ=Y*10.
I=II+2
J=JJ+2
N=J-1
P=10.*X-II
Q=10.*Y-JJ
15 P2=P*P
Q2=Q*Q
PQ=P*Q
HP=.5*P
HQ=.5*Q
HQ2=.5*Q2
HP2=.5*P2
A1=HP2-HQ
A2=HP2+HP
A3=1.+PQ-P2-Q2
A4=HP2-PQ+HP
A5=HQ2-PQ+HQ
REW=A1*TR(I,N )+A2*TR(I-1,J)+A3*TR(I,J)+A4*TR(I+1,J)+A5*TR(I,J+1) QUIC0030
1+PQ*TR(I+1,J+1) QUIC0040
IF(KI.LE.0) GO TO 8 QUIC0050
5 AIMW=A1*TI(I,N )+A2*TI(I-1,J)+A3*TI(I,J)+A4*TI(I+1,J)+A5*TI(I,J+1) QUIC0060
1)+PQ*TI(I+1,J+1) QUIC0070
AIMW=AIMW*AKI QUIC0080
GOTO 8 QUIC0090
2 A1=X*X -Y*Y
A2=2.*X*Y
A3=A2*A2
A4=A1-.27525E1 QUIC0110
A5=A1-2.72474E QUIC0120
D1=.5124242/(A4*A4+A3) QUIC0130
D2=.0E176536/( A5*A5+A3) QUIC0140
REW=D1*(A2*X-A4*Y)+D2*(A2*X-A5*Y) QUIC0150
IF(KI.LE.0) GO TO 8 QUIC0160
7 AIMW=C1*(A4*X +A2*Y)+D2*(A5*X+A2*Y) QUIC0170
AIMW=AIMW*AKI QUIC0180
GOTO 8 QUIC0190
3 A1=(X*X -Y*Y )*2.
A2=4.*X*Y
A4=A1-1.
D1=1.1283792/(A4*A4+A2*A2) QUIC0200
REW=D1*(A2*X-A4*Y) QUIC0210
IF(KI.LE.0) GO TO 8 QUIC0220
9 AIMW=C1*(A4*X+A2*Y) QUIC0230
AIMW=AIMW*AKI QUIC0240
8 RETURN QUIC0250
END QUIC0260

```

APPENDIX III. SAMPLE PROBLEM

A. Listing of Input

SIMB TEST PROBLEM WITH 40M 238U DATA

3	5	9	1	0	0	0	0	0	-1	1	1	0
5.74E-07	7.40E-12	566.0		386.0		0.999				0.0030		
(F10.3,6F6.3)												
458.136	0.864	0.025	0.536	0.017	0.149	0.005						
458.344	0.888	0.026	0.580	0.018	0.146	0.005						
458.552	0.901	0.026	0.550	0.017	0.138	0.004						
458.761	0.834	0.024	0.542	0.017	0.149	0.005						
458.970	0.869	0.025	0.580	0.018	0.143	0.004						
459.179	0.906	0.026	0.542	0.017	0.157	0.005						
459.388	0.866	0.025	0.582	0.018	0.141	0.004						
459.597	0.849	0.024	0.541	0.017	0.146	0.004						
459.806	0.862	0.025	0.558	0.017	0.150	0.005						
460.016	0.887	0.025	0.529	0.016	0.151	0.005						
460.225	0.843	0.024	0.535	0.017	0.153	0.005						
460.435	0.871	0.025	0.570	0.018	0.154	0.005						
460.645	0.893	0.025	0.604	0.019	0.152	0.005						
460.855	0.858	0.025	0.552	0.017	0.151	0.005						
461.065	0.871	0.025	0.577	0.018	0.154	0.005						
461.275	0.873	0.025	0.565	0.017	0.149	0.005						
461.486	0.878	0.025	0.559	0.017	0.160	0.005						
461.697	0.906	0.026	0.560	0.017	0.159	0.005						
461.907	0.862	0.024	0.563	0.018	0.155	0.005						
462.118	0.817	0.024	0.551	0.017	0.144	0.005						
462.329	0.806	0.023	0.453	0.015	0.103	0.003						
462.540	0.778	0.023	0.381	0.014	0.059	0.003						
462.752	0.665	0.021	0.242	0.010	0.020	0.002						
462.960	0.542	0.018	0.116	0.007	0.004	0.001						
463.175	0.501	0.017	0.066	0.005	0.003	0.001						
463.386	0.510	0.017	0.091	0.006	0.005	0.001						
463.598	0.635	0.020	0.167	0.008	0.013	0.001						
463.811	0.734	0.022	0.263	0.010	0.033	0.002						
464.023	0.782	0.023	0.403	0.014	0.062	0.003						
464.235	0.851	0.025	0.473	0.015	0.090	0.003						
464.448	0.843	0.024	0.489	0.016	0.107	0.004						
464.660	0.858	0.025	0.497	0.016	0.114	0.004						
464.873	0.854	0.024	0.560	0.018	0.115	0.004						
465.086	0.874	0.025	0.542	0.017	0.120	0.004						
465.299	0.846	0.025	0.501	0.016	0.128	0.004						
465.512	0.896	0.026	0.528	0.016	0.123	0.004						
465.726	0.916	0.027	0.531	0.017	0.127	0.004						
465.939	0.840	0.024	0.517	0.016	0.128	0.004						
466.153	0.826	0.024	0.529	0.017	0.122	0.004						
466.366	0.858	0.025	0.573	0.018	0.130	0.004						
466.581	0.853	0.024	0.546	0.017	0.130	0.004						
466.795	0.871	0.025	0.524	0.016	0.127	0.004						

467.009	0.839	0.024	0.504	0.016	0.123	0.004
467.223	0.879	0.025	0.523	0.016	0.125	0.004
467.438	0.877	0.025	0.511	0.016	0.129	0.004
467.653	0.856	0.024	0.511	0.016	0.129	0.004
467.867	0.871	0.025	0.531	0.017	0.136	0.004
468.082	0.875	0.025	0.565	0.018	0.133	0.004
468.297	0.835	0.024	0.539	0.017	0.134	0.004
468.513	0.873	0.025	0.533	0.016	0.144	0.005
468.728	0.898	0.026	0.577	0.018	0.140	0.004
468.944	0.839	0.024	0.542	0.017	0.140	0.004
469.159	0.852	0.025	0.529	0.017	0.141	0.004
469.375	0.842	0.024	0.551	0.017	0.137	0.004
469.591	0.849	0.024	0.542	0.017	0.136	0.004
469.808	0.875	0.025	0.559	0.017	0.139	0.004
470.024	0.867	0.025	0.556	0.017	0.143	0.004
470.240	0.860	0.025	0.556	0.017	0.140	0.004
470.457	0.837	0.024	0.582	0.018	0.141	0.004
470.674	0.890	0.026	0.564	0.018	0.142	0.004
470.891	0.876	0.025	0.521	0.016	0.142	0.004
471.108	0.372	0.025	0.571	0.018	0.149	0.005
471.325	0.871	0.025	0.565	0.017	0.143	0.004
471.542	0.872	0.025	0.553	0.017	0.141	0.004
471.760	0.866	0.025	0.575	0.018	0.148	0.005
471.978	0.891	0.026	0.521	0.016	0.142	0.004
472.195	0.887	0.025	0.564	0.017	0.141	0.004
472.413	0.919	0.026	0.568	0.018	0.141	0.004
472.632	0.927	0.027	0.566	0.017	0.150	0.005
472.850	0.894	0.026	0.560	0.017	0.147	0.005
473.068	0.886	0.026	0.578	0.018	0.147	0.004
473.287	0.838	0.024	0.577	0.018	0.147	0.005
473.506	0.852	0.024	0.544	0.017	0.146	0.004
473.724	0.842	0.024	0.539	0.017	0.151	0.005
473.943	0.879	0.025	0.563	0.018	0.148	0.005
474.163	0.901	0.026	0.568	0.018	0.144	0.004
474.382	0.881	0.025	0.526	0.016	0.148	0.005
474.602	0.892	0.025	0.564	0.018	0.142	0.004
474.821	0.862	0.025	0.571	0.018	0.149	0.005
475.041	0.892	0.026	0.575	0.018	0.160	0.005
475.261	0.847	0.024	0.527	0.016	0.149	0.004
475.481	0.897	0.025	0.589	0.018	0.147	0.004
475.701	0.878	0.025	0.541	0.017	0.158	0.005
475.922	0.866	0.025	0.572	0.018	0.164	0.005
476.142	0.870	0.025	0.572	0.018	0.157	0.005
476.363	0.862	0.024	0.557	0.017	0.162	0.005
476.584	0.835	0.024	0.582	0.018	0.155	0.005
476.805	0.839	0.024	0.584	0.018	0.159	0.005

477.026	0.864	0.025	0.558	0.018	0.155	0.005
477.247	0.824	0.024	0.538	0.017	0.147	0.005
477.469	0.876	0.026	0.522	0.017	0.130	0.004
477.690	0.831	0.025	0.444	0.015	0.099	0.004
477.912	0.746	0.023	0.346	0.013	0.047	0.002
478.134	0.656	0.021	0.218	0.010	0.015	0.001
478.356	0.522	0.020	0.119	0.007	0.004	0.001
478.579	0.604	0.019	0.117	0.007	0.007	0.001
478.801	0.560	0.021	0.201	0.009	0.017	0.001
479.023	0.750	0.022	0.298	0.011	0.041	0.002
479.246	0.841	0.024	0.395	0.013	0.072	0.003
479.469	0.856	0.025	0.473	0.015	0.097	0.003
479.692	0.835	0.024	0.562	0.018	0.115	0.004
479.915	0.860	0.025	0.540	0.017	0.121	0.004
480.139	0.843	0.024	0.523	0.016	0.132	0.004
480.362	0.824	0.024	0.532	0.016	0.133	0.004
480.586	0.839	0.024	0.501	0.016	0.142	0.004
480.810	0.885	0.026	0.541	0.017	0.136	0.004
481.034	0.867	0.025	0.539	0.017	0.138	0.004
481.258	0.867	0.025	0.577	0.018	0.139	0.004
481.482	0.859	0.024	0.520	0.016	0.139	0.004
481.707	0.884	0.026	0.541	0.017	0.141	0.004
481.931	0.857	0.024	0.556	0.017	0.151	0.005
482.156	0.890	0.025	0.529	0.016	0.145	0.004
482.381	0.853	0.024	0.550	0.017	0.133	0.004
482.606	0.909	0.026	0.547	0.017	0.142	0.004
482.831	0.834	0.024	0.528	0.016	0.148	0.005
483.056	0.861	0.025	0.542	0.017	0.137	0.004
483.282	0.835	0.024	0.568	0.017	0.141	0.004
483.508	0.898	0.026	0.567	0.017	0.141	0.004
483.734	0.903	0.026	0.543	0.017	0.142	0.004
483.960	0.847	0.024	0.565	0.017	0.146	0.004
484.186	0.876	0.025	0.522	0.016	0.143	0.004
484.412	0.890	0.026	0.532	0.017	0.141	0.004
484.639	0.853	0.024	0.512	0.016	0.140	0.004
484.865	0.874	0.025	0.549	0.017	0.135	0.004
485.092	0.880	0.025	0.518	0.016	0.124	0.004
485.319	0.902	0.026	0.526	0.016	0.115	0.004
485.546	0.893	0.026	0.503	0.016	0.129	0.004
485.773	0.844	0.024	0.548	0.017	0.139	0.004
486.001	0.850	0.024	0.531	0.016	0.136	0.004
486.229	0.833	0.024	0.581	0.018	0.143	0.004
486.456	0.871	0.025	0.548	0.017	0.151	0.005
486.684	0.886	0.025	0.538	0.016	0.150	0.005
486.912	0.888	0.025	0.557	0.017	0.159	0.005
487.141	0.870	0.025	0.560	0.017	0.148	0.004
487.369	0.833	0.024	0.570	0.018	0.151	0.005
487.597	0.901	0.026	0.542	0.017	0.153	0.005
487.826	0.879	0.025	0.547	0.017	0.143	0.004

488.055	0.860	0.024	0.535	0.017	0.130	0.004
488.284	0.856	0.025	0.518	0.016	0.112	0.004
488.513	0.854	0.025	0.482	0.016	0.078	0.003
488.743	0.818	0.024	0.377	0.013	0.057	0.002
488.972	0.801	0.023	0.392	0.014	0.052	0.002
489.202	0.851	0.025	0.428	0.014	0.068	0.003
489.432	0.844	0.024	0.483	0.016	0.095	0.003
489.662	0.862	0.025	0.524	0.017	0.130	0.004
489.892	0.859	0.025	0.588	0.018	0.141	0.004
490.123	0.896	0.025	0.526	0.016	0.155	0.005
490.353	0.886	0.026	0.548	0.017	0.149	0.005
490.584	0.846	0.024	0.593	0.018	0.146	0.004
490.814	0.860	0.024	0.540	0.017	0.152	0.005
491.045	0.852	0.024	0.557	0.017	0.157	0.005
491.277	0.895	0.026	0.543	0.017	0.160	0.005
491.508	0.906	0.025	0.588	0.018	0.153	0.005
491.740	0.907	0.026	0.570	0.018	0.155	0.005
491.971	0.897	0.026	0.575	0.018	0.156	0.005
492.203	0.865	0.025	0.562	0.017	0.153	0.005
492.435	0.836	0.024	0.578	0.018	0.150	0.005
492.667	0.893	0.025	0.571	0.018	0.149	0.004
492.899	0.867	0.025	0.580	0.018	0.158	0.005
493.132	0.864	0.024	0.568	0.018	0.154	0.005
493.365	0.889	0.025	0.540	0.016	0.153	0.005
493.597	0.883	0.025	0.549	0.017	0.158	0.005
493.830	0.902	0.026	0.568	0.017	0.154	0.005
494.063	0.912	0.026	0.608	0.019	0.149	0.004
494.297	0.888	0.025	0.554	0.017	0.159	0.005
494.530	0.892	0.025	0.566	0.017	0.158	0.005
494.764	0.865	0.025	0.564	0.017	0.148	0.004
494.998	0.880	0.025	0.556	0.017	0.160	0.005
495.231	0.857	0.025	0.587	0.018	0.156	0.005

BLANK CARD
BLANK CARD

0.012395	0.05208	0.17536				
0.0	0.0	0.0				
0.0	0.0	0.0				
(3F10.3)						
1.000	0.9184	236.01	300.0			
	0	1 1.0	1.0	0.04906	0.981	0.0230
397.4	0.00640	0.0252				
410.2	0.02060	0.0226				

433.7	0.00998	0.0235
462.8	0.00550	0.0235
478.3	0.00380	0.0235
518.3	0.05160	0.0244
535.2	0.04700	0.0235

	1	0 1,0	1.0
466.8	0.00010	0.0236	
485.0	0.00012	0.0236	
488.2	0.00062	0.0241	

0.0

0 0 0
1 1 0
0 0 0
0 2
0 0 0
0 0 0
0 0 0
2 0 2
2 0 2
0 0 0
0 0 0

2 0 2
2 0 2
2 0 2

1

BLANK CARD

BLANK CARD
BLANK CARD
BLANK CARD

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BLANK CARD

BLANK CARD
BLANK CARD

B. Listing of Output

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S1OB TEST PROBLEM WITH 40M 238L DATA
FIXED POINT INPUTS   3   5   9   1   0   0   0   0   0   0   -1   0   1   1   0
FLOATING POINT INPUTS  0.574E-06  0.740E-11  566.   386.   0   0.999   1   0
NUMBER OF TRANSMISSION VALUES   5C7
MAXIMUM ADDRESS OF F-ARRAY   176E
MAXIMUM ADDRESS OF G-ARRAY   591
TRUNCATION LIMITS   386.00   566.00

INPUT RESONANCE PARAMETERS

NUCLEAR SPECIES= 1 REDUCED MOMENTUM= 0.21875E-02 NUCLEAR RADIUS= 0.83874
COUPLER WIDTH= 0.78623E-62 NUMBER OF ANGULAR MOMENTS= 2
FRACTIONAL ABUNDANCE= 1.00000 EFFECTIVE RADIUS= 0.9184

ANGULAR MOMENTUM= 0 INTERFERENCE PARAMETER= 1 SPIN STATISTICAL FACTOR= 1.000 POTENTIAL SCATTERING FRACTION= 1.000
STRENGTH-FUNCTION= 0.49000E-01 AVERAGE NEUTRON-WIDTH= 0.98170 AVERAGE CAPTURE-WIDTH= 0.23000E-01

NUMBER OF LEVELS= 7
      RESONANCE ENERGY    CAPTURE-WIDTH    NEUTRON-WIDTH
      397.40    0.25200E-01    0.64000E-02
      410.20    0.22600E-01    0.20600E-01
      433.70    0.23500E-01    0.99800E-02
      462.80    0.23500E-01    0.55000E-02
      478.30    0.23500E-01    0.38000E-02
      518.30    0.24400E-01    0.51600E-01
      535.20    0.23800E-01    0.47000E-01

ANGULAR MOMENTUM= 1 INTERFERENCE PARAMETER= 0 SPIN STATISTICAL FACTOR= 1.000 POTENTIAL SCATTERING FRACTION= 1.000
STRENGTH-FUNCTION= 0.0 AVERAGE NEUTRON-WIDTH= 0.0 AVERAGE CAPTURE-WIDTH= 0.0

NUMBER OF LEVELS= 3
      RESONANCE ENERGY    CAPTURE-WIDTH    NEUTRON-WIDTH
      466.80    0.23600E-01    0.10000E-03
      485.00    0.23600E-01    0.12000E-03
      488.20    0.24100E-01    0.62000E-03

ITERATION NUMBER 1
      NPS          ETA        CHIOLD        CHINEW
      0           1.0000     29.000      4.8829

SAMPLE-THICKNESSES
      OLD VALUE        NEW VALUE        ERROR
      0.12395E-01
      0.52080E-01
      0.17536

NORMALISATION-ERRORS
      OLD VALUE        NEW VALUE        ERROR
      0.0            -0.60741E-02    0.48846D-02
      0.0            -0.29360E-01    0.53139D-02
      0.0

TRANSMISSION-BACKGROUNDS
      OLD VALUE        NEW VALUE        ERROR
      0.0
      0.0
      0.0
  
```

RESONANCE PARAMETERS

NUCLEAR SPECIES = 1 NUMBER OF ANGULAR MOMENTA = 2

FRACTIONAL ABUNDANCE AND RADIUS

OLD VALUE	NEW VALUE	ERROR
1.0000 0.91840	0.9E370	0.12906D-02

ANGULAR MOMENTUM = 0 NUMBER OF LEVELS= 7

RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
(ONLY VARIED LEVELS ARE LISTED)		
462.80 0.23500E-01 0.55019E-02	462.12 0.39651E-02	0.11517E-01 0.21574E-03
478.30 0.23500E-01 0.38005E-02	47E.42 0.37049E-02	0.12477E-01 0.14500E-03

ANGULAR MOMENTUM = 1 NUMBER OF LEVELS= 3

RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
(ONLY VARIED LEVELS ARE LISTED)		
466.80 0.23600E-01 0.10004E-03	46E.51 0.49464E-04	0.12985 0.24433E-04
485.00 0.23600E-01 0.12010E-03	48E.26 0.7E360E-04	0.11205 0.24801E-04
488.20 0.24100E-01 0.62093E-03	48E.69 0.29111E-03	0.27767E-01 0.41450E-04

AUXILIARY PARAMETERS

OLD VALUE	NEW VALUE	ERROR
0.0	-0.33570	0.13253

ITERATION NUMBER 2

NPS	ETA	CHIOLD	CHINEW
0	1.0000	4.8829	2.0742

SAMPLE-THICKNESSES

OLD VALUE	NEW VALUE	ERROR
0.12395E-01		
0.52080E-01		
0.17536		

NORMALISATION-ERRORS

OLD VALUE	NEW VALUE	ERROR
-0.60741D-02	-0.26567E-02	0.32031D-02
-0.29360D-01	-0.22132E-01	0.36255D-02
0.0		

TRANSMISSION-BACKGROUNDS

OLD VALUE	NEW VALUE	ERROR
0.0		
0.0		
0.0		

RESONANCE PARAMETERS

NUCLEAR SPECIES = 1 NUMBER OF ANGULAR MOMENTA = 2

FRACTIONAL ABUNDANCE AND RADIALS

OLD VALUE	NEW VALUE	ERROR
1.0000		
0.95370	0.94888	0.92928D-03

ANGULAR MOMENTUM = 0 NUMBER OF LEVELS= 7

RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
-----------	-----------	-------

(ONLY VARIED LEVELS ARE LISTED)

463.12	463.17	0.74882E-02
0.22500E-01		
0.39653E-02	0.51063E-02	0.88958E-04
478.42	478.43	0.86925E-02
0.23500E-01		
0.37049E-02	0.39649E-02	0.96005E-04

ANGULAR MOMENTUM = 1 NUMBER OF LEVELS= 3

RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
-----------	-----------	-------

(ONLY VARIED LEVELS ARE LISTED)

466.91 0.23600E-01 0.49502E-04	467.15 0.5290EE-04	0.18469 0.16739E-04
485.26 0.23600E-01 0.78376E-04	485.33 0.12665E-03	0.12528 0.17750E-04
488.69 0.24100E-01 0.29152E-03	489.15 0.64901E-03	0.33424E-01 0.18594E-04

AUXILIARY PARAMETERS

OLD VALUE	NEW VALUE	ERROR
-0.33570	-0.22924E-01	0.99935D-01

ITERATION NUMBER 3

NPS	ETA	CHIOLD	CHINEW
0	1.0000	2.0742	1.0611

SAMPLE-THICKNESSES

OLD VALUE	NEW VALUE	ERROR
0.12395E-01 0.52080E-01 0.17536		

NORMALISATION-ERRORS

OLD VALUE	NEW VALUE	ERROR
-0.28567D-02 -0.22132D-01 0.0	-0.2110EE-02 -0.21063E-01	0.23008D-02 0.26021D-02

TRANSMISSION-BACKGROUNDS

OLD VALUE	NEW VALUE	ERROR
0.0 0.0 0.0		

RESONANCE PARAMETERS

NUCLEAR SPECIES = 1 NUMBER OF ANGULAR MOMENTA = 2
 FRACTIONAL ABUNDANCE AND RADIUS

OLD VALUE	NEW VALUE	ERROR
1.0000 0.94888	0.94863	0.66121D-03

ANGULAR MOMENTUM = 0 NUMBER OF LEVELS= 7
 RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE NEW VALUE ERROR

(ONLY VARIED LEVELS ARE LISTED)

463.17 0.23500E-01 0.51063E-02	463.17 0.53836E-02	0.50667E-02 0.84385E-04
478.43 0.23500E-01 0.39649E-02	478.43 0.39813E-02	0.60386E-02 0.72857E-04

ANGULAR MOMENTUM = 1 NUMBER OF LEVELS= 3
 RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
467.15 0.23600E-01 0.52912E-04	467.16 0.55953E-04	0.12355 0.11985E-04
485.33 0.23600E-01 0.12864E-03	485.30 0.13023E-03	0.55287E-01 0.13155E-04
485.15 0.24100E-01 0.64846E-03	485.67 0.72674E-03	0.13038E-01 0.18745E-04

AUXILIARY PARAMETERS

OLD VALUE	NEW VALUE	ERROR
-0.22924D-01	-0.174C0E-01	0.70507D-01

ITERATION NUMBER 4

NPS	ETA	CHIOLD	CHINEW
0	1.0000	1.0611	0.97770

SAMPLE-THICKNESSES

OLD VALUE	NEW VALUE	ERROR
0.12395E-01		
0.52080E-01		
0.17536		

NORMALISATION-ERRORS

OLD VALUE	NEW VALUE	ERROR
-0.21108D-02	-0.19608E-02	0.22108D-02
-0.21063D-01	-0.20653E-01	0.25023D-02
0.0		

TRANSMISSION-BACKGROUNDS

OLD VALUE	NEW VALUE	ERROR
0.0		
0.0		
0.0		

RESONANCE PARAMETERS

NUCLEAR SPECIES = 1 NUMBER OF ANGULAR MOMENTA = 2

FRACTIONAL ABUNDANCE AND RADIALS

OLD VALUE	NEW VALUE	ERROR
1.0000		
0.94863	0.94810	0.63565D-03

ANGULAR MOMENTUM = C NUMBER OF LEVELS= 7

RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
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(ONLY VARIED LEVELS ARE LISTED)

463.17	463.17	0.48384E-02
0.23500E-01		
0.53836E-02	0.53979E-02	0.86178E-04
478.43	478.43	0.57896E-02
0.23500E-01		
0.39813E-02	0.39905E-02	0.70193E-04

ANGULAR MOMENTUM = 1 NUMBER OF LEVELS= 3
 RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
(ONLY VARIED LEVELS ARE LISTED)		
467.18 0.23600E-01 0.55954E-04	467.18 0.56053E-04	0.11257 0.11568E-04
485.30 0.23600E-01 0.13023E-03	485.30 0.13524E-03	0.52450E-01 0.12646E-04
488.87 0.24100E-01 0.72682E-03	488.91 0.82585E-03	0.11597E-01 0.19243E-04

AUXILIARY PARAMETERS

OLD VALUE	NEW VALUE	ERROR
-0.17400D-01	0.55976E-01	0.67549D-01

ITERATION NUMBER 5

NPS	ETA	CHIOLD	CHINEW
0	1.0000	0.97770	0.97676

SAMPLE-THICKNESSES

OLD VALUE	NEW VALUE	ERROR
0.12395E-01		
0.5208CE-01		
0.17536		

NORMALISATION-ERRORS

OLD VALUE	NEW VALUE	ERROR
-0.19608D-02	-0.15473E-02	0.22102D-02
-0.20693D-01	-0.20634E-01	0.25027D-02
0.0		

TRANSMISSION-BACKGROUNDS

OLD VALUE	NEW VALUE	ERROR
0.0		
0.0		
0.0		

RESONANCE PARAMETERS

NUCLEAR SPECIES = 1 NUMBER OF ANGULAR MOMENTA = 2

FRACTIONAL ABUNDANCE AND RADIUS

OLD VALUE	NEW VALUE	ERROR
1.0000		
0.94810	0.94810	0.63482D-03

ANGULAR MOMENTUM = 0 NUMBER OF LEVELS= 7

RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
(ONLY VARIED LEVELS ARE LISTED)		
463.17	463.17	0.48367E-02
0.23500E-01	0.53983E-02	0.86427E-04
0.52979E-02		
478.43	47E.43	0.57741E-02
0.23500E-01	0.39907E-02	0.70242E-04
0.39905E-02		

ANGULAR MOMENTUM = 1 NUMBER OF LEVELS= 3

RESONANCE-ENERGY,CAPTURE-WIDTH,NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
(ONLY VARIED LEVELS ARE LISTED)		
467.18	467.18	0.11233
0.23600E-01	0.56053E-04	0.11565E-04
0.56053E-04	0.56062E-04	
485.30	48E.30	0.50458E-01
0.23600E-01	0.13524E-03	0.12664E-04
0.13524E-03	0.13532E-03	
488.91	48E.91	0.10758E-01
0.24100E-01	0.82584E-03	0.21053E-04
0.82584E-03	0.83286E-03	

AUXILIARY PARAMETERS

OLD VALUE	NEW VALUE	ERROR
0.55976D-01	C.57396E-01	0.67436D-01

STOP ITERATIONS BECAUSE CONVERGENCE IS TOO SLOW

ENERGY	CALCULATION	EXPERIMENT	ERROR	ATOMS PER BARN
458.14	0.8700 0.5500 0.1433	0.8640 0.5360 0.1490	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
458.34	0.8702 0.5605 0.1436	0.8880 0.5800 0.1460	0.0260 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
458.55	0.8704 0.5610 0.1442	0.9010 0.5500 0.1380	0.0260 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
458.76	0.8706 0.5616 0.1447	0.8340 0.5420 0.1490	0.0240 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
458.97	0.8708 0.5621 0.1452	0.8690 0.5800 0.1430	0.0250 0.0180 0.0040	0.12395E-01 0.52080E-01 0.17536
459.18	0.8710 0.5628 0.1457	0.9060 0.5420 0.1570	0.0260 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
459.39	0.8713 0.5634 0.1463	0.8660 0.5820 0.1410	0.0250 0.0180 0.0040	0.12395E-01 0.52080E-01 0.17536
459.60	0.8716 0.5641 0.1470	0.8490 0.5410 0.1460	0.0240 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
459.81	0.8719 0.5645 0.1477	0.8620 0.5580 0.1500	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
460.02	0.8722 0.5658 0.1485	0.8870 0.5290 0.1510	0.0250 0.0160 0.0050	0.12395E-01 0.52080E-01 0.17536
460.22	0.8726 0.5668 0.1494	0.8430 0.5350 0.1530	0.0240 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
460.43	0.8730 0.5679 0.1504	0.8710 0.5700 0.1540	0.0250 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
460.64	0.8735 0.5692 0.1516	0.8930 0.6040 0.1520	0.0250 0.0190 0.0050	0.12395E-01 0.52080E-01 0.17536
460.85	0.8740 0.5697 0.1525	0.8580 0.5520 0.1510	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
461.06	0.8747 0.5625 0.1546	0.8710 0.5770 0.1540	0.0250 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
461.27	0.8754 0.5646 0.1566	0.8730 0.5650 0.1490	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
461.49	0.8763 0.5670 0.1588	0.8780 0.5590 0.1600	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
461.70	0.8769 0.5677 0.1605	0.9080 0.5600 0.1590	0.0260 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
461.91	0.8753 0.5650 0.1582	0.8620 0.5630 0.1550	0.0240 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
462.12	0.8646 0.5418 0.1436	0.8170 0.5510 0.1440	0.0240 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
462.33	0.8315 0.4761 0.1694	0.8060 0.4530 0.1030	0.0230 0.0150 0.0030	0.12395E-01 0.52080E-01 0.17536
462.54	0.7601 0.3586 0.0632	0.7780 0.3810 0.0590	0.0230 0.0140 0.0030	0.12395E-01 0.52080E-01 0.17536
462.75	0.6539 0.2191 0.0257	0.6650 0.2420 0.0200	0.0210 0.0100 0.0030	0.12395E-01 0.52080E-01 0.17536
462.96	0.5510 0.1126 0.0069	0.5420 0.1160 0.0040	0.0180 0.0070 0.0030	0.12395E-01 0.52080E-01 0.17536
463.17	0.5015 0.0691 0.0017	0.5010 0.0660 0.0030	0.0170 0.0050 0.0030	0.12395E-01 0.52080E-01 0.17536
463.39	0.5309 0.0916 0.0032	0.5100 0.0910 0.0050	0.0170 0.0060 0.0030	0.12395E-01 0.52080E-01 0.17536
463.60	0.6195 0.1726 0.0124	0.6350 0.1670 0.0130	0.0200 0.0080 0.0030	0.12395E-01 0.52080E-01 0.17536
463.81	0.7201 0.2885 0.0329	0.7340 0.2630 0.0330	0.0220 0.0100 0.0030	0.12395E-01 0.52080E-01 0.17536
464.02	0.7940 0.3958 0.0619	0.7820 0.4030 0.0620	0.0230 0.0140 0.0030	0.12395E-01 0.52080E-01 0.17536

464.23	0.8333	0.8510	0.0250	0.12395E-01
	0.4655	0.4730	0.0150	0.52080E-01
	0.0684	0.0900	0.0030	0.17536
464.45	0.8499	0.8430	0.0240	0.12395E-01
	0.4998	0.4890	0.0160	0.52080E-01
	0.1056	0.1070	0.0040	0.17536
464.66	0.8561	0.8580	0.0250	0.12395E-01
	0.5142	0.4970	0.0160	0.52080E-01
	0.1146	0.1140	0.0040	0.17536
464.87	0.8588	0.8540	0.0240	0.12395E-01
	0.5209	0.5600	0.0180	0.52080E-01
	0.1194	0.1150	0.0040	0.17536
465.09	0.8604	0.8740	0.0250	0.12395E-01
	0.5249	0.5420	0.0170	0.52080E-01
	0.1225	0.1200	0.0040	0.17536
465.30	0.8615	0.8460	0.0250	0.12395E-01
	0.5278	0.5010	0.0160	0.52080E-01
	0.1247	0.1280	0.0040	0.17536
465.51	0.8624	0.8960	0.0260	0.12395E-01
	0.5300	0.5280	0.0160	0.52080E-01
	0.1265	0.1230	0.0040	0.17536
465.73	0.8631	0.9160	0.0270	0.12395E-01
	0.5318	0.5310	0.0170	0.52080E-01
	0.1280	0.1270	0.0040	0.17536
465.94	0.8636	0.8400	0.0240	0.12395E-01
	0.5333	0.5170	0.0160	0.52080E-01
	0.1291	0.1280	0.0040	0.17536
466.15	0.8640	0.8260	0.0240	0.12395E-01
	0.5341	0.5290	0.0170	0.52080E-01
	0.1298	0.1220	0.0040	0.17536
466.37	0.8639	0.8580	0.0250	0.12395E-01
	0.5340	0.5730	0.0180	0.52080E-01
	0.1297	0.1300	0.0040	0.17536
466.58	0.8633	0.8530	0.0240	0.12395E-01
	0.5324	0.5460	0.0170	0.52080E-01
	0.1284	0.1300	0.0040	0.17536
466.79	0.8621	0.8710	0.0250	0.12395E-01
	0.5294	0.5240	0.0160	0.52080E-01
	0.1261	0.1270	0.0040	0.17536
467.01	0.8611	0.8390	0.0240	0.12395E-01
	0.5268	0.5040	0.0160	0.52080E-01
	0.1240	0.1230	0.0040	0.17536
467.22	0.8610	0.8790	0.0250	0.12395E-01
	0.5266	0.5230	0.0160	0.52080E-01
	0.1238	0.1250	0.0040	0.17536
467.44	0.8622	0.8770	0.0250	0.12395E-01
	0.5295	0.5110	0.0160	0.52080E-01
	0.1261	0.1290	0.0040	0.17536
467.65	0.8635	0.8560	0.0240	0.12395E-01
	0.5340	0.5110	0.0160	0.52080E-01
	0.1298	0.1290	0.0040	0.17536
467.87	0.8655	0.8710	0.0250	0.12395E-01
	0.5381	0.5310	0.0170	0.52080E-01
	0.1332	0.1360	0.0040	0.17536
468.08	0.8665	0.8750	0.0250	0.12395E-01
	0.5408	0.5650	0.0180	0.52080E-01
	0.1354	0.1330	0.0040	0.17536
468.30	0.8671	0.8350	0.0240	0.12395E-01
	0.5422	0.5390	0.0170	0.52080E-01
	0.1366	0.1340	0.0040	0.17536
468.51	0.8674	0.8730	0.0250	0.12395E-01
	0.5430	0.5330	0.0160	0.52080E-01
	0.1373	0.1440	0.0050	0.17536
468.73	0.8676	0.8980	0.0260	0.12395E-01
	0.5436	0.5770	0.0180	0.52080E-01
	0.1378	0.1400	0.0040	0.17536
468.94	0.8678	0.8390	0.0240	0.12395E-01
	0.5441	0.5420	0.0170	0.52080E-01
	0.1382	0.1400	0.0040	0.17536
469.16	0.8680	0.8520	0.0250	0.12395E-01
	0.5446	0.5290	0.0170	0.52080E-01
	0.1386	0.1410	0.0040	0.17536
469.38	0.8681	0.8420	0.0240	0.12395E-01
	0.5450	0.5510	0.0170	0.52080E-01
	0.1390	0.1370	0.0040	0.17536
469.59	0.8683	0.8490	0.0240	0.12395E-01
	0.5455	0.5420	0.0170	0.52080E-01
	0.1394	0.1360	0.0040	0.17536
469.81	0.8684	0.8750	0.0250	0.12395E-01
	0.5459	0.5590	0.0170	0.52080E-01
	0.1397	0.1390	0.0040	0.17536
470.02	0.8686	0.8670	0.0250	0.12395E-01
	0.5463	0.5560	0.0170	0.52080E-01
	0.1401	0.1430	0.0040	0.17536
470.24	0.8688	0.8600	0.0250	0.12395E-01
	0.5467	0.5560	0.0170	0.52080E-01
	0.1404	0.1400	0.0040	0.17536
470.46	0.8689	0.8370	0.0240	0.12395E-01
	0.5471	0.5820	0.0180	0.52080E-01
	0.1408	0.1410	0.0040	0.17536

477.03	0.8763	0.8640	0.0250	0.12395E-01
	0.5671	0.5580	0.0180	0.52080E-01
477.25	0.1591	0.1550	0.0050	0.17536
	0.8730	0.8240	0.0240	0.12395E-01
	0.5563	0.5380	0.0170	0.52080E-01
477.47	0.1537	0.1470	0.0050	0.17536
	0.8583	0.8760	0.0260	0.12395E-01
	0.5266	0.5220	0.0170	0.52080E-01
	0.1234	0.1300	0.0040	0.17536
477.69	0.8190	0.8310	0.0250	0.12395E-01
	0.4456	0.4440	0.0150	0.52080E-01
	0.0547	0.0990	0.0040	0.17536
477.91	0.7471	0.7460	0.0230	0.12395E-01
	0.3278	0.3460	0.0130	0.52080E-01
	0.0496	0.0470	0.0030	0.17536
478.13	0.6656	0.6560	0.0210	0.12395E-01
	0.2046	0.2180	0.0100	0.52080E-01
	0.0182	0.0150	0.0030	0.17536
478.36	0.5986	0.6220	0.0250	0.12395E-01
	0.1304	0.1190	0.0070	0.52080E-01
478.58	0.0051	0.0040	0.0030	0.17536
	0.5995	0.6040	0.0190	0.12395E-01
	0.1303	0.1170	0.0070	0.52080E-01
478.80	0.0044	0.0070	0.0030	0.17536
	0.6591	0.6600	0.0210	0.12395E-01
	0.1995	0.2010	0.0090	0.52080E-01
479.02	0.0143	0.0170	0.0030	0.17536
	0.7399	0.7500	0.0220	0.12395E-01
	0.3090	0.2980	0.0110	0.52080E-01
479.25	0.0372	0.0410	0.0030	0.17536
	0.8047	0.8410	0.0240	0.12395E-01
	0.4135	0.3950	0.0130	0.52080E-01
479.47	0.0694	0.0720	0.0030	0.17536
	0.8407	0.8580	0.0250	0.12395E-01
	0.4819	0.4730	0.0150	0.52080E-01
479.69	0.0984	0.0970	0.0030	0.17536
	0.8559	0.8350	0.0240	0.12395E-01
	0.5147	0.5620	0.0180	0.52080E-01
479.91	0.1164	0.1150	0.0040	0.17536
	0.8615	0.8600	0.0250	0.12395E-01
	0.5280	0.5400	0.0170	0.52080E-01
480.14	0.1252	0.1210	0.0040	0.17536
	0.8638	0.8430	0.0240	0.12395E-01
	0.5337	0.5230	0.0160	0.52080E-01
480.36	0.1295	0.1320	0.0040	0.17536
	0.8650	0.8240	0.0240	0.12395E-01
	0.5369	0.5320	0.0160	0.52080E-01
480.59	0.1321	0.1330	0.0040	0.17536
	0.8655	0.8390	0.0240	0.12395E-01
	0.5391	0.5010	0.0160	0.52080E-01
480.81	0.1340	0.1420	0.0040	0.17536
	0.8665	0.8850	0.0260	0.12395E-01
	0.5409	0.5410	0.0170	0.52080E-01
481.03	0.1355	0.1360	0.0040	0.17536
	0.8671	0.8670	0.0250	0.12395E-01
	0.5423	0.5390	0.0170	0.52080E-01
481.26	0.1367	0.1380	0.0040	0.17536
	0.8676	0.8670	0.0250	0.12395E-01
	0.5435	0.5770	0.0180	0.52080E-01
481.48	0.1377	0.1390	0.0040	0.17536
	0.8680	0.8590	0.0240	0.12395E-01
	0.5446	0.5200	0.0160	0.52080E-01
481.71	0.1386	0.1390	0.0040	0.17536
	0.8683	0.8840	0.0260	0.12395E-01
	0.5455	0.5410	0.0170	0.52080E-01
481.93	0.1394	0.1410	0.0040	0.17536
	0.8686	0.8570	0.0240	0.12395E-01
	0.5463	0.5560	0.0170	0.52080E-01
482.16	0.1401	0.1510	0.0050	0.17536
	0.8689	0.8900	0.0250	0.12395E-01
	0.5471	0.5290	0.0160	0.52080E-01
482.38	0.1407	0.1450	0.0040	0.17536
	0.8691	0.8530	0.0240	0.12395E-01
	0.5477	0.5500	0.0170	0.52080E-01
482.61	0.1413	0.1330	0.0040	0.17536
	0.8694	0.9090	0.0260	0.12395E-01
	0.5483	0.5470	0.0170	0.52080E-01
482.83	0.1418	0.1420	0.0040	0.17536
	0.8696	0.8340	0.0240	0.12395E-01
	0.5489	0.5280	0.0160	0.52080E-01
483.06	0.1423	0.1480	0.0050	0.17536
	0.8698	0.8610	0.0250	0.12395E-01
	0.5494	0.5420	0.0170	0.52080E-01
483.28	0.1428	0.1370	0.0040	0.17536
	0.8700	0.8350	0.0240	0.12395E-01
	0.5499	0.5680	0.0170	0.52080E-01
483.51	0.1432	0.1410	0.0040	0.17536
	0.8701	0.8980	0.0260	0.12395E-01
	0.5504	0.5670	0.0170	0.52080E-01
	0.1436	0.1410	0.0040	0.17536

483.73	0.8703	0.9030	0.0260	0.12395E-01
	0.5508	0.5430	0.0170	0.52080E-01
	0.1440	0.1420	0.0040	0.17536
483.96	0.8704	0.8470	0.0240	0.12395E-01
	0.5510	0.5650	0.0170	0.52080E-01
	0.1442	0.1460	0.0040	0.17536
484.19	0.8702	0.8760	0.0250	0.12395E-01
	0.5506	0.5220	0.0160	0.52080E-01
	0.1439	0.1430	0.0040	0.17536
484.41	0.8695	0.8900	0.0260	0.12395E-01
	0.5486	0.5320	0.0170	0.52080E-01
	0.1421	0.1410	0.0040	0.17536
484.64	0.8675	0.8530	0.0240	0.12395E-01
	0.5435	0.5120	0.0160	0.52080E-01
	0.1376	0.1400	0.0040	0.17536
484.86	0.8643	0.8740	0.0250	0.12395E-01
	0.5352	0.5490	0.0170	0.52080E-01
	0.1310	0.1350	0.0040	0.17536
485.09	0.8611	0.8800	0.0250	0.12395E-01
	0.5269	0.5180	0.0160	0.52080E-01
	0.1242	0.1240	0.0040	0.17536
485.32	0.8599	0.9020	0.0260	0.12395E-01
	0.5239	0.5260	0.0160	0.52080E-01
	0.1218	0.1150	0.0040	0.17536
485.55	0.8618	0.8930	0.0260	0.12395E-01
	0.5265	0.5030	0.0160	0.52080E-01
	0.1255	0.1290	0.0040	0.17536
485.77	0.8653	0.8440	0.0240	0.12395E-01
	0.5378	0.5480	0.0170	0.52080E-01
	0.1332	0.1390	0.0040	0.17536
486.00	0.8686	0.8500	0.0240	0.12395E-01
	0.5465	0.5310	0.0160	0.52080E-01
	0.1404	0.1360	0.0040	0.17536
486.23	0.8707	0.8330	0.0240	0.12395E-01
	0.5518	0.5810	0.0180	0.52080E-01
	0.1449	0.1430	0.0040	0.17536
486.46	0.8716	0.8710	0.0250	0.12395E-01
	0.5642	0.5480	0.0170	0.52080E-01
	0.1470	0.1510	0.0050	0.17536
486.68	0.8719	0.8860	0.0250	0.12395E-01
	0.5551	0.5380	0.0160	0.52080E-01
	0.1476	0.1500	0.0050	0.17536
486.91	0.8721	0.8880	0.0250	0.12395E-01
	0.5555	0.5570	0.0170	0.52080E-01
	0.1482	0.1590	0.0050	0.17536
487.14	0.8722	0.8700	0.0250	0.12395E-01
	0.5558	0.5600	0.0170	0.52080E-01
	0.1484	0.1480	0.0040	0.17536
487.37	0.8721	0.8330	0.0240	0.12395E-01
	0.5557	0.5700	0.0180	0.52080E-01
	0.1484	0.1510	0.0050	0.17536
487.60	0.8716	0.9010	0.0260	0.12395E-01
	0.5544	0.5420	0.0170	0.52080E-01
	0.1473	0.1530	0.0050	0.17536
487.83	0.8695	0.8790	0.0250	0.12395E-01
	0.5489	0.5470	0.0170	0.52080E-01
	0.1428	0.1430	0.0040	0.17536
488.05	0.8630	0.8600	0.0240	0.12395E-01
	0.5326	0.5350	0.0170	0.52080E-01
	0.1306	0.1300	0.0040	0.17536
488.28	0.8491	0.8560	0.0250	0.12395E-01
	0.4593	0.5180	0.0160	0.52080E-01
	0.1478	0.1120	0.0040	0.17536
488.51	0.8288	0.8540	0.0250	0.12395E-01
	0.4516	0.4820	0.0160	0.52080E-01
	0.0793	0.0780	0.0030	0.17536
488.74	0.8109	0.8180	0.0240	0.12395E-01
	0.4114	0.3770	0.0130	0.52080E-01
	0.0572	0.0570	0.0030	0.17536
488.97	0.8271	0.8010	0.0230	0.12395E-01
	0.4029	0.3920	0.0140	0.52080E-01
	0.0528	0.0520	0.0030	0.17536
489.20	0.8201	0.8510	0.0250	0.12395E-01
	0.4321	0.4280	0.0140	0.52080E-01
	0.0683	0.0680	0.0030	0.17536
489.43	0.8411	0.8440	0.0240	0.12395E-01
	0.4802	0.4830	0.0160	0.52080E-01
	0.3962	0.0950	0.0030	0.17536
489.66	0.8586	0.8620	0.0250	0.12395E-01
	0.5219	0.5240	0.0170	0.52080E-01
	0.1233	0.1300	0.0040	0.17536
489.89	0.8683	0.8690	0.0250	0.12395E-01
	0.5459	0.5880	0.0180	0.52080E-01
	0.1408	0.1410	0.0040	0.17536

490.12	0.8721	0.8960	0.0250	0.12395E-01
	0.5658	0.5260	0.0160	0.52080E-01
490.35	0.1487	0.1550	0.0050	0.17536
	0.8734	0.8860	0.0260	0.12395E-01
	0.5590	0.5480	0.0170	0.52080E-01
490.58	0.1514	0.1490	0.0050	0.17536
	0.8737	0.8460	0.0240	0.12395E-01
	0.5600	0.5930	0.0180	0.52080E-01
490.81	0.1523	0.1460	0.0040	0.17536
	0.8739	0.8600	0.0240	0.12395E-01
	0.5605	0.5400	0.0170	0.52080E-01
491.04	0.1527	0.1520	0.0050	0.17536
	0.8740	0.8520	0.0240	0.12395E-01
	0.5608	0.5570	0.0170	0.52080E-01
491.28	0.1530	0.1570	0.0050	0.17536
	0.8742	0.8950	0.0260	0.12395E-01
	0.5612	0.5430	0.0170	0.52080E-01
491.51	0.1533	0.1600	0.0050	0.17536
	0.8743	0.9060	0.0250	0.12395E-01
	0.5615	0.5880	0.0180	0.52080E-01
491.74	0.1536	0.1530	0.0050	0.17536
	0.8744	0.9070	0.0260	0.12395E-01
	0.5618	0.5700	0.0180	0.52080E-01
491.97	0.1539	0.1550	0.0050	0.17536
	0.8745	0.8970	0.0260	0.12395E-01
	0.5621	0.5750	0.0180	0.52080E-01
492.20	0.1542	0.1560	0.0050	0.17536
	0.8746	0.8650	0.0250	0.12395E-01
	0.5624	0.5620	0.0170	0.52080E-01
	0.1545	0.1530	0.0050	0.17536

492.43	0.8747	0.8360	0.0240	0.12395E-01
	0.5627	0.5780	0.0180	0.52080E-01
492.67	0.1547	0.1500	0.0050	0.17536
	0.8748	0.8930	0.0250	0.12395E-01
	0.5630	0.5710	0.0180	0.52080E-01
492.90	0.1550	0.1490	0.0040	0.17536
	0.8750	0.8670	0.0250	0.12395E-01
	0.5633	0.5800	0.0180	0.52080E-01
493.13	0.1553	0.1580	0.0050	0.17536
	0.8751	0.8640	0.0240	0.12395E-01
	0.5636	0.5680	0.0180	0.52080E-01
493.36	0.1556	0.1540	0.0050	0.17536
	0.8752	0.8890	0.0250	0.12395E-01
	0.5639	0.5400	0.0160	0.52080E-01
493.60	0.1558	0.1530	0.0050	0.17536
	0.8753	0.8830	0.0250	0.12395E-01
	0.5642	0.5490	0.0170	0.52080E-01
493.83	0.1561	0.1580	0.0050	0.17536
	0.8754	0.9020	0.0260	0.12395E-01
	0.5645	0.5680	0.0170	0.52080E-01
494.06	0.1564	0.1540	0.0050	0.17536
	0.8755	0.9120	0.0260	0.12395E-01
	0.5648	0.6080	0.0190	0.52080E-01
494.30	0.1567	0.1490	0.0040	0.17536
	0.8756	0.8880	0.0250	0.12395E-01
	0.5651	0.5540	0.0170	0.52080E-01
494.53	0.1570	0.1590	0.0050	0.17536
	0.8757	0.8920	0.0250	0.12395E-01
	0.5654	0.5660	0.0170	0.52080E-01
494.76	0.1573	0.1580	0.0050	0.17536
	0.8759	0.8650	0.0250	0.12395E-01
	0.5657	0.5640	0.0170	0.52080E-01
495.00	0.1576	0.1480	0.0040	0.17536
	0.8760	0.8800	0.0250	0.12395E-01
	0.5660	0.5560	0.0170	0.52080E-01
495.23	0.1579	0.1600	0.0050	0.17536
	0.8761	0.8570	0.0250	0.12395E-01
	0.5663	0.5870	0.0180	0.52080E-01
	0.1582	0.1560	0.0050	0.17536

C. Plots, generated by local utilities

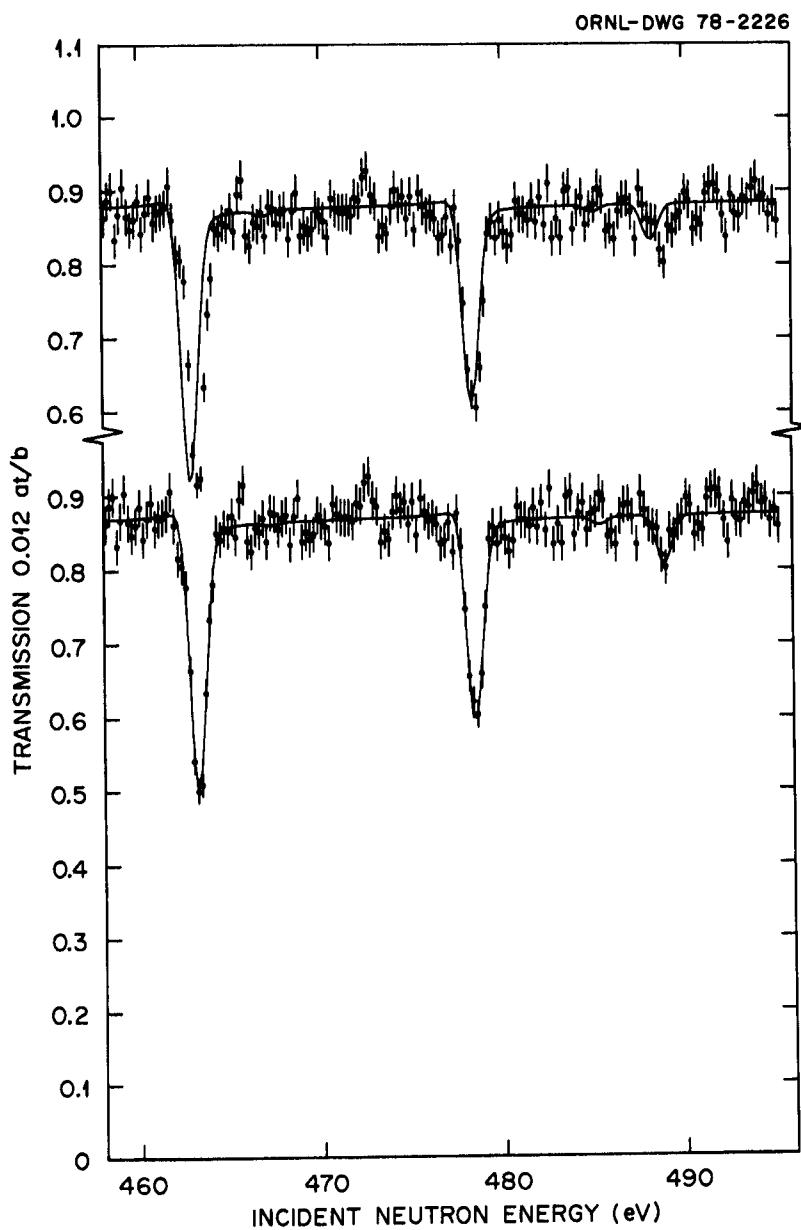


Fig. 1. Transmission of a 0.012 at/b sample of ^{238}U . This figure is generated in connection of the sample problem discussed in the appendix. The upper curve represents the transmission curve computed with the initial guesses. The lower curve is computed with the parameters obtained from the simultaneous fit to three sample thicknesses. The data fitted were obtained from reference 1.

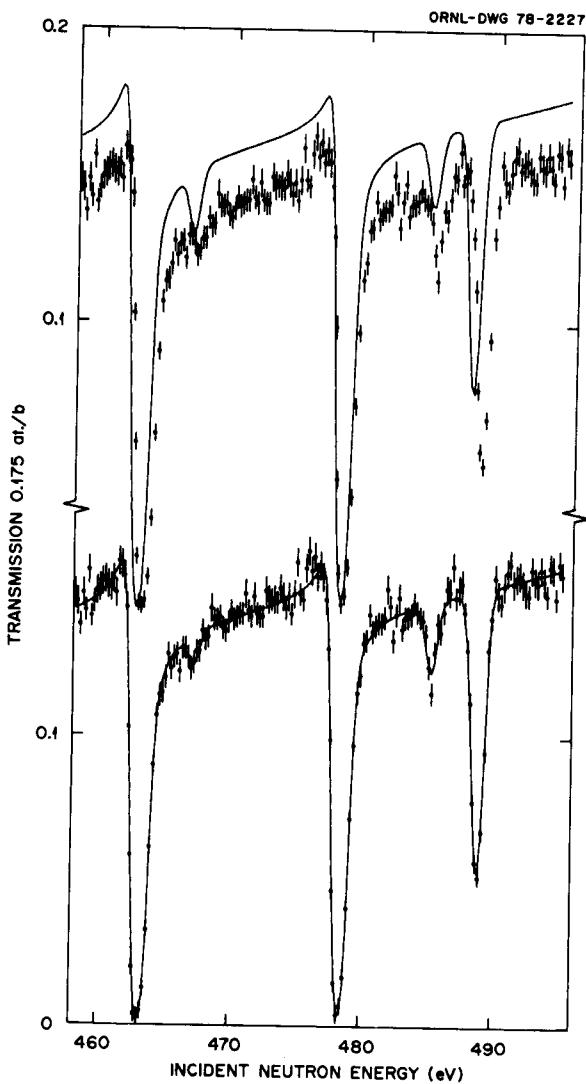


Fig. 2. Transmission of a 0.052 at/b sample of ^{238}U . This figure is generated in connection of the sample problem discussed in the appendix. The upper curve represents the transmission curve computed with the initial guesses. The lower curve is computed with the parameters obtained from the simultaneous fit to three sample thicknesses. The data fitted were obtained from reference 1.

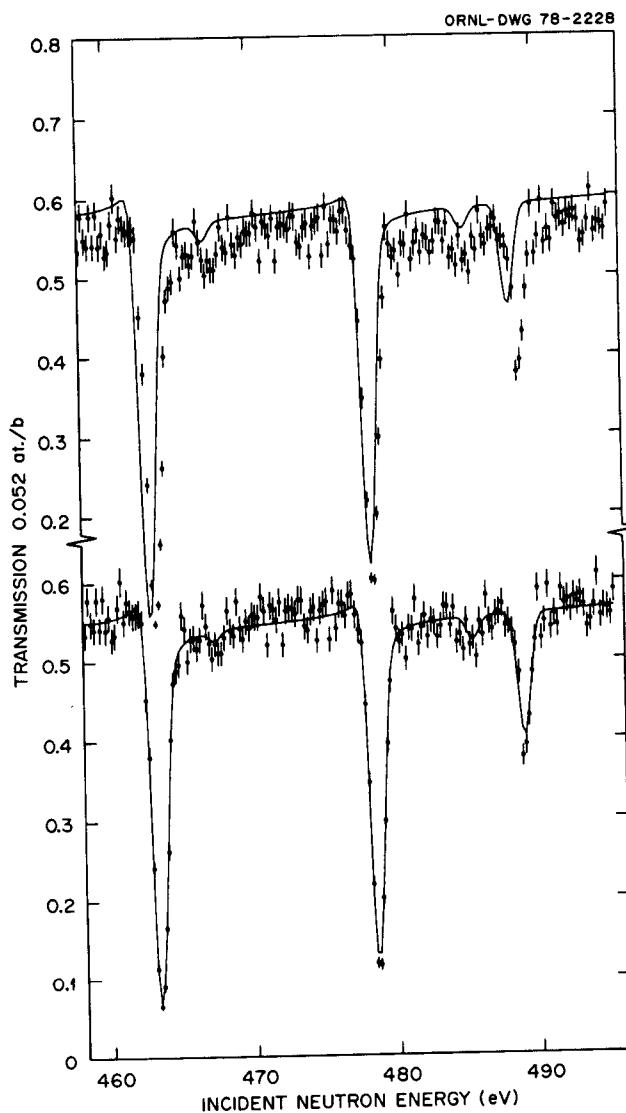


Fig. 3. Transmission of a 0.175 at/b sample of ^{238}U . This figure is generated in connection of the sample problem discussed in the appendix. The upper curve represents the transmission curve computed with the initial guesses. The lower curve is computed with the parameters obtained from the simultaneous fit to three sample thicknesses. The data fitted were obtained from reference 1.

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