288
6-14-78
UC-79d plus ENDF
Dewitt

28.146

ORNL/TM-6286
ENDF-261

MASTER

**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

OAK RIDGE NATIONAL LABORATORY
OPERATED BY UNION CARBIDE CORPORATION • FOR THE DEPARTMENT OF ENERGY

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
Price: Printed Copy \$6.00; Microfiche \$3.00

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, contractors, subcontractors, or their employees, makes any warranty, express or implied, nor assumes any legal liability or responsibility for any third party's use or the results of such use of any information, apparatus, product or process disclosed in this report, nor represents that its use by such third party would not infringe privately owned rights.

Contract No. W-7405-eng-26

Neutron Physics Division

SIOB:* A FORTAN 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

NOTICE MN ONLY

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

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

Date Published: May 1978

Prepared by the
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
for the
DEPARTMENT OF ENERGY

NOTICE

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

**THIS PAGE
WAS INTENTIONALLY
LEFT BLANK**

CONTENTS

	<u>Page</u>
ABSTRACT.	v
I. INTRODUCTION.	1
II. BRIEF DESCRIPTION OF THE PROGRAM.	2
III. CALCULATED RESOLUTION BROADENED TRANSMISSION.	4
IV. TOTAL CROSS-SECTION EXPRESSIONS	6
A. <u>The Single-Level-Breit-Wigner Formula</u>	7
B. <u>The Multilevel-Breit-Wigner Formula</u>	8
C. <u>Truncation Effects</u>	10
D. <u>The Total Cross-Section Trial Function</u>	11
E. <u>Doppler Broadening</u>	13
V. LEAST-SQUARE-FIT ALGORITHM.	13
VI. DIMENSIONS OF THE PROGRAM	17
VII. VARIABLE PARAMETERS AND FLAGS	18
ACKNOWLEDGMENTS	19
REFERENCES.	20
APPENDIX I. INPUT DATA AND THEIR FUNCTIONS	22
APPENDIX II. FORTRAN LISTING OF SIØB PROGRAM AND SUBPROGRAMS . . .	28
APPENDIX III. SAMPLE PROLEM.	
A. <u>Listing of Input</u>	46
B. <u>Listing of Output</u>	51
C. <u>Plots, Generated by Local Utilities</u>	65

**THIS PAGE
WAS INTENTIONALLY
LEFT BLANK**

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 SIOB

1. 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:

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

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

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:

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

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 $\mu = 72.3 \text{ eV}^{1/2} \text{ } \mu\text{S/m}$. 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

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

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:

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

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 $\phi_\ell(\hat{ka})$ 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,

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

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,

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

where

$$G_r = \sum_{s \neq r} \Gamma_{ns}^0 \frac{g_{rs}}{g_{rs}^2 + h_{rs}^2}, \quad (16)$$

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

Angular Momentum ℓ	Shift-factor $S_\ell(\rho)$	Penetration Factor $P_\ell(\rho)$	Phase Shift $\phi_\ell(\rho)$
0	0	ρ	ρ
1	$-\frac{1}{1 + \rho^2}$	$\frac{\rho^3}{1 + \rho^2}$	$\rho - \tan^{-1} \rho$
2	$-\frac{18 + 3\rho^2}{9 + 3\rho^2 + \rho^4}$	$\frac{\rho^5}{9 + 3\rho^2 + \rho^4}$	$\rho - \tan^{-1}\left(\frac{3\rho}{3 - \rho^2}\right)$
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 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

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

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

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

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 $\epsilon = (1 - e)^{-1} \approx .582$. 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:

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

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

where $NS2$ nuclear species NS contribute to the cross section and the parameters η_{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:

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

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

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

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

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} , $\hat{a}_{NS}$ 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 $\hat{a}_{NS}$ 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

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

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

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

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

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

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 $\phi[p^{(1)}]$ is smaller or equal to $\phi[p^{(0)}]$ 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 $\phi[p^{(1)}]$ is larger than $\phi[p^{(0)}]$, Eq. (33) is replaced by:

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

where I is the identity matrix ($I_{kl} = \delta_{kl}$) 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 η_{NS} and effective scattering radii $\hat{\alpha}_{NS}$ 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 $\tau_{NT}\eta_{NS}$ determines the areal density and only one of the two parameters τ_{NT} or η_{NS} can be varied.

ACKNOWLEDGMENTS

The authors wish to acknowledge many helpful discussions and encouragement particularly from G. A. Auchampaugh, D. Horen, D. Larson, F. G. Perey, R. R. Spencer and H. Weigmann. The help of J. Craven was indispensable in implementing the program to the IBM 360 through the ORELA PDP-10.

REFERENCES

1. D. K. Olsen, G. de Saussure, R. B. Perez, E. G. Silver, F. C. Difilippo, R. W. Ingle and H. Weaver, Nucl. Sci. and Eng. 62, 479(1977) and D. K. Olsen, G. de Saussure, R. B. Perez, F. C. Difilippo, R. W. Ingle and H. Weaver, "150-m Measurement of 0.880- to 100.0-keV Neutron Transmissions through Four Samples of ^{238}U ," ORNL/TM-5915 (ENDF-255) 1977.
2. G. F. Auchampaugh, "Multi, A FORTRAN Code for Least-Square Fitting of Neutron Cross-Section Data Using the Reich-Moore Multilevel Formalism," LA-5473-MC (March 1974).
3. H. Derrien and M. Alix, "Programme d'Analyse des Sections Efficaces Neutroniques des Noyaux Fissiles dans le Domaine des Resonances par un Formalisme Multiniveaux," CEA-N-1564 (October 1972).
4. F. H. Fröhner, Formanalysenprogramm zur Bestimmung von Resonanzparametern aus mehreren Transmissionsdatensätzen Gleichzeitig Nach der Methode der Kleinsten Quadrate," Arbeitsbericht Nr. 97 KFK, (Jan. 1976).
5. S. E. Atta and J. A. Harvey, "Numerical Analysis of Neutron Resonances," ORNL-3205 (1961).
6. H. Weigmann, R. L. Macklin and J. A. Harvey, Phys. Rev. C 14, 1328 (1976).
7. F. H. Fröhner and E. Haddad, Nucl. Phys. 71, 129(1965).
8. A. Michaudon, Reactor Sci. Technology 17, 168(1963).
9. A. Michaudon and P. Ribon, J. Phys. Radium 22, 712 (1961).
10. J. Rainwater *et al.*, Rev. Sci. Inst. 31, 481 (1960).
11. G. de Saussure *et al.*, "Simultaneous Measurements of the Neutron Fission and Capture Cross Sections for ^{235}U for Incident Neutron Energies from 0.4 to 3 keV," ORNL/TM-1804 (Nov. 1967); and references contained therein.
12. Salzer, Zucker and Capuano, N.B.S. Journ. of Res., 48, 111(1952).
13. G. Breit and E. P. Wigner, Phys. Rev. 49, 519(1936).
14. H. A. Bethe, Rev. Mod. Phys. 9, 69(1937).
15. D. Garber, C. Dunford and S. Pearlstein, "Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF," ENDF-102 (Oct. 1975, revised June 76).

16. M. F. James and J. S. Story, "Contribution of Negative Energy and Distant Resonances in the Resolved Resonance Region," in Nuclear Data for Reactors, Vol. I, p. 359, International Atomic Energy Agency; Vienna (1967).
17. G. de Saussure, D. K. Olsen and R. B. Perez, Nucl. Sci. and Eng. 61, 496 (1976).
18. A. W. Solbrig, Am. J. Phys. 29, 257 (1961).
19. The authors are indebted to C. Durston (ANL) who brought to their attention this very fast routine described in H. Henryson II, B. J. Toppel and C. G. Stenberg, "MC²-2: A Code to Calculate Fast Neutron Spectra and Multigroup Cross-Sections," ANL-8144 (ENDF-239) June 1976, p. 237.
20. D. W. Marquardt, J. Soc. Indust. Appl. Math, 11, 431(63).
21. D. D. Morrison, "Methods for Nonlinear Least Squares Problems and Convergence Proofs, Tracking Program and Orbit Determination," Proc. JPL Seminar (1960), p. 1.
22. H. Rutishauser, "Solution of Eigenvalue Problems with the L-R Transformation," NBS Applied Math Series, 49(1958).
23. J. H. Wilkinson, J. Ass. Comput. Mach., 8, 281(1961).
24. D. K. Faddeev, and V. N. Faddeeva (1963), "Computational Methods of Linear Algebra" (translated by Robert C. Williams from a Russian book of 1960). San Francisco: W. H. Freeman and Co., 620 pp. 114.

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 Cards

A. Fixed point switches and floating point constants.

1st card:	Format (9A8)	Legend
2nd card:	Format (15I4)	<i>NT2, IT2, NGS, NAUX, JERR, JCAL, JRES,</i> <i>JPAR, LPAR, LMAT, MPAR, LPLT, LDAT, JPLY,</i> <i>JKEV</i>
3rd card:	Format (6F11.3)	<i>BE2, CE3, EH, EL, RATIØ, DTMIN</i>

B. Transmission data.

4. Format Card:	Format (9A8)	<i>FMDAT</i>
-----------------	--------------	--------------

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) $LJ, INT, GSJ, FR, STRE, GNA, GAV$
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 (40F2.0) $F_{\tau_1}, \dots, F_{\tau_{NT_2}}$

18. Flags for Normalizations: Format (40F2.0) $FE_1, \dots, FE_{NT_2}$
19. Flags for Backgrounds: Format (40F2.0) $FB_1, \dots, FB_{N^2}$
20. Flags of Nuclear Species: Format (2F2.0) $FFRS, FAHAT$
21. Flags of Level Parameters: Format (3F2.0) $FE_0, \Gamma_n, \Gamma_\gamma$
22. Terminate each J sequence with a blank card.
23. Terminate resonance parameters with a blank card.
24. Flags for auxiliary parameters: Format (40F2.0) $F\gamma_1, \dots, F\gamma_{NAUX}$

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>L</i> <i>PAR</i> =2	The initial guesses are printed before the iteration loop and the final values after the loop.
<i>L</i> <i>PAR</i> =-1	The initial guesses and final values are not printed.
<i>L</i> <i>MAT</i> ≤0	The parameter-covariance matrix is not printed
<i>L</i> <i>MAT</i> >0	The parameter-covariance matrix is printed
<i>M</i> <i>PAR</i> <0	The final values of the parameters are punched
<i>M</i> <i>PAR</i> ≥0	The final values of the parameters are not punched
<i>L</i> <i>PLT</i> <0	No plot-punched cards generated
<i>L</i> <i>PLT</i> ≥0	Final plot-punched cards generated
<i>L</i> <i>PLT</i> >0	Plot-punched cards generated at each iteration (These punched cards are used with a local utility program to generate plots)
<i>L</i> <i>DAT</i> ≤0	Calculated and measured transmissions not printed
<i>L</i> <i>DAT</i> >0	Final calc. and meas. transmissions printed
<i>L</i> <i>DAT</i> >1	Calc. and meas. transmissions printed at each iteration
<i>J</i> <i>PLY</i> ≠0	Transmissions are channel-broadened by Eq. 7 Section III
<i>J</i> <i>PLY</i> =0	Channel broadening is not done
<i>J</i> <i>KEV</i> =0	All energy inputs are in eV
<i>J</i> <i>KEV</i> ≠0	All energy inputs are in keV
<i>BE</i> 2 and <i>CE</i> 3	Parameters used in computing the resolution width of <i>JRES</i> =0; see Eq. 4 of Section III
<i>EH</i> , <i>EL</i>	Parameters used in computing the contribution of a picket-fence of levels, see Eq. 20 and 21 of Section IV D
<i>RATI</i> ∅	Convergence parameters: the iteration loop is terminated if $\chi^2_{\text{new}} > \text{RATI}\emptyset * \chi^2_{\text{old}}$

<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, δT_1, T₂, δT_2, ...</i>	Energy, transmission through first sample, error, transmission through second sample, error...
$\tau_i, i=1, NT2$	Sample thickness, see Eq. 1, Section III
$\epsilon_i, i=1, NT2$	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_γ 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 $S, \langle \Gamma_n^0 \rangle$ and Γ_α in Eq. 20, 21 and 22 of Section IV C. If STRF=0, the picket-fence contribution is ignored.

$E_0, \Gamma_n, \Gamma_\gamma$

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 $\tau_i, \epsilon_i, \beta_i$, are *FRS*, *AHAT*, $E_0, \Gamma_n, \Gamma_\gamma$ 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,
1 IFN2,IFB1,IFB2,IFS1,IF2,IG1,IG2
COMMON/KAD/LN1,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/IEV/IE1,IE2,IE3,IEC1,IGS,NGT
COMMON/LEV/JFLAG,NS2,NAUX,JL(10),NRL(10,10),MDM(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,6,7,0/
DATA FMAPB/8H(8P10,5),8*8H
DATA FMCAT/8H(F10,5,1,8H4F5,3),7*8H
DATA FMPAR/8H(E11,5,2,8H2X,2E11,8H5),6*8H
DATA FMFLG/8H(4CF2,0),8*8H
DATA NGSP,NAUXF,AKP,B4/1,1,002196771,00034465/
DATA ROP,RIP,AWRIP/.123,00,236,01/
DATA PI/3.141593/
DATA RATIO/.999/
DATA IPILOT/0/
DATA AKPCVT,B4CVT/31.62278,0.0010/
DATA IRTN/0/
1 READ(IT1,101)(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(IT1,102)NT2,IT2,NGS,NAUX,JERR,JCAL,JRES,JPAR,LPAR,LMAT,MPAR,
1 LPLT,LDAT,JPLY,JKEV
C READ FLOATING POINT INPUT
READ(IT1,103)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=NAUXF
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(IT1,101)(FM(I),I=1,9)
IF(ICMPARE(FM(1),8H
,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(IT1,FMDAT)F(IE),(F(IE+NT),F(IE+NT2+NT),NT=1,N
1 NT2)
IF(JERR.NE.0) READ(IT1,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(IT1,101)(FM(I),I=1,9)
IF(ICMPARE(FM(1),8H
,8).EQ.0) GO TO 9
DO 7 I=1,9
7 FMAPB(I)=FM(I)
C READ SAMPLE THICKNESSES IN ATOMS PER EARN (APB)
9 IPT2=IE-1
READ(IT1,FMAPB)(F(IP),IP=IP1,IPT2)
C READ TRANSMISSION-NORMALISATION ERRORS
IPN1=IPT2+1
IPN2=IPT2+NT2
READ(IT1,FMAPB)(F(IP),IP=IPN1,IPN2)

```

```

C   READ TRANSMISSION BACKGROUNDS
    IPB1=IPN2+1
    IPB2=IPN2+NT2
    READ(IT1,FMAFB)(F(IF),IP=IPB1,IPB2)
    IE=IPB2+1
C   READ FORMAT FOR RESONANCE-PARAMETERS
    READ(IT1,101)(FM(I),I=1,9)
    IF(ICMPARE(FM(1),8),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(IT1,104)FRS,AHAT,AWRI,TEMP,DEL,RN,AK
    IF(FRS.EQ.0.) GO TO 19
    JL(NS2)=0
    F(IE)=FHS
    F(IE+1)=AHAT
    IE=IE+2
    IF(AWRI.EQ.0.) AWRI=AWRIP
    IF(TEMP.NE.0.) CEL=SQRT(B4*TEMP/AWRI)
    DELTA(NS2)=DEL
    IF(RN.EQ.0.) RN=FCP*(AWRI**3.33)+RIP
    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(IT1,106)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(IT1,FMPAR)E0,GN,GG
    IF(JPAR.EQ.1) READ(IT1,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(IT1,104)(F(IF),IP=IE,IP2)
C   READ FORMAT FOR FLAGS
    READ(IT1,101)(FM(I),I=1,9)
    IF(ICMPARE(FM(1),8),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(IT1,FMFLG)(F(IF),IF=IF1,IFT2)
C   READ FLAGS TO VARY NORMALISATIONS
    IFN1=IFT2+1
    IFN2=IFT2+NT2
    READ(IT1,FMFLG)(F(IF),IF=IFN1,IFN2)
C   READ FLAGS TO VARY BACKGROUNDS
    IFB1=IFN2+1
    IFB2=IFN2+NT2
    READ(IT1,FMFLG)(F(IF),IF=IFB1,IFB2)
    IFS1=IFB2+1
    IFE2=IFS1
C   READ FLAGS TO VARY PARAMETERS
    DO 27 NS=1,NS2
    READ(IT1,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(IT1,FMFLG)(F(IF+N),N=1,3)

```

```

25 IF=IF+3
26 CONTINUE
27 READ(ITI,FMFLG)
   READ(ITI,FMFLG)
   IF2=IF+NAUX
   IF=IF+1
   READ(ITI,FMFLG)(F(I),I=IF,IF2)
C   SET EH AND EL IF EH=0.
   IF(EH.EQ.0.) EL=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(IFT2+NT).NE.0.) NVN=NVN+1
     IF(F(IFN2+NT).NE.0.) NVB=NVB+1
29 CONTINUE
   NVP=0
   DO 31 IF=IFS1,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) GC 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) GC TO 40
   IE=IPS1
   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=MOD(NS,J)
       INT=INTL(NS,J)
       CSJ=GSFIN(NS,J)
       FR=FRL(NS,J)
       STRF=STRFL(NS,J)
       GNA=GNAL(NS,J)
       GAV=GAVL(NS,J)
       NR2=NRNL(NS,J)
       WRITE(ITO,233)LJ,INT,GSJ,FR,STRF,GNA,GAV,NR2
       IF(NR2.EQ.0) GC TO 37
       WRITE(ITO,236)
     DO 35 NR=1,NR2
       E0=F(IE)
       GG=F(IE+1)
       GN=F(IE+2)*PEN(LJ,AKRN*SQR(ABS(E0)))
       IE=IE+3
35 WRITE(ITO,235)E0,GG,GN
   WRITE(ITO,237)
37 CONTINUE
40 CONTINUE
   IF(IRTN.EQ.1) GC TO 70
C   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.

```

```

41 LM=LM+1
   JFLAG=0
   PHI=0.
   JV=0
   CALL FHINEQ(JV)
   PHIOLD=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,N
1T2)
44 CONTINUE
46 CONTINUE
   WRITE(ITO,208)I1
   CALL MVP
   IF(PH1.GT.RATIO*PHIOLD) 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
   IPLCT=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,N
1T2)
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,FMAP8)(F(IP),IP=IP1,IPT2)
   WRITE(ITC,FMAP8)(F(IP),IP=IPN1,IPN2)
   WRITE(ITC,FMAP8)(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=RAC(NS)
   AK=AKC(NS)
   AKRN=AK*RN
   AWRI=C.
   TEMP=C.
   WRITE(ITC,104)FRS,AHAT,AWRI,TEMP,DEL,RN,AK
   JL2=JL(NS)

```



```

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,100)J,INT,GSJ,FR,STRF,GAV
NR2=NRL(NS,J)
IF(NR2.EQ.C) GO TO 62
DO 61 NR=1,NR2
EO=F(IE)
GG=F(IE+1)
GN=F(IE+2)*PEN(J,AKHN*SCRT(ABS(EO)))
IE=IE+3
IF(JPAR.EQ.C) WRITE(ITC,FMPAR)EO,GN,GG
IF(JPAR.EQ.1) WRITE(ITC,FMPAR)EO,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(ITO,235)
IRTN=1
GO TO 34
70 IRTN=C
71 CONTINUE
READ(ITI,102)IGCTC
IF(IGCTO.EQ.C)CALL EXIT
IF(IGCTO.FO.1)CALL FRRCR
IF(IGCTO.EQ.2)GO TO 1
101 FORMAT(9A8,18)
102 FORMAT(20I4)
103 FORMAT(7G11.3)
104 FORMAT(7G11.3)
105 FORMAT(2G11.3,5I11)
106 FORMAT(2I11,5G11.3)
201 FORMAT(1H1,'COMMON TOO SMALL',4I20)
202 FORMAT(1H0,'STOP ITERATIONS BECAUSE CONVERGENCE IS TOO SLOW')
203 FORMAT(1H ,08X,7(1X,F10.7,5H APB ))
204 FORMAT(1H1,9X,'ENERGY',11X,'CALCULATION' 4X,'EXPERIMENT',
1 8X,'ERROR',8X,'ATCMS PER EARN',/)
205 FORMAT(1H ,G20.5,3F15.4,G20.5/(21X,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',2G16.5)
217 FORMAT(1H0,'NUMBER OF TRANSMISSION VALUES',I8,/, 'MAXIMUM ADDRESS 0
1 F-ARRAY',I9,/, 'MAXIMUM ADDRESS OF G-ARRAY',I9)
222 FORMAT(1H0,'FIXED POINT INPUTS ',20I4)
223 FORMAT(1H ,FLGATING POINT INPUTS ',7G11.3)
225 FORMAT(1H0,////////,15X,'INPUT RESONANCE PARAMETERS',///)
231 FORMAT(1H0,2X,'NUCLEAR SPECIES ',I3,5X,
1'REDUCED MOMENTUM='G12.5,5X,
2'NUCLEAR RADIUS='C12.5,/,
38X,'DEPLETER WIDTH='G12.5,5X,
4'NUMBER OF ANGULAR MOMENTA='I3,/,
58X,'FRACTIONAL ABUNDANCE='F7.4,5X,
6'EFFECTIVE RADIUS='F7.4,/)
233 FORMAT(1H0,4X,'ANGULAR MOMENTUM='I2,5X,
1'INTERFERENCE PARAMETER='I2,5X,
2'SPIN STATISTICAL FACTOR='F6.3,5X,
3'POTENTIAL SCATTERING FRACTION='F6.3,/,
410X,'STRENGTH-FUNCTION='G12.5,5X,
5'AVERAGE NEUTRON-WIDTH='G12.5,5X,
6'AVERAGE CAPTURE-WIDTH='G12.5,///,10X,
7'NUMBER OF LEVELS='I4)
236 FORMAT(1H0,15X,'RESONANCE ENERGY',5X,'CAPTURE-WIDTH',5X,'NEUTRON-W
1IDTH',/)
235 FORMAT(14X,3G18.5)
237 FORMAT(1H0)
239 FORMAT(1H1,'FINAL RESONANCE PARAMETERS',///)
301 FORMAT(2GA4)
END

```

```

SUBROUTINE PHINEQ(JV)
C   REQUIRES RES(E,JRES),SIG(E,JV),BGR(E,NT),WEIGHT(NT,IE)
REAL * 8 D
DIMENSION C(1)
DIMENSION A(55),X(45)
COMMON F(1)
COMMON/VAR/G(1)
COMMON/IAD/IP1, IPT2, IPN1, IPN2, IPB1, IPB2, IPS1, IP2, IF1, IFT2, IFN1,
1 IFN2, IFB1, IFB2, IF51, IF2, IG1, IG2
COMMON/KAC/LM1, LS1, MV1, MM1, MS1, MS2, KV1, KG1, KG2
COMMON/NAD/NVT, NV1, NVB, NVP, NV2, NT2
COMMON/INDX/JERF, JCAL, JRES, JPAR, LPAR, LMAT, MPAR, LPLT, LOAT, JPLY, JKEV
COMMON/IE/IE1, IE2, IE3, IEC1, IGS, NGT
COMMON/FLT/BE2, CE3, EH, EL, PHI, DOFINV, DTMIN
EQUIVALENCE(C(1),G(1))
DATA A/ 1.0000E-01, 6.6667E-01, 1.6667E-01, 5.3333E-01, 2.2208E-01,
2 1.1257E-02, 4.5714E-01, 2.4012E-01, 3.0757E-02, 5.4827E-04,
3 4.0635E-01, 2.4417E-01, 4.9916E-02, 2.7891E-03, 2.2345E-05,
4 3.6941E-01, 2.4224E-01, 6.6139E-02, 6.7203E-03, 1.9576E-04,
5 8.1218E-07, 3.4099E-01, 2.3787E-01, 7.9169E-02, 1.1771E-02,
6 6.8124E-04, 1.1527E-05, 2.7226E-08, 3.1826E-01, 2.3246E-01,
7 8.9418E-02, 1.7366E-02, 1.5674E-03, 5.6421E-05, 5.9754E-07,
8 8.5856E-10, 2.9954E-01, 2.2671E-01, 9.7406E-02, 2.3087E-02,
9 2.8589E-03, 1.6849E-04, 4.0127E-06, 2.8080E-08, 2.5843E-11,
A 2.8377E-01, 2.2094E-01, 1.0360E-01, 2.8667E-02, 4.5072E-03,
B 3.7850E-04, 1.5351E-05, 2.5322E-07, 1.2204E-09, 7.4828E-13/
DATA X/ 1.22474460, 0.95857251, 2.02018261, 0.81628788, 1.67355156,
2 2.65196133, 0.72355098, 1.46855259, 2.26658058, 3.19099331,
3 0.65680963, 1.32655716, 2.02594757, 2.78328991, 3.66847134,
4 0.60576391, 1.22005463, 1.85310841, 2.51973629, 3.24660873,
5 4.10133839, 0.56506962, 1.13611603, 1.71999264, 2.32573223,
6 2.96716555, 3.66994953, 4.49999142, 0.53163302, 1.06764889,
7 1.61252362, 2.17350292, 2.75776291, 3.37893200, 4.06194687,
8 4.87134457, 0.50352019, 1.01036835, 1.52417088, 2.04923153,
9 2.59112467, 3.15784931, 3.76218700, 4.42853260, 5.22027206/
C   LOOP CVER ENERGIES
IP0=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 CVER 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=SIG(ENG,JV)
C   LOOP CVER TRANSMISSION-SAMPLES
K=KG1
DO 57 NT=1, NT2
APN=F(IP0+NT)
TR=ANG*EXP(-APN*CS)
TN=(1.+F(IPT2+NT))*TR
IF(NG.EQ.1) G(K)=F(IPN2+NT)*BGR(E,NT)
G(K)=G(K)+TN
C   LOOP CVER 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+NVB
DO 56 NV=1, NVP
IF(NG.EQ.1) G(KNV)=0.
G(KNV)=G(KNV)-APN*TN*G(KV)
KNV=KNV+1

```

```

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
C 59 CONTINUE
   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)
   DTN=F(IE+NT)-G(K)
   DTNW=CTN*W
   PHI=PHI+DTN*DTNW
   IF(JV.LT.0) GO TO 65
C   DERIVATIVES OF TRANSMISSION-BACKGROUND
   K1=K+NVT+NVN+1
   NTC=1
   DO 61 IF=IFB1,IFB2
   IF(F(IF).EQ.0.) GO TO 61
   G(K1)=0.
   IF(NTC.EQ.NT) G(K1)=BGR(E,NT)
   K1=K1+1
C 61 NTC=NTC+1
   NORMAL EQUATIONS
   L=LM1
   DO 63 NA=1,NV2
   GKNA=G(K+NA)
   D(NA)=D(NA)+DTNW*GKNA
   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+IE2
   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.C41667*(F(IT+IE3)+F(IT-IE3)+22.0*F(IT))
70 PHI=PHI+WEIGHT(NT,IE)*(F(IE+NT)-F(IT))*2
71 IFC=IEC+IE2
   RETURN
   END

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

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

FUNCTION WEIGHT(NT,IE)
COMMON F(1)
COMMON/NAC/NVT,NVN,NVE,NVP,NV2,NT2
COMMON/FLT/BE2,CE3,EH,EL,PHI,DOFINV,DTMIN
COMMON/INDX/JERR,JCAL,JRES,JPAR,LPAR,LMAT,MPAR,LPLT,LDAT,JPLY,JKEV
DT=F(IE+NT+NT2)
IF(CT.CE.DTMIN) GO TO 10
DT=DTMIN
F(IE+NT+NT2)=DTMIN
10 WEIGHT=1.0/(DT*DT)
RETURN
END

```

```

SUBROUTINE MVP
C   REQUIRES SLV(NV2)
C   MVP DCES A P-SEARCH IF NEEDED
C   SAVE OLD CHISQUARE
REAL * 8 D
DIMENSION C(1)
COMMON F(1)
COMMON/VAR/G(1)
COMMON/IAD/IP1,IP2,IPN1,IPN2,IPB1,IPB2,IPS1,IP2,IF1,IFT2,IFN1,
1 IFN2,IFB1,IFB2,IFS1,IF2,IG1,IG2
COMMON/KAD/LM1,LS1,NV1,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),MM(10,10),INL(10,10)
COMMON/FLT/BE2,CE3,EH,EL,PHI,DOFINV,DTMIN
COMMON/FLD/AK0(10),CO(10),RAD(10),DELTA(10)
COMMON/FL2/GSPIN(10,10),GAVL(10,10),STRFL(10,10),FRL(10,10)
EQUIVALENCE(C(1),G(1))
DATA ITI,ITO/5,6/
DATA EPP,NPSMAX/.C33,10/
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 EQLATIONS
19 CALL SLV(NV2)
C   GAUGE ETA, IF NPS=0 SAVE ORIGINAL PARAMETERS
ETA=1.
IF=IF1
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).EQ.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=IF1
LS=LS1
MV=MV1
DO 27 IP=IP1,IP2
IF(F(IF).EQ.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)
CHISC=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)=CHISC*D(LM)
IF(LA.NE.LB) GO TO 29
D(MS)=DSQRT(D(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(CHISC.GT.CHIOLD) GO TO 51
WRITE(ITO,201)
WRITE(ITO,202)NFS,ETA,CHIOLD,CHISC
C   PRINT SAMPLE THICKNESSES
WRITE(ITO,221)
WRITE(ITO,203)
IF=IF1
MS=MS1
MV=MV1
DO 33 IP=IP1,IP2
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

```

```

32 WRITE(ITO,204)F(IF)
33 IF=IF+1
C PRINT NORMALISATION-ERRORS
  WRITE(ITO,226)
  WRITE(ITO,203)
  DO 82 IP=IPN1,IFN2
    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,IFB2
    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=RAC(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=MCN(NS,J)
      NR2=NRL(NS,J)
      WRITE(ITO,232)LJ,NR2
      IF(NR2.EQ.0) GO TO 46
      WRITE(ITO,226)
      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(ABS(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

```

```

43 IF=IF+1
46 CONTINUE
C AUXILIARY PARAMETERS
WRITE(ITO,226)
WRITE(ITO,203)
DO 45 N=1,NAUX
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.
MMO=MM1-1
GG=0.
DO 55 LA=1,NV2
SUM=0.
NM=MMO+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 C(LM1)
61 LM=LM1
MM=MM1
DO 63 LA=1,NV2
DO 63 LB=LA,NV2
D(LM)=D(MM)
IF(LA.EQ.LB) C(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 CHIOLO
CHISO=CHICLO
IF=IF1
MV=MV1
DO 75 IP=IP1,IP2
IF(F(IF).EQ.C.) 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,'CHIOLO',14X,
1'CHINew',/)
202 FORMAT(1H ,110.6X,3G20.5,/)
203 FURMAT(1H0.9X,'CLC VALUE',11X,'NEW VALUE',14X,
1'ERROR',/)
204 FORMAT(1H ,6G20.5)
205 FORMAT(1H0,'CAN DC NO GOOD. SURRY')
211 FORMAT(1H )
221 FORMAT(1H0.5X,'SAMPLE-THICKNESSES')
222 FORMAT(1H0.5X,'TRANSMISSION-BACKGROUNDS')
224 FORMAT(1H0.5X,'FRACTICNAL ABUNDANCE AND RADIUS')
225 FORMAT(1H0.5X,'RESCNANCE-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 MUMENTUM =',I2.5X,
7'NUMBER OF LEVELS='I4)
END

```

```

SUBROUTINE SLV(N)
IMPLICIT REAL * 8 (A-H,O-Y)
COMMON/VAH/F(1)
REAL * 8 F
IF(N-1) 1,2,3
1 WRITE(6,101)
101 FORMAT (1H0,'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+M
DO 5 LM=1,M1
A=A+F(KL)*F(KM)
J=N-LM
KL=KL+J
5 KM=KM+J
6 T=F(K)-A
IF(L.EQ.M) GO TO 5
IF(T.EQ.0.) GO TO 7
WRITE(6,102)T
102 FORMAT (1H0,'FAILURE IN SLV T= ',G20.5)
7 D=DSORT(T)
F(K)=D
GO TO 10
9 F(K)=1/D
10 K=K+1
K=N+1
F(K)=1./F(K)
DO 12 L=2,N
K=K+N-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-M
KL=LK+J
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 18 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(ZEC,ETA,U0,V0) AND FNS(VE,N)
C   FOR JV.GE.C COMPUTES DERIVATIVES
C   FOR JFLAG=C RECCMPLTES INTERFERENCE TERMS
COMMON F(1)
COMMON/VAR/G(1)
COMMON/IAC/IP1,IP2,IPN1,IPN2,IPB1,IPB2,IPS1,IP2,IF1,IFT2,IFN1,
1 IFN2,IFB1,IFB2,IFS1,IF2,IG1,IG2
COMMON/KAC/LM1,LS1,MV1,MM1,MS1,MS2,KV1,KG1,KG2
COMMON/NAD/NVT,AVN,NVB,NVP,NV2,NT2
COMMON/INDX/JERF,JCAL,JRES,JPAR,LPAR,LMAT,MPAR,LPLT,LDAT,JPLY,JKEV
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/AK0(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=AK0(NS)*RAD(NS)
DO 20 J=1,JL2
NR2=NRL(NS,J)
IF(NR2.EQ.0) GO TO 20
INT=IAL(NS,J)
IF(INT.EQ.0) GO TO 13
LJ=MOM(NS,J)
IPO=IP
13 DO 15 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,RHOR)
F(K)=0.
F(K+1)=0.
GR=GNR*PENR
14 IPS=IPO
DO 17 MS=1,NR2
IF(MS.EQ.NR) GO TO 17
ES=F(IPS)
GNS=F(IPS+2)
RHOS=AKRNS*SQRT(AES(ES))
GS=GNS*PENR
DL=ER-ES-(SHF(LJ,RHOS)-SHFR)*GNS
GH=.5*(GAR+F(IPS+1)+GR+GS)
TEMP=GNS/(CL*DL+GT*GH)
F(K)=F(K)+TEMP*GH
F(K+1)=F(K+1)+TEMP*CL
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=AK0(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)
SQPIDE=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
  KVVJ=0.
  KV=KV+1
31 IF=IF+2
C SUM OVER ANGULAR-MOMENTA
33 DO 49 J=1,JL2
  LJ=MCN(NS,J)
  GSJ=GSPIN(NS,J)
  INT=INL(NS,J)
  NR2=NRL(NS,J)
  PHIL2=PHI2(LJ,RHCFAT)
  SIN2=SIN(PHIL2)
  COS2=COS(PHIL2)

  PENL=FEN(LJ,RFC)
  SHFL=SHF(LJ,RFC)
  CFG=CFNS*GSJ
  FPF=FPF(NS,J)
  SIGJ=C.
  IF(FR.EQ.0.) GO TO 34
  ALJ=2*LJ+1
  CCOS=1.-CCS2
  IF(COS2.GT..999) CCOS=2.*(SIN(.5*PHIL2)**2)
  SIGJ=ALJ*CCOS*FPF
34 CONTINUE
  IF(KVR.NE.0) GKVR=0.
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
C CONTRIBUTION OF RESONANCES
  UU 47 NH=1,NR2
  ER=F(IP)
  GAR=F(IP+1)
  GNR=F(IP+2)
  IP=IP+3
  GN=GNR*PENL
  RHR=AKRNS*SORT(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
  HH=HR-PFA
36 CONTINUE
  IF(JV.GE.0) FLAG=F(IF)+F(IF+1)+F(IF+2)
  IF(DEI.NE.0) GO TO 37
  DENINV=1./(GH*GH+CL*DL)
  U=GH*DENINV
  V=UL*DENINV
  IF(FLAG.EQ.0.) GO TO 39
  DPI=-(U+U)*V

```

```

DP2=(U+V)*(U-V)
GO TO 39
37 ETA=GH*DE
ZED=CL*DE
CALL SVS(ZED,ETA,LO,V0)
U=SQPIDE*UC
V=SQPIDE*V0
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 RADIUS 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*DP1-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.) GO TO 45
UN=DP1*SHIFT-.5*DP2*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,RHOMAT)
49 SIGS=SIGS+SIGJ
IF(JV.LT.C) GC TO 55
IF(KVR.NE.0) G(KVR)=(CFNS+CFNS)*AKNS*GKVJ
IF(KVN.NE.C) G(KVN)=SIGS*CNS
59 SIG=SIG+SIGS*CFNS
C CONTRIBUTION OF AUXILIARY PARAMETERS
DO 69 N=1,NALX
SIG=SIG+F(IP)*FNS(VE,E,N)
IF(JV.LT.0) GC TO 69
C DERIVATIVES W.R.T. AUXILIARY PARAMETERS
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.+RHOSQ*(3.+RHOSQ))
RETURN
3 IF(LJ.NE.3) CALL ERROR
RHO4=RHOSQ*RHOSQ
DPH=(RHO4+RHC4)/(RHOSQ+2.)/
1 (225.+45.*RHOSQ+RHO4*(6.+RHOSQ))
RETURN
END

```

```

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

```

```

FUNCTION DSHF(LJ,RHC)
  IF(LJ.NE.0) GO TO 1
  DSHF=0.
  RETURN
1 RHO SQ=RHO*RHO
  IF(LJ.NE.1) GO TO 2
  DSHF=RHO/((1.+RHC SC)**2)
  RETURN
2 IF(LJ.NE.2) GO TO 3
  TEMP=9.+RHC SC*(3.+RHO SQ)
  DSHF=3.*RHC*(TEMP+5.*RHO SQ)/(TEMP*TEMP)
  RETURN
3 IF(LJ.NE.3) CALL ERROR
  RHO4=RHO SQ*RHO SQ
  RHO6=RHO4*RHC SC
  TEMP=225.+45.*RHO SQ+6.*RHO4+RHO6
  DSHF=1687.5+500.*RHC SC+382.5*RHO4+RHO6*(30.+RHO SQ)
  DSHF=6.*RHC*DSHF/(TEMP*TEMP)
  RETURN
END

```

```

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

```

```

FUNCTION FNS(VE,E,N)
  COMMON/FLT/BE2,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=(EH-EL+VE)/((EH-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)
COMMON/TRI/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 W(REZ,AIM1,REW,AIMW)
REW=0.
AIMW=C.
AIMZ=ABS (AIM1)
IF (REZ)27,20C1,27
2001 IF(AIM1)27,20C2,27
2002 REW=1.
RETURN
27 R2=REZ*REZ
A12=AIMZ*AIMZ
ABREZ=ABS (REZ)
IF(ABREZ+1.25*AIMZ-5.C)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
102 IF(AEREZ+1.863636*AIMZ-4.1)111,111,104
103 IF(AIMZ-1.5)116,120,120
104 IF(AIMZ-1.4)115,115,101
105 IF(ABREZ+1.07317*AIMZ-4.4)119,119,118
106 IF(AEREZ-2.7)127,128,128
107 IF(AEREZ-3.1)106,106,108
108 IF(ABREZ-3.4)125,130,130
109 IF(R2+1.12*A12-5.76)103,107,107
110 IF(R2+1.7227*A12-4.41)125,126,126
111 IF(R2+1.71*A12-2.89)113,109,109
112 IF(R2+1.69*A12-1.69)123,124,124
113 IF(R2+2.0408*A12-1.0)114,112,112
114 IF(R2+1.5625*A12-.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
2) KW=2
   AIMZ=AIM1
   GO TO 200
15 KW=1
   IF(AIM1)2000,15C,15C
2000 KW=2
      AIMZ=AIM1
      GO TO 200
C WA IS OBTAINED FROM ASYMPTOTIC 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=-1.1283752*AIMZ
   D=1.1283752*REZ
   AM=RV-1.
   AAK=1.
   K=0
11 AJTEMP=2.*AAK
   TEMP4=(1.-AJTEMP)*AJTEMP
   AJP=RV-(4.*AAK+1.)
   GO TO 40
41 AAK=AAK+1.
   K=K+1
   PR=REW
   PI=AIMW
12 AMAGN=TEMPM**2+TEMEL**2
   REW=(TEMPC*TEMPM+TEMPC*TEMEL)/AMAGN
   AIMW=(TEMPM*TEMPC-TEMEL*TEMPC)/AMAGN
   IF(ABS (REW-PR)-1.E-6)665,11,11
665 IF(ABS (AIMW-PI)-1.E-6)65,11,11
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=0.
   JSIG=C
   G=0.
   H=0.
   EL=0.
   A=1.
   AM=1.
   SIGP=1.5
   EXPON=EXP (TEMP2*AJ)
   EXPC=EXPON*CCS (TEMP2*AK)
   EXP6=-EXPON*6IN (TEMP2*AK)
   SIG2P=2.*SIGP
4 AJ4SIG=4.*AJSIG
   AJ4SM1=AJ4SIG-1.
   TEMP3=1./(AJ4SM1*(AJ4SIG+3.))
   TT4=SIG2P*(2.*AJSIG-1.)
   TEMP4=TT4/(AJ4SM1*(AJ4SIG+1.)*(AJ4SIG-3.)*AJ4SM1)
   AJP=AJP+TEMP3
   GO TO 40
42 AJSIG=AJSIG+1.
   JSIG=JSIG+1
6 TEMP7=(AM*AM+EL*EL)*1.7724539
   REF=(AIMZ*(C*AM+D*EL)-REZ*(AM*C-C*EL))/
1 TEMP7/TEMP1
   AIMF=(AIMZ*(AM*C-C*EL)+REZ*(C*AM +D*EL))/TEMP7/TEMP1
   PR=REW
   PI=AIMW
   REW=EXPON-REF
   AIMW=EXPON-AIMF
   IF(ABS (REW-PR)=1.E-6)664,7,7
664 IF(ABS (AIMW-PI)-1.E-6)64,7,7
64 RETURN
7 SIG2P=2.*AJSIG
   GO TO 4
40 TEMPC=AJP*C+TEMP4*A-AK*D
   TEMPD=AJP*D+TEMP4*B+AK*C
   TEMEL=AJP*EL+TEMP4*H+AK*AM
   TEMPM=AJP*AM+TEMP4*G-AK*EL
   A=C
   B=D
   G=AM
   H=EL
   C=TEMPC
   D=TEMPC
   AM=TEMPM
   EL=TEMEL
   IF(ABS (TEMPM)+ABS (TEMEL)-1.0E15)49,43,43

```

```

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

```

```

SUBROUTINE QUICKW (AX,Y ,REW,AIMW)
COMMON/TRI/TR(62,62),TI(62,62),KI
AKI=SIGN(1.,AX)
X=ABS(AX)
TEST=X*X+Y*Y
IF (TEST.LT.36.)GO TC 10
IF (TEST.LT.144.)GO TO 2
IF (TEST.LT.10000.)GO TO 3
A1=1./((1.7724535*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=HQ2-HQ
   A2=HP2-HP
   A3=1.+PQ-P2-Q2
   A4=HP2-PQ+HQ
   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)
   1+PQ*TR(I+1,J+1)
   IF (KI.LE.0) GO TO 8
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)
   1+PQ*TI(I+1,J+1)
   AIMW=AIMW*AKI
   GOTO 8
2 A1=X*X -Y*Y
   A2=2.*X*Y
   A3=A2*A2
   A4=A1-.2752551
   A5=A1-2.724745
   D1=.5124242/(A4*A4+A3)
   D2=.05176536/(A5*A5+A3)
   REW=D1*(A2*X-A4*Y)+D2*(A2*X-A5*Y)
   IF (KI.LE.0) GO TO 8
7 AIMW=C1*(A4*X +A2*Y)+D2*(A5*X+A2*Y)
   AIMW=AIMW*AKI
   GOTO 8
3 A1=(X*X -Y*Y )*2.
   A2=4.*X*Y
   A4=A1-1.
   D1=1.1283792/(A4*A4+A2*A2)
   REW=D1*(A2*X-A4*Y)
   IF (KI.LE.0) GO TO 8

9 AIMW=C1*(A4*X+A2*Y)
   AIMW=AIMW*AKI
8 RETURN
END

```

QUIC0030
 QUIC0040
 QUIC0050
 QUIC0060
 QUIC0070
 QUIC0080
 QUIC0100
 QUIC0110
 QUIC0120
 QUIC0130
 QUIC0140
 QUIC0150
 QUIC0160
 QUIC0170
 QUIC0180
 QUIC0190
 QUIC0200
 QUIC0210
 QUIC0220
 QUIC0230
 QUIC0240
 QUIC0250
 QUIC0260
 QUIC0270
 QUIC0280
 QUIC0290
 QUIC0300
 QUIC0310
 QUIC0320
 QUIC0330
 QUIC0340
 QUIC0350
 QUIC0360
 QUIC0370
 QUIC0380
 QUIC0390
 QUIC0400
 QUIC0410
 QUIC0420
 QUIC0430
 QUIC0440
 QUIC0450
 QUIC0460
 QUIC0470
 QUIC0480
 QUIC0490
 QUIC0500
 QUIC0520
 QUIC0530
 QUIC0540
 QUIC0550
 QUIC0560
 QUIC0570
 QUIC0580
 QUIC0600

APPENDIX III. SAMPLE PROBLEM

A. Listing of Input

SIDE TEST PROBLEM WITH 40M 238U DATA

3	5	9	1	0	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	0.908	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
462.961	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	0.587	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	0.622	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	0.660	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	0.858	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	0.865	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	0.869	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	

BLANK CARD

BLANK CARD
BLANK CARD
BLANK CARD

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

BLANK CARD

2 0 2
2 0 2
2 0 2

BLANK CARD

BLANK CARD
BLANK CARD

BLANK CARD
BLANK CARD

1

RESONANCE PARAMETERS

NUCLEAR SPECIES = 1 NUMBER OF ANGULAR MOMENTA = 2

FRACTIONAL ABUNDANCE AND RADIUS

OLD VALUE	NEW VALUE	ERROR
1.0000		
0.91840	0.95370	0.129060-02

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	463.12	0.11517E-01
0.23500E-01		
0.55019E-02	0.35651E-02	0.21574E-03
478.30	478.42	0.12477E-01
0.23500E-01		
0.38005E-02	0.37049E-02	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	466.61	0.12985
0.23600E-01		
0.10004E-03	0.49464E-04	0.24433E-04
485.80	485.26	0.11205
0.23600E-01		
0.12010E-03	0.78360E-04	0.24801E-04
488.20	488.29	0.27767E-01
0.24100E-01		
0.60000E-03	0.20111E-03	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	-0.28567E-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 RADIUS

OLD VALUE	NEW VALUE	ERROR
1.0000		
0.95370	0.94868	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
0.23500E-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	467.15	0.18469
0.23600E-01		
0.49502E-04	0.52908E-04	0.16739E-04
485.26	485.33	0.12528
0.23600E-01		
0.78376E-04	0.12865E-03	0.17750E-04
488.69	489.15	0.33424E-01
0.24100E-01		
0.29152E-03	0.64901E-03	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		
0.62080E-01		
0.17536		

NORMALISATION-ERRORS

OLD VALUE	NEW VALUE	ERROR
-0.28567D-02	-0.21106E-02	0.23008D-02
-0.22132D-01	-0.21063E-01	0.26021D-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		
0.94888	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	463.17	0.50667E-02
0.23500E-01		
0.51063E-02	0.53836E-02	0.84385E-04
478.43	478.43	0.60386E-02
0.23500E-01		
0.39649E-02	0.39813E-02	0.72857E-04

ANGULAR MOMENTUM = 1 NUMBER OF LEVELS = 3

RESONANCE-ENERGY, CAPTURE-WIDTH, NEUTRON-WIDTH

OLD VALUE	NEW VALUE	ERROR
(ONLY VARIED LEVELS ARE LISTED)		
467.15	467.15	0.12355
0.23600E-01		
0.52912E-04	0.55953E-04	0.11985E-04
485.33	485.30	0.55287E-01
0.23600E-01		
0.12864E-03	0.13023E-03	0.13155E-04
485.15	485.87	0.13038E-01
0.24100E-01		
0.64846E-03	0.72674E-03	0.18745E-04

AUXILIARY PARAMETERS

OLD VALUE	NEW VALUE	ERROR
-0.22924D-01	-0.17400E-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	-0.18406E-02	0.22108D-02
-0.21063D-01	-0.20693E-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 RADIUS

OLD VALUE	NEW VALUE	ERROR
1.0000		
0.94863	0.94810	0.63565D-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	0.48384E-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	467.18	0.11257
0.23600E-01		
0.55954E-04	0.56053E-04	0.11568E-04
485.30	485.30	0.52450E-01
0.23600E-01		
0.13023E-03	0.13524E-03	0.12646E-04
488.87	488.91	0.11597E-01
0.24100E-01		
0.72682E-03	0.82566E-03	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		
0.52080E-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		
0.53979E-02	0.53583E-02	0.86427E-04
478.43	478.43	0.57741E-02
0.23500E-01		
0.35905E-02	0.35907E-02	0.70242E-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	467.18	0.11233
0.23600E-01		
0.56053E-04	0.56062E-04	0.11565E-04
485.30	485.30	0.50458E-01
0.23600E-01		
0.12524E-03	0.12532E-03	0.12664E-04
488.91	488.91	0.10750E-01
0.24100E-01		
0.82584E-03	0.82286E-03	0.21053E-04

AUXILIARY PARAMETERS

OLD VALUE	NEW VALUE	ERROR
0.55976D-01	0.57396E-01	0.67436D-01

STOP ITERATIONS BECAUSE CONVERGENCE IS TOO SLOW

ENERGY	CALCULATION	EXPERIMENT	ERROR	ATOMS PER BARN
458.14	0.8700	0.8640	0.0250	0.12395E-01
	0.5500	0.5360	0.0170	0.52080E-01
	0.1433	0.1490	0.0050	0.17536
458.34	0.8702	0.8880	0.0260	0.12395E-01
	0.5505	0.5800	0.0180	0.52080E-01
	0.1438	0.1460	0.0050	0.17536
458.55	0.8704	0.9010	0.0260	0.12395E-01
	0.5510	0.5500	0.0170	0.52080E-01
	0.1442	0.1380	0.0040	0.17536
458.76	0.8706	0.8340	0.0240	0.12395E-01
	0.5516	0.5420	0.0170	0.52080E-01
	0.1447	0.1490	0.0050	0.17536
458.97	0.8708	0.8690	0.0250	0.12395E-01
	0.5521	0.5800	0.0180	0.52080E-01
	0.1452	0.1430	0.0040	0.17536
459.18	0.8710	0.9060	0.0260	0.12395E-01
	0.5528	0.5420	0.0170	0.52080E-01
	0.1457	0.1570	0.0050	0.17536
459.39	0.8713	0.8660	0.0250	0.12395E-01
	0.5534	0.5820	0.0180	0.52080E-01
	0.1463	0.1410	0.0040	0.17536
459.60	0.8716	0.8490	0.0240	0.12395E-01
	0.5541	0.5410	0.0170	0.52080E-01
	0.1470	0.1460	0.0040	0.17536
459.81	0.8719	0.8620	0.0250	0.12395E-01
	0.5549	0.5580	0.0170	0.52080E-01
	0.1477	0.1500	0.0050	0.17536
460.02	0.8722	0.8870	0.0250	0.12395E-01
	0.5552	0.5290	0.0160	0.52080E-01
	0.1485	0.1510	0.0050	0.17536
460.22	0.8726	0.8430	0.0240	0.12395E-01
	0.5566	0.5350	0.0170	0.52080E-01
	0.1494	0.1530	0.0050	0.17536
460.43	0.8730	0.8710	0.0250	0.12395E-01
	0.5579	0.5700	0.0180	0.52080E-01
	0.1504	0.1540	0.0050	0.17536
460.64	0.8735	0.8930	0.0250	0.12395E-01
	0.5592	0.6040	0.0190	0.52080E-01
	0.1516	0.1520	0.0050	0.17536
460.85	0.8740	0.8580	0.0250	0.12395E-01
	0.5607	0.5520	0.0170	0.52080E-01
	0.1529	0.1510	0.0050	0.17536
461.06	0.8747	0.8710	0.0250	0.12395E-01
	0.5625	0.5770	0.0180	0.52080E-01
	0.1546	0.1540	0.0050	0.17536
461.27	0.8754	0.8730	0.0250	0.12395E-01
	0.5646	0.5650	0.0170	0.52080E-01
	0.1565	0.1490	0.0050	0.17536
461.49	0.8763	0.8780	0.0250	0.12395E-01
	0.5670	0.5590	0.0170	0.52080E-01
	0.1588	0.1600	0.0050	0.17536
461.70	0.8769	0.9080	0.0260	0.12395E-01
	0.5687	0.5600	0.0170	0.52080E-01
	0.1605	0.1590	0.0050	0.17536
461.91	0.8753	0.8620	0.0240	0.12395E-01
	0.5650	0.5630	0.0180	0.52080E-01
	0.1582	0.1550	0.0050	0.17536
462.12	0.8646	0.8170	0.0240	0.12395E-01
	0.5418	0.5510	0.0170	0.52080E-01
	0.1436	0.1440	0.0050	0.17536
462.33	0.8315	0.8060	0.0230	0.12395E-01
	0.4761	0.4530	0.0150	0.52080E-01
	0.1094	0.1030	0.0030	0.17536
462.54	0.7601	0.7780	0.0230	0.12395E-01
	0.3588	0.3810	0.0140	0.52080E-01
	0.0632	0.0590	0.0030	0.17536
462.75	0.6539	0.6650	0.0210	0.12395E-01
	0.2191	0.2420	0.0100	0.52080E-01
	0.0257	0.0200	0.0030	0.17536
462.96	0.5510	0.5420	0.0180	0.12395E-01
	0.1126	0.1160	0.0070	0.52080E-01
	0.0069	0.0040	0.0030	0.17536
463.17	0.5015	0.5010	0.0170	0.12395E-01
	0.0091	0.0060	0.0050	0.52080E-01
	0.0017	0.0030	0.0030	0.17536
463.39	0.5309	0.5100	0.0170	0.12395E-01
	0.0916	0.0910	0.0060	0.52080E-01
	0.0032	0.0050	0.0030	0.17536
463.60	0.6195	0.6350	0.0200	0.12395E-01
	0.1726	0.1670	0.0080	0.52080E-01
	0.0124	0.0130	0.0030	0.17536
463.81	0.7201	0.7340	0.0220	0.12395E-01
	0.2005	0.2030	0.0100	0.52080E-01
	0.0325	0.0330	0.0030	0.17536
464.02	0.7540	0.7820	0.0230	0.12395E-01
	0.3958	0.4030	0.0140	0.52080E-01
	0.0619	0.0620	0.0030	0.17536

464.23	0.8333 0.4666 0.0888	0.8510 0.4730 0.0900	0.0250 0.0150 0.0030	0.12395E-01 0.52080E-01 0.17536
464.45	0.8499 0.4998 0.1056	0.8430 0.4890 0.1070	0.0240 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
464.66	0.8561 0.5142 0.1146	0.8580 0.4970 0.1140	0.0250 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
464.87	0.8588 0.5209 0.1194	0.8540 0.5600 0.1150	0.0240 0.0180 0.0040	0.12395E-01 0.52080E-01 0.17536
465.09	0.8604 0.5249 0.1225	0.8740 0.5420 0.1200	0.0250 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
465.30	0.8615 0.5278 0.1247	0.8460 0.5010 0.1280	0.0250 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
465.51	0.8624 0.5300 0.1265	0.8960 0.5280 0.1230	0.0260 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
465.73	0.8631 0.5318 0.1280	0.9160 0.5310 0.1270	0.0270 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
465.94	0.8636 0.5333 0.1291	0.8400 0.5170 0.1280	0.0240 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
466.15	0.8640 0.5341 0.1298	0.8260 0.5290 0.1220	0.0240 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
466.37	0.8639 0.5340 0.1297	0.8580 0.5730 0.1300	0.0250 0.0180 0.0040	0.12395E-01 0.52080E-01 0.17536
466.58	0.8633 0.5324 0.1284	0.8530 0.5460 0.1300	0.0240 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
466.79	0.8621 0.5294 0.1261	0.8710 0.5240 0.1270	0.0250 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
467.01	0.8611 0.5268 0.1240	0.8390 0.5040 0.1230	0.0240 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
467.22	0.8610 0.5266 0.1238	0.8790 0.5230 0.1250	0.0250 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
467.44	0.8622 0.5295 0.1261	0.8770 0.5110 0.1290	0.0250 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
467.65	0.8636 0.5340 0.1296	0.8560 0.5110 0.1290	0.0240 0.0160 0.0040	0.12395E-01 0.52080E-01 0.17536
467.87	0.8655 0.5381 0.1332	0.8710 0.5310 0.1360	0.0250 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
468.08	0.8665 0.5400 0.1354	0.8750 0.6660 0.1330	0.0250 0.0180 0.0040	0.12395E-01 0.52080E-01 0.17536
468.30	0.8671 0.5422 0.1366	0.8350 0.5390 0.1340	0.0240 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
468.51	0.8674 0.5430 0.1373	0.8730 0.5330 0.1440	0.0250 0.0160 0.0050	0.12395E-01 0.52080E-01 0.17536
468.73	0.8676 0.5436 0.1378	0.8980 0.5770 0.1400	0.0260 0.0180 0.0040	0.12395E-01 0.52080E-01 0.17536
468.94	0.8676 0.5441 0.1382	0.8390 0.5420 0.1400	0.0240 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
469.16	0.8680 0.5446 0.1386	0.8520 0.5290 0.1410	0.0250 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
469.38	0.8681 0.5460 0.1390	0.8420 0.5510 0.1370	0.0240 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
469.59	0.8683 0.5455 0.1394	0.8490 0.5420 0.1360	0.0240 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
469.81	0.8684 0.5459 0.1397	0.8750 0.5590 0.1390	0.0250 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
470.02	0.8686 0.5463 0.1401	0.8670 0.5560 0.1430	0.0250 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
470.24	0.8688 0.5467 0.1404	0.8600 0.5560 0.1400	0.0250 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
470.46	0.8689 0.5471 0.1408	0.8370 0.5820 0.1410	0.0240 0.0180 0.0040	0.12395E-01 0.52080E-01 0.17536

470.67	0.8651	0.8900	0.0260	0.12395E-01
	0.5475	0.5640	0.0180	0.52080E-01
	0.1411	0.1420	0.0040	0.17536
470.89	0.8692	0.8760	0.0250	0.12395E-01
	0.5479	0.5210	0.0160	0.52080E-01
	0.1415	0.1420	0.0040	0.17536
471.11	0.8694	0.8720	0.0250	0.12395E-01
	0.5483	0.5710	0.0180	0.52080E-01
	0.1418	0.1490	0.0050	0.17536
471.32	0.8695	0.8710	0.0250	0.12395E-01
	0.5487	0.5650	0.0170	0.52080E-01
	0.1421	0.1430	0.0040	0.17536
471.54	0.8697	0.8720	0.0250	0.12395E-01
	0.5491	0.5530	0.0170	0.52080E-01
	0.1425	0.1410	0.0040	0.17536
471.76	0.8698	0.8660	0.0250	0.12395E-01
	0.5455	0.5750	0.0180	0.52080E-01
	0.1428	0.1480	0.0050	0.17536
471.98	0.8659	0.8910	0.0260	0.12395E-01

	0.5459	0.5210	0.0160	0.52080E-01
	0.1432	0.1420	0.0040	0.17536
472.19	0.8701	0.8870	0.0250	0.12395E-01
	0.5503	0.5640	0.0170	0.52080E-01
	0.1435	0.1410	0.0040	0.17536
472.41	0.8702	0.9190	0.0260	0.12395E-01
	0.5507	0.5680	0.0180	0.52080E-01
	0.1439	0.1410	0.0040	0.17536
472.63	0.8704	0.9270	0.0270	0.12395E-01
	0.5511	0.5660	0.0170	0.52080E-01
	0.1442	0.1500	0.0050	0.17536
472.85	0.8706	0.8940	0.0260	0.12395E-01
	0.5515	0.5600	0.0170	0.52080E-01
	0.1446	0.1470	0.0050	0.17536
473.07	0.8707	0.8860	0.0260	0.12395E-01
	0.5519	0.5780	0.0180	0.52080E-01
	0.1450	0.1470	0.0040	0.17536
473.29	0.8709	0.8380	0.0240	0.12395E-01
	0.5524	0.5770	0.0180	0.52080E-01
	0.1454	0.1470	0.0050	0.17536
473.51	0.8711	0.8520	0.0240	0.12395E-01
	0.5528	0.5440	0.0170	0.52080E-01
	0.1458	0.1460	0.0040	0.17536
473.72	0.8712	0.8420	0.0240	0.12395E-01
	0.5533	0.5390	0.0170	0.52080E-01
	0.1462	0.1510	0.0050	0.17536
473.94	0.8714	0.8790	0.0250	0.12395E-01
	0.5538	0.5630	0.0180	0.52080E-01
	0.1467	0.1480	0.0050	0.17536
474.16	0.8716	0.9010	0.0260	0.12395E-01
	0.5544	0.5680	0.0180	0.52080E-01
	0.1472	0.1440	0.0040	0.17536
474.38	0.8718	0.8810	0.0250	0.12395E-01
	0.5549	0.5260	0.0160	0.52080E-01
	0.1477	0.1480	0.0050	0.17536
474.60	0.8721	0.8920	0.0250	0.12395E-01
	0.5555	0.5640	0.0180	0.52080E-01
	0.1482	0.1420	0.0040	0.17536
474.82	0.8723	0.8620	0.0250	0.12395E-01
	0.5562	0.5710	0.0180	0.52080E-01
	0.1488	0.1490	0.0050	0.17536
475.04	0.8726	0.8920	0.0260	0.12395E-01
	0.5568	0.5750	0.0180	0.52080E-01
	0.1494	0.1600	0.0050	0.17536
475.26	0.8728	0.8470	0.0240	0.12395E-01
	0.5576	0.5270	0.0160	0.52080E-01
	0.1501	0.1490	0.0040	0.17536
475.48	0.8732	0.8970	0.0250	0.12395E-01
	0.5585	0.5890	0.0180	0.52080E-01
	0.1509	0.1470	0.0040	0.17536
475.70	0.8735	0.8780	0.0250	0.12395E-01
	0.5594	0.5410	0.0170	0.52080E-01
	0.1517	0.1580	0.0050	0.17536
475.92	0.8739	0.8660	0.0250	0.12395E-01
	0.5605	0.5720	0.0180	0.52080E-01
	0.1527	0.1640	0.0050	0.17536
476.14	0.8744	0.8700	0.0250	0.12395E-01
	0.5617	0.5720	0.0180	0.52080E-01
	0.1539	0.1570	0.0050	0.17536
476.36	0.8749	0.8620	0.0240	0.12395E-01
	0.5632	0.5570	0.0170	0.52080E-01
	0.1552	0.1620	0.0050	0.17536
476.58	0.8756	0.8350	0.0240	0.12395E-01
	0.5650	0.5820	0.0180	0.52080E-01
	0.1569	0.1550	0.0050	0.17536
476.80	0.8762	0.8390	0.0240	0.12395E-01
	0.5668	0.5840	0.0180	0.52080E-01
	0.1586	0.1590	0.0050	0.17536

477.03	0.8763	0.8640	0.0250	0.12395E-01
	0.5671	0.5580	0.0180	0.52080E-01
	0.1591	0.1550	0.0050	0.17536
477.25	0.8730	0.8240	0.0240	0.12395E-01
	0.5553	0.5380	0.0170	0.52080E-01
	0.1537	0.1470	0.0050	0.17536
477.47	0.8583	0.8760	0.0260	0.12395E-01
	0.5266	0.5220	0.0170	0.52080E-01
	0.1334	0.1300	0.0040	0.17536
477.69	0.8190	0.8310	0.0250	0.12395E-01
	0.4460	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
	0.3272	0.3460	0.0130	0.52080E-01
	0.0496	0.0470	0.0030	0.17536
478.13	0.6556	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	0.0200	0.12395E-01
	0.1304	0.1190	0.0070	0.52080E-01
	0.0051	0.0040	0.0030	0.17536
478.58	0.5555	0.6040	0.0190	0.12395E-01
	0.1303	0.1170	0.0070	0.52080E-01
	0.0044	0.0070	0.0030	0.17536
478.80	0.6391	0.6600	0.0210	0.12395E-01
	0.1595	0.2010	0.0090	0.52080E-01
	0.0143	0.0170	0.0030	0.17536
479.02	0.7355	0.7500	0.0220	0.12395E-01
	0.2090	0.2980	0.0110	0.52080E-01
	0.0372	0.0410	0.0030	0.17536
479.25	0.8047	0.8410	0.0240	0.12395E-01
	0.4135	0.3950	0.0130	0.52080E-01
	0.0654	0.0720	0.0030	0.17536
479.47	0.8407	0.8580	0.0250	0.12395E-01
	0.4619	0.4730	0.0150	0.52080E-01
	0.0584	0.0970	0.0030	0.17536
479.69	0.8555	0.8350	0.0240	0.12395E-01
	0.5147	0.5620	0.0180	0.52080E-01
	0.1164	0.1150	0.0040	0.17536
479.91	0.8615	0.8600	0.0250	0.12395E-01
	0.5280	0.5400	0.0170	0.52080E-01
	0.1252	0.1210	0.0040	0.17536
480.14	0.8632	0.8430	0.0240	0.12395E-01
	0.5337	0.5230	0.0160	0.52080E-01
	0.1295	0.1320	0.0040	0.17536
480.36	0.8650	0.8240	0.0240	0.12395E-01
	0.5365	0.5320	0.0160	0.52080E-01
	0.1221	0.1330	0.0040	0.17536
480.59	0.8655	0.8390	0.0240	0.12395E-01
	0.5351	0.5010	0.0160	0.52080E-01
	0.1340	0.1420	0.0040	0.17536
480.81	0.8665	0.8850	0.0260	0.12395E-01
	0.5409	0.5410	0.0170	0.52080E-01
	0.1255	0.1360	0.0040	0.17536
481.03	0.8671	0.8670	0.0250	0.12395E-01
	0.5423	0.5390	0.0170	0.52080E-01
	0.1367	0.1380	0.0040	0.17536
481.26	0.8676	0.8670	0.0250	0.12395E-01
	0.5435	0.5770	0.0180	0.52080E-01
	0.1377	0.1390	0.0040	0.17536
481.48	0.8680	0.8590	0.0240	0.12395E-01
	0.5446	0.5200	0.0160	0.52080E-01
	0.1386	0.1390	0.0040	0.17536
481.71	0.8683	0.8840	0.0260	0.12395E-01
	0.5455	0.5410	0.0170	0.52080E-01
	0.1394	0.1410	0.0040	0.17536
481.93	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
	0.1407	0.1450	0.0040	0.17536
482.38	0.8691	0.8530	0.0240	0.12395E-01
	0.5477	0.5500	0.0170	0.52080E-01
	0.1412	0.1330	0.0040	0.17536
482.61	0.8694	0.9090	0.0260	0.12395E-01
	0.5483	0.5470	0.0170	0.52080E-01
	0.1418	0.1420	0.0040	0.17536
482.83	0.8696	0.8340	0.0240	0.12395E-01
	0.5489	0.5280	0.0160	0.52080E-01
	0.1423	0.1480	0.0050	0.17536
483.06	0.8698	0.8610	0.0250	0.12395E-01
	0.5494	0.5420	0.0170	0.52080E-01
	0.1428	0.1370	0.0040	0.17536
483.28	0.8700	0.8350	0.0240	0.12395E-01
	0.5499	0.5680	0.0170	0.52080E-01
	0.1432	0.1410	0.0040	0.17536
483.51	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
	0.1378	0.1400	0.0040	0.17536
484.86	0.8643	0.8740	0.0250	0.12395E-01
	0.5252	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
	0.5285	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
	0.5278	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
	0.5542	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
	0.1478	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
	0.4590	0.5180	0.0160	0.52080E-01
	0.1678	0.1120	0.0040	0.17536
488.51	0.8282	0.8540	0.0250	0.12395E-01
	0.4512	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	0.8071	0.8010	0.0230	0.12395E-01
	0.4029	0.3920	0.0140	0.52080E-01
	0.0522	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
	0.4602	0.4830	0.0160	0.52080E-01
	0.0962	0.0950	0.0030	0.17536
489.66	0.8586	0.8620	0.0250	0.12395E-01
	0.5215	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 0.5558 0.1487	0.8960 0.5260 0.1550	0.0250 0.0160 0.0050	0.12395E-01 0.52080E-01 0.17536
490.35	0.8734 0.5590 0.1514	0.8860 0.5480 0.1490	0.0260 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
490.58	0.8737 0.5600 0.1523	0.8460 0.5930 0.1460	0.0240 0.0180 0.0040	0.12395E-01 0.52080E-01 0.17536
490.81	0.8739 0.5605 0.1527	0.8600 0.5400 0.1520	0.0240 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
491.04	0.8740 0.5608 0.1530	0.8520 0.5570 0.1570	0.0240 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
491.28	0.8742 0.5612 0.1533	0.8950 0.5430 0.1600	0.0260 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
491.51	0.8743 0.5615 0.1536	0.9060 0.5880 0.1530	0.0250 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
491.74	0.8744 0.5618 0.1536	0.9070 0.5700 0.1550	0.0260 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
491.97	0.8745 0.5621 0.1542	0.8970 0.5750 0.1560	0.0260 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
492.20	0.8746 0.5624 0.1545	0.8650 0.5620 0.1530	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
492.43	0.8747 0.5627 0.1547	0.8360 0.5780 0.1500	0.0240 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
492.67	0.8748 0.5630 0.1550	0.8930 0.5710 0.1490	0.0250 0.0180 0.0040	0.12395E-01 0.52080E-01 0.17536
492.90	0.8750 0.5633 0.1553	0.8670 0.5800 0.1580	0.0250 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
493.13	0.8751 0.5636 0.1556	0.8640 0.5680 0.1540	0.0240 0.0180 0.0050	0.12395E-01 0.52080E-01 0.17536
493.36	0.8752 0.5639 0.1558	0.8890 0.5400 0.1530	0.0250 0.0160 0.0050	0.12395E-01 0.52080E-01 0.17536
493.60	0.8753 0.5642 0.1561	0.8830 0.5490 0.1580	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
493.83	0.8754 0.5645 0.1564	0.9020 0.5680 0.1540	0.0260 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
494.06	0.8755 0.5648 0.1567	0.9120 0.6080 0.1490	0.0260 0.0190 0.0040	0.12395E-01 0.52080E-01 0.17536
494.30	0.8756 0.5651 0.1570	0.8880 0.5540 0.1590	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
494.53	0.8757 0.5654 0.1573	0.8920 0.5660 0.1580	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
494.76	0.8759 0.5657 0.1576	0.8650 0.5640 0.1480	0.0250 0.0170 0.0040	0.12395E-01 0.52080E-01 0.17536
495.00	0.8760 0.5660 0.1575	0.8800 0.5560 0.1800	0.0250 0.0170 0.0050	0.12395E-01 0.52080E-01 0.17536
495.23	0.8761 0.5663 0.1582	0.8570 0.5870 0.1560	0.0250 0.0180 0.0050	0.12395E-01 0.52080E-01 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.

**THIS PAGE
WAS INTENTIONALLY
LEFT BLANK**

ORNL/TM-6286
 ENDF-261
 Dist. Category UC-79d

INTERNAL DISTRIBUTION

1. L. S. Abbott	38.-52. D. K. Olsen
2. G. T. Chapman	53. R. W. Peelle
3. J. Craven	54. F. G. Perey
4-18 G. de Saussure	55. R. B. Perez
19. J. K. Dickens	56. S. Raman
20. F. C. Difilippo	57. E. G. Silver
21. G. F. Flanagan	58. R. R. Spencer
22. G. Goldstein (consultant)	59. M. L. Tobias
23. R. Gwin	60. J. H. Todd
24. J. Halperin	61. H. Weaver
25. J. A. Harvey	62. C. R. Weisbin
26. N. W. Hill	63. L. W. Weston
27. D. J. Horen	64. R. Q. Wright
28. R. W. Ingle	65. A. Zucker
29. C. H. Johnson	66. P. Greebler (consultant)
30. E. H. Kobisk	67. W. B. Lowenstein (consultant)
31. D. C. Larson	68. R. E. Uhrig (consultant)
32. R. L. Macklin	69. R. Wilson (consultant)
33. F. C. Maienschein	70.-71. Central Research Library
34. B. F. Maskewitz	72. ORNL Y-12 Technical Library
35. A. G. Mitchell	Document Reference Section
36. M. Mizumoto	73.-74. Laboratory Records Department
37. G. L. Morgan	75. ORNL Patent Office
	76. Laboratory Records (RC)

EXTERNAL DISTRIBUTION

77. DOE Oak Ridge Operations, Research and Technical Support Division,
 P. O. Box E, Oak Ridge, Tennessee 37830: Director
78. DOE Oak Ridge Operations, Reactor Division, P. O. Box E, Oak Ridge,
 Tennessee 37830: Director
- 79.-80. DOE Division of Reactor Research and Development, Washington, DC
 20545: Director
- 81.-368. For distribution as shown in TID-4500 Distribution Category UC-79d,
 Liquid Metal Fast Breeder Reactor Physics - Base (62 copies -
 ENDF distribution)