663298

DP-1278

ENDF-152

AEC RESEARCH AND DEVELOPMENT REPORT

FLANGE II (Version 71-1)

A CODE TO PROCESS THERMAL NEUTRON DATA FROM AN ENDF/B TAPE

H. C. HONECK
D. R. FINCH

DUPONT
REG. U.S. PAT. OFF.

Savannah River Laboratory

Aiken, South Carolina

Printed in the United States of America
Available from
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151
Price: Printed Copy $3.00; Microfiche $0.95

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Mathematics and Computers
(TID-4500, UC-32)

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A CODE TO PROCESS THERMAL NEUTRON DATA FROM AN ENDF/B TAPE

by

Henry C. Honeck
Donald R. Finch

Approved by

H. C. Honeck, Research Manager
Computer Applications Division

October 1971

E. I. DU PONT DE NEMOURS & COMPANY
SAVANNAH RIVER LABORATORY
AIKEN, S. C. 29801

CONTRACT AT(07-2)-1 WITH THE
UNITED STATES ATOMIC ENERGY COMMISSION

ABSTRACT

The FLANGE II (Version 71-1) computer code processes data for smooth cross sections, resonance parameters, angular distributions, and thermal scattering law from an ENDF/B-II or ENDF/B-III data tape for use in thermal spectrum calculations. Options are available in the code to produce pointwise or group-averaged cross sections for up to 200 energy points or groups, and Legendre angular distributions up to P_5 order. Resonance contributions in the thermal region are computed as infinitely dilute, Doppler broadened values. This report describes the theory, methods, application, and utilization of FLANGE II in creating thermal cross sections from ENDF/B-II and ENDF/B-III library data.

ACKNOWLEDGMENT

The original FLANGE II code was developed in 1966 by H. C. Honeck at the U. S. Atomic Energy Commission in Washington, D. C. with the assistance of Y. D. Naliboff and Dale Houston of Gulf General Atomics Corporation, San Diego, California. Several modifications and corrections to the original code were made by D. R. Finch between 1967 and 1970. Version 71-1 of FLANGE II contains new features by D. R. Finch with theoretical guidance for the short collision time approximation by G. M. Borgonovi of Gulf Energy & Environmental Systems, Inc.

CONTENTS

1. INTRODUCTION

This report describes the code FLANGE II (Version 71-1) developed to process data for thermal neutron cross sections, resonance parameters, angular distributions, and scattering law from the ENDF/B-II or ENDF/B-III library into multigroup cross sections and scattering kernels. Sections 1 through 5 of this report give a brief description of the code, the physical and numerical theory, and operating instructions. Sections 6 and 7 describe in detail the numerical procedures. Section 8 describes an auxiliary code for use with FLANGE II.

FLANGE II is written in FORTRAN IV and is designed for use on a computer with about 40K of fast core storage and 3 tapes (plus systems tapes). Larger core storages or disk memories can be easily used to increase the speed of the code. The code is designed to handle up to 200 energy groups and Legendre moments up to P_5.

The input data on the ENDF/B tape can be summarized as follows (only data needed for thermal calculations are listed here):

- ν (neutrons/fission), radioactive decay data, fission product yields.
- Cross sections of the form $\sigma^x(E,T)$, where E is the neutron energy, T is the material temperature, and x denotes elastic, inelastic, scattering (elastic and inelastic), absorption, fission, total, or (n,γ).
- Angular distributions of the form $\sigma^x(E,\mu,T)$, where μ is the cosine of the scattering angle, and x denotes elastic, inelastic, or scattering.
- The thermal neutron scattering law, $S(\alpha,\beta,T)$, which is represented as a tabulated part plus analytic parts of the free gas or diffusive motion form.
- Resolved resonance parameters in the single or multi-level Breit-Wigner representation.

The user of FLANGE II supplies a group structure (energy mesh) and the desired temperature of the material. FLANGE II then computes, prints, and punches

$$\sigma^{y}(E_i)$$

$$\sigma_{\ell}^{x}(E_i)$$

$$\sigma_{\ell}^{in}(E_i \rightarrow E_j)$$

where ℓ denotes the order of the Legendre expansion; E_i and E_j are points on the user's energy mesh; y denotes absorption, fission, total, or transport; x denotes elastic, inelastic, or scattering; and in denotes inelastic. The cross sections $\sigma^{y}(E_i)$ and $\sigma_{\ell}^{x}(E_i)$ may be either evaluated at the points in the input energy mesh or averaged over the input group structure. The scattering kernels $\sigma_{\ell}^{in}(E_i \rightarrow E_j)$ are evaluated only at the input energy points. The diagonals of the kernels can be adjusted so that when they are integrated to yield a cross section, they yield the inelastic or elastic plus inelastic cross section. If $\sigma_{\ell}^{in}(E)$ is not given on the ENDF/B input tape, a high accuracy integration can be done to compute it directly from the scattering law.

The code computes only Legendre moments of angular distributions. The code is written in the form of separate links, and additional links can be conveniently added. Later extensions of the code could be links to handle point angular distributions, special links to produce results of direct interest to experimentalists, and links for compressing large scattering kernels to few group kernels via a B_{ℓ} calculation.

2. DESCRIPTION OF THE PHYSICS

2.1 NOMENCLATURE

Symbol	Definition	Unit
E	Neutron energy	ev
E', E	Initial and final neutron energies	ev
E_i	Characteristic energy of the i^{th} energy group	ev
E_i^b	Lower energy boundary of the i^{th} energy group	ev
W_i	Integration weight for the i^{th} energy group	ev
$\sigma(E)$	Cross section	barns
$d\sigma/d\Omega$	Differential cross section	barns/steradian
$d^2\sigma/d\Omega dE$	Differential cross section	barns/steradian-ev
μ	Cosine of the scattering angle in the laboratory system	
$\sigma(E,\mu)$	Differential cross section defined by $\sigma(E,\mu) = 2\pi d\sigma/d\Omega$	barns
$\sigma(E'\rightarrow E,\mu)$	Differential cross section defined by $\sigma(E'\rightarrow E,\mu) = 2\pi d^2\sigma/d\Omega dE$	barns/ev
t,a,s,f,in, el,tr,γ	Superscripts denoting total, absorption, scattering, fission, inelastic, elastic, transport, and (n,γ)	
ℓ	Subscript denoting the Legendre order	
$P_\ell(\mu)$	Legendre polynomial of order ℓ	
T	Material temperature	°K
kT	Material temperature, $k = 0.86166 \times 10^{-4}$ ev/°K	ev
T_0	Reference temperature = 293.62°K	
kT_0	Reference temperature = 0.0253 ev/°K	
$f_\ell(E)$	Coefficient in a Legendre expansion	
$p(E,\mu)$	Angular scattering probability	
$S(\alpha,\beta)$	Thermal scattering law	

2.2 ENDF/B INPUT TAPE

The quantities contained on the ENDF/B input tape are described briefly in this section and in more detail in the specification of the ENDF/B formats.[1]

The ENDF/B tape is organized by material, file, and section. For a particular material, the file numbers run from 1 to 7, and each file contains a particular type of information.

File	Type of Information
1	Description of the material, comments, ν (neutrons/fission), fission yields, and radioactive decay data
2	Resolved and unresolved resonance parameters
3	Smooth cross sections, $\sigma(E,T)$
4	Angular distributions, $p(E,\mu,T)$, expressed as tabulations or Legendre expansions
5	Secondary energy distributions, $p(E'\rightarrow E,T)$
6	Secondary energy angle correlations, $p(E'\rightarrow E,\mu,T)$
7	Thermal scattering law, $S(\alpha,\beta,T)$

The dependence of the above quantities on the material temperature is also included where appropriate. Files 5 and 6 are intended primarily for high energy data, and are not used by FLANGE II.

Each file is divided into sections. The sections which may occur in File 1 are:

Section	Description
451	Hollerith comment cards describing the data and material
452	$\nu(E)$ (neutrons/fission) expressed as a tabulation or polynomial in E
453	Radioactive decay constants for this isotope and neutron-induced reaction products of this isotope
454	Fission product yield data

All of the above quantities (if present on the tape) are processed by FLANGE II. $\nu(E)$ is evaluated at E = 0 and stored for later use.

File 2 contains resolved resonance parameters from which contributions to capture, fission, and elastic scattering are computed where applicable.

Files 3, 4, and 7 are divided as follows:

Section	File 3	File 4	File 7
1	$\sigma^{t}(E,T)$	-	-
2	$\sigma^{el}(E,T)$	$p^{el}(E,\mu,T)$	-
4	$\sigma^{in}(E,T)$	$p^{in}(E,\mu,T)$	$S(\alpha,\beta,T)$
18	$\sigma^{f}(E,T)$	-	-
29	$\sigma^{s}(E,T)$	$p^{s}(E,\mu,T)$	-
102	$\sigma^{\gamma}(E,T)$	-	-

Here, scattering (superscript s) means elastic plus inelastic. The $p(E,\mu,T)$ are defined by

$$\frac{d\sigma(E,\mu,T)}{d\Omega} = \frac{\sigma(E,T)}{2\pi} p(E,\mu,T)$$

and $p(E,\mu,T)$ may be represented by a tabulation or a Legendre expansion. The scattering law on File 7 is represented as a tabulation and/or analytic terms of the free gas or diffusion type. The short collision time approximation is used to extend tabular values to higher energies.

The table above contains the maximum amount of data of use for thermal calculation which could be given on the tape. In most cases, many of the items will be missing. When sufficient data are given, FLANGE II can compute items not given on the tape. For example, $\sigma^{in}(E,T)$ and $p^{in}(E,\mu,T)$ can be computed from $S(\alpha,\beta,T)$; $\sigma^{s}(E,T)$ can be computed from $\sigma^{el}(E,T)$ and $\sigma^{in}(E,T)$; and $\sigma^{t}(E,T)$ can be computed from $\sigma^{s}(E,T)$ and $\sigma^{a}(E,T)$. The tape should contain sufficient information to allow computation of all required quantities. The user must be aware of what quantities are actually given on the tape and then instruct FLANGE II what quantities are to be derived.

2.3 INPUT ENERGY MESH

The user must supply a description of the neutron energy space in which the calculations are to be done. Three sets of numbers are required. Let i denote a region of energy (group).

E_i^b Lower energy boundary (ev) of the i^{th} group

E_i Characteristic energy (ev) of the i^{th} group lying between the lower boundary (E_i^b) and the upper boundary (E_{i+1}^b) of the group

W_i Integration weight (ev) for the i^{th} group such that the integral of a function f(E) over the group is well approximated by $f(E_i)W_i$

Several methods may be used to specify these numbers. For example, the user may:

- Give an arbitrary list of the E_i
- Give an arbitrary list of the E_i^b
- Specify energy regions in which the E_i^b will be assigned on the basis of equal spacing in energy or lethargy (ln E)
- Use the above methods but change the word energy to reduced velocity, $x = \sqrt{E/kT_o}$

2.4 CROSS SECTIONS

The user specifies the cross section desired and whether the cross section is to be read from the input ENDF/B tape or to be derived from other cross sections. The user specifies the material temperature, and as the appropriate cross section $\sigma(E,T)$ is read from the ENDF/B tape, it is automatically evaluated at the desired temperature. Thus, the temperature dependence has been removed, and the resulting cross section is denoted by $\sigma(E)$. Resolved resonance contributions are included where required as infinitely dilute values. Doppler broadening is included in the resonance calculations.

A series of test numbers are used as input to describe how a specific cross section is to be obtained. One test number for each type of cross section is illustrated in the following table:

Cross Section	Value of the Test Number 1	2	3
$\sigma^t(E)$	ENDF/B tape	$\sigma^s(E) + \sigma^a(E)$	-
$\sigma^{el}(E)$	ENDF/B tape	$\sigma^s(E) - \sigma^{in}(E)$	-
$\sigma^{in}(E)$	ENDF/B tape	$\sigma^s(E) - \sigma^{el}(E)$	$S(\alpha,\beta)$
$\sigma^f(E)$	ENDF/B tape	-	-
$\sigma^a(E)$	$\sigma^f(E) + \sigma^\gamma(E)$ ($\sigma^\gamma(E)$ from ENDF/B tape)	$\sigma^t(E) - \sigma^s(E)$	-
$\sigma^s(E)$	ENDF/B tape	$\sigma^{el}(E) + \sigma^{in}(E)$	-

If the test number is 1, the cross section is read from the ENDF/B tape; if it is 2, the cross section is computed from other cross sections; and if it is 3 (inelastic only), it is computed from $S(\alpha,\beta)$.

A second series of test numbers are input by the user to describe the averaging and output procedures. If the test is positive, the cross section will be printed and punched; if negative, only printing will occur. If the absolute value of the test is 1, the cross section will be evaluated on the input energy mesh, so that the output will be the numbers $\sigma_i = \sigma(E_i)$. If the absolute value of the test is 2, the cross section will be averaged over the input energy group, so that the output will be the numbers

$$\overline{\sigma}_i = \int_{E^b_i}^{E^b_{i+1}} dE\sigma(E)/(E^b_{i+1} - E^b_i)$$

This latter feature is essential for elastic cross sections of crystalline materials. Group averaging of the inelastic cross section can be done if it is read from the ENDF/B tape, but not if it is computed from the scattering law.

A transport cross section (with or without absorption) can also be computed, printed, and punched. For fissionable isotopes, the quantities η_i and α_i are also computed and printed.

2.5 ANGULAR DISTRIBUTIONS

The present version of FLANGE II computes Legendre moments of the angular distribution (up to P_5) from $S(\alpha,\beta)$, and accepts Legendre moments or tabulated distributions from the ENDF/B tape.

The data given on File 4 of the ENDF/B tape are $p(E,\mu,T)$ in the Legendre expansion form

$$p(E,\mu,T) = \sum_{\ell=0}^{LX} \frac{2\ell+1}{2} f_\ell(E,T) P_\ell(\mu)$$

or as tabular values of $p(E,\mu,T)$. As before, as each $f_\ell(E,T)$ is read from the tape or obtained by fitting the tabular values, it is evaluated at the desired temperature to obtain $f_\ell(E)$. The appropriate cross section, $\sigma(E)$, is obtained from File 3. FLANGE II processes these data into Legendre cross sections, $\sigma_\ell(E)$, defined by

$$\frac{d\sigma(E,\mu)}{d\Omega} = \frac{1}{2\pi} \sigma(E,\mu)$$

$$\sigma(E,\mu) = \sum_{\ell=0}^{LX} \frac{2\ell+1}{2} \sigma_\ell(E) P_\ell(\mu)$$

$$\sigma_\ell(E) = \sigma(E) f_\ell(E)$$

The same series of test numbers used for cross sections are used here with their same meaning.

Legendre Cross Section	Value of the Test Number		
	1	2	3
$\sigma_\ell^{el}(E)$	ENDF/B tape	$\sigma_\ell^{s}(E) - \sigma_\ell^{in}(E)$	-
$\sigma_\ell^{in}(E)$	ENDF/B tape	$\sigma_\ell^{s}(E) - \sigma_\ell^{el}(E)$	$S(\alpha,\beta)$
$\sigma_\ell^{s}(E)$	ENDF/B tape	$\sigma_\ell^{el}(E) + \sigma_\ell^{in}(E)$	-

If resonance parameters are defined that overlap the input energy mesh, these contributions are added to the elastic scattering if the test number is 1. An option allows this contribution to be calculated from the resonance formulas or taken as only the potential scattering term.

The second test number again indicates the desired printing, punching, and averaging procedure. Thus, the computed quantities may be either $\sigma_{\ell i} = \sigma_\ell(E_i)$, or

$$\overline{\sigma}_{\ell i} = \int_{E_i^b}^{E_{i+1}^b} dE\sigma_\ell(E)/(E_{i+1}^b - E_i^b)$$

The product $\sigma(E)f_\ell(E) = \sigma_\ell(E)$ is averaged over the group, rather than $f_\ell(E)$.

As mentioned in Section 2.4, a transport cross section can be computed from either

$$\sigma_i^{tr} = \sigma_{0i}^s - \sigma_{1i}^s$$

or

$$\sigma_i^{tr} = \sigma_i^a + \sigma_{0i}^s - \sigma_{1i}^s$$

where the $\sigma_{\ell i}^s$ and σ_i^a are the cross sections defined above and may be either point or averaged numbers.

2.6 SCATTERING KERNELS

The present version of FLANGE II computes Legendre moments of the scattering kernel (up to P_5) from the scattering law on File 7 on the ENDF/B tape.

The scattering law contained on the ENDF/B tape consists of a fully tabulated $S(\alpha,\beta)$ plus the parameters needed to specify analytic terms to be added to the tabulated scattering law. FLANGE II will handle the tabulation and analytic terms of the free gas or diffusive type. The tabulation may be extended to higher energy transfers using the short collision time approximation.[2] The effective temperature of the scatterer must be specified to use this feature.

The scattering kernel is related to the scattering law by

$$\frac{d^2\sigma^{in}(E'\to E,\mu,T)}{d\Omega dE} = \frac{\sigma_b}{4\pi kT}\sqrt{\frac{E}{E'}}\, e^{-\beta/2} S(\alpha,\beta,T)$$

where $\alpha = (E' + E - 2\mu\sqrt{EE'})/AkT$

$\beta = (E - E')/kT$

The Legendre moments of the kernel, $\sigma_\ell^{in}(E'\to E)$, are defined by

$$\sigma^{in}(E'\to E,\mu) = 2\pi \frac{d^2\sigma^{in}(E'\to E,\mu)}{d\Omega dE}$$

$$= \sum_{\ell=0}^{LX} \frac{2\ell+1}{2}\sigma_\ell^{in}(E'\to E)P_\ell(\mu)$$

$$\sigma_\ell^{in}(E'\to E) = \frac{\sigma_b}{2kT}\sqrt{\frac{E}{E'}}\, e^{-\beta/2}\int_{-1}^{1} d\mu P_\ell(\mu) S(\alpha,\beta)$$

FLANGE II computes these integrals and the kernels

$$\sigma_{\ell ij}^{in} = \sigma_\ell^{in}(E_i\to E_j)$$

for $0 \leqslant \ell \leqslant 5$, and the E_i and E_j refer to the input energy mesh.

The inelastic cross sections can be computed from

$$\sigma_{\ell i}^{in} = \sigma_\ell^{in}(E_i) = \int_0^\infty dE\sigma_\ell^{in}(E_i\to E)$$

The E_i refers to the input energy mesh, but the integration over final energies E is independent of the input energy mesh.

It is often desirable to renormalize the kernels by adjusting the diagonal terms so that when integrated, they will give some desired cross section. Let $\sigma_{\ell i}^*$ be the cross section obtained from the kernel before adjustment:

$$\sigma_{\ell i}^* = \sum_j \sigma_{\ell ij}^{in} W_j$$

Let $\sigma^{x}_{\ell i}$ be the cross section used for normalization, and $\sigma^{x}_{\ell ij}$ be the kernel after normalization:

$$\sigma^{x}_{\ell ij} = \sigma^{in}_{\ell ij} + \delta_{ij}(\sigma^{x}_{\ell i} - \sigma^{*}_{\ell i})/W_i$$

The following renormalizations are allowed:

$\sigma^{x}_{\ell i} = \sigma^{*}_{\ell i}$ No renormalization

$= \sigma^{in}_{\ell i}$ Normalized to the computed or input inelastic cross section

$= \sigma^{s}_{\ell i}$ Normalized to the input elastic plus the computed or input inelastic cross section

3. NUMERICAL PROCEDURES

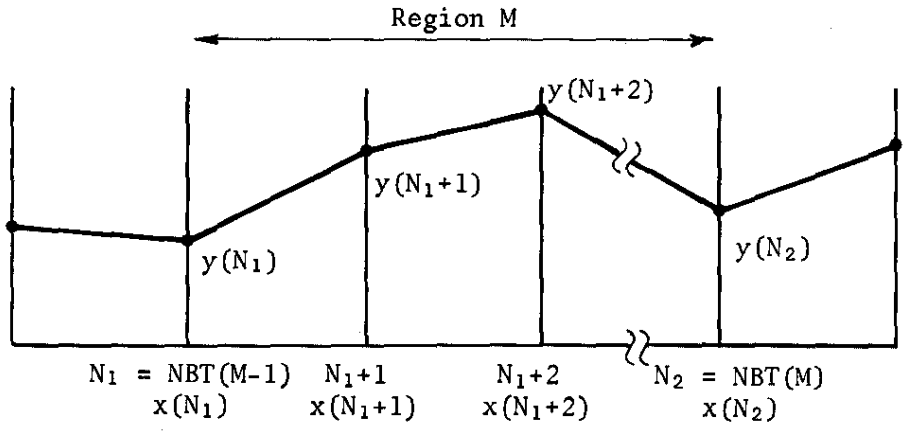
The numerical procedures used in FLANGE II are described briefly in this section. A more detailed description is given in Sections 6 and 7.

3.1 TABULATED FUNCTIONS

Nearly all data stored on an ENDF/B tape are in the form of a tabulated function, $y(x)$, which might represent $\sigma(E)$, $\sigma_\ell(E)$, or $S(\alpha,\beta)$ at a particular β. The quantities used to represent the function are:

- X(N) - List of values of x (or E)
- Y(N) - List of values of y (or σ) evaluated at X(N)
- NP - Number of values of x (and y) given
- NBT(M) - Breakpoint table giving the upper N value associated with the M^{th} region of x
- JNT(M) - Interpolation code used in the M^{th} region of x
- NR - Number of interpolation regions of x

The following sketch illustrates the use of these tabulated functions.



Let the N^{th} panel be the space between X(N) and X(N+1). Then, in the sketch above, panels N_1, N_1+1, ..., N_2-1 belong to region M. A region is defined as a consecutive set of panels in which the same interpolation method is used in each panel. The interpolation code JNT(M) indicates how intermediate values are to be obtained. For simplicity, let (x_1,y_1) and (x_2,y_2) denote the end points of a panel.

JNT	Interpolation Formula
1	$y = y_1$
2	$y = y_1 + (y_2-y_1)(x-x_1)/(x_2-x_1)$
3	$y = y_1 + (y_2-y_1)\ln(x/x_1)/\ln(x_2/x_1)$
4	$\ln(y) = \ln(y_1) + \ln(y_2/y_1)(x-x_1)/(x_2-x_1)$
5	$\ln(y) = \ln(y_1) + \ln(y_2/y_1)\ln(x/x_1)/\ln(x_2/x_1)$

3.2 INTERPOLATION PROCEDURES

In certain cases, the interpolation code given may be correct for the original data, but subsequent manipulation of the data makes the interpolation code ambiguous. For example, in the calculation of Legendre cross sections, the original data for $\sigma(E)$ may specify ln-ln interpolation, and the original data for $f_\ell(E)$ may specify linear interpolation. Since $\sigma_\ell(E) = \sigma(E)f_\ell(E)$, a decision must be made as to what E mesh and interpolation are to be used. Since $\sigma(E)$ probably varies more rapidly than $f_\ell(E)$, the E mesh and interpolation are used for $\sigma(E)$, and $f_\ell(E)$ is evaluated on this mesh. The $f_\ell(E)$ may be negative or zero, and logarithmic interpolation is meaningless. The code automatically senses such conditions and will change the interpolation code in an appropriate manner. Thus, if JNT = 4 or 5, and y_1 or y_2 is negative or zero, Codes 3 or 4 will automatically be used. If JNT = 3 or 5, and x_1 or x_2 is negative or zero, Codes 2 or 4 will be used. All interpolations and the logic described above are in subroutine TERP1, which interpolates a single point.

As indicated in the illustration above, it is often necessary to compute an entire table by interpolation in another table. Subroutine TERP2 is used for this purpose. The procedure would be trivial were it not for the possibility of discontinuities in y(x) (indicated by two successive values of y with the same value of x). Such discontinuities appear in thermal elastic scattering cross sections for crystalline materials, and at the end points of energy regions described by resonance parameters. TERP2 will look for such discontinuities and treat them properly.

Tabular $S(\alpha,\beta)$ data cannot be interpolated accurately as a function of temperature using the two-point interpolation formulas described in Section 3.1. A four-point Lagrangian interpolation formula is used in these cases and is discussed in detail in Section 7.2.1.

3.3 ENERGY AVERAGING OF CROSS SECTIONS

As indicated in Section 2, the cross sections $\sigma_\ell(E)$ may be either evaluated at points of the input energy mesh or averaged over an input energy group. For this latter case, integration formulas are needed. Since the data to be averaged will always be tabulated, the required formulas are integrals over a portion of a panel. The integral of a group is then found from the sum of integrals over appropriate panels or parts of panels.

Let (x_3,y_3) and (x_4,y_4) be the end points of a panel, and x_1 and x_2 be the integration limits. The integrals are then given by

$$B = \int_{x_1}^{x_2} y(x)dx$$

Interpolation Code 1

$$B = (x_2-x_1)y_3$$

Interpolation Code 2

$$B = (x_2-x_1)\left[a + \frac{1}{2}\, b(x_2+x_1)\right]$$

$$b = (y_4-y_3)/(x_4-x_3)$$

$$a = y_3-bx_3$$

Interpolation Code 3

$$B = (x_2-x_1)\left[y_3 + b\, \ln \frac{x_1}{x_3}\right] + bx_1\left[1 + \frac{x_2}{x_1}\,(\ln \frac{x_2}{x_1} - 1)\right]$$

$$b = (y_4-y_3)/\ln\frac{x_4}{x_3}$$

$$\left[1 + \frac{x_2}{x_1}\left(\ln\frac{x_2}{x_1} - 1\right)\right] = \frac{1}{2}z^2\left[1 - \frac{1}{3}z + \frac{1}{6}z^2 - \frac{1}{10}z^3\right], \quad |z| \leq 0.15$$

$$z = (x_2 - x_1)/x_1$$

Interpolation Code 4

$$B = e^{a+bx_1}(e^z-1)/b, \quad |z| > 0.1$$

$$B = e^{a+bx_1}(x_2-x_1)\left(1 + \frac{1}{2}z + \frac{1}{6}z^2\right) \quad |z| \leq 0.1$$

$$b = \ln\frac{y_4}{y_3}/(x_4-x_3)$$

$$a = \ln(y_3) - bx_3$$

$$z = (x_2-x_1)b$$

Interpolation Code 5

$$B = y_3x_1\left(\frac{x_1}{x_3}\right)^b \frac{1}{b+1}\left[\left(\frac{x_2}{x_1}\right)^{b+1} - 1\right]$$

$$b = \ln\frac{y_4}{y_3}/\ln\frac{x_4}{x_3}$$

$$\frac{1}{b+1}\left[\left(\frac{x_2}{x_1}\right)^{b+1} - 1\right] = \ln\frac{x_2}{x_1}\left(1 + \frac{1}{2}z + \frac{1}{6}z^2\right), \quad |z| \leq 0.1$$

$$z = (b+1)\ln(x_2/x_1)$$

3.4 α MESH FOR $S(\alpha,\beta)$

The scattering law data on the ENDF/B tape are arranged in the following way. For the first value of $\beta_1 (= 0)$, there is a table of $S(\alpha,\beta_1)$ versus α. Next, there is a table of $S(\alpha,\beta_2)$ versus α, and so forth. In general, the α mesh used to describe S is different for each value of β. The procedure used is

to define a "fine" α mesh and to evaluate S by interpolation on this fine α mesh. All calculations are then done with the S calculated on the fine α mesh, and it is assumed that ln(S) is linear in α between tabulated values.

The fine α mesh, α_i, is defined by

$$\alpha_i = \alpha_0 \rho_0^{i-1}, \qquad 1 \leq i \leq IALX$$

where $\rho_0 = 1.03$ and IALX = 300 are preset constants. If E_{max} is the largest energy in the input energy mesh, and A is the mass used to calculate α, then $\alpha_{max} = 4E_{max}/AkT$ is the largest α that will be needed. α_0 is computed so that the largest α in the fine mesh will be less than α_{max}.

$$\alpha_0 = \alpha_{max}/\rho_0^{IALX-2}$$

If $E_{max} = 1.0$ ev, kT = 0.025 ev, A = 1, and $\alpha_{max} = 160$, then $\alpha_0 = 0.024$.

Definition of the fine α mesh in this manner has two advantages. First, the S for all β are evaluated on the same α mesh so that interpolation in β is greatly simplified. Second, the use of a constant expansion ratio ρ_0 permits large savings in computation time through the use of fast table look-up procedures for the α integrations.

Generally the tabulated α mesh for large β values will not span the entire range of the fine mesh α's. This can lead to ignoring some scattering contributions for large energy transfers. The required $S(\alpha,\beta)$ values for these large β's may be added using the short collision form of the $S(\alpha,\beta)$.

3.5 α INTEGRATION OF $S(\alpha,\beta)$

In the calculation of Legendre moments, integrations over μ can be transformed into integrations over α.

$$\sigma_\ell(E' \to E) = \frac{A\sigma_b}{4E'} e^{-\beta/2} \int_{\alpha_L}^{\alpha_H} d\alpha S(\alpha,\beta) \sum_{n=0}^{\ell} W_{\ell n} \alpha^n$$

The $W_{\ell n}$ are expansion coefficients of $P_\ell(\mu)$ in powers of α and depend on E and E'. The main calculation is that of the α moments

of $S(\alpha,\beta)$; since the limits α_L and α_H include many tabulated points, the moments can be expressed as the sum of contributions from each "panel," or the region between two tabulated points.

Consider one panel bounded by the points (α_3,y_3) and (α_4,y_4), where $y = \ln(S)$. Let α_1 and α_2 denote the end points of the integration for this panel. Since it is assumed that $\ln(S)(= y)$ is linear in α between tabulated points,

$$y = a+b\alpha$$

$$b = (y_4-y_3)/(\alpha_4-\alpha_3)$$

$$a = y_3-b\alpha_3$$

and the required integral is

$$h_n = \int_{\alpha_1}^{\alpha_2} d\alpha\ \alpha^n e^{a+b\alpha}$$

By suitable transformation,

$$h_n = S_1\alpha_1^{n+1}G_n(c,\rho)$$

where $$G_n(c,\rho) = \left(\frac{\rho+1}{2}\right)^{n+1}\left[\gamma F_0(c) + n\gamma^2 F_1(c) + \frac{1}{2}n(n-1)\gamma^3 F_2(c)\right]$$

$$F_k(c) = \frac{e^c}{c^{k+1}}\int_{-c}^{c} dy\ y^k e^y$$

$$\rho = \alpha_2/\alpha_1$$

$$c = b\gamma(\alpha_1+\alpha_2)/2$$

$$\gamma = (\rho-1)/(\rho+1)$$

This formula can be used for starting panels ($\alpha_1 = \alpha_L$, $\alpha_2 = \alpha_4$), intermediate panels ($\alpha_1 = \alpha_3$, $\alpha_2 = \alpha_4$), and end panels ($\alpha_1 = \alpha_3$, $\alpha_2 = \alpha_H$). For intermediate panels, $\rho = \rho_0$ which is a constant for all panels, and $c = 1/2(y_4-y_3)$. The function $G_n(c,\rho_0)$ depends only on c, and can be tabulated for fast evaluation.

Several numerical approximations are used to speed up the evaluation of the α integrals. They have been selected to be accurate to a relative precision of 3.3×10^{-5}.

3.6 FINAL ENERGY INTEGRATION OF THE KERNEL

Legendre inelastic cross sections are obtained from

$$\sigma_\ell^{in}(E') = \int_0^\infty dE \sigma_\ell^{in}(E' \to E)$$

The E' refer to the input energy mesh, but the final energy integration is completely independent of the input energy mesh and depends only on the β mesh given for the scattering law. Two successive β points (β_L and β_H) are selected; the region between β_L and βH is a panel. The integral given above is then the sum of integrals over each panel. A downscattering part (E<E') and upscattering part (E>E') must be considered for each panel, and three different types of panels are considered.

The panel $\beta_L = 0$ contributes heavily to the cross section and may contain a singularity. A variable y is proportional to the neutron velocity and is scaled to be zero at $\beta = \beta_L$ and unity at $\beta = \beta_H$. The kernel is evaluated at the points $y_1 = 1/8$, $y_2 = 1/4$, $y_3 = 1/2$, and $y_4 = 1$. The resulting values of the kernel are denoted by H_1, H_2, H_3, and H_4. These four values are fit to the function

$$H(y) = \frac{a}{\ln \frac{1}{2}} \ln(y) + b + cy + dy^2$$

and H(y) is then integrated over the panel.

$$I = \int_{E'}^{E'+kT\beta_H} dE H(E) = 2kT\Delta \int_0^1 dy (x_0 + y\Delta) H(y)$$

$$= 2kT\Delta x_0 (0.58791H_1 - 0.58440H_2 + 0.84776H_3 + 0.14873H_4)$$

$$+ 2kT\Delta^2 (0.07291H_1 - 0.12758H_2 + 0.39712H_3 + 0.15755H_4)$$

$$x_0 = \sqrt{E'/kT}$$

$$\Delta = x_4 - x_0$$

$$x_4 = \sqrt{\beta_H + E'/kT}$$

The above equation is used for upscattering. For downscattering, Δ is redefined to be positive, and the sign of the second term of the integral is set negative.

For intermediate values of β, three points equally spaced in velocity in the panel are used. Again y is proportional to the velocity and scaled so that $y_1 = 0$ at $\beta = \beta_L$, $y_3 = 1$ at $\beta = \beta_H$, and $y_2 = 1/2(y_1+y_3)$. The corresponding values of the kernel are H_1, H_2, and H_3. These three values are fit to the function

$$H(y) = a + by + cy^2$$

and H(y) is then integrated over the panel.

$$I = \frac{1}{3} kT\Delta x_1 (H_1 + 4H_2 + H_3) + \frac{1}{3} kT\Delta^2 (2H_2 + H_3)$$

$$x_1 = \sqrt{\beta_L + E'/kT}$$

$$\Delta = x_3 - x_1$$

$$x_3 = \sqrt{\beta_H + E'/kT}$$

The above equation is used for upscattering. For downscattering, Δ is redefined to be positive, and the sign of the second term of the integral is set negative.

For large values of β, only the end points of the panel, H_1 and H_2 are used, and it is assumed that the function is exponential in character. Thus,

$$I = \int_{E_1}^{E_2} dEH(E) = (E_2 - E_1)(H_2 - H_1)/\ln \frac{H_2}{H_1}$$

$$E_1 = E' + kT\beta_L \qquad E_2 = E' + kT\beta_H$$

Many special cases to the above formulas are considered in detail in a later section. For example, downscattering will have to be terminated when E = 0, which may occur in the middle of a panel. Also, Legendre moments may change sign so that terms involving logarithms must be changed.

4. DESCRIPTION OF CODE

4.1 GENERAL STRUCTURE AND OPERATION

FLANGE II is written in ASA Standard FORTRAN (FORTRAN IV) and is designed to be used on a computer with at least 40K of available fast storage plus three tapes. It has been written as a main program plus large subprograms which can easily be made links of a chain or overlay program. The subprograms will be referred to as links here. The various parts of the FLANGE II code are:

Main Program - Processes the input data, sets up the input energy mesh, and controls the calling of the links listed below.

Link 1 - Processes Files 1, 2, 3, and 4 from the ENDF/B input tape. Cross sections and angular distributions are evaluated (or averaged) on the input energy mesh, Legendre components are computed, and the results (if complete) are printed and punched. The results are also stored on tape NSTA for use in Link 2.

Link 2 - Processes File 7 from the ENDF/B input tape. The scattering law is integrated to form Legendre components of the scattering kernel, the inelastic cross sections are computed, the cross sections from tape NSTA are read (and completed if necessary), and the scattering kernels are printed and punched.

4.2 TAPE ASSIGNMENTS

The following tapes are used. The tape numbers are symbolic and are stored in CØMMØN/BLØCK1/. The values are assigned at the start of the main program.

NIN - Systems input tape

NØUT - Systems print output tape

NPUN - Systems punch output tape

LIB - ENDF/B library tape, modes 1, 2, or 3

NSTA - Scratch tape used to transmit cross sections from Link 1 to Link 2. Disk storage should be used in place of this tape if available.

NSTB - Scratch tape used in Link 2 to store the scattering kernels in the order calculated. Disk storage should be used in place of this tape if available.

4.3 ERROR STOPS

Errors are signaled on the output by a message "FLANGE II ERRØR STØP NUMBER xxx," where xxx is a three-digit integer describing the error. The list of these numbers, the subroutine in which the error occurred, and a description of the error are given below.

Number	Subroutine	Description
21	EMESH	NEG larger than 200
22	EMESH	NEVT not 1 or 2
23	EMESH	METH not 1, 2, or 3
24	EMESH	KX not in range 1-20
25	EMESH	Zero groups/region specified
26	EMESH	NEG not equal to the sum of groups specified for each region
27	EMESH	Energy range breakpoint table out of order
99	RREC	Library tape data set not defined
100	RREC	Record type called for not valid
101	RREC	Library tape mode not 1, 2, or 3
102	RREC	T not in range of specified data
103	RREC	Interpolation table too long or of zero length
104	RREC	List length too long or of zero length
105	RREC	Data length too long or less than 2 points
106	RREC	Improper temperature dependence
107	RREC	MAT, MF, MT incorrect for List, TAB1, TAB2, or Hollerith records
110	ECSI	Wrong interpolation code given
120	ACS	Zero group width specified
122	ACS	Interpolation table incorrect
130	TERP2	x table not in increasing order

Number	Subroutine	Description
131	TERP2	x table not in increasing order
132	TERP2	Interpolation table incorrect
133	TERP1	Interpolation table incorrect
134	TERP1	Zero or negative value cannot be interpolated by logs
135	SRCH	Section not on library, or library out of order
136	PRØF4	Angular data given in CM (center of mass) system
138	PRØF4	Internal tape error on NSTA
139	PRØF4	E interpolation table incorrect on File 4
200	SRCH7	No File 7 on library
223	REATS	Temperature out of range given on library
224	REATS	Improper T dependence, lists different lengths
225	REATS	More than 1000 $S(\alpha,\beta)$ given for one β
226	REATS	More than 100 entries in α interpolation table
230	PRØF7	Improper β interpolation table
231	PRØF7	Scattering law not given
232	KERC	Improper β interpolation table
233	KERC	$S(\alpha,\beta)$ not integrable at small α
234	KERA	Analytic $S(\alpha,\beta)$ not specified
235	KERA	$S(\alpha,\beta)$ not integrable at low α

5. INPUT/OUTPUT DESCRIPTION

The following section describes the input and output data for FLANGE II. The input data consist of the ENDF/B library tape (Mode 1, 2, or 3) and two decks of cards (the problem definition input and the input energy mesh).

5.1 PROBLEM DEFINITION INPUT

All input data are read by the main program. The problem definition input is read by subroutine INPUT. The input data are listed below, and are stored in CØMMØN/BLØCK3/.

Card	Columns	Format	Symbol	Description
1	1-72	18A4	(TITLE(N) N=1,18)	72-character Hollerith description of the calculation
2	1-10	I10	LABEL	Label that is supposed to appear at the ENDF/B tape. If LABEL = 0, label will not be checked.
	11-20	I10	MAT	Material number to be processed from the ENDF/B tape
	21-30	E10.0	FID	Seven-digit integer (written in floating point) used to identify the punched output for this material
	31-40	E10.0	T	Desired temperature (°K)
	41-50	E10.0	TEFF	Effective temperature for short collision time approximation (°K)
	51-60	I10	MØDE	Tape mode (1, 2, or 3 — defaults to 3)
3	1-10	I10	LINK1	Flag indicating whether Link 1 is to be used or not; 0 = no, 1 = yes
	11-20	I10	LINK2	Same as above, but for Link 2
4	1-10	I10	LX	Maximum Legendre order (0-5) desired
	11-20	I10	LMESH	= 0, read new energy mesh = 1, use energy mesh of previous problem

Card	Columns	Format	Symbol	Description
4	21-30	I10	LRSCT	= 0, if material is not to be treated as a resonance scatterer, = 1 otherwise
	31-50	20X	-	
	51-60	I10	LPDD	= 1, print and punch decay data = 0, ignore = -1, print decay data
	61-70	I10	LPFP	= 1, print and punch fission product yields = 0, ignore = -1, print fission product yields
5	1-10	I10	LABS	= 0, ignore $\sigma^a(E)$ = 1, read $\sigma^\gamma(E)$ from ENDF/B tape and compute $\sigma^a(E) = \sigma^\gamma(E) + \sigma^f(E)$ = 2, compute $\sigma^a(E) = \sigma^t(E) - \sigma^s(E)$
	11-20	I10	LPABS	= -2, print group avg $\sigma^a(E)$ = -1, print $\sigma^a(E)$ = 0, ignore = 1, print and punch $\sigma^a(E)$ = 2, print and punch group avg $\sigma^a(E)$
	21-30	I10	LFISS	= 0, ignore $\sigma^f(E)$ = 1, read $\sigma^f(E)$ from ENDF/B tape
	31-40	I10	LPFIS	= -2, print group avg $\sigma^f(E)$ = -1, print $\sigma^f(E)$ = 0, ignore = 1, print and punch $\sigma^f(E)$ = 2, print and punch group $\sigma^f(E)$
	41-50	I10	LPTØT	= 0, ignore $\sigma^t(E)$ = 1, read $\sigma^t(E)$ from ENDF/B tape = 2, compute $\sigma^t(E) = \sigma^a(E) + \sigma^s(E)$
	51-60	I10	LPTØT	= -2, print group avg $\sigma^t(E)$ = -1, print $\sigma^t(E)$

Card	Columns	Format	Symbol	Description
5	51-60	I10	LPTØT	= 0, ignore
				= 1, print and punch $\sigma^t(E)$
				= 2, print and punch group avg $\sigma^t(E)$
	61-70	I10	LPTR	= -2, compute and print $\sigma^{tr}(E) = \sigma^a(E) + \sigma_0^s(E) - \sigma_1^s(E)$
				= -1, compute and print $\sigma^{tr}(E) = \sigma_0^s(E) - \sigma_1^s(E)$
				= 0, ignore
				= 1, compute, print and punch $\sigma^{tr}(E) = \sigma_0^s(E) - \sigma_1^s(E)$
				= 2, compute, print, and punch $\sigma^{tr}(E) = \sigma^a(E) + \sigma_0^s(E) - \sigma_1^s(E)$
6	1-10	I10	LELAS	= 0, ignore $\sigma^{el}(E)$
				= 1, read $\sigma_\ell^{el}(E)$ and $p_\ell^{el}(E,\mu)$ from ENDF/B tape
				= 2, compute $\sigma_\ell^{el}(E) = \sigma_\ell^s(E) - \sigma_\ell^{in}(E)$
	11-20	I10	LPEL	= -2, print group avg $\sigma_\ell^{el}(E)$
				= -1, print $\sigma_\ell^{el}(E)$
				= 0, ignore
				= 1, print and punch $\sigma_\ell^{el}(E)$
				= 2, print and punch group avg $\sigma_\ell^{el}(E)$
	21-30	I10	LINEL	= 0, ignore $\sigma_\ell^{in}(E)$
				= 1, read $\sigma_\ell^{in}(E)$ and $p_\ell^{in}(E,\mu)$ from ENDF/B
				= 2, compute $\sigma_\ell^{in}(E) = \sigma_\ell^s(E) - \sigma_\ell^{el}(E)$
				= 3, compute $\sigma_\ell^{in}(E)$ from $S(\alpha,\beta)$
	31-40	I10	LPIN	= -2, print group avg $\sigma_\ell^{in}(E)$
				= -1, print $\sigma_\ell^{in}(E)$
				= 0, ignore

Card	Columns	Format		Description
6	31-40	I10	LPIN	= 1, print and punch $\sigma_\ell^{in}(E)$ = 2, print and punch group avg $\sigma_\ell^{in}(E)$
	41-50	I10	LSCAT	= 0, ignore $\sigma_\ell^{s}(E)$ = 1, read $\sigma_\ell^{s}(E)$ and $p_\ell^{s}(E,\mu)$ from ENDF/B = 2, compute $\sigma_\ell^{s}(E) = \sigma_\ell^{in}(E) + \sigma_\ell^{el}(E)$
	51-60	I10	LPSC	= -2, print group avg $\sigma_\ell^{s}(E)$ = -1, print $\sigma_\ell^{s}(E)$ = 0, ignore = 1, print and punch $\sigma_\ell^{s}(E)$ = 2, print and punch group avg $\sigma_\ell^{s}(E)$
7	1-10	I10	LTSL	= 0, ignore scattering kernels = 1, ignore scattering kernels = 3, compute scattering kernels = 4, compute scattering kernels and normalize to exact σ_ℓ^{in} = 5, compute scattering kernels and normalize to $\sigma_\ell^{s}(E)$
	11-20	I10	LPTSL	= -2, print scattering kernels = -1, ignore print and punch = 0, ignore print and punch = 1, punch scattering kernels = 2, print and punch kernels
	21-30	I10	LBND	Signal to compute only bound component of molecule. Also divides σ_b by its value, i.e., $\sigma_b = \sigma_b/LBND$.

5.2 INPUT ENERGY MESH

Text Symbol	Code Symbol	Description
i	I	Index numbering energy groups
NEG	NEG	Number of energy groups
E_i	E(I)	Characteristic energy of the i^{th} group(ev)
E_i^*	EB(I)	Lower energy limit of the i^{th} group

Text Symbol	Code Symbol	Description
v_i	V(I)	Reduced characteristic velocity of the i^{th} group $v_i = \sqrt{E_i}/0.0253$
v_i^*	VB(I)	Lower reduced velocity limit of the i^{th} group $v_i^* = \sqrt{E_i^*}/0.0253$
W_i	W(I)	Energy integration weight for the i^{th} group
Δ_i	DEL(I)	Group width used for both energy and velocity calculations
k	K	Index numbering regions to be subdivided into groups
K	KX	Number of regions
M_k	MK	Number of groups to be distributed in the k^{th} region
B_k	BPT(K)	Upper boundary of the k^{th} region

The mesh can be specified in any one of six ways:

1. The mesh is computed from an input table of energy regions and number of groups to be assigned per region.
2. Energy group widths are read in and the characteristic energies are computed as being at the center of each group.
3. Energy group widths and characteristic energies are read in and artificial group boundaries are computed.
4. Same as 1 but using velocity.
5. Same as 2 but using velocity.
6. Same as 3 but using velocity.

Current practice at GGA is to use 2 (but 3 was used in the past), and at BNL and SRL to use 5. Two tests are used:

NEVT = 1, energy input
= 2, reduced velocity input

METH = 1, regions and groups per region input
= 2, group widths input
= 3, group widths and characteristic energy (velocity) input

In all cases a complete energy and velocity mesh will be computed and stored. The six cases will be described separately.

NEVT = 1, METH = 1

The energy range of interest is divided in K regions numbered 1, 2, ..., k, ..., K. Let B_k be the upper bound of the k^{th} region, and M_k the number of groups to be distributed in the k^{th}region. If $M_k > 0$, a constant mesh spacing is used within the region. If $M_k < 0$, the group boundary expands by a factor for each successive group in the region.

To illustrate the procedure, let k be the region under consideration, and let i denote the last group boundary computed. Thus, E_i^* is the upper limit of the $k\text{-}1^{st}$ range and the lower limit of the k^{th} range. For $M_k > 0$, compute

$$\Delta_k = (B_k - B_{k-1})/M_k$$

$$E_i^* = B_{k-1}$$

$$E_{i+1}^* = E_i^* + \Delta_k$$

$$E_{i+2}^* = E_i^* + 2\Delta_k$$

$$\vdots$$

$$E_{i+M_k}^* = E_i^* + M_k\Delta_k = B_k$$

For $M_k < 0$, set $M_k = -M_k$, and compute

$$\Delta_k = (B_k/B_{k-1})^{1/M_k}$$

$$E_i^* = B_{k-1}$$

$$E_{i+1}^* = \Delta_k E_i^*$$

$$E_{i+2}^* = \Delta_k^2 E_i^*$$

$$\vdots$$

$$E_{i+M_k}^* = \Delta_k^{M_k} E_i^* = B_k$$

The $|M_k|$ must add up to NEG, the total number of energy groups.

The group boundaries are established, and the characteristic energy, integration weight, and reduced velocities are computed from:

$$E_i = \frac{1}{2}(E_i^* + E_{i+1}^*)$$

$$W_i = E_{i+1}^* - E_i^*$$

$$v_i^* = \sqrt{E_i^*}/0.253$$

$$v_i = \sqrt{E_i}/0.0253$$

NEVT = 1, METH = 2

A low energy cutoff (EVL) and the group widths W_i (taken to be the same as the integration weights) are read in. The group boundaries are computed from

$$E_1^* = EVL$$

$$E_i^* = E_{i-1}^* + W_{i-1}$$

The remaining quantities are computed from

$$E_i = \frac{1}{2}(E_i^* + E_{i+1}^*)$$

$$v_i^* = \sqrt{E_i^*}/0.0253$$

$$v_i = \sqrt{E_i}/0.0253$$

NEVT = 1, METH = 3

The characteristic energies E_i and integration weights are read in. Presumably, the weights were selected for some high accuracy integration scheme and may not resemble group widths. Group boundaries are required to average simple cross sections. Group boundaries (arbitrarily) are selected as the midpoint between characteristic energies. Thus

$$E_i^* = \frac{1}{2}(E_{i-1} + E_i)$$

$$E_1^* = EVL$$

$$E_{NEG+1}^* = \frac{3}{2}E_{NEG} - \frac{1}{2}E_{NEG-1}$$

$$v_i = \sqrt{E_i}/0.0253$$

$$v_i^* = \sqrt{E_i^*}/0.0253$$

NEVT = 2, METH = 1

The method is the same as for NEVT = 1, METH = 2 except that all quantities (including EVL, B_k) refer to reduced velocity. Thus for $M_k > 0$

$$\Delta_k = (B_k - B_{k-1})/M_k$$

$$v_i^* = B_{k-1}$$

$$v_{i+1}^* = v_i^* + \Delta_k$$

$$v_{i+2}^* = v_i^* + 2\Delta_k$$

$$\vdots$$

$$v_{i+M_k}^* = v_i^* + M_k\Delta_k = B_k$$

For $M_k < 0$, set $M_k = -M_k$,

$$\Delta_k = (B_k/B_{k-1})^{1/M_k}$$

$$v_i^* = B_{k-1}$$

$$v_{i+1}^* = \Delta_k v_i^*$$

$$v_{i+2}^* = \Delta_k^2 v_i^*$$

$$\vdots$$

$$v_{i+M_k}^* = \Delta_k^{M_k} v_i^* = B_k$$

$$v_i = \frac{1}{2}(v_i^* + v_{i+1}^*)$$

$$E_i = 0.0253 v_i^2$$

$$E_i^* = 0.0253v_i^{*2}$$

$$W_i = E_{i+1}^* - E_i^*$$

NEVT = 2, METH = 2

The method is the same as for NEVT = 2, METH = 1 except that all quantities (EVL, W_i) refer to reduced velocity. Thus

$$v_1^* = EVL$$

$$v_1^* = v_{i-1}^* + W_{i-1}$$

$$v_i = \frac{1}{2}(v_i^* + v_{i+1}^*)$$

$$E_i = 0.0253v_i^2$$

$$E_i^* = 0.0253v_i^{*2}$$

$$W_i = E_{i+1}^* - E_i^*$$

W_i read in refers to velocity but is recomputed to refer to energy.

NEVT = 2, METH = 3

The method is the same as for NEVT = 1, METH = 3 except that all quantities (including EVL and W_i) refer to velocity.

$$v_i^* = EVL$$

$$v_i^* = \frac{1}{2}(v_{i-1} + v_i)$$

$$v_{NEG+1}^* = \frac{3}{2}v_{NEG} - \frac{1}{2}v_{NEG-1}$$

$$E_i = 0.0253v_i^2$$

$$E_i^* = 0.0253v_i^{*2}$$

$$W_i = 0.0506v_iW_i \text{ (input)}$$

W_i on input refers to velocity but is recomputed to refer to energy.

The following cards are used to describe the input energy mesh. These cards follow the problem definition cards.

Card	Columns	Format	Symbol	Description
8	1-10	I10	NEG	Number of energy groups (≤200)
	11-20	I10	NEVT	= 1, mesh input in energy units = 2, mesh input in reduced velocity units
	21-30	I10	METH	= 1, region data are input = 2, group widths are input = 3, group widths and characteristics are input
	31-40	I10	NPNT	= 0, ignore = 1, print energy mesh = 2, print and punch energy mesh
	41-50	E10.5	EVL	Low energy (if NEVT = 1) or velocity (in NEVT = 2) cutoff
	51-70	5A4	(HØL(N) N=1,5)	20-character description of the energy mesh. See description of the punching.

The remaining cards depend on the values of METH and NEVT.

NEVT = 1, METH = 1

Card	Columns	Format	Symbol	Description
9	1-10	I10	KX	Energy of energy regions (≤20)
	11-20	I10	MINT(1)	Number of groups in Region 1. If MINT(1) > 0, equal energy spacing. If MINT(1) < 0, equal lethargy spacing.
	21-30	E10.5	BPT(1)	Upper energy limit of Region 1
	31-40	I10	MINT(2)	Same as above, but for Region 2
	41-50	E10.5	BPT(2)	Same as above, but for Region 2
	⋮	⋮	⋮	⋮

The pattern above is repeated until all KX regions have been specified. The second and remaining cards start in Column 11.

NEVT = 1, METH = 2

Card	Columns	Format	Symbol	Description
9	-	7E10.5	(W(I),I=1 NEG)	List of energy group widths (ev) in order of increasing group number
	-	7E10.5	(E(I),I=1 NEG)	List of characteristic group energies (ev) in increasing order
	-	7E10.5	(W(I),I=1 NEG)	Integration weights (ev)

Cards for NEVT = 2 follow the same description as for NEVT = 1, except the word "energy" is changed to read "reduced velocity."

5.3 OUTPUT

The printed output (on tape NØUT) is clearly labeled and will not be described here.

There are three types of punched output: energy mesh, scattering kernels, and cross sections.

The energy mesh is punched if the input number is NPNT = 2. Two decks of cards are obtained. If NEVT = 1 (energy mesh), the first deck is the energy points E_i, and the second deck the integration weights, W_i. If NEVT = 2 (velocity mesh), the first deck is the velocity points v_i, and the second deck is the velocity integration weights defined by $W_i/0.0506v_i$. The punching of one deck is done in subroutine PUNCH3. Each card of the deck has the same structure.

Columns	Format	Description
1-70	7F10.7	Seven values of the data
73-76	A4	First four characters of the Hollerith description of the mesh. See input description.
77-78	I2	Integer describing the data = 1, energy points = 2, energy integration weights = 3, velocity points = 4, velocity integration weights
79-80	I2	Sequence number

The punched card format for scattering kernels was devised by John Suich at SRL and is used at GGA, SRL, and BNL. A card is divided into 11 fields.

Field	Columns	Format	Description
1	1	I1	Legendre order (0-9)
2	2-4	I3	Final energy group index (J) of the first data word on this card
3	5-7	I3	Initial energy group index of the data on this card
4	8	-	Blank
5	9-20	E12.4	$\sigma_\ell(I \rightarrow J)$
6	21-32	E12.4	$\sigma_\ell(I \rightarrow J+1)$
7	33-44	E12.4	$\sigma_\ell(I \rightarrow J+2)$
8	45-56	E12.4	$\sigma_\ell(I \rightarrow J+3)$
9	57-68	E12.4	$\sigma_\ell(I \rightarrow J+4)$
10	69-76	F8.0	Isotopic or material designation, FID
11	77-80	I4	Deck sequence number

The zero values will not be read from the above cards, but the array will be cleared prior to loading the kernel deck. It is only necessary to punch the non-zero values of the kernel on these cards. Each card is uniquely identified as to its location in the array.

Each deck is headed by a card in the format given above. The fields on this card are:

Field	Description
1	Same as before
2	Smallest group index = 1
3	Largest group index = NEG
4	Same
5	Temperature (°K)
6-9	Not used
10	Same as before
11	Same as before

With a slight modification, the above card format is also used to punch cross sections and Legendre moments. The character "c" punched in Field 4 signals this type of data. Field 2 is used to denote the type of cross section data given, and the number is the same as the MT (reaction type) number given on the ENDF/B tape.

6. DETAILED DESCRIPTION OF LINK 1

6.1 OVERALL OPERATION

Link 1 is divided into five major sections (subroutines PRØF1, PRØF2, PRØF3, PRØF4, and PLEAT). The operation of these sections are described generally here and in detail in later sections. The five major sections perform the following operation:

PRØF1 Prints documentation information, decay data, and fission product yield data. Evaluates ν (neutrons/fission) at E = 0.0 ev.

PRØF2 Calculates infinitely dilute (Doppler broadened) capture fission, and scattering cross sections from resolved resonance parameters. Group averages are produced as required.

PRØF3 Group averages or interpolates all smooth cross sections specified by test numbers to be taken from the ENDF/B tape.

PRØF4 Combines smooth cross sections and Legendre moments taken from the ENDF/B tape and produces group-averaged or interpolated Legendre cross sections for elastic, inelastic, and total scattering.

PLEAT Completes the cross sections based on the set of test numbers described in Section 2.4. This operation is performed only if Link 2 is not to be executed.

Cross sections to be printed or punched are done so in this routine.

6.1.1 Internal Energy Mesh

To properly generate the contributions to elastic, inelastic, and total scattering from File 3 cross sections with possible contributions from File 2 resonance parameters, an internal energy mesh is defined. This mesh contains energy points at which Files 3 and 2 cross sections are evaluated. Interpolation between points is assumed ln-ln, but may be easily changed if required. The number of points is chosen to enable the sharp Bragg peaks in some crystalline moderator material to be adequately represented.

The mesh contains IENX points (= 1000) equally spaced in lethargy between the low and high energies of the input mesh. The lethargy increment is defined from

$$\Delta u = \ln\left(\frac{E^*_{NEG+1}}{E^*_1}\right)/(IENX-1)$$

and the points from

$$E'_i = E^*_{NEG+1}\exp\left[-\ln\left(\frac{E^*_{NEG+1}}{E^*_1}\right) + (i-1)\Delta u\right] \quad i = 1, IENX$$

In PRØF2, contributions to elastic scattering cross sections from resonances are generated on the internal energy mesh and written to tape NSTA. In PRØF3, cross sections for elastic, inelastic, and total scattering are generated and written on tape NSTA. Tape NSTA is read in PRØF4 and the cross sections used to generate the Legendre cross sections for each reaction.

6.1.2 Common Storage

Common storage is divided into five named blocks designated BLØCK1, BLØCK2, ..., BLØCK5. BLØCK1, BLØCK3, and BLØCK4 are the same throughout the code. BLØCK2 common changes throughout the code to provide temporary storage as required. BLØCK5 is the same within each link of the code and is used for cross section storage. The details of each common block are given below for Link 1.

BLØCK1

NIN	Input data set number
NØUT	Output data set number
NPUN	Punch data set number
LIBØ	Not presently used. Data set number of interfaced library for output.
LIB	Data set number of ENDF/B tape
NSTA	Data set number of scratch tape A
NSTB	Data set number of scratch tape B

MØDE	Mode of ENDF/B tape = 1, binary standard format = 2, binary alternate format = 3, BCD format
DUMA(2)	Not used
LINK1	Flag to indicate execution of Link 1 (0 - no; 1 - yes)
LINK2	Flag to indicate execution of Link 2 (0 - no; 1 - yes)
LINK3	Not used
LINK4	Not used
LINK5	Not used
LINK6	Not used
LINK7	Not used
DUMB(33)	Not used

BLØCK3

LABEL	ENDF/B tape label requested
MATS	ENDF/B material number
T	Temperature (°K) at which cross sections are required
TEV	kT = temperature (ev) at which cross sections are required
LX	Highest Legendre scattering order requested (≤ 5)
LXPØ	LX + 1
FID	Floating point output identification number for numbered output
TITLE(18)	72-character description and page heading
LPDD	Test flag on decay data (453)
LPFP	Test flag on fission product yield data (454)
LABS	Test flag for processing absorption cross section
LPABS	Test flag for printing, punching, and group averaging in absorption cross section
LFISS	Test flag for processing fission cross sections
LPFIS	Test flag for printing, punching, and group averaging fission cross sections

LTØT	Test flag for processing total cross sections
LPTØT	Test flag for printing, punching, and group averaging total cross sections
LPTR	Test flag defining transport cross sections
LELAS	Test flag for processing elastic scattering cross sections
LPEL	Test flag for printing, punching, and group averaging elastic scattering cross sections
LINEL	Test flag for processing inelastic scattering cross section
LPIN	Test flag for printing, punching, and group averaging inelastic scattering cross sections
LSCAT	Test flag for processing total scattering cross sections
LPSC	Test flag for printing, punching, and group averaging total scattering cross sections
LTSL	Test flag for computing and normalizing thermal scattering matrices
LPTSL	Test flag for printing and punching thermal scattering matrices
LMESH	Test flag indicating whether to read new energy mesh or use old mesh (0 - yes; 1 - no)
VNU	Value of ν at E = 0.0 from Section 452 of File 1
LSTRP	Not used
LBND	Test flag indicating only the bound principal scatterer is to be calculated from $S(\alpha,\beta)$ data
LSCØL	Test flag indicating short collision time approximation to $S(\alpha,\beta)$ is used (0 - no; 1 - yes)
TEFF	Effective temperature (°K) to be used in short collision time equations
LRP	Test flag showing presence of resolved resonance parameters for a material (0 - no; 1 - yes)
LRSCT	Test flag indicating scattering should be computed from resonance formula (0 - no; 1 - yes)
DUMC(31)	Not used

BLØCK4

NEG	Number of energy groups in mesh
E(200)	Characteristic energy of each group (ev)

EB(201)	Lower boundary energy of each group (ev)
V(200)	Characteristic reduced velocity of each group (m/sec)
VB(201)	Lower boundary reduced velocity for each group (m/sec)
W(200)	Integration weight for each group
IENX	Number of points in internal energy mesh

BLØCK5

ZA	ENDF/B ZA designation for material
AWR	Atomic mass ratio of material to neutron mass
L1H	Test flag L1 in ENDF/B record
L2H	Test flag L2 in ENDF/B record
N1H	Test flag N1 in ENDF/B record
N2H	Test flag N2 in ENDF/B record
NBT(100)	Interpolation breakpoint table in ENDF/B record
INT(100)	Interpolation code table in ENDF/B record
X(4000)	Independent variable table in ENDF/B tabular record
Y(4000)	Dependent variable table in ENDF/B tabular record
B(4000)	ENDF/B LIST record table
XA(200)	Absorption cross section for each group (barns)
XF(200)	Fission cross section for each group (barns)
XT(200)	Total cross sections for each group (barns)
XTR(200)	Transport cross sections for each group (barns)
XRC(200)	Resonance contribution to capture cross section for each group (barns)
XRF(200)	Resonance contribution to fission cross section for each group (barns
XRS(200)	Resonance contribution to elastic scattering cross section for each group (barns)
XSE(200,6)	Elastic scattering cross section for each group and Legendre order (barns/ev)

XSI(200,6)	Inelastic scattering cross section for each group and Legendre order (barns/ev)
XSS(200,6)	Total scattering cross section for each group and Legendre order (barns/ev)

BLØCK2 - Normal

TSA(2000)	Temporary storage
TSB(200,5)	Temporary storage
TSC(1000)	Temporary storage
TSD(1000)	Temporary storage
TSE(2500)	Temporary storage

BLØCK2 - PRØF1

TSA(2000)	Temporary storage
TSB(200,5)	Temporary storage

BLØCK2 - PRØF2

TSA(1000)	Temporary storage
TSB(1000)	Temporary storage
TSC(1000)	Temporary storage
TSD(1000)	Temporary storage

BLØCK2 - PRØF4

XSEC(1000)	Cross section on internal energy mesh (barns)
EN(1000)	Energies of internal energy mesh (ev)
TMP(1000,5)	Legendre cross section on internal energy mesh (ℓ = 1, ..., 5)
TM(400)	Transformation matrix from CM to LAB (center of mass to laboratory coordinate systems) for Legendre coefficients
BS(10)	Temporary storage of Legendre coefficients

6.2 FILE 1 PROCESSING

Subroutine PRØF1 processes data from File 1 of the ENDF/B tape. These consist of documentation (451), neutron yield/fission (452), radioactive decay data (453), and fission product yield data (454). For all of these reactions except neutron yield/fission, the only operation is to print the information and/or punch cards for input to another program. Documentation (451) is

always printed, and test numbers are specified for decay data (453) and fission yield data (454) to determine what is done.

The total neutrons/fission (452) may be specified by one of two representations on the ENDF/B tape. Either a series expansion of the form

$$\nu(E) = \sum_{n=1}^{NC} C_n E^{n-1}$$

or as a tabular array of $\nu(E)$ versus E. FLANGE II evaluates the thermal ν as that value that occurs at E = 0. This corresponds to C_0 in the above expansion or the value of $\nu(E)$ that occurs at the lowest energy in a tabulation.

6.3 FILE 2 PROCESSING

Thermal cross sections are often represented by resolved resonance parameters rather than as tabular cross sections. This method is economical in terms of the volume of numbers required to represent a cross section. Subroutine PRØF2 calculates the contributions to capture, fission, and elastic scattering cross sections from resolved resonances. This calculation is restricted to single level Breit-Wigner resonance parameters, and may contain the interference scattering term. All cross sections produced are infinitely dilute and contain Doppler broadening for the specified temperature.

The method used is to generate the cross sections on the internal energy mesh described in Section 6.1.1 using the equations in Section 6.3.1. The resulting cross sections are interpolated or group averaged, as specified by test flags, and added to the capture, fission, and elastic scattering cross sections as specified. The scattering component may be calculated under one of two assumptions specified by test flag LRSCT.

- The scattering is represented by its potential scattering cross section which is the normal case for heavy isotopes (LRSCT = 0).

- The scattering is represented by the cross sections calculated from the resonance formulas which is more normal for light isotopes (LRSCT $\neq$ 0).

The scattering cross section on the internal mesh is written to scratch tape NSTA for transfer to File 4. It is identified by a negative reaction-type number to indicate it is to be added to the elastic scattering cross section.

6.3.1 Resonance Formulas Without Doppler Broadening

The equations[1,3] used to calculate cross sections from Breit-Wigner parameters at 0°K are those recommended for use by the Resonance Region Subcommittee of the Cross Section Evaluation Working Group. The cross sections for scattering, capture, and fission are given as follows for a single level representation.

$$\sigma_s(E) = \sum_{\ell=0}^{\substack{\text{All}\\ \ell \text{ states}}} \left\{ \frac{4\pi(2\ell+1)\sin^2\phi_\ell}{k^2} + \frac{\pi}{k^2} \sum_{J=1}^{\substack{\text{All}\\ J \text{ states}}} g_J \sum_{r=1}^{\substack{\text{Number}\\ \text{resonances}}} \right.$$

$$\left. \times \frac{\Gamma_{nr}^2 \cos 2\phi_\ell - 2\Gamma_{nr}(\Gamma_{\gamma r}+\Gamma_{fr})\sin^2\phi_\ell + 2(E-E_r')\sin 2\phi_\ell}{(E-E_r')^2 + (\frac{\Gamma_r}{2})^2} \right\}$$

$$\sigma_\gamma(E) = \sum_{\ell=0}^{\substack{\text{All}\\ \ell \text{ states}}} \frac{\pi}{k^2} \sum_{J=1}^{\substack{\text{All}\\ J \text{ states}}} g_J \sum_{r=1}^{\substack{\text{All}\\ \text{resonances}}} \frac{\Gamma_{nr}\,\Gamma_{\gamma r}}{(E-E_r')^2 + (\frac{\Gamma_r}{2})^2}$$

$$\sigma_f(E) = \sum_{\ell=0}^{\substack{\text{All}\\ \ell \text{ states}}} \frac{\pi}{k^2} \sum_{J}^{\substack{\text{All}\\ J \text{ states}}} g_J \sum_{r=1}^{\substack{\text{All}\\ \text{resonances}}} \frac{\Gamma_{nr}\,\Gamma_{fr}}{(E-E_r')^2 + (\frac{\Gamma_r}{2})^2}$$

where

E = energy at which cross section is evaluated (ev)

E_r = resonance energy (ev)

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

I = target nuclear spin

J = compound nuclear spin

$\Gamma_{nr} = P_\ell(E)\Gamma_{nr}(|E_r|)/P_\ell(|E_r|)$

$\Gamma_{nr}(|E_r|)$ = neutron width (ev)

P_ℓ = penetration factor

$$P_0 = \rho$$

$$P_1 = \frac{\rho^3}{1 + \rho^2}$$

$$P_2 = \frac{\rho^5}{9 + 3\rho^2 + \rho^4}$$

$\rho = ka$

a = channel radius (10^{-12} cm) = $\frac{1.23(A)^{1/3} + 0.8}{10}$

A = atomic mass ratio of target nucleus to neutron

$k = 2.196771 \frac{A}{A+1} \sqrt{E} \times 10^{-3}$

$\Gamma_r = \Gamma_{nr}(E) + \Gamma_{\gamma r} + \Gamma_{fr}$

$\Gamma_{\gamma r}$ = radiation width (ev)

Γ_{fr} = fission width (ev)

$$E_r' = E_r + \frac{S_\ell(|E_r|) - S_\ell(E)}{2P_\ell(|E_r|)} \Gamma_{nr}(|E_r|)$$

S_ℓ = shift factor

$$S_0 = 0$$

$$S_1 = \frac{-1}{1 + \rho^2}$$

$$S_2 = \frac{-18 - 3\rho^2}{9 + 3\rho^2 + \rho^4}$$

ϕ_ℓ = phase shift

$$\phi_0 = \hat{\rho}$$

$$\phi_1 = \hat{\rho} - \tan^{-1} \hat{\rho}$$

$$\phi_2 = \hat{\rho} - \tan^{-1} \frac{3\hat{\rho}}{3 - \hat{\rho}^2}$$

$\hat{\rho} = k\hat{a}$

$\hat{a}$ = effective scattering radius (10^{-12} cm)

If multilevel Breit-Wigner parameters are provided, the following term is added to the $\sigma_s(E)$ to include level-level interference:

$$\sum_{\substack{\text{All}\\ \ell \text{ states}}} \frac{\pi}{k^2} \sum_{\substack{\text{All}\\ J \text{ states}}} g_J \sum_{\substack{\text{All resonances}\\ \text{in state } J}} \sum_{r=2}$$

$$\times \sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns}[(E-E'_r)(E-E'_s) + \frac{1}{4}\Gamma_r\Gamma_s]}{[(E-E'_r)^2 + (\frac{\Gamma_r}{2})^2][(E-E'_s)^2 + (\frac{\Gamma_s}{2})^2]}$$

6.3.2 Resonance Formulas with Doppler Broadening

The formulas used when a non-zero temperature is specified are the same as used in the MC^2 program.[4] These formulas do not include the level-level terms as used in Section 6.3.1; however, the interference term with potential scattering is included. The cross sections for scattering, capture, and fission are given as follows.

$$\sigma_s(E) = \sum_{\substack{\ell=0\\ \ell \text{ states}}}^{\text{All}} \left\{ \frac{4\pi}{k^2}(2\ell+1)\sin^2\phi_\ell \right.$$

$$+ \frac{4\pi}{k^2}\left(\frac{A+1}{A}\right)^2 \sum_{\substack{\text{All}\\ J \text{ states}}} g_J \sum_{\substack{\text{All } J\\ \text{resonances}}} \frac{\Gamma_{nr}(|E_r|)}{\Gamma_r(|E_r|)}\Psi(\xi,x)$$

$$\left. + 4\pi\hat{a}\frac{A+1}{ak_0} \sum_{\substack{\text{All}\\ J \text{ states}}} g_J \sum_{\substack{\text{All } J\\ \text{resonances}}} \frac{\Gamma_{nr}(|E_r|)}{\Gamma_r(|E_r|)}\chi(\xi,x) \right\}$$

$$\sigma_\gamma(E) = \sum_{\substack{\ell=0\\ \ell \text{ states}}}^{\text{All}} \frac{4\pi}{k_0^2}\left(\frac{A+1}{A}\right)^2 \sum_{\substack{\text{All}\\ J \text{ states}}} g_J \sum_{\substack{\text{All } J\\ \text{resonances}}}$$

$$\times \left(\frac{|E_r|}{E}\right)^{1/2} \frac{\Gamma_{nr}(|E_r|)\Gamma_{\gamma r}(|E_r|)}{\Gamma_r^2(|E_r|)}\Psi(\xi,x)$$

$$\sigma_f(E) = \sum_{\ell=0}^{\text{All } \ell \text{ states}} \frac{4\pi}{k_0^2}\left(\frac{A+1}{A}\right)^2 \sum_{J}^{\text{All } J \text{ states}} g_J \sum_{r=1}^{\text{All J resonances}} \times \left(\frac{|E_r|}{E}\right)^{1/2} \frac{\Gamma_{nr}(|E_r|)\Gamma_{fr}(|E_r|)}{\Gamma_r^2(E_r)} \Psi(\xi,x)$$

where

E = energy at which cross section is evaluated (ev)

E_r = resonance energy (ev)

$g_J = \frac{2J+1}{2(2I+1)}$ = statistical spin factor

I = target nucleus spin

J = compound nucleus spin

$\Gamma_{nr}(|E_r|)$ = neutron width (ev)

$\Gamma_{\gamma r}(|E_r|)$ = radiation width (ev)

$\Gamma_{fr}(|E_r|)$ = fission width (ev)

$\Gamma_r(|E_r|) = \Gamma_{nr} + \Gamma_{\gamma r} + \Gamma_{fr}$

A = atomic mass ratio of target nucleus to neutron mass

$k = 2.196771\left(\frac{A}{A+1}\right)\sqrt{E} \times 10^{-3}$

$k_0 = 2.196771\left(\frac{A}{A+1}\right)\sqrt{E_r} \times 10^{-3}$

ϕ_ℓ = phase shift

$\phi_0 = \hat{\rho}$

$\phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho}$

$\phi_2 = \hat{\rho} - \tan^{-1}\frac{3\hat{\rho}}{3 - \hat{\rho}^2}$

$\hat{\rho} = k\hat{a}$

$\hat{a}$ = spin dependent scattering length (10^{-12} cm)

$\left.\begin{matrix}\Psi(\xi,x)\\ \chi(\xi,x)\end{matrix}\right\}$ = Doppler broadened line shape functions

$$\xi = \left(\frac{A\Gamma_r^2}{4|E_r|T}\right)^{1/2} = \frac{\Gamma_r}{\Delta}$$

$$\Delta = \text{Doppler width (ev)} = \left(\frac{4|E_r|T}{A}\right)^{1/2}$$

T = temperature (ev)

$$x = \frac{2(E - E_r)}{\Gamma_r}$$

The Doppler line shape functions are evaluated using the complex probability integral function W.[5] These quantities are related through the expressions

$$\Psi(\xi,x) = \frac{\xi\sqrt{\pi}}{2}\ \mathrm{ReW}\left(\frac{\xi x}{2},\frac{\xi}{2}\right)$$

$$\chi(\xi,x) = \xi\sqrt{\pi}\ \mathrm{ImW}\left(\frac{\xi x}{2},\frac{\xi}{2}\right)$$

The probability integral function is evaluated directly from convergent series and asymptotic expansions given in Reference 5.

6.4 FILE 3 PROCESSING

Subroutine PRØF3 performs interpolation or group averaging of smooth components of cross sections contained in ENDF/B File 3. The reactions considered are:

Reaction	Section
$\sigma^t(E,T)$ total	1
$\sigma^{el}(E,T)$ elastic	2
$\sigma^{in}(E,T)$ inelastic	4
$\sigma^f(E,T)$ fission	18
$\sigma^s(E,T)$ total scattering	29
$\sigma^\gamma(E,T)$ (n,γ)	102

A call is made to subroutine PRØF3 for each reaction shown in the table. PRØF3 first examines the test flags to determine whether to process the section, then returns or continues. If it continues, it first searches the tape for the required cross section. If not found, error stop 135 occurs. If found, the cross section is interpolated for the correct temperature. If the specified temperature is outside the range of the data, error stop 102 occurs.

When the required data are attained, they are stored as an ENDF/B TAB1 record in /BLØCK5/ common. The cross section may be interpolated at the characteristic energies of each group or averaged over the energy range of each group as specified by the test flags. Interpolation is performed by subroutine TERP2, and group averaging is performed by subroutine ACS.

If the cross section is elastic, inelastic, or total scattering the cross sections are interpolated on the internal energy mesh using subroutine TERP2. These cross sections are then written to tape NSTA with the section number as an identifier for use in File 4.

6.5 FILE 4 PROCESSING

Subroutine PRØF4 calculates Legendre cross sections up to order P_5 using smooth cross sections passed to it from PRØF2 and PRØF3 and angular distribution data from File 4 of the ENDF/B tape. Elastic, inelastic, or total scattering is calculated depending on the test flags specified in input.

When a scattering cross section is to be processed, the first step is to locate and read the P_0 order cross sections tabulated on the internal energy mesh from tape NSTA. These tabulations were written in PRØF3. For elastic scattering, a further search of tape NSTA is made to locate possible contributions from resonance scattering which are added to the smooth cross sections from PRØF3. The cross sections are stored in BLØCK2 in array XSEC(N) with the corresponding internal energy mesh in BLØCK2 array EN(N).

The probability that a neutron with energy E and temperature T will scatter through an angle whose cosine is μ for a particular scattering process is given in File 4 of the ENDF/B tape as either an expansion in Legendre polynomials in the form

$$p(E,\mu,T) = \sum_{\ell=0}^{LX} \frac{2\ell+1}{2} f_\ell(E,T) P_\ell(\mu)$$

or a tabular table of $p(E,\mu_i,T)$ versus μ_i. The desired Legendre cross sections $\sigma_\ell(E)$ are given by

$$\sigma_\ell(E) = \sigma(E) f_\ell(E)$$

where $\sigma(E)$ is the P_0 cross section and $f_\ell(E)$ is the Legendre coefficient of order ℓ. The differenctial angular cross section for scattering is related to $\sigma_\ell(E)$ by

$$\frac{d\sigma(E,\mu)}{d\Omega} = \frac{1}{2\pi} \sum_{\ell=0}^{LX} \frac{2\ell+1}{2} \sigma_\ell(E) P_\ell(\mu)$$

In File 4 of the ENDF/B tape the angular distribution may be specified in either the center of mass (CM) system or the laboratory (LAB) system. The required cross sections are for the LAB system: hence whenever possible a transformation is made, otherwise an error stop occurs. Normally a transformation matrix is given for eleastic Legendre moments when specified in the CM system. The LAB moments are related to the CM moments by the following equation.[1]

$$f_\ell^{lab}(E) = \sum_{m=0}^{NM} u_{\ell m} f_m^{CM}(E)$$

where the $u_{\ell m}$ are the elements of the transformation matrix and are stored in array TM(400) in BLØCK2.

If the angular distribution is tabular, the Legendre moments may be derived by integrating the tabular distribution for a specified number of Legendre polynomials. These moments are given by

$$f_\ell(E) = \int_{-1}^{+1} p(E,\mu)\ P_\ell(\mu)\ d\mu$$

This definition is valid for both the LAB and CM systems.

PRØF4 will process angular distributions in either Legendre expansion or tabular form in the LAB system. Only the Legendre expansion form is acceptable for CM data and the transformation matrix must be supplied. Any data not meeting these restrictions will lead to an error stop.

After the required P_0 cross sections are retrieved from tape NSTA the angular distribution at the first energy is read, converted into LAB system Legendre moments, and stored. The calculation of the Legendre cross sections is arranged so that the angular distribution data are read only once. At any time two distributions corresponding to E_{high} and E_{low} are maintained in core. Legendre moments for each energy on the internal mesh between E_{high} and E_{low} are obtained by interpolation. After Legendre cross sections are tabulated at all energy points between E_{high} and E_{low} the distribution at E_{low} is moved to E_{high} and a new E_{low} distribution is read. The process continues until Legendre cross sections are obtained for all orders and all energy points on the internal mesh. These Legendre cross sections will be array TMP(1000,5) in BLØCK2 common.

The Legendre cross sections are now interpolated or group averaged as specified by the test flags to obtain the final cross sections.

6.6 COMPLETING THE CROSS SECTION SET

Subroutine PLEAT is executed only if LINK2 of the code is not executed. Its function is to complete the cross sections specified by the test flags as being derived from other cross sections. If LINK2 of the code is being executed, all cross sections computed and stored in BLØCK5 common are written as tape NSTA for transfer. A second subroutine PLEAT2 in LINK2 will then perform the operations necessary to complete the cross sections.

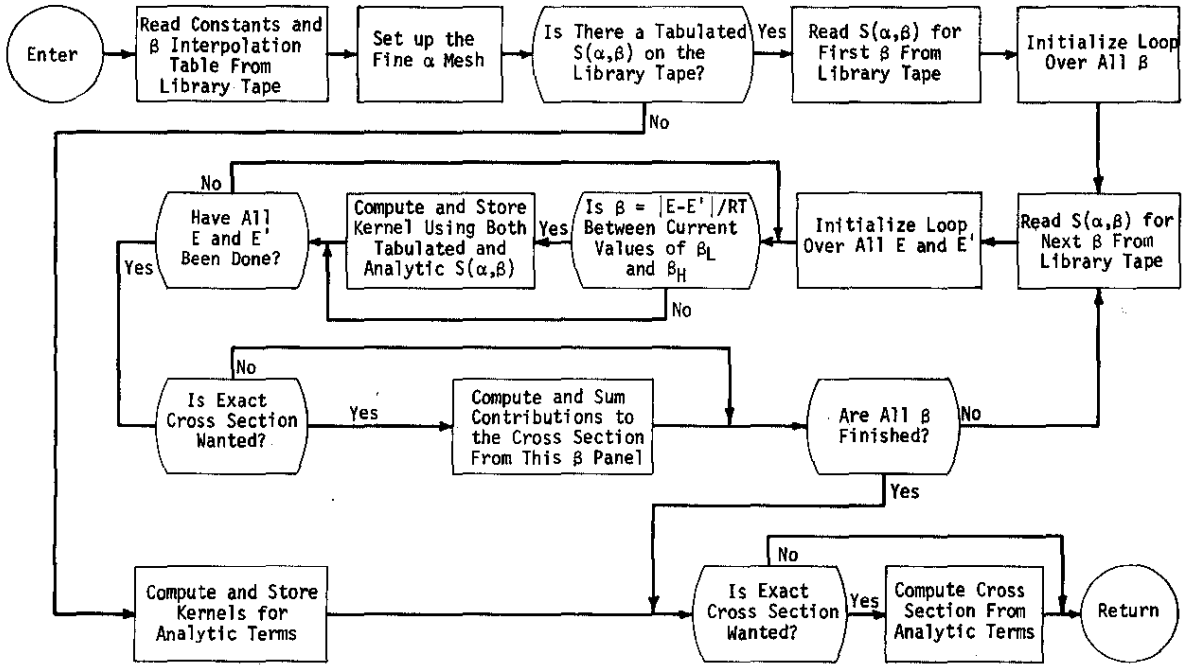
The test flags and computing operations performed by PLEAT are described in detail in Section 2.4. Any mutually exclusive set of test flags will lead to an error stop.

After the operations necessary to complete the cross sections are performed, PLEAT then prints and/or punches all cross sections as indicated by the second set of test flags.

7. DETAILED DESCRIPTION OF LINK 2

7.1 OVERALL OPERATION

Link 2 is divided into three sections (subroutines PRØF7, PLEAT2, and REKØN). Operation of each section is described below, and a flow diagram for PRØF7 is given here.



Flow Diagram for PRØF7

It is assumed that on entering Link 2, Link 1 has been executed and the resulting cross sections are stored on tape NSTA. Link 2 then operates as follows:

PRØF7 - The tabulated scattering law $S(\alpha,\beta)$ is read one β at a time from the ENDF/B tape. Two successive β values form a panel, and the scattering kernels and cross sections are computed for each panel as it is read in. These results are stored in the fast

memory if room is available, or dumped onto tape NSTB. Analytic terms are also evaluated and added to the results from the tabulated $S(\alpha,\beta)$. The short collision approximation is used to extend the tabular $S(\alpha,\beta)$ table when requested.

PLEAT2 - If all required cross sections were obtained in Link 1, they are read in from tape NSTA and stored for use in normalizing the scattering kernels. If the inelastic cross section was computed in Link 2 (and not read in Link 1), the cross sections are read from tape NSTA and the inelastic cross section is added to complete the set. The cross sections are then printed, punched, and stored for use in normalizing the scattering kernels.

REKØN - The scattering kernels (in the order in which they were computed) are brought in from core or tape storage, re-ordered, normalized, printed, and punched.

7.2 STORAGE ALLOCATION

7.2.1 Storage of $S(\alpha,\beta,T)$

The scattering law, $S(\alpha,\beta,T)$, is stored on the library tape in the following manner.

1. Heading record giving the test LAT.

2. Record giving σ_b and A for the tabulated law, and the constants for the analytic laws.

3. Record giving the number of β values given (NBETA) and a table telling how to interpolate between values of β.

4. Record giving pairs of $\alpha,S(\alpha,\beta,T)$ for the first β and the first temperature, and a table telling how to interpolate between values of α.

5. Record giving values of $S(\alpha,\beta,T)$ for the first β and the second temperature (same α and interpolation as for the first temperature).

6. Repeat of Item 5 until all temperatures are given.

7. Repeat of Items 4 and 5 until all temperatures and all β are given.

The first three records are read and processed in PRØF7. The remaining records are read and processed in REATS.

The calculation is arranged so that the $S(\alpha,\beta,T)$ is read from the library tape only once. Since the entire array probably cannot be fit into core storage, only two consecutive values of β are stored at one time. The data for the first two values of β are read in, and all computations of kernels and cross sections that involve this range of β are done. The data for the high value of β are then moved to the area used to store data for the low value of β, and a new set of data for the next β are read from the library. The computations involving this β range are done, and the process is repeated until all β have been processed. This logic is contained in PRØF7.

Consider the steps involved in reading the data for one β from the library. Since the α mesh for one value of β may be different from the α mesh for another value of β, it is convenient to evaluate the scattering law on a single α mesh for all β. This common α mesh is called the "fine" α mesh and is computed in the following manner. Let IALX (= 300) be the number of points in the "fine" α mesh, and ρ_0 (= 1.03) be an expansion ratio. Denote the "fine" α mesh by α_i.

$$\alpha_i = \alpha_0 \rho_0^{i-1}$$

The α_0 is selected by requiring that $\alpha_{IALX} < \alpha_{max}$, where $\alpha_{max} = 4E_{max}/AT$, and E_{max} is the largest energy in the input energy mesh. Then

$$\alpha_0 = \alpha_{max}/\rho_0^{IALX-2}$$

For E_{max} = 1 ev, kT = 0.025 ev, A = 1, ρ_0 = 1.03, and IALX = 300, then α_{max} = 160, and α_0 = 0.024.

Let β_H and β_L denote the high and low values of β contained in storage. Define

$$SA(I) = S(\alpha_i,\beta_L,T)$$

$$ASA(I) = \ln S(\alpha_i,\beta_L,T)$$

$$SB(I) = S(\alpha_i,\beta_H,T)$$

$$ASB(I) = \ln S(\alpha_i,\beta_H,T)$$

$$ALP(I) = \alpha_i$$

where T denotes the input temperature.

The first step in subroutine REATS is to move SB→SA, ASB→ASA, and $\beta_H \rightarrow \beta_L$. The next step is to read a record containing the new $\beta = \beta_H$, pairs of $[\alpha_n, S(\alpha_n,\beta,T)]$, and a table for interpolating between the α_n. The α_n is the α mesh contained on the library tape of this β. These data are stored in

$$TSA(N) = \alpha_n$$

$$TSB(N) = S(\alpha_n,\beta,T)$$

The temperature used to define α and β on the library tape may have been the actual temperature (LAT = 0) or a constant equal to 0.0253 ev. (LAT = 1). If the latter, the β and α_n are scaled by the factor 0.0253/kT to achieve the proper β and α_n at temperature T.

The $S(\alpha_n,\beta,T)$ are now interpolated on the "fine" α mesh and stored in array TSD(I,4) and T4 is set equal to T. Because the α_n mesh in TSA(N) for a temperature T may not span the same range as the "fine" α mesh, the option is available to use the short collision approximation to supply the additional non-zero $S(\alpha_i,\beta,T)$ values on the "fine" α mesh. If the short collision approximation is not used, then "fine" α mesh interpolation is performed by subroutine TERP2. If the short collision approximation is used, the effective temperature for the short collision approximation equation

$$S_{sc}(\alpha_i,\beta,T,T_{eff}) = \frac{e^{\frac{\beta}{2}} \; e^{-\frac{T}{4\alpha_i T_{eff}}(\alpha_i+\beta)^2}}{\sqrt{4\pi\alpha_i T_{eff}/T}}$$

is supplied, and the interpolation is performed by subroutine TERP3. The values in TSD(I,4) are tested and set to values $>1.0 \times 10^{-33}$.

Temperature T4 is now compared to the requested temperature. If equal, the values of $S(\alpha_i,\beta,T)$ stored in TSD(I,4) are stored in SB(I) and the natural log in ASB(I). If the requested temperature is greater than T4, the values in the TSD(I,K) array are all moved back one position, and the temperature is stored backwards as

$$TSD(I,1) = TSD(I,2) \qquad T1 = T2$$

$$TSD(I,2) = TSD(I,3) \qquad T2 = T3$$

$$TSD(I,3) = TSD(I,4) \qquad T3 = T4$$

A new set of $S(\alpha_n,B,T)$ are now read into TSB(N) at a new temperature T. T4 is set to T and the α_n mesh is corrected for the new temperature as $\alpha_n = \alpha_n T3/T4$. The $S(\alpha_n,\beta,T)$ are again interpolated on the "fine" α mesh as described above. The process is continued until four sets of $S(\alpha_i,\beta,T)$ are stored in array TSD(I,K) corresponding to four temperatures T1 through T4. If possible, the requested temperature is made to be in the range $T2 < T < T3$. If T equals any of the four temperatures, it is accepted as interpolated and stored in SB(I) as described above.

A four-point Lagrangian interpolation is now performed to obtain the $S(\alpha_i,\beta,T)$ required according to

$$SB(I) = A_1\ TSD(I,1) + A_2\ TSD(I,2) + A_3\ TSD(I,3) + A_4\ TSD(I,4)$$

where

$$A_1 = (T-T2)(T-T3)(T-T4)/(T1-T2)(T1-T3)(T1-T4)$$

$$A_2 = (T-T1)(T-T3)(T-T4)/(T2-T1)(T2-T3)(T2-T4)$$

$$A_3 = (T-T1)(T-T2)(T-T4)/(T3-T1)(T3-T2)(T3-T4)$$

$$A_4 = (T-T1)(T-T2)(T-T3)/(T4-T1)(T4-T2)(T4-T3)$$

If only three temperatures are available in the data, a three-point Lagrangian interpolation is used according to

$$SB(I) = A_2\ TSD(I,2) + A_3\ TSD(I,3) + A_4\ TSD(I,4)$$

where

$$A_2 = (T-T3)(T-T4)/(T2-T3)(T2-T4)$$

$$A_3 = (T-T2)(T-T4)/(T3-T2)(T3-T4)$$

$$A_4 = (T-T2)(T-T3)/(T4-T2)(T4-T3)$$

If only two temperatures are available in the data, the standard two-point interpolation codes are used with subroutine TERP1.

The final step is to store the natural log of SB(I) in array ASB(I).

The method of interpolation described here is designed to provide as exact a method of temperature interpolation as is possible over the entire range of values of $S(\alpha,\beta,T)$. Generally as β becomes large (>10) the $S(\alpha,\beta,T)$ changes with temperature by factors as large as 100/°K while simultaneously becoming

smaller in magnitude. At some value of β the entire interpolation scheme will break down due to the large-scale factors on temperature. This effect is computer dependent and typically occurs between β values of 30 to 40. Once such a limit is reached it is no longer possible to generate accurate $S(\alpha,\beta)$ tables at intermediate temperatures between the tabulated temperatures. This restriction does not, however, apply to the temperatures at which the $S(\alpha,\beta)$ are tabulated since no interpolation is done beyond transforming to the "fine" α mesh. A method of circumventing the restrictions produced by these interpolation errors is described in Section 8.

7.2.2 Cross Section Storage

Manipulation of cross sections is done by subroutine PLEAT2. Cross sections processed by Link 1 are stored on tape NSTA. These are read into the storage block SBB, completed, printed, punched, and the appropriate cross section for the normalization of the kernels is computed and stored. The completing, printing, and punching are identical to that described previously for Link 1.

This process occurs following the computation of the kernels and inelastic cross sections in PRØF7, and prior to reorganization of the kernels in REKØN. The exact inelastic cross section is obtained from Files 3 and 4 of the library tape or computed from $S(\alpha,\beta)$. It is stored in XSI(N,L). An approximate cross section is computed during the computation of the kernels.

$$\sigma_\ell^*(E_i) = \sum_{j=1}^{NEG} \sigma_\ell(E_i \rightarrow E_j) W_j$$

where W_j is the integration weight for the j^{th} group. This approximate cross section is stored in XINA(N,L). The test LTSL is used to indicate how the kernels are to be normalized. The array XINE(N,L) is to be set up with the cross section wanted to normalize the kernels.

LTSL = 3 No renormalization desired
XINE(N,L) = XINA(N,L)

LTSL = 4 Normalize to the inelastic cross section
XINE(N,L) = XSI(N,L)

LTSL = 5 Normalize to the total (Elastic + inelastic) cross section XINE(N,L) = XSS(N,L)

When the ordered kernel is set up by REKØN, the diagonal element will be changed by adding.

$$[XINE(N,L) - XINA(N,L)]/W(N)$$

7.2.3 Storage of the Scattering Kernel

Allowance is made for a large input energy mesh (≤200 points). A single kernel might require 20,100 entries, and six Legendre components might require 120,600 entries. A fast and efficient method is needed to transfer data between fast core storage and bulk storage. Two one-dimensional arrays (SBA and SBB) are used for this purpose, and subroutine STØRK handles all transfers between core storage and tape.

If NEG is the number of energy groups, a full kernel requires NEG*NEG storage locations. Because of the detailed balance condition, only the upper half matrix (downscattering plus diagonal terms) is required, or NEG*(NEG+1)/2 storage locations.

Since the kernels are calculated in the order of increasing β and since all of the data may not be contained in fast core storage, the data are collected and stored in array SBA as the data are calculated. If LX is the maximum Legendre order, and LXPØ = LX+1, then LXPØ locations are needed for each term of the kernel. Let I denote the initial energy group, J denote the final energy group, and S(L) denote the kernel. Combine the I and J into C = 1000J+I. The string of numbers

$$C,S(1),S(2),\ldots,S(LXPØ)$$

is stored sequentially in SBA(K). Since there are LXPØ+1 numbers in the string, K is incremented by LXPØ+1 after storage of the string. SBA is presently dimensioned for 4623 locations. The following table gives the largest value of NEG which can be held in SBA.

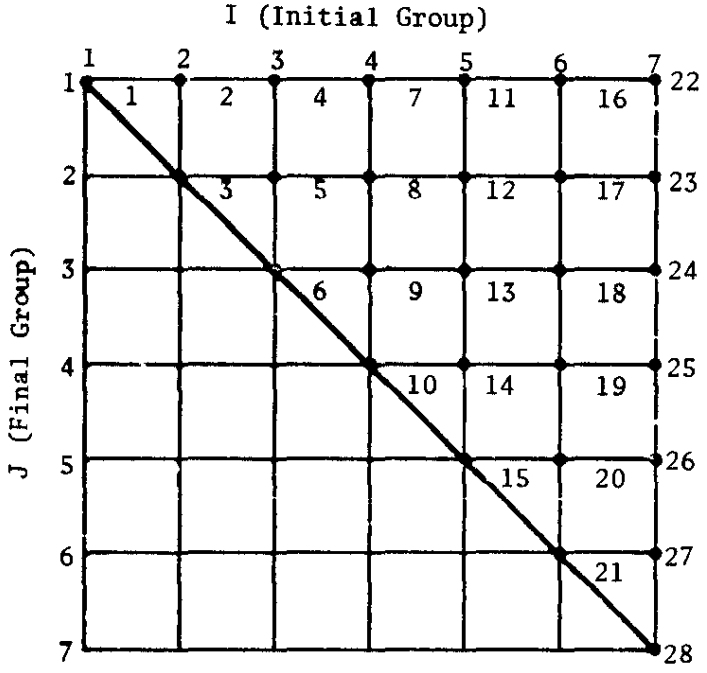
LX	LXPO+1	Max Number of (I,J) Entries	Max NEG
0	2	2311	67
1	3	1541	55
2	4	1155	47
3	5	924	42
4	6	770	38
5	7	660	35

If the actual NEG does not exceed the values given in the above table, all kernels can be contained in fast core storage and tapes are not used.

If NEG exceeds the values given in the table, the array SBA will automatically be dumped onto tape NSTB whenever the array is full. Thus, if LX = 5, and NEG = 200 (the maximum problem), 120,600 entries are required which would use 26 full arrays and 1 partial array. 27 blocks would be dumped on tape NSTB, and end-of-file written, and the tape rewound.

Frequently, many off-diagonal terms are very small and can be ignored. A criterion EPSK ($= 10^{-8}$) is used to reject these terms. This rejection is done in STØRK and all Legendre components must be less than EPSK for the terms to be rejected.

Next the kernels are brought back into core storage, properly ordered, normalized, printed, and punched. These operations are done in subroutine REKØN which uses STØRK to fetch numbers from tape or core storage. The properly ordered kernel is contained in array SBB which is dimensioned at 5151. Only one Legendre moment kernel is stored in SBB at one time. The kernel is a two-dimensional array, and SBB is a one-dimensional array. Consider the following diagram (illustrated for NEG = 7).



Each point shown above represents an element of the kernel which is stored. Let K denote the location in array SBB. The number by each point is this value of K. The number of entries up to

and including column I is 1/2[I(I+1)], and the number of entries between and including columns IA and IB is

$$KX = 1/2[IB(IB+1) - IA(IA-1)]$$

If NEG $\leq$ 101, 1/2[NEG(NEG+1)] $\leq$ 5151, and the entire kernel will fit into SBB. If NEG > 101, several passes are made. For example, suppose NEG = 200. Four passes are required:

Pass	IA	IB	KX (Storage Used)
1	1	101	5151
2	102	143	5145
3	144	175	5104
4	176	200	4700

The location K for a particular combination I,J is given by

$$K = 1/2[I(I-1)] - 1/2[IA(IA-1)] + J$$

Thus, I = 127, J = 53 would require Pass 2, IA = 102, and K = 2903.

The calculation proceeds in the following manner. The entire tape NSTB is read, block by block, into SBA. The P_0 components are extracted and stored in SBB. If NEG $\leq$ 101, the entire kernel will fit into SBB. If NEG > 101, only the terms for I $\leq$ 101 are stored. The contents of SBB are normalized, printed, and punched, and tape NSTB is rewound. If NEG > 101, the tape is again read, and the P_0 components for 102 $\leq$ I $\leq$ 143 are stored in SBB. These are normalized, printed, punched, and NSTB is rewound. This is repeated until the entire P_0 kernel has been processed. The entire operation is repeated for the P_1 component, and so forth. The following table gives the number of times tape NSTB will be read.

Range of NEG	Maximum Legendre Component Requested					
	P_0	P_1	P_2	P_3	P_4	P_5
1-35	0	0	0	0	0	0
36-38	0	0	0	0	0	6
39-42	0	0	0	0	5	6
43-47	0	0	0	4	5	6
48-55	0	0	3	4	5	6
56-67	0	2	3	4	5	6
68-101	1	2	3	4	5	6
102-143	2	4	6	8	10	12
144-175	3	6	9	12	15	18
176-200	4	8	12	16	20	24

7.2.4 Common Storage

Labeled common storage is used and designated by BLØCK1, BLØCK2, ..., BLØCK5. BLØCK1, BLØCK3, and BLØCK4 are the same as in Link 1.

BLØCK2

TSA(1000)	Temporary storage
TSB(1000)	Temporary storage
TSD(300,4)	Temporary storage

BLØCK 5

BETL	β_L, the lower β value of the two currently in storage (see PRØF7, REATS)
BETH	β_H, the higher β value of the two currently in storage (see PRØF7, REATS)
EPSK	Test ($=10^{-8}$) used to reject terms in the kernels (see Section 7.2.3)
LAT	Test indicating whether the actual temperature (LAT = 0) or the value 0.0253 ev (LAT = 1) was used on the library tape to define α and β
AMASS	A, the mass ratio used to compute α for a tabulated scattering law
SIGB	σ_b, the bound atom cross section (barns) used with the tabulated scattering law. If $\sigma_b = 0$, no tabulation is given, only analytic terms are given.
IALX	= 300, the number of α used for the fine α mesh. This should correspond to the dimensions of ALP, SA, ASA, SB, ASB.
RHØ	ρ_0, the expansion ratio (= 1.03) for the fine α mesh (see 7.2.3)
ARHØ	ln ρ_0, (see 7.2.3)
ALPHØ	α_0, first α value in the fine α mesh (see 7.2.3)
XINE(200,6)	XINE(N,L), the exact inelastic scattering cross section $\sigma_\ell^{in}(E_H)$, L = ℓ+1, computed from $S(\alpha,\beta)$ (see PRØF7)

XINA(200,6)	XINA(N,L), an approximate inelastic scattering cross section $\sigma^*_\ell(E_N)$, L = ℓ+1, computed from the calculated kernel (see 7.2.2 and PRØF7)
KMXA	= 4623, the length of array SBA
KMXB	= 5151, the length of array SBB
SBA(4623)	Storage block (see 7.2.3)
SBB(5151)	Storage block (see 7.2.3)
ALP(300)	ALP(I) contains α_i (see 7.2.1)
SA(300)	SA(I) contains $S(\alpha_i,\beta_L)$ (see 7.2.1)
ASA(300)	ASA(I) contains ln $S(\alpha_i,\beta_L)$ (see 7.2.1)
SB(300)	SB(I) contains $S(\alpha_i,\beta_H)$ (see 7.2.1)
ASB(300)	ASB(I) contains ln $S(\alpha_i,\beta_H)$ (see 7.2.1)
SBC(200,6)	SBC(N,L), the inelastic scattering kernel $\sigma_\ell(E_N \rightarrow E_N+\beta_L)$, L = ℓ+1, used in the calculation of the inelastic cross section (see FEINT)
SBD(200,6)	SBD(N,L), the inelastic scattering kernel $\sigma_\ell(E_N \rightarrow E_N-\beta_L)$, L = ℓ+1, used in the calculation of the inelastic cross section (see FEINT)
XSE(200,6) XSI(200,6) XSS(200,6) XA(200) XF(200) XT(200) XTR(200)	Cross sections computed and defined in Link 1 which are transmitted from Link 1 to Link 2 via tape NSTA. See Section 6 for their definition and PLEAT2 for the way they are used in Link 2.

Many of these arrays are equivalent to SBB. The following table summarizes this equivalence.

SBB(1)	=	ALP	= XA
SBB(301)	=	SA	= XF
SBB(601)	=	ASA	= XT
SBB(901)	=	SB	= XTR
SBB(1201)	=	ASB	
SBB(1501)	=	SBC	= XSE
SBB(2701)	=	SBD	= XSI
SBB(3901)	=		= XSS

7.3 CALCULATION OF THE SCATTERING KERNELS

7.3.1 General Method

The scattering kernels are calculated from

$$\sigma_\ell(E'\to E) = \frac{\sigma_b}{4\pi kT}\sqrt{\frac{E}{E'}}\, e^{-\beta/2}\int_{-1}^{1} d\mu S(\alpha,\beta)P_\ell(\mu)$$

$$\alpha = (E + E' - 2\mu\sqrt{EE'})/AkT$$

This equation is rewritten so that the integration is over α instead of μ.

$$\sigma_\ell(E'\to E) = \frac{A\sigma_b}{4E'}\, e^{-\beta/2}\int_{\alpha_L}^{\alpha_H} d\alpha S(\alpha,\beta)P_\ell(\mu)$$

$$\alpha_L = (E + E' - 2\sqrt{EE'})/AkT$$

$$\alpha_H = (E + E' + 2\sqrt{EE'})/AkT$$

$P_\ell(\mu)$ is expanded in powers of α.

$$P_\ell(\mu) = \sum_{n=0}^{\ell} W_{\ell n}\alpha^n$$

The final expression for the kernel is then

$$\sigma_\ell(E'\to E) = \frac{A\sigma_b}{4E'} e^{-\beta/2} \sum_{n=0}^{\ell} W_{\ell n}H_n$$

$$H_n = \int_{\alpha_L}^{\alpha_H} d\alpha\ \alpha^n S(\alpha,\beta)$$

7.3.2 Coefficients $W_{\ell n}$

The coefficients $W_{\ell n}$ can be obtained straightforward by expanding $P_\ell(\mu)$ in a power series.

$$P_\ell(\mu) = \sum_{k=0}^{\ell} a_k^\ell(\gamma_0-\gamma_1\alpha)^k$$

$$\mu = \gamma_0-\gamma_1\alpha, \qquad \gamma_0 = (E' + E)/2\sqrt{EE'}, \qquad \gamma_1 = AkT/2\sqrt{EE'}$$

The a_k^ℓ satisfy the recursion formulas

$$a_0^{\ell+1} = -\frac{\ell}{\ell+1} a_0^{\ell-1}$$

$$a_k^{\ell+1} = \frac{2\ell+1}{\ell+1} a_{k-1}^{\ell} - \frac{\ell}{\ell+1} a_k^{\ell-1}, \qquad 1 \leqslant k \leqslant \ell-1$$

$$a_\ell^{\ell+1} = \frac{2\ell+1}{\ell+1} a_{\ell-1}^{\ell}$$

$$a_{\ell+1}^{\ell+1} = \frac{2\ell+1}{\ell+1} a_\ell^{\ell}$$

The a_k^ℓ for $\ell \leq 5$ are given in the following table:

ℓ \ k	0	1	2	3	4	5
0	1					
1	0	1				
2	-1/2	0	3/2			
3	0	-3/2	0	5/2		
4	3/8	0	-30/8	0	35/8	
5	0	15/8	0	-70/8	0	63/8

Next use the binomial expansion to obtain

$$(\gamma_0-\gamma_1\alpha)^k = \sum_{m=0}^{k} \binom{k}{m} \gamma_0^k (-\gamma_1)^{m-k} \alpha^{m-k}$$

Change index and insert

$$W_{\ell n} = (-\gamma_1)^n \sum_{j=0}^{\ell-n} b_{jn}^\ell \gamma_0^j$$

$$b_{jn}^\ell = \binom{j+n}{n} a_{j+n}^\ell$$

The b_{jn}^{ℓ} for $\ell \leq 5$ are given in the following table:

ℓ	n \ j	0	1	2	3	4	5
0	0	1					
1	0	0	1				
	1	1					
2	0	-1/2	0	3/2			
	1	0	3				
	2	3/2					
3	0	0	-3/2	0	5/2		
	1	-3/2	0	15/2			
	2	0	15/2				
	3	5/2					
4	0	3/8	0	-15/4	0	35/8	
	1	0	-15/2	0	35/2		
	2	-15/4	0	105/4			
	3	0	35/2				
	4	35/8					
5	0	0	15/8	0	-35/4	0	63/8
	1	15/8	0	-105/4	0	315/8	
	2	0	-105/4	0	315/4		
	3	-35/4	0	315/4			
	4	0	315/8				
	5	63/8					

7.3.3 Tabulated $S(\alpha,\beta)$

The method of calculating the α moments is discussed in detail. The representation of $S(\alpha,\beta)$ is given in this section for a tabulated function and in Section 7.3.4 for an analytic function.

Assume that $S(\alpha,\beta)$ for two consecutive values of β are in storage. Denote the lower value of β by β_L, and the upper by β_H. Also given are initial and final energies, E' and E, such that $\beta = |E' - E|/kT$ lies between β_L and β_H. For both the upper and lower values of β, the scattering law $S(\alpha,\beta)$ and $y = \ln[S(\alpha,\beta)]$ are evaluated on an α mesh defined by

$$\alpha_i = \alpha_0 \rho_0^{i-1}, \qquad 1 \leq i \leq IALX$$

where ρ_0, and IALX are preset constants. If E_{max} is the largest energy in the input and A is the mass used to define α, then α_0 is computed from

$$\alpha_{max} = 4E_{max}/AkT < \alpha_{IALX} = \alpha_0 \rho_0^{IALX-1}$$

$$\alpha_0 = \alpha_{max}/\rho_0^{IALX-2}$$

If E_{max} = 1 ev, kT = 0.025 ev, IALX = 300, ρ_0 = 1.03 and A = 1, then α_{max} = 160 and α_0 = 0.024.

The upper and lower integration limits are computed from

$$\alpha_L = (E' + E - 2\sqrt{EE'})/AkT$$

$$\alpha_H = (E' + E + 2\sqrt{EE'})/AkT$$

A low index, IL, is computed from

$$IL = 1 + \ln(\alpha_L/\alpha_0)/\ln(\rho_0)$$

so that $\alpha_{IL} \leq \alpha_L < \alpha_{IL+1}$. A value IL = 0 implies that $\alpha_L < \alpha_0$.

Similarly, a high index is computed from

IH = Smaller of [IALX-1, $1 + \ln(\alpha_H/\alpha_0)/\ln(\rho_0)$]

so that $\alpha_{IH} \leq \alpha_H < \alpha_{IH+1}$, but does not fall outside the table.

Finally the values of $S(\alpha,\beta)$ for $\alpha_{IL} \leq \alpha \leq \alpha_{IH+1}$ and for the specific β are obtained by interpolation between the values given at β_L and β_H. Let ICØDE denote the interpolation code.

ICØDE = 1, $S(\alpha,\beta) = S(\alpha,\beta_L)$

ICØDE = 2, $S(\alpha,\beta) = S(\alpha,\beta_L) + (\beta-\beta_L)[S(\alpha,\beta_H) - S(\alpha,\beta_L)]/(\beta_H-\beta_L)$

ICØDE = 3, $S(\alpha,\beta) = S(\alpha,\beta_L) + \ln(\beta/\beta_L)[S(\alpha,\beta_H) - S(\alpha,\beta_L)]/\ln(\beta_H/\beta_L)$

ICØDE = 4, $\ln[S(\alpha,\beta)] = \ln[S(\alpha,\beta_L)] + (\beta-\beta_L)\ln[S(\alpha,\beta_H)/S(\alpha,\beta_L)]/(\beta_H-\beta_L)$

ICØDE = 5, $\ln[S(\alpha,\beta)] = \ln[S(\alpha,\beta_L)] + \ln(\beta/\beta_L)\ln[S(\alpha,\beta_H)/S(\alpha,\beta_L)]/\ln(\beta_H/\beta_L)$

If ICØDE = 3 or 5, and $\beta_L = 0$, ICØDE is automatically changed to 2.

The equations and logic given above are contained in subroutine KERC, statements 10-220.

7.3.4 Analytic $S(\alpha,\beta)$

Analytic formulas for the free gas or diffusive motion laws may be used to calculate $S(\alpha,\beta)$. The procedure is to evaluate the formulas on an α mesh so that the same numerical integration procedures can be used as are used for tabulated functions.

Let A' be the mass associated with the analytic formula. Then

$$\alpha_L = (E' + E - 2\sqrt{EE'})/A'kT$$

$$\alpha_H = (E' + E + 2\sqrt{EE'})/A'kT$$

Define a new lower α mesh limit

$$\alpha_0' = \alpha_0 A/A'$$

and let

$$\alpha_1' = \text{Larger of } (\alpha_0', \alpha_L)$$

Define a new α mesh from

$$\alpha_i' = \alpha_0' \rho_0^{i-1}, \qquad 1 \leqslant i \leqslant \text{IALX}$$

The analytic formulas are then evaluated on this mesh.

$$S(\alpha,\beta) = \frac{1}{\sqrt{4\pi\alpha}} \exp\left[-\frac{\alpha^2 + \beta^2}{4\alpha}\right] \qquad \text{(Free Gas)}$$

$$S(\alpha,\beta) = \frac{2d\alpha}{\pi}\left[c^2 + \frac{1}{4}\right] e^{2dc\alpha} K_1(x)/x \qquad \text{(Diffusion)}$$

$$x = \left[\left(c^2 + \frac{1}{4}\right)(\beta^2 + 4d^2\alpha^2)\right]^{1/2}$$

The equations and logic given above are contained in subroutine KERA, statements 10-290.

7.3.5 Short Collision Time Approximation to $S(\alpha,\beta)$

It is sometimes of interest to treat scattering systems accounting for scattering to energies of 3 to 5 ev. The analytic formulas of Section 7.3.4 may be used directly for these cases; however, the tabular $S(\alpha,\beta)$ scatterer rarely exceeds β values corresponding 1 to 2 ev energy transfers; hence it is not possible to generate scattering components to the higher energies. Provision is made to allow the tabular $S(\alpha,\beta)$ for a scatterer to be extended to larger energy transfers using the short collision time approximation.[2]

The utilization of the short collision time approximation requires specification of an effective moderator temperature for the scatterer. This temperature is defined by the equation

$$\frac{kT_{eff}}{\hbar} = 1/2 \int_0^\infty f(\omega)\omega \coth \frac{\hbar\omega}{2kT} d\omega$$

where $f(\omega)$ is the generalized frequency spectrum, and $\hbar\omega = E_0 - E$ is the energy gained by the scattering system.

When the effective temperature for the scatter is specified, the short collision time approximation to $S(\alpha,\beta)$ is given by

$$S(\alpha,\beta,T,T_{eff}) = \frac{e^{\frac{\beta}{2}} e^{-\frac{T}{4\alpha T_{eff}}(\alpha+\beta)^2}}{\sqrt{4\pi\alpha T_{eff}/T}}$$

A mesh is chosen for β that spans the region between the maximum tabular β and that β value required to account for all energy transfers for the input energy mesh. If an effective temperature for the scatterer is not specified, the $S(\alpha,\beta)$ is assumed zero for all β above the maximum tabulated β.

The short collision time approximation is quite useful in extending the range of a scattering kernel to higher energies. There are, however, limitations in the range of energies over which it may be used. These are computer dependent limitations related to the number of significant digits a particular machine can carry, and to the type of interpolation that is used.

Examination of the short collision time approximation to $S(\alpha,\beta)$ above shows that for large β ($\tilde{=}$ 200) the amplitude of $S(\alpha,\beta)$ for fixed α, T, and T_{eff} is small. Further, as β becomes

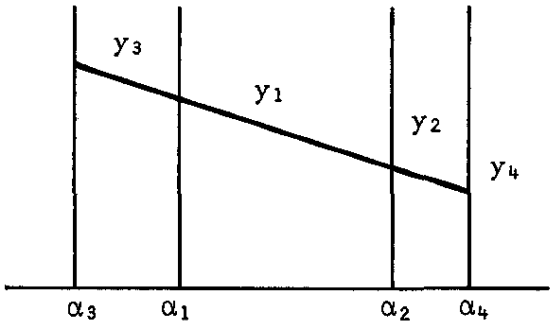
larger the $S(\alpha,\beta)$ can change by orders of magnitude for a fractional change in β. This leads to errors in interpolating between tabular sets of $S(\alpha,\beta)$ at β_L and β_H. Not only is the interpolation used important, but for a given interpolation method the machine word significance limits the accuracy. Ultimately these factors limit the energy range over which the short collision time approximation can be used, the exact limitations being computer dependent.

The best method for interpolation of the $S(\alpha,\beta)$ table generated at high β values would be a three- or four-point Lagrangian interpolation similar to that described in Section 7.2.1. However, the short collision time approximation is only used to extend the tabular (α,β) table and does not justify the more difficult interpolation that would be required to use the Lagrangian method. Instead an interpolation code of ICØDE = 4 is used as described in Section 7.3.3 as the better of the several two-point interpolation schemes. This allows the integration over α to be performed in the same manner as for the tabular $S(\alpha,\beta)$; however, the accuracy of the interpolation method places an upper limit on the energy to which it may be applied.

7.3.6 Basic α Integration

The integral extends from α_L to α_H, and since $S(\alpha,\beta)$ is tabulated, this α range extends over many tabulated points or panels. In this section integration over one panel is described, and in later sections how the results are to be summed over all panels is indicated.

A schematic of a typical panel is given below.



Let $y = \ln(S)$, and hence y is linear in α in the panel whose end points are (α_3,y_3), (α_4,y_4). The desired range of integration is (α_1,α_2). If this panel were the starting panel, $\alpha_1 = \alpha_L$, $\alpha_2 = \alpha_4$; if it were a full panel, $\alpha_1 = \alpha_3$, $\alpha_2 = \alpha_4$; and if it were the last panel, $\alpha_1 = \alpha_3$, $\alpha_2 = \alpha_H$. Let

$$y = a + b\alpha$$

$$b = (y_4 - y_3)/(\alpha_4 - \alpha_3)$$

$$a = y_3 - b\alpha_3$$

and the required integral becomes

$$h_n = \int_{\alpha_1}^{\alpha_2} d\alpha\ \alpha^n e^{a+b\alpha}$$

Let

$$\bar{\alpha} = (\alpha_1+\alpha_2)/2, \qquad x = (\alpha-\bar{\alpha})/\bar{\alpha}$$

$$\rho = \alpha_2/\alpha_1, \qquad \gamma = (\rho-1)/(\rho+1)$$

Expand

$$\alpha^n = \bar{\alpha}^n(1+x)^n = \bar{\alpha}^n\left[1 + nx + \frac{1}{2}n(n-1)x^2 + \frac{1}{6}n(n-1)(n-2)x^3 + \ldots\right]$$

Neglect the last term (and higher terms). The error involved is summarized in the following table.

Relative Error ($\times 10^5$)

n	ρ = 1.02	ρ = 1.03	ρ = 1.04	ρ = 1.05
3	0.1	0.3	0.8	1.6
4	0.4	1.4	3.2	6.2
5	1.0	3.4	8.0	15.6
6	2.0	6.8	16.0	31.2

Since the limitations $\rho \leq 1.03$ and $n \leq 5$ are used in the code, the accuracy is 3.4×10^{-5}.

Define $y = b\bar{\alpha}x$

$c = b\bar{\alpha}\gamma$

Then

$$h_n' = S_1 \alpha_1^{n+1} G_n(c,\rho)$$

$$G_n(c,\rho) = \left(\frac{\rho+1}{2}\right)^{n+1}\left[\gamma F_0(c) + n\gamma^2 F_1(c) + \frac{1}{2}\, n(n-1)\gamma^3 F_2(c)\right]$$

$$F_k(c) = \frac{e^c}{c^{k+1}} \int_{-c}^{c} dy\; y^k e^y$$

$$F_0(c) = \frac{1}{c}\,(e^{2c} - 1)$$

$$= 2e^c\left(1 + \frac{1}{6}\, c^2\right), \qquad c \leqslant 0.20$$

$$F_1(c) = \frac{1}{c}\,(e^{2c} + 1) - \frac{1}{c}\, F_0(c)$$

$$= \frac{2}{3}\, ce^c\left(1 + \frac{1}{10}\, c^2\right), \qquad c \leqslant 0.20$$

$$F_2(c) = \frac{1}{c}\,(e^{2c} - 1) - \frac{2}{c}\, F_1(c)$$

$$= \frac{2}{3}\, e^c\left(1 + \frac{3}{10}\, c^2\right), \qquad c \leqslant 0.20$$

where the approximate expression is accurate to 3.3×10^{-5} if $c \leqslant 0.20$.

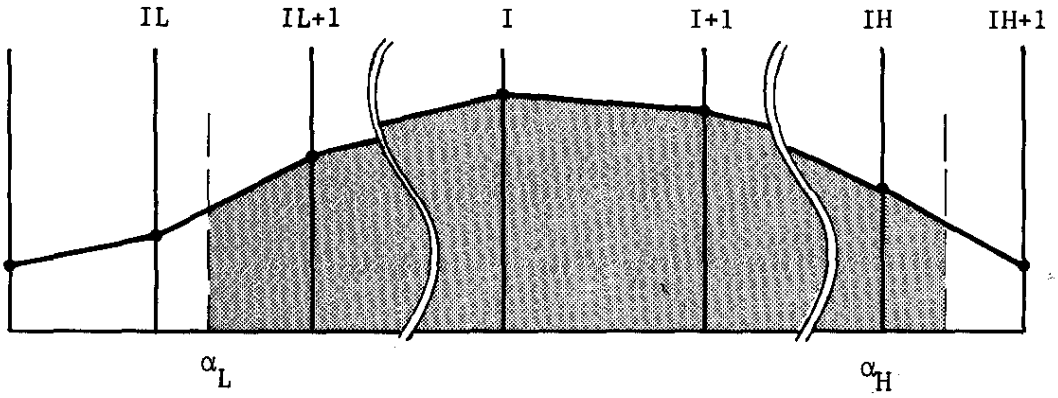
Two subroutines are used to calculate $G_n(c,\rho)$. GNCR calculates $G_n(c,\rho)$ from the above formulas and is used to calculate end panels. For intermediate panels $\rho = \alpha_4/\alpha_3 = \rho_0$, which is a constant for all intermediate panels. Thus, $G_n(c,\rho_0)$ is actually a function only if c and ρ_0 can be tabulated for rapid evaluation. Subroutine GNC sets up tables of $G_n(c,\rho_0)$ at $c' = \pm 0.04(k-1)$, $k = 1, 100$. Three-point quadratic interpolation is used to obtain intermediate values. The combination of three-point quadratic interpolation and $\Delta c = 0.04$ leads to an error less than 3×10^{-5} (the error is approximately $1/2\ (\Delta c)^3$).

7.3.7 Summation of the α Moments

The quantities needed in Section 7.3.1 to calculate the kernels are the moments

$$H_n = \int_{\alpha_L}^{\alpha_H} d\alpha\ \alpha^n S(\alpha,\beta)$$

where $S(\alpha,\beta)$ and $y = \ln[S(\alpha,\beta)]$ at fixed β are tabulated at the points α_i. The region between tabulated points is called a "panel."



Formulas for the integrals over one panel were developed in Section 7.3.6. These formulas are applied to the panels shown in the illustration above. Thus, the summation for all panels is

$$H_n = \sum_{I=IL}^{IH} h_n^I$$

The following cases are to be considered.

Starting Panel (I = IL)

$$h_n^{IL} = S_{IL} e^{b(\alpha_L - \alpha_{IL})} \alpha_L^{n+1} G_n(c,\rho)$$

$$\rho = \alpha_{IL+1}/\alpha_L$$

$$b = (y_{IL+1} - y_{IL})/(\alpha_{IL+1} - \alpha_{IL})$$

$$c = \frac{1}{2} b(\alpha_{IL+1} - \alpha_L)$$

If IL = 0, α_L lies below the limits of the table. In this region $S(\alpha,\beta)$ is assumed to vary like α^k, where k and the constant of proportionality are determined from the first two tabulated points.

$$S(\alpha,\beta) = S_1(\alpha/\alpha_0)^k, \qquad k = (y_2-y_1)/\ln(\rho_0)$$

$$h_n^0 = \frac{S_1}{n+k+1}\left[\alpha_x^{n+k+1} - \alpha_L^{n+k+1}/\alpha_0^k\right]$$

where α_x is the smaller of α_0 and α_H.

Intermediate Panel

$$h_n^I = S_I\alpha_I^{n+1}G_n(c,\rho_0)$$

$$c = \frac{1}{2}(y_{I+1} - y_I)$$

End Panel

$$h_n^I = S_{IH}\alpha_{IH}^{n+1}G_n(c,\rho)$$

$$\rho = \alpha_H/\alpha_{IH}$$

$$b = (y_{IH+1} - y_{IH})(\alpha_{IH+1} - \alpha_{IH})$$

$$c = \frac{1}{2} b(\alpha_H - \alpha_{IH})$$

The equations and logic described above are contained in subroutines KERC and KERA, statements 300-450.

7.4 CROSS SECTION CALCULATION

7.4.1 General Method

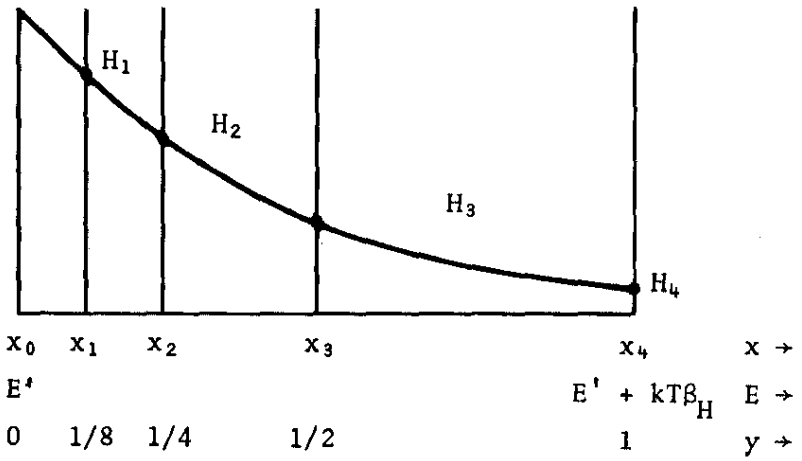
The cross sections are defined by

$$\sigma_\ell(E') = \int_0^\infty dE \sigma_\ell(E' \to E)$$

The final energy integration mesh is determined by the β mesh used to tabulate $S(\alpha,\beta)$ and is independent of the input energy mesh. Again, the E space is represented by a discrete set of points and the region between points is called a "panel." Three different types of panels are considered.

7.4.2 Method for Small β

The region near $\beta = 0$ contributes most heavily to the cross section and may contain a singularity. Consider the panel bounded by $\beta_L = 0$ and β_H for the case where the neutron gains energy (upscattering).



In this region of small β the scattering law varies like α^k, where $k \simeq 1$ for bound motion, $k \simeq -1/2$ for gas motion, and $k \approx -1$ for diffusive motion. The $P_\ell(\mu)$ can be expanded in powers of α so that the scattering kernel will contain terms like

$$I = \int_{\alpha_L}^{\alpha_H} d\alpha \;\; \alpha^{k+\ell} = \frac{1}{k+\ell+1}\left[\alpha_H^{k+\ell+1} - \alpha_L^{k+\ell+1}\right], \quad k+\ell+1 \neq 0$$

$$= \ln(\alpha_H/\alpha_L), \qquad k+\ell+1 = 0$$

Define a dimensionless velocity $x = \sqrt{E/kT}$. Then

$$\alpha_L = \frac{1}{A}(x-x')^2$$

$$\alpha_H = \frac{1}{A}(x+x')^2$$

and the integral above will be proportional to

$$I_m = \frac{1}{m}\left[(x+x')^m - (x-x')^m\right]$$

$$m = 2(k+\ell+1), \; m \neq 0$$

or

$$I_0 = \ln\left|\frac{x+x'}{x-x'}\right|, \; m = 0$$

Considering the possible values of k and ℓ, the possible values of m are m = 0, 1, 2, 3, ...

Referring to the above diagram, let

$x_0 = \sqrt{E'/kT}$

$x_4 = \sqrt{\beta_H + E/kT}$

$\Delta = x_4 - x_0 \qquad y = (x-x_0)/\Delta$

$x_1 = x_0 + 1/8\Delta \qquad y_1 = 1/8 \qquad y_0 = 0$

$x_2 = x_0 + 1/4\Delta \qquad y_2 = 1/4 \qquad y_4 = 1$

$x_3 = x_0 + 1/2\Delta \qquad y_3 = 1/2$

Let H(E) represent $\sigma_\ell(E' \to E)$ for a fixed E' and ℓ, and H_1, H_2, H_3, H_4 represent H(E) at the points x_1, x_2, x_3, x_4. The approximation to the true function is

$$H(y) = \frac{a}{\ln \frac{1}{2}} \ln(y) + b + cy + dy^2$$

which corresponds to taking m = 0, 1, 2, 3 in the discussions above. The coefficients are selected by fitting H(y) to the points H_1, H_2, H_3, H_4. The results are:

$$d = \frac{32}{9}(-2H_1 + 5H_2 - 4H_3 + H_4)$$

$$c = 4(4H_1 - 9H_2 + 6H_3 - H_4)$$

$$b = \frac{1}{9}(-80H_1 + 164H_2 - 88H_3 + 13H_4)$$

$$a = \frac{1}{3}(8H_1 - 14H_2 + 7H_3 - H_4)$$

Next calculate the integral over the panel.

$$I = \int_{E'}^{E'+Tk\beta_H} dEH(E) = 2Tk\Delta \int_0^1 dy(x_0 + y\Delta)H(y)$$

$$= 2kT\Delta x_0 \left(\frac{a}{\ln 2} + b + \frac{1}{2}c + \frac{1}{3}d\right)$$

$$+ 2kT\Delta^2 \left(\frac{a}{4 \ln 2} + \frac{1}{2}b + \frac{1}{3}c + \frac{1}{4}d\right)$$

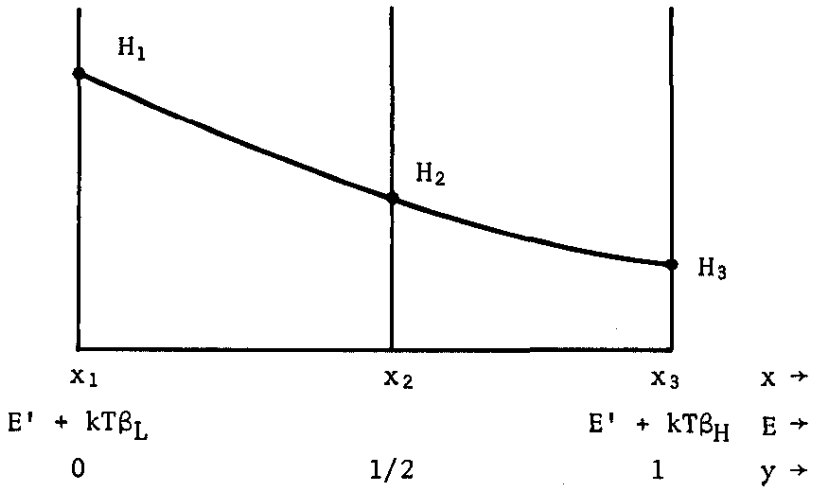
$$= 2kT\Delta x_0(0.58791H_1 - 0.58440H_2 + 0.84776H_3 + 0.14873H_4)$$

$$+ 2kT\Delta^2(0.07291H_1 - 0.12758H_2 + 0.39712H_3 + 0.15755H_4)$$

In the case where the neutron loses energy (downscattering) redefine $\Delta = x_0 - x_4$ so that Δ and y is positive. The integration formula can again be used by changing the sign of the second term. If $E'-Tk\beta_H < 0$, x_4 and H_4 are set to 0.

7.4.3 Method for Intermediate β

A second type of integration scheme is used for intermediate values of β. Again, consider upscattering.



Using the same notation as before,

$x_1 = \sqrt{\beta_L + E'/kT}$ $\qquad$ $y_1 = 0$

$x_3 = \sqrt{\beta_H + E'/kT}$ $\qquad$ $y_2 = 1/2$

$x_2 = x_1 + 1/2\Delta$ $\qquad$ $y_3 = 1$

$\Delta = x_3 - x_1$ $\qquad$ $y = (x-x_1)/\Delta$

Assume that

$$H(y) = a + by + cy^2$$

where the coefficients are obtained by fitting H(y) to the points H_1, H_2, and H_3. Thus,

$$a = H_1$$

$$b = -3H_1 + 4H_2 - H_3$$

$$c = 2(H_1 - 2H_2 + H_3)$$

Calculate the integral over the panel.

$$I = \int_{E'+kT\beta_L}^{E'+kT\beta_H} dEH(E) = 2kT\Delta \int_0^1 dy(x_1 + y\Delta)H(y)$$

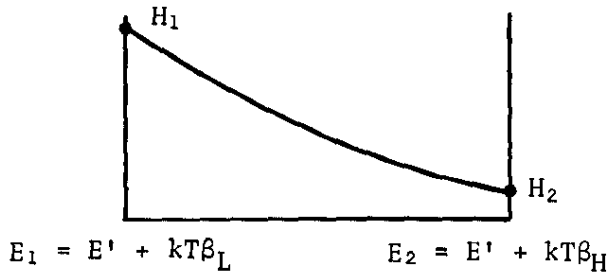
$$= 2kT\Delta x_1(a + \frac{1}{2}b + \frac{1}{3}c) + 2kT\Delta^2(\frac{1}{2}a + \frac{1}{3}b + \frac{1}{4}c)$$

$$= \frac{1}{3}kT\Delta x_1(H_1 + 4H_2 + H_3) + \frac{1}{3}kT\Delta^2(2H_2 + H_3)$$

In the downscattering case, redefine $\Delta = x_1 - x_3$ so that Δ and y are positive. The integration formula given above can again be used by changing the sign of the second term. If $E'-kT\beta_L < 0$, the integral is ignored. If $E'-kT\beta_H < 0$, x_3 and H_3 are set to zero.

7.4.4 Method for Large β

A third type of integration scheme is used for large values of β. Again consider upscattering.



Assume that

$$H(E) = e^{a+bE}$$

$$b = \ln(H_2/H_1)/(E_2 - E_1)$$

$$a = \ln(H_1) - bE_1$$

The integral over the panel is given by

$$I = \int_{E_1}^{E_2} dE H(E) = (E_2-E_1)(H_2-H_1)/\ln(H_2/H_1)$$

If $\varepsilon = (H_2 - H_1)/H_1$ and $|\varepsilon| \leq 0.05$, use

$$I = (E_2 - E_1)H_1/(1 + \frac{1}{2}\varepsilon + \frac{1}{3}\varepsilon^2)$$

which is accurate to 3.3×10^{-5}.

In the downscattering case, reverse E_1 and E_2. If $E_2 < 0$, set $E_2 = 0$, assume H(E) is linear, and

$$I = \frac{1}{2} E_1 H_1$$

Difficulties may arise with this third type of integration scheme since Legendre moments may be negative. If both H_1 and H_2 are negative, exponential integration is used with $|H_1|$ and $|H_2|$, and the answer set negative. If H_1 and H_2 are of opposite sign, a linear form is used.

$$I = \frac{1}{2} |E_2 - E_1| (H_1 + H_2)$$

The equations and logic described in this section are contained in subroutines FEINT and FEINA.

7.4.5 Tabulated $S(\alpha,\beta)$

All three of the preceding integration formulas are used for tabulated $S(\alpha,\beta)$ in subroutine FEINT. The β limits are those specified in the tabulation. The first formula (log + quadratic) is used in the first panel (β near zero). The second formula (quadratic) is used in the next three panels, and the last formula (experimental) is used in the remaining panels. It would be better to provide an automatic switch between the quadratic and exponential formulas, but a suitable switching criterion has yet to be found. If switching on the value of β rather than the panel number is desired, statement 200 in FEINT should be changed.

Since the tabulated scattering law may lead to structure in the kernel, it is not safe to apply a convergence criterion to stop the integration. Therefore, all panels specified for the tabulation are used.

7.4.6 Analytic $S(\alpha,\beta)$

Only the first (log + quadratic) and third (exponential) integration formulas are used for analytic scattering law in subroutine FEINA since the behavior is nearly exponential except near $\beta = 0$. The panel limits are selected in the following way. If $x = \sqrt{E/kT}$, it has been found in practice that a $\Delta x = 0.1$ is a reasonable mesh spacing for integrating a hydrogen gas kernel. A characteristic multiplier of x in the free gas kernel is $2\sqrt{A}/(A+1)$, and starting Δx is

$$\Delta x = 0.2\sqrt{A}/(A+1)$$

where A is the mass associated with the analytic law. This value is used for both free gas laws and diffusive motion laws, but its adequacy for the latter case has yet to be established.

If $x' = \sqrt{E'/kT}$, the limits of the first panel are then

$x' \leqslant x \leqslant x'+\Delta x$ (Upscattering)

$x' \geqslant x \geqslant x'-\Delta x$ (Downscattering)

and the first (log + quadratic) integration formula is used.

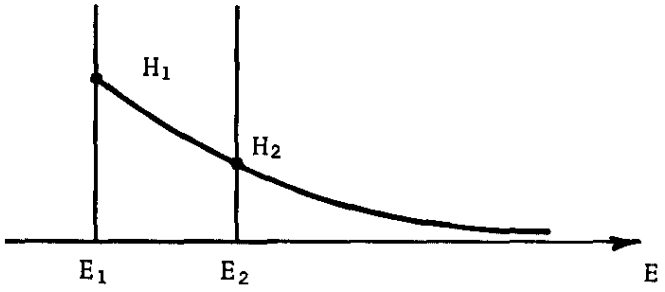
For the remaining panels, the width is uniformly expanded by 5%. If k is the panel number, Δx_k is the width and x_k is the lower bound,

$$\Delta x_k = 1.05\Delta x_{k-1}$$

$$x_k = x_{k-1} + \Delta x_{k-1}$$

The third (exponential) integration formula is used for these panels.

Since the analytic functions are monotonically decreasing on either side of the peak at $\beta = 0$, a convergence criterion can be specified and the integration terminated. Consider first the upscattering part of the isotropic kernel which will be decaying exponentially for large β.



Assume that the panel shown above is the last calculated and that the current value of the integral is I. If

$$b = \ln(H_2/H_1)/(E_2 - E_1)$$

then the integral from E_2 to infinity is estimated to be

$$I_\infty - I = -H_2/b$$

If $|H_2/bI| \leq 10^{-5}$, and if $b < 0$, the integral is assumed to have converged, the quantity H_2/b is added to the integral, and the integration terminated. This test is not made until the fifth panel has been done. The integration is also terminated if more than 200 panels are required to integrate the upscattering part.

The same method is applied to the downscattering part, but here $b > 0$.

TEST PROBLEM 2

Problem 2 is an example of generating a scattering kernel for H bound in H_2O using the short collision approximation to extend the tabular $S(\alpha,\beta)$ mesh to 3.5 ev. The energy mesh for this problem contains 15 groups and was chosen to provide a short illustrative problem rather than for physical reasons. Input cards and printed output are shown below.

TEST PROBLEM 2 INPUT CARDS

```
H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV                    TST2  10
  6007    1002 123456.   296.0    1440.0         3                  TST2  20
     1       1       0       0         0       0       0           TST2  30
     5       0       0       0         0       0                   TST2  40
     0       0       0       0         2      -1      -1           TST2  50
     0       0       3      -1         2                           TST2  60
     4      -2       2                                             TST2  70
    15       1       1       1   0.00005 MESH TO 3.5 EV            TST2  80
     1      15  3.5                                                TST2  90
```

TEST PROBLEM 2 OUTPUT

```
FLANGE II ( VERSION 71-1 )
**************************
 H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV
TAPE LABELED  6C07      ENDF/B NO.  10C2     OUTPUT FID   123456.
TEMPERATURE  296.00(KELVIN)      EFFECTIVE TEMPERATURE FOR SHORT COLLISION 1440.00(KELVIN)
LINKS USED (0=NO, 1=YES)
LINK1  LINK2  LINK3  LINK4  LINK5  LINK6  LINK7
  1      1      0      0      0      0      0
MAX LEGENDRE ORDER = 5
DATA REQUESTED
--------------
              LPDD = 0
              LPFP = 0
  LABS = 0    LPABS= 0
  LFISS= 0    LPFIS= 0
  LTOT = 2    LPTOT=-1
              LPTR =-1
  LELAS= 0    LPEL = 0    LRSCT= 0
  LINEL= 3    LPIN =-1
  LSCAT= 2    LPSC = 0
  LTSL = 4    LPTSL=-2    LEND = 2
ENERGY AND VELOCITY MESH - MESH TO 3.5 EV
  NEG= 15   NEVT=1   METH=1   EVL= 0.0000500
GROUP     ENERGY      VELOCITY      WEIGHT      E BOUNDARY  V BOUNDARY
-----   ----------  ----------  ----------  ----------  ----------
                                                0.0000500   0.0444554
  1      0.1167149   2.1478443   0.2333299
                                                0.2333799   3.0371857
  2      0.3500448   3.7196455   0.2333300
                                                0.4667099   4.2949991
  3      0.5833745   4.8019028   0.2333300
                                                0.7000398   5.2601852
  4      0.8167048   5.6816196   0.2333300
                                                0.9333698   6.0738840
  5      1.0500345   6.4423075   0.2333297
                                                1.1666994   6.7907724
  6      1.2833643   7.1222086   0.2333298
                                                1.4000292   7.4388914
  7      1.5166941   7.7426338   0.2333298
                                                1.6333590   8.0349007
  8      1.7500238   8.3169041   0.2333298
                                                1.8666887   8.5896530
  9      1.9833536   8.8540049   0.2333298
                                                2.1000185   9.1106892
 10      2.2166834   9.3603382   0.2333298
                                                2.3333483   9.6034994
 11      2.4500132   9.8406525   0.2333298
                                                2.5666780  10.0722246
 12      2.6833429  10.2985907   0.2333298
                                                2.8000078  10.5200872
 13      2.9166727  10.7370148   0.2333298
                                                3.0333376  10.9496460
 14      3.1500025  11.1582270   0.2333298
                                                3.2666674  11.3629780
 15      3.3833332  11.5641069   0.2333326
                                                3.5000000  11.7617989
```

LIBRARY TAPE LABELED 6C07
SCATTERING LAW AND CRCSS SECTIONS FOR H2O(1002) AND D2O(1004)

MATERIAL DESCRIPTION
THERMAL SCATTERING LAW DATA COMPUTED AT BNL USING GA CODE GASKET
USING INCOHERENT APPROX WITH EXPERIMENTAL ROTATIONAL FREQUENCY
BAND ACCORDING TC HAYWCOD PLUS TWO DISCRETE VIBRATIONAL MODES.
DATA TABULATED FOR 8 TEMPERATURES %296,350,400,450,500,60C,800,
1000 DEG K<

123456. H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV

CROSS SECTIONS AT T= 296.CO K

GRP	E(EV)	ABSORPTION	INELASTIC	ELASTIC	SCATTERING	TOTAL	TRANSPORT
1	0.116715	0.0	0.32463E 02	0.0	0.32463E 02	0.32463E 02	0.21341E 02
2	0.350045	0.0	0.24720E 02	0.0	0.24720E 02	0.24720E 02	0.13197E 02
3	0.583375	0.0	0.22214E 02	0.0	0.22214E 02	0.22214E 02	0.10752E 02
4	0.816705	0.0	C.21425E C2	0.0	0.21425E 02	C.21425E 02	0.96716E 01
5	1.C50035	0.0	0.20995E 02	0.0	0.20995E 02	0.20995E 02	0.89785E 01
6	1.283364	0.0	0.20815E 02	0.0	0.20815E 02	0.20815E 02	0.86260E 01
7	1.516694	0.0	C.20542E 02	0.0	0.20542E 02	0.20542E 02	0.82242E 01
8	1.750024	0.0	0.20591E 02	0.0	0.20591E 02	C.20591E 02	0.81999E 01
9	1.983354	0.0	C.20352E 02	0.0	0.20352E 02	0.20352E 02	0.78353E 01
10	2.216683	0.0	C.20347E 02	0.0	0.20347E 02	0.20347E 02	0.76733E 01
11	2.450013	0.0	0.20323E C2	0.0	0.20323E 02	0.20323E 02	0.7575dE 01
12	2.683343	0.0	0.20325E 02	0.0	0.20325E 02	C.20325E 02	0.75442E 01
13	2.916673	0.0	C.20325E 02	0.0	0.20325E 02	0.20325E 02	0.75160E 01
14	3.150002	0.0	0.20325E 02	0.0	0.20325E 02	C.20325E 02	0.74859E 01
15	3.383333	0.0	C.20323E 02	0.0	0.20323E 02	0.20323E 02	0.74553E 01

123456. H BOUND IN H2O - 296 DEG K - ENERGY MESH TC 3.5 EV

INELASTIC LEGENDRE CROSS SECTICNS AT T= 296.00 K

GRP	E(EV)	SIGMA C	SIGMA 1 (MU-BAR)	SIGMA 2	SIGMA 3	SIGMA 4	SIGMA 5
1	0.116715	0.32463E 02	0.11122E C2 (0.34260)	0.28390E 01	0.63923E 00	0.15849E 00	0.64228E-01
2	0.350045	0.24720E 02	C.11613E C2 (0.46977)	0.39132E 01	0.95205E 00	0.15079E 00	0.47613E-01
3	0.583375	0.22214E 02	0.11462E C2 (0.51597)	0.42402E 01	0.11940E C1	0.21828E 00	-0.10859E-01
4	0.816705	0.21425E 02	C.11753E C2 (0.54858)	0.45927E 01	0.13231E 01	0.26467E 00	-0.97763E-02
5	1.050035	0.20995E 02	0.12016E 02 (0.57235)	0.47720E 01	0.13444E C1	0.21412E 00	-0.27254E-01
6	1.283364	0.20815E 02	0.12189E 02 (0.58560)	0.49465E 01	0.13274E 01	0.13924E 00	-0.14360E 00
7	1.516694	0.20542E 02	0.12318E C2 (0.59964)	0.50079E 01	0.12853E 01	0.67272E-01	-0.12482E 00
8	1.750024	0.20591E 02	C.12391E 02 (0.60178)	0.50937E 01	0.12697E 01	-0.92039E-03	-0.19073E 00
9	1.983354	0.20352E 02	0.12517E 02 (0.61501)	0.51268E 01	0.12256E 01	-0.60116E-01	-0.22221E 00
10	2.216683	0.20347E 02	0.12674E 02 (0.62288)	0.52354E 01	0.11819E 01	-0.10948E 00	-0.22411E 00
11	2.450013	0.20323E 02	0.12748E 02 (0.62724)	0.53383E 01	0.11364E 01	-0.23651E 00	-0.30276E 00
12	2.683343	0.20325E 02	C.12780E 02 (0.62882)	0.53839E 01	0.11239E 01	-0.33067E 00	-0.36993E 00
13	2.916673	0.20325E 02	0.12809E 02 (0.63022)	0.53837E 01	0.11122E 01	-0.38896E 00	-0.44483E 00
14	3.150002	0.20325E 02	C.12839E 02 (0.63168)	C.53744E 01	0.10921E C1	-0.42362E 00	-0.49651E 00
15	3.383333	0.20323E C2	C.12867E 02 (0.63315)	0.53718E 01	0.10651E 01	-0.44801E 00	-0.51575E 00

123456. H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV

LEGENDRE SCATTERING CROSS SECTIONS AT T= 296.00 K

GRP	E(EV)	SIGMA 0	SIGMA 1 (MU-BAR)	SIGMA 2	SIGMA 3	SIGMA 4	SIGMA 5
1	0.116715	0.32463E 02	0.11122E 02 (0.34260)	0.28390E 01	0.63923E 00	0.15849E 00	0.64228E-01
2	0.350045	0.24720E 02	0.11613E C2 (0.46977)	0.39132E 01	0.95205E 00	0.15079E 00	0.47613E-01
3	0.583375	0.22214E 02	0.11462E C2 (0.51597)	0.42402E 01	0.11940E C1	0.21828E 00	-0.10859E-01
4	0.816705	0.21425E 02	C.11753E 02 (0.54858)	0.45927E 01	0.13231E 01	0.26467E 00	-0.97763E-02
5	1.050035	0.20995E 02	C.12016E 02 (0.57235)	0.47720E 01	0.13444E C1	0.21412E 00	-0.27254E-01
6	1.283364	0.20815E 02	0.12189E C2 (0.58560)	0.49465E 01	0.13274E 01	0.13924E 00	-0.14360E 00
7	1.516694	0.20542E 02	0.12318E C2 (0.59964)	0.50079E 01	0.12853E 01	0.67272E-01	-0.12482E 00
8	1.750024	0.20591E 02	C.12391E 02 (0.60178)	0.50937E 01	0.12697E 01	-0.92039E-03	-0.19073E 00
9	1.983354	0.20352E 02	0.12517E 02 (0.61501)	0.51268E 01	0.12256E 01	-0.60116E-01	-0.22221E 00
10	2.216683	0.20347E 02	0.12674E 02 (0.62288)	0.52354E 01	0.11819E 01	-0.10948E 00	-0.22411E 00
11	2.450013	0.20323E 02	C.12748E 02 (0.62724)	0.53383E 01	0.11364E 01	-0.23651E 00	-0.30276E 00
12	2.683343	0.20325E 02	0.12780E 02 (0.62882)	0.53839E 01	0.11239E 01	-0.33067E 00	-0.36993E 00
13	2.916673	0.20325E 02	0.12809E 02 (0.63022)	0.53837E 01	0.11122E 01	-0.38896E 00	-0.44483E 00
14	3.150002	0.20325E 02	C.12839E 02 (0.63168)	0.53744E 01	0.10921E 01	-0.42362E 00	-0.49651E 00
15	3.383333	0.20323E 02	C.12867E 02 (0.63315)	0.53718E 01	0.10651E 01	-0.44801E 00	-0.51575E 00

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 123456.      H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV

L= 0 SCATTERING KERNEL NORMALIZED TO SIGMA INELASTIC

GROUP   1   INITIAL E= 0.1167149   L= 0
    1  0.13911E 03

GROUP   2   INITIAL E= 0.3500448   L= 0
    1  0.54962E 02      2  0.50976E 02

GROUP   3   INITIAL E= 0.5833745   L= 0
    1  0.28683E 02      2  0.36392E 02    3  0.30126E 02

GROUP   4   INITIAL E= 0.8167048   L= 0
    1  0.20947E 02      2  0.23707E 02    3  0.26051E 02   4  0.21113E 02

GROUP   5   INITIAL E= 1.0500345   L= 0
    1  0.16349E 02      2  0.18904E 02    3  0.18704E 02   4  0.20265E 02   5  0.15754E 02

GROUP   6   INITIAL E= 1.2833643   L= 0
    1  0.13312E 02      2  0.15431E 02    3  0.15630E 02   4  0.15390E 02   5  0.16581E 02   6  0.12865E 02

GROUP   7   INITIAL E= 1.5166941   L= 0
    1  0.11184E 02      2  0.13060E 02    3  0.13183E 02   4  0.13259E 02   5  0.13063E 02   6  0.14031E 02
    7  0.10258E 02

GROUP   8   INITIAL E= 1.7500238   L= 0
    1  0.96221E 01      2  0.11290E 02    3  0.11449E 02   4  0.11452E 02   5  0.11503E 02   6  0.11343E 02
    7  0.12160E 02      8  0.94305E 01

GROUP   9   INITIAL E= 1.9833536   L= 0
    1  0.83133E 01      2  0.98956E 01    3  0.10078E 02   4  0.10130E 02   5  0.10115E 02   6  0.10155E 02
    7  0.10021E 02      8  0.10730E 02    9  0.77872E 01

GROUP  10   INITIAL E= 2.2166834   L= 0
    1  0.76169E 01      2  0.88389E 01    3  0.89597E 01   4  0.90387E 01   5  0.90738E 01   6  0.90552E 01
    7  0.90883E 01      8  0.89738E 01    9  0.96002E 01  10  0.71567E 01

GROUP  11   INITIAL E= 2.4500132   L= 0
    1  0.68895E 01      2  0.81592E 01    3  0.79112E 01   4  0.81250E 01   5  0.81848E 01   6  0.82141E 01
    7  0.81954E 01      8  0.82240E 01    9  0.81242E 01  10  0.86859E 01  11  0.63878E 01

GROUP  12   INITIAL E= 2.6833429   L= 0
    1  0.62890E 01      2  0.74476E 01    3  0.75662E 01   4  0.72410E 01   5  0.74246E 01   6  0.74758E 01
    7  0.75020E 01      8  0.74843E 01    9  0.75096E 01  10  0.74211E 01  11  0.79306E 01  12  0.58143E 01

GROUP  13   INITIAL E= 2.9166727   L= 0
    1  0.57848E 01      2  0.68503E 01    3  0.69589E 01   4  0.69740E 01   5  0.66673E 01   6  0.68331E 01
    7  0.68769E 01      8  0.69030E 01    9  0.68865E 01  10  0.69093E 01  11  0.68298E 01  12  0.72962E 01
   13  0.53376E 01

GROUP  14   INITIAL E= 3.1500025   L= 0
    1  0.53555E 01      2  0.63416E 01    3  0.64420E 01   4  0.64556E 01   5  0.64590E 01   6  0.61756E 01
    7  0.63281E 01      8  0.63699E 01    9  0.63923E 01  10  0.63770E 01  11  0.63977E 01  12  0.63257E 01
   13  0.67558E 01     14  0.49302E 01

GROUP  15   INITIAL E= 3.3833532   L= 0
    1  0.49855E 01      2  0.59033E 01    3  0.59965E 01   4  0.60089E 01   5  0.60118E 01   6  0.60137E 01
    7  0.57506E 01      8  0.58923E 01    9  0.59309E 01  10  0.59519E 01  11  0.59376E 01  12  0.59567E 01
   13  0.58907E 01     14  0.62898E 01   15  0.45793E 01
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 123456.      H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV

L= 1 SCATTERING KERNEL NORMALIZED TO SIGMA INELASTIC

GROUP   1   INITIAL E= 0.1167149   L= 1
    1  0.47663E 02

GROUP   2   INITIAL E= 0.3500448   L= 1
    1  0.77751E 01      2  0.41991E 02

GROUP   3   INITIAL E= 0.5833745   L= 1
    1  0.18757E 01      2  0.18846E 02    3  0.28398E 02

GROUP   4   INITIAL E= 0.8167048   L= 1
    1  0.18054E 01      2  0.98100E 01    3  0.17600E 02  4  0.21154E 02

GROUP   5   INITIAL E= 1.0500345   L= 1
    1  0.13369E 01      2  0.71220E 01    3  0.10912E 02  4  0.15312E 02  5  0.16815E 02

GROUP   6   INITIAL E= 1.2833643   L= 1
    1  0.94828E 00      2  0.52089E 01    3  0.83541E 01  4  0.10400E 02  5  0.13327E 02  6  0.14002E 02

GROUP   7   INITIAL E= 1.5166941   L= 1
    1  0.73688E 00      2  0.40385E 01    3  0.64444E 01  4  0.83011E 01  5  0.95869E 01  6  0.11730E 02
    7  0.11953E 02

GROUP   8   INITIAL E= 1.7500238   L= 1
    1  0.60130E 00      2  0.32624E 01    3  0.52078E 01  4  0.66499E 01  5  0.78964E 01  6  0.87807E 01
    7  0.10447E 02      8  0.10261E 02

GROUP   9   INITIAL E= 1.9833536   L= 1
    1  0.56208E 00      2  0.26864E 01    3  0.43142E 01  4  0.55269E 01  5  0.65049E 01  6  0.74094E 01
    7  0.80535E 01      8  0.94049E 01    9  0.91817E 01

GROUP  10   INITIAL E= 2.2166834   L= 1
    1  0.84568E 00      2  0.22971E 01    3  0.36289E 01  4  0.46697E 01  5  0.55216E 01  6  0.62367E 01
    7  0.69269E 01      8  0.74152E 01    9  0.85453E 01 10  0.82294E 01

GROUP  11   INITIAL E= 2.4500132   L= 1
    1  0.72739E 00      2  0.21157E 01    3  0.31057E 01  4  0.39948E 01  5  0.47407E 01  6  0.53830E 01
    7  0.59315E 01      8  0.64775E 01    9  0.68589E 01 10  0.78259E 01 11  0.74716E 01

GROUP  12   INITIAL E= 2.6833429   L= 1
    1  0.63431E 00      2  0.18451E 01    3  0.27937E 01  4  0.34456E 01  5  0.41110E 01  6  0.46835E 01
    7  0.51896E 01      8  0.56248E 01    9  0.60687E 01 10  0.63734E 01 11  0.72162E 01 12  0.67880E 01

GROUP  13   INITIAL E= 2.9166727   L= 1
    1  0.55949E 00      2  0.16277E 01    3  0.24644E 01  4  0.31315E 01  5  0.35752E 01  6  0.41076E 01
    7  0.45658E 01      8  0.49772E 01    9  0.53313E 01 10  0.56999E 01 11  0.59479E 01 12  0.66932E 01
   13  0.62166E 01

GROUP  14   INITIAL E= 3.1500025   L= 1
    1  0.49837E 00      2  0.14498E 01    3  0.21951E 01  4  0.27893E 01  5  0.32885E 01  6  0.35998E 01
    7  0.40430E 01      8  0.44207E 01    9  0.47629E 01 10  0.50567E 01 11  0.53682E 01 12  0.55730E 01
   13  0.62400E 01     14  0.57379E 01

GROUP  15   INITIAL E= 3.3833332   L= 1
    1  0.44762E 00      2  0.13022E 01    3  0.19714E 01  4  0.25050E 01  5  0.29533E 01  6  0.33454E 01
    7  0.35679E 01      8  0.39468E 01    9  0.42649E 01 10  0.45548E 01 11  0.48026E 01 12  0.50695E 01
   13  0.52408E 01     14  0.58437E 01   15  0.53313E 01
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 123456.      H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV

L= 2 SCATTERING KERNEL NORMALIZED TO SIGMA INELASTIC

GROUP   1   INITIAL E= 0.1167149   L= 2
    1  0.12170E 02

GROUP   2   INITIAL E= 0.3500448   L= 2
    1 -0.68511E 01     2  0.23622E 02

GROUP   3   INITIAL E= 0.5833745   L= 2
    1 -0.36062E 01     2  0.15064E 01   3  0.20271E 02

GROUP   4   INITIAL E= 0.8167048   L= 2
    1 -0.20838E 01     2 -0.16166E 01   3  0.64396E 01  4  0.16943E 02

GROUP   5   INITIAL E= 1.0500345   L= 2
    1 -0.17072E 01     2 -0.17853E 01   3  0.18335E 01  4  0.79253E 01  5  0.14184E 02

GROUP   6   INITIAL E= 1.2833643   L= 2
    1 -0.14625E 01     2 -0.20437E 01   3  0.45500E 00  4  0.36415E 01  5  0.81438E 01  6  0.12405E 02

GROUP   7   INITIAL E= 1.5166941   L= 2
    1 -0.12334E 01     2 -0.20194E 01   3 -0.46395E 00  4  0.19777E 01  5  0.44696E 01  6  0.79089E 01
    7  0.10823E 02

GROUP   8   INITIAL E= 1.7500238   L= 2
    1 -0.10637E 01     2 -0.18945E 01   3 -0.88187E 00  4  0.82607E 00  5  0.28552E 01  6  0.48012E 01
    7  0.75200E 01     8  0.96672E 01

GROUP   9   INITIAL E= 1.9833536   L= 2
    1 -0.92929E 00     2 -0.17796E 01   3 -0.10832E 01  4  0.18443E 00  5  0.16794E 01  6  0.33355E 01
    7  0.48809E 01     8  0.70931E 01   9  0.85901E 01

GROUP  10   INITIAL E= 2.2166834   L= 2
    1 -0.70540E 00     2 -0.16089E 01   3 -0.11904E 01  4 -0.21440E 00  5  0.95758E 00  6  0.22190E 01
    7  0.35811E 01     8  0.48314E 01   9  0.66743E 01 10  0.78927E 01

GROUP  11   INITIAL E= 2.4500132   L= 2
    1 -0.65132E 00     2 -0.13422E 01   3 -0.11676E 01  4 -0.47523E 00  5  0.46505E 00  6  0.14896E 01
    7  0.25522E 01     8  0.36871E 01   9  0.47159E 01 10  0.62813E 01 11  0.73235E 01

GROUP  12   INITIAL E= 2.6833429   L= 2
    1 -0.60477E 00     2 -0.12898E 01   3 -0.11150E 01  4 -0.58291E 00  5  0.11949E 00  6  0.96306E 00
    7  0.18496E 01     8  0.27510E 01   9  0.37090E 01 10  0.45685E 01 11  0.59197E 01 12  0.67859E 01

GROUP  13   INITIAL E= 2.9166727   L= 2
    1 -0.56440E 00     2 -0.12367E 01   3 -0.11349E 01  4 -0.67659E 00  5 -0.75545E-01  6  0.57691E 00
    7  0.13213E 01     8  0.20899E 01   9  0.28615E 01 10  0.36802E 01 11  0.44075E 01 12  0.55896E 01
   13  0.62341E 01

GROUP  14   INITIAL E= 3.1500025   L= 2
    1 -0.52846E 00     2 -0.11846E 01   3 -0.11372E 01  4 -0.76467E 00  5 -0.24718E 00  6  0.32862E 00
    7  0.92096E 00     8  0.15767E 01   9  0.22469E 01 10  0.29136E 01 11  0.36208E 01 12  0.42434E 01
   13  0.52894E 01    14  0.57547E 01

GROUP  15   INITIAL E= 3.3833332   L= 2
    1 -0.49701E 00     2 -0.11343E 01   3 -0.11280E 01  4 -0.82305E 00  5 -0.38473E 00  6  0.11926E 00
    7  0.64265E 00     8  0.11776E 01   9  0.17571E 01 10  0.23455E 01 11  0.29265E 01 12  0.35435E 01
   13  0.40817E 01    14  0.50164E 01  15  0.53793E 01
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 123456.      H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV

L= 3 SCATTERING KERNEL NORMALIZED TO SIGMA INELASTIC

GROUP   1   INITIAL E= 0.1167149   L= 3
    1  0.27410E 01

GROUP   2   INITIAL E= 0.3500448   L= 3
    1 -0.34601E 01     2  0.75416E 01

GROUP   3   INITIAL E= 0.5833745   L= 3
    1 -0.65714E 00     2 -0.55816E 01   3  0.11356E 02

GROUP   4   INITIAL E= 0.8167048   L= 3
    1 -0.41955E 00     2 -0.37318E 01   3 -0.15628E 01  4  0.11385E 02

GROUP   5   INITIAL E= 1.0500345   L= 3
    1 -0.43312E 00     2 -0.27815E 01   3 -0.28791E 01  4  0.13047E 01  5  0.10551E 02

GROUP   6   INITIAL E= 1.2833643   L= 3
    1 -0.34192E 00     2 -0.23953E 01   3 -0.28946E 01  4 -0.12474E 01  5  0.29067E 01  6  0.96609E 01

GROUP   7   INITIAL E= 1.5166941   L= 3
    1 -0.25539E 00     2 -0.19624E 01   3 -0.26522E 01  4 -0.19891E 01  5  0.76413E-01  6  0.37499E 01
    7  0.87408E 01

GROUP   8   INITIAL E= 1.7500238   L= 3
    1 -0.20641E 00     2 -0.16170E 01   3 -0.25808E 01  4 -0.23592E 01  5 -0.10106E 01  6  0.10059E 01
    7  0.41675E 01     8  0.80418E 01

GROUP   9   INITIAL E= 1.9833536   L= 3
    1 -0.18156E 00     2 -0.13751E 01   3 -0.22959E 01  4 -0.23711E 01  5 -0.16442E 01  6 -0.19981E 00
    7  0.16312E 01     8  0.43459E 01   9  0.73465E 01

GROUP  10   INITIAL E= 2.2166834   L= 3
    1 -0.26151E 00     2 -0.11982E 01   3 -0.20575E 01  4 -0.22735E 01  5 -0.18785E 01  6 -0.96907E 00
    7  0.42189E 00     8  0.20440E 01   9  0.43879E 01 10  0.68493E 01

GROUP  11   INITIAL E= 2.4500132   L= 3
    1 -0.22578E 00     2 -0.11465E 01   3 -0.18307E 01  4 -0.21409E 01  5 -0.19483E 01  6 -0.13470E 01
    7 -0.40134E 00     8  0.88520E 00   9  0.23115E 01 10  0.43518E 01 11  0.63617E 01

GROUP  12   INITIAL E= 2.6833429   L= 3
    1 -0.19906E 00     2 -0.10248E 01   3 -0.16741E 01  4 -0.19616E 01  5 -0.19353E 01  6 -0.15400E 01
    7 -0.86239E 00     8  0.55774E-01   9  0.12261E 01 10  0.24798E 01 11  0.42711E 01 12  0.59809E 01

GROUP  13   INITIAL E= 2.9166727   L= 3
    1 -0.17808E 00     2 -0.92428E 00   3 -0.15362E 01  4 -0.18316E 01  5 -0.18334E 01  6 -0.16251E 01
    7 -0.11379E 01     8 -0.44744E 00   9  0.41703E 00 10  0.14750E 01 11  0.25801E 01 12  0.41658E 01
   13  0.56423E 01

GROUP  14   INITIAL E= 3.1500025   L= 3
    1 -0.15803E 00     2 -0.83815E 00   3 -0.14146E 01  4 -0.17231E 01  5 -0.17719E 01  6 -0.15985E 01
    7 -0.12956E 01     8 -0.77455E 00   9 -0.10193E 00 10  0.70008E 00 11  0.16550E 01 12  0.26332E 01
   13  0.40479E 01    14  0.53202E 01

GROUP  15   INITIAL E= 3.3833332   L= 3
    1 -0.14359E 00     2 -0.76368E 00   3 -0.13060E 01  4 -0.16192E 01  5 -0.17085E 01  6 -0.16051E 01
    7 -0.13320E 01     8 -0.98303E 00   9 -0.45876E 00 10  0.18192E 00 11  0.92081E 00 12  0.17837E 01
   13  0.26535E 01    14  0.39246E 01  15  0.50204E 01
```

```
 123456.      H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV

L= 4 SCATTERING KERNEL NORMALIZED TO SIGMA INELASTIC

GROUP   1   INITIAL E= 0.1167149   L= 4
    1  0.67952E 00

GROUP   2   INITIAL E= 0.3500448   L= 4
    1 -0.22943E 00     2  0.87675E CC

GROUP   3   INITIAL E= 0.5833745   L= 4
    1  0.51937E 00     2 -C.484C3E C1   3  0.52573E 01

GROUP   4   INITIAL E= C.8167048   L= 4
    1  0.13253E 00     2 -C.13017E C1   3 -C.45023E 01  4  0.68063E 01

GROUP   5   INITIAL E= 1.0500345   L= 4
    1  0.34614E-01     2 -0.78632E 00   3 -0.28542E 01  4 -C.26079E 01  5  0.71317E 01

GROUP   6   INITIAL E= 1.2833643   L= 4
    1  0.59067E-01     2 -0.57052E CC   3 -0.21773E 01  4 -0.28171E 01  5 -0.91757E 00 6  0.70201E 01

GROUP   7   INITIAL E= 1.5166941   L= 4
    1  0.70161E-01     2 -C.29068E CC   3 -0.17268E 01  4 -0.26242E 01  5 -0.21642E 01 6  0.31578E 00
    7  C.67082E 01

GROUP   8   INITIAL E= 1.75CC238   L= 4
    1  0.64205E-01     2 -0.13208E CC   3 -0.12518E 01  4 -0.23373E 01  5 -0.24451E 01 6 -0.14140E 01
    7  C.11665E 01     8  0.63455E C1

GROUP   9   INITIAL E= 1.9833536   L= 4
    1  0.65486E-01     2 -C.43994E-C1   3 -0.91891E 00  4 -0.19187E 01  5 -0.24249E 01 6 -0.20164E 01
    7 -C.74213E 00     8  C.17416E C1   9  0.6CCC1E 01

GROUP  10   INITIAL E= 2.2166834   L= 4
    1 -0.12828E-01     2 -0.51132E-02   3 -0.67999E 00  4 -0.15671E 01  5 -0.21712E 01 6 -0.22289E 01
    7 -0.15316E 01     8 -C.18867E CC   9  0.21256E 01 10  0.57904E 01

GROUP  11   INITIAL E= 2.4500132   L= 4
    1  0.95343E-02     2 -C.20008E 00   3 -0.52931E 00  4 -0.12777E 01  5 -0.18987E 01 6 -0.21488E 01
    7 -0.19134E 01     8 -0.10723E C1   9  0.25162E 00 10  0.23780E 01 11  0.53872E 01

GROUP  12   INITIAL E= 2.6833429   L= 4
    1  0.81808E-02     2 -0.13258E 00   3 -0.6C538E 00  4 -0.10599E 01  5 -0.16405E 01 6 -0.19862E 01
    7 -0.19793E 01     8 -C.15659E C1   9 -0.66693E 00 10  0.59632E 00 11  C.25394E 01 12  0.50754E 01

GROUP  13   INITIAL E= 2.9166727   L= 4
    1  0.10554E-01     2 -0.89321E-C1   3 -0.47731E 00  4 -0.10060E 01  5 -0.14136E 01 6 -0.17950E 01
    7 -0.19231E 01     8 -0.17433E C1   9 -0.12285E 01 10 -0.32097E 00 11  0.86400E 00 12  0.26374E 01
   13  C.48179E 01

GROUP  14   INITIAL E= 3.15CC025   L= 4
    1  0.21356E-01     2 -0.52344E-C1   3 -0.37835E 00  4 -0.84459E 00  5 -0.12998E 01 6 -0.15948E 01
    7 -C.18072E 01     8 -0.17777E C1   9 -0.14863E 01 10 -C.91930E 00 11 -0.30812E-C1 12  0.10707E 01
   13  0.269C8E 01    14  0.45924E 01

GROUP  15   INITIAL E= 3.3833332   L= 4
    1  0.13175E-01     2 -0.23712E-01   3 -0.29685E 00  4 -0.71056E 00  5 -0.11342E 01 6 -0.14749E 01
    7 -0.16496E 01     8 -C.17321E C1   9 -0.15931E 01 10 -C.12326E 01 11 -0.64430E 00 12  0.21027E 00
   13  C.12296E 01    14  C.27129E 01  15  0.44058E 01
```

```
 123456.      H BOUND IN H2O - 296 DEG K - ENERGY MESH TO 3.5 EV

L= 5 SCATTERING KERNEL NORMALIZED TO SIGMA INELASTIC

GROUP   1   INITIAL E= 0.1167149   L= 5
    1  0.27528E 00

GROUP   2   INITIAL E= 0.3500448   L= 5
    1  0.22507E 00     2 -C.20508E-01

GROUP   3   INITIAL E= 0.5833745   L= 5
    1  0.23697E 00     2 -0.19852E C1   3  0.17025E 01

GROUP   4   INITIAL E= 0.8167048   L= 5
    1 -0.42617E-02     2  C.5398CE CC   3 -0.38746E 01  4  0.32978E 01

GROUP   5   INITIAL E= 1.0500345   L= 5
    1  0.17644E-01     2  0.26773E CO   3 -0.94176E 00  4 -0.36975E 01  5  0.42375E 01

GROUP   6   INITIAL E= 1.2833643   L= 5
    1  0.13150E-01     2  C.23412E CC   3 -0.48378E 00  4 -0.19856E 01  5 -0.27926E 01  6  0.43996E 01

GROUP   7   INITIAL E= 1.5166941   L= 5
    1  0.15668E-01     2  C.32190E CO   3 -0.16702E 00  4 -0.13954E 01  5 -0.22860E 01  6 -0.18150E 01
    7  C.47911E 01

GROUP   8   INITIAL E= 1.7500238   L= 5
    1  0.42361E-01     2  C.29638E CC   3  0.12751E 00  4 -0.90234E 00  5 -0.19258E 01  6 -0.21507E 01
    7 -C.96716E 00     8  C.46624E C1

GROUP   9   INITIAL E= 1.9833536   L= 5
    1  0.58354E-01     2  0.28606E CO   3  0.24981E 00  4 -0.44800E 00  5 -0.14856E 01  6 -0.20937E 01
    7 -0.18260E 01     8 -C.28494E CC   9  0.45518E 01

GROUP  10   INITIAL E= 2.2166834   L= 5
    1 -C.35715E-01     2  0.26530E CC   3  0.32415E 00  4 -0.16944E 00  5 -0.10105E 01  6 -0.18098E 01
    7 -C.20315E 01     8 -0.14454E C1   9  0.24738E 00 10  0.47050E 01

GROUP  11   INITIAL E= 2.4500132   L= 5
    1  0.65480E-01     2  0.157C9E CO   3  0.34450E 00  4  0.24568E-01  5 -0.65991E 00  6 -0.14059E 01
    7 -C.19227E 01     8 -C.18471E C1   9 -0.10716E 01 10  0.65719E 00 11  0.43606E 01

GROUP  12   INITIAL E= 2.6833429   L= 5
    1  0.27658E-01     2  C.17636E 00   3  0.17991E 00  4  0.12750E 00  5 -0.38932E 00  6 -0.10599E 01
    7 -C.16282E 01     8 -C.18951E C1   9 -0.16085E 01 10 -C.73080E 00 11  0.97069E 00 12  0.42440E 01

GROUP  13   INITIAL E= 2.9166727   L= 5
    1  0.34557E-01     2  C.16079E 00   3  0.22637E 00  4  0.20386E-01  5 -0.21581E 00  6 -0.76654E 00
    7 -0.13309E 01     8 -C.17153E C1   9 -0.17836E 01 10 -0.13547E 01 11 -0.43140E 00 12  0.12094E 01
   13  C.40403E 01

GROUP  14   INITIAL E= 3.1500025   L= 5
    1  0.57747E-01     2  C.16118E CO   3  0.24731E 00  4  0.11578E 00  5 -0.23033E 00  6 -0.55396E 00
    7 -0.10537E 01     8 -0.14859E C1   9 -0.17087E 01 10 -0.16271E 01 11 -0.11066E 01 12 -0.17364E 00
   13  C.13903E 01    14  0.38396E C1

GROUP  15   INITIAL E= 3.3833332   L= 5
    1  0.16474E-02     2  C.15289E CC   3  0.26200E 00  4  0.18381E 00  5 -0.92698E-01  6 -0.49364E 00
    7 -C.83022E 00     8 -0.12467E C1   9 -0.15513E 01 10 -0.16418E 01 11 -0.14506E 01 12 -0.87466E 00
   13  C.45866E-01    14  0.15266E C1  15  0.37983E 01
```

APPENDIX B – KERINT SAMPLE PROBLEM

A sample problem for the KERINT code is shown below. The problem is based on four-group scattering kernels up to P_3 Legendre order. Kernels are input at temperatures of 296, 350, and 400 degrees Kelvin. One output kernel is generated at a temperature of 320 degrees Kelvin using Lagrangian interpolation between the input temperature points. Input cards, printed output, and punched output are shown below.

KERINT TEST PROBLEM INPUT CARDS

```
                3          1          3          6  296.0     350.0     400.0
   320.0
0  1  4     296.0000                                                    100.   1
0  1  1   1.5336E 03  0.0          0.0          0.0          0.0        100.   2
0  1  2   2.4722E 02  1.8678E 02  0.0          0.0          0.0        100.   3
0  1  3   2.9186E 01 -5.2174E 01  6.7203E 01   0.0          0.0        100.   4
0  1  4   1.9236E 01  3.2982E 01  3.7361E 01   4.8618E 01   0.0        100.   5
8
1  1  4     296.0000                                                    100.   1
1  1  1   2.9430E 02  0.0          0.0          0.0          0.0        100.   2
1  1  2  -1.2089E 01  7.6304E 01  0.0          0.0          0.0        100.   3
1  1  3  -1.0711E 00  2.6299E 00  4.9855E 01   0.0          0.0        100.   4
1  1  4  -1.3521E-01  2.0590E 00  2.2205E 01   3.5996E 01   0.0        100.   5
8
2  1  4     296.0000                                                    100.   1
2  1  1   4.5001E 01  0.0          0.0          0.0          0.0        100.   2
2  1  2  -1.2712E 01  2.0355E 01  0.0          0.0          0.0        100.   3
2  1  3  -6.4969E-01 -5.1351E 00  2.2647E 01   0.0          0.0        100.   4
2  1  4  -4.8521E-01 -3.0207E 00  4.8136E 00   2.2087E 01   0.0        100.   5
8
3  1  4     296.0000                                                    100.   1
3  1  1   7.4199E 00  0.0          0.0          0.0          0.0        100.   2
3  1  2  -2.8404E 00  4.2747E 00  0.0          0.0          0.0        100.   3
3  1  3   1.1826E-01 -4.4959E-01  5.7110E 00   0.0          0.0        100.   4
3  1  4  -2.3636E-02 -6.2900E-01 -6.4328E 00   1.5396E 01   0.0        100.   5
8
```

```
0  1  4     350.0000                                                    100.   1
0  1  1   1.4080E 03  0.0           0.0           0.0           0.0     100.   2
0  1  2   2.4653E 02  1.8770E 02    0.0           0.0           0.0     100.   3
0  1  3   2.9252E 01  5.1996E 01    6.7547E 01    0.0           0.0     100.   4
0  1  4   1.9211E 01  3.2953E 01    3.7650E 01    4.8550E 01    0.0     100.   5
8
1  1  4     350.0000                                                    100.   1
1  1  1   3.0660E 02  0.0           0.0           0.0           0.0     100.   2
1  1  2  -1.1184E 01  7.6351E 01    0.0           0.0           0.0     100.   3
1  1  3  -1.0129E 00  2.6801E 00    4.9868E 01    0.0           0.0     100.   4
1  1  4  -1.2940E-01  2.0733E 00    2.2170E 01    3.6067E 01    0.0     100.   5
8
2  1  4     350.0000                                                    100.   1
2  1  1   5.4561E 01  0.0           0.0           0.0           0.0     100.   2
2  1  2  -1.2486E 01  2.0603E 01    0.0           0.0           0.0     100.   3
2  1  3  -6.9019E-01 -5.1577E 00    2.2697E 01    0.0           0.0     100.   4
2  1  4  -4.8544E-01 -3.0007E 00    4.9056E 00    2.1570E 01    0.0     100.   5
8
3  1  4     350.0000                                                    100.   1
3  1  1   1.0516E 01  0.0           0.0           0.0           0.0     100.   2
3  1  2  -2.8399E 00  4.4641E 00    0.0           0.0           0.0     100.   3
3  1  3   9.6219E-02 -5.8430E-01    5.8183E 00    0.0           0.0     100.   4
3  1  4  -1.9590E-02 -6.3109E-01   -6.3061E 00    1.5265E 01    0.0     100.   5
8
0  1  4     400.0000                                                    100.   1
0  1  1   1.2827E 03  0.0           0.0           0.0           0.0     100.   2
0  1  2   2.4612E 02  1.8852E 02    0.0           0.0           0.0     100.   3
0  1  3   2.9270E 01  5.1778E 01    6.7862E 01    0.0           0.0     100.   4
0  1  4   1.9135E 01  3.2840E 01    3.7893E 01    4.8483E 01    0.0     100.   5
8
1  1  4     400.0000                                                    100.   1
1  1  1   3.1859E 02  0.0           0.0           0.0           0.0     100.   2
1  1  2  -1.0127E 01  7.6318E 01    0.0           0.0           0.0     100.   3
1  1  3  -9.5205E-01  2.7490E 00    4.9842E 01    0.0           0.0     100.   4
1  1  4  -1.1753E-01  2.0884E 00    2.2136E 01    3.6082E 01    0.0     100.   5
8
2  1  4     400.0000                                                    100.   1
2  1  1   6.4641E 01  0.0           0.0           0.0           0.0     100.   2
2  1  2  -1.2385E 01  2.0786E 01    0.0           0.0           0.0     100.   3
2  1  3  -7.2571E-01 -5.1586E 00    2.2726E 01    0.0           0.0     100.   4
2  1  4  -4.8469E-01 -2.9712E 00    4.9812E 00    2.1855E 01    0.0     100.   5
8
3  1  4     400.0000                                                    100.   1
3  1  1   1.3269E 01  0.0           0.0           0.0           0.0     100.   2
3  1  2  -2.8343E 00  4.5947E 00    0.0           0.0           0.0     100.   3
3  1  3   7.3984E-02 -7.0395E-01    5.9089E 00    0.0           0.0     100.   4
3  1  4  -2.7226E-02 -6.3372E-01   -6.1643E 00    1.5117E 01    0.0     100.   5
8
9
```

PRINTED OUTPUT FROM KERINT

```
L = 0 SCATTERING KERNEL FOR ZA =    100. AT T =  320.00 DEG K

GROUP   1  L = 0
    1  C.14790E 04

GROUP   2  L = 0
    1  0.24688E 03     2  C.18719E 03

GROUP   3  L = 0
    1  0.29221E 02     2  0.52102E C2     3  0.67356E 02

GROUP   4  L = 0
    1  0.19232E 02     2  C.32981E C2     3  0.37493E 02     4  0.48588E 02


L = 1 SCATTERING KERNEL FOR ZA =    100. AT T =  320.00 DEG K

GROUP   1  L = 1
    1  C.29968E 03

GROUP   2  L = 1
    1 -C.11717E 02     2  0.76335E C2

GROUP   3  L = 1
    1 -0.10462E 01     2  C.26491E C1     3  0.49866E 02

GROUP   4  L = 1
    1 -0.13353E 00     2  0.20651E C1     3  0.22190E 02     4  0.36035E 02


L = 2 SCATTERING KERNEL FOR ZA =    100. AT T =  320.00 DEG K

GROUP   1  L = 2
    1  C.49080E 02

GROUP   2  L = 2
    1 -0.12597E 02     2  C.20472E C2

GROUP   3  L = 2
    1 -0.66796E 00     2 -C.51479E C1     3  0.22672E 02

GROUP   4  L = 2
    1 -0.48545E 00     2 -C.30133E C1     3  0.48558E 01     4  0.22036E 02


L = 3 SCATTERING KERNEL FOR ZA =    100. AT T =  320.00 DEG K

GROUP   1  L = 3
    1  C.88117E 01

GROUP   2  L = 3
    1 -C.28409E 01     2  0.43651E C1

GROUP   3  L = 3
    1  0.10872E 00     2 -C.51016E CC     3  0.57599E 01

GROUP   4  L = 3
    1 -0.20262E-01     2 -0.62983E 00     3 -0.63799E 01     4  0.15341E 02
```

PUNCHED OUTPUT FROM KERINT

```
 0  1  4   0.3200E 03                                                    100.   1
*0  1  1   1.4790E 03  0.0          0.0          0.0          0.0       100.   2
 0  1  2   2.4688E 02  1.8719E 02  0.0          0.0          0.0       100.   3
 0  1  3   2.9221E 01  5.2102E 01  6.7356E 01  0.0          0.0       100.   4
 0  1  4   1.9232E 01  3.2981E 01  3.7493E 01  4.8588E 01  0.0       100.   5
 1  1  4   0.3200E 03                                                    100.   1
 1  1  1   2.9968E 02  0.0          0.0          0.0          0.0       100.   2
 1  1  2  -1.1717E 01  7.6335E 01  0.0          0.0          0.0       100.   3
 1  1  3  -1.0462E 00  2.6491E 00  4.9866E 01  0.0          0.0       100.   4
 1  1  4  -1.3353E-01  2.0651E 00  2.2190E 01  3.6035E 01  0.0       100.   5
 2  1  4   0.3200E 03                                                    100.   1
 2  1  1   4.9080E 01  0.0          0.0          0.0          0.0       100.   2
 2  1  2  -1.2597E 01  2.0472E 01  0.0          0.0          0.0       100.   3
 2  1  3  -6.6796E-01 -5.1479E 00  2.2672E 01  0.0          0.0       100.   4
 2  1  4  -4.8545E-01 -3.0133E 00  4.8558E 00  2.2036E 01  0.0       100.   5
 3  1  4   0.3200E 03                                                    100.   1
 3  1  1   8.8117E 00  0.0          0.0          0.0          0.0       100.   2
 3  1  2  -2.8409E 00  4.3651E 00  0.0          0.0          0.0       100.   3
 3  1  3   1.0872E-01 -5.1016E-01  5.7599E 00  0.0          0.0       100.   4
 3  1  4  -2.0262E-02 -6.2983E-01 -6.3799E 00  1.5341E 01  0.0       100.   5
```

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8. AUXILIARY CODE KERINT

8.1 INTRODUCTION

In Section 7.2.1 limitations on the temperature interpolation of $S(\alpha,\beta,T)$ were described. These restrictions were based on inaccuracies that arise in temperature interpolation due to rapidly changing values of $S(\alpha,\beta,T)$ and computer word length. Generally these restrictions allow accurate interpolations at any temperature only for energy meshes whose maximum energy transfer is <0.85 ev at room temperature. An example of such a dependence is shown in the following table for moderator H_2O (ENDF/B MAT = 1002).

P_0 Total Scattering Cross Section (barns) for Moderator H_2O (MAT = 1002)

Temperature, °K	Energy, ev			
	1.0	0.625	0.1	0.025
296[a]	46.141	47.718	71.485	111.53
300	57.309	47.736	71.501	111.60
310	62.153	47.767	71.546	111.80
320	56.912	47.784	71.589	112.00
330	51.536	47.796	71.633	112.20
340	48.035	47.809	71.674	112.40
350[a]	46.235	47.823	71.718	112.61

a. A temperature at which $S(\alpha,\beta)$ is tabulated.

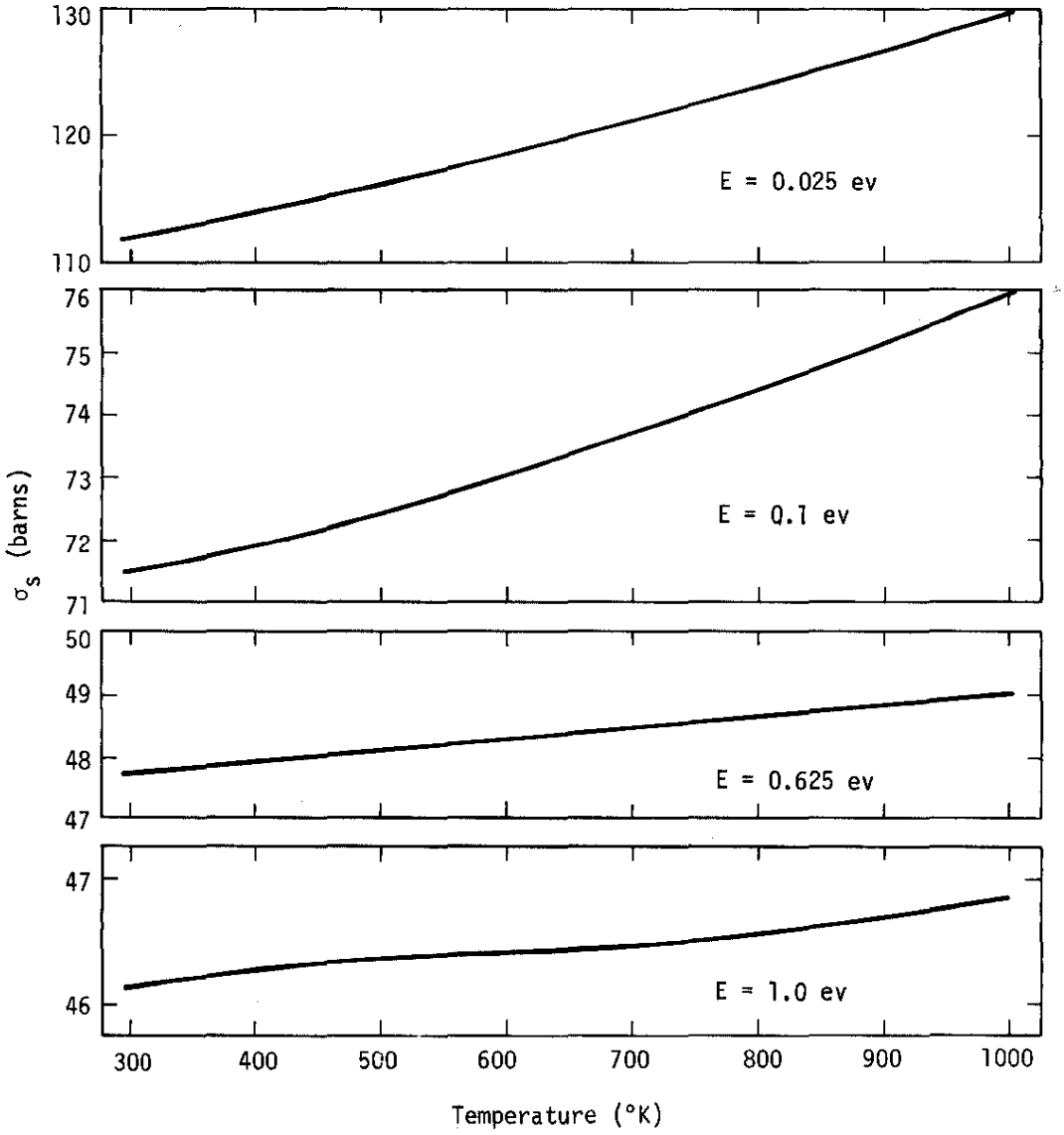
Some materials however have tabular $S(\alpha,\beta)$ data that correspond to larger energy transfer ($\cong$ 2 ev) at room temperature. For these materials the temperature interpolation methods used in FLANGE II will lead to significant errors in kernels and cross sections for energy group with energies >0.85 ev and temperatures between the tabulated temperature on the ENDF/B tape.

An alternative method of obtaining kernels at intermediate temperature is provided by the code KERINT. The restrictions on temperature interpolation do not apply to temperatures at which the $S(\alpha,\beta)$ are tabulated on the ENDF/B tape and it is possible to generate kernels with energy transfers limited only by the accuracy that can be maintained in the short collision time approximation (generally $\cong$ 4.0 ev at room temperature). Several scattering kernels may be generated, therefore, at the temperature at which the $S(\alpha,\beta)$ is tabulated, then code KERINT will interpolate

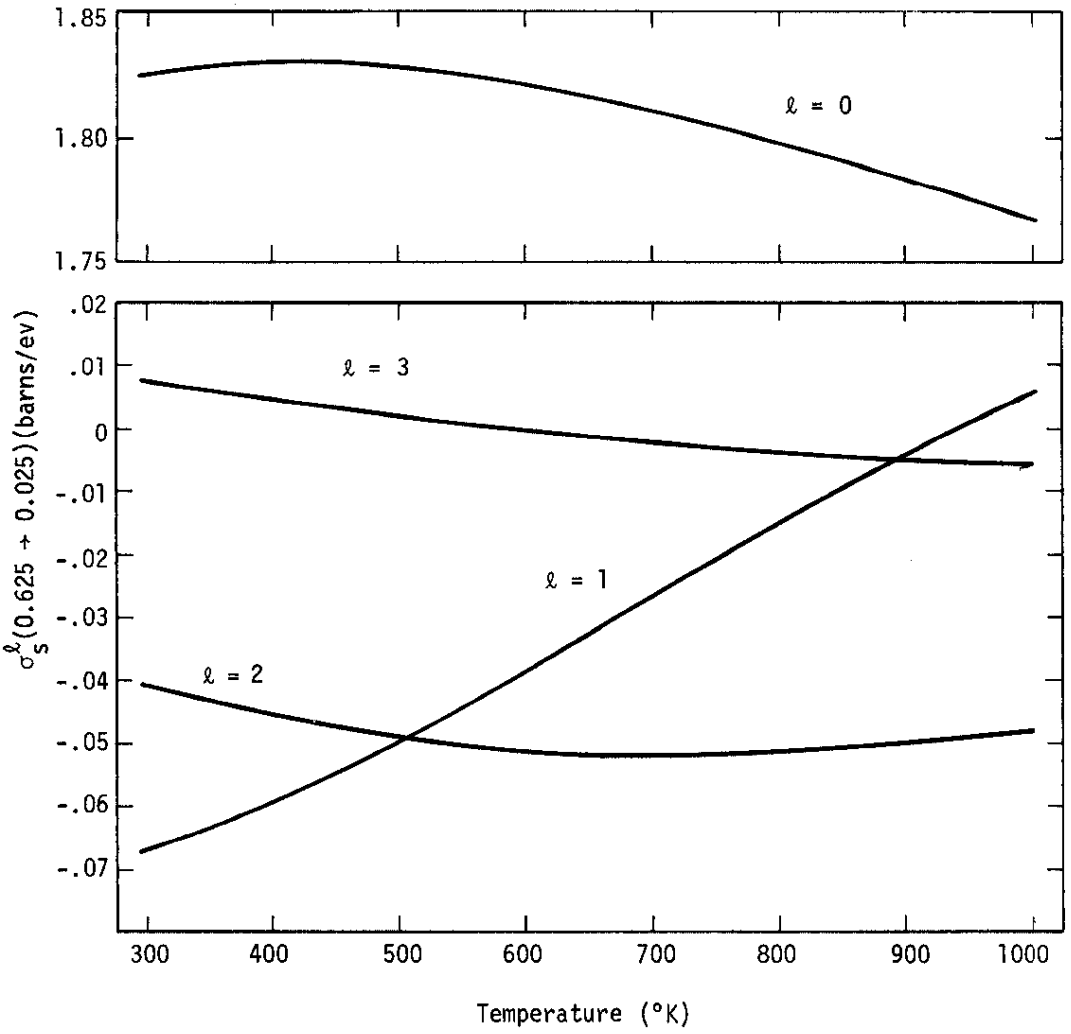
the kernel directly at intermediate temperatures. Two-point and three-point temperature interpolations are provided with a choice of interpolation methods.

8.2 TEMPERATURE DEPENDENCE OF CROSS SECTIONS AND KERNEL ELEMENTS

Unlike the $S(\alpha,\beta)$, the scattering cross sections and kernel elements are smooth functions of temperature. A diagram of the temperature dependence of the P_0 scattering cross section for molecular H_2O (MAT = 1002) as a function of temperature for several energies is given below.



Similarly a diagram of the differential scattering cross section for scattering from 0.625 to 0.025 ev is shown below as a function of Legendre scattering order.



From these diagrams it is clear that two-point temperature interpolation of the kernels should be sufficient for molecular H_2O. Three-point temperature interpolation is probably better, however, for cases where Bragg scattering peaks may shift as a function of temperature (as is the case for ZrH, Be, BeO, and graphite).

8.3 INTERPOLATION CODES

Several possible interpolation codes are built into KERINT for both two- and three-point temperature interpolations. The two-point interpolation codes are described in Section 3.1 and summarized below and identified by flag ICODE.

8.3.1 Two-Point Interpolation Codes

ICØDE=1 $\sigma(T)$ linear in T

$$\sigma(T) = \sigma(T_1) + [\sigma(T_2) - \sigma(T_1)]\ [(T - T_1)/(T_2 - T_1)]$$

ICØDE=2 $\ell n[\sigma(T)]$ linear in T

$$\sigma(T) = \sigma(T_1) + [\sigma(T_2) - \sigma(T_1)]\ [\ln(T/T_1)/\ln(T_2/T_1)]$$

ICØDE=3 $\sigma(T)$ linear in ln(T)

$$\ln[\sigma(T)] = \ln[\sigma(T_1)] + \ln[\sigma(T_2)/\sigma(T_1)]\ [(T - T_1)/(T_2 - T_1)]$$

ICØDE=4 $\ln[\sigma(T)]$ linear in ln(T)

$$\ln[\sigma(T)] = \ln[\sigma(T_1)] + \ln[\sigma(T_2)/\sigma(T_1)]\ [\ln(T/T_1)/\ln(T_2/T_1)]$$

Two three-point interpolation codes are available described below and identified by flag ICODE.

8.3.2 Three-Point Interpolation Codes

ICODE=5 Three-point least squares fit to form $\sigma(T) = Ae^{BT}$

$$\ln \sigma(T) = \frac{\left(\sum_{i=1}^{3} T_i^2 - T \sum_{i=1}^{3} T_i\right)\left(\sum_{i=1}^{3} \ln[(\sigma(T_i)]\right)}{\left(3 \sum_{i=1}^{3} T_i^2\right) - \left(\sum_{i=1}^{3} T_i\right)^2}$$

$$+ \frac{\left(3T - \sum_{i=1}^{3} T_i\right)\left(\sum_{i=1}^{3} T_i \ln[\sigma(T_i)]\right)}{\left(3 \sum_{i=1}^{3} T_i^2\right) - \left(\sum_{i=1}^{3} T_i\right)^2}$$

ICODE=6 Three-point Lagrangian to polynomial form
$\sigma(T) = A + BT + CT^2$

$$\sigma(T) = (T-T_2)(T-T_3)\sigma(T_1)/(T_1-T_2)(T_1-T_3)$$
$$+ (T-T_1)(T-T_3)\sigma(T_2)/(T_2-T_1)(T_2-T_3)$$
$$+ (T-T_1)(T-T_2)\sigma(T_3)/(T_3-T_1)(T_3-T_2)$$

A comparison of the six interpolation codes is made in the next table for molecular H_2O (MAT = 1002) at E = 0.625 ev and T = 320°K. The values may be compared to the exact value of 47.784 barns shown in the table of Section 8.1. Temperatures at which kernels were generated were 296, 350, and 400°K.

ICODE	σ_2 at 0.625 ev and 320°K	$\frac{\text{Correct-Interpolated}}{\text{Correct}} \times 100$
1	47.7647	0.040
2	47.7668	0.036
3	47.7647	0.040
4	47.7668	0.036
5	47.7636	0.042
6	47.7671	0.035

8.4 DESCRIPTION OF KERINT

KERINT contains a main program and four subroutines. The main program is divided generally into three functions: reading and checking input, reading and storing kernels using one scratch tape NSTA if required, and interpolating and punching the interpolated kernel.

8.4.1 Data Set Assignments

The following data sets are used and their values are stored in COMMON/TAPES/. Numbers are assigned in the main program.

NIN - System input = 5

NOUT - System output = 6

NPUN - System punch = 7

NTSA - Scratch data set (disk, drum, or tape) = 3

8.4.2 Error Stops

Errors are handled by subroutine ERROR which prints a full message. These are the following:

1. "THE NUMBER OF INPUT TEMPERATURES IS LE 0" - Check the input cards and specify what temperature kernels will be read into the code.

2. "THE NUMBER OF OUTPUT TEMPERATURES IS LE 0" - No temperatures have been specified for kernels to be generated. Check input cards.

3. "NUMBER OF OUTPUT TEMPERATURES GT 20" - Kernels may be generated at only 20 temperatures on output.

4. "INTERPOLATION CODE LE 0 OR GT 6" - An incorrect interpolation code is specified in the input.

5. "END OF FILE OCCURRED ON THE READER BEFORE END OF INPUT" - More input kernels were expected than were in the input deck.

6. "KERNELS HAVE INCONSISTENT NUMBERS OF GROUPS" - A kernel was read specifying a different number of groups than the previous kernels.

7. "A KERNEL HAS A TEMPERATURE DIFFERENT FROM THE SPECIFIED TABULATED TEMPERATURES" - A kernel was read with a temperature that did not agree with those specified.

8. "TWO TEMPERATURES ARE IDENTICAL" - Two kernels specified as tabulated temperatures are identical.

8.4.3 Kernel Storage

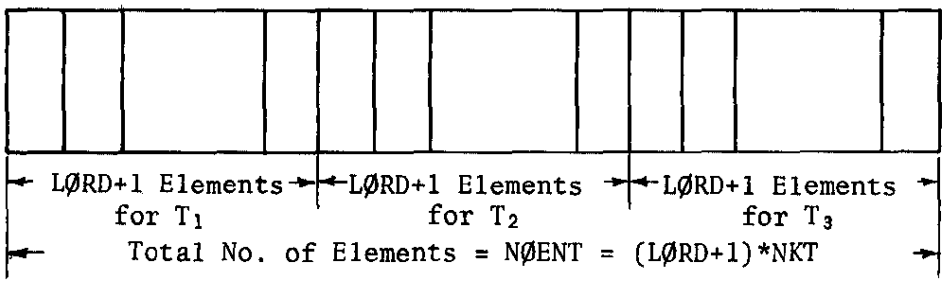
Storage of a kernel for interpolation purposes presents a data handling problem. FLANGE II generates scattering kernels for ~~emergency~~ meshes up to 200 points; however, because it generates only the downscattering part of the kernel this corresponds to 20,100 transfer elements for each Legendre order and temperature. For interpolation purposes it is desirable to store kernels for all Legendre orders and temperatures simultaneously to obtain all desired output temperatures from a single pass through the code. The storage necessary to do this for a 200-group energy mesh, P_5 Legendre kernels, and three-point temperature interpolation is 361,800 single precision words. This amount of fast core storage is not available; hence a system utilizing a single scratch data set (NSTA) is used.

All data are stored in a singly indexed array. This array gives values of the initial and final energy groups for which transfer elements are given. The array values are defined as

$$IN(I) = 1000*NI+NF \qquad (I=1,NUMB)$$

where IN(I) is the array value, NI is the initial group index, NF is the final group index, and NUMB is the number of array values for a given set of transfer matrices. The maximum value of NUMB is 20,100.

The transfer elements for a set of matrices by Legendre order and temperature are stored in pages of data, each page containing a fixed number of entries. If the Legendre order specified is LØRD and there are NKT temperatures (=2, or 3) a typical entry is diagrammed below.



For each entry in the IN(I) array there will be a segment of a data page as diagrammed above for the indicated initial to final group transfers. These are stored sequentially in the data pages starting with the first entry IN(1) to the last entry, IN(NUMB) each having length NOENT = (LØRD+1)*NKT. Each page of data can store JMAX(= 9600) words of data; hence, each page can store NØPP = JMAX/NØENT entries.

The procedure to store the kernels then is the following: The IN(I) array and NUMB are set to zero. NSTA is rewound, data page NPAGE is set to 1, and the page values X(J) are set to zero. The first kernel is read in the format that FLANGE II punches. As each element is read, array IN(I) is checked to see if this transfer element has been read. If it has not been read, a new entry in IN(I) is created, the appropriate area is reserved in X(J), and data for the particular transfer element are stored by temperature and Legendre order. As each data page is filled up it is written to NSTA with the page number attached. The first kernel must reserve all data space, and care must be taken to assure that new transfer elements do not occur in subsequent kernels.

After the first kernel is read NSTA is rewound. Each subsequent kernel element is then read, the appropriate location in the data pages is determined, and data are stored by temperature and Legendre order. The method of location is as follows:

- Array IN(I) is searched until the proper initial and final energy groups are found. Designate this value IX.
- The page number on which the data entry resides is determined from IPAGE = IX/NØPP+1 where NØPP is the number of data entries/page.
- The proper page is brought into core from NSTA.
- The position of the entry on the page is determined from IPT = IX-(IPAGE-1)*NØPP.
- The first word of the entry on the page is determined from IWD = (IPT-1)*NØENT+1 where NØENT = (LØRD+1)NKT.

Each kernel element is stored in the above manner as it is read from a card.

8.5 INPUT/OUTPUT DESCRIPTION

8.5.1 Input

The input to KERINT contains 1 to 4 input cards plus scattering kernels for each Legendre order and temperature specified. The required data are as follows.

Number	Columns	Format	Mnemonic	Description
1	1-10	I10	NKT	Number of temperatures at which kernels are input (= 2 or 3)
	11-20	I10	NT	Number of temperatures at which kernels will be interpolated (≤20)
	21-30	I10	LØRD	Highest Legendre order contained in input kernels (≤5)
	31-40	I10	ICØDE	Interpolation code (Section 8.3)
	41-50	E10.0	T1	Temperature (°K) of first set of kernels
	51-60	E10.0	T2	Temperature (°K) of second set of kernels
	61-70	E10.0	T3	Temperature (°K) of third set of kernels
2-4		8E10.0	T(I)	NT temperatures at which kernels will be interpolated (°K)

The above cards are followed by (LØRD+1)*NKT scattering kernels each corresponding to one Legendre order at one temperature (T1, T2, or T3). Each kernel is followed by a blank card with an 8-punch in Column 1 to signal the end of a kernel.

The last card of a problem is a blank card with a 9-punch in Column 1.

An example of an input deck for KERINT is shown in Appendix B.

8.5.2 Output

For each temperature T(I) specified on input a kernel for each Legendre order $P_0 \rightarrow P_{LØRD}$ will be punched in the format described in Section 5.3 for scattering kernels. A printout similar to that for FLANGE II will be produced for each kernel at each temperature. An example of this printout is shown in Appendix B.

9. REFERENCES

1. *Data Formats and Procedures for the ENDF Neutron Cross Section Library.* Edited by M. K. Drake, Brookhaven National Lab., Upton, N. Y. USAEC Report BNL 50274 (T-601) (ENDF 102, Vol. I) (1970).

2. G. M. Borgonovi. *Neutron Scattering Kernel Calculations at Epithermal Energies.* USAEC Report GA-9950, General Atomic, Inc., San Diego, Calif. (1970).

3. J. E. Lynn. *The Theory of Neutron Resonance Reactions.* Chapter VII, Clarendon Press, Oxford (1968).

4. B. J. Toppel, A. L. Rago, and D. M. O'Shea. *MC^2 - A Code to Calculate Multigroup Cross Sections.* USAEC Report ANL-7318, Argonne National Lab., Ill. (1967).

5. D.M. O'Shea and H.C. Thacher. "Computation of Resonance Line Shape Functions." Trans. Am. Nucl. Soc. 6, 36 (June 1963).

EQN/bch/mp

APPENDIX A – FLANGE II SAMPLE PROBLEMS

Two sample problems are shown for use in checking the code and as illustrations of its use.

TEST PROBLEM 1

Problem 1 is an example of obtaining group-averaged cross sections with no scattering matrices being generated. The energy mesh for this problem is the standard 30-group THERMØS code mesh. The material is uranium-235 taken from ENDF/B-II (MAT = 1102 from tape 201). Input cards and printed output are shown below.

TEST PROBLEM 1 INPUT CARDS

```
U-235 AT 0 DEG K - MAT 1102 - GROUP AVERAGED CROSS SECTIONS          TST1  10
  201    1102   0.0    0.0                  3                      TST1  20
    1       0                                                      TST1  30
    1       0      0                                               TST1  40
    1      -2      1      -2          1      -1          -2        TST1  50
    1      -2      0       0          2      -2                    TST1  60
    0       0      0                                               TST1  70
   30       2      2       1    0.05  THERMOS V MESH                TST1  80

 0.1     0.1     0.1     0.1     0.1     0.1     0.1               TST1  90
 0.1     0.1     0.1     0.1     0.1     0.1     0.1               TST1 100
 0.1     0.11    0.12    0.13    0.14    0.145   0.165             TST1 110
 0.19    0.22    0.255   0.295   0.34    0.39    0.445             TST1 120
 0.505   0.57                                                      TST1 130
```

TEST PROBLEM 1 OUTPUT

```
FLANGE II ( VERSION 71-1 )
**************************

 U-235 AT 0 DEG K - MAT 1102 - GROUP AVERAGED CROSS SECTIONS

TAPE LABELED   201     ENDF/B NO.  1102     OUTPUT FID        0.

TEMPERATURE    0.0 (KELVIN)     EFFECTIVE TEMPERATURE FOR SHORT COLLISION    0.0 (KELVIN)

LINKS USED (0=NO, 1=YES)
LINK1  LINK2  LINK3  LINK4  LINK5  LINK6  LINK7
  1      0      0      0      0      0      0

MAX LEGENDRE ORDER = 1

DATA REQUESTED
--------------
              LPDD = 0
              LPFP = 0
  LABS = 1    LPABS=-2
  LFISS= 1    LPFIS=-2
  LTOT = 1    LPTOT=-1
              LPTR =-2
  LELAS= 1    LPEL =-2    LRSCT= 0
  LINEL= 0    LPIN = 0
  LSCAT= 2    LPSC =-2
  LTSL = 0    LPTSL= 0    LBND = 0

ENERGY AND VELOCITY MESH -  THERMOS V MESH

  NEG= 30   NEVT=2   METH=2   EVL= 0.0500000

GROUP     ENERGY      VELOCITY     WEIGHT     E BOUNDARY  V BOUNDARY
-----  ----------  ----------  ----------  ----------  ----------
                                                0.0000632   0.0500000
  1       0.0002530   0.0999999   0.0005060
                                                0.0005692   0.1499999
  2       0.0010120   0.1999999   0.0010120
                                                0.0015812   0.2499999
  3       0.0022770   0.2999998   0.0015180
                                                0.0030992   0.3499998
  4       0.0040480   0.3999998   0.0020240
                                                0.0051232   0.4499998
  5       0.0063250   0.4999998   0.0025300
                                                0.0076532   0.5499998
  6       0.0091080   0.5999994   0.0030360
                                                0.0106892   0.6499997
  7       0.0123970   0.6999993   0.0035420
                                                0.0142312   0.7499997
  8       0.0161920   0.7999992   0.0040480
                                                0.0182792   0.8499997
  9       0.0204930   0.8999996   0.0045540
                                                0.0228332   0.9499996
 10       0.0253000   0.9999990   0.0050600
                                                0.0278932   1.0499992
 11       0.0306129   1.0999985   0.0055660
                                                0.0334592   1.1499987
 12       0.0364319   1.1999979   0.0060720
                                                0.0395311   1.2499981
 13       0.0427568   1.2999973   0.0065779
                                                0.0461091   1.3499975
 14       0.0495878   1.3999968   0.0070839
```

				0.0531930	1.4499969
15	0.0569247	1.4999962	0.0075900		
				0.0607830	1.5499964
16	0.0651730	1.6049957	0.0089334		
				0.0697163	1.6599960
17	0.0748471	1.7199955	0.0104437		
				0.0801601	1.7799959
18	0.0861214	1.8449955	0.0121363		
				0.0922964	1.9099951
19	0.0991855	1.9799948	0.0140262		
				0.1063226	2.0499945
20	0.1139759	2.1249937	0.0155727		
				0.1218953	2.1949940
21	0.1312305	2.2749935	0.0190148		
				0.1409101	2.3599939
22	0.1524829	2.4549932	0.0236022		
				0.1645123	2.5499935
23	0.1790117	2.6599932	0.0256110		
				0.1941233	2.7699928
24	0.2124051	2.8974924	0.0373862		
				0.2315095	3.0249920
25	0.2546369	3.1724911	0.0473557		
				0.2788652	3.3199911
26	0.3081548	3.4899902	0.0600416		
				0.3389068	3.6599903
27	0.3759819	3.8549900	0.0760740		
				0.4149808	4.0499897
28	0.4618304	4.2724895	0.0962037		
				0.5111846	4.4949894
29	0.5702278	4.7474890	0.1213123		
				0.6324969	4.9999886
30	0.7066566	5.2849884	0.1524296		
				0.7849265	5.5699883

LIBRARY TAPE LABELED 201
ENDF/B TAPE 201 (5/13/70)

MATERIAL DESCRIPTION
U-235 CSEWG EVAL-SEP69 LEGNARD,ALTER,LUBITZ %RE-EVAL<
AI-AEC-MEMO-12916 DIST-JAN70 REV-APR70
* * * * * *
URANIUM-235
VARIOUS INDIVIDUALS CONTRIBUTED TO TE EVALUATION OF
THE CROSS SECTIONS FOR THIS MATERIAL

B.R..LEGNARD %BNW<- CROSS SECTIONS BELOW 1.0 EV
H.ALTER AND C.L.DUNFORD- CROSS SETIONS ABOVE 15 KEV
C.LUBITZ- THE ORIGINAL DATA SET %MAT#1044<
E.PENNINGTON- UNRESOLVED RESONANCE PARAMETERS
AND THE FISSILE AND FERTILE TASK FORCE %JUNE-AUG.,1969<
* * * * * *
MAT#1102 IS A PARTIAL RE-EVALUATION OF DATA IN MAT#1044
THE TOTAL AND ALL PARTIAL CROSS SECTIONS FOR NEUTRON ENERGIES
BELOW 1.0 EV WERE PROVEDIED BY B.R.LEGNARD,JR.%UNPUBLISHED MEMO
TO CSEWG%AUG.1969<.
THE PARTIAL X-SEC WERE OBTAINED BY STARTING WITH DATA GIVEN IN
MAT#1044 AND MODIFYING THE SHAPE AND MAGNITUDE OF THESE DATA TO
CONFORM TO THE 2200 M/SEC PARAMETERS %INCLUDING G FACTORS< THAT
WERE OBTAINED DURING THE 1969 IAEA EVALUATION GROUP %SEE- HANNA
ET AL, ATOMIC ENERGY REVIEW, VOL VII, NO.4, 1969<.
* * * * * *

```
THE 2200 M/SEC PARAMETERS ARE
          TOTAL   #    694.276
          ELASTIC#     15.776
          FISSICN#    580.200
          N,GAMMA#     98.300
          NU      #     2.423     TOTAL %DELAYED PLUS PROMPT<
          ALPHA   #     0.16942
          ETA     #     2.07196
*         *          *          *          *          *
BELOW 1.0 EV DATA GIVEN IN FILE 3 %SMOOTH X-SEC<.
BETWEEN 1.0 AND 64.5 DATA GIVEN AS SLBW RESOLVED RESONANCE
PARAMETER PLUS BACKGROUND X-SEC IN FILE 3.
BETWEEN 64.5 EV AND 24.8 KEV  ALL DATA GIVEN IN  FILE 2 %LRF#2,
ENERGY DEPENDENT REDUCED NEUTRON WIDTHS AND FISSICN WIDTHS<.
ABOVE   24.8 KEV ALL DATA GIVEN IN FILE 3.
*         *          *          *          *          *
BELCW 0.4 EV FISSION X-SEC BASED CN DATA OF B.R.LEONARD%FROM
SCISRS TAPE< AND THAT OF C.D.BOWMAN ET AL%UCRL-1460<. N,GAMMA
BASED ON ALPHA*FISSION,WHERE ALPHA TAKEN FROM GRAPH IN BNL-325
PAGE 92-235-33 %FOR ENERGIES BETWEEN 0.07 TO 0.4 EV<.
*         *          *          *          *          *
BETWEEN 0.4 EV AND 3.0 KEV THE CAPTURE AND FISSION X-SEC BASED ON
DATA OF G.DESAUSSURE ET AL%ORNL-RPI,1966<. FROM 3.0 KEV TC 15 KEV
CAPTURE AND FISSICN BASED CN EVAL. BY SCHMIDT%KFK-120, PART-II,
1962<. ABOVE 15 KEV ALL PARTIAL CROSS SECTIONS BASED CN EVAL. BY
ALTER AND DUNFORD%AI<,%AI-AEC-MEMO-12916,JAN.1970<
*** NOTE* FISSICN CROSS FRCM EVAL. BY DAVEY %N.S.E. 26,149%1966<
   AND N.S.E. 32,35%1968<<.***
*         *          *          *          *          *
RESOLVED RESONANCE PARAMETERS OBTAINED BY SIMULTANEOUS FIT TO
CAPTURE AND FISSICN CROSS SECTION %ORNL-RPI,1966 DATA<
A POTENTIAL SCATTERING X-SEC OF  10 BARNS WAS USED IN FIT.
*         *          *          *          *          *
UNRESOLVED RESONANCE PARAMETERS WERE OBTAINED BY E. PENNINGTON
%ANL<. FINE GROUP AVERAGED CROSS SECTICNS WERE OBTAINED FROM
RECOMMEND KAPL DATA %NOT MAT#1044 DATA<. ENERGY DEPENDENT AVERAGE
RESONANCE PARAMETERS WERE OBTAINED AND ARE INCLUDED IN FILE 2 AS
LRU# 2, LRF # 2.
*         *          *          *          *          *
ENERGY DEPENDENCE OF NU TAKEN FROM KFK-120 PART-1
SIMPLE FISSION SPECTRUM USED T# 1.30 MEV AT THERMAL
T%E< FROM FORMULA BY  TERRELL  3/2*T%E<#0.75 &0.65%NU%E<&1.0<**.5
*         *          *          *          *          *
FISSION PRODUCT YIELD DATA FROM  RECOMMENDED VALUES OF M.E.MEEK
AND B.F.RIDER, APED-5398-A, REVISED %OCT.1968<
YIELDS NORMALIZED FOR A SUM # 2.0000
*         *          *          *          *          *
ANGULAR DISTRIBUTIONS FOR ELASTIC SCATTERING FROM EVAL. BY %AI<
MT#251,252,253 CALC. FRCM  ANG. DISTR DATA
ANG. DISTR. OF NEUTRONS FRCM INELASTIC SCAT ASSUMMED TC BE
ISOTROPIC IN C.M. SYSTEM
*         *          *          *          *          *
DATA MODIFIED TO CONFORM TO ENDF/B-II FORMATS %APRIL, 1970<
*         *          *          *          *          *
INFINITE DILUTICN RESONANCE INTEGRALS %ABOVE 0.5 EV<
          FISSICN #  298.40 BARNS
          N,GAMMA #  142.40 BARNS
          ELASTIC #  165.60 BARNS
*         *          *          *          *          *
INELASTIC LEVEL CROSS SECTICN FROM EVAL. BY PARKER %AWRE O-82/63<
*         *          *          *          *          *
      NOTE       NOTE       NOTE       NOTE
CROSS SECTION SHOULD BE COMPUTED FROM RESOLVED RESONANCE
PARAMETERS IN FIVE EV INTERVALS, 0 TC 5, 5 TO 10, ETC.  IN EACH
INTERVAL USE ONLY RESONANCES IN THE ENCLOSING FIFTEN VOLT
INTERVAL, I.E., -5 TC 10, 0 TO 15, 5 TO 20, ETC. USING ANY OTHER
RECIPE PRODUCES SMALL INCONSISTENCY WITH DATA ON WHICH RESONANCE
PARAMETERS ARE BASED. %EXCEPTION--- USE NEGATIVE ENERGY RESONANCE
UP TO 10 EV.<
      ----       ----       ----       ----       ----
```

0. U-235 AT 0 DEG K - MAT 1102 - GROUP AVERAGED CROSS SECTIONS

NU=2.42300 T= 0.0 K

GRP	E(EV)	SIGMA ABS	SIGMA FISS	ALPHA	ETA
1	0.000253	0.72417E 04	0.61593E 04	0.17574	2.06084
2	0.001012	0.36154E 04	0.30752E 04	0.17567	2.06095
3	0.002277	0.23995E 04	0.20414E 04	0.17545	2.06134
4	0.004048	0.17930E 04	0.15256E 04	0.17526	2.06167
5	0.006325	0.14262E 04	0.12139E 04	0.17488	2.06234
6	0.009108	0.11803E 04	0.10050E 04	0.17435	2.06327
7	0.012397	0.10025E 04	0.85462E 03	0.17306	2.06554
8	0.016192	0.86826E 03	0.74109E 03	0.17161	2.06810
9	0.020493	0.76308E 03	0.65197E 03	0.17042	2.07020
10	0.025300	0.67835E 03	0.58006E 03	0.16945	2.07191
11	0.030613	0.60859E 03	0.52070E 03	0.16879	2.07308
12	0.036432	0.55012E 03	0.47078E 03	0.16855	2.07351
13	0.042757	0.50041E 03	0.42818E 03	0.16870	2.07325
14	0.049588	0.45756E 03	0.39136E 03	0.16916	2.07243
15	0.056925	0.42025E 03	0.35925E 03	0.16979	2.07131
16	0.065173	0.38606E 03	0.32976E 03	0.17073	2.06965
17	0.074847	0.35370E 03	0.30178E 03	0.17204	2.06733
18	0.086121	0.32392E 03	0.27594E 03	0.17389	2.06407
19	0.099186	0.29682E 03	0.25230E 03	0.17644	2.05959
20	0.113976	0.27283E 03	0.23079E 03	0.18217	2.04962
21	0.131230	0.25091E 03	0.21115E 03	0.18831	2.03902
22	0.152483	0.23251E 03	0.19397E 03	0.19871	2.02134
23	0.179012	0.21943E 03	0.18094E 03	0.21270	1.99801
24	0.212405	0.21772E 03	0.17636E 03	0.23449	1.96275
25	0.254637	0.23265E 03	0.18648E 03	0.24759	1.94214
26	0.308155	0.22448E 03	0.18155E 03	0.23651	1.95954
27	0.375982	0.15344E 03	0.13005E 03	0.17983	2.05368
28	0.461830	0.10425E 03	0.92413E 02	0.12805	2.14795
29	0.570228	0.78664E 02	0.71009E 02	0.10779	2.18723
30	0.706657	0.65119E 02	0.59294E 02	0.09824	2.20625

0. U-235 AT 0 DEG K - MAT 1102 - GROUP AVERAGED CROSS SECTIONS

CROSS SECTIONS AT T= 0.0 K

GRP	E(EV)	ABSORPTION	INELASTIC	ELASTIC	SCATTERING	TOTAL	TRANSPORT
1	0.000253	0.72417E 04	0.0	0.15910E 02	0.15910E 02	0.72573E 04	0.72576E 04
2	0.001012	0.36154E 04	0.0	0.15905E 02	0.15905E 02	0.36336E 04	0.36313E 04
3	0.002277	0.23995E 04	0.0	0.15898E 02	0.15898E 02	0.24153E 04	0.24154E 04
4	0.004048	0.17930E 04	0.0	0.15888E 02	0.15888E 02	0.18088E 04	0.18088E 04
5	0.006325	0.14262E 04	0.0	0.15876E 02	0.15876E 02	0.14420E 04	0.14421E 04
6	0.009108	0.11803E 04	0.0	0.15861E 02	0.15861E 02	0.11962E 04	0.11961E 04
7	0.012397	0.10025E 04	0.0	0.15844E 02	0.15844E 02	0.10183E 04	0.10183E 04
8	0.016192	0.86826E 03	0.0	0.15824E 02	0.15824E 02	0.88411E 03	0.88404E 03
9	0.020493	0.76308E 03	0.0	0.15801E 02	0.15801E 02	0.77900E 03	0.77884E 03
10	0.025300	0.67835E 03	0.0	0.15776E 02	0.15776E 02	0.69428E 03	0.69408E 03
11	0.030613	0.60859E 03	0.0	0.15749E 02	0.15749E 02	0.62439E 03	0.62429E 03
12	0.036432	0.55012E 03	0.0	0.15719E 02	0.15719E 02	0.56586E 03	0.56580E 03
13	0.042757	0.50041E 03	0.0	0.15686E 02	0.15686E 02	0.51609E 03	0.51605E 03
14	0.049588	0.45756E 03	0.0	0.15652E 02	0.15652E 02	0.47324E 03	0.47317E 03
15	0.056925	0.42025E 03	0.0	0.15614E 02	0.15614E 02	0.43587E 03	0.43582E 03
16	0.065173	0.38606E 03	0.0	0.15573E 02	0.15573E 02	0.40165E 03	0.40159E 03
17	0.074847	0.35370E 03	0.0	0.15525E 02	0.15525E 02	0.36911E 03	0.36918E 03
18	0.086121	0.32392E 03	0.0	0.15469E 02	0.15469E 02	0.33936E 03	0.33935E 03
19	0.099186	0.29682E 03	0.0	0.15406E 02	0.15406E 02	0.31219E 03	0.31218E 03
20	0.113976	0.27283E 03	0.0	0.15336E 02	0.15336E 02	0.28815E 03	0.28812E 03
21	0.131230	0.25091E 03	0.0	0.15253E 02	0.15253E 02	0.26606E 03	0.26612E 03
22	0.152483	0.23251E 03	0.0	0.15154E 02	0.15154E 02	0.24756E 03	0.24762E 03
23	0.179012	0.21943E 03	0.0	0.15032E 02	0.15032E 02	0.23352E 03	0.23442E 03
24	0.212405	0.21772E 03	0.0	0.14889E 02	0.14889E 02	0.23203E 03	0.23256E 03
25	0.254637	0.23265E 03	0.0	0.14771E 02	0.14771E 02	0.24750E 03	0.24737E 03
26	0.308155	0.22448E 03	0.0	0.14753E 02	0.14753E 02	0.24465E 03	0.23920E 03
27	0.375982	0.15344E 03	0.0	0.14599E 02	0.14599E 02	0.16695E 03	0.16799E 03
28	0.461830	0.10425E 03	0.0	0.14300E 02	0.14300E 02	0.11760E 03	0.11851E 03
29	0.570228	0.78664E 02	0.0	0.13967E 02	0.13967E 02	0.92230E 02	0.92591E 02
30	0.706657	0.65119E 02	0.0	0.13606E 02	0.13606E 02	0.78391E 02	0.78686E 02

0. U-235 AT 0 DEG K - MAT 1102 - GROUP AVERAGED CROSS SECTIONS

ELASTIC LEGENDRE CROSS SECTIONS AT T= 0.0 K

GRP	E(EV)	SIGMA 0	SIGMA 1	(MU-BAR)	SIGMA 2	SIGMA 3	SIGMA 4	SIGMA 5
1	0.000253	0.15910E 02	0.45517E-01	(0.00286)	0.0	0.0	0.0	0.0
2	0.001012	0.15905E 02	0.45503E-01	(0.00286)	0.0	0.0	0.0	0.0
3	0.002277	0.15898E 02	0.45483E-01	(0.00286)	0.0	0.0	0.0	0.0
4	0.004048	0.15888E 02	0.45456E-01	(0.00286)	0.0	0.0	0.0	0.0
5	0.006325	0.15876E 02	0.45421E-01	(0.00286)	0.0	0.0	0.0	0.0
6	0.009108	0.15861E 02	0.45378E-01	(0.00286)	0.0	0.0	0.0	0.0
7	0.012397	0.15844E 02	0.45328E-01	(0.00286)	0.0	0.0	0.0	0.0
8	0.016192	0.15824E 02	0.45271E-01	(0.00286)	0.0	0.0	0.0	0.0
9	0.020493	0.15801E 02	0.45207E-01	(0.00286)	0.0	0.0	0.0	0.0
10	0.025300	0.15776E 02	0.45135E-01	(0.00286)	0.0	0.0	0.0	0.0
11	0.030613	0.15749E 02	0.45056E-01	(0.00286)	0.0	0.0	0.0	0.0
12	0.036432	0.15719E 02	0.44970E-01	(0.00286)	0.0	0.0	0.0	0.0
13	0.042757	0.15686E 02	0.44877E-01	(0.00286)	0.0	0.0	0.0	0.0
14	0.049588	0.15652E 02	0.44778E-01	(0.00286)	0.0	0.0	0.0	0.0
15	0.056925	0.15614E 02	0.44672E-01	(0.00286)	0.0	0.0	0.0	0.0
16	0.065173	0.15573E 02	0.44553E-01	(0.00286)	0.0	0.0	0.0	0.0
17	0.074847	0.15525E 02	0.44417E-01	(0.00286)	0.0	0.0	0.0	0.0
18	0.086121	0.15469E 02	0.44257E-01	(0.00286)	0.0	0.0	0.0	0.0
19	0.099186	0.15406E 02	0.44076E-01	(0.00286)	0.0	0.0	0.0	0.0
20	0.113976	0.15336E 02	0.43874E-01	(0.00286)	0.0	0.0	0.0	0.0
21	0.131230	0.15253E 02	0.43638E-01	(0.00286)	0.0	0.0	0.0	0.0
22	0.152483	0.15154E 02	0.43353E-01	(0.00286)	0.0	0.0	0.0	0.0
23	0.179012	0.15032E 02	0.43005E-01	(0.00286)	0.0	0.0	0.0	0.0
24	0.212405	0.14889E 02	0.42596E-01	(0.00286)	0.0	0.0	0.0	0.0
25	0.254637	0.14771E 02	0.42258E-01	(0.00286)	0.0	0.0	0.0	0.0
26	0.308155	0.14753E 02	0.42206E-01	(0.00286)	0.0	0.0	0.0	0.0
27	0.375982	0.14599E 02	0.41768E-01	(0.00286)	0.0	0.0	0.0	0.0
28	0.461830	0.14300E 02	0.40911E-01	(0.00286)	0.0	0.0	0.0	0.0
29	0.570228	0.13967E 02	0.39959E-01	(0.00286)	0.0	0.0	0.0	0.0
30	0.706657	0.13606E 02	0.38926E-01	(0.00286)	0.0	0.0	0.0	0.0

0. U-235 AT 0 DEG K - MAT 1102 - GROUP AVERAGED CROSS SECTIONS

LEGENDRE SCATTERING CROSS SECTIONS AT T= 0.0 K

GRP	E(EV)	SIGMA 0	SIGMA 1	(MU-BAR)	SIGMA 2	SIGMA 3	SIGMA 4	SIGMA 5
1	0.000253	0.15910E 02	0.45517E-01	(0.00286)	0.0	0.0	0.0	0.0
2	0.001012	0.15905E 02	0.45503E-01	(0.00286)	0.0	0.0	0.0	0.0
3	0.002277	0.15898E 02	0.45483E-01	(0.00286)	0.0	0.0	0.0	0.0
4	0.004048	0.15888E 02	0.45456E-01	(0.00286)	0.0	0.0	0.0	0.0
5	0.006325	0.15876E 02	0.45421E-01	(0.00286)	0.0	0.0	0.0	0.0
6	0.009108	0.15861E 02	0.45378E-01	(0.00286)	0.0	0.0	0.0	0.0
7	0.012397	0.15844E 02	0.45328E-01	(0.00286)	0.0	0.0	0.0	0.0
8	0.016192	0.15824E 02	0.45271E-01	(0.00286)	0.0	0.0	0.0	0.0
9	0.020493	0.15801E 02	0.45207E-01	(0.00286)	0.0	0.0	0.0	0.0
10	0.025300	0.15776E 02	0.45135E-01	(0.00286)	0.0	0.0	0.0	0.0
11	0.030613	0.15749E 02	0.45056E-01	(0.00286)	0.0	0.0	0.0	0.0
12	0.036432	0.15719E 02	0.44970E-01	(0.00286)	0.0	0.0	0.0	0.0
13	0.042757	0.15686E 02	0.44877E-01	(0.00286)	0.0	0.0	0.0	0.0
14	0.049588	0.15652E 02	0.44778E-01	(0.00286)	0.0	0.0	0.0	0.0
15	0.056925	0.15614E 02	0.44672E-01	(0.00286)	0.0	0.0	0.0	0.0
16	0.065173	0.15573E 02	0.44553E-01	(0.00286)	0.0	0.0	0.0	0.0
17	0.074847	0.15525E 02	0.44417E-01	(0.00286)	0.0	0.0	0.0	0.0
18	0.086121	0.15469E 02	0.44257E-01	(0.00286)	0.0	0.0	0.0	0.0
19	0.099186	0.15406E 02	0.44076E-01	(0.00286)	0.0	0.0	0.0	0.0
20	0.113976	0.15336E 02	0.43874E-01	(0.00286)	0.0	0.0	0.0	0.0
21	0.131230	0.15253E 02	0.43638E-01	(0.00286)	0.0	0.0	0.0	0.0
22	0.152483	0.15154E 02	0.43353E-01	(0.00286)	0.0	0.0	0.0	0.0
23	0.179012	0.15032E 02	0.43005E-01	(0.00286)	0.0	0.0	0.0	0.0
24	0.212405	0.14889E 02	0.42596E-01	(0.00286)	0.0	0.0	0.0	0.0
25	0.254637	0.14771E 02	0.42258E-01	(0.00286)	0.0	0.0	0.0	0.0
26	0.308155	0.14753E 02	0.42206E-01	(0.00286)	0.0	0.0	0.0	0.0
27	0.375982	0.14599E 02	0.41768E-01	(0.00286)	0.0	0.0	0.0	0.0
28	0.461830	0.14300E 02	0.40911E-01	(0.00286)	0.0	0.0	0.0	0.0
29	0.570228	0.13967E 02	0.39959E-01	(0.00286)	0.0	0.0	0.0	0.0
30	0.706657	0.13606E 02	0.38926E-01	(0.00286)	0.0	0.0	0.0	0.0