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NTIS

871

**An Integrated System for Production of Neutronics and
Photonics Calculational Constants
Volume 17, Part B**

**PROGRAM SIGMA1 (VERSION 77-1): DOPPLER BROADEN
EVALUATED CROSS SECTIONS IN THE EVALUATED
NUCLEAR DATA FILE/VERSION B
(ENDF/B) FORMAT**

D. E. Cullen

January 12, 1977

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**LAWRENCE
LIVERMORE
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University of California - Livermore

MASTER

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Foreword

The total cross section probability (TCP) system is designed to process evaluated neutron cross section data into a continuous energy or multigroup form. In the following figure, we have described the function of each of the computer codes in the TCP system by contrasting the form of the data before and after code processing.

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PROGRAM SIGMA1 (VERSION 77-1): DOPPLER BROADEN EVALUATED CROSS SECTIONS IN THE EVALUATED NUCLEAR DATA FILE/VERSION B (ENDF/B) FORMAT

Abstract

We have designed a code, SIGMA1, to Doppler broaden evaluated cross sections in the ENDF/B format. The code can only be applied to tabulated data that vary linearly in energy and cross section between tabulated points. This report describes the methods used in the code and serves as a user's guide to the code.

Method

DOPPLER BROADENING

Doppler broadening refers to a change in cross section resulting from thermal motion, rotation, and vibration of nuclei in a target material. The SIGMA1 method¹ may be used to Doppler broaden cross sections for any particle (e.g., neutron, proton, deuteron, etc.) incident at nonrelativistic energies upon a target in which the free-atom approximation is valid.

The SIGMA1 method is extensively described in Ref. 1. We have briefly described the method below, starting from the well-known free-atom Doppler broadening equations in which energy [Eq. (1)] and speed [Eq. (2)] are the independent variables:

$$\sigma_{\text{E}}^{\text{D}}(E,T) = \frac{1}{2} \left(\frac{A}{kT} \right)^{1/2} \int_0^{\infty} |v_{\text{r}}^{\text{D}}(E_{\text{r}},0)| dE_{\text{r}} \left[\exp\{-\alpha(\sqrt{E} - \sqrt{E_{\text{r}}})^2\} + \exp\{-\alpha(\sqrt{E} + \sqrt{E_{\text{r}}})^2\} \right] \quad (1)$$

$$V^{\text{D}}(V,T) = \frac{1}{V} \left(\frac{A}{2\pi} \right)^{1/2} \int_0^{\infty} |v_{\text{r}}^{\text{D}}(V_{\text{r}},0)| V_{\text{r}} dV_{\text{r}} \left[\exp\{-\alpha(V - V_{\text{r}})^2\} + \exp\{-\alpha(V + V_{\text{r}})^2\} \right] \quad (2)$$

where

$$\alpha = \frac{A}{kT} \quad ; \quad \beta = \frac{M}{2kT} \quad ; \quad A = \frac{M}{m}$$

and

m = projectile mass (e.g., neutron, proton, alpha, etc.)

$\sqrt{E}$ = projectile velocity

$V = |v|$ = projectile speed

$$E = \frac{1}{2}mV^2 = \text{projectile energy}$$

$$M = \text{target nuclei mass}$$

$$\vec{V}_T = \text{target velocity}$$

$$V_T = |\vec{V}_T| = \text{target speed}$$

$$E_T = \frac{1}{2}MV_T^2 = \text{target energy}$$

$$A = M/m = \text{atomic weight ratio (target mass/projectile mass)}$$

$$\vec{V}_r = \vec{V} - \vec{V}_T = \text{relative velocity}$$

$$V_r = |\vec{V}_r| = \text{relative speed}$$

$$E_r = \frac{1}{2}mV_r^2 = \text{relative energy of the neutron as "seen" by the target}$$

$$\sigma(V,0) = \text{cold (0 K) cross section}$$

$$\sigma(V,T) = \text{Doppler broadened cross section}$$

By changing variables in Eq. (2) so that

$$\begin{aligned} y^2 &= (E - E_r) = 2V^2 \\ x^2 &= (E_r - E_T) = 2V_r^2 \end{aligned} \quad (3)$$

the Doppler broadening equation becomes

$$\sigma(y, T_2) = \frac{1}{y^2} \left(\frac{1}{\pi} \right)^{1/2} \int_0^\infty x^2 \sigma(x, T_1) \{ \exp[-(x - y)^2] - \exp[-(x + y)^2] \} dx. \quad (4)$$

The ensuing development can be simplified by defining

$$\sigma^*(y, T_2) = \frac{1}{y^2} \left(\frac{1}{\pi} \right)^{1/2} \int_0^\infty x^2 \sigma(x, T_1) \exp[-(x - y)^2] dy \quad (5)$$

and noting that the Doppler broadened cross section is

$$\sigma(y, T_2) = \sigma^*(y, T_2) - \sigma^*(-y, T_2). \quad (6)$$

Next, we will assume that the cross section to be Doppler broadened is given as a table of cross sections and their corresponding energies. Values between the tabulated points will be assumed to vary linearly in energy and cross section:

$$\sigma(E, T_1) = \left[\frac{E - E_k}{E_{k+1} - E_k} \right] \sigma_{k+1} + \left[\frac{E_{k+1} - E}{E_{k+1} - E_k} \right] \sigma_k = A_k + B_k E \quad : \quad E \in (E_k, E_{k+1}) \quad (7)$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{\sigma} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2} + \frac{1}{\sigma} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2} \right) \quad (10)$$

where the data are x and the μ and σ are fitted parameters. Since the $\mu = 0$ and $\sigma = 1$ (10) reduces to the Gaussian distribution, the Gaussian distribution is a special case of the generalized Gaussian distribution. If we use the data x and μ and σ with the generalized form of the table are fitted data, then the generalized form of the table are fitted data, then Eq. (10) becomes

$$f(x) = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{\sigma} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2} + \frac{1}{\sigma} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2} \right) \quad (11)$$

where the variance $\sigma^2 = x^2 + y^2$ and collecting terms in powers of x , we get

$$f(x) = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{\sigma} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2} + \frac{1}{\sigma} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2} \right) \quad (12)$$

Equation (12) can be defined exactly in terms of the functions

$$F^n(a) = F^n(a) + F^n(b) \quad (13)$$

$$F^n(a) = \frac{1}{\sqrt{2\pi}} \int_0^a z^n \exp(-z^2) dz \quad (14)$$

where

$$n = 0, 1, 2, 3, 4, \dots \quad (15)$$

These functions can easily be shown to satisfy the recursion relationship

$$F^n(a) = \left(\frac{n-1}{2} \right) F^{n-2}(a) + \left(\frac{1}{2} \right) a^{n-1} \exp(-a^2) + \left(\frac{1}{2} \right) \frac{1}{n+1} \quad (16)$$

By explicitly evaluating Eq. (12) for $n = 0$ and 1, as well as by applying the recursion relationship, we can derive the required functions

$$F^0(a) = \text{ERF}(a) \quad (17)$$

$$F^1(a) = \left(\frac{1}{\sqrt{2\pi}} \right) \{ 1 - \exp(-a^2) \} \quad (18)$$

although the reaction rate is becoming smoother, the same may not be true of the cross section because the two differ by a factor of V/V_1 (i.e., $\sigma(V,V) = R(V,T)/V$). To ensure that this low-energy $1/V$ tail does not prevent the cross section from being linear-linear interpolatable, all we have to do is choose an energy grid for the broadened data that is the same as the energy grid for the unbroadened data, except that the latter is supplemented by an additional set of energy points. These additional points should be added in such a way that between any two energy points of the final energy grid, the difference between linear-linear and $1/V$ variations in the cross section is always less than some allowable error ϵ .

Consider two possible representations of the same cross section: a $1/V$ variation and a linear-linear variation in energy. By insisting that the two representations agree exactly at the two ends of an interval $V(V_1, V_2)$ and that $V_2 = SV_1$, we get

$$\begin{aligned}\sigma_1(V) &= \frac{1}{V} \quad (1/V \text{ variation}) \\ \sigma_2(V) &= \frac{1}{V} + \frac{(V_2^2 - V_1^2)}{V_1^3 S(S+1)} \quad \left(\begin{array}{l} \text{linear-linear in } V \\ \text{cross section-energy} \end{array} \right) \\ V &= V_1 + SV_1.\end{aligned}\tag{17}$$

The fractional difference between these two representations is

$$\delta(V) = \frac{\sigma_1(V) - \sigma_2(V)}{\sigma_1(V)} = 1 - \frac{V^3 - V_1^2}{V_1^3 S(S+1)} = \frac{V}{V_1}$$

and the variation in the fractional difference is

$$\frac{d}{dV} \delta(V) = \frac{V^2 - V_1^2}{V_1^3 S(S+1)} = \frac{1}{V_1}.\tag{18}$$

Therefore, the point of maximum difference and the value of the difference at that point are

$$\begin{aligned}V_{\max} &= V_1 \left[\frac{1}{3} (1 + S + S^2) \right]^{1/2} \\ (\delta_{\max}) &= 1 - \left(\frac{1}{3} \right)^{1/2} \left(\frac{1}{S(S+1)} \right)^{3/2}\end{aligned}\tag{19}$$

Note (V_{max}) is independent of V , and only depends on s , the spacing between tabulated points. This means that a $1/V$ variation can be represented by a linear-linear variation in energy to within any allowable error ϵ , simply by ensuring that the energies for successive tabulated values are within $S^2 E$ of one another (independent of E).

Table I illustrates the typical factor (S) required for a number of allowable tolerances (ϵ), when ϵ is in the range 0.1 to 2.0%. The table also shows the number of points that would be required to space points $S^2 E$ apart between 10^{-5} eV and 20 MeV. For example, an allowable tolerance of 0.5% would require 124 points or roughly 10 per energy decade.

Table I. Linear-Linear approximation of a $1/V$ cross section.

Tolerance	Factor	Points ^a
0.001	1.0530	276
0.002	1.0757	195
0.003	1.0935	160
0.004	1.1087	139
0.005	1.1223	124
0.006	1.1347	110
0.007	1.1463	100
0.008	1.1571	90
0.009	1.1674	83
0.010	1.1772	88
0.011	1.1865	84
0.012	1.1956	81
0.013	1.2043	78
0.014	1.2128	75
0.015	1.2210	72
0.016	1.2290	70
0.017	1.2367	68
0.018	1.2444	66
0.019	1.2518	65
0.020	1.2591	63

^a Points to span 10^{-5} eV to 20 MeV.

Therefore, to ensure that the Doppler broadened cross sections are linear-linear interpolatable, we must start from the same energy points as the 0 K data and supplement this grid in any interval where the points are more widely spaced than S^2 (where S^2 depends on the allowable error %).

TRUNCATING THE INTEGRATION RANGE

Although the algorithm as previously described can exactly evaluate the Doppler broadened cross section, it can be a costly procedure since the calculational time can vary as the square of the number of points used to represent a given reaction. To reduce the cost, we can use the strongly convergent Gaussian character of the Doppler broadening kernel to truncate the Doppler broadening integral. Because of the exponential term $\exp[-(x - y)^2]$ [see Eq. (5)], the major contribution to the integral $x\sigma(0, \infty)$ is from an interval centered about y ; the interval is defined by $x\sigma(y - N, y + N)$. Therefore, it is only necessary to integrate over this interval. The truncation procedure should recognize that although $\exp[-(x - y)^2]$ is rapidly decreasing, the term $x^2\sigma(x, T)$ can be rapidly increasing, particularly $\sigma(x, T)$ in the resonance region. Therefore, the truncation procedure should be:

$$\int_0^{\infty} x^2 \sigma(x, T) \exp[-(x - y)^2] dx = \int_{y-N}^{y+N} x^2 \sigma(x, T) \exp[-(x - y)^2] dx + R(y), \quad (20)$$

$$R(y) = \int_0^{y-N} x^2 \sigma(x, T) \exp[-(x - y)^2] dx + \int_{y+N}^{\infty} x^2 \sigma(x, T) \exp[-(x - y)^2] dx \quad (21)$$

$$R(y) \approx 2 \int_N^{\infty} (Z + y)^2 \exp(-Z^2) dZ \quad (22)$$

If we assume that the cross section will vary no more than four orders of magnitude (10^4) and that the error will be no more than 0.1%, then we can safely truncate the integral when $N = 4$. Thus, the truncated integral should only be extended over those intervals in which at least one end is within four units of y . In particular, the second term $\sigma^*(y, T_2)$ [Eq. (6)] need not be calculated unless $y \leq 4$.

Limitations and Assumptions

The program nonselectively Doppler broadens all sections of file 3 data on the original ENDF/B format tape (i.e., all sections between the tape label

card and the tape end card),³ except for the parameters $\bar{u}$, $\bar{z}$, and γ (MT = 251-253).

The program only uses the ENDF/B BCD format (as opposed to binary) and copies all sections except file 3 as hollerith. As such, the program may be used on data in the ENDF/b - 1, II, III, IV or V format, since all sections of file 3 data are identical in all ENDF/B versions.

The program reads and Doppler broadens the data a page at a time, so there is no limit to the number of points in any section (i.e., each section may be described by any number of points).

The program is written entirely in FORTRAN-IV and can be easily modified to run on any medium-sized computer.

We recommend the LINEAR program as the best way to linearize data in the ENDF/B format.⁴ If the data do not vary linearly in energy and cross section between tabulated points, the program will check the interpolation law and abort.

During Doppler broadening, three pages of data are core resident: the page being broadened, the page below it in energy, and the page above it in energy. If at any time the integral extends beyond the limits of these pages, the cross section is extended as a constant and an "EXTENSION" warning message is printed out, advising the user of the maximum temperature step allowable to avoid "EXTENSION." In this case we recommend rerunning the program by bootstrapping the cross section up to the final temperature, in temperature steps smaller than or equal to that recommended in the "EXTENSION" message.

The program will automatically select the energy grid consistent with the input-allowable error to avoid problems resulting from the onset of the low energy 1/V cross section. If an allowable error of less than 0.1% is specified, it will be used for output thinning, but maximum energy point spacing will be based on 0.1%.

If the original ENDF/B data are given at a temperature that is higher than the final temperature, the section will not be Doppler broadened and the original temperature will be left in the section. If the original ENDF/B data are given at a temperature between 0 K and the final temperature, the program will broaden the data by the temperature difference (see Bootstrapping).

In the unresolved resonance region, starting from energy-averaged cross sections the SIGMA1 algorithm will conserve the averages and return the same values. This program does not use unresolved parameters directly.

Requirements

The I/O units are defined as follows:

<u>Filename</u> *	<u>Unit</u>	<u>Description</u>
INPUT	5	Input card
OUTPUT	6	Output report
ENDFIN	21	Evaluated data to be Doppler broadened in the ENDF/B format
ENDFOUT	22	Doppler broadened evaluated data in the ENDF/B format
SCRATCH	23	Scratch file

All read and write statements use variable I/O unit numbers. To convert to any other set of unit numbers, it is necessary to redefine the unit numbers as described in the program listing.

The program, when run on the Livermore CDC-7600, requires 21 000 words of small core memory and 6 000 words of large core memory (I/O buffers). It takes 0.9 min to Doppler broaden ENDL-76⁵ tape 6 from 0 to 300 K and to thin the output to 0.1% accuracy [it takes 9.44 min to Doppler broaden the entire ENDL-76⁵ library (88 complete evaluations) from 0 to 300 K and thin the output to 0.1% accuracy].

Input Cards

The program requires a single input card to define the allowable fractional error.

<u>Card</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
1	1 - 11	E11.4	Fractional output thinning criteria
	12 - 22	F11.4	Output Kelvin temperature

To Doppler broaden to 300 K and thin the output to 0.5% the following input card is required:

5.0000E-03 3.0000E+02

* The filenames apply to the program run at Livermore. Disk files that have these names will be used by the program.

A 0.0 thinning criteria means that there will not be any output thinning but there will be maximum output spacing in order to keep the result within 0.1' of 1/V.

Example Output

Table 2 presents the output that results from Doppler broadening ENDF-76 tape 6 to 300 K and thinning the output to 0.1'. Figures 2 through 5 illustrate the wide range of applications of the SIGMA code. Note that it can be applied to Doppler broadening at

- Reactor core-like temperatures (300 - 2000 K) (Fig. 2)
- Controlled thermonuclear reactor core and stellar temperatures (1 eV-10 keV)* (Fig. 3)
- Initially constant cross sections from 0.01 eV to 10 MeV (Fig. 4)
- Initially 1/V cross section from 0.01 eV to 10 MeV (Fig. 5)

* For those who are unfamiliar with the convention of expressing temperature in eV, note the unit of KT is energy and can be used to describe temperature (e.g., 1 eV $\sim$ 12000 K; 10 keV $\sim$ 1.2×10^8 K).

Table 2. Example output listing.

DOPPLER BROADEN ENDF/B CROSS SECTIONS (SIGMA 77-1)							
THINNING CRITERIA-- 1.00000- 3							
TEMPERATURE----- 3.00000+ 2 KELVIN							
LAPE LABEL							
LAWRENCE LIVERMORE EVALUATED LIBRARY (ENDL) 2/10/76							
ZA	MAT	MT	KELVIN	Q-VALUE	POINTS	POINTS	
			IN	EV	IN	OUT	
90231	7163	1	0.	+ 0	0.	+ 0	246 220
90231	7163	2	0.	+ 0	0.	+ 0	4. 72
90231	7163	4	0.	+ 0	0.	+ 0	22 22
90231	7163	16	0.	+ 0	-5.12000+ 6	19	19
90231	7163	17	0.	+ 0	-1.19100+ 7	11	11
90231	7163	18	0.	+ 0	1.80000+ 8	152	195
90231	7163	37	0.	+ 0	-1.71500+ 7	5	4
90231	7163	91	0.	+ 0	0.	+ 0	22 22
90231	7163	102	0.	+ 0	6.43000+ 6	139	193
90231	7163	251	0.	+ 0	0.	+ 0	20 20
90231	7163	252	0.	+ 0	0.	+ 0	20 19
90231	7163	253	0.	+ 0	0.	+ 0	20 19
MAT TOTALS					718	806	
90232	7164	1	0.	+ 0	0.	+ 0	6248 5316
90232	7164	2	0.	+ 0	0.	+ 0	2983 2898
90232	7164	4	0.	+ 0	0.	+ 0	62 51
90232	7164	16	0.	+ 0	-6.34000+ 6	17	16
90232	7164	17	0.	+ 0	-1.15600+ 7	8	8
90232	7164	18	0.	+ 0	1.70000+ 8	36	34
90232	7164	37	0.	+ 0	-1.83500+ 7	2	2
90232	7164	91	0.	+ 0	0.	+ 0	62 51
90232	7164	102	0.	+ 0	4.79000+ 5	5535	5451
90232	7164	251	0.	+ 0	0.	+ 0	14 13
90232	7164	252	0.	+ 0	0.	+ 0	14 14
90232	7164	253	0.	+ 0	0.	+ 0	14 14
MAT TOTALS					14995	13868	
90233	7165	1	0.	+ 0	0.	+ 0	296 220
90233	7165	2	0.	+ 0	0.	+ 0	43 72
90233	7165	4	0.	+ 0	0.	+ 0	21 21
90233	7165	16	0.	+ 0	-4.78300+ 6	19	19
90233	7165	17	0.	+ 0	-1.12200+ 7	14	14
90233	7165	18	0.	+ 0	1.80000+ 8	130	174
90233	7165	37	0.	+ 0	-1.63400+ 7	5	4
90233	7165	91	0.	+ 0	0.	+ 0	21 21
90233	7165	102	0.	+ 0	6.18000+ 6	121	157
90233	7165	251	0.	+ 0	0.	+ 0	16 15
90233	7165	252	0.	+ 0	0.	+ 0	16 15
90233	7165	253	0.	+ 0	0.	+ 0	16 16
MAT TOTALS					718	748	
92233	7166	1	0.	+ 0	0.	+ 0	2884 2353
92233	7166	2	0.	+ 0	0.	+ 0	343 352
92233	7166	4	0.	+ 0	0.	+ 0	32 30
92233	7166	16	0.	+ 0	-5.90000+ 6	12	11

Table 2. (Continued).

92233	7166	17	0.	+ 0	-1.31800+	7	6	5
92233	7166	18	0.	+ 0	1.80000+	8	1613	1608
92233	7166	91	0.	+ 0	0.	+ 0	32	30
92233	7166	102	0.	+ 0	6.84000+	6	1954	1949
92233	7166	251	0.	+ 0	0.	+ 0	21	21
92233	7166	252	0.	+ 0	0.	+ 0	21	21
92233	7166	253	0.	+ 0	0.	+ 0	21	20
----- MAT TOTALS -----							6939	6400
92234	7167	1	0.	+ 0	0.	+ 0	188	190
92234	7167	2	0.	+ 0	0.	+ 0	37	57
92234	7167	4	0.	+ 0	0.	+ 0	19	17
92234	7167	16	0.	+ 0	-6.84000+	6	13	13
92234	7167	17	0.	+ 0	-1.25900+	7	7	7
92234	7167	18	0.	+ 0	1.80000+	3	40	40
92234	7167	91	0.	+ 0	0.	+ 0	19	17
92234	7167	102	0.	+ 0	5.31000+	6	128	166
92234	7167	251	0.	+ 0	0.	+ 0	29	28
92234	7167	252	0.	+ 0	0.	+ 0	29	29
92234	7167	253	0.	+ 0	0.	+ 0	29	27
----- MAT TOTALS -----							538	591
92235	7168	1	0.	+ 0	0.	+ 0	2293	2293
92235	7168	2	0.	+ 0	0.	+ 0	235	264
92235	7168	4	0.	+ 0	0.	+ 0	28	27
92235	7168	16	0.	+ 0	-5.23000+	6	15	15
92235	7168	17	0.	+ 0	-1.30000+	7	7	7
92235	7168	18	0.	+ 0	1.00000+	8	1511	1585
92235	7168	37	0.	+ 0	-1.78900+	7	3	3
92235	7168	91	0.	+ 0	0.	+ 0	28	27
92235	7168	102	0.	+ 0	6.55000+	6	767	837
92235	7168	251	0.	+ 0	0.	+ 0	29	27
92235	7168	252	0.	+ 0	0.	+ 0	29	29
92235	7168	253	0.	+ 0	0.	+ 0	29	28
----- MAT TOTALS -----							4974	5142
92236	7169	1	0.	+ 0	0.	+ 0	179	77
92236	7169	2	0.	+ 0	0.	+ 0	35	54
92236	7169	4	0.	+ 0	0.	+ 0	21	19
92236	7169	16	0.	+ 0	-6.55000+	6	14	14
92236	7169	17	0.	+ 0	-1.18500+	7	8	8
92236	7169	18	0.	+ 0	1.80000+	8	40	71
92236	7169	91	0.	+ 0	0.	+ 0	21	19
92236	7169	102	0.	+ 0	5.12000+	6	127	183
92236	7169	251	0.	+ 0	0.	+ 0	27	28
92236	7169	252	0.	+ 0	0.	+ 0	29	29
92236	7169	253	0.	+ 0	0.	+ 0	29	28
----- MAT TOTALS -----							532	634
92237	7170	1	0.	+ 0	0.	+ 0	285	226
92237	7170	2	0.	+ 0	0.	+ 0	48	71
92237	7170	4	0.	+ 0	0.	+ 0	22	21
92237	7170	16	0.	+ 0	-5.12000+	6	11	11
92237	7170	17	0.	+ 0	-1.15700+	7	7	7
92237	7170	18	0.	+ 0	1.90000+	8	81	113
92237	7170	91	0.	+ 0	0.	+ 0	22	21

Table 2. (Continued).

92237	7170	102	0.	+ 0	6.14000+	6	174	216
92237	7170	251	0.	+ 0	0.	+ 0	21	20
92237	7170	252	0.	+ 0	0.	+ 0	21	21
92237	7170	253	0.	+ 0	0.	+ 0	21	21

MAT TOTALS							713	730

92238	7171	1	0.	+ 0	0.	+ 0	1744	1565
92238	7171	2	0.	+ 0	0.	+ 0	453	464
92238	7171	4	0.	+ 0	-4.50000+	4	72	61
92238	7171	16	0.	+ 0	-6.04000+	6	15	15
92238	7171	17	0.	+ 0	-1.14500+	7	9	9
92238	7171	18	0.	+ 0	-1.80000+	8	41	40
92238	7171	37	0.	+ 0	-1.78200+	7	3	3
92238	7171	51	0.	+ 0	-4.50000+	4	21	21
92238	7171	52	0.	+ 0	-1.48000+	5	13	13
92238	7171	53	0.	+ 0	-3.03000+	5	8	8
92238	7171	54	0.	+ 0	-6.80000+	5	17	17
92238	7171	55	0.	+ 0	-7.32000+	5	16	16
92238	7171	56	0.	+ 0	-8.27000+	5	13	13
92238	7171	57	0.	+ 0	-9.30000+	5	14	14
92238	7171	58	0.	+ 0	-9.67000+	5	12	12
92238	7171	59	0.	+ 0	-1.00000+	6	12	12
92238	7171	60	0.	+ 0	-1.04100+	6	12	12
92238	7171	61	0.	+ 0	-1.05000+	6	12	12
92238	7171	62	0.	+ 0	-1.12000+	6	12	12
92238	7171	63	0.	+ 0	-1.15000+	6	10	10
92238	7171	64	0.	+ 0	-1.22000+	6	11	11
92238	7171	65	0.	+ 0	-1.27000+	6	10	10
92238	7171	66	0.	+ 0	-1.30000+	6	9	9
92238	7171	67	0.	+ 0	-1.36000+	6	9	9
92238	7171	68	0.	+ 0	-1.41000+	6	8	8
92238	7171	69	0.	+ 0	-1.43700+	6	9	9
92238	7171	70	0.	+ 0	-1.47000+	6	11	11
92238	7171	71	0.	+ 0	-1.62500+	6	13	13
92238	7171	72	0.	+ 0	-1.87500+	6	11	11
92238	7171	91	0.	+ 0	0.	+ 0	22	22
92238	7171	102	0.	+ 0	4.80000+	6	1473	1519
92238	7171	251	0.	+ 0	0.	+ 0	28	27
92238	7171	252	0.	+ 0	0.	+ 0	29	26
92238	7171	253	0.	+ 0	0.	+ 0	28	25

MAT TOTALS							4179	4039

TABLE TOTALS							3+306	32958

Fig. 2. Doppler broadening of the ^{233}U total cross section for reactor-like temperatures ($T = 0 - 10\,000\text{ K}$).

Fig. 3. Doppler broadening of the cross section in Fig. 2 to stellar or CTR core temperatures ($KT = 0$ to 10 keV).

Fig. 4. Doppler broadening of an initially constant cross section from temperatures of 1 eV to 1 MeV. The results agree with theoretical predictions over the entire energy range.

Fig. 5. Doppler broadening of an initially $1/v$ cross section. Although the cross section should be temperature independent, it does not deviate until well above 100 keV - and then only at extremely low energies.

Error Messages

In the following error messages the underlined items are variables.

EXTENSION

CROSS SECTION EXTENSION CAN BE AVOIDED BY THINNING DATA OR DOPPLER BROADENING IN STEPS OF LESS THAN 2.7419+6 KELVIN

The Doppler integrals have extended beyond the three pages of core resident data. This normally occurs only for large temperature changes. Doppler broaden to the final temperature in steps (in the above example each step is not to exceed about 2.7×10^6 K).

INTERPOLATION LAW IS NOT LINEAR-LINEAR

EXECUTION TERMINATED

The data in the ENDF/B format must be linear-linear interpolatable for valid Doppler broadening by SIGMA1. Convert the data to linear-linear form using program LINEAR.⁴

Operation at LLL

At Livermore a compiled, loaded, ready-to-execute version of the program is available from the photostore as file

.193025:PROGRAMS:SAVSIG

The program is small enough (21 000 words of SCM, 6 000 words of LCM) to run at standby during the daytime as file

SAVSIG / 1 S

The program will automatically use disk files (see Requirements).

Program Listing

```

PROGRAM SIGMA1 (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
1 TAPE21,TAPE22,TAPE23)
SIG00010
SIG00020
SIG00030
SIG00040
SIG00050
SIG00060
SIG00070
SIG00080
SIG00090
SIG00100
SIG00110
SIG00120
SIG00130
SIG00140
SIG00150
SIG00160
SIG00170
SIG00180
SIG00190
SIG00200
SIG00210
SIG00220
SIG00230
SIG00240
SIG00250
SIG00260
SIG00270
SIG00280
SIG00290
SIG00300
SIG00310
SIG00320
SIG00330
SIG00340
SIG00350
SIG00360
SIG00370
SIG00380
SIG00390
SIG00400
SIG00410
SIG00420
SIG00430
SIG00440
SIG00450
SIG00460
SIG00470
SIG00480
SIG00490
SIG00500
SIG00510
SIG00520
SIG00530
SIG00540
SIG00550
SIG00560
SIG00570
SIG00580
SIG00590
SIG00600

```

THIS PROGRAM IS DESIGNED TO READ SECTIONS OF FILE 3 ENDF B
 DATA THAT HAVE ALREADY BEEN CONVERTED TO LINEAR-LINEAR
 INTERPOLATION IN ENERGY AND CROSS SECTION. THE DATA IS THEN
 DOPPLER BROADENED, THINNED AND OUTPUT IN THE ENDF B FORMAT.

THE PROGRAM ONLY USES THE ENDF B BCD FORMAT AND COPIES ALL
 SECTIONS EXCEPT FILE 3 AS HOLEPITH. AS SUCH IT MAY BE USED ON
 DATA IN THE ENDF B 1, 11, 111, IV OR V FORMAT SINCE A SECTION
 OF FILE 3 DATA IS IDENTICAL IN ALL ENDF B VERSIONS.

THE PROGRAM OPERATES NON-SELECTIVELY ON AN ENTIRE ENDF B TAPE
 (ALL CARD IMAGES BETWEEN THE TAPE LABEL AND THE TAPE END CARD).
 ALL SECTIONS OF FILE 3, EXCEPT MU-BAR, XI OR GAMMA (MT=253
 ARE BROADENED. ALL SECTIONS ARE THINNED (INCLUDING MT=253).

THE PROGRAM BROADENS A PAGE OF DATA AT A TIME (1 PAGE=100 POINTS).
 USING A PAGES OF DATA AT THE ORIGINAL TEMPERATURE. THE PAGE
 BEING BROADENED. THE PAGE BELOW IT IN ENERGY AND THE PAGE
 ABOVE IT IN ENERGY. OPERATING IN THIS MANNER THERE IS NO LIMIT
 TO THE NUMBER OF POINTS IN A SECTION.

THE ENERGY GRID FOR THE DOPPLER BROADENED CROSS SECTIONS IS
 SELECTED TO INSURE THAT THE BROADENED DATA IS LINEAR-LINEAR
 INTERPOLATABLE. AS SUCH THE ENERGY GRID FOR THE BROADENED
 DATA MAY NOT BE THE SAME AS THE ENERGY GRID FOR THE ORIGINAL
 UNBROADENED DATA.

IF THE ORIGINAL DATA IS NOT AT ZERO KELVIN THE PROGRAM
 WILL BROADEN THE DATA BY THE EFFECTIVE TEMPERATURE DIFFERENCE TO
 THE FINAL TEMPERATURE. IF THE DATA IS ALREADY AT A TEMPERATURE
 THAT IS HIGHER THAN THE FINAL TEMPERATURE DOPPLER BROADENING
 IS NATURALLY NOT PERFORMED AND THE TEMPERATURE IN THE SECTION
 IS LEFT AT ITS ORIGINAL VALUE.

THE PRESENT VERSION ONLY DOPPLER BROADENS TO ONE FINAL TEMPERATURE.
 IF THERE IS SUFFICIENT INTEREST EXPRESSED BY USERS FUTURE
 VERSIONS MAY BROADEN TO MULTIPLE TEMPERATURES. PLEASE
 CONTACT THE AUTHOR IF YOU ARE INTERESTED IN A MULTIPLE
 TEMPERATURE OPTION.

INPUT FILES

```

C      UNIT DESCRIPTION
C      -----
C      5 INPUT CARDS
C      21 SOURCE FILE (DATA AT ORIGINAL TEMPERATURE)
C      23 SCRATCH FILE FOR BROADEN DATA
C
C      OUTPUT FILES
C      -----
C      UNIT DESCRIPTION
C      -----
C      6 OUTPUT REPORT
C      22 RESULT FILE (DATA AT FINAL TEMPERATURE)
C      23 SCRATCH FILE FOR BROADENED DATA
C
C      INPUT CARDS
C      -----
C      CARD COLS. FORMAT DESCRIPTION
C      -----
C      1 1-11 E11.4 FRACTIONAL THINNING CRITERIA
C      (I.E. 0.5 PER-CENT = 0.005)
C      1 12-22 E11.4 FINAL KELVIN TEMPERATURE
C
C      EXAMPLE INPUT
C      -----
C      TO DOPPLER BROADEN TO 293 KELVIN (ROOM TEMPERATURE) AND THEN
C      THE BROADENED DATA TO 0.5 PER-CENT (0.005 AS A FRACTION), THE
C      FOLLOWING INPUT CARD SHOULD BE USED.
C
C      5.0000E+03 2.9300E+02
C
C      THE PROGRAM MAY BE USED TO THIN DATA, WITHOUT DOPPLER
C      BROADENING BY SPECIFYING A TEMPERATURE OF ZERO, AS FOLLOWS.
C
C      5.0000E+03 0.0000E+00
C
C      LINEARIZING AND/OR THINNING DATA CAN BE DONE MORE EFFICIENTLY
C      USING THE PROGRAM LINEAR (UCRL-50400, VOL. 17, PART B BY C. P. L. ET AL.)
C
C      INTEGER OTAPE,OUTP,SCR
C      COMMON/HEADER/C1H,C2H,L1H,L2H,N1H,N2H,MATH,MFH,MTF,NOSEQ
C      COMMON/FILLER/DUMMY(17),MATD,MFD,MTD
C      COMMON/UNITS/OUTP,INP,ITAPE,OTAPE,SCR
C      COMMON/HOTS/ALPHA,TEMPK,TEMPF,ERTHIN,N2TOT,N2OTIC
C      COMMON/MATTOT/MATIN,MATOUT
C      COMMON/NORMIT/XNORM161,KSIGN161,KEXP16
C      COMMON/CONTACT/OVP1,OVP12,ATOP
C      COMMON/EXTEND/MESS,MEAT,DTMAX
C
C      --- DEFINE ZERO TO FILL MFTM AND NOSEQ FIELDS OF LABEL RECORD.
C      DATA IZERO/0/
C
C      --- DEFINE PORTIONS OF PI TO DEFINE PI ACCURATELY ON VARIOUS
C      COMPUTERS.
C      DATA PI1/3.14159/
C      DATA PI2/9.2653E-5/
C      DATA PI3/5.8979E-10/
C      DATA PI4/3.2384E-15/
C
C      DEFINE ALL 1.0 UNITS TO CHANGE UNIT ASSIGNMENTS FOR ANY
C      OTHER INSTALLATION. MERELY CHANGE THE FOLLOWING DEFINITION
C      TO SUIT YOURSELF, WHERE APPROPRIATE.

```

```

C      INP  = INPUT CARD                      51001217
C      OUTP = OUTPUT LISTING FILE             51001227
C      ITAPE = DATA IN ENDF/B FORMAT AT ORIGINAL TEMPERATURE 51001232
C      OTAPE = DATA IN ENDF/B FORMAT AT FINAL TEMPERATURE   51001242
C      SCR   = SCRATCH FILE                   51001255
C                                              51001265
C      IF YOU WISH TO ALLOW FOR VARIABLE UNIT ASSIGNMENTS MERELY 51001278
C      ACTIVATE THE SECOND INPUT FORM ALREADY LISTED AS A COMMENT 51001280
C      CARD BELOW (THE FORMAT IS ALREADY COMPATIBLE)           51001290
C                                                              51001305
C      INP=5
C      OUTP=6
C      ITAPE=21
C      OTAPE=22
C      SCR=23
C      51001310
C      51001320
C      51001330
C      51001340
C      51001350
C      51001360
C-----READ RUN PARAMETERS (2E11,4)
C      READ(INP,5000) ERTHIN,TEMPK
C      51001370
C      51001380
C      51001390
C      51001400
C      51001410
C      51001420
C      51001430
C      51001440
C      51001450
C      51001460
C      51001470
C      51001480
C      51001490
C      51001500
C      51001510
C      51001520
C      51001530
C      51001540
C      51001550
C      51001560
C      51001570
C      51001580
C      51001590
C      51001600
C      51001610
C      51001620
C      51001630
C      51001640
C      51001650
C      51001660
C      51001670
C      51001680
C      51001690
C      51001700
C      51001710
C      51001720
C      51001730
C      51001740
C      51001750
C      51001760
C      51001770
C      51001780
C      51001790
C      51001800

```

```

WRITE(OTAPE,5010) (XNORM(I),KSIGN(I),KEXP(I),L=1,2),
1 L1H,L2H,N1H,N2H,MATH,MFH,MTD,NOSEQ
C-----CHECK FOR SECTION OF FILE 3 DATA.
IF(MFH-3) 60,50,60
C-----FILE 3 LOCATED. PROCESS SECTION
50 CALL FILE3
C-----SKIP TO END OF SECTION.
60 READ(OTAPE,5030) DUMMY,MATD,MFD,MTD,
NOSEQ=NATSEQ(NOSEQ)
IF(MTD) 80,80,70
70 WRITE(OTAPE,5030) DUMMY,MATD,MFD,MTD,NOSEQ
GO TO 60
80 WRITE(OTAPE,5020) MATD,MFD,MTD,NOSEQ
GO TO 10
C-----END CARD READ AND WRITTEN.
C---- WRITE TOTALS FOR LAST MATERIAL.
90 WRITE(OUTP,5040) MATIN,MATOUT
C-----LIST TOTAL NUMBER OF FILE 3 POINTS READ AND WRITTEN.
WRITE(OUTP,5050) N2TOT1,N2TOT0
C---- WRITE WARNING MESSAGE IF CROSS SECTION EXTENSION USED.
IF(DTMAX.LE.0.0) GO TO 100
CALL NORMAL(DTMAX,XNORM(1),KSIGN(1),KEXP(1))
WRITE(OUTP,6020) XNORM(1),KSIGN(1),KEXP(1)
C---- CLOSE FILE AND TERMINATE.
100 END FILE OTAPE
REWIND OTAPE
REWIND OTAPE
CALL EXIT
5010 FORMAT(2I11,4,4I11,14,12,13,15)
5010 FORMAT(2I18,5,A1,12),4I11,14,12,13,15)
5020 FORMAT(6X,14,12,13,15)
5030 FORMAT(16A4,A2,14,12,13,15)
5040 FORMAT(2X,54(IH-1)/32X,10HMT TOTALS,217/2X,54(IH-1))
5050 FORMAT(2X,54(IH-1)/32X,11HTAPE TOTALS,217/2X,54(IH-1))
6000 FORMAT(39H1 DOPPLER BROADENING/8 CROSS SECTIONS,
1 1H-1 SIGMA) 77 1) 2X,54(IH-1)/
2 2X,19HTHINNING CRITERIA--FB,5,A1,12)
3 2X,19HTEMPERATURE-----FB,5,A1,12,7H KELVIN,2X,54(IH-1))
6010 FORMAT(2X,10HTAPE LABEL,2X,16A4,A2,14,2X,54(IH-1))
1 2X,5H 2A,5H MAT,5H M,6X,6HKELVIN,5X,7H0-VALUE,
2 7H POINTS,7H POINTS)
3 2X,2HIN,10X,2HEX,7H IN,7H OUT,2X,54(IH-1))
6020 FORMAT(1/11H EXTENSION:2X,9H-1)
1 4H CROSS SECTION EXTENSION CAN BE AVOIDED BY:
2 4H THINNING DATA OR DOPPLER BROADENING IN STEPS
3 14H IF LESS THAN,FB,5,A1,12,7H KELVIN)
END
SUBROUTINE FILES
C
C MAIN ROUTINE IS DESIGNED TO LOAD DATA INTO THE CORE AND DOPPLER
C BROADENING A PAGE AT A TIME. (1) PAGE=1000 POINTS. IF THE SECTION
C IS 1000 OR LESS POINTS THE ENTIRE OPERATION IS PERFORMED IN CORE.
C IF THE SECTION IS OVER 1000 POINTS IT IS WRITTEN ONTAPE IN A
C FILE WHICH CAN LATER BE READ BY TABFIN.
C
INTEGER OMP,OCR,TOCHI
COMMON INDEL,LOW,KHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,
1 INDEL,NPAGE,INCR1,NLEFT,NPAGE,LOLOW,LOON
COMMON TEMP,NTOT1,NTOT0,INT200
100000000 ALPHA,TEMP,TEMP,ERTH,N,N2TOT1,N2TOT0

```

```

S1G01810
S1G01820
S1G01830
S1G01840
S1G01850
S1G01860
S1G01870
S1G01880
S1G01890
S1G01900
S1G01910
S1G01920
S1G01930
S1G01940
S1G01950
S1G01960
S1G01970
S1G01980
S1G01990
S1G02000
S1G02010
S1G02020
S1G02030
S1G02040
S1G02050
S1G02060
S1G02070
S1G02080
S1G02090
S1G02100
S1G02110
S1G02120
S1G02130
S1G02140
S1G02150
S1G02160
S1G02170
S1G02180
S1G02190
S1G02200
S1G02210
S1G02220
S1G02230
S1G02240
S1G02250
S1G02260
S1G02270
S1G02280
S1G02290
S1G02300
S1G02310
S1G02320
S1G02330
S1G02340
S1G02350
S1G02360
S1G02370
S1G02380
S1G02390
S1G02400

```


READ LITARE,50101 (NBTK),INT(K),K+1,N1)	51003010
C - INSURE DATA IS LINEAR-LINEAR INTERPOLABLE.	51003020
DO 60 K=1,N1	51003030
IF (INT(K).NE.2) GO TO 70	51003040
60 CONTINUE	51003050
GO TO 80	51003060
C - NOT LINEAR-LINEAR. TERMINATE EXECUTION.	51003070
70 WRITE (OUTP,5050) IZA,MATH,MTH	51003080
CALL EXIT	51003090
5. SET BROADENING INDICES TO MIDDLE PAGE.	51003100
80 NLOW=NPAGE+1	51003110
NHIGH=2*NPAGE	51003120
C - SET INDEX TO LOADED POINTS AT BEGINNING OF MIDDLE PAGE.	51003130
KLOW=NLOW	51003140
C - SET THINNING CONVERGED INDEX TO FIRST POINT IN CORE.	51003150
KCON=NLOW	51003160
5. SET INDICES TO LOAD MIDDLE AND LAST PAGE.	51003170
NLOW=NLOW	51003180
NHIGH=2*NPAGE	51003190
5. INITIALIZE SECTION FLAGS.	51003200
NR=1 AND	51003210
IF (NR.NE.1) NR=1	51003220
NLEFT=0	51003230
NEMAKE	51003240
5. LOAD NEXT PAGE OF DATA AT ORIGINAL TEMPERATURE	51003250
90 CALL READPR	51003260
5. SET INDEX TO LOADED POINTS TO LAST POINT LOADED.	51003270
KHIGH=NRIGH	51003280
IF (NRIGH.NE.NHIGH) NRIGH=NHIGH	51003290
5. SHOULD DATA BE DOPPLER BROADENED....	51003300
DO 100 K=NRIGH+1,100 TO 120	51003310
5. DOPPLER BROADENED DATA TO BROADENED LOCATIONS. NO BROADENING	51003320
IF (E=0) ENERGY HAS NOT BEEN CONVERTED TO SPEED AND THEREFORE	51003330
DO NOT NEED BE RE CONVERTED DURING THIS STEP	51003340
DO 100 K=NLOW,NHIGH	51003350
100 CONTINUE	51003360
5. IF NR=1	51003370
NR=1	51003380
5. BROADEN POINTS IN MIDDLE PAGE	51003390
100 CALL BROADN	51003400
5. THIN BROADENED POINTS.	51003410
150 CALL THINB	51003420
5. DEFINE NUMBER OF POINTS LEFT ON PAGE AFTER THINNING.	51003430
NH=NRIGH-KLOW+1	51003440
IF (ORIGINAL DATA IS ONE PAGE OR LESS) OUTPUT SECTION	51003450
5. DERIVED FROM CORE.	51003460
IF (NRIGH.NE.NHIGH) GO TO 140	51003470
5. NEMAKE=1,NPAGE GO TO 180	51003480
5. OVERWRITE OUTPUT TO SCRATCH.	51003490
200 DO 100 WRITE (OUTP,KR) (K+1,SB(K),K+1,NLOW,NHIGH)	51003500
INCREASE COUNT OF POINTS TO OUTPUT.	51003510
K=K+1	51003520
5. HAVE THE LAST P. BEEN BROADENED....	51003530
DO 100 K=NRIGH+1,100 TO 180	51003540
5. HAVE UNCONVERGED THINNING POINTS OR ANY IN THE SECTION	51003550
IMMEDIATELY IN FRONT OF THE NEXT PAGE TO BE BROADENED. AFTER THAT	51003560
ALL K BROADENED THEN REMAINING POINTS PLUS THE BROADENED DATA	51003570
WILL BE TREATED AS ONE SET OF POINTS FOR THINNING.	51003580
DO 100 K=NRIGH+1,100 TO 180	51003590
5. HAVE ALL THINNING	51003600

```

      150 KKKKK=1
      160 KKK=0
      170 KKK=1
      180 KKK=1
      190 KKK=1
      200 KKK=1
      210 KKK=1
      220 KKK=1
      230 KKK=1
      240 KKK=1
      250 KKK=1
      260 KKK=1
      270 KKK=1
      280 KKK=1
      290 KKK=1
      300 KKK=1
      310 KKK=1
      320 KKK=1
      330 KKK=1
      340 KKK=1
      350 KKK=1
      360 KKK=1
      370 KKK=1
      380 KKK=1
      390 KKK=1
      400 KKK=1
      410 KKK=1
      420 KKK=1
      430 KKK=1
      440 KKK=1
      450 KKK=1
      460 KKK=1
      470 KKK=1
      480 KKK=1
      490 KKK=1
      500 KKK=1
      510 KKK=1
      520 KKK=1
      530 KKK=1
      540 KKK=1
      550 KKK=1
      560 KKK=1
      570 KKK=1
      580 KKK=1
      590 KKK=1
      600 KKK=1
      610 KKK=1
      620 KKK=1
      630 KKK=1
      640 KKK=1
      650 KKK=1
      660 KKK=1
      670 KKK=1
      680 KKK=1
      690 KKK=1
      700 KKK=1
      710 KKK=1
      720 KKK=1
      730 KKK=1
      740 KKK=1
      750 KKK=1
      760 KKK=1
      770 KKK=1
      780 KKK=1
      790 KKK=1
      800 KKK=1
      810 KKK=1
      820 KKK=1
      830 KKK=1
      840 KKK=1
      850 KKK=1
      860 KKK=1
      870 KKK=1
      880 KKK=1
      890 KKK=1
      900 KKK=1
      910 KKK=1
      920 KKK=1
      930 KKK=1
      940 KKK=1
      950 KKK=1
      960 KKK=1
      970 KKK=1
      980 KKK=1
      990 KKK=1
      1000 KKK=1

```

```

COMMON /HOTS/ALPHA,TEMPK,TEMPER,ERTHIN,N2TOT1,N2TOT2
COMMON /HITS/OUTP,INP,ITAPE,OTAPE,SCR
COMMON /INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,
1 N2IN,N2MADE,N2OUT,NLEFT,NPAGE,JJLOW,JJHIGH
COMMON /INLER/IFILL,NFILL,NLEFT,TOOH1
COMMON /X/30061,5130061,XOUT12551,100130061,XOUT12551,BREAL,1002
1 EINT12551,5INT12551
COMMON /XIN/2401,XIN12401
5 SET UP LOOP OVER POINTS TO LOAD INTO ORIGINAL TEMPERATURE ARRAY.
60 JG K MLOW,MHIGH
7 IF NO MORE POINTS IN CORE READ NEXT PAGE (IF ANY).
8 IF IFILL LE NFILL GO TO 20
9 IF NLEFT GT NFILL GO TO 10
10 IF NLEFT LE 01 GO TO 80
11 NLEFT=NLEFT-1
12 READ ITAPE,5050 (XIN11,XIN111,1,NFILL)
13 IFILL=1
14 DETERMINE IF DATA WILL BE DOPPLER BROADENED (IF NOT MAXIMUM
15 ENERGY SPACING IS NOT REQUIRED).
20 IF (TOOH1) 30,40,50
30 NO DOPPLER BROADENING IF THRESHOLD OVER 1.00E+000*KT AL.
40 TOOH1=0
50 IF (ALPHA*(IN11-5E+0000000.0)/TOOH1)
60 TO 50
7 CHECK FOR MAXIMUM ALLOWABLE ENERGY SPACING.
80 IF (XIN12401-LE XNEXT) GO TO 50
9 INTERPOLATE TO INSERT POINT AT MAXIMUM ALLOWABLE ENERGY SPACING.
XK=XNEXT
XK1=XNEXT-XKMI*(XIN12401-5XMI)/(XIN12401-XKMI)
60 TO 60
7 ENERGY SPACING OK.
50 XK1=XIN12401
60 IF (XIN12401)
70 IFILL=IFILL+1
80 XKMI=XK1
90 XKMI=XK1
100 XNEXT=DEMAX*XKMI
11 IF NLEFT GT 0 AND (IFILL GT NFILL + NLEFT*2)
GO TO 40
80 END OF DATA TABLE.
80 MHIGH=K-1
NLEFT=0
90 N2MADE=N2MADE+MHIGH-MLOW+1
RETURN
ENTRY MAXDE
1 ENTRY POINT TO DEFINE MAXIMUM ALLOWABLE ENERGY SPACING.
CON 2.0/SQRT(1.0-3.0)*3.0
1 1.0
01 0.01
FRUSE=ERTHIN
IF (ERTHIN LT 0.001) FRUSE=0.001
1 1 01
BOTTOM=1+1
TOP=BOTTOM+1.0
FRS=ABS(1.0-CON*TOP/SQRT(TOP)*BOTTOM)
IF (FRS LE FRUSE) 110,120,100
110 IF (L1 LT 1.0E-06) GO TO 120

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      T=T*DT
      DT=0.1*DT
      GO TO 100
120  DEMAX=T*T
      RETURN
5000  FORMAT(6E11.4)
      END
      SUBROUTINE BROADEN
C
C      GIVEN A CROSS SECTION THAT IS DESCRIBED BY A TABLE OF
C      X'S VS. X AND LINEAR-LINEAR INTERPOLATION BETWEEN POINTS
C      THIS ROUTINE WILL EXACTLY DOPPLER BROADENING THE CROSS
C      SECTION AT A PORTION OF THE ENERGIES CORRESPONDING TO THE
C      ORIGINAL CROSS SECTION (APPROXIMATELY THE MIDDLE THIRD).
C
C      INPUT PARAMETERS
C      KLOW =INDEX TO FIRST POINT LOADED IN CORE.
C      KHIGH =INDEX TO LAST POINT LOADED IN CORE.
C      NLOW =INDEX TO FIRST POINT TO BROADEN.
C      NHIGH =INDEX TO LAST POINT TO BROADEN.
C      MLOW =INDEX TO FIRST POINT JUST LOADED.
C      MHIGH =INDEX TO LAST POINT JUST LOADED.
C      X =TABLE OF ENERGIES CORRESPONDING TO S.
C      S =TABLE OF CROSS SECTIONS AT INITIAL TEMPERATURE.
C      CK =SCRATCH ARRAY TO USE FOR SLOPE BETWEEN POINTS IN (X,S).
C      EB =TABLE OF ENERGIES CORRESPONDING TO SB.
C      SB =TABLE OF CROSS SECTION BROADENED TO TEMPK.
C      ALPHA =DOPPLER WIDTH ((1505.3*AWC)/TEMPK)
C
C      THE POINTS JUST LOADED (MLOW,MHIGH) ARE CONVERTED TO SPEED
C      LIKE TERMS AND SLOPES BETWEEN POINTS COMPUTED. THE TABLE OF
C      POINTS (KLOW,KHIGH) IS USED TO BROADEN THE RESULT TABLE
C      (NLOW,NHIGH).
C
C      THE CORE TABLES MAY BE CONSIDERED TO BE COMPOSED OF PAGES OF
C      1002 POINTS EACH. THREE PAGES ARE USED FOR THE DATA AT THE
C      ORIGINAL TEMPERATURE (X,S,CK) (9018 WORDS) AND ONE PAGE
C      IS USED FOR THE BROADENED CROSS SECTION (SB).
C
C      DURING ONE PASS OF THIS ROUTINE A PAGE OF DOPPLER BROADENED
C      CROSS SECTIONS WILL BE CREATED AT THE ENERGIES CORRESPONDING
C      TO THOSE IN THE MIDDLE PAGE OF THE DATA AT THE ORIGINAL
C      TEMPERATURE.
C
C      ONCE THE BROADENED DATA ARE CREATED THE DATA AT THE
C      ORIGINAL TEMPERATURE IN THE FIRST PAGE IS NO LONGER NEEDED.
C      AND THE ENERGIES CORRESPONDING TO THE BROADENED CROSS
C      SECTIONS ARE STORED IN THE FIRST PAGE OF (CK) FOR LATER
C      TRIPPING IN ROUTINE THINB.
C
C      IN ORDER TO ALLOW THE SAME INDICES TO BE USED FOR BOTH
C      THE ORIGINAL AND BROADENED DATA TWO DUMMY ARRAYS (EB,SB)
C      ARE DEFINED ONE PAGE IN FRONT OF THE LOCATIONS THAT WILL
C      BE USED TO STORE THE BROADENED DATA.
C
C      COMMON/INDEX/KLOW,KHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,
C      N2IN,NPMAD,N2GOT,N2LEFT,NPAGE,JJLOW,JJLOW,ILOW
C      COMMON/HEADER/EB,AWC,L1H,L2H,N1H,N2H,MATH,MFH,M1H,N2SG
C      COMMON/LEADER/L1,L2,L1,L2,N1,N2,MAT,MF,MT
C      COMMON/HOTS/ALPHA,TEMPK,TEMPER,ERHIN,N2TOT1,N2TOT2

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COMMON/ERFEX/P/EXPERT	51005410
COMMON/CONTACT/OVP1,OVP12,ATOP	51005420
COMMON/INDICE/KNOW,KLOW,KLPI,KHMI	51005430
COMMON/EXTEND/MESS,MEXT,DTMAX	51005440
COMMON X(3006),S(3006),EOUT(255),CK(3006),SGUT(255),SBPEAL(150),	51005450
LEIN(255),SIN(255)	51005460
DIMENSION IB(2004),SB(2004)	51005470
EQUIVALENCE (S(2260),EB),CK(2260),SB)	51005480
C	51005490
C CONVERT FROM ENERGY TO SPEED AND DEFINE SLOPES BETWEEN POINTS.	51005500
C	51005510
C-----CONVERT ENERGIES TO SPEED LIKE TERMS.	51005520
DO 10 N=ML0W,MHIGH	51005530
10 X(N)=SQRT(ALPHA*X(N))	51005540
C-----DEFINE THE NUMBER OF INTERVALS AND COMPUTE SLOPE IN	51005550
C-----EACH INTERVAL.	51005560
KLPI=KLOW+1	51005570
KHMI=KHIGH-1	51005580
ML=MLOW	51005590
IF(MLOW.GT.KLOW) ML=ML-1	51005600
MHI=MHIGH-1	51005610
XXLAST=X(ML)**2	51005620
DO 30 KNOW=ML,MHI	51005630
XXNOW=X(KNOW+1)**2	51005640
DX=XXNOW-XXLAST	51005650
IF(DX.LE.0.0) GO TO 20	51005660
CK(KNOW)=S(KNOW+1)-S(KNOW)+DX	51005670
GO TO 30	51005680
20 CK(KNOW)=0.0	51005690
30 XLAST=XXNOW	51005700
C	51005710
C TEST FOR CROSS SECTION EXTENSION	51005720
C	51005730
C-----TEST LOWER LIMIT FOR ALL PAGES BEYOND SECOND.	51005740
MEXT=MEXT+1	51005750
IF(MEXT.LE.3) GO TO 40	51005760
DX=X(1003)-X(1)	51005770
IF(DX.LE.ATOP) GO TO 50	51005780
C TEST UPPER LIMIT FOR ALL PAGES BUT LAST ONE.	51005790
40 IF(IN2LEFT.LE.0) GO TO 60	51005800
DX=X(3006)-X(2004)	51005810
IF(DX.GT.ATOP) GO TO 60	51005820
C-----DEFINE MAXIMUM ALLOWABLE TEMPERATURE CHANGE TO AVOID	51005830
C-----CROSS SECTION EXTENSION.	51005840
50 DX=DX/ATOP	51005850
DTMAX2=TEMPF*DX*DX	51005860
IF(DTMAX.LE.0.0.OR.DTMAX2.LT.DTMAX) DTMAX=DTMAX2	51005870
C-----SET FLAG TO PRINT OUT MESSAGE WITH SECTION	51005880
MESS=2	51005890
C	51005900
C BROADEN DATA. SPECIAL TREATMENT FOR LOW ENERGY.	51005910
C	51005920
60 KNOW=NLOW	51005930
IF(X(NLOW).GT.ATOP) GO TO 70	51005940
CALL BROADL	51005950
IF(KNOW.GT.NHIGH) RETURN	51005960
70 CALL BROADH	51005970
RETURN	51005980
END	51005990
SUBROUTINE BROADL	51006000


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C      - - - - - DEFINE CONSTANTS FOR THIS POINT.
      BMY=B*Y
      BPY=B*Y
      RBMY=R*AT10N(BMY)
      RBPY=R*AT10N(BPY)
      EXBMY=EXP(-BMY*BMY)
      EXBPY=EXP(-BPY*BPY)
      SO=ERF(C/RBMY,EXBMY)-ERF(C/RBPY,EXBPY)
      EM=EXBMY+EXBPY
      EP=L*EM+EXBPY
      BEMYE=B*EM+Y*EP
      F2B=Y*A*(SO+OVP)*BEMYE
      DUMMY1=DUMMY1+0.5*(SILNOW+1)*(F2A-F2B)
      IF(BMY.GT.ATOP) GO TO 30
10    CONTINUE
C      - - - - - CONTINUE CROSS SECTION AS CONSTANT TO X=INFINITY
20    DUMMY1=DUMMY1+SIKHIGH*F2B
      RE INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES
30    R=AT10N(Y2)
      EXP1=EXP(Y2*Y2)
      F2A=Y*A*(1.0+ERF(C/R,EXPERF1)+OVP)/2*Y
      NO INTERVALS BELOW CURRENT FIRST POINT.
      IF(SILNOW.EQ.KLOW) GO TO 50
      GET 100 OVER OVER INTERVALS BELOW CURRENT POINT
      KLOW=KLOW
      DUM1=DUM1+K*SIKLOW
      UNDO=UNDO+1
      A=K*SIKLOW
      CALL CALF1 FROM A * INTEGRAL
      EXP1=EXP1
C      - - - - - DEFINE CONSTANTS FOR THIS POINT.
      YMA=Y+A
      YPA=Y+A
      RYMA=R*AT10N(YMA)
      RYPA=R*AT10N(YPA)
      EXYMA=EXP(-YMA*YMA)
      EXYPA=EXP(-YPA*YPA)
      SO1=ERF(C/RYMA,EXYMA)-ERF(C/RYPA,EXYPA)
      EM1=EXYMA+EXYPA
      EP1=L*EM1+EXYPA
      BEMYE1=B*EM1+Y*EP1
      F2A1=Y*A*(SO1+OVP)*BEMYE1
      DUMMY1=DUMMY1+0.5*(NEW1+1)*(F2A-F2A1)
      IF(YMA.GT.ATOP) GO TO 60
40    CONTINUE
C      - - - - - CONTINUE CROSS SECTION AS CONSTANT TO X=INFINITY
50    R=AT10N(Y2)
      EXP1=EXP(Y2*Y2)
      DUMMY1=DUMMY1+KLOW*(Y2-YA)*OVP*ERF(C/R,EXPERF1)
      F2A=Y*A*(1.0+ERF(C/R,EXPERF1)+OVP)/2*Y
      DEFINE BE-ADDED CROSS SECTION
      KLOW=KLOW+K*SIKLOW
      UNDO=UNDO+1
C      - - - - - CONTINUE CORRELATED LINE TERMS RE-START ENERGY
      L=K*SIKLOW*UNDO
      RE=L*SIKLOW*ALPHA
      KLOW=KLOW+L
      RE=RE+L
      RE=RE+RE*ALPHA

```


[illegible]


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      GO TO 70
C-----THREE OR MORE POINTS ALL WITH THE SAME ENERGY. KEEP NEXT
C-----POINT IF NOT THE SAME CROSS SECTION AS LAST POINT.
      50 IF(SB(JHIGH).EQ.SB(ILOW)) GO TO 70
C-----AT LEAST ONE POINT IN INTERVAL FAILS TEST. SAVE LAST POINT
C-----WITHIN THE INTERVAL.
      60 JHIGH=JHIGH+1
         XB(JHIGH)=XB(NM1)
         SB(JHIGH)=SB(NM1)
C-----RESET LOWER LIMIT OF INTERVAL THAT CAN BE THINNED.
         ILOW=N
      70 CONTINUE
C-----IS THIS THE END OF THE ENTIRE TABLE (ALL POINTS BROADENED).
      IF(NHIGH.LT.KHIGH) GO TO 80
C-----YES. MOVE LAST POINT IN TABLE TO THINNED TABLE.
         JHIGH=JHIGH+1
         XB(JHIGH)=XB(NHIGH)
         SB(JHIGH)=SB(NHIGH)
         RETURN
C-----NO. DETERMINE NUMBER OF UNCONVERGED POINTS LEFT OVER FROM
C-----THINNING.
         80 KLEFT=NHIGH-ILOW+1
C-----WILL REMAINING POINTS FIT INTO (XGUT,YOUT).
         IF(KLEFT.LE.255) GO TO 90
C-----NO. THIN INTERMEDIATE POINTS BETWEEN ILOW AND NHIGH BY SIMPLE
C-----RESETTING LOWER THINNING INDEX.
         ILOW=NHIGH
         RETURN
C-----YES. SAVE LAST CONVERGED POINT IN CORE TO SERVE AS PLOT OF W
C-----THINNING OF NEXT PAGE OF DATA.
         90 ILOW=ILOW-1
            JHIGH=JHIGH-1
            RETURN
         END
         SUBROUTINE TABFIN
C
C   THIS ROUTINE IS DESIGNED TO COPY THE SECTION OF BROADENED AND TH
C   THINNED DATA FROM THE CORE OR SCRATCH FILE TO THE RESULT FILE IN
C   THE ENDF B FORMAT.
C
      INTEGER OTAPE,OUTP,SCR
      COMMON/UNITS/OUTP,INF,ITAPE,OTAPE,SCR
      COMMON/TERP/NBT(200),INT(200)
      COMMON/HEADER/C1H,C2H,L1H,L2H,N1H,N2H,MATH,MFH,MTH,NOSF
      COMMON/LEADER/C1,C2,L1,L2,N1,N2,MA,MP,MT
      COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,KLOW,KHIGH
      COMMON/IN,NZPIN,NZMADE,NZOUT,NZLEFT,NPAGE,JULOK,ILOW
      COMMON/X(3006),S(3006),XOUT(255),CK(3006),YOUT(255),XBEA
      COMMON/L(1255),SIN(255)
      COMMON/NORM/IT,XNORM(6),KSIGN(6),KEXP(6)
      DIMENSION XP(1257),YP(1257),XB(2256),SB(2256)
      EQUIVALENCE (S(12560),XB),CK(12560),SB),XB,XBEA,XOUT,XBEA
C----- DEFINE NUMBER OF POINTS TO OUTPUT.
      NZ=NZOUT
C----- SET INTERPOLATION LAW TO LINEAR LINEAR OVER ENTIRE TABLE
      NBT(1)=NZOUT
      INT(1)=
      INT(2)=
      INT(3)=
C----- INCREMENT SEQUENCE NUMBER AND WRITE LEADING INTERPOLATION LA
      NBT(N+1)=NBT(N)+NOSF

```



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111 CALL NORMAL(XB(1),XNORM(1),KSIGN(1),KEXP(1))
112 CALL NORMAL(XB(2),XNORM(2),KSIGN(2),KEXP(2))
113 GO TO (130,140),ILEFT
130 WRITE(OTAPE,5030) (XNORM(I),KSIGN(I),KEXP(I),I=1,I2)
1 MAT,ME,MT,NOSEQ
140 GO TO 150
141 WRITE(OTAPE,5040) (XNORM(I),KSIGN(I),KEXP(I),I=1,I2)
1 MAT,ME,MT,NOSEQ
C----- F SWATCH FILE WAS USED RE-POSITION FOR NEXT TABLE
150 IF(INZMADE.GT.NPAGED)REWIND SCR
RETURN
5000 FORMAT(2(F8.5,A1,I2),4(I1,I4,I2,I3,I5)
5010 FORMAT(2(I1),4(X,I4,I2,I3,I5)
5020 FORMAT(6(F8.5,A1,I2),I4,I2,I3,I5)
5030 FORMAT(2(F8.5,A1,I2),4(X,I4,I2,I3,I5)
5040 FORMAT(4(F8.5,A1,I2),I2(X,I4,I2,I3,I5)
END
SUBROUTINE NORMAL(X,XNORM,KSIGN,KEXP)
C
C CONVERT FLOATING POINT NUMBER TO NORMAL FORM FOR OUTPUT
C OUTPUT WILL BE IN THE FORM X.YXXXXX*10**N, WHICH GIVES
C AN ADDITIONAL DIGIT OF ACCURACY WHEN COMPARED WITH
C FORTRAN OUTPUT. IN ADDITION THE OUTPUT WILL BE COMPATIBLE
C INDEPENDENT (I.E. SAME ON IBM, CD, UNIVAC ETC)
C
C INTEGER PLUS
C DEFINE TWO POSSIBLE SIGNS FOR EXPONENT.
DATA PLUS/1H+/
DATA MINUS/1H-/
C COMPUTE SIGNED EXPONENT FROM ABSOLUTE VALUE.
XABS=ABS(X)
C IF NUMBER IS 0.0 DEFINE 0.00000E+0
IF(XABS)50,50,10
C DEFINE EXPONENT TO NORMALIZE MANTISSA.
10 KEXP=ALOG10(XABS)
SHIFT=10.0**KEXP
XNORM=XABS*SHIFT
IF(XNORM.GE.0.999995)GO TO 20
KEXP=KEXP-1
SHIFT=SHIFT*10.0
GO TO 30
20 IF(XNORM.LT.0.999995)GO TO 30
KEXP=KEXP+1
SHIFT=10.0*SHIFT
C COMPUTE SIGNED MANTISSA.
30 XNORM=X*SHIFT
C----- DEFINE SIGN OF EXPONENT AND INSURE EXPONENT IS EVEN.
IF(KEXP)40,60,60
40 KSIGN=MINUS
KEXP=KEXP-1
RETURN
C X IS 0.0, DEFINE AS 0.00000E+0
50 XNORM=0.0
KEXP=0
60 KSIGN=PLUS
RETURN
END
END SUBROUTINE NEXTSEQ(NOSEQ)

```

1	DEFINE NEXT SEQUENCE NUMBER SUB-ENTRY B OUTPUT, ALLOW FOR	000000
2	MORE THAN 100000 CARDS PER EVALUATION BY RESERVING NUMBER	000000
3	TO 1 EVERY TIME 100000 IS REACHED.	000000
4		000000
5	NNNNNNNN	000000
6	IF>NNNNNNNNNNNN	000000
7	NNNNNNNN	000000
8	RETURN	000000
9	END	000000

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