27
5/28/79
240 HTLS

MASTER

UCRL-50400
Vol 21, Pt. C

AN INTEGRATED SYSTEM FOR PRODUCTION OF NEUTRONICS AND PHOTONICS CALCULATIONAL CONSTANTS VOLUME 21, PART C

PROGRAM SIGNAL (VERSION 79-1): DOPPLER-BROADEN
EVALUATED CROSS SECTIONS IN THE LIVERMORE-EVALUATED
NUCLEAR DATA LIBRARY (ENDL) FORMAT

D. E. Cullen

March 17, 1979

Work performed under the auspices of the U.S. Department of
Energy by the UCLLL under contract number W-7405-ENG-48.

LAWRENCE LIVERMORE LABORATORY

University of California / Livermore, California 94550

UCRL-50400 Vol. 21, Part C

AN INTEGRATED SYSTEM FOR PRODUCTION OF NEUTRONICS AND PHOTONICS CALCULATIONAL CONSTANTS

**PROGRAM SIGNAL (VERSION 79-1): DOPPLER-BROADEN
EVALUATED CROSS SECTIONS IN THE LIVERMORE-EVALUATED
NUCLEAR DATA LIBRARY (ENDL) FORMAT**

D. E. Cullen

MS. date: March 17, 1979

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

89

FOREWORD

The UCRL-50400 series describes an integrated and computer-oriented system for the production and application of neutronics and photonics calculational constants.

The system must supply reliable up-to-date data, select specific types of data on request, provide output in a variety of forms (ultimately in the form of input to other computer codes), and function rapidly and efficiently. The system has now been developed to a point where we are achieving these goals.

The UCRL-50400 series, *An Integrated System for Production of Neutronics and Photonics Calculational Constants*, comprises the following volumes:

- Vol. 1, Part A, Rev. 3, *ECSIL: A System for Storage, Retrieval, and Display of Experimental Neutron Data*, September 1976.
- Vol. 1, Part B, *Program ECSX4 (Version 78-1): Conversion of Experimentally Measured Cross-Section Data from the Four-Center-Exchange (X-4) Format to the Livermore ECSIL Format*, December 1978.
- Vol. 2, Rev. 2, *A Bibliography of the Experimental Data of Neutron-Induced Interactions*, July 1976.
- Vol. 3, Rev. 2, *An Index of Experimental Data of Neutron-Induced Interactions*, July 1976.
- Vol. 4, *Evaluated Nuclear Cross-Section Library*, April 1971.
- Vol. 5, Part A, Rev. 1, *CLYDE: A Code for the Production of Calculational Constants from Nuclear Data*, September 1975.
- Vol. 5, Part B, Rev. 1, *Relativistic Transformations between Center-of-Mass and Laboratory Systems for Two-Body Nuclear Reactions*, April 1978.
- Vol. 6, Rev. 2, *Tables and Graphs of Photon-Interaction Cross Sections from 1 keV and 100 MeV*, December 1978.
- Vol. 7, Part A, Rev. 1, *Major Neutron-Induced Interactions ($Z \leq 55$): Graphical, Experimental Data*, July 1976.
- Vol. 7, Part B, Rev. 1, *Major Neutron-Induced Interactions ($Z > 55$): Graphical, Experimental Data*, July 1976.
- Vol. 8, Part A, Rev. 1, *Supplemental Neutron-Induced Interactions ($Z \leq 35$): Graphical, Experimental Data*, July 1976.
- Vol. 8, Part B, Rev. 1, *Supplemental Neutron-Induced Interactions ($Z > 35$): Graphical, Experimental Data*, July 1976.
- Vol. 9, *Thresholds of Nuclear Reactions Induced by Neutrons, Photons, Deutrons, Tritons, and Alpha Particles*, September 1970.
- Vol. 10, Rev. 1, *Tabulated Experimental Data for Neutron-Induced Interactions*, July 1976.
- Vol. 11, *Experimental Data, Indexes, and Techniques of Obtaining a Selected Set of Neutron Resonance Parameters*, May 1972.
- Vol. 12, *An Atlas of Resolved Neutron Resonance Parameters*, July 1972.
- Vol. 13, *An Atlas of Unresolved Neutron Resonance Parameters*, September 1972.
- Vol. 14, *TARTNP: A Coupled Neutron-Photon Monte Carlo Transport Code*, February 1976.
- Vol. 15, Part A, *The LLL Evaluated-Nuclear-Data Library (ENDL): Evaluation Techniques, Reaction Index, and Descriptions of Individual Evaluations*, September 1975.
- Vol. 15, Part B, *The LLL Evaluated-Nuclear-Data Library (ENDL): Graphs of Cross Sections from the Library*, October 1978.
- Vol. 15, Part C, *The LLL Evaluated-Nuclear-Data Library (ENDL): Translation of ENDF Neutron-Induced Interaction Data into the ENDF/B Format*, April 1976.
- Vol. 15, Part D, *The LLL Evaluated-Nuclear-Data Library (ENDL): Descriptions of Individual Evaluations for $Z = 0-98$* , May 1978.
- Vol. 16, Rev. 2, *Tabular and Graphical Presentation of 175 Neutron-Group Constants Derived from the LLL Evaluated-Nuclear-Data Library (ENDL)*, October 1978.
- Vol. 17, Part A, *Program LINEAR (Version 77-1): Linearize Data in the Evaluated-Nuclear-Data File/Version B (ENDF/B) Format*, January 1977.

- Vol. 17, Part B, *Program SIGMA1 (Version 77-1): Doppler Broaden Evaluated Cross Sections in the Evaluated-Nuclear-Data File/Version B (ENDF/B) Format*, January 1977.
- Vol. 17, Part C, *Program RECENT: Reconstruction of Energy-Dependent Cross Sections from Resonance Parameters in the ENDF/B Format*, 1979.
- Vol. 17, Part D, *Program GROUPIE: Calculation of Self-Shielded Cross Sections and Multiband Parameters for Evaluated Data in the ENDF/B Format*, 1979.
- Vol. 17, Part E, *Program EVALPLOT: Plot Data in the Evaluated-Nuclear-Data File/Version B (ENDF/B) Format*, February 1979.
- Vol. 18, *ACTL: Evaluated Neutron Activation Cross-Section Library*, 1979.
- Vol. 19, *Neutron-Induced Angular and Energy Distributions: Graphical Experimental Data*, April 1977.
- Vol. 20, *Bonderenko Self-Shielded Cross Sections and Multiband Parameters Derived from the LLL Evaluated-Nuclear-Data Library (ENDL)*, July 1978.
- Vol. 21, Part A, *Maxwell-Averaged Reaction Rates ($\overline{\sigma v}$) for Selected Reactions between Ions with Atomic Mass ≤ 11* , February 1979.

CONTENTS

Abstract	1
Method	1
Doppler Broadening	1
Bootstrapping	4
Representations of Broadened Cross Sections	5
Effect on Threshold Reactions	7
Truncating the Integration Range	8
Program Operation	8
Limitations and Assumptions	9
Requirements	10
Input Cards	10
Example Output	11
Error Messages	22
Operation at LLL	22
Conversion to Other Installations	23
Program Listing	24
References	51

AN INTEGRATED SYSTEM FOR PRODUCTION OF NEUTRONICS AND PHOTONICS CALCULATIONAL CONSTANTS

ABSTRACT

We have designed a code, SIGMAL, to Doppler-broaden evaluated cross sections in the ENDL format. This code can Doppler-broaden cross sections that result from neutrons, protons, deuterons, tritons, ^3He , or alpha particles incident on any target nuclei. The code allows broadening to up to 100 final temperatures, either directly from the initial temperature or by bootstrapping to successively higher temperatures.

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 SIGMAL method¹ may be used to Doppler-broaden cross sections for any particle (e.g., neutron, proton, deuteron, etc.) incident—at nonrelativistic energies—on a target in which the free-atom approximation is valid.

The SIGMAL 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

$$\sqrt{E}\sigma(E, T) = \frac{1}{2} \left(\frac{\alpha}{\pi E} \right)^{1/2} \int_0^\infty [\sqrt{E_r}\sigma(E_r, 0)] dE_r \{ \exp[-\alpha(\sqrt{E} - \sqrt{E_r})^2] - \exp[-\alpha(\sqrt{E} + \sqrt{E_r})^2] \} \quad (1)$$

$$V\sigma(V, T) = \frac{1}{V} \left(\frac{\beta}{\pi} \right)^{1/2} \int_0^\infty [V_r\sigma(V_r, 0)] V_r dV_r \{ \exp[-\beta(V - V_r)^2] - \exp[-\beta(V + V_r)^2] \} \quad (2)$$

where

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

and

m = projectile mass (e.g., neutron, proton, alpha, etc.)
 $\bar{V}$ = projectile velocity
 $V = |\bar{V}|$ = projectile speed
 $E = 1/2mV^2$ = projectile energy
 M = target nuclei mass
 $\bar{V}_T$ = target velocity
 $V_T = |\bar{V}_T|$ = target speed
 $E_T = 1/2MV_T^2$ = target energy
 $A = M/m$ = atomic weight ratio (target mass/projectile mass)
 $\bar{V}_r = \bar{V} - \bar{V}_T$ = relative velocity
 $V_r = |\bar{V}_r|$ = relative speed
 $E_r = 1/2mV_r^2$ = relative energy of the neutron as "seen" by the target
 $\sigma(V, 0)$ = cold (0 K) cross section
 $\sigma(V, T)$ = Doppler-broadened cross section.

By changing variables in Eq. (2) so that

$$\begin{aligned}
 y^2 &= \alpha E = \beta V^2 \\
 x^2 &= \alpha E_r = \beta V_r^2
 \end{aligned}
 \tag{3}$$

the Doppler-broadening equation becomes

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

The ensuing development can be simplified by defining

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

and noting that the Doppler-broadened cross section is

$$\sigma(y, T_2) = \sigma^*(y, T_2) - \sigma^*(-y, T_2) .
 \tag{6}$$

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 as a linear function of energy and cross section:

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

$$\sigma(x, T_1) = A_k + C_k x^2 : x \in (x_k, x_{k+1}) \quad (8)$$

Since tabulated cross sections span only a finite energy range (e.g., 10^{-5} eV to 20 MeV), we will also assume that the cross section will be continued as constant outside the range of the table. If we make these assumptions (data within the energy range of the table are linear; data outside the energy range of the table are constant), then Eq. (5) becomes

$$\sigma^*(y, T_2) = \frac{1}{y^2} \left(\frac{1}{\pi} \right)^{1/2} \sum_k \int_{x_k}^{x_{k+1}} x^2 (A_k + C_k x^2) \exp[-(x - y)^2] dx \quad (9)$$

By changing variables to $Z = x - y$ and collecting terms in powers of Z , we get

$$\begin{aligned} \sigma^*(y, T_2) = \frac{1}{y^2} \left(\frac{1}{\pi} \right)^{1/2} \sum_k \int_{x_k - y}^{x_{k+1} - y} [C_k Z^4 + 4C_k y Z^3 + (A_k + 6C_k y^2) Z^2 + (2A_k y + 4C_k y^3) Z \\ + (A_k y^2 + C_k y^4)] \exp(-Z^2) dZ \end{aligned} \quad (10)$$

Equation (10) can be defined exactly in terms of the functions

$$H^n(a, b) = F^n(a) - F^n(b) \quad (11)$$

$$F^n(a) = \frac{2}{\sqrt{\pi}} \int_0^a Z^n \exp(-Z^2) dZ \quad (12)$$

where

$$n = 0, 1, 2, 3, 4 \quad .$$

These functions can easily be shown to satisfy the recursion relationship

$$F^n(a) = \frac{(n-1)}{2} F^{n-2}(a) - \left(\frac{1}{\pi}\right)^{1/2} a^{n-1} \exp(-a^2) + \left(\frac{1}{\pi}\right)^{1/2} \delta_{n,1} . \quad (13)$$

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

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

$$F^1(a) = \left(\frac{1}{\pi}\right)^{1/2} [1 - \exp(-a^2)] \quad (14)$$

$$F^2(a) = \frac{1}{2} \text{ERF}(a) - \frac{a}{\sqrt{\pi}} \exp(-a^2)$$

$$F^3(a) = \left(\frac{1}{\pi}\right)^{1/2} [1 - (1 + a^2) \exp(-a^2)]$$

$$F^4(a) = \frac{3}{4} \text{ERF}(a) - \left(\frac{1}{\pi}\right)^{1/2} \left(\frac{3a}{2} + a^3\right) \exp(-a^2) .$$

With the definition of these functions, the algorithm describing the Doppler-broadened cross section at any arbitrary energy is complete.

BOOTSTRAPPING

The Doppler-broadening equations can be slightly generalized if we recognize that not only can they be used to broaden cross sections from 0 K to a temperature T K, but can also be used to broaden cross sections from any temperature T_1 K to any higher temperature T_2 K (Ref. 2). For example, it is possible to start from experimentally measured data at room temperature (293 K) and Doppler-broaden it to 600 K, which in turn can be broadened to 1000 K, etc. For each of these steps to be independent, the Doppler-broadening equations must be in the laboratory system (as opposed to the center-of-mass system) and the above definition of E_r must be used. The generalized equations are:

$$V\sigma(V, T_2) = \frac{1}{V} \left(\frac{\beta}{\pi}\right)^{1/2} \int_0^\infty [V_r \sigma(V_r, T_1)] V_r dV_r \{ \exp[-\beta(V - V_r)^2] - \exp[-\beta(V + V_r)^2] \} : \quad (15)$$

$$\beta = \frac{M}{2k(T_2 - T_1)} ,$$

$$\sqrt{E}\sigma(E, T_2) = \frac{1}{2} \left(\frac{\alpha}{\pi E}\right)^{1/2} \int_0^\infty [\sqrt{E_r} \sigma(E_r, T_1)] dE_r \times \{ \exp[-\alpha(\sqrt{E} - \sqrt{E_r})^2] - \exp[-\alpha(\sqrt{E} + \sqrt{E_r})^2] \} : \quad (16)$$

$$\alpha = \frac{A}{k(T_2 - T_1)} ,$$

where the V_r and E_r associated with the T_1 K cross sections $\sigma(V_r, T_1)$ and $\sigma(E_r, T_1)$ are merely the laboratory speed and energy, respectively, of the neutron.

REPRESENTATIONS OF BROADENED CROSS SECTIONS

If the programs that produce multigroup and continuous Monte Carlo data from evaluated cross-section libraries (the library data being subject to linear-linear interpolation) are to be applicable to Doppler-broadened cross sections, the latter cross sections must also be subject to linear-linear interpolation. Although the Doppler-broadening algorithm described above allows the cross section to be calculated at any given energy, it does not guarantee that the broadened cross section is subject to linear-linear interpolation between any two given energies. Use of an iterative scheme, such as interval halving, can be prohibitively expensive. Use of the same energy grid that was used to represent the unbroadened cross section can lead to pitfalls. For example, the 0-K hydrogen-elastic cross section is roughly 20 barns from 10^{-5} eV to 1 keV. Linear variation in energy and cross section can be used to define the 0-K cross section from 10^{-5} eV to 1 keV and to calculate Doppler-broadened cross sections at 10^{-5} eV and 1 keV. The broadened cross section is certainly not subject to linear-linear interpolation between these two energies. Large errors will result if a multigroup processing code assumes that it is. Figure 1 illustrates this error by comparing linear-linear variation to a $1/V$ cross section variation between 0.01 and 100 eV. The figure speaks for itself as far as the errors that would occur.

Although Doppler-broadening is a smoothing process, it is the reaction rate, not the cross section, that is becoming smoother. Therefore, if the energy grid that represents the unbroadened reaction rate is sufficiently dense, the smoother Doppler-broadened reaction rate can be adequately represented on the same energy grid. At higher energies ($\alpha E \gg 1$), this smoothing process applies equally well to the cross section. However, at lower energies, 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 $1/V$ [i.e., $\sigma(V, T) = R(V, T)/V$]. To ensure that this low-energy $1/V$ tail does not prevent the cross section from being in a form subject to linear-linear interpolation, 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_1, V_2 and that $V_2 = SV_1$, we get

$$\begin{aligned}\sigma_1(V) &= \frac{1}{V} \text{ (1/V variation)} \\ \sigma_2(V) &= \frac{1}{V} - \frac{(V^2 - V_1^2)}{V_1^3 S(S+1)} \text{ (linear-linear in cross section-energy)} \\ V\epsilon(V_1, SV_1) &, \end{aligned} \tag{17}$$

The fractional difference between these two representations is

$$\epsilon(V) = \frac{\sigma_1(V) - \sigma_2(V)}{\sigma_1(V)} = 1 - \frac{V^3 - VV_1^2}{V_1^3 S(S+1)} - \frac{V}{V_1}$$

FIG. 1. Linearized $1/V$ cross section.

and the variation in the fractional difference is

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

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

$$V_{max} = V_1 \left[\frac{1}{3} (1 + S + S^2) \right]^{1/2}$$

$$\epsilon(V_{max}) = 1 - \left(\frac{2}{3} \right) \left(\frac{1}{3} \right)^{1/2} \frac{(1 + S + S^2)^{3/2}}{S(S + 1)} \quad (19)$$

Note $\epsilon(V_{max})$ is dependent of V_1 and depends only 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 1 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.

Therefore, to ensure that the Doppler-broadened cross sections are subject to linear-linear interpolation, 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 $S^2 E$ (where S^2 depends on the allowable error ϵ).

TABLE 1. Linear-linear approximation of a 1/V cross section.

Tolerance	Factor	Points ^a	Tolerance	Factor	Points ^a
0.001	1.0530	276	0.011	1.1865	84
0.002	1.0757	195	0.012	1.1956	81
0.003	1.0935	160	0.013	1.2043	78
0.004	1.1087	139	0.014	1.2128	75
0.005	1.1223	124	0.015	1.2210	72
0.006	1.1347	114	0.016	1.2290	70
0.007	1.1463	105	0.017	1.2367	68
0.008	1.1571	99	0.018	1.2444	66
0.009	1.1674	93	0.019	1.2518	65
0.010	1.1772	88	0.020	1.2591	63

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

EFFECT ON THRESHOLD REACTIONS

In a cold medium, a particle-target nucleus reaction will not occur if the particle's laboratory energy stays below the threshold energy level for that particular reaction. However, as we heat the medium, it is possible for the motions of a given particle and target nucleus to result in a combined energy above the threshold, even if the laboratory energy of the particle is less than the threshold energy. The effect is that if we Doppler-broaden to define cross sections in a hot medium for particle laboratory energies, the thresholds of threshold reactions shift to lower and lower energies as the temperature of the medium is raised to higher and higher temperatures.

The effect of Doppler-broadening on thresholds is negligible as long as $KT, AE \ll I$, where

A = weight ratio of target to projectile nucleus,

I = energy of the threshold,

T = temperature of the medium; e.g., kelvin,

KT = temperature of the medium in energy units; e.g., keV.

Generally this effect is very small at reaction-like temperatures ($T = 300-1500$ K; $KT = 0.025-0.1$ eV) and can be ignored. However, in fusion applications (e.g., controlled thermonuclear reactions, CTR), KT is measured in keV and threshold shifts can be quite large.

Program SIGMAL will automatically shift thresholds to new effective values whenever KT is not much less than AE , but maintains the original threshold energy otherwise.

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 of the integral $\sigma(x, \infty)$ is from an interval centered about y ; the interval is defined by $\sigma(y-N, y+N)$. 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 $x^2\sigma(x, T)$ may be rapidly increasing, particularly $\sigma(x, T)$ in the resonance region. Therefore, the truncation procedure should be:

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

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

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

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 $y \leq 4$.

PROGRAM OPERATION

On input the user may specify how accurately to represent the Doppler-broadened cross sections, whether or not bootstrapping should be used, and a list of up to 100 temperatures to which cross sections should be broadened. Each temperature may be defined as either merely a step in the bootstrapping process (no output in the ENDL format) or as a temperature at which the Doppler-broadened cross sections should be output.

All data except cross sections ($I = 0$), for n, p, d, t, ^3He , or alpha incident ($Y_1 = 1$ to 6) are copied from the ENDL format original file to the Doppler-broadened file. As such, the final ENDL format file will contain all the data for any evaluation, with the cross sections Doppler-broadened and all other data unaffected.

Each section of ENDL cross section data (i.e., each reaction) is handled separately. The cross section at the original temperature is read from the ENDL format file and Doppler-broadened to the first temperature. If output is requested at this temperature, the broadened data are output in the ENDL format. During the broadening process, either the original unbroadened cross sections (no bootstrapping) or the Doppler-broadened cross sections (bootstrapping) are saved either in core or on a scratch disk file. The cross sections for the next temperature are then obtained using the saved cross section (either original or last step of broadened data). The cycle of broadening/saving and output (or no output) is repeated for all temperatures for one reaction before proceeding to the next reaction. The output is in the form of an ENDL section, separately for each temperature.

LIMITATIONS AND ASSUMPTIONS

The program non-selectively Doppler-broadens all cross section data on the original ENDL format file (i.e., all sections with $I = 0$ and $Y_1 = 1$ to 6).³ This program does not require the evaluations to be in any particular order; e.g., the data may be in ZA order, I order, etc.

The program only uses the ENDL BCD format (as opposed to the binary library format) and copies all sections except cross section as Hollerith. As such, the program may be used to obtain complete evaluations containing broadened cross sections as well as the original angular distributions, energy distributions, etc.

The program can Doppler-broaden cross sections from neutrons, protons, deuterons, tritons, ^3He , or alpha particles incident on any target nuclei.

The programs may be used to Doppler-broaden cross sections to up to 100 final temperatures. The cross sections for each final temperature may be calculated either from the original cross sections (as read from the ENDL format file) or they may be bootstrapped from the cross sections obtained during the last temperature step. In the bootstrapping mode, each temperature may be identified as either merely a step in the bootstrapping process (no ENDL format output) or as a real temperature for which output is required. If the bootstrapping mode is not being used, all temperatures identified as bootstrapping steps (no output) will be ignored.

Cross sections are computed for temperatures in the order in which the temperatures are input; i.e., the program does not sort the temperatures into ascending order. Therefore, in the bootstrapping mode, the temperatures should be input in ascending numerical order.

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—up to 500 000 points per section).³

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

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 ENDL data³ 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 ENDL data³ 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:

<i>Filename</i>	<i>Description</i>
INPUT	Input cards
OUTPUT	Output cards
ENDLIN	Evaluated data in the ENDL format (to be broadened)
SCRD001	Scratch file—used only for multiple temperatures
SCRD002	Scratch file—used only for bootstrapping

The program, when run on the Livermore CDC-7600, required 32 K₁₀ words of small core memory and 6 K₁₀ of large core memory (I/O buffers). To execute the sample problem described in the following sections (15 evaluations broadened to 300 and 600 Kelvin and thinned to 0.1% accuracy) required a total running time of 0.35 minutes (i.e., less than one second per evaluation per temperature).

INPUT CARDS

The input format is as follows:

<i>Card</i>	<i>Columns</i>	<i>Format</i>	<i>Description</i>
1	1-11	E11.4	Fractional output thinning criteria (i.e., 0.5% = 0.005)
	12-22	I11	Temperature input (of following cards)* = 0 MeV = 1 K
	23-33	I11	Bootstrapping option = 0, no bootstrapping = 1, bootstrapping
2-N	1-11	E11.4	Temperature (in MeV or kelvin depending on the temperature units on first input card)
	12-22	I11	Bootstrap set flag = 0, broaden to this temperature and output = 1, broaden to this temperature only to allow bootstrapping to the next temperature. No input for this temperature.

*The user may select to input temperature in either MeV or kelvin units.

To Doppler-broaden data to 300 and 600 Kelvin without bootstrapping, and to thin the output to 0.1% accuracy, the following input cards are required:

```
1.00000 - 03      1      0
3.00000 + 02      0
6.00000 + 02      0
```

EXAMPLE OUTPUT

See the program listing for an example of the use of bootstrapping and bootstrapping steps.

Table 2 is the output report that resulted from using the above input cards to Doppler-broaden 15 ENDL evaluations. This entire execution took only 0.35 minutes of CDC-7600 time. Figures 2-5 illustrate the wide range of applications of the SIGMAL code. Note that it can be applied to Doppler-broaden at

- Reactor core-like temperatures (300-10000 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)

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

*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 $\sim 12\,000\text{ K}$; 10 keV $\sim 1.2 \times 10^8\text{ K}$).

ENDL-7166

92-U-233

FIG. 3. Doppler-broadening of the cross section in Fig. 2 to stellar or CTR core temperatures ($KT = 0$ to 10 keV; $T = 0$ to 1.2×10^8 K).

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 at extremely low energies.

Table 2. Example output for Doppler-broadened ENDF evaluation.

1 DOPPLER BROADEN ENDF CROSS SECTIONS (SIGMAL 79-1)

THINNING CRITERIA-- 1.00000- 3
 TEMPERATURE UNITS-- KELVIN
 BOOTSTRAP OPTION--- OFF
 TEMPERATURE(S)----- 2.59044- 8 MEV 3.00000+ 2 KELVIN
 5.18088- 8 5.00000+ 2

ZA	Y1	C	Q-VALUE MEV	TEMP. IN MEV	TEMP. OUT MEV	POINTS IN	POINTS OUT	MESSAGES
1001	1	10	0.	+ 0 0.	+ 0 2.59044- 8	99	172	
1001	1	10	0.	+ 0 0.	+ 0 5.18088- 8	0	178	
1001	1	46	2.22470+ 0 0.	+ 0 2.59044- 8		219	224	
1001	1	46	2.22470+ 0 0.	+ 0 5.18088- 8		0	224	
ZA TOTALS						318	798	
1002	1	12	0.	+ 0 0.	+ 0 2.59044- 8	40	106	
1002	1	10	0.	+ 0 0.	+ 0 5.18088- 8	0	114	
1002	1	12	-2.23000+ 0 0.	+ 0 2.59044- 8		12	12	
1002	1	12	-2.23000+ 0 0.	+ 0 5.18088- 8		0	12	
1002	1	46	6.25000+ 0 0.	+ 0 2.59044- 8		72	122	
1002	1	46	6.25000+ 0 0.	+ 0 5.18088- 8		0	124	
ZA TOTALS						124	490	
3006	1	10	0.	+ 0 0.	+ 0 2.59044- 8	55	111	
3006	1	10	0.	+ 0 0.	+ 0 5.18088- 8	0	118	
3006	1	12	-5.66000+ 0 0.	+ 0 2.59044- 8		5	5	
3006	1	12	-5.66000+ 0 0.	+ 0 5.18088- 8		0	5	
3006	1	22	-1.46000+ 0 0.	+ 0 2.59044- 8		26	24	
3006	1	22	-1.46000+ 0 0.	+ 0 5.18088- 8		0	24	
3006	1	22	-1.46000+ 0 0.	+ 0 2.59044- 8		22	20	
3006	1	22	-1.46000+ 0 0.	+ 0 5.18088- 8		0	20	
3006	1	40	-2.73000+ 0 0.	+ 0 2.59044- 8		14	14	
3006	1	40	-2.73000+ 0 0.	+ 0 5.18088- 8		0	14	
3006	1	42	4.79000+ 0 0.	+ 0 2.59044- 8		301	294	
3006	1	42	4.79000+ 0 0.	+ 0 5.18088- 8		0	294	
3006	1	46	7.26000+ 0 0.	+ 0 2.59044- 8		271	267	
3006	1	46	7.26000+ 0 0.	+ 0 5.18088- 8		0	267	
ZA TOTALS						694	1477	
5010	1	10	0.	+ 0 0.	+ 0 2.59044- 8	44	96	
5010	1	10	0.	+ 0 0.	+ 0 5.18088- 8	0	103	
5010	1	11	0.	+ 0 0.	+ 0 2.59044- 8	9	8	
5010	1	11	0.	+ 0 0.	+ 0 5.18088- 8	0	8	
5010	1	11	0.	+ 0 0.	+ 0 2.59044- 8	9	9	
5010	1	11	0.	+ 0 0.	+ 0 5.18088- 8	0	9	
5010	1	11	0.	+ 0 0.	+ 0 2.59044- 8	6	6	
5010	1	11	0.	+ 0 0.	+ 0 5.18088- 8	0	6	
5010	1	11	0.	+ 0 0.	+ 0 2.59044- 8	6	6	
5010	1	11	0.	+ 0 0.	+ 0 5.18088- 8	0	6	
5010	1	11	0.	+ 0 0.	+ 0 2.59044- 8	5	5	
5010	1	11	0.	+ 0 0.	+ 0 5.18088- 8	0	5	
5010	1	12	-8.44000+ 0 0.	+ 0 2.59044- 8		4	4	
5010	1	12	-8.44000+ 0 0.	+ 0 5.18088- 8		0	4	
5010	1	23	-6.02000+ 0 0.	+ 0 2.59044- 8		5	5	
5010	1	23	-6.02000+ 0 0.	+ 0 5.18088- 8		0	5	

Table 2. (Continued.)

5010	1	43	3.30000-	1	0.	+ 0	2.59044- 8	13	13
5010	1	43	3.30000-	1	0.	+ 0	5.18088- 8	0	13
5010	1	45	2.80000+	0	0.	+ 0	2.59044- 8	322	317
5010	1	45	2.80000+	0	0.	+ 0	5.18088- 8	0	317
5010	1	46	1.14500+	1	0.	+ 0	2.59044- 8	56	134
5010	1	46	1.14500+	1	0.	+ 0	5.18088- 8	0	141
ZA TOTALS								479	1220
5011	1	10	0.	+ 0	0.	+ 0	2.59044- 8	55	107
5011	1	10	0.	+ 0	0.	+ 0	5.18088- 8	0	114
5011	1	11	0.	+ 0	0.	+ 0	2.59044- 8	9	9
5011	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	9
5011	1	11	0.	+ 0	0.	+ 0	2.59044- 8	11	11
5011	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	11
5011	1	11	0.	+ 0	0.	+ 0	2.59044- 8	9	8
5011	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	8
5011	1	11	0.	+ 0	0.	+ 0	2.59044- 8	5	5
5011	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	5
5011	1	12	-1.14600+	1	0.	+ 0	2.59044- 8	3	3
5011	1	12	-1.14600+	1	0.	+ 0	5.18088- 8	0	3
5011	1	40	-1.07200+	1	0.	+ 0	2.59044- 8	3	3
5011	1	40	-1.07200+	1	0.	+ 0	5.18088- 8	0	3
5011	1	42	-9.56000+	0	0.	+ 0	2.59044- 8	3	3
5011	1	42	-9.56000+	0	0.	+ 0	5.18088- 8	0	3
5011	1	45	-6.64000+	0	0.	+ 0	2.59044- 8	5	5
5011	1	45	-6.64000+	0	0.	+ 0	5.18088- 8	0	5
5011	1	46	3.37000+	0	0.	+ 0	2.59044- 8	35	113
5011	1	46	3.37000+	0	0.	+ 0	5.18088- 8	0	118
ZA TOTALS								137	546
6012	1	10	0.	+ 0	0.	+ 0	2.59044- 8	123	169
6012	1	10	0.	+ 0	0.	+ 0	5.18088- 8	0	175
6012	1	11	0.	+ 0	0.	+ 0	2.59044- 8	21	20
6012	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	20
6012	1	27	-7.36000+	0	0.	+ 0	2.59044- 8	9	9
6012	1	27	-7.36000+	0	0.	+ 0	5.18088- 8	0	9
6012	1	27	-7.36000+	0	0.	+ 0	2.59044- 8	4	4
6012	1	27	-7.36000+	0	0.	+ 0	5.18088- 8	0	4
6012	1	27	-7.36000+	0	0.	+ 0	2.59044- 8	6	6
6012	1	27	-7.36000+	0	0.	+ 0	5.18088- 8	0	6
6012	1	27	-7.36000+	0	0.	+ 0	2.59044- 8	4	4
6012	1	27	-7.36000+	0	0.	+ 0	5.18088- 8	0	4
6012	1	27	-7.36000+	0	0.	+ 0	2.59044- 8	4	4
6012	1	27	-7.36000+	0	0.	+ 0	5.18088- 8	0	4
6012	1	27	-7.36000+	0	0.	+ 0	2.59044- 8	3	3
6012	1	27	-7.36000+	0	0.	+ 0	5.18088- 8	0	3
6012	1	40	-1.25800+	1	0.	+ 0	2.59044- 8	4	4
6012	1	40	-1.25800+	1	0.	+ 0	5.18088- 8	0	4
6012	1	41	-1.37200+	1	0.	+ 0	2.59044- 8	4	4
6012	1	41	-1.37200+	1	0.	+ 0	5.18088- 8	0	4
6012	1	45	-5.70000+	0	0.	+ 0	2.59044- 8	11	10
6012	1	45	-5.70000+	0	0.	+ 0	5.18088- 8	0	10
6012	1	46	4.94600+	0	0.	+ 0	2.59044- 8	11	86
6012	1	46	4.94600+	0	0.	+ 0	5.18088- 8	0	91
ZA TOTALS								204	657
7014	1	10	0.	+ 0	0.	+ 0	2.59044- 8	409	450

Table 2. (Continued.)

7014	1	10	0.	+ 0 0.	+ 0	5.18088- 8	0	155
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	27	24
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	24
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	24	22
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	22
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	22	19
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	19
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	21	21
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	21
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	20	18
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	18
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	19	19
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	19
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	19	16
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	16
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	19	18
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	18
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	17	16
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	16
7014	1	11	0.	+ 0 0.	+ 0	2.59044- 8	15	15
7014	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	15
7014	1	12	-1.05500+	1 0.	+ 0	2.59044- 8	10	9
7014	1	12	-1.05500+	1 0.	+ 0	5.18088- 8	0	9
7014	1	20	-7.55000+	0 0.	+ 0	2.59044- 8	11	9
7014	1	20	-7.55000+	0 0.	+ 0	5.18088- 8	0	9
7014	1	40	6.26000-	1 0.	+ 0	2.59044- 8	340	415
7014	1	40	6.26000-	1 0.	+ 0	5.18088- 8	0	421
7014	1	41	-5.32000+	0 0.	+ 0	2.59044- 8	18	16
7014	1	41	-5.32000+	0 0.	+ 0	5.18088- 8	0	16
7014	1	42	4.00000+	0 0.	+ 0	2.59044- 8	24	22
7014	1	42	4.00000+	0 0.	+ 0	5.18088- 8	0	22
7014	1	45	-1.50000-	1 0.	+ 0	2.59044- 8	229	209
7014	1	45	-1.50000-	1 0.	+ 0	5.18088- 8	0	209
7014	1	46	1.08300+	1 0.	+ 0	2.59044- 8	50	130
7014	1	46	1.08300+	1 0.	+ 0	5.18088- 8	0	137

					7A TOTALS	1294	2915	
8016	1	10	0.	+ 0 0.	+ 0	2.59044- 8	264	312
8016	1	10	0.	+ 0 0.	+ 0	5.18088- 8	0	318
8016	1	11	0.	+ 0 0.	+ 0	2.59044- 8	9	8
8016	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	8
8016	1	11	0.	+ 0 0.	+ 0	2.59044- 8	21	20
8016	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	20
8016	1	11	0.	+ 0 0.	+ 0	2.59044- 8	18	18
8016	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	16
8016	1	11	0.	+ 0 0.	+ 0	2.59044- 8	13	13
8016	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	13
8016	1	11	0.	+ 0 0.	+ 0	2.59044- 8	7	7
8016	1	11	0.	+ 0 0.	+ 0	5.18088- 8	0	7
8016	1	12	-1.56700+	1 0.	+ 0	2.59044- 8	3	3
8016	1	12	-1.56700+	1 0.	+ 0	5.18088- 8	0	3
8016	1	20	-1.21200+	1 0.	+ 0	2.59044- 8	4	4
8016	1	20	-1.21200+	1 0.	+ 0	5.18088- 8	0	4
8016	1	26	-7.15000+	0 0.	+ 0	2.59044- 8	10	10
8016	1	26	-7.15000+	0 0.	+ 0	5.18088- 8	0	10
8016	1	40	3.61000+	0 0.	+ 0	2.59044- 8	13	13
8016	1	40	-9.61000+	0 0.	+ 0	5.18088- 8	0	13
8016	1	41	-9.89000+	0 0.	+ 0	2.59044- 8	4	4
8016	1	41	-9.89000+	0 0.	+ 0	5.18088- 8	0	4

Table 2. (Continued.)

8016	1	45	-2.21000+	0	0.	+ 0	2.59044- 8	56	56
8016	1	45	-2.21000+	0	0.	+ 0	5.18088- 8	0	56
ZA TOTALS								422	936
13027	1	10	0.	+ 0	0.	+ 0	2.59044- 8	1713	1755
13027	1	10	0.	+ 0	0.	+ 0	5.18088- 8	0	1758
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	17	17
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	17
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	53	53
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	53
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	50	50
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	50
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	36	36
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	36
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	51	51
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	51
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	51	51
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	51
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	38	37
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	37
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	27	27
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	27
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	34	34
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	34
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	53	53
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	53
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	46	46
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	46
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	35	35
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	35
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	32	32
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	32
13027	1	11	0.	+ 0	0.	+ 0	2.59044- 8	30	30
13027	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	30
13027	1	12	-1.30570+	1	0.	+ 0	2.59044- 8	14	14
13027	1	12	-1.30570+	1	0.	+ 0	5.18088- 8	0	14
13027	1	40	-1.82780+	0	0.	+ 0	2.59044- 8	147	146
13027	1	40	-1.82780+	0	0.	+ 0	5.18088- 8	0	146
13027	1	41	-6.04600+	0	0.	+ 0	2.59044- 8	24	24
13027	1	41	-6.04600+	0	0.	+ 0	5.18088- 8	0	24
13027	1	42	-1.08840+	1	0.	+ 0	2.59044- 8	14	14
13027	1	42	-1.08840+	1	0.	+ 0	5.18088- 8	0	14
13027	1	45	-3.13160+	0	0.	+ 0	2.59044- 8	32	32
13027	1	45	-3.13160+	0	0.	+ 0	5.18088- 8	0	32
13027	1	46	7.73000+	0	0.	+ 0	2.59044- 8	168	233
13027	1	46	7.73000+	0	0.	+ 0	5.18088- 8	0	236
ZA TOTALS								2665	5546
14000	1	10	0.	+ 0	0.	+ 0	2.59044- 8	871	915
14000	1	10	0.	+ 0	0.	+ 0	5.18088- 8	0	921
14000	1	11	0.	+ 0	0.	+ 0	2.59044- 8	17	16
14000	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	16
14000	1	11	0.	+ 0	0.	+ 0	2.59044- 8	13	13
14000	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	13
14000	1	11	0.	+ 0	0.	+ 0	2.59044- 8	190	189
14000	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	189
14000	1	12	-8.48400+	0	0.	+ 0	2.59044- 8	6	6
14000	1	12	-8.48400+	0	0.	+ 0	5.18088- 8	0	6

Table 2. (Continued.)

14000	1	20	-1.15730+	1	0.	+ 0	2.59044- 8	50	50
14000	1	20	-1.15730+	1	0.	+ 0	5.18088- 8	0	50
14000	1	40	-2.89320+	0	0.	+ 0	2.59044- 8	369	347
14000	1	40	-2.89320+	0	0.	+ 0	5.18088- 8	0	347
14000	1	41	-9.35830+	0	0.	+ 0	2.59044- 8	81	81
14000	1	41	-9.35830+	0	0.	+ 0	5.18088- 8	0	81
14000	1	45	3.27000-	2	0.	+ 0	2.59044- 8	73	360
14000	1	45	-3.27000-	2	0.	+ 0	5.18088- 8	0	360
14000	1	46	8.76800+	0	0.	+ 0	2.59044- 8	46	121
14000	1	46	8.76800+	0	0.	+ 0	5.18088- 8	0	125
ZA TOTALS								2016	4206
67165	1	10	0.	+ 0	0.	+ 0	2.59044- 8	3372	3331
67165	1	10	0.	+ 0	0.	+ 0	5.18088- 8	0	3292
67165	1	11	0.	+ 0	0.	+ 0	2.59044- 8	20	19
67165	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	19
67165	1	12	-7.99000+	0	0.	+ 0	2.59044- 8	16	16
67165	1	12	-7.99000+	0	0.	+ 0	5.18088- 8	0	16
67165	1	13	-1.46700+	1	0.	+ 0	2.59044- 8	7	7
67165	1	13	-1.46700+	1	0.	+ 0	5.18088- 8	0	7
67165	1	46	6.24000+	0	0.	+ 0	2.59044- 8	4662	4671
67165	1	46	6.24000+	0	0.	+ 0	5.18088- 8	0	4546
ZA TOTALS								8077	15924
79197	1	10	0.	+ 0	0.	+ 0	2.59044- 8	126	158
79197	1	10	0.	+ 0	0.	+ 0	5.18088- 8	0	165
79197	1	11	0.	+ 0	0.	+ 0	2.59044- 8	20	19
79197	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	19
79197	1	12	-8.06000+	0	0.	+ 0	2.59044- 8	12	12
79197	1	12	-8.06000+	0	0.	+ 0	5.18088- 8	0	12
79197	1	13	-1.47500+	1	0.	+ 0	2.59044- 8	5	5
79197	1	13	-1.47500+	1	0.	+ 0	5.18088- 8	0	5
79197	1	40	4.00000-	2	0.	+ 0	2.59044- 8	12	10
79197	1	40	4.00000-	2	0.	+ 0	5.18088- 8	0	10
79197	1	45	7.03000+	0	0.	+ 0	2.59044- 8	6	6
79197	1	45	7.03000+	0	0.	+ 0	5.18088- 8	0	6
79197	1	46	6.51000+	0	0.	+ 0	2.59044- 8	3583	3609
79197	1	46	6.51000+	0	0.	+ 0	5.18088- 8	0	3558
ZA TOTALS								3764	7594
90232	1	10	0.	+ 0	0.	+ 0	2.59044- 8	2983	2899
90232	1	10	0.	+ 0	0.	+ 0	5.18088- 8	0	2853
90232	1	11	0.	+ 0	0.	+ 0	2.59044- 8	62	51
90232	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	51
90232	1	12	-6.34000+	0	0.	+ 0	2.59044- 8	17	16
90232	1	12	-6.34000+	0	0.	+ 0	5.18088- 8	0	16
90232	1	13	-1.15600+	1	0.	+ 0	2.59044- 8	8	8
90232	1	13	-1.15600+	1	0.	+ 0	5.18088- 8	0	8
90232	1	14	-1.83500+	1	0.	+ 0	2.59044- 8	2	2
90232	1	14	-1.83500+	1	0.	+ 0	5.18088- 8	0	2
90232	1	15	1.70000+	2	0.	+ 0	2.59044- 8	34	34
90232	1	15	1.70000+	2	0.	+ 0	5.18088- 8	0	34
90232	1	46	4.79000+	0	0.	+ 0	2.59044- 8	5535	5451
90232	1	46	4.79000+	0	0.	+ 0	5.18088- 8	0	5434
ZA TOTALS								8641	16859

Table 2. (Continued.)

92235	1	10	0.	+ 0	0.	+ 0	2.59044- 8	235	264
92235	1	10	0.	+ 0	0.	+ 0	5.18088- 8	0	265
92235	1	11	0.	+ 0	0.	+ 0	2.59044- 8	25	25
92235	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	25
92235	1	12	-5.23000+	0	0.	+ 0	2.59044- 8	16	16
92235	1	12	-5.23000+	0	0.	+ 0	5.18088- 8	0	16
92235	1	13	-1.20000+	1	0.	+ 0	2.59044- 8	7	7
92235	1	13	-1.20000+	1	0.	+ 0	5.18088- 8	0	7
92235	1	14	-1.78900+	1	0.	+ 0	2.59044- 8	3	3
92235	1	14	-1.78900+	1	0.	+ 0	5.18088- 8	0	3
92235	1	15	1.80000+	2	0.	+ 0	2.59044- 8	1511	1585
92235	1	15	1.80000+	2	0.	+ 0	5.18088- 8	0	1582
92235	1	46	6.55000+	0	0.	+ 0	2.59044- 8	767	837
92235	1	46	6.55000+	0	0.	+ 0	5.18088- 8	0	836

ZA TOTALS 2564 5471

92238	1	10	0.	+ 0	0.	+ 0	2.59044- 8	453	465
92238	1	10	0.	+ 0	0.	+ 0	5.18088- 8	0	470
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	22	22
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	22
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	21	21
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	21
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	13	13
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	13
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	8	8
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	8
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	17	17
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	17
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	16	16
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	16
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	13	13
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	13
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	14	14
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	14
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	12	12
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	12
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	12	12
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	12
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	12	12
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	12
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	12	12
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	12
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	10	10
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	10
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	11	11
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	11
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	10	10
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	10
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	9	9
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	9
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	9	9
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	9
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	8	8
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	8
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	9	9
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	9
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	11	11

Table 2. (Continued.)

92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	11
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	13	13
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	13
92238	1	11	0.	+ 0	0.	+ 0	2.59044- 8	11	11
92238	1	11	0.	+ 0	0.	+ 0	5.18088- 8	0	11
92238	1	12	-6.04000+	0	0.	+ 0	2.59044- 8	15	15
92238	1	12	-6.04000+	0	0.	+ 0	5.18088- 8	0	15
92238	1	13	-1.14500+	1	0.	+ 0	2.59044- 8	9	9
92238	1	13	-1.14500+	1	0.	+ 0	5.18088- 8	0	9
92238	1	14	-1.78200+	1	0.	+ 0	2.59044- 8	3	3
92238	1	14	-1.78200+	1	0.	+ 0	5.18088- 8	0	3
92238	1	15	1.80000+	2	0.	+ 0	2.59044- 8	41	40
92238	1	15	1.80000+	2	0.	+ 0	5.18088- 8	0	40
92238	1	46	4.80000+	0	0.	+ 0	2.59044- 8	1473	1520
92238	1	46	4.80000+	0	0.	+ 0	5.18088- 8	0	1524

ZA TOTALS 2279 4683

TAPE TOTALS 33678 69322

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).

SCRATCH MAXIMUM PAGE COUNT EXCEEDED

EXECUTION TERMINATED

The scratch disk file is designed to allow each section to include up to 500 000 points. In the unlikely event that this limit is exceeded, this error message is printed out.

OPERATION AT LLL

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

.193025:PROGRAMS:SIGNAL

The program is small enough (32 000 words of SCM, 6 000 words of LCM) to run at standby during the daytime as file

SIGNAL / 1 S

The program will automatically use disk files as illustrated in Fig. 6.

FIG. 6. Linear operations.

CONVERSION TO OTHER INSTALLATIONS

This edition of the code is designed for operation at Lawrence Livermore Laboratory on a CDC 7600 computer. It uses special I/O routines to avoid the inefficiency of FORTRAN binary reads and writes. All points in the code that use these special routines are preceded and followed by comment cards of the form,

C**** LTSS*****

to indicate the Livermore time sharing system. For conversion to standard FORTRAN binary I/O, the required statements are included in the program as comment cards and can easily be activated. Alternatively, by recognizing all of these points one can easily implement his own direct disk access routines, which are equivalent to those used at Livermore. If FORTRAN binary I/O is used, subroutines

IONAME

FILEIO

WAIT

are not required.

PROGRAM LISTING

EXAMPLE OUTPUT

PROGRAM SIGNAL (INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT, 1 TAPE21, TAPE22, TAPE23, TAPE24)	SIG00010
	SIG00020
PROGRAM SIGNAL	SIG00030
VERSION 79-1 (MARCH 1979)	SIG00040
	SIG00050
WRITTEN BY DERMOTT E. CULLEN	SIG00060
L-71	SIG00070
UNIVERSITY OF CALIFORNIA	SIG00080
LAWRENCE LIVERMORE LABORATORY	SIG00090
P.O. BOX 808	SIG00100
LIVERMORE, CALIFORNIA	SIG00110
TELEPHONE 415-447-1100 X-3134	SIG00120
	SIG00130
	SIG00140
THIS PROGRAM IS DESIGNED TO READ EVALUATED CROSS SECTION DATA IN THE ENDL FORMAT, DOPPLER BROADEN, THIN AND OUTPUT CROSS SECTIONS IN THE ENDL FORMAT.	SIG00150
	SIG00160
	SIG00170
	SIG00180
THIS PROGRAM CAN HANDLE NEUTRONS, PROTONS, DEUTERONS, TRITONS, HELIUM-3 OR ALPHA PARTICLES INCIDENT ON ANY TARGET NUCLEUS.	SIG00190
	SIG00200
	SIG00210
THIS PROGRAM ONLY USES THE ENDL CARD IMAGE FORMAT (SEE UCRL-50400 VOLUME 4) AND COPIES ALL DATA EXCEPT CROSS SECTIONS (I=0, YIENDL=1 TO 6). FOR EXAMPLE, ALL ANGULAR AND ENERGY DISTRIBUTIONS WILL BE COPIED, UNCHANGED TO THE BROADENED DATA FILE (ENDLOUT).	SIG00220
	SIG00230
	SIG00240
	SIG00250
	SIG00260
THE PROGRAM OPERATES NON-SELECTIVELY ON AN ENTIRE ENDL FORMAT DISK FILE. EACH ORIGINAL SECTION OF CROSS SECTIONS WILL BE DOPPLER BROADENED AND THINNED.	SIG00270
	SIG00280
	SIG00290
	SIG00300
THIS VERSION OF THE CODE ALLOWS EACH SECTION TO BE DOPPLER BROADENED TO UP TO 100 FINAL TEMPERATURES. ALL TEMPERATURES ARE INPUT IN EITHER MEV OR KELVIN (E.G. 293 KELVIN CORRESPONDS TO KT = 0.0253 EV. SIMILARLY 11,581 KELVIN CORRESPONDS TO KT = 1 EV).	SIG00310
	SIG00320
	SIG00330
	SIG00340
	SIG00350
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 TEMPERATURE. THIS FEATURE MAY BE USED INCLUDE THE COLD (KT=0) CROSS SECTIONS IN THE OUTPUT FILE.	SIG00360
	SIG00370
	SIG00380
	SIG00390
	SIG00400
	SIG00410
	SIG00420
	SIG00430
WHEN DOPPLER BROADENING TO A SERIES OF SUCCESSIVELY HIGHER TEMPERATURES THE USER MAY MINIMIZE RUNNING TIME BY USING THE DOPPLER BROADENED CROSS SECTION FROM THE LAST TEMPERATURE TO DEFINE THE DOPPLER BROADENED CROSS SECTION AT THE NEXT HIGHEST TEMPERATURE. THIS PROCESS, CALLED BOOTSTRAPPING, CAN SAVE RUNNING TIME, BUT ERRORS IN THE CROSS SECTION CAN ACCUMULATE (I.E. BOOTSTRAPPING THROUGH A SERIES OF 20 TEMPERATURES EACH OF WHICH IS ACCURATE TO WITHIN 1 PER-CENT CAN LEAD TO A COMBINED ERROR OF 20 PER-CENT AT THE HIGHEST TEMPERATURE). BOOTSTRAPPING IS ONLY RECOMMENDED FOR DOPPLER BROADENING VERY LARGE CROSS SECTION SET (I.E. A REACTION DESCRIBED BY 3000 OR MORE ENERGY VS. CROSS SECTION PAIRS). EVEN IN THIS CASE ONLY A FEW TEMPERATURE STEPS SHOULD BE USED.	SIG00440
	SIG00450
	SIG00460
	SIG00470
	SIG00480
	SIG00490
	SIG00500
	SIG00510
	SIG00520
	SIG00530
	SIG00540
	SIG00550
	SIG00560
	SIG00570
THE TEMPERATURES TO BROADEN TO, CAN BE IDENTIFIED AS EITHER REAL TEMPERATURES THAT OUTPUT ARE REQUIRED FOR OR MERELY AS STEPS IN THE BOOTSTRAPPING PROCESS. FOR EXAMPLE, IF ONE WISHES TO	SIG00580
	SIG00590
	SIG00600

C	OBTAIN THE DOPPLER BROADENED CROSS SECTION AT 1 KEV ONE MAY	SIG00610
C	OPTIMIZE RUNNING TIME BY DOPPLER BROADENING TO 1, 10, 100 AND	SIG00620
C	1000 EV. BY BOOTSTRAPPING, AND TO ONLY OUTPUT THE 1 KEV CROSS	SIG00630
C	SECTIONS.	SIG00640
C		SIG00650
C	CROSS SECTIONS AT EACH TEMPERATURES THAT ARE OUTPUT ARE OUTPUT	SIG00660
C	AS SEPERATE SECTIONS IN THE ENDL FORMAT. THE TEMPERATURE OF EACH	SIG00670
C	SECTION IS INDICATED IN COLUMNS 59-70 OF THE FIRST HEADER CARD	SIG00680
C	OF EACH ENDL SECTION (TEMPERATURE IS IN MEV-STANDARD ENDL UNITS).	SIG00690
C		SIG00700
C	THE PROGRAM BROADENS A PAGE OF DATA AT A TIME (1 PAGE=1002 POINTS)	SIG00710
C	USING 3 PAGES OF DATA AT THE ORIGINAL TEMPERATURE (THE PAGE	SIG00720
C	BEING BROADENED, THE PAGE BELOW IT IN ENERGY AND THE PAGE	SIG00730
C	ABOVE IT IN ENERGY). OPERATING IN THIS MANNER THERE IS NO LIMIT	SIG00740
C	TO THE NUMBER OF POINTS IN A SECTION.	SIG00750
C		SIG00760
C	THE ENERGY GRID FOR THE DOPPLER BROADENED CROSS SECTIONS IS	SIG00770
C	SELECTED TO INSURE THAT THE BROADENED DATA IS LINEAR-LINEAR	SIG00780
C	INTERPOLATABLE. AS SUCH THE ENERGY GRID FOR THE BROADENED	SIG00790
C	DATA MAY NOT BE THE SAME AS THE ENERGY GRID FOR THE ORIGINAL	SIG00800
C	UNBROADENED DATA.	SIG00810
C		SIG00820
C	THE THINNING CRITERIA MAY BE USED TO FORCE THE CROSS SECTION AT	SIG00830
C	FINAL TEMPERATURES TO BE ON THE SAME ENERGY GRID BY SPECIFYING	SIG00840
C	0.0 AS THE THINNING CRITERIA. IN THIS CASE THE PROGRAM WILL SET	SIG00850
C	UP AN ENERGY GRID TO GUARANTEE CROSS SECTIONS ACCURATE TO WITHIN	SIG00860
C	0.1 PER-CENT AND WILL NOT THIN THE RESULTANT GRID ON OUTPUT.	SIG00870
C	THE ONLY EXCEPTION TO THIS RULE IS THRESHOLD REACTIONS, SINCE	SIG00880
C	AT SUCCESSIVELY HIGHER TEMPERATURES THE EFFECTIVE THRESHOLD	SIG00890
C	WILL EXTEND TO LOWER AND LOWER ENERGIES. THIS PROBLEM CAN BE	SIG00900
C	ELIMINATED BY HAVING ENERGY POINTS AT $1.0E-11$ MEV AND THE	SIG00910
C	THRESHOLD WITH THE CROSS SECTION EQUAL TO ZERO AT BOTH POINTS.	SIG00920
C		SIG00930
C	INPUT FILES	SIG00940
C	-----	SIG00950
C	FILENAME DESCRIPTION	SIG00960
C	-----	SIG00970
C	INPUT INPUT PARAMETERS	SIG00980
C	ENDLIN EVALUATED DATA IN THE ENDL CARD IMAGE FORMAT	SIG00990
C	SCRD001 SCRATCH FILE (ONLY USED FOR MULTIPLE TEMPERATURES)	SIG01000
C	SCRD002 SCRATCH FILE (ONLY USED FOR BOOTSTRAPPING)	SIG01010
C		SIG01020
C	OUTPUT FILES	SIG01030
C	-----	SIG01040
C	FILENAME DESCRIPTION	SIG01050
C	-----	SIG01060
C	OUTPUT OUTPUT REPORT	SIG01070
C	ENDLOUT DOPPLER BROADENED, THINNED EVALUATED DATA IN THE	SIG01080
C	ENDL CARD IMAGE FORMAT	SIG01090
C	SCRD001 SCRATCH FILE (ONLY USED FOR MULTIPLE TEMPERATURES)	SIG01100
C	SCRD002 SCRATCH FILE (ONLY USED FOR BOOTSTRAPPING)	SIG01110
C		SIG01120
C	INPUT CARDS	SIG01130
C	-----	SIG01140
C	CARD COLS. FORMAT DESCRIPTION	SIG01150
C	-----	SIG01160
C	1 1-11 F11.4 FRACTIONAL THINNING CRITERIA	SIG01170
C	(I.E. 0.5 PER-CENT = 0.005)	SIG01180
C	12-22 I11 TEMPERATURE UNITS	SIG01190
C	= 0 MEV	SIG01200

C			= 1 KELVIN	SIG01210
C	23-33	111	BOOTSTRAPPING OPTION	SIG01220
C			= 0 NO BOOTSTRAPPING	SIG01230
C			= 1 BOOTSTRAP	SIG01240
C	2-N	1-11 E11.4	TEMPERATURE IN MEV OR KELVIN (SEE	SIG01250
C			TEMPERATURE UNITS INDICATOR, ABOVE)	SIG01260
C	12-22	111	BOOTSTRAP STEP FLAG	SIG01270
C			= 0 BROADEN TO THIS TEMPERATURE AND OUTPUT	SIG01280
C			= 1 BROADEN TO THIS TEMPERATURE ONLY TO	SIG01290
C			ALLOW BOOTSTRAPPING TO NEXT HIGHEST	SIG01300
C			TEMPERATURE. NO OUTPUT FOR THIS	SIG01310
C			TEMPERATURE.	SIG01320
C				SIG01330
C			EACH CARD AFTER THE FIRST ONE SPECIFIES A SINGLE TEMPERATURE	SIG01340
C			TO WHICH EACH SECTION OF CROSS SECTION DATA SHOULD BE	SIG01350
C			BROADENED. UP TO 100 TEMPERATURES MAY BE SPECIFIED (I.E.	SIG01360
C			UP TO 101 INPUT CARDS MAY BE IN THE INPUT FILE). IF MORE THAN	SIG01370
C			100 TEMPERATURES ARE SPECIFIED, ONLY THE FIRST 100 WILL BE	SIG01380
C			USED. THE BOOTSTRAP STEP WITH EACH TEMPERATURE ALLOWS THE USER	SIG01390
C			TO INDICATE WHICH TEMPERATURES SHOULD BE USED MERELY AS STEPS	SIG01400
C			IN THE BOOTSTRAPPING PROCESS AND WHICH ARE ACTUALLY REQUIRED	SIG01410
C			AS OUTPUT.	SIG01420
C				SIG01430
C			EXAMPLE INPUT	SIG01440
C			-----	SIG01450
C			THE FOLLOWING INPUT CARDS ARE REQUIRED IN ORDER TO OBTAIN	SIG01460
C			DOPPLER BROADENED CROSS SECTIONS AT 0, 20, 2000 AND 200000 EV	SIG01470
C			TEMPERATURE. BOOTSTRAPPING WILL BE USED AND THE TEMPERATURES	SIG01480
C			2, 200 AND 20000 EV WILL BE USED AS BOOTSTRAP STEPS, WITHOUT	SIG01490
C			OUTPUT. ALL TEMPERATURES WILL BE ENTERED IN MEV (AS OPPOSED	SIG01500
C			TO KELVIN) AND THE BROADENED CROSS SECTIONS WILL BE THINNED	SIG01510
C			TO AN ACCURACY OF 0.1 PER-CENT (0.001 EXPRESSED AS A FRACTION).	SIG01520
C				SIG01530
C	1.00000-03	0	1	SIG01540
C	0.0			SIG01550
C	00000-06	1		SIG01560
C	2.00000-05			SIG01570
C	2.00000-04	1		SIG01580
C	2.00000-03			SIG01590
C	2.00000-02	1		SIG01600
C	2.00000-01			SIG01610
C				SIG01620
C			NOTE THAT ALL TEMPERATURES HAVE BEEN INPUT IN MEV. THE 0 MEV	SIG01630
C			TEMPERATURE IS USED TO INCLUDE THE COLD CROSS SECTIONS IN THE	SIG01640
C			FINAL BROADENED DATA FILE (ENDLOUT).	SIG01650
C				SIG01660
C			REAL MEV2EV,MEV2K	SIG01670
C			INTEGER OTAPE,OUTP,FLAG72,ZAENDL,YIENDL,YOENDL,CENDL,STEPS	SIG01680
C			1,BLANK,STEPIT,FLAG17	SIG01690
C			COMMON/HEAD1/ZAENDL,YIENDL,YOENDL,ATWT,DATE,FLAG,ELEVEL,HALFLIFE	SIG01700
C			1,TEMPIN,TMPOUT,FLAG72	SIG01710
C			COMMON/HEAD2/CENDL,IENDL,SENDL,QENDL,XIENDL(4)	SIG01720
C			COMMON/WEIGHT/AWR	SIG01730
C			COMMON/FILLER/DUMMY(17),MATD,MFD,MTD	SIG01740
C			COMMON/UNITS/OUTP,INP,ITAPE,OTAPE	SIG01750
C			COMMON/HOTS/ALPHA,TEMPK,ERTHIN,NTOT1,NTOT2	SIG01760
C			COMMON/JERZY/STEPS(100),TMPMEV(100),NTEMP,ITEMP	SIG01770
C			COMMON/NORMIT/XNORM(6),KSIGN(6),KEXP(6)	SIG01780
C			COMMON/CONTAC/OVPI,OVPI2,ATOP	SIG01790
C			COMMON/EXTEND/MESS1,MEXT1,DIMAX	SIG01800

COMMON/FILTOT/KTOTI,KTOTO	SIG01810
COMMON/ITCH/IADR(2),ISCR(2),NSCR(100,2),IPAGE(2),IPGMAX(2),	SIG01820
I IBOOTS,IUSE,ISAVE	SIG01830
COMMON/CONVRT/MEV2EV,EV2MEV,MEV2K,BOLTZM	SIG01840
COMMON/MINIE/ETHRES,EMIN	SIG01850
DIMENSION AWRY(6),BOOTS(2),UNITIN(2,2),FLAGIT(3),STEPIT(3),	SIG01860
I IGNOR(3),CARD(18)	SIG01870
DATA LEN/0/	SIG01880
DATA IERR/0/	SIG01890
C-----DEFINE ATOMIC WEIGHT OF INCIDENT PARTICLES.	SIG01900
DATA AWRY(1)/1.0037,1.0078,2.014,3.017,3.016,4.0026/	SIG01910
C-----DEFINE BOOTSTRAP OPTION ON OR OFF.	SIG01920
DATA BOOTS/3HOFF,3H ON/	SIG01930
C-----DEFINE TEMPERATURE INPUT UNITS.	SIG01940
DATA UNITIN/4H M,2HEV,4HKELV,2HIN/	SIG01950
C-----DEFINE FLAG FOR BOOTSTRAP STEPS.	SIG01960
DATA BLANK/1H /	SIG01970
DATA STEPIT/4HNO 0.4HUTPU,1HT/	SIG01980
DATA IGNOR/4HIGNO,4HRED ,1H /	SIG01990
C-----DEFINE PORTIONS OF P1 TO DEFINE P1 ACCURATELY ON VARIOUS	SIG02000
C-----COMPUTERS.	SIG02010
DATA P11/3.1415/	SIG02020
DATA P12/9.2653E-5/	SIG02030
DATA P13/5.8979E-10/	SIG02040
DATA P14/3.2384E-15/	SIG02050
C-----CREATE DROP FILE.	SIG02060
CALL DROPIT(7H+SIGMAL)	SIG02070
C-----DEFINE ALL I/O UNITS.	SIG02080
INP=5	SIG02090
OUTP=6	SIG02100
ITAPE=21	SIG02110
OTAPE=22	SIG02120
ISCR(1)=23	SIG02130
ISCR(2)=24	SIG02140
C-----OPEN INPUT FILE AND CREATE OUTPUT FILE.	SIG02150
CALL IOFILE(INP,5HINPUT,LEN,1,2,IERR)	SIG02160
CALL IOFILE(OUTP,6HOUTPUT,200000,2,2,IERR)	SIG02170
C-----DEFINE BOLTZMANN CONSTANT IN EV/DEGREE KELVIN	SIG02180
C----- (ASSUMING ENERGY WILL BE EXPRESSED IN EV AND THE ATOMIC	SIG02190
C-----WEIGHT RATIO WILL BE EXPRESSED IN ATOMIC MASS UNITS (AMU)).	SIG02200
C-----BELOW CONSTANT IS BASED ON 0.0253 EV = 293 KELVIN TIMES THE	SIG02210
C-----BOLTZMANN CONSTANT.	SIG02220
BOLTZM=8.6348E-05	SIG02230
C-----DEFINE FACTOR TO CONVERT FROM MEV TO EV AND EV TO MEV.	SIG02240
MEV2EV=1.0E+06	SIG02250
EV2MEV=1.0E-06	SIG02260
C-----DEFINE MINIMUM ENERGY OF INTEREST (IN EV).	SIG02270
EMIN=1.0E-05	SIG02280
C-----DEFINE MINIMUM THRESHOLD ENERGY (IN EV).	SIG02290
ETHRES=1.0	SIG02300
C-----DEFINE CONVERSION FACTOR FROM TEMPERATURE IN MEV TO KELVIN.	SIG02310
MEV2K=MEV2EV/BOLTZM	SIG02320
C-----INITIALIZE SCRATCH INDICES.	SIG02330
ISAVE=1	SIG02340
IUSE=1	SIG02350
C-----READ AND LIST RUN PARAMETERS.	SIG02360
READ(INP,5000) ERTHIN,KELVIN,IBOOTS	SIG02370
IF(KELVIN.NE.0) KELVIN=1	SIG02380
IF(IBOOTS.NE.0) IBOOTS=1	SIG02390
CALL NORMAL(ERTHIN,XNORM(1),KSIGN(1),KEXP(1))	SIG02400

WRITE(OUTP,6000) XNORM(1),KSIGN(1),KEXP(1)	SIG02410
1,UNITIN(1,KELVIN+1),UNITIN(2,KELVIN+1),BOOTS(1BOOTS+1)	SIG02420
DO 60 NTEMP=1,100	SIG02430
10 READ(INP,5000) TMPMEV(NTEMP),STEPS(NTEMP)	SIG02440
IF(NEOF(INP).NE.0) GO TO 70	SIG02450
C-----IF REQUIRED CONVERT TEMPERATURE FROM KELVIN TO MEV.	SIG02460
IF(KELVIN.GT.0) TMPMEV(NTEMP)=TMPMEV(NTEMP)/MEV2K	SIG02470
C-----LIST TEMPERATURE IN MEV AND KELVIN.	SIG02480
CALL NORMAL(TMPMEV(NTEMP),XNORM(2),KSIGN(2),KEXP(2))	SIG02490
TEMPK=MEV2K*TMPMEV(NTEMP)	SIG02500
CALL NORMAL(TEMPK,XNORM(3),KSIGN(3),KEXP(3))	SIG02510
FLAGIT(1)=BLANK	SIG02520
FLAGIT(2)=BLANK	SIG02530
FLAGIT(3)=BLANK	SIG02540
IF(STEPS(NTEMP).LE.0) GO TO 30	SIG02550
IF(1BOOTS.LE.0) GO TO 20	SIG02560
FLAGIT(1)=STEPIT(1)	SIG02570
FLAGIT(2)=STEPIT(2)	SIG02580
FLAGIT(3)=STEPIT(3)	SIG02590
GO TO 30	SIG02600
20 FLAGIT(1)=IGNOR(1)	SIG02610
FLAGIT(2)=IGNOR(2)	SIG02620
FLAGIT(3)=IGNOR(3)	SIG02630
30 IF(NTEMP.GT.1) GO TO 40	SIG02640
WRITE(OUTP,6002) (XNORM(1),KSIGN(1),KEXP(1),11=2,3)	SIG02650
1,FLAGIT	SIG02660
GO TO 50	SIG02670
40 WRITE(OUTP,6005) (XNORM(1),KSIGN(1),KEXP(1),11=2,3)	SIG02680
1,FLAGIT	SIG02690
C-----IGNOR BOOTSTRAPPING STEP, IF BOOTSTRAPPING OPTION IS NOT ON.	SIG02700
50 IF(STEPS(NTEMP).GT.0.AND.1BOOTS.LE.0) GO TO 10	SIG02710
60 CONTINUE	SIG02720
NTEMP=101	SIG02730
70 NTEMP=NTEMP-1	SIG02740
FLAG72=0	SIG02750
C- --TERMINATE IF NO TEMPERATURES GIVEN.	SIG02760
IF(NTEMP.GT.0) GO TO 80	SIG02770
WRITE(OUTP,6030)	SIG02780
CALL EXIT	SIG02790
80 WRITE(OUTP,6010)	SIG02800
C-----DEFINE ALL I/O UNITS AND DISK FILE NAMES.	SIG02810
CALL IONAME	SIG02820
C-----DEFINE REQUIRED CONSTANTS.	SIG02830
ATOP=4.0	SIG02840
P1=PI1+PI2+PI3+PI4	SIG02850
OVPI=1.0/SQRT(P1)	SIG02860
OVPI2=2.0*OVPI	SIG02870
C-----INITIALIZE MAXIMUM ALLOWABLE TEMPERATURE STEP (TO AVOID	SIG02880
C-----CROSS SECTION EXTENSION)	SIG02890
DTMAX=0.0	SIG02900
C-----INITIALIZE TOTAL NUMBER OF POINTS READ AND WRITTEN.	SIG02910
KTOT1=0	SIG02920
KTOTO=0	SIG02930
C-----DEFINE MAXIMUM ALLOWABLE ENERGY SPACING.	SIG02940
CALL MAXDE	SIG02950
C-----READ AND WRITE FIRST HEAD CARD.	SIG02960
90 IF(FLAG72.EQ.2) GO TO 150	SIG02970
READ(ITAPE,5020) ZAENDL,YIENDL,YOENDL,ATHT,DATE,FLAG,ELEVEL.	SIG02980
1 HALFLIFE,TEMPIN	SIG02990
IF(NEOF(ITAPE).NE.0.OR.ZAENDL.GE.400000) GO TO 150	SIG03000

READ(1TAPE,5030) CENDL,IENDL,SENDL,QENDL,XIENDL	SIG03010
IF(NOE(1TAPE).NE.0) GO TO 150	SIG03020
C-----READ AND WRITE SECOND HEAD CARD.	SIG03030
C-----COPY DATA IF IT IS NOT A CROSS SECTION (IENDL=1) OR NOT FOR A	SIG03040
C-----DEFINED INCIDENT PARTICLE (YIENDL=1 TO 6)	SIG03050
IF(IENDL.EQ.0.AND.YIENDL.GE.1.AND.YIENDL.LE.6) GO TO 140	SIG03060
C-----SECTION IS NOT CROSS SECTIONS. COPY IT.	SIG03070
TMPOUT=TEMPIN	SIG03080
CALL HEADOUT	SIG03090
100 READ(1TAPE,5035) CARD,FLAG72	SIG03100
IF(NOE(1TAPE)) 150,110,150	SIG03110
110 IF(FLAG72) 120,120,130	SIG03120
120 WRITE(1TAPE,5035) CARD	SIG03130
GO TO 100	SIG03140
130 WRITE(1TAPE,5060) FLAG72	SIG03150
GO TO 90	SIG03160
C-----DEFINE ATOMIC WEIGHT RATIO OF TARGET TO PROJECTILE.	SIG03170
140 AWR=ATWT/AWRY(IYIENDL)	SIG03180
C-----BROADEN CROSS SECTION.	SIG03190
CALL BROADS	SIG03200
GO TO 90	SIG03210
C	SIG03220
C	SIG03230
C	SIG03240
C	SIG03250
C-----WRITE TOTALS FOR LAST MATERIAL.	SIG03260
150 IF(NTOTI.LE.0) GO TO 160	SIG03270
WRITE(OUTP,5040) NTOTI,NTOTO	SIG03280
C-----INCREMENT TOTALS FOR ENTIRE FILE.	SIG03290
KTOTI=KTOTI+NTOTI	SIG03300
KTOTO=KTOTO+NTOTO	SIG03310
C-----LIST TOTAL NUMBER OF BROADENED POINTS READ AND WRITTEN.	SIG03320
160 WRITE(OUTP,5050) KTOTI,KTOTO	SIG03330
C-----WRITE WARNING MESSAGE IF CROSS SECTION EXTENSION USED.	SIG03340
IF(DTMAX.LE.0.0) GO TO 170	SIG03350
CALL NGRMAL(DTMAX/MEV2K,XNORM(1),KSIGN(1),KEXP(1))	SIG03360
CALL NORMAL(DTMAX,XNORM(2),KSIGN(2),KEXP(2))	SIG03370
WRITE(OUTP,6020) (XNORM(1),KSIGN(1)),(11=1,2)	SIG03380
C-----OUTPUT END OF DATA CARD TO ENDOUT.	SIG03390
170 WRITE(1TAPE,5010)	SIG03400
C-----END FILE AND CLOSE ENDF/B FORMAT OUTPUT FILE.	SIG03410
CALL IOFILE(1TAPE,7HENDLOUT,LEN,3,2,IERR)	SIG03420
C-----DESTROY ANY SCRATCH FILES THAT WERE CREATED.	SIG03430
IF(NTEMP.GT.1) CALL IOFILE(1SCR(1),7HSCR0001,LEN,8,4,IERR)	SIG03440
IF(1BOOTS.GT.0) CALL IOFILE(1SCR(2),7HSCR0002,LEN,8,4,IERR)	SIG03450
CALL EXIT	SIG03460
5000 FORMAT(11,4,2111)	SIG03470
5010 FORMAT(6H200000,65X,1H2)	SIG03480
5020 FORMAT(16,213,E12.5,17,13,3E12.5)	SIG03490
5030 FORMAT(12,213,6E12.5)	SIG03500
5035 FORMAT(17A4,A3,11)	SIG03510
5040 FORMAT(2X,B7(1H-)/44X,10H ZA TOTALS,217/2X,B7(1H-))	SIG03520
5050 FORMAT(2X,B7(1H-)/43X,11HTAPE TOTALS,217/2X,B7(1H-))	SIG03530
5060 FORMAT(71X,11)	SIG03540
6000 FORMAT(37H1 DOPPLER BROADEN ENDL CROSS SECTIONS,	SIG03550
1 14H (SIGMAL 79-1)/2X,B7(1H-)/	SIG03560
2 2X,19HTHINNING CRITERIA--,F8.5,A1,12/	SIG03570
3 2X,19HTEMPERATURE UNITS--,5X,A4,A2/	SIG03580
3 2X,19HBOOTSTRAP OPTION--,8X,A3)	SIG03590
6002 FORMAT(2X,19HTEMPERATURE(S)-----,F8.5,A1,12,4H MEV,	SIG03600

1 IX,F8.5,A1,12,7H KELVIN,IX,2A4,A1)	SIG03610
6005 FORMAT(2IX,F8.5,A1,12,5X,F8.5,A1,12,8X,2A4,A1)	SIG03620
6010 FORMAT(2X,87(1H-))	SIG03630
1 2X,6H ZA,5H Y1,5H C,5X,7HQ-VALUE,4X,8HTEMP. IN,	SIG03640
2 3X,9HTEMP. OUT,7H POINTS,7H POINTS,2X,8HMESSAGES/	SIG03650
2 27X,3HMEV,9X,3HMEV,9X,3HMEV,7H IN,7H OUT/2X,87(1H-))	SIG03660
6020 FORMAT(///11H EXTENSION/2X,9(1H-))	SIG03670
1 43H CROSS SECTION EXTENSION CAN BE AVOIDED BY/	SIG03680
2 46H THINNING DATA OR DOPPLER BROADENING IN STEPS/	SIG03690
3 14H OF LESS THAN,F8.5,A1,12,6H MEV (,F8.5,A1,12,8H KELVIN))	SIG03700
6030 FORMAT(2X,40HNO TEMPERATURE(S)...EXECUTION TERMINATED)	SIG03710
END	SIG03720
SUBROUTINE BROADS	SIG03730
C	SIG03740
C THIS ROUTINE IS DESIGNED TO LOAD DATA INTO THE CORE AND DOPPLER	SIG03750
C BROADEN IT A PAGE AT A TIME (1 PAGE=1002 POINTS). IF THE SECTION	SIG03760
C IS 1002 OR LESS POINTS THE ENTIRE OPERATION IS PERFORMED IN CORE.	SIG03770
C IF THE SECTION IS OVER 1002 POINTS IT IS WRITTEN ONTO A SCRATCH	SIG03780
C FILE WHICH CAN LATER BE READ BY TABFIN.	SIG03790
C	SIG03800
REAL MEV2EV,MEV2K	SIG03810
INTEGER OUTP,OTAPE,ZAENDL,YIENDL,YOENDL,CENDL,SENDL,STEPS	SIG03820
COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,	SIG03830
1 NOW1,N2MAOE,NOWO,N2LEFT,NPAGE,JJLOW,ILOW	SIG03840
COMMON/HOTS/ALPHA,TEMPK,ERTHIN,NTOT1,NTOTO	SIG03850
COMMON/JERZY/STEPS(100),TMPMEV(100),NTEMP,ITEMP	SIG03860
COMMON/HEAD1/ZAENDL,YIENDL,YOENDL,ATWT,DATE,FLAG,ELEVEL,HALFLIFE	SIG03870
1,TEMPIN,TMPOUT,FLAG72	SIG03880
COMMON/HEAD2/CENDL,IENDL,SENDL,QENDL,XIENDL(4)	SIG03890
COMMON/WEIGHT/AWR	SIG03900
COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT	SIG03910
COMMON/UNITS/OUTP,INP,ITAPE,OTAPE	SIG03920
COMMON/NORMIT/XNORM(6),KSIGN(6),KEXP(6)	SIG03930
COMMON/FILLER/IFILL,NFILL,NLEFT,NODOPE,ITHRES	SIG03940
COMMON/SAVER/JSAVE,NSAVE	SIG03950
COMMON/EXTEND/MESS1,MEXT,DTMAX	SIG03960
COMMON/CONTAC/OVPI,OVPI2,ATOP	SIG03970
COMMON/FILTOT/KTOT1,KTOTO	SIG03980
COMMON/ITCH/IADR(2),ISCR(2),NSCR(100,2),IPAGE(2),IPGMAX(2),	SIG03990
1 (BOOTS,1USE,ISAVE	SIG04000
COMMON/CONVRT/MEV2EV,EV2MEV,MEV2K,BOLTZM	SIG04010
COMMON/PAGEIN/XIN(6000),YIN(6000)	SIG04020
COMMON/LASTEP/XNEXT	SIG04030
COMMON/MINNIE/ETHRES,EMIN	SIG04040
COMMON X(3006),S(3006),XOUT(255),CK(3006),YOUT(255),YBREAL(1002),	SIG04050
1 EIN(255),SIN(255)	SIG04060
DIMENSION XB(2004),SB(2004),MESSAG(3,2,2)	SIG04070
EQUIVALENCE (CK(2260),SB),(S(2260),XB)	SIG04080
C-----DEFINE CROSS SECTION EXTENSION MESSAGE.	SIG04090
DATA MESSAG/	SIG04100
1 1H,1H,1H,	SIG04110
2 4HEXTE,4HNSIO,1HN,	SIG04120
3 1H,1H,1H,	SIG04130
4 4HNO 0,4HUTPU,1HT/	SIG04140
C-----INITIALIZE LAST MAT FOUND	SIG04150
DATA LASTZA/-100000/	SIG04160
C-----SET UP LOOP OVER TEMPERATURES.	SIG04170
LOWOUT=0	SIG04180
DO 200 ITEMP=1,NTEMP	SIG04190
C-----INITIALIZE NEXT ENERGY FOR MINIMUM ENERGY SPACING.	SIG04200

XNEXT=0.0	SIG04210
C-----INITIALIZE DISK ADDRESS AND PAGE COUNT.	SIG04220
IADR(1)=0	SIG04230
IADR(2)=0	SIG04240
IPAGE(1)=0	SIG04250
IPAGE(2)=0	SIG04260
JSAVE=0	SIG04270
C-----INITIALIZE FLAG TO DOPPLER BRADEN SECTION.	SIG04280
NODOPE=-1	SIG04290
C-----DEFINE EFFECTIVE TEMPERATURE IN KELVIN.	SIG04300
TEMPK=MEV2K*(TMPMEV(ITEMP)-TEMPIN)	SIG04310
C-----IF NO TEMPERATURE INCREASE SKIP THIS TEMPERATURE.	SIG04320
IF(TEMPK.GT.0.0) GO TO 10	SIG04330
C-----NO DOPPLER BROADENING. ALLOW ONE SECTION WITHOUT BROADENING	SIG04340
C-----TO BE LISTED.	SIG04350
NODOPE=1	SIG04360
LOWOUT=LOWOUT+1	SIG04370
IF(LOWOUT-1) 20,20,200	SIG04380
C-----DEFINE GAUSSIAN WIDTH.	SIG04390
10 ALPHA=AWR/(BOLTZM*TEMPK)	SIG04400
C-----DEFINE TEMPERATURE OF SECTION BEING OUTPUT (EITHER ORIGINAL	SIG04410
C-----TEMPERATURE OF SECTION OR TEMPERATURE TO WHICH SECTION WILL BE	SIG04420
C-----BROADENED, WHICHEVER IS HIGHER).	SIG04430
20 TMPOUT=TEMPIN	SIG04440
IF(TMPOUT.LT.TMPMEV(ITEMP)) TMPOUT=TMPMEV(ITEMP)	SIG04450
C-----IF SECTION WILL BE OUTPUT, WRITE SECTION HEAD CARDS.	SIG04460
IF(STEPS(ITEMP).LE.0) CALL HEADOUT	SIG04470
C-----INITIALIZE PAGE COUNT FOR CROSS SECTION EXTENSION TEST.	SIG04480
MEXT=0	SIG04490
C-----INITIALIZE FLAG NOT TO PRINT OUT MESSAGE WITH SECTION.	SIG04500
MESS1=1	SIG04510
C-----DEFINE PAGE SIZE (BY CHANGING DIMENSION, COMMON STATEMENTS	SIG04520
C-----AND THIS NUMBER THE SIZE OF THE CORE TABLES MAY BE CHANGED).	SIG04530
NPAGE=1002	SIG04540
C-----INITIALIZE TOTAL NUMBER OF POINTS FOR OUTPUT, INPUT AND LEFT	SIG04550
C-----FOR INPUT.	SIG04560
NOWO=0	SIG04570
NOWI=0	SIG04580
N2LEFT=100000	SIG04590
C-----SET BROADENING INOICES TO MIDDLE PAGE.	SIG04600
NLOW=NPAGE+1	SIG04610
NHIGH=2*NPAGE	SIG04620
C-----SET INDEX TO LOADED POINTS AT BEGINNING OF MIDDLE PAGE.	SIG04630
KLOW=NLOW	SIG04640
C-----SET THINNING CONVERGED INDEX TO FIRST POINT IN CORE.	SIG04650
JJLOW=NLOW	SIG04660
C-----SET INDICES TO LOAD MIDDLE AND LAST PAGE.	SIG04670
MLOW=NLOW	SIG04680
MHIGH=3*NPAGE	SIG04690
C-----INITIALIZE SECTION FLAGS.	SIG04700
NFILL=6000	SIG04710
IFILL=NFILL+1	SIG04720
NLEFT=100000	SIG04730
N2MADE=0	SIG04740
C-----LOAD NEXT PAGE OF DATA AT ORIGINAL TEMPERATURE.	SIG04750
30 CALL FILLUP	SIG04760
C-----SET INDEX TO LOADED POINTS TO LAST POINT LOADED.	SIG04770
KHIGH=MHIGH	SIG04780
IF(NHIGH.GT.MHIGH) NHIGH=MHIGH	SIG04790
C-----SHOULD DATA BE DOPPLER BROADENED....	SIG04800

40 IF(NODOPE.LE.0) GO TO 60	SIG04810
C-----COPY UNBROADENED DATA TO BROADENED LOCATIONS (NO BROADENING).	SIG04820
C-----NOTE...ENERGY HAS NOT BEEN CONVERTED TO SPEED AND THEREFORE	SIG04830
C-----SHOULD NOT BE RE-CONVERTED DURING THIS STEP.	SIG04840
DO 50 K=NLOW,NHIGH	SIG04850
XB(K)=X(K)	SIG04860
50 SB(K)=S(K)	SIG04870
GO TO 70	SIG04880
C-----BROADEN POINTS IN MIDDLE PAGE	SIG04890
60 CALL BROADN	SIG04900
C-----THIN BROADENED POINTS.	SIG04910
70 CALL THINB	SIG04920
C-----IF THRESHOLD REACTION AND FIRST ENERGY POINT IS ABOVE MINIMUM	SIG04930
C-----ENERGY, INSURE CROSS SECTION IS ZERO AT NEW EFFECTIVE THRESHOLD.	SIG04940
IF(ITHRES.GT.0.AND.NOWO.LE.0.AND.XB(JLOW).GT.1.1*EMIN)	SIG04950
1 SB(JLOW)=0.0	SIG04960
C-----INCREMENT COUNTS OF POINTS OUTPUT.	SIG04970
JJ=JHIGH-JLOW+1	SIG04980
NOWO=NOWO+JJ	SIG04990
C-----IF SECTION WILL BE OUTPUT, WRITE THINNED POINTS.	SIG05000
IF(STEPS(ITEMP).GT.0) GO TO 90	SIG05010
DO 80 J=JLOW,JHIGH	SIG05020
DUME=EV2MEV*XB(J)	SIG05030
CALL NORMAL(DUME,XNORM(1),KSIGN(1),KEXP(1))	SIG05040
CALL NORMAL(SB(J),XNORM(2),KSIGN(2),KEXP(2))	SIG05050
80 WRITE(OTAPE,5020) (XNORM(I),KSIGN(I),KEXP(I),I=1,2)	SIG05060
C*	SIG05070
C* IF BOOTSTRAPPING AND THIS IS NOT THE LAST TEMPERATURE, SAVE	SIG05080
C* BROADENED CROSS SECTIONS EITHER IN CORE OR ON SCRATCH.	SIG05090
C*	SIG05100
90 IF(1BOOTS.LE.0.OR.1TEMP.GE.NTEMP) GO TO 140	SIG05110
C-----IF ALL INPUT POINTS HAVE NOT YET BEEN USED POINTS MUST BE SAVED	SIG05120
C-----ON SCRATCH.	SIG05130
IF(N2LEFT.GT.0) GO TO 130	SIG05140
C- ---FIRST PAGE WILL ALWAYS FIT IN CORE. SUM OF FIRST AND SECOND	SIG05150
C- --PAGES MAY FIT (IF THEY DO COMBINE THEM INTO ONE PAGE). MORE THAN	SIG05160
C-----TWO PAGES INDICATES POINTS ALREADY BEING WRITTEN TO SCRATCH.	SIG05170
IF(IPAGE(ISAVE)-1) 110,100,130	SIG05180
C-----IF FIRST PAGE OF POINTS WENT TO SCRATCH THE REMAINDER MUST.	SIG05190
100 IF(JSAVE.LE.0) GO TO 130	SIG05200
C-----DETERMINE IF BOTH PAGES WILL FIT IN CORE.	SIG05210
IF(JSAVE+JJ.LE.6000) GO TO 110	SIG05220
C-----MOVE POINTS, THAT HAVE ALREADY BEEN SAVED, FROM CORE TO	SIG05230
C-----SCRATCH.	SIG05240
CALL OBLOCK(ISCR(ISAVE),IADR(ISAVE),XIN,JSAVE)	SIG05250
CALL OBLOCK(ISCR(ISAVE),IADR(ISAVE),YIN,JSAVE)	SIG05260
GO TO 130	SIG05270
C-----SAVE POINTS IN CORE. SET COUNTERS TO INDICATE ONE PAGE IN CORE.	SIG05280
110 DO 120 J2=JLOW,JHIGH	SIG05290
JSAVE=JSAVE+1	SIG05300
XIN(JSAVE)=XB(J2)	SIG05310
120 YIN(JSAVE)=SB(J2)	SIG05320
IPAGE(ISAVE)=1	SIG05330
NSCR(I,ISAVE)=JSAVE	SIG05340
GO TO 140	SIG05350
C-----INCREMENT PAGE COUNT. SAVE POINT COUNT. STORE DATA ON SCRATCH.	SIG05360
130 IPAGE(ISAVE)=IPAGE(ISAVE)+1	SIG05370
NSCR(IPAGE(ISAVE),ISAVE)=JJ	SIG05380
CALL OBLOCK(ISCR(ISAVE),IADR(ISAVE),XB(JLOW),JJ)	SIG05390
CALL OBLOCK(ISCR(ISAVE),IADR(ISAVE),SB(JLOW),JJ)	SIG05400

```

C-----HAS THE LAST POINT BEEN BROADENED....
  140 IF(NHIGH.GE.KHIGH) GO TO 180
C-----NO. SAVE UNCONVERGED THINNING POINTS (IF ANY) IN THE LOCATIONS
C-----IMMEDIATELY IN FRONT OF THE NEXT PAGE TO BE BROADENED (AFTER NEXT
C-----PAGE IS BROADENED THESE REMAINING POINTS PLUS THE BROADENED PAGE
C-----MAY BE TREATED AS ONE SET OF POINTS FOR THINNING).
  IF(LOW.GT.NHIGH) GO TO 160
  KK=NLOW-1-(NHIGH-LOW)
  JJLOW=KK
  DO 150 K=LOW,NHIGH
  XB(KK)=XB(K)
  SB(KK)=SB(K)
  150 KK=KK+1
C-----SHIFT REMAINING UNBROADENED POINTS ONE PAGE FORWARD IN CORE.
  160 KK=0
  DO 170 K=NLOW,KHIGH
  KK=KK+1
  X(KK)=X(K)
  S(KK)=S(K)
  170 CK(KK)=CK(K)
C-----SET INDEX TO LOADED POINTS TO BEGINNING OF TABLE.
  KLOW=1
C-----SET INDEX TO NEXT AVAILABLE LOCATION FOR LOADING.
  MLOW=KK+1
C-----ARE THERE ANY MORE POINTS STILL TO READ....
  IF(N2LEFT.GT.0) GO TO 30
C-----NO. SET INDEX TO LAST LOADED POINT.
  KHIGH=KK
C-----SET INDEX TO BROADEN ALL REMAINING POINTS.
  NHIGH=KHIGH
  GO TO 40
C-----ENTIRE TABLE HAS BEEN BROADENED AND OUTPUT.
C-----WRITE REPORT OF SECTION.
  180 IF(ZAENDL.EQ.LASTZA) GO TO 190
  IF(LASTZA.GT.0) WRITE(OUTP,5040) NTOTI,NTOTO
C-----INCREMENT TOTALS FOR ENTIRE FILE.
  KTOTI=KTOTI+NTOTI
  KTOTO=KTOTO+NTOTO
C-----INITIALIZE TOTALS FOR NEXT MATERIAL.
  NTOTI=0
  NTOTO=0
  LASTZA=ZAENDL
C-----WRITE REPORT FOR SECTION.
  190 CALL NORMAL(QENDL,XNORM(1),KSIGN(1),KEXP(1))
  CALL NORMAL(TEMPIN,XNORM(2),KSIGN(2),KEXP(2))
  CALL NORMAL(TMPMEV(ITEMP),XNORM(3),KSIGN(3),KEXP(3))
  MESS2=1
  IF(STEPS(ITEMP).GT.0) MESS2=2
  WRITE(OUTP,5030) ZAENDL,YIENDL,CENDL,
  1 (XNORM(L),KSIGN(L),KEXP(L),L=1,3),NOWI,NOWO,
  1 (MESSAG(L,MESS2,2),L=1,3), (MESSAG(L,MESS1,1),L=1,3)
C-----INCREMENT TOTALS FOR ENTIRE MATERIAL.
  NTOTI=NTOTI+NOWI
  IF(STEPS(ITEMP).LE.0) NTOTO=NTOTO+NOWO
C-----IF BOOTSTRAPPING DEFINE NEW INITIAL TEMPERATURE.
  IF(1BOOTS.GT.0) TEMPIN=TMPMEV(ITEMP)
C-----IF SECTION IS OUTPUT, WRITE SECTION END SENTINEL.
  IF(STEPS(ITEMP).LE.0) WRITE(OTAPE,5010)
  IPGMAX(1SAVE)=IPAGE(1SAVE)
C-----SWITCH SCRATCH INDICES.

```

SIG05410
 SIG05420
 SIG05430
 SIG05440
 SIG05450
 SIG05460
 SIG05470
 SIG05480
 SIG05490
 SIG05500
 SIG05510
 SIG05520
 SIG05530
 SIG05540
 SIG05550
 SIG05560
 SIG05570
 SIG05580
 SIG05590
 SIG05600
 SIG05610
 SIG05620
 SIG05630
 SIG05640
 SIG05650
 SIG05660
 SIG05670
 SIG05680
 SIG05690
 SIG05700
 SIG05710
 SIG05720
 SIG05730
 SIG05740
 SIG05750
 SIG05760
 SIG05770
 SIG05780
 SIG05790
 SIG05800
 SIG05810
 SIG05820
 SIG05830
 SIG05840
 SIG05850
 SIG05860
 SIG05870
 SIG05880
 SIG05890
 SIG05900
 SIG05910
 SIG05920
 SIG05930
 SIG05940
 SIG05950
 SIG05960
 SIG05970
 SIG05980
 SIG05990

11=ISAVE	SIG06010
ISAVE=IUSE	SIG06020
IUSE=11	SIG06030
200 CONTINUE	SIG06040
RETURN	SIG06050
5010 FORMAT(71X,1H1)	SIG06060
5020 FORMAT(F8.5,A1,12,F8.5,A1,12)	SIG06070
5030 FORMAT(2X,16,215,3(1X,F8.5,A1,12),217,1X,2A4,A1,2X,2A4,A1)	SIG06080
5040 FORMAT(2X,87(1H-)/44X,10H ZA TOTALS,217/2X,87(1H-))	SIG06090
END	SIG06100
SUBROUTINE FILLUP	SIG06110
C	SIG06120
C LOAD NEXT PAGE OR PAGES OF CROSS SECTIONS AT THE ORIGINAL	SIG06130
C TEMPERATURE INTO CORE. INSURE THAT THE MAXIMUM ENERGY	SIG06140
C SPACING REQUIRED FOR LINEAR-LINEAR INTERPOLATABLE DOPPLER	SIG06150
C BROADENED DATA IS NOT EXCEEDED.	SIG06160
C	SIG06170
C THE DATA IS READ FROM THE ENDLIN FILE FOR THE FIRST TEMPERATURE.	SIG06180
C IF MULTIPLE TEMPERATURES, DATA WILL STILL BE IN XIN AND YIN FOR	SIG06190
C SUCCESSIVE TEMPERATURES (IF LESS THAN 6001 POINTS) OR ON SCRATCH	SIG06200
C DISK FILE (IF OVER 6000 POINTS).	SIG06210
C	SIG06220
REAL MEV2EV	SIG06230
INTEGER FLAG72	SIG06240
COMMON/HOTS/ALPHA,TEMPK,ERTHIN,NTOT1,NTOT0	SIG06250
COMMON/JERZY/STEPS(100),TMPMEV(100),NTEMP,ITEMP	SIG06260
COMMON/UNITS/OUTP,INP,ITAPE,OTAPE	SIG06270
COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,	SIG06280
I NOWI,NZMADE,NOWO,NZLEFT,NPAGE,JJLOW,ILOW	SIG06290
COMMON/ITCH/IADR(2),ISCR(2),NSCR(100,2),IPAGE(2),IPGMAX(2),	SIG06300
I IBOOTS,IUSE,ISAVE	SIG06310
COMMON/FILLER/IFILL,NFILL,NLEFT,NODOPE,ITHRES	SIG06320
COMMON/SAVER/JSAVE,NSAVE	SIG06330
COMMON/CONTAC/OVPI,OVPI2,ATOP	SIG06340
COMMON/HEAD1/ZAENDL,YIENDL,YOENDL,ATWT,DATE,FLAG,ELEVEL,HALFLIFE	SIG06350
I,TEMPIN,TMPOUT,FLAG72	SIG06360
COMMON/CONVRT/MEV2EV,EV2MEV,MEV2K,BOLTZM	SIG06370
COMMON/LASTEP/XNEXT	SIG06380
COMMON/MINNIE/ETHRES,EMIN	SIG06390
COMMON X(3006),S(3006),XOUT(255),CK(3006),YOUT(255),YBREAL(1002),	SIG06400
I EIN(255),SIN(255)	SIG06410
COMMON/PAGEIN/XIN(6000),YIN(6000)	SIG06420
C-----DEFINE MINIMUM ENERGY SPACING, ALLOWING FOR ROUND-OFF DURING	SIG06430
C-----BOOTSTRAPPING.	SIG06440
DEMAXI=DEMAX	SIG06450
IF(ITEMP.GT.1).AND.IBOOTS.GT.0) DEMAXI=1.00000001*DEMAXI	SIG06460
C-----SET UP LOOP OVER POINTS TO LOAD INTO ORIGINAL TEMPERATURE ARRAY.	SIG06470
DO 150 KPT=MLOW,MHIGH	SIG06480
C-----IF NO MORE POINTS IN CORE READ NEXT PAGE (IF ANY).	SIG06490
IF(IFILL.LE.NFILL) GO TO 90	SIG06500
IF(NLEFT.LE.0) GO TO 160	SIG06510
C-----FOR FIRST TEMPERATURE READ FROM ENDLIN. FOR ALL OTHER	SIG06520
C-----TEMPERATURES DATA IS EITHER IN CORE OR CAN BE READ FROM SCRATCH.	SIG06530
IF(ITEMP.LE.1) GO TO 20	SIG06540
IPAGE(IUSE)=IPAGE(IUSE)+1	SIG06550
NFILL=NSCR(IPAGE(IUSE),IUSE)	SIG06560
IF(IPGMAX(IUSE).GT.1) GO TO 10	SIG06570
C-----DATA IS ENTIRELY CORE RESIDENT. SET FLAG TO SHOW NO MORE TO READ.	SIG06580
NLEFT=0	SIG06590
GO TO 80	SIG06600

C-----OVER 6000 DATA POINTS. READ FROM SCRATCH.	SIG06610
10 CONTINUE	SIG06620
CALL IBLOCK(ISCRT(IUSE),IADR(IUSE),XIN,NFILL)	SIG06630
CALL IBLOCK(ISCRT(IUSE),IADR(IUSE),YIN,NFILL)	SIG06640
IF(IPAGE(IUSE).GE.IPGMAX(IUSE)) NLEFT=0	SIG06650
GO TO 80	SIG06660
C-----READ DATA FROM ENDL FORMAT FILE.	SIG06670
20 CONTINUE	SIG06680
DO 40 I=1,NFILL	SIG06690
READ(ITAPE,5020) XIN(I),YIN(I),FLAG72	SIG06700
IF(NOEOT(ITAPE).EQ.0) GO TO 30	SIG06710
FLAG72=2	SIG06720
GO TO 50	SIG06730
30 IF(FLAG72.GT.0) GO TO 50	SIG06740
40 XIN(I)=MEV2EV*XIN(I)	SIG06750
GO TO 60	SIG06760
50 NLEFT=0	SIG06770
NFILL=I-1	SIG06780
C-----IF MORE THAN ONE TEMPERATURE DATA MUST BE SAVED.	SIG06790
60 IF(NTMP.LE.1) GO TO 70	SIG06800
C-----IF BOOTSTRAPPING CROSS SECTIONS. NO NEED TO SAVE INITIAL DATA.	SIG06810
IF(IROOTS.GT.0) GO TO 70	SIG06820
IPAGE(ISAVE)=IPAGE(ISAVE)+1	SIG06830
NSCRT(IPAGE(ISAVE),ISAVE)=NFILL	SIG06840
C-----IF INITIAL DATA IS ALL CORE RESIDENT, NO NEED TO WRITE ON SCRATCH.	SIG06850
IF(IPAGE(ISAVE).LE.1.AND.NLEFT.LE.0) GO TO 70	SIG06860
C-----OVER 6000 DATA POINTS. WRITE TO SCRATCH.	SIG06870
CALL OBLOCK(ISCRT(ISAVE),IADR(ISAVE),XIN,NFILL)	SIG06880
CALL OBLOCK(ISCRT(ISAVE),IADR(ISAVE),YIN,NFILL)	SIG06890
70 NOWI=NOWI+NFILL	SIG06900
80 IFILL=1	SIG06910
C-----DETERMINE IF DATA WILL BE DOPPLER BROADENED (IF NOT MAXIMUM	SIG06920
C-----ENERGY SPACING IS NOT REQUIRED).	SIG06930
90 IF(NODOPE) 100,120,110	SIG06940
C-----NO DOPPLER BROADENING IF THRESHOLD OVER 1,000,000*KT/A.	SIG06950
0 NODOPE=1	SIG06960
ITHRES=0	SIG06970
AX=ALPHA*XIN(1)	SIG06980
IF(AX.GE.1000000.0) GO TO 130	SIG06990
NODOPE=0	SIG07000
C-----IF THIS IS A THRESHOLD REACTION DOPPLER BROADENING WILL SHIFT THE	SIG07010
C-----THRESHOLD TO A LOWER ENERGY EFFECTIVE THRESHOLD. CREATE EXTRA DATA	SIG07020
C-----POINTS BELOW THE ORIGINAL THRESHOLD AT WHICH THE INITIAL CROSS	SIG07030
C-----SECTION IS ZERO. POSITION THE SUB-THRESHOLD POINTS TO INSURE THE	SIG07040
C-----CROSS SECTION AT THE LOWEST ENERGY WILL BE ZERO AFTER DOPPLER	SIG07050
C-----BROADENING (NEW EFFECTIVE THRESHOLD).	SIG07060
IF(XIN(1).LT.ETHRES) GO TO 130	SIG07070
ITHRES=1	SIG07080
V=SQRT(AX)-ATOP	SIG07090
XNEXT=V*V/ALPHA	SIG07100
IF(XNEXT.LT.ETHRES.OR.V.LE.0.0) XNEXT=EMIN	SIG07110
X(KPT)=XNEXT	SIG07120
S(KPT)=0.0	SIG07130
GO TO 140	SIG07140
C-----NO BROADENING. USE MINIMUM ENERGY SPACING IF UNIFORM OUTPUT	SIG07150
C-----ENERGY GRID IS REQUESTED (INDICATED BY ERTHIN=0.0).	SIG07160
110 IF(ERTHIN.GT.0.0.OR.XNEXT.LE.0.0) GO TO 130	SIG07170
C-----CHECK FOR MAXIMUM ALLOWABLE ENERGY SPACING.	SIG07180
120 IF(XIN(1FILL).LE.XNEXT) GO TO 130	SIG07190
C-----INTERPOLATE TO INSERT POINT AT MAXIMUM ALLOWABLE ENERGY SPACING.	SIG07200

X(KPT)=XNEXT	SIG07210
S(KPT)=SKPTM1+(XNEXT-XKPTM1)*(YIN(IFILL)-SKPTM1)/	SIG07220
1 (XIN(IFILL)-XKPTM1)	SIG07230
GO TO 140	SIG07240
C-----ENERGY SPACING O K	SIG07250
130 X(KPT)=XIN(IFILL)	SIG07260
S(KPT)=YIN(IFILL)	SIG07270
IFILL=IFILL+1	SIG07280
140 XKPTM1=X(KPT)	SIG07290
SKPTM1=S(KPT)	SIG07300
150 XNEXT=DEMAX1*XKPTM1	SIG07310
IF(NLEFT.LE.0.AND. IFILL.GT.NFILL) N2LEFT=0	SIG07320
GO TO 170	SIG07330
C-----END OF DATA TABLE.	SIG07340
160 MHIGH=KPT-1	SIG07350
N2LEFT=0	SIG07360
170 N2MADE=N2MADE+(MHIGH-MLDW)+1	SIG07370
RETURN	SIG07380
ENTRY MAXDE	SIG07390
C	SIG07400
C ENTRY POINT TO DEFINE MAXIMUM ALLOWABLE ENERGY SPACING.	SIG07410
C	SIG07420
CON=2.0*SQRT(1.0/3.0)/3.0	SIG07430
T=1.2	SIG07440
DT=0.1	SIG07450
ERUSE=ERTHIN	SIG07460
IF(ERTHIN.LT.0.001) ERUSE=0.001	SIG07470
180 T=T-DT	SIG07480
BOTTOM=T*T+T	SIG07490
TOP=BOTTOM+1.0	SIG07500
ERS=ABS(1.0-CON*TOP*SQRT(TOP)/BOTTOM)	SIG07510
IF(ERS-ERUSE) 190,200,180	SIG07520
190 IF(DT.LT.1.0E-06) GO TO 200	SIG07530
T=T+DT	SIG07540
DT=0.1*DT	SIG07550
GO TO 180	SIG07560
200 DEMAX=T*T	SIG07570
RETURN	SIG07580
5020 FORMAT(2E11.4,49X,11)	SIG07590
END	SIG07600
SUBROUTINE BROADN	SIG07610
C	SIG07620
C GIVEN A CROSS SECTION THAT IS DESCRIBED BY A TABLE OF	SIG07630
C X/S VS. X AND LINEAR-LINEAR INTERPOLATION BETWEEN POINTS	SIG07640
C THIS ROUTINE WILL EXACTLY DOPPLER BROADENING THE CROSS	SIG07650
C SECTION AT A PORTION OF THE ENERGIES CORRESPONDING TO THE	SIG07660
C ORIGINAL CROSS SECTION (APPROXIMATELY THE MIDDLE THIRD).	SIG07670
C	SIG07680
C INPUT PARAMETERS	SIG07690
C KLOW =INDEX TO FIRST POINT LOADED IN CORE.	SIG07700
C KHIGH =INDEX TO LAST POINT LOADED IN CORE.	SIG07710
C NLOW =INDEX TO FIRST POINT TO BROADEN.	SIG07720
C NHIGH =INDEX TO LAST POINT TO BROADEN.	SIG07730
C MLOW =INDEX TO FIRST POINT JUST LOADED.	SIG07740
C MHIGH =INDEX TO LAST POINT JUST LOADED.	SIG07750
C X =TABLE OF ENERGIES CORRESPONDING TO S.	SIG07760
C S =TABLE OF CROSS SECTIONS AT INITIAL TEMPERATURE.	SIG07770
C CK =SCRATCH ARRAY TO USE FOR SLOPE BETWEEN POINTS IN (X,S).	SIG07780
C EB =TABLE OF ENRGIES CORRESPONDING TO SB.	SIG07790
C SB =TABLE OF CROSS SECTIONS BROADENED TO TEMPK.	SIG07800

C	ALPHA =DOPPLER WIDTH ((1505.3*AWR/TEMPK)	SIG07810
C		SIG07820
C	THE POINTS JUST LOADED (MLOW,MHIGH) ARE CONVERTED TO SPEED	SIG07830
C	LIKE TERMS AND SLOPES BETWEEN POINTS COMPUTED. THE TABLE OF	SIG07840
C	POINTS (KLOW,KHIGH) IS USED TO BROADEN THE RESULT TABLE	SIG07850
C	(NLOW,NHIGH).	SIG07860
C		SIG07870
C	THE CORE TABLES MAY BE CONSIDERED TO BE COMPOSED OF PAGES OF	SIG07880
C	1002 POINTS EACH. THREE PAGES ARE USED FOR THE DATA AT THE	SIG07890
C	ORIGINAL TEMPERATURE (X,S,CK) (9018 WORDS) AND ONE PAGE	SIG07900
C	IS USED FOR THE BROADENED CROSS SECTION (SB).	SIG07910
C		SIG07920
C	DURING ONE PASS OF THIS ROUTINE A PAGE OF DOPPLER BROADENED	SIG07930
C	CROSS SECTIONS WILL BE CREATED AT THE ENERGIES CORRESPONDING	SIG07940
C	TO THOSE IN THE MIDDLE PAGE OF THE DATA AT THE ORIGINAL	SIG07950
C	TEMPERATURE.	SIG07960
C		SIG07970
C	ONCE THE BROADENED DATA ARE CREATED THE DATA AT THE	SIG07980
C	ORIGINAL TEMPERATURE IN THE FIRST PAGE IS NO LONGER NEEDED	SIG07990
C	AND THE ENERGIES CORRESPONDING TO THE BROADENED CROSS	SIG08000
C	SECTIONS ARE STORED IN THE FIRST PAGE OF (CK) FOR LATER	SIG08010
C	THINNING IN ROUTINE THINB.	SIG08020
C		SIG08030
C	IN ORDER TO ALLOW THE SAME INDICES TO BE USED FOR BOTH	SIG08040
C	THE ORIGINAL AND BROADENED DATA TWO DUMMY ARRAYS (EB,SB)	SIG08050
C	ARE DEFINED ONE PAGE IN FRONT OF THE LOCATIONS THAT WILL	SIG08060
C	BE USED TO STORE THE BROADENED DATA.	SIG08070
C		SIG08080
C	COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,	SIG08090
C	I NOWI,N2MADE,NOWO,N2LEFT,NPAGE,JJLOW,ILOW	SIG08100
C	COMMON/HEAD1/ZAENDL,YIENDL,YOENDL,ATWT,DATE,FLAG,ELEVEL,HALFLIFE	SIG08110
C	I,TEMPIN,TMPOUT,FLAG72	SIG08120
C	COMMON/HEAD2/CENDL,IENDL,SENDL,QENDL,XIENDL(4)	SIG08130
C	COMMON/WEIGHT/AWR	SIG08140
C	COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT	SIG08150
C	COMMON/HOTS/ALPHA,TEMPK,ERTHIN,NTOTI,NTOTO	SIG08160
C	COMMON/JERZY/STEPS(100),TMPMEV(100),NTEMP,ITEMP	SIG08170
C	COMMON/ERFEXP/EXPERF	SIG08180
C	COMMON/CONTAC/OVP1,OVP12,ATOP	SIG08190
C	COMMON/INDICE/KNOW,LNOW,KLP1,KHMI	SIG08200
C	COMMON/EXTEND/MESS1,MEXT,DTMAX	SIG08210
C	COMMON X(3006),S(3006),EOUT(255),CK(3006),SOUT(255),SBREAL(1002),	SIG08220
C	I EIN(255),SIN(255)	SIG08230
C	DIMENSION EB(2004),SB(2004)	SIG08240
C	EQUIVALENCE (S(2260),EB),(CK(2260),SB)	SIG08250
C		SIG08260
C	CONVERT FROM ENERGY TO SPEED AND DEFINE SLOPES BETWEEN POINTS.	SIG08270
C		SIG08280
C	C-----CONVERT ENERGIES TO SPEED LIKE TERMS.	SIG08290
C	DO 10 N=MLOW,MHIGH	SIG08300
C	10 X(N)=SQRT(ALPHA*X(N))	SIG08310
C	C-----DEFINE THE NUMBER OF INTERVALS AND COMPUTE SLOPE IN	SIG08320
C	C-----EACH INTERVAL.	SIG08330
C	KLP1=KLOW+1	SIG08340
C	KHMI=KHIGH-1	SIG08350
C	ML=MLOW	SIG08360
C	IF (ML.GT.KLOW) ML=ML-1	SIG08370
C	MHMI=MHIGH-1	SIG08380
C	XXLAST=X(ML)**2	SIG08390
C	DO 30 KNGW=ML,MHMI	SIG08400

XXNOW=X(KNOW+1)**2	SIG08410
DX=XXNOW-XXLAST	SIG08420
IF(DX.LE.0.0) GO TO 20	SIG08430
CK(KNOW)=(S(KNOW+1)-S(KNOW))/DX	SIG08440
GO TO 30	SIG08450
20 CK(KNOW)=0.0	SIG08460
30 XXLAST=XXNOW	SIG08470
C	SIG08480
C TEST FOR CROSS SECTION EXTENSION	SIG08490
C	SIG08500
C-----TEST LOWER LIMIT FOR ALL PAGES BEYOND SECOND.	SIG08510
MEXT=MEXT+1	SIG08520
IF(MEXT.LE.3) GO TO 40	SIG08530
DX=X(1003)-X(1)	SIG08540
IF(DX.LE.ATOP) GO TO 50	SIG08550
C-----TEST UPPER LIMIT FOR ALL PAGES BUT LAST ONE.	SIG08560
40 IF(N2LEFT.LE.0) GO TO 60	SIG08570
DX=X(3006)-X(2004)	SIG08580
IF(DX.GT.ATOP) GO TO 60	SIG08590
C-----DEFINE MAXIMUM ALLOWABLE TEMPERATURE CHANGE TO AVOID	SIG08600
C-----CROSS SECTION EXTENSION.	SIG08610
50 DX=DX/ATOP	SIG08620
DTMAX2=TEMPK*DX*DX	SIG08630
IF(DTMAX.LE.0.0.OR.DTMAX2.LT.DTMAX) DTMAX=DTMAX2	SIG08640
C-----SET FLAG TO PRINT OUT MESSAGE WITH SECTION	SIG08650
MESS1=2	SIG08660
C	SIG08670
C BROADEN DATA. SPECIAL TREATMENT FOR LOW ENERGY.	SIG08680
C	SIG08690
60 KNOW=NLOW	SIG08700
IF(X(NLOW).GT.ATOP) GO TO 70	SIG08710
CALL BROADL	SIG08720
IF(KNOW.GT.NHIGH) RETURN	SIG08730
70 CALL BROADH	SIG08740
RETURN	SIG08750
END	SIG08760
SUBROUTINE BROADL	SIG08770
C	SIG08780
C LOW ENERGY DOPPLER BROADENING ROUTINE. THIS ROUTINE WILL	SIG08790
C BE USED TO DOPPLER BROADEN ALL CROSS SECTIONS AT ENERGIES	SIG08800
C WHERE AE/KT IS LESS THAN OR EQUAL TO 16. ANY POINT WITH A	SIG08810
C HIGHER ENERGY WILL BE PASSED ON TO ROUTINE BROADH.	SIG08820
C	SIG08830
C THE ROUTINE HAS BEEN DESIGNED WITH NO SUBROUTINE CALLS	SIG08840
C IN ORDER TO MINIMIZE RUNNING TIME. THE ARITHMETIC	SIG08850
C STATEMENT FUNCTIONS RATION(A) AND ERFC(R,EXPERF) WILL	SIG08860
C BE COMPILED AS IN LINE CODING BY VIRTUALLY ANY FORTRAN	SIG08870
C COMPILER, AND AS SUCH DO NOT REPRESENT FUNCTION CALLS.	SIG08880
C	SIG08890
C COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,	SIG08900
1 NOW1,N2MADE,NOW0,N2LEFT,NPAGE,JJLOW,ILOW	SIG08910
COMMON/HEAD1/ZAENDL,YIENDL,YOENDL,ATWT,DATE,FLAG,ELEVEL,HALFLIFE	SIG08920
1,TEMPIN,TEMPOUT,FLAG72	SIG08930
COMMON/HEAD2/CENDL,IENDL,SENDL,QENDL,XIENDL(4)	SIG08940
COMMON/WEIGHT/AWR	SIG08950
COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT	SIG08960
COMMON/HOTS/ALPHA,TEMPK,ERTHIN,NTOTI,NTOTO	SIG08970
COMMON/JERZY/STEPS(100),THPMEV(100),NTEMP,ITEMP	SIG08980
COMMON/ERFEXP/EXPERF	SIG08990
COMMON/CONTAC/OVPI,OVPI2,ATOP	SIG09000

COMMON/INDICE/KNOW,LOW,KLP1,KHM1	SIG09010
COMMON X(3006),S(3006),EOUT(255),CK(3006),SOUT(255),SBREAL(1002),	SIG09020
1 EIN(255),SIN(255)	SIG09030
DIMENSION EB(2004),SB(2004)	SIG09040
EQUIVALENCE (S(2260),EB),(CK(2260),SR)	SIG09050
C	SIG09060
C COMPLEMENTARY ERROR FUNCTION DEFINITION.	SIG09070
C	SIG09080
C-----DEFINE CONSTANTS FOR COMPLEMENTARY ERROR FUNCTION	SIG09090
DATA A1,A2,A3,A4,A5/0.254829592,-0.284496736,1.421413741,	SIG09100
1 -1.453152027,1.061405429/	SIG09110
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR RATIONAL ARGUMENT	SIG09120
C-----OF COMPLEMENTARY ERROR FUNCTION.	SIG09130
RATION(A)=1./((1.+0.3275911*A)	SIG09140
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR COMPLEMENTARY	SIG09150
C-----STATEMENT FUNCTION.	SIG09160
ERFC(R,EXPERF)=((((A5*R+A4)*R+A3)*R+A2)*R+A1)*R*EXPERF	SIG09170
C	SIG09180
C SET UP LOOP TO DOPPLER BROADEN CROSS SECTIONS.	SIG09190
C	SIG09200
DO 150 KNOW=LOW,NHIGH	SIG09210
C-----INITIALIZE INTEGRAL AND CONSTANTS.	SIG09220
Y=X(KNOW)	SIG09230
IF(Y.GT.ATOP) RETURN	SIG09240
C-----INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES.	SIG09250
C-----DEFINE ALL REQUIRED CONSTANTS FOR POINT.	SIG09260
Y2=2.0*Y	SIG09270
YY=Y*Y	SIG09280
YYA=0.5*YY	SIG09290
C-----INITIALIZE INTEGRALS.	SIG09300
DUMMY1=0.0	SIG09310
IF(Y2.LE.ATOP) GO TO 10	SIG09320
ERFCY2=0.0	SIG09330
F2B=YYA+OVPI2*Y	SIG09340
GO TO 20	SIG09350
0 R=RATION(Y2)	SIG09360
EXPERF=EXP(-Y2*Y2)	SIG09370
ERFCY2=ERFC(R,EXPERF)	SIG09380
F2B=YYA*(1.0-ERFCY2)+OVPI2*Y	SIG09390
C*	SIG09400
C* INTEGRATE OVER ALL ENERGY INTERVALS ABOVE THE CURRENT ENERGY	SIG09410
C* POINT.	SIG09420
C*	SIG09430
C-----NO INTERVALS ABOVE THE LAST POINT.	SIG09440
20 IF(KNOW.EQ.KHIGH) GO TO 70	SIG09450
C-----SET UP LOOP OVER INTERVALS ABOVE CURRENT ONE.	SIG09460
DO 60 LNOW=KNOW,KHM1	SIG09470
B=X(LNOW+1)	SIG09480
C-----TEST FOR END OF RANGE OF INTEGRATION.	SIG09490
BMY=B-Y	SIG09500
IF(BMY.LE.ATOP) GO TO 30	SIG09510
C-----EXTEND INTEGRAL FROM CURRENT POINT TO INFINITY.	SIG09520
DUMMY1=DUMMY1+0.5*(S(LNOW+1)+S(LNOW))*F2B	SIG09530
GO TO 80	SIG09540
C-----SAVE VALUES FROM LAST INTERGAL.	SIG09550
30 F2A=F2B	SIG09560
RBMY=RATION(BMY)	SIG09570
EXBMY=EXP(-BMY*BMY)	SIG09580
C-----TEST FOR END OF RANGE OF INTEGRATION OF SECOND INTEGRAL.	SIG09590
BPY=B+Y	SIG09600

RBPY=RATION(BPY)	SIG09610
IF(BPY.LE.ATOP) GO TO 40	SIG09620
EXBPY=0.0	SIG09630
GO TO 50	SIG09640
40 FXBPY=EXP(-BPY*BPY)	SIG09650
50 F2B=YYA*(ERFC(RBMY,EXBMY)-ERFC(RBPY,EXBPY))+	SIG09660
1 OVPI*(B*(EXBMY-EXBPY)+Y*(EXBMY+EXBPY))	SIG09670
60 DUMMY1=DUMMY1+0.5*(S(LNOW+1)+S(LNOW))*(F2A-F2B)	SIG09680
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=INFINITY.	SIG09690
70 DUMMY1=DUMMY1+S(KHIGH)*F2B	SIG09700
C-----RE-INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES	SIG09710
80 F2A=-YYA*(1.0+ERFCY2)+OVPI2*Y	SIG09720
C*	SIG09730
C* INTEGRATE OVER ALL ENERGY INTERVALS BELOW THE CURRENT ENERGY	SIG09740
C* POINT.	SIG09750
C*	SIG09760
C-----NO INTERVALS BELOW FIRST POINT.	SIG09770
IF(KNOW.EQ.KLOW) GO TO 130	SIG09780
C-----SET UP LOOP OVER INTERVALS BELOW CURRENT POINT.	SIG09790
LNOW=KNOW	SIG09800
DO 120 LL=KLP1,KNOW	SIG09810
LNOW=LNOW-1	SIG09820
A=X(LNOW)	SIG09830
C-----TEST FOR END OF RANGE OF INTEGRATION.	SIG09840
YMA=Y-A	SIG09850
IF(YMA.LE.ATOP) GO TO 90	SIG09860
C-----DEFINE REMAINING INTEGRAL AS ZERO.	SIG09870
DUMMY1=DUMMY1-0.5*(S(LNOW+1)+S(LNOW))*F2A	SIG09880
GO TO 150	SIG09890
C-----SAVE VALUES FROM LAST INTEGRAL.	SIG09900
90 F2B=F2A	SIG09910
C-----DEFINE EXPONENTIAL FOR FIRST INTEGRAL.	SIG09920
RYMA=RATION(YMA)	SIG09930
EXYMA=EXP(-YMA*YMA)	SIG09940
C --- DEFINE CONTRIBUTION FROM SECOND INTEGRAL.	SIG09950
YPA=Y+A	SIG09960
RYPY=RATION(YPA)	SIG09970
IF(YPA.LE.ATOP) GO TO 100	SIG09980
EXYPA=0.0	SIG09990
GO TO 110	SIG10000
100 EXYPA=EXP(-YPA*YPA)	SIG10010
C-----ADD CONTRIBUTION FROM CURRENT INTERVAL.	SIG10020
110 F2A=-YYA*(ERFC(RYMA,EXYMA)+ERFC(RYPY,EXYPA))+	SIG10030
1 OVPI*(A*(EXYMA-EXYPA)+Y*(EXYMA+EXYPA))	SIG10040
120 DUMMY1=DUMMY1+0.5*(S(LNOW+1)+S(LNOW))*(F2A-F2B)	SIG10050
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=0.0	SIG10060
130 IF(Y.LE.ATOP) GO TO 140	SIG10070
DUMMY1=DUMMY1-S(KLOW)*F2A	SIG10080
GO TO 150	SIG10090
140 R=RATION(Y)	SIG10100
EXPERF=EXP(-YY)	SIG10110
DUMMY1=DUMMY1+S(KLOW)*((-YYA*2.0*ERFC(R,EXPERF)	SIG10120
1 +OVPI2*Y*EXPERF)-F2A)	SIG10130
C-----DEFINE BROADENED CROSS SECTION.	SIG10140
150 SB(KNOW)=0.5*DUMMY1/YY	SIG10150
C-----CONVERT SPEED LIKE TERMS BACK TO ENERGY.	SIG10160
DO 160 N=NLOW,NHIGH	SIG10170
160 EB(N)=X(N)**2/ALPHA	SIG10180
KNOW=NHIGH+1	SIG10190
RETURN	SIG10200

COMMON/INDICE/KNOW,NLOW,KLP1,KHM1	SIG09010
COMMON X(3006),S(3006),EOUT(255),CK(3006),SCUT(255),SBREAL(1002),	SIG09020
I EIN(255),SIN(255)	SIG09030
DIMENSION EB(2004),SB(2004)	SIG09040
EQUIVALENCE (S(2260),EB),(CK(2260),SR)	SIG09050
C	SIG09060
C COMPLEMENTARY ERROR FUNCTION DEFINITION.	SIG09070
C	SIG09080
C-----DEFINE CONSTANTS FOR COMPLEMENTARY ERROR FUNCTION	SIG09090
DATA A1,A2,A3,A4,A5/0.254829592,-0.284496736,1.421413741,	SIG09100
I -1.453152027,1.061405429/	SIG09110
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR RATIONAL ARGUMENT	SIG09120
C-----OF COMPLEMENTARY ERROR FUNCTION.	SIG09130
RATION(A)=1./((1.+0.3275911*A)	SIG09140
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR COMPLEMENTARY	SIG09150
C-----STATEMENT FUNCTION.	SIG09160
ERFC(R,EXPERF)=((((A5*R+A4)*R+A3)*R+A2)*R+A1)*R*EXPERF	SIG09170
C	SIG09180
C SET UP LOOP TO DOPPLER BROADEN CROSS SECTIONS.	SIG09190
C	SIG09200
DO 150 KNOW=NLOW,NHIGH	SIG09210
C-----INITIALIZE INTEGRAL AND CONSTANTS.	SIG09220
Y=X(KNOW)	SIG09230
IF(Y.GT.ATOP) RETURN	SIG09240
C-----INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES.	SIG09250
C-----DEFINE ALL REQUIRED CONSTANTS FOR POINT.	SIG09260
Y2=2.0*Y	SIG09270
YY=Y*Y	SIG09280
YYA=0.5+YY	SIG09290
C-----INITIALIZE INTEGRALS.	SIG09300
DUMMY1=0.0	SIG09310
IF(Y2.LE.ATOP) GO TO 10	SIG09320
ERFCY2=0.0	SIG09330
F2B=YYA+OVPI2*Y	SIG09340
GO TO 20	SIG09350
0 R=RATION(Y2)	SIG09360
EXPERF=EXP(-Y2*Y2)	SIG09370
ERFCY2=ERFC(R,EXPERF)	SIG09380
F2B=YYA*(1.0-ERFCY2)+OVPI2*Y	SIG09390
C*	SIG09400
C* INTEGRATE OVER ALL ENERGY INTERVALS ABOVE THE CURRENT ENERGY	SIG09410
C* POINT.	SIG09420
C*	SIG09430
C-----NO INTERVALS ABOVE THE LAST POINT.	SIG09440
20 IF(KNOW.EQ.KHIGH) GO TO 70	SIG09450
C-----SET UP LOOP OVER INTERVALS ABOVE CURRENT ONE.	SIG09460
DO 60 LNOW=KNOW,KHM1	SIG09470
B=X(LNOW+1)	SIG09480
C-----TEST FOR END OF RANGE OF INTEGRATION.	SIG09490
BMY=B-Y	SIG09500
IF(BMY.LE.ATOP) GO TO 30	SIG09510
C-----EXTEND INTEGRAL FROM CURRENT POINT TO INFINITY.	SIG09520
DUMMY1=DUMMY1+0.5*(S(LNOW+1)+S(LNOW))*F2B	SIG09530
GO TO 80	SIG09540
C-----SAVE VALUES FROM LAST INTERGAL.	SIG09550
30 F2A=F2B	SIG09560
RBMY=RATION(BMY)	SIG09570
EXBMY=EXP(-BMY*BMY)	SIG09580
C-----TEST FOR END OF RANGE OF INTEGRATION OF SECOND INTEGRAL.	SIG09590
BPY=B+Y	SIG09600

RBPY=RATION(BPY)	SIG09610
IF(BPY.LE.ATOP) GO TO 40	SIG09620
EXBPY=0.0	SIG09630
GO TO 50	SIG09640
40 FXBPY=EXP(-BPY*BPY)	SIG09650
50 F2B=YYA*(ERFC(RBMY,EXBMY)-ERFC(RBPY,EXBPY))+	SIG09660
1 OVPI*(B*(EXBMY-EXBPY)+Y*(EXBMY+EXBPY))	SIG09670
60 DUMMY1=DUMMY1+0.5*(S(LNOW+1)+S(LNOW))*(F2A-F2B)	SIG09680
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=INFINITY.	SIG09690
70 DUMMY1=DUMMY1+S(KHIGH)*F2B	SIG09700
C-----RE-INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES	SIG09710
80 F2A=-YYA*(1.0+ERFCY2)+OVPI2*Y	SIG09720
C*	SIG09730
C* INTEGRATE OVER ALL ENERGY INTERVALS BELOW THE CURRENT ENERGY	SIG09740
C* POINT.	SIG09750
C*	SIG09760
C-----NO INTERVALS BELOW FIRST POINT.	SIG09770
IF(KNOW.EQ.KLOW) GO TO 130	SIG09780
C-----SET UP LOOP OVER INTERVALS BELOW CURRENT POINT.	SIG09790
LNOW=KNOW	SIG09800
DO 120 LL=KLPI,KNOW	SIG09810
LNOW=LNOW-I	SIG09820
A=X(LNOW)	SIG09830
C-----TEST FOR END OF RANGE OF INTEGRATION.	SIG09840
YMA=Y-A	SIG09850
IF(YMA.LE.ATOP) GO TO 90	SIG09860
C-----DEFINE REMAINING INTEGRAL AS ZERO.	SIG09870
DUMMY1=DUMMY1-0.5*(S(LNOW+1)+S(LNOW))*F2A	SIG09880
GO TO 150	SIG09890
C-----SAVE VALUES FROM LAST INTEGRAL.	SIG09900
90 F2B=F2A	SIG09910
C-----DEFINE EXPONENTIAL FOR FIRST INTEGRAL.	SIG09920
RYMA=RATION(YMA)	SIG09930
EXYMA=EXP(-YMA*YMA)	SIG09940
C-----DEFINE CONTRIBUTION FROM SECOND INTEGRAL.	SIG09950
YPA=Y+A	SIG09960
RYPY=RATION(YPA)	SIG09970
IF(YPA.LE.ATOP) GO TO 100	SIG09980
EXYPA=0.0	SIG09990
GO TO 110	SIG10000
100 EXYPA=EXP(-YPA*YPA)	SIG10010
C-----ADD CONTRIBUTION FROM CURRENT INTERVAL.	SIG10020
110 F2A=-YYA*(ERFC(RYMA,EXYMA)+ERFC(RYPY,EXYPA))+	SIG10030
1 OVPI*(A*(EXYMA-EXYPA)+Y*(EXYMA+EXYPA))	SIG10040
120 DUMMY1=DUMMY1+0.5*(S(LNOW+1)+S(LNOW))*(F2A-F2B)	SIG10050
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=0.0	SIG10060
130 IF(Y.LE.ATOP) GO TO 140	SIG10070
DUMMY1=DUMMY1-S(KLOW)*F2A	SIG10080
GO TO 150	SIG10090
140 R=RATION(Y)	SIG10100
EXPERF=EXP(-YY)	SIG10110
DUMMY1=DUMMY1+S(KLOW)*((-YYA*2.0*ERFC(R,EXPERF)	SIG10120
1 +OVPI2*Y*EXPERF)-F2A)	SIG10130
C-----DEFINE BROADENED CROSS SECTION.	SIG10140
150 SB(KNOW)=0.5*DUMMY1/YY	SIG10150
C-----CONVERT SPEED LIKE TERMS BACK TO ENERGY.	SIG10160
DO 160 N=NLON,NHIGH	SIG10170
160 EB(N)=X(N)**2/ALPHA	SIG10180
KNOW=NHIGH+1	SIG10190
RETURN	SIG10200

END	SIG10210
SUBROUTINE BROADH	SIG10220
C	SIG10230
C HIGH ENERGY DOPPLER BROADENING ROUTINE. THIS ROUTINE WILL	SIG10240
C BE USED TO DOPPLER BROADEN ALL CROSS SECTIONS AT ENERGIES	SIG10250
C WHERE AE/KT IS GRATER THAN 16. ANY POINT WITH A LOWER	SIG10260
C ENERGY WILL ALREADY HAVE BEEN DOPPLER BROADENED BY	SIG10270
C ROUTINE BROADL.	SIG10280
C	SIG10290
C THE ROUTINE HAS BEEN DESIGNED WITH NO SUBROUTINE CALLS	SIG10300
C IN ORDER TO MINIMIZE RUNNING TIME. THE ARITHMETIC	SIG10310
C STATEMENT FUNCTIONS RATION(A) AND ERFC(R,EXPERF) WILL	SIG10320
C BE COMPILED AS IN LINE CODING BY VIRTUALLY ANY FORTRAN	SIG10330
C COMPILER, AND AS SUCH DO NOT REPRESENT FUNCTION CALLS.	SIG10340
C	SIG10350
COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,	SIG10360
I NOW1,N2MADE,NOWO,N2LEFT,NPAGE,JJLOW,ILOW	SIG10370
COMMON/HEAD1/ZAENDL,YIENDL,YOENDL,ATWT,DATE,FLAG,ELEVEL,HALFLIFE	SIG10380
I,TEMPIN,IMPOUT,FLAG72	SIG10390
COMMON/HEAD2/CENDL,IENDL,SENDL,QENDL,XIENDL(4)	SIG10400
COMMON/WEIGHT/AWR	SIG10410
COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT	SIG10420
COMMON/HOTS/ALPHA,TEMPK,ERTHIN,NTOTI,NTOTO	SIG10430
COMMON/JERZY/STEPS(100),TMPMEV(100),NTEMP,ITEMP	SIG10440
COMMON/ERFEXP/EXPERF	SIG10450
COMMON/CONTAC/OVP1,OVP12,ATOP	SIG10460
COMMON/INDICE/KNOW,LNOW,KLP1,KHM1	SIG10470
COMMON X(3006),S(3006),ECUT(255),CK(3006),SOUT(255),SBREAL(1002),	SIG10480
I E1N(255),S1N(255)	SIG10490
DIMENSION EB(2004),SB(2004)	SIG10500
EQUIVALENCE (S(2260),EB),(CK(2260),SB)	SIG10510
C	SIG10520
C COMPLEMENTARY ERROR FUNCTION DEFINITION.	SIG10530
C	SIG10540
C- ---DEFINE CONSTANTS FOR COMPLEMENTARY ERROR FUNCTION	SIG10550
DATA A1,A2,A3,A4,A5/0.254829592,-0.284496736,1.421413741,	SIG10560
1 -1.453152027,1.061405429/	SIG10570
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR RATIONAL ARGUMENT	SIG10580
C-----OF COMPLEMENTARY ERROR FUNCTION.	SIG10590
RATION(A)=1./((1.+0.327591)*A)	SIG10600
C-----DEFINE ARITHMETIC STATEMENT FUNCTION FOR COMPLEMENTARY	SIG10610
C-----STATEMENT FUNCTION.	SIG10620
ERFC(R,EXPERF)=((1+((A5*R+A4)*R+A3)*R+A2)*R+A1)*R*EXPERF	SIG10630
C	SIG10640
C SET UP LOOP TO DOPPLER BROADEN CROSS SECTIONS.	SIG10650
C	SIG10660
NNLOW=KNOW	SIG10670
DO 90 KNOW=NNLOW,NHIGH	SIG10680
C-----INITIALIZE INTEGRAL AND CONSTANTS.	SIG10690
Y=X(KNOW)	SIG10700
C-----INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES.	SIG10710
C-----DEFINE ALL REQUIRED CONSTANTS FOR POINT.	SIG10720
YY=Y*Y	SIG10730
BB=YY	SIG10740
YYA=0.5+YY	SIG10750
YYB=YY*(YY+3.0)+0.75	SIG10760
YYC=2.0*(YY+1.0)	SIG10770
YYD=YY+1.5	SIG10780
C-----INITIALIZE INTEGRALS.	SIG10790
DUMMY1=0.5	SIG10800

DUMMY2=0.0	SIG10810
F2B=YYA*OVPI2*Y	SIG10820
F4B=YYB*OVPI2*Y*YYC	SIG10830
C*	SIG10840
C* INTEGRATE OVER ALL ENERGY INTERVALS ABOVE THE CURRENT ENERGY	SIG10850
C* POINT.	SIG10860
C*	SIG10870
C-----NO INTERVALS ABOVE THE LAST POINT.	SIG10880
IF(KNOW.EQ.KHIGH) GO TO 30	SIG10890
C-----SET UP LOOP OVER INTERVALS ABOVE CURRENT ONE.	SIG10900
DO 20 LNOW=KNOW,KHIGH	SIG10910
B=X(LNOW+1)	SIG10920
BMY=B-Y	SIG10930
IF(BMY.LE.ATOP) GO TO 10	SIG10940
DUMMY1=DUMMY1+S(LNOW)*F2B	SIG10950
DUMMY2=DUMMY2+CK(LNOW)*(F4B-BB*F2B)	SIG10960
GO TO 40	SIG10970
C-----SAVE VALUES FROM LAST INTERVAL	SIG10980
10 F2A=F2B	SIG10990
F4A=F4B	SIG11000
C-----DEFINE CONSTANTS FOR THIS POINT.	SIG11010
AA=BB	SIG11020
BB=B*B	SIG11030
BPY=B*Y	SIG11040
R=RAT10N(BMY)	SIG11050
EXPERF=EXP(-BMY*BMY)	SIG11060
S0=ERFC(R,EXPERF)	SIG11070
F2B=YYA*S0+OVPI*BPY*EXPERF	SIG11080
F4B=YYB*S0+OVPI*(BPY*(BB+YYD)+Y)*EXPERF	SIG11090
S1=F2A-F2B	SIG11100
DUMMY1=DUMMY1+S(LNOW)*S1	SIG11110
20 DUMMY2=DUMMY2+CK(LNOW)*((F4A-F4B)-AA*S1)	SIG11120
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=INFINITY.	SIG11130
30 DUMMY1=DUMMY1+S(KHIGH)*F2B	SIG11140
C---RE-INITIALIZE INTEGRALS TO ZERO DISTANCE VALUES	SIG11150
0 AA=YY	SIG11160
F2A=-YYA+OVPI2*Y	SIG11170
F4A=-YYB+OVPI2*Y*YYC	SIG11180
C*	SIG11190
C* INTEGRATE OVER ALL ENERGY INTERVALS BELOW THE CURRENT ENERGY	SIG11200
C* POINT.	SIG11210
C*	SIG11220
C-----NO INTERVALS BELOW CURRENT FIRST POINT.	SIG11230
IF(KNOW.EQ.KLOW) GO TO 70	SIG11240
C-----SET UP LOOP OVER INTERVALS BELOW CURRENT POINT.	SIG11250
LNOW=KNOW	SIG11260
DO 60 LL=KLPI,KNOW	SIG11270
LNOW=LNOW-1	SIG11280
A=X(LNOW)	SIG11290
YMA=Y-A	SIG11300
IF(YMA.LE.ATOP) GO TO 50	SIG11310
DUMMY1=DUMMY1-S(LNOW+1)*F2A	SIG11320
DUMMY2=DUMMY2-CK(LNOW)*(F4A-AA*F2A)	SIG11330
GO TO 90	SIG11340
C-----SAVE VALUES FROM LAST INTEGRAL.	SIG11350
50 F2B=F2A	SIG11360
F4B=F4A	SIG11370
C-----DEFINE CONSTANTS FOR THIS POINT.	SIG11380
BB=AA	SIG11390
AA=A*A	SIG11400

YPA=Y+A	SIG11410
R=RATION(YMA)	SIG11420
EXPERF=EXP(-YMA*YMA)	SIG11430
S0=-ERFC(R,EXPERF)	SIG11440
F4A=YYB*S0*OVPI*(YPA*(AA+YYD)+Y)*EXPERF	SIG11450
S1=F2A-F2B	SIG11460
DUMMY1=DUMMY1+S(LNOW+1)*S1	SIG11470
60 DUMMY2=DUMMY2+CK(LNOW)*((F4A-F4B)-BB*S1)	SIG11480
C-----CONTINUE CROSS SECTION AS CONSTANT TO X=0.0	SIG11490
70 IF(Y.LE.ATOP) GO TO 80	SIG11500
DUMMY1=DUMMY1-S(KLOW)*F2A	SIG11510
GO TO 90	SIG11520
80 R=RATION(Y)	SIG11530
EXPERF=EXP(-YY)	SIG11540
DUMMY1=DUMMY1+S(KLOW)*((-YYA*ERFC(R,EXPERF)	SIG11550
1 +OVPI*Y*EXPERF)-F2A)	SIG11560
C-----DEFINE BROADENED CROSS SECTION.	SIG11570
90 SB(KNOW)=0.5*(DUMMY1+DUMMY2)/YY	SIG11580
C-----CONVERT SPEED LIKE TERMS BACK TO ENERGY.	SIG11590
DO 100 N=NLOW,NHIGH	SIG11600
100 EB(N)=X(N)**2/ALPHA	SIG11610
RETURN	SIG11620
END	SIG11630
SUBROUTINE THINB	SIG11640
C	SIG11650
C	SIG11660
C GIVEN A FUNCTION REPRESENTED BY X AND S COORDINATES	SIG11670
C AND LINEAR-LINEAR INTERPOLATION BETWEEN POINTS, THIS	SIG11680
C ROUTINE WILL REMOVE ALL EXTRANEIOUS POINTS THAT LIE WITHIN A	SIG11690
C GIVEN ACCURACY OF THE FUNCTION BASED UPON INTERPOLATION	SIG11700
C FROM SURROUNDING POINTS.	SIG11710
C	SIG11720
C DURING ONE PASS THIS ROUTINE WILL THIN ANY UNCONVERGED POINTS	SIG11730
C FROM THE LAST BROADENED PAGE PLUS THE CURRENT BROADENED PAGE.	SIG11740
C AT THE END OF THE CURRENT PAGE THE LAST CONVERGED POINT AND ALL	SIG11750
C UNCONVERGED POINTS WILL BE LEFT IN THE CORE TO BE THINNED WITH	SIG11760
C THE NEXT PAGE (UNLESS THE END OF THE TABLE IS REACHED IN WHICH	SIG11770
C CASE THE LAST POINT IS CONVERGED).	SIG11780
C	SIG11790
C	SIG11800
COMMON/UNITS/OUTP,INP,ITAPE,OTAPE	SIG11810
COMMON/INDEX/JLOW,JHIGH,KLOW,KHIGH,MLOW,MHIGH,NLOW,NHIGH,	SIG11820
1 NCH,N2MADE,NCHD,N2LEFT,NPAGE,JJLOW,ILLOW	SIG11830
COMMON/LEADER/C1,C2,L1,L2,N1,N2,MAT,MF,MT	SIG11840
COMMON/HOTS/ALPHA,TEMPK,ERTHIN,NTOT1,NTOT0	SIG11850
COMMON/JERZY/STEPS(100),TMPMEV(100),NTEMP,ITEMP	SIG11860
COMMON X(3006),S(2259),XB(3006),YOUT(255),SB(2004),	SIG11870
1 EIN(255),SIN(255)	SIG11880
C-----IF ALLOWABLE ERROR IS NOT POSITIVE NO THINNING CAN BE	SIG11890
C-----PERFORMED ON THE TABLE.	SIG11900
IF(ERTHIN.LE.0.0) GO TO 10	SIG11910
C-----AT LEAST 3 POINTS REQUIRED FOR THINNING.	SIG11920
IF(NHIGH-NLOW.GE.2) GO TO 20	SIG11930
C-----SET THINNED INDICES EQUAL TO ORIGINAL INDICES AND RETURN.	SIG11940
10 JLOW=JJLOW	SIG11950
JHIGH=NHIGH	SIG11960
ILLOW=NHIGH+1	SIG11970
RETURN	SIG11980
C-----INITIALIZE THINNED INDICES TO AUTOMATICALLY ACCEPT FIRST POINT.	SIG11990
20 JLOW=JJLOW	SIG12000
JHIGH=JJLOW	

C-----INITIALIZE INDEX TO NEXT CANDIDATE FOR THINNING.	SIG12010
ILOW=JLOW+1	SIG12020
C-----SET UP LOOP OVER ALL OTHER POINTS.	SIG12030
NBOI=JLOW+2	SIG12040
DO 50 N=NBOI,NHIGH	SIG12050
C-----DEFINE INDEX TO LAST CANDIDATE FOR THINNING.	SIG12060
NM1=N-1	SIG12070
C-----DEFINE CHANGE IN ENERGY AND CHECK FOR THREE (OR MORE)	SIG12080
C-----SUCCESSIVE POINTS ALL WITH THE SAME ENERGY.	SIG12090
DXB=XB(N)-XB(JHIGH)	SIG12100
IF(DXB.LE.0.0) GO TO *0	SIG12110
C-----DEFINE SLOPE BETWEEN LAST ACCEPTED POINT AND END OF	SIG12120
C-----INTERVAL.	SIG12130
SLOPE=(SB(N)-SB(JHIGH))/DXB	SIG12140
C-----TEST ALLOWABLE ERROR AT ALL INTERVENING POINTS.	SIG12150
DO 30 K=ILOW,NM1	SIG12160
YP=SB(JHIGH)+SLOPE*(XB(K)-XB(JHIGH))	SIG12170
IF(ABS(YP-SB(K)).GT.ERTHIN*SB(K)) GO TO 50	SIG12180
30 CONTINUE	SIG12190
C-----ALL INTERVENING POINTS CAN BE THINNED. EXTEND INTERVAL TO	SIG12200
C-----THIN BY ONE MORE POINT.	SIG12210
GO TO 60	SIG12220
C-----THREE OR MORE POINTS ALL WITH THE SAME ENERGY. KEEP NEXT	SIG12230
C-----POINT IF NOT THE SAME CROSS SECTION AS LAST POINT.	SIG12240
40 IF(SB(JHIGH).EQ.SB(ILOW)) GO TO 60	SIG12250
C-----AT LEAST ONE POINT IN INTERVAL FAILS TEST. SAVE LAST POINT	SIG12260
C-----WITHIN THE INTERVAL.	SIG12270
50 JHIGH=JHIGH+1	SIG12280
XB(JHIGH)=XB(NM1)	SIG12290
SB(JHIGH)=SB(NM1)	SIG12300
C-----RESET LOWER LIMIT OF INTERVAL THAT CAN BE THINNED.	SIG12310
ILOW=N	SIG12320
60 CONTINUE	SIG12330
C-----IS THIS THE END OF THE ENTIRE TABLE (ALL POINTS BROADENED)....	SIG12340
IF(NHIGH.LT.KHIGH) GO TO 70	SIG12350
C- --YES. MOVE LAST POINT IN TABLE TO THINNED TABLE.	SIG12360
JHIGH=JHIGH+1	SIG12370
XB(JHIGH)=XB(NHIGH)	SIG12380
SB(JHIGH)=SB(NHIGH)	SIG12390
RETURN	SIG12400
C-----NO. DETERMINE NUMBER OF UNCONVERGED POINTS LEFT OVER FROM	SIG12410
C-----THINNING.	SIG12420
70 KLEFT=NHIGH-ILOW+1	SIG12430
C-----WILL REMAINING POINTS FIT INTO (XOUT,YOUT)	SIG12440
IF(KLEFT.LE.255) GO TO 80	SIG12450
C-----NO. THIN INTERMEDIATE POINTS BETWEEN ILOW AND NHIGH BY SIMPLY	SIG12460
C-----RESETTING LOWER THINNING INDEX.	SIG12470
ILOW=NHIGH	SIG12480
RETURN	SIG12490
C-----YES. SAVE LAST CONVERGED POINT IN CORE TO SERVE AS PIVOT FOR	SIG12500
C-----THINNING OF NEXT PAGE OF DATA.	SIG12510
80 ILOW=ILOW-1	SIG12520
JHIGH=JHIGH-1	SIG12530
RETURN	SIG12540
END	SIG12550
SUBROUTINE NORMAL(X,XNORM,KSIGN,KEXP)	SIG12560
C	SIG12570
C CONVERT FLOATING POINT NUMBER TO NORMAL FORM FOR OUTPUT.	SIG12580
C OUTPUT WILL BE IN THE FORM X.XXXXX+/-NN, WHICH GIVES	SIG12590
C AN ADDITIONAL DIGIT OF ACCURACY WHEN COMPARED TO E11.4	SIG12600

```

C      FORTRAN OUTPUT. IN ADDITION: THE
C      INDEPENDENT (I.E. SAME ON IBM,
C
C      INTEGER PLUS
C      ----DEFINE TWO POSSIBLE SIGNES F-
C      DATA PLUS/1H+/
C      DATA MINUS/1H-/
C      ----COMPUTE SIGNED EXPONENT FROM
C      XABS=ABS(X)
C      ----IF NUMBER IS 0.0 DEFINE 0.
C      IF(XABS) 50,50,10
C      ----DEFINE EXPONENT TO NORMALIZE
C      10 KEXP=ALOG10(XABS)
C      SHIFT=10.0**KEXP
C      XNORM=XABS/SHIFT
C      IF(XNORM.GE.0.999995) GO TO
C      KEXP=KEXP-1
C      SHIFT=SHIFT/10.0
C      GO TO 30
C      20 IF(XNORM.LT.9.999995) GO TO
C      KEXP=KEXP+1
C      SHIFT=10.0*SHIFT
C      ----COMPUTE SIGNED MANTISSA.
C      30 XNORM=X/SHIFT
C      ----DEFINE SIGN OF EXPONENT AND
C      IF(KEXP) 40,60,70
C      40 KSIGN=MINUS
C      KEXP= KEXP
C      RETURN
C      ----X IS 0.0. DEFINE AS 0.00000+
C      50 XNORM=0.0
C      60 KEXP=0
C      70 KSIGN=PLUS
C      RETURN
C      END
C      SUBROUTINE HEADOUT
C
C*      OUTPUT SECTION HEAD CARDS.
C
C*      INTEGER ZAENDL,YIENDL,YOENDL,CENDL,SEN
C      1,OF,FLAG
C      COMMON/UNITS/OUTP,INP,ITAPE,OTAPE
C      COMMON/CONVRT/MEV2EV,EV2MEV,MEV2K,BOLTZM
C      COMMON/NORMIT/XNORM(6),KSIGN(6),KEXP(6)
C      COMMON/HEAD1/ZAENDL,YIENDL,YOENDL,ATHT,DATE
C      1,TEMPIN,TMPOUT,FLAG72
C      COMMON/HEAD2/CENDL,IENDL,SENDL,QENDL,XIENDL(4)
C
C*      OUTPUT FIRST CARD OF A SECTION
C*
C*      CALL NORMAL(ATHT,XNORM(1),KSIGN(1),KEXP(1))
C*      CALL NORMAL(ELEVEL,XNORM(2),KSIGN(2),KEXP(2))
C*      CALL NORMAL(HALFLIFE,XNORM(3),KSIGN(3),KEXP(3))
C*      CALL NORMAL(TMPOUT,XNORM(4),KSIGN(4),KEXP(4))
C*      WRITE(OTAPE,5000) ZAENDL,YIENDL,YOENDL,XNORM(1),KSIGN(1),
C*      1 DATE,FLAG,(XNORM(1),KSIGN(1),KEXP(1),1=2,4)
C
C*      OUTPUT SECOND LINE OF SECTION
C*
C*      CALL NORMAL(QENDL,XNORM(1),KSIGN(1),KEXP(1))

```

DO 10 I=2,5	SIG13210
10 CALL NORMAL(XIENDL(I-1),XNORM(I),KSIGN(I),KEXP(I))	SIG13220
WRITE(OTAPE,5010) CENDL,IENDL,SENDL,(XNORM(I),KSIGN(I),KEXP(I))	SIG13230
I,I=1,5)	SIG13240
RETURN	SIG13250
5000 FORMAT(16,213,1X,F8.5,A1,12,17,13,3(1X,F8.5,A1,12))	SIG13260
5010 FORMAT(12,213,6(1X,F8.5,A1,12))	SIG13270
END	SIG13280
SUBROUTINE IONAME	SIG13290
C	SIG13300
C DEFINE ALL I/O UNITS AND DISK FILE NAMES.	SIG13310
C	SIG13320
INTEGER OUTP,OTAPE	SIG13330
COMMON/UNITS/OUTP,INP,ITAPE,OTAPE	SIG13340
COMMON/ITCH/IADR(2),ISCR(2),NSCR(100,2),IPAGE(2),IPGMAX(2),	SIG13350
I IBOOTS,IUSE,ISAVE	SIG13360
COMMON/HOTS/ALPHA,TEMPK,ERTHIN,NTOT),NTOTO	SIG13370
COMMON/JERZY/STEPS(100),TMPMEV(100),NTEMP,ITEMP	SIG13380
DATA LENS/500000/	SIG13390
DATA IERR/0/	SIG13400
IADR(1)=0	SIG13410
IADR(2)=0	SIG13420
INTO=OUTP	SIG13430
OUTP=59	SIG13440
CALL IOFILE(ITAPE,6HENDLIN,LEN,1,2,IERR)	SIG13450
LEN=3*LEN*NTEMP	SIG13460
IF (LEN.LT.100000) LEN=100000	SIG13470
IF (LEN.GT.2000000) LEN=2000000	SIG13480
CALL IOFILE(OTAPE,7HENDLOUT,LEN,2,2,IERR)	SIG13490
IF (NTEMP.LE.1) GO TO 10	SIG13500
CALL IOFILE(ISCR(1),7HSCR001,LENS,2,4,IERR)	SIG13510
IF (IBOOTS.LE.0) GO TO 10	SIG13520
CALL IOFILE(ISCR(2),7HSCR002,LENS,2,4,IERR)	SIG13530
IUSE=2	SIG13540
10 OUTP=INTO	SIG13550
RETURN	SIG13560
END	SIG13570
SUBROUTINE DROPIT(NAME)	SIG13580
C	SIG13590
C CREATE DROP FILE ON CDC-7600 OR CRAY-1. ON CRAY-1 ASSIGN TELETYPE.	SIG13600
C	SIG13610
C***** EXPORT *****	SIG13620
C RETURN	SIG13630
C***** EXPORT *****	SIG13640
C***** CDC-7600 *****	SIG13650
C CALL CHANGE(NAME)	SIG13660
C***** CDC-7600 *****	SIG13670
C***** CRAY-1 *****	SIG13680
CALL DROPFILE(0)	SIG13690
CALL MSGLINK(59,1)	SIG13700
C***** CRAY-1 *****	SIG13710
RETURN	SIG13720
END	SIG13730
SUBROUTINE IBLOCK(ISCR,IADR,X,IX)	SIG13740
C	SIG13750
C ALL I/O TO AND FROM SCRATCH IS HANDLED BY THIS ROUTINE.	SIG13760
C	SIG13770
INTEGER OUTP	SIG13780
COMMON/UNITS/TTY,OUTP,INP,ITAPE,OTAPE,SCR	SIG13790
DIMENSION X(1)	SIG13800

DATA IERR/0/	SIG13810
DATA XDUM/0.0/	SIG13820
C	SIG13830
C BUFFER IN A BLOCK OF WORDS FROM SCRATCH FILE.	SIG13840
C	SIG13850
C***** EXPORT *****	SIG13860
C IF(IADR.EQ.0) END FILE ISCR	SIG13870
C IF(IADR.EQ.0) REWIND ISCR	SIG13880
C READ(ISCR) (X(I),I=1,IX)	SIG13890
C GO TO 20	SIG13900
C***** EXPORT *****	SIG13910
C BUFFER IN(ISCR,0) (X(I),X(IX),IADR)	SIG13920
C GO TO 10	SIG13930
C ENTRY OBLOCK(ISCR,IADR,X,IX)	SIG13940
C	SIG13950
C BUFFER OUT A BLOCK OF WORDS TO SCRATCH FILE.	SIG13960
C	SIG13970
C***** EXPORT *****	SIG13980
C IF(IADR.EQ.0) REWIND ISCR	SIG13990
C WRITE(ISCR) (X(I),I=1,IX)	SIG14000
C GO TO 20	SIG14010
C***** EXPORT *****	SIG14020
C BUFFER OUT(ISCR,0) (X(I),X(IX),IADR)	SIG14030
C	SIG14040
C DELAY UNTIL ALL I/O IS COMPLETED.	SIG14050
C	SIG14060
C***** CRAY-1 *****	SIG14070
C 10 IF(IOSTATUS(ISCR,IERR)) 30,20,30	SIG14080
C***** CRAY-1 *****	SIG14090
C***** CDC-7600 *****	SIG14100
C 10 IF(UNIT,ISCR) 10,20,30,30	SIG14110
C***** CDC-7600 *****	SIG14120
C	SIG14130
C I/O IS COMPLETE. INCREMENT DISK ADDRESS FOR NEXT I/O OPERATION	SIG14140
C	SIG14150
C 0 IADR=IADR+IX	SIG14160
C RETURN	SIG14170
C ENTRY SBLOCK(ISCR,IADR,X,IX)	SIG14180
C	SIG14190
C SKIP A PAGE OF DATA ON SCRATCH FILE. FOR RANDOM ACCESS JUST	SIG14200
C ADVANCE DISK ADDRESS. FOR LINEAR ACCESS READ ONE WORD FROM	SIG14210
C NEXT RECORD (TO SKIP RECORD) AND ADVANCE ADDRESS.	SIG14220
C	SIG14230
C***** EXPORT *****	SIG14240
C IF(IADR.EQ.0) END FILE ISCR	SIG14250
C IF(IADR.EQ.0) REWIND ISCR	SIG14260
C READ(ISCR) XDUM	SIG14270
C***** EXPORT *****	SIG14280
C IADR=IADR+IX	SIG14290
C RETURN	SIG14300
C	SIG14310
C ERROR DURING I/O OPERATION.	SIG14320
C	SIG14330
C 30 WRITE(OUTP,5900)	SIG14340
C CALL EXIT	SIG14350
C 5900 FORMAT(41H SCRATCH I/O ERROR...EXECUTION TERMINATED)	SIG14360
C END	SIG14370
C SUBROUTINE IOFILE(UNIT,NAME,LENGTH,IOPS,ITYPE,IERR)	SIG14380
C	SIG14390
C THIS ROUTINE IS DESIGNED TO HANDLE ALL I/O DEVICE ASSIGNMENTS.	SIG14400

```

C      FILE OPENING AND CLOSING AS WELL AS END OF FILES AND LAST BUFFER SIG14410
C      UNLOADING. SIG14420
C      ARGUMENTS SIG14430
C      ----- SIG14440
C      NAME      DESCRIPTION SIG14450
C      ----- SIG14460
C      UNIT      LOGICAL UNIT NUMBER (E.G. UNIT=5 BEFORE READ(5,5000)) SIG14470
C      NAME      DISK FILE NAME (E.G. NAME=SHINPUT ) SIG14480
C      LENGTH    DISK FILE SIZE (FOR OPENS THIS ROUTINE WILL DEFINE THE SIG14490
C                  SIZE OF THE FILE OPENED. FOR CREATES THE USER MUST
C                  SPECIFY THE SIZE OF THE FILE). SIG14500
C      IOPS      OPERATION INDEX DEFINED AS FOLLOWS.... SIG14510
C                  = 1 OPEN FILE SIG14520
C                  = 2 CREATE FILE SIG14530
C                  = 3 END FILE, EMPTY BUFFER, CLOSE AND RELEASE FILE. SIG14540
C                  = 4 END FILE, CLOSE AND RELEASE FILE. SIG14550
C                  = 5 CLOSE AND RELEASE FILE. SIG14560
C                  = 6 NO LONGER USED SIG14570
C                  = 7 NO LONGER USED SIG14580
C                  = 8 DESTROY FILE (USUALLY SCRATCH AT END OF RUN) SIG14590
C                  = 9 END FILE SIG14600
C                  =10 REWIND SIG14610
C      IITYPE    SPECIFIES TYPE OF FILE ON CRAY-1 SIG14620
C                  = 1 - SEQUENTIAL (BINARY-LINEAR) SIG14630
C                  = 2 - TEXT SIG14640
C                  = 3 - HARD COPY (OUTPUT LISTING) SIG14650
C                  = 4 - ABSOLUTE (BINARY-RANDOM ACCESS) SIG14660
C                  NOT USED ON THE CDC-7600 SIG14670
C      IERR      ERROR FLAG RETURNED BY THIS ROUTINE (=0 O.K., SIG14680
C                  =1 ERROR) SIG14690
C
C      IN ADDITION THIS ROUTINE USES LABELLED COMMON/UNITS/ TO DEFINE
C      AN OUTPUT UNIT FOR ERROR MESSAGES. IF IITY IS GREATER THAN ZERO
C      ERROR MESSAGES WILL BE WRITTEN ON THIS UNIT NUMBER. FOR OPEN
C      AND CREATE ADDITIONAL CONVENTIONS ARE USED... SIG14700
C      OPEN - IF IITY=ONLINE (TELETYPE) THIS ROUTINE WILL CONTINUE TO SIG14710
C              TRY TO OPEN THE FILE. SIG14720
C      CREATE - IF IITY IS GREATER THAN 0 (ERROR MESSAGE WRITTEN) THIS
C              ROUTINE WILL CONTINUE TO TRY TO CREATE THE FILE. SIG14730
C
C      INTEGER IITY,ONLINE,UNIT SIG14740
C      COMMON/UNITS/TTY SIG14750
C-----DEFINE UNIT NUMBER FOR ON LINE MESSAGES. SIG14760
C      DATA ONLINE/59/ SIG14770
C      IPASS=0 SIG14780
C      IERR=0 SIG14790
C      GO TO (10,20,30,30,40,90,90,50,60,70),IOPS SIG14800
C***** EXPORT ***** SIG14810
C 10 RETURN SIG14820
C 20 RETURN SIG14830
C 30 END FILE UNIT SIG14840
C 40 RETURN SIG14850
C 50 RETURN SIG14860
C***** EXPORT ***** SIG14870
C***** CDC-7600 ***** SIG14880
C 10 CALL ASSIGN(UNIT,NAME) SIG14890
C CALL NOPAGE(UNIT) SIG14900
CERRA CALL DEVICE(4,HOPEN,NAME,LENGTH,IERR) SIG14910
C IF(IERR.LE.0.OR.IERR.EQ.2) GO TO 80 SIG14920
C                                     SIG14930
C                                     SIG14940
C                                     SIG14950
C                                     SIG14960
C                                     SIG14970
C                                     SIG14980
C                                     SIG14990
C                                     SIG15000

```

C	IF(IPASS.LE.0.AND.TTY.GT.0.AND.TTY.NE.UNIT) WRITE(TTY,5900) NAME	SIG15010
C	IF(TTY.NE.ONLINE) GO TO 90	SIG15020
C	IPASS=1	SIG15030
C	GO TO ERRA	SIG15040
C	20 CALL ASSIGN(UNIT,NAME)	SIG15050
C	CALL NOPAGE(UNIT)	SIG15060
CERRB	CALL DEVICE(7HDESTROY,NAME,IERR)	SIG15070
C	CALL DEVICE(6HCREATE,NAME,LENGTH,IERR)	SIG15080
C	IF(IERR.EQ.0) GO TO 80	SIG15090
C	IF(IPASS.EQ.0.AND.TTY.GT.0.AND.TTY.NE.UNIT) WRITE(TTY,5900) NAME	SIG15100
C	IF(TTY.LE.0) GO TO 90	SIG15110
C	IPASS=1	SIG15120
C	GO TO ERRA	SIG15130
C	30 IF(ITYPE.EQ.4) GO TO 40	SIG15140
C	END FILE UNIT	SIG15150
C	IF(IOPS.EQ.4) CALL EMPTY(UNIT)	SIG15160
C	40 CALL DEVICE(6HCLOSE,NAME,IERR)	SIG15170
C	IF(IERR.EQ.0) GO TO 80	SIG15180
C	IF(TTY.GT.0.AND.TTY.NE.UNIT) WRITE(TTY,5910) NAME	SIG15190
C	GO TO 90	SIG15200
C	50 CALL DEVICE(7HDESTROY,NAME,IERR)	SIG15210
C	IF(IERR.EQ.0) GO TO 80	SIG15220
C	IF(TTY.GT.0.AND.TTY.NE.UNIT) WRITE(TTY,5520) NAME	SIG15230
C	GO TO 90	SIG15240
C5900	FORMAT(IX,A10,21H INITIALIZATION ERROR)	SIG15250
C5910	FORMAT(IX,A10,14H CLOSING ERROR)	SIG15260
C5920	FORMAT(IX,A10,14H DESTROY ERROR)	SIG15270
C*****	CDC-7600 *****	SIG15280
C*****	CRAY-1 *****	SIG15290
	10 CALL OPEN(UNIT,NAME,ITYPE,LENGTH,ERRA)	SIG15300
	GO TO 80	SIG15310
ERRA	IF(IPASS.LE.0.AND.TTY.GT.0.AND.TTY.NE.UNIT) WRITE(TTY,5900) NAME	SIG15320
	IF(TTY.NE.ONLINE) GO TO 90	SIG15330
	IPASS=1	SIG15340
	GO TO 10	SIG15350
	0 CALL DESTROY(NAME)	SIG15360
	CALL CREATE(UNIT,NAME,ITYPE,LENGTH,ERRB)	SIG15370
	GO TO 80	SIG15380
ERRB	IF(IPASS.LE.0.AND.TTY.GT.0.AND.TTY.NE.UNIT) WRITE(TTY,5900) NAME	SIG15390
	IF(TTY.LE.0) GO TO 90	SIG15400
	IPASS=1	SIG15410
	GO TO 20	SIG15420
	30 IF(ITYPE.NE.4) END FILE UNIT	SIG15430
	40 CALL CLOSE(UNIT)	SIG15440
	GO TO 80	SIG15450
	50 CALL DESTROY(NAME)	SIG15460
	GO TO 80	SIG15470
	5900 FORMAT(IX,A10,21H INITIALIZATION ERROR)	SIG15480
C*****	CRAY-1 *****	SIG15490
	60 END FILE UNIT	SIG15500
	GO TO 80	SIG15510
	70 REWIND UNIT	SIG15520
	GO TO 90	SIG15530
	80 IERR=0	SIG15540
	RETURN	SIG15550
	90 IERR=1	SIG15560
	RETURN	SIG15570
	END	SIG15580
	FUNCTION NOEOF(ITAPE)	SIG15590
C		SIG15600


```

C      TEST FOR END OF FILE ON LOGICAL UNIT NUMBER 1TAPE.
C      = 0 NO EOF
C      = 1 EOF
C
C      DATA IERR/0/
C***** CRAY-1 *****
C      IF (IOSTATUS(1TAPE,IERR)) 10,20,10
C***** CRAY-1 *****
C***** CDC-7600 *****
C      IF (EOF,1TAPE) 10,20
C***** CDC-7600 *****
10 NOEOF=1
   RETURN
20 NOEOF=0
   RETURN
END

```

```

SIG15610
SIG15620
SIG15630
SIG15640
SIG15650
SIG15660
SIG15670
SIG15680
SIG15690
SIG15700
SIG15710
SIG15720
SIG15730
SIG15740
SIG15750
SIG15760

```

REFERENCES

1. D. E. Cullen and C. R. Weishin, *Nuc. Sci. and Eng.* **60**, 199-229 (1976).
2. R. V. Meghrebian and D. K. Holmes, *Reactor Analysis* (McGraw-Hill Book Company, New York, 1960), p. 137.
3. R. J. Howerton et al., *The LLL Evaluated Nuclear Data Library (ENDL)*, Lawrence Livermore Laboratory, Rept. UCRL-50400, Vol. 15, Parts A, B, and C (1976).