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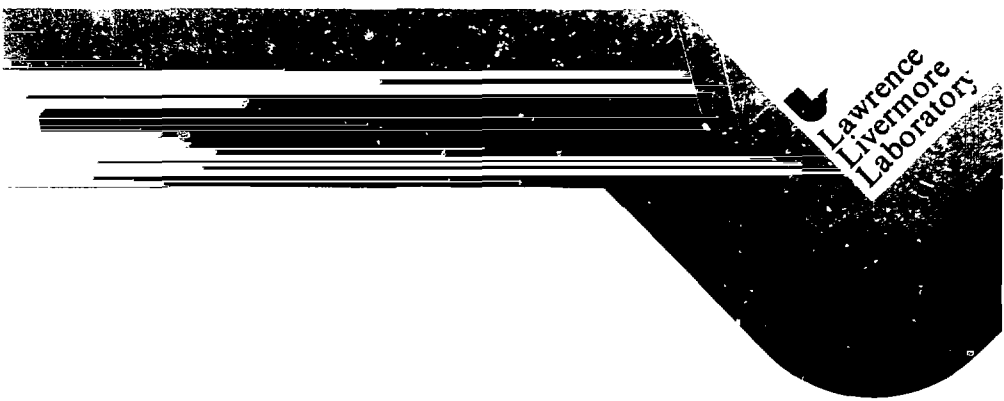
Part B, Rev. 2

Program SIGMA1 (version 79-1): Doppler broaden evaluated cross sections in the evaluated nuclear data file/version B (ENDF/B) format

D. E. Cullen

October 31, 1979



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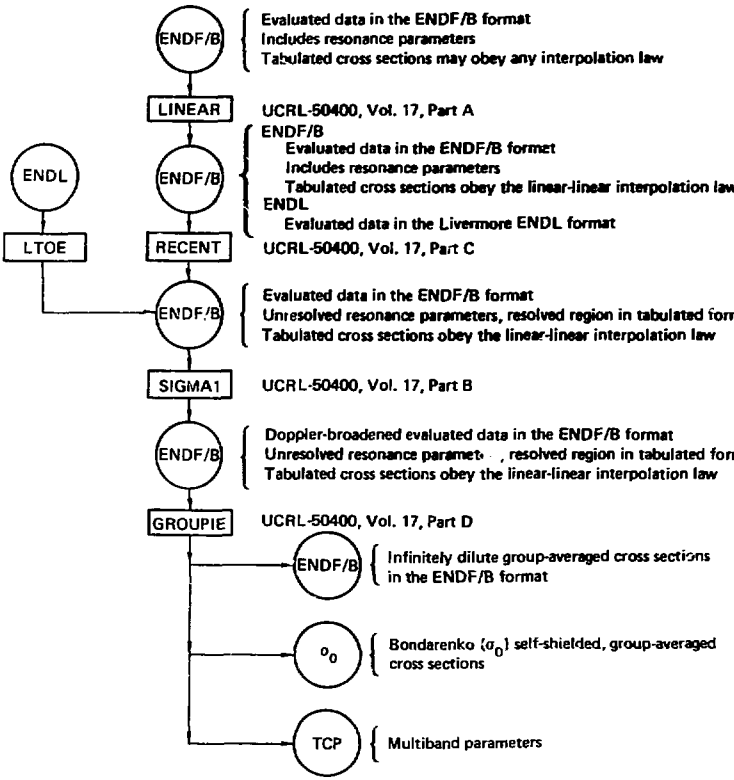
FOREWORD

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



Plots of evaluated cross sections in the ENDF/B format can be obtained at any stage of the above processing by using the EVALPLOT program (UCRL-50400, Vol. 17, Part E). Comparisons between evaluated cross sections in the ENDF/B format and experimental data in the ECSIL format can be obtained by using the ECSPLT program (UCRL-50400, Vol. 1, Part A).

CONTENTS

PROGRAM SIGMA1 (VERSION 79-1): DOPPLER BROADEN EVALUATED CROSS SECTIONS IN THE EVALUATED NUCLEAR DATA FILE/VERSION B (ENDF/B) FORMAT

ABSTRACT

Program SIGMA1 Doppler-broadens evaluated cross sections in the ENDF/B format. The program requires that input cross sections be tabulated as linearly interpolable functions of energy in ENDF/B File 3; broadened cross sections, in this same form, replace the original values in the output tape. This report describes the methods used in the code and serves as a user's guide. A listing of the source deck is available on request.

NEW FEATURES IN THE 1979 EDITION

The following features are new in the 1979 edition: (1) provision for an energy-dependent allowable error--this can be used to emphasize energy regions of interest and to reflect the accuracy with which cross sections are known; (2) retrieval of evaluations by up to 100 ranges of ZA or MAT; (3) more accurate representation of output energies by using up to nine digits; (4) versions for the CDC-7600 and the CRAY-1, with standard treatment of I/O by use of subroutines in all programs in the total cross section probability (TCP) system.

INTRODUCTION

There exist several widely used, highly detailed libraries of evaluated neutron cross sections. Associated with these libraries are programs that use these data to produce multigroup and continuous Monte Carlo data. For efficiency in coding many of these programs require that cross sections, which are tabulated as functions of energy in the data libraries, be subject to linear-linear interpolation.

The existence of these libraries of evaluated neutron data, and of their associated computer codes, has made it desirable to develop a code to

Doppler-broaden linear-linear tabulated cross sections and to output the results in linear-linear tabulated form. Program SIGMA1 does this.

SIGMA1 replaces cross sections stored in File 3 of data in the ENDF/B format[1] with Doppler-broadened cross sections. The ENDF/B tapes must be run with program LINEAR[2] before running with SIGMA1 to ensure that the File 3 data are linearly interpolable.

METHOD

DOPPLER BROADENING

Doppler broadening, in the context of this report, refers to a change in cross section resulting from thermal motion (translation, rotation, and vibration) of nuclei in a target material. The SIGMA1 method[3] can be used to Doppler-broaden cross sections for any particle (e.g., neutron, proton, deuteron) incident--at nonrelativistic energies--on a target in which the free-atom approximation is valid.

The SIGMA1 method is extensively described in Ref. 3. We briefly describe 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:

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

$$v\sigma(v,T) = \frac{1}{v}\left(\frac{\beta}{\pi}\right)^{\frac{1}{2}}\int_0^\infty \left[v_r\sigma(v_r,0)\right]v_r dv_r \left\{\exp\left[-\beta(v - v_r)^2\right] - \exp\left[-(v + v_r)^2\right]\right\}, \quad (2)$$

where

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

and

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

v = projectile velocity,

$v = |v|$ = projectile speed,

$E = \frac{1}{2}mv^2$ = projectile energy,

M = target nucleus mass,

v_T = target velocity,

$v_T = |v_T|$ = target speed,

$E_T = \frac{1}{2}Mv_T^2$ = target energy,

$v_r = v - v_T$ = relative velocity,

$v_r = |v_r|$ = relative speed,

$E_r = \frac{1}{2}mv_r^2$ = relative energy of projectile as seen by the target,

$\sigma(E,0)$, $\sigma(v,0)$ = cold (0-K) cross sections, and

$\sigma(E,T)$ $\sigma(v,T)$ = Doppler-broadened cross sections.

By a change of variables in Eq. (2) so that

$$y^2 = \alpha E = \beta v^2$$

and

$$x^2 = \alpha E_r = \beta v_r^2, \tag{3}$$

the equation becomes

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

where, for now, $T_1 = 0$ and T_2 is an arbitrary temperature.

The development below is simplified by defining the quantity

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

and noting that the Doppler-broadened cross section is then given by

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

Next we assume that the cross section to be Doppler broadened is given as a table of cross section vs energy, and that values between tabulated points vary linearly with energy and cross section:

$$\sigma(E,T_1) = \frac{E - E_k}{E_{k+1} - E_k}\sigma_{k+1} + \frac{E_{k+1} - E}{E_{k+1} - E_k}\sigma_k = A_k + B_kE, \qquad E_k \leq E \leq E_{k+1} \quad , \tag{7}$$

or

$$\sigma(x,T_1) = A_k + C_kx^2, \qquad x_k \leq x \leq x_{k+1} \quad . \tag{8}$$

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

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

By changing variables to $z = x - y$ and collecting terms in powers of z we obtain

$$\sigma^*(y,T_2) = \frac{1}{y^2}\left(\frac{1}{\pi}\right)^{\frac{1}{2}} \sum_k \int_{x_k-y}^{x_{k+1}-y} \left[C_k z^4 + 4C_k y z^3 + (A_k + 6C_k y^2)z^2\right.$$

$$\left. + (2A_k y + 4C_k y^3)z + (A_k y^2 + C_k y^4)\right]\exp(-z^2)dz \quad . \qquad (10)$$

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

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

and

$$F^n(a) = \frac{2}{\pi^{\frac{1}{2}}}\int_0^a z^n \exp(-z^2)dz \quad , \qquad (12)$$

with

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

In terms of the H^n Eq. (10) becomes

$$\sigma^*(y,T_2) = \frac{1}{2y^2} \sum_k C_k H^4(z_{k+1},z_k) + 4C_k y H^3(z_{k+1},z_k)$$

$$+ (A_k + 6C_k y)H^2(z_{k+1},z_k)$$

$$+ (2A_k y + 4C_k y^3)H^1(z_{k+1},z_k) + (A_k y^2 + C_k y^4)H^0(z_{k+1},z_k) \quad , \qquad (13)$$

where

$$Z_{k+1} = x_{k+1} - y \quad ,$$

$$Z_k = x_k - y \quad .$$

The functions $F^n(a)$ satisfy the recursion relation

$$F^n(a) = \frac{(n-1)}{2} F^{n-2}(a) - \left(\frac{1}{\pi}\right)^{\frac{1}{2}} a^{n-1} \exp(-a^2) + \left(\frac{1}{\pi}\right)^{\frac{1}{2}} \delta_{n,1} \quad , \tag{14}$$

where $\delta_{n,1}$ is the Kronecker delta.

By evaluating Eq. (12) for n = 0 and 1, and by applying the recursion relation with n = 2, 3, and 4, we obtain the required functions

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

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

$$F^2(a) = \frac{1}{2} \text{erf}(a) - \frac{a}{\pi^{\frac{1}{2}}} \exp(-a^2) \quad ,$$

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

and

$$F^4(a) = \frac{3}{4} \text{erf}(a) - \left(\frac{1}{\pi}\right)^{\frac{1}{2}} \left(\frac{3a}{2} + a^3\right) \exp(-a^2) \quad . \tag{15}$$

This completes the algorithm for determining the Doppler-broadened cross section at any arbitrary energy.

BOOTSTRAPPING

The Doppler-broadening equations can be used to broaden cross sections from 0 K to a temperature T K. Suitably generalized, they can also be used to broaden cross sections from any temperature T_1 to any higher temperature T_2 (Ref. 4). For example experimentally measured data at room temperature (293 K) can be Doppler broadened to 600 K, the resulting data 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

$$v\sigma(v,T_2) = \frac{1}{v}\left(\frac{\beta}{\pi}\right)^{\frac{1}{2}} \int_0^\infty \left[v_r\sigma(v_r,T_1)\right] v_r dv_r \times \left\{\exp\left[-\beta(v - v_r)^2\right] - \exp\left[-\beta(v + v_r)^2\right]\right\}, \qquad (16)$$

where

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

and

$$E^{\frac{1}{2}}\sigma(E,T_2) = \frac{1}{2}\left(\frac{\alpha}{\pi E}\right)^{\frac{1}{2}} \int_0^\infty \left[E_r^{\frac{1}{2}}\sigma(E_r,T_1)\right] dE_r \times \left\{\exp\left[-\alpha(E^{\frac{1}{2}} - E_r^{\frac{1}{2}})^2\right] - \exp\left[-\alpha(E^{\frac{1}{2}} + E_r^{\frac{1}{2}})^2\right]\right\}, \qquad (17)$$

where

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

the v_r and E_r associated with the cross sections $\sigma(v_r,T_1)$ and $\sigma(E_r,T_1)$ are the laboratory speed and energy of the projectile, respectively.

ENERGY GRID FOR BROADENED CROSS SECTIONS

If programs that produce multigroup and continuous Monte Carlo data from evaluated cross section libraries (in which the data are subject to linear-linear interpolation) are to be used with Doppler-broadened cross sections, those cross sections must also be linearly interpolable; large errors can result if they are not. Figure 1 shows the great discrepancy between a 1/v cross section and values obtained by linear-linear interpolation between energies that are too far apart. 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 linearly interpolable between energies.

Even using the same energy grid that was used to represent the unbroadened cross section can lead to pitfalls. This is because while Doppler broadening smooths out resonance peaks, reducing the number of points needed for linear interpolability, it also introduces a 1/v dependence (which extends to higher and higher projectile energies as the target temperature is increased), increasing the number of points needed. Figure 4 shows this effect. For example the 0-K elastic cross section for neutrons on hydrogen is roughly constant, at about 20 barns, between 10^{-5} eV and 1 keV, so that the cross section can be linearly interpolated between these energies. When this cross section is broadened to 10 000 K about 50 points must be inserted between these energies to retain linear interpolability to 1%. (On the other hand Doppler broadening makes reaction rates more nearly constant, as well as smoother, so they can be adequately represented on the same energy grid as the cold reaction rates.)

SIGMA1 uses the 0-K energy grid as the basis for the output energy grid, but inserts energy points as necessary to retain linear interpolability. The use of an interval-halving algorithm to insert the points would be very expensive of computer time. To develop a faster algorithm for inserting points, we assume (as in Fig. 1) a 1/v cross section σ_1, with values $\sigma_1(v_1) = 1/v_1$ and $\sigma_1(v_2) = 1/v_2$ at the ends of an interval (v_1, v_2), and a cross section σ_2

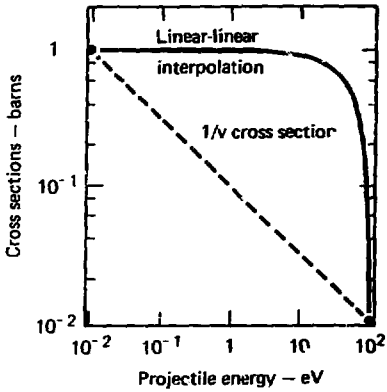


FIG. 1. Comparison of a 1/v cross section (which appears as a straight line in this log-log plot) with the incorrect cross section that results from linear-linear interpolation between energies that are very far apart.

that obeys linear-linear interpolation in energy and that agrees with σ_1 at the end points. If we write $v_2 = Sv_1$, these two cross sections have the forms

$$\sigma_1(v) = \frac{1}{v} \quad , \quad \text{(1/v variation)}$$

$$\sigma_2(v) = \frac{1}{v_1} - \frac{\left(v^2 - v_1^2\right)}{v_1^3 S(S+1)} \qquad \left(\begin{array}{l}\text{linear-linear in} \\ \text{cross section and energy}\end{array}\right) . \tag{18}$$

The fractional error at any speed v is

$$\varepsilon(v) = \frac{\sigma_1(v) - \sigma_2(v)}{\sigma_1(v)} = 1 - \frac{v^3 - vv_1^2}{v_1^3 S(S+1)} - \frac{v}{v_1} \quad ,$$

and the derivative of the fractional error with respect to v is

$$\frac{d\epsilon}{dv} = \frac{3v^2 - v_1^2}{v_1^3 S(S+1)} - \frac{1}{v_1} \quad . \tag{19}$$

The point of maximum ϵ, and the value of ϵ at that point, are thus

$$v_{max} = v_1 \left[\frac{1}{3}(1 + S + S^2)\right]^{\frac{1}{2}}$$

and

$$\epsilon(v_{max}) = 1 - \frac{2}{3}\left(\frac{1}{3}\right)^{1/2} \frac{\left(1 + S + S^2\right)^{3/2}}{S(S+1)} \leq 0, \qquad v_1 \leq v \leq v_2 \quad . \tag{20}$$

It is clear from Fig. 1 that ϵ is always a negative quantity.

Note that $\epsilon(v_{max})$ is independent of v and depends only on S, the spacing factor between tabulated points. This means that a 1/v variation can be represented by a linear-linear variation in energy, to within fractional error ϵ, simply by ensuring that successive tabulated energy values are within a factor S^2 of one another (where S depends on ϵ, but not on E). SIGMA1 starts from the same energy points as the 0-K data and supplements this grid in any interval where the points are more widely spaced than a factor S^2. A thinning algorithm[2] then removes points not actually required for linear interpolability.

Table 1 gives the spacing factor [obtained from Eq. (20)] required for fractional errors ϵ in the range 0.1 to 2.0%. The table also shows the number of points required to space points a factor S^2 apart between 10^{-5} eV and 20 MeV. For example a tolerance of 0.5% would require 124 points (counting the end points) or roughly 10 per energy decade; the points would be spaced a factor of about $(1.1223)^2 = 1.2596$ apart.

TABLE 1. Point-spacing requirements for linear interpolability with a 1/v cross section. For a fractional error no greater than ε, energy points must be spaced a factor S^2 apart. To span 10^{-5} eV to 20 MeV requires the number of points given (counting end points).

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

TRUNCATING THE INTEGRATION RANGE

Although the algorithm previously described can evaluate the Doppler-broadened cross section exactly, this would be a costly procedure since the calculation time varies as the square of the number of points used to represent each reaction. To reduce the cost, we use the strongly convergent Gaussian character of the Doppler-broadening kernel to truncate the Doppler-broadening integral of Eq. (15). Because of the exponential term $\exp[-(x - y)^2]$

we expect the major contribution to the integral from some interval ±N centered on y; that is, the integration will be over values of x from y - N to y + N. A procedure for determining N must recognize that although $\exp\left[-(x - y)^2\right]$ is rapidly decreasing the term for $x^2\sigma(x,T)$ may be rapidly increasing; this is particularly true for $\sigma(x,T)$ in the resonance region.

We write the integral of Eq. (5) in truncated form,

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

$$= \frac{1}{y^2\pi^{\frac{1}{2}}}\int_{y-N}^{y+N} x^2\sigma(x,T_1)\exp\left[-(x - y)^2\right]dx + R(y) \quad , \qquad (21)$$

where

$$R(y) = \frac{1}{y^2\pi^{\frac{1}{2}}}$$

$$\times\left\{\int_0^{y-N} x^2\sigma(x,T_1)\exp\left[-(x - y)^2\right]dx + \int_{y+N}^{\infty} x^2\sigma(x,T_1)\exp\left[-(x - y)^2\right]dx\right\} . \qquad (22)$$

We note that

$$R(y) \leq \frac{1}{y^2\pi^{\frac{1}{2}}}\sigma_{max}$$

$$\times\left\{\int_0^{y-N} x^2\exp\left[-(x - y)^2\right]dx + \int_{y+N}^{\infty} x^2\exp\left[-(x - y)^2\right]dx\right\} ; \qquad (23)$$

changing variables (to Z = y - x in the first integral and to Z = x - y in the second) we obtain

$$R(y) \leq \frac{1}{y^2\pi^{\frac{1}{2}}} \sigma_{max} \left\{ \int_N^y (y - z)^2 e^{-z^2} dz + \int_N^y (y + z)^2 e^{-z^2} dz \right\} . \qquad (24)$$

For the first integral we have

$$\int_N^y (y - z)^2 e^{-z^2} dz < \int_N^y (y + z)^2 e^{-z^2} dz < \int_N^\infty (y + z)^2 e^{-z^2} dz ,$$

so that

$$R(y) \leq \frac{2}{y^2\pi^{\frac{1}{2}}} \sigma_{max} \int_N^\infty (y + z)^2 e^{-z^2} dz . \qquad (25)$$

The fractional error made by truncating at N is therefore

$$\varepsilon(y) = \frac{R(y)}{\sigma(y)} \leq \frac{2}{y^2\pi^{\frac{1}{2}}} \frac{\sigma_{max}}{\sigma(y)} \int_N^\infty (y + z)^2 e^{-z^2} dz . \qquad (26)$$

We assume that $\sigma_{max}/\sigma(y) = 10^4$, and seek a value of N such that $\varepsilon \leq 0.001$; N = 4 accomplishes this safely. 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 this means that the second term in Eq. (6), $\sigma^*(-y,T_2)$, need not be evaluated at all unless $y \leq 4$.

PROGRAM USE--GENERAL

LIMITATIONS AND ASSUMPTIONS

SIGMA1 uses only the ENDF/B BCD format (as opposed to binary). It copies all sections except File 3 as Hollerith. The program can therefore be used on data in the ENDF/B-I, II, III, IV or V formats, since all sections of File 3 data are identical in all versions of ENDF/B.

The program reads and Doppler-broadens the data a page at a time, so there is virtually no limit to the number of points in any section (i.e., each reaction can be described by up to 500 000 points).

SIGMA1 does not update the reaction index in File 1, Section 451 of each evaluation (see Ref. 1). This will not affect the user unless he has a program that uses the index to perform random access. In this case program DICTION[6] should be used to create an up-to-date reaction index after SIGMA1 is used.

Evaluations can be in MAT or ZA order. SIGMA1 assumes that the data are in order of increasing MAT or ZA, whichever is used as the retrieval criterion. The program stops searching when it finds an evaluation with a MAT or ZA value that exceeds the highest requested value.

SIGMA1 is written entirely in Fortran IV and can be easily modified to run on any medium-sized computer.

SIGMA1 requires that input data in the ENDF/B format obey the linear-linear interpolation law; the program will abort if this condition is not met. Program LINEAR[2] is the best way to linearize data in the ENDF/B format.

During Doppler broadening three pages of data are in core at any given time: 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 constant and a warning message ("EXTENSION") is printed out advising the user of the maximum temperature step allowable to avoid "EXTENSION." In this case rerun the program, bootstrapping the cross section up to the final temperature in temperature steps smaller than or equal to the step size recommended in the "EXTENSION" message.

The program selects 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 error of less than 0.1% is specified it will be used for output thinning, but maximum energy-point spacing will be based on 0.1%.

If the original ENDF/B data are given at a temperature higher than the final temperature, the section will not be Doppler-broadened; the data for the original temperature will be left in the section. If the original data are given at a temperature between 0 K and the final temperature, the program will correctly broaden the data to the final temperature (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. SIGMA1 does not use unresolved-resonance parameters directly.

REQUIREMENTS

The I/O units are defined as follows:

Filename*	Unit	Description
INPUT	5	Input card
OUTPUT	6	Output report
ENDFIN	21	Evaluated data (in the ENDF/B format) to be Doppler broadened
ENDFOUT	22	Doppler-broadened data (in the ENDF/B format)
SCRSIG	23	Scratch file

All read and write statements use variable I/O unit numbers. To convert to any other set of unit numbers, redefine the unit numbers on the program card and at the beginning of the program (see Appendix).

The program requires approximately 28 000 words of core storage on either the LLL CDC-7600 or the CRAY-1. The program executes approximately twice as fast on the CRAY-1 as on the CDC-7600. On the CRAY-1, for example, the program requires 0.35 minutes to Doppler-broaden ENDL-78[5] Tape 6 from 0 to 300 K and to thin the output to 0.1% accuracy. It takes about 4 minutes to Doppler broaden the entire ENDL-78 library (88 complete evaluations) from 0 to 300 K and thin the output to 0.1% accuracy.

PROGRAM USE--DETAILS

REQUESTING EVALUATED DATA FOR DOPPLER BROADENING

Evaluations can be requested either by MAT number[1] or by ZA, where ZA = 1000Z + A for an isotope and ZA = 1000Z for an element. Up to 100 ranges of

*The filenames apply to the program at LLL. Disk files with these names will be used by the program.

MAT or ZA can be requested. The ENDF/B data are assumed to be in increasing MAT or ZA order, whichever criterion the user specifies for retrieval. All evaluations that meet the selection criteria will be processed by this program; all other evaluations will be skipped. Processing is ended when an evaluation with a MAT (or ZA) is found that exceeds the highest requested value. For example if the user requests all materials with MAT numbers between 1000 and 1100, or between 1200 and 1300, processing is ended as soon as an evaluation with a MAT number higher than 1300 is found; the program assumes the ENDF/B data are in MAT order and does not search any further.

To simplify requests for individual evaluations, as opposed to evaluations in ranges of MAT or ZA, SIGMA1 has been written so that if only a minimum MAT or ZA is specified, only an evaluation with that MAT or ZA will be searched for. For example to process ^{238}U, searching by ZA, one need only specify the lower limit ZA = 92238 and make no entry for the upper limit. (See Input Cards for details.)

SIGMA1 outputs the entire evaluation, not just File 3 cross sections; e.g., angular and energy distributions, if present, will also be output. Thus the output from this program is complete and in a form that can be used directly in subsequent processing codes.

ENDF/B MINIMUM ENERGY SPACING

Normally, output in the ENDF/B format that is written with a Fortran write in E11.4 format yields numbers accurate to 5 digits; e.g., 123.456789 is output as 1.2346E 2. For the many narrow resonances in heavy isotopes (such as ^{232}Th, ^{238}U, and ^{240}Pu) more than 5 digits are needed to distinguish between successive energies (cross sections do not present a problem).

The accuracy of the ENDF/B format has been extended to six digits in many codes--including this one--by writing floating point output in a E11.4 format that has an additional digit of accuracy instead of the "E"; e.g., 123.456789 is output as 1.23457+2. This format is called 6-digit E11.4 format.

In SIGMA1 the user can further extend the accuracy of the energy output in the ENDF/B format to as many as nine digits by writing energies in Fortran "F" format. Under this option the format will vary from F11.8 to F11.0 depending on the energy. For energies between 1 eV and 100 MeV this option gives nine digits of accuracy; for energies between 10^{-3} and 1 eV the accuracy

varies from six to nine digits, which is at least as good as using the 6-digit E11.4 format; below 10^{-3} eV and above 100 MeV 6-digit E11.4 format is used.

In SIGMA1, during interval halving, any interval so short that the energies at the two ends of the interval cannot be distinguished is not subdivided further. For example the energies 123.45651 and 123.45749 are indistinguishable in 6-digit E11.4 ENDF/B output format, in which they are both equal to 1.23457+2; an interval with these energies as endpoints would not be subdivided.

SPECIFYING MAXIMUM FRACTIONAL ERROR

The maximum fractional error used in thinning can be specified by an energy-dependent error law, represented by up to twenty (energy, error) pairs. The energies must be in ascending order, in eV; errors must be positive decimal fractions (not percents). If only one pair is given the error is taken as constant for all energies. If more than one pair is given the error is taken to vary linearly between tabulated values and to be constant outside of the energy limits given.

For example the following error law specifies 0.1% accuracy below 100 eV, accuracy varying linearly from 0.1% at 100 eV to 1% at 1 keV, and 1% accuracy above 1 keV:

energy, eV	fractional error
0.0	0.001
100.0	0.001
1000.	0.01
1.0E+10	0.01

[The form above makes clear how error is to vary over the entire energy range of interest; however, because of the convention that errors are taken as constant outside the energy range specified, the first and last of the four (energy, error) pairs above could be left out. Thus the error law

energy, eV	fractional error
100.0	0.001
1000.0	0.01

is exactly equivalent to the one above, which uses four energy-error pairs.]

The error law can be used to tailor output for specific applications. For example the error law given above can be used to obtain very accurate (0.1%) cross sections for ^{238}U and yet minimize the number of data points used to represent the many narrow resonances between about 1 and 3 keV.

INPUT CARDS

Card	Columns	Format	Description
1	1-11	I11	Retrieval criterion (0 indicates MAT, 1 indicates ZA).
	12-22	I11	Minimum energy spacing (0 indicates 6-digit minimum energy spacing for calculations, 6-digit E11.4 output; 1 indicates 9-digit minimum energy spacing for calculations, 6-digit E11.4 output; 2 indicates 9-digit minimum energy spacing for calculations, variable 9-digit F format output).
	23-33	E11.4	Output Kelvin temperature.
vary	1-11	I11	Minimum MAT or ZA.
	12-22	I11	Maximum MAT or ZA (blank, for single evaluation). Up to 100 MAT or ZA ranges can be specified, one range per card. The list is terminated by a blank card.
vary	1-11	E11.4	Energy for File 3 error law.
	12-22	E11.4	Error for File 3 error law.

The File 3 error law can be described by up to 20 (energy, error) pairs, one pair per card. The input for the law is terminated by a blank card. If only one point is given the error law is assumed to be constant over the entire range. The energies must be in ascending order, in eV; errors must be positive decimal fractions (not percents).

ERROR MESSAGES

1. 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 data in core. This normally occurs only for large temperature changes. Doppler broaden to the final temperature in steps (in the above example each step must be smaller than about 2.7×10^6 K).

2. INTERPOLATION LAW IS NOT LINEAR-LINEAR
EXECUTION TERMINATED

The data in the ENDF/B format must be subject to linear-linear interpolation for valid Doppler broadening by SIGMA1. Convert the data to linear-linear form with program LINEAR.[2]

3. SCRATCH MAXIMUM PAGE COUNT EXCEEDED
EXECUTION TERMINATED

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

4. OVER 100 RANGES--EXECUTION TERMINATED
A maximum of 100 MAT or ZA ranges is allowed.

5. OVER 20 RANGES--EXECUTION TERMINATED
The error law may be described by no more than 20 (energy, error) pairs.

6. ERROR MUST BE POSITIVE--EXECUTION TERMINATED
Iteration will not converge unless the errors in the error law are positive.

7. ENERGIES MUST BE IN ASCENDING ORDER--EXECUTION TERMINATED
8. ENDFIN INITIALIZATION ERROR
9. ENDFOUT CLOSING ERROR
10. SCRSIG DESTROY ERROR

These errors indicate that the program is having trouble locating, creating, closing, or destroying a disk file. If the program cannot

initialize ENDFIN it indicates the ENDF/B format data is either not on disk or has the wrong filename. If the program cannot initialize ENDFOUT or SCRSIG it is having trouble locating disk space in order to create a file; it will keep trying.

11. SCRATCH I/O ERROR--EXECUTION TERMINATED

This can only occur if an evaluation generates more than 500 000 data points and exceeds the present disk file allocation of 1 000 000 words, or if there is a computer problem. In the former case increase the allowable error, so as to generate fewer points, and re-run. In the latter case try again.

INPUT AND OUTPUT EXAMPLES

EXAMPLE INPUT

The input cards shown below correspond to the following problem:

Consider ^{235}U, which is MAT 1261. Retrieve it by MAT number. Use 9-digit energy spacing for the accuracy of the calculation, and 6-digit output. Doppler broaden the data to 300 K. Insert data points and thin to the following accuracies: between 0 and 100 eV use 0.1% accuracy; between 100 eV and 1 keV very accuracy between 0.1 and 1.0%; above 1 keV use 1% accuracy.

The required input cards are

```
                                        0                   1                   300.0
                                    1261
(blank card terminates request list)
                                0.                  0.001
                            100.                    0.0001
                        1000.                       0.01
                    1.000000+09                     0.01
(blank card terminates file 3 error law)
```

EXAMPLE OUTPUT LISTING

The following listing results from Doppler broadening ENDL-76 Tape 6 to 300 K and thinning the output to 0.1%. Figures 2 through 5 illustrate the wide range of applications of the SIGMA1 code:

- Fig. 2 shows broadening of the ^{233}U total cross section to reactor-core temperatures (300--10 000 K).
- Fig. 3 shows broadening of the ^{233}U total cross section to controlled-thermonuclear-reactor (CTR) and stellar temperatures (1 eV--10 keV)*.
- Fig. 4 shows broadening of a constant cross section at 0 K to temperatures ranging from 1 eV to 1 MeV.
- Fig. 5 shows broadening of a 1/v cross section at 0 K to temperatures ranging from 1 eV to 1 MeV.

OPERATION

OPERATION AT LLL

At Livermore compiled, loaded, ready-to-execute versions of this program are available from the photostore file for either the CDC-7600, with the command

.193025:PROGRAMS [SIGMA1 INSIGMA1] ,

or for the CRAY-1, with the command

.193025:PROGRAMS:CRAY-1 [SIGMA1 INSIGMA1].

---

*Some readers may be unfamiliar with the practice of expressing temperatures in eV, which arises because the dimension of kT is energy. From Boltzmann's constant $k = 1.38 \times 10^{-23}$ joule per Kelvin = 8.62×10^{-5} eV per Kelvin we obtain, e.g., the equivalences 1 eV ≈ 12 000 K and 10 keV ≈ 1.2×10^{8} K.

1 DOPPLER BROADEN ENDF/B CROSS SECTIONS (SIGMA1 73-1)

RETRIEVAL CRITERIA---------- MAT
MINIMUM ENERGY SPACING------- 6 DIGITS
ENERGY OUTPUT FORMAT--------- STANDARD
TEMPERATURE---------- 3.00000+ 2 KELVIN
MAT RANGES---------- MINIMUM MAXIMUM
0 9999
ALLOWABLE ERROR---------- ENERGY ERROR
0. + 0 1.00000- 3
1.00000+ 9 1.00000- 3

TAPE LABEL

LAWRENCE LIVERMORE EVALUATED LIBRARY (ENDL) 6/01/78 6

ZA	MAT	MT		KELVIN IN	Q-VALUE EV	POINTS IN	POINTS OUT
90231	7863	1	0.	+ 0 0.	+ 0	246	220
90231	7863	2	0.	+ 0 0.	+ 0	43	72
90231	7863	4	0.	+ 0 0.	+ 0	22	22
90231	7863	16	0.	+ 0 -5.12000+	6	19	19
90231	7863	17	0.	+ 0 -1.19100+	7	11	11
90231	7863	18	0.	+ 0 1.80000+	8	152	195
90231	7863	37	0.	+ 0 -1.71500+	7	5	4
90231	7863	91	0.	+ 0 0.	+ 0	22	22
90231	7863	102	0.	+ 0 6.43000+	6	138	183
90231	7863	251	0.	+ 0 0.	+ 0	20	20
90231	7863	252	0.	+ 0 0.	+ 0	20	19
90231	7863	253	0.	+ 0 0.	+ 0	20	19
				MAT TOTALS		718	806
90232	7864	1	0.	+ 0 0.	+ 0	6261	5323
90232	7864	2	0.	+ 0 0.	+ 0	2983	2898
90232	7864	4	0.	+ 0 0.	+ 0	62	51
90232	7864	16	0.	+ 0 -6.34000+	6	17	16
90232	7864	17	0.	+ 0 -1.15600+	7	8	8
90232	7864	18	0.	+ 0 1.70000+	8	34	34
90232	7864	37	0.	+ 0 -1.83500+	7	2	2
90232	7864	91	0.	+ 0 0.	+ 0	62	51
90232	7864	102	0.	+ 0 4.79000+	6	5535	5451
90232	7864	251	0.	+ 0 0.	+ 0	14	13
90232	7864	252	0.	+ 0 0.	+ 0	14	14
90232	7864	253	0.	+ 0 0.	+ 0	14	13
				MAT TOTALS		15006	13874
90233	7865	1	0.	+ 0 0.	+ 0	296	219
90233	7865	2	0.	+ 0 0.	+ 0	43	72
90233	7865	4	0.	+ 0 0.	+ 0	21	21
90233	7865	16	0.	+ 0 -4.78000+	6	19	19
90233	7865	17	0.	+ 0 -1.12200+	7	14	14
90233	7865	18	0.	+ 0 1.80000+	8	130	174
90233	7865	37	0.	+ 0 -1.63400+	7	5	4
90233	7865	91	0.	+ 0 0.	+ 0	21	21
90233	7865	102	0.	+ 0 6.18000+	6	121	157
90233	7865	251	0.	+ 0 0.	+ 0	16	15
90233	7865	252	0.	+ 0 0.	+ 0	16	15
90233	7865	253	0.	+ 0 0.	+ 0	16	16
				MAT TOTALS		718	747

92233	7866	1	0.	+ 0	0.	+ 0	2884	2353		
92233	7866	2	0.	+ 0	0.	+ 0	343	352		
92233	7866	4	0.	+ 0	0.	+ 0	32	30		
92233	7866	16	0.	+ 0	-5.90000	+ 6	12	11		
92233	7866	17	0.	+ 0	-1.31800	+ 7	6	5		
92233	7866	18	0.	+ 0	1.80000	+ 8	1613	1608		
92233	7866	91	0.	+ 0	0.	+ 0	32	30		
92233	7866	102	0.	+ 0	6.84000	+ 6	1954	1949		
92233	7866	251	0.	+ 0	0.	+ 0	21	21		
92233	7866	252	0.	+ 0	0.	+ 0	21	21		
92233	7866	253	0.	+ 0	0.	+ 0	21	20		
					MAT TOTALS		6939	6400		
92234	7867	1	0.	+ 0	0.	+ 0	188	190		
92234	7867	2	0.	+ 0	0.	+ 0	37	57		
92234	7867	4	0.	+ 0	0.	+ 0	19	17		
92234	7867	16	0.	+ 0	-6.84000	+ 6	13	13		
92234	7867	17	0.	+ 0	-1.25900	+ 7	7	7		
92234	7867	18	0.	+ 0	1.80000	+ 8	40	40		
92234	7867	91	0.	+ 0	0.	+ 0	19	17		
92234	7867	102	0.	+ 0	5.31000	+ 6	128	166		
92234	7867	251	0.	+ 0	0.	+ 0	29	28		
92234	7867	252	0.	+ 0	0.	+ 0	29	29		
92234	7867	253	0.	+ 0	0.	+ 0	29	27		
					MAT TOTALS		538	591		
92235	7868	1	0.	+ 0	0.	+ 0	2294	2292		
92235	7868	2	0.	+ 0	0.	+ 0	235	264		
92235	7868	4	0.	+ 0	0.	+ 0	25	25		
92235	7868	16	0.	+ 0	-5.230(	+ 6	16	16		
92235	7868	17	0.	+ 0	-1.200(	+ 7	7	7		
92235	7868	18	0.	+ 0	1.80000	+ 8	1511	1585		
92235	7868	37	0.	+ 0	-1.78900	+ 7	3	3		
92235	7868	91	0.	+ 0	0.	+ 0	25	25		
92235	7868	102	0.	+ 0	6.55000	+ 6	767	837		
92235	7868	251	0.	+ 0	0.	+ 0	29	27		
92235	7868	252	0.	+ 0	0.	+ 0	29	29		
92235	7868	253	0.	+ 0	0.	+ 0	29	27		
					MAT TOTALS		4970	5137		
92236	7869	1	0.	+ 0	0.	+ 0	179	176		
92236	7869	2	0.	+ 0	0.	+ 0	35	58		
92236	7869	4	0.	+ 0	0.	+ 0	21	19		
92236	7869	16	0.	+ 0	-6.55000	+ 6	14	14		
92236	7869	17	0.	+ 0	-1.18500	+ 7	8	8		
92236	7869	18	0.	+ 0	1.80000	+ 8	40	71		
92236	7869	91	0.	+ 0	0.	+ 0	21	19		
92236	7869	102	0.	+ 0	5.12000	+ 6	127	183		
92236	7869	251	0.	+ 0	0.	+ 0	29	28		
92236	7869	252	0.	+ 0	0.	+ 0	29	29		
92236	7869	253	0.	+ 0	0.	+ 0	29	28		
					MAT TOTALS		532	633		

93237	1263	56	0.	+	0	-2.24000+	5	30	25
93237	1263	57	0.	+	0	-2.68000+	5	27	24
93237	1263	58	0.	+	0	-3.05000+	5	25	23
93237	1263	59	0.	+	0	-3.32000+	5	24	20
93237	1263	60	0.	+	0	-3.69000+	5	21	19
93237	1263	61	0.	+	0	-3.71000+	5	19	17
93237	1263	91	0.	+	0	-3.32000+	5	128	70
93237	1263	102	0.	+	0	5.49000+	6	316	214
93237	1263	251	0.	+	0	0.	+ 0	39	38
93237	1263	252	0.	+	0	0.	+ 0	39	37
93237	1263	253	0.	+	0	0.	+ 0	39	39
						MAT TOTALS		2171	1392
22000	1286	1	0.	+	0	0.	+ 0	1305	1043
22000	1286	2	0.	+	0	0.	+ 0	913	898
22000	1286	3	0.	+	0	0.	+ 0	444	397
22000	1286	4	0.	+	0	-2.44000+	5	48	47
22000	1286	16	0.	+	0	-1.16300+	7	6	6
22000	1286	51	0.	+	0	-9.87000+	5	39	38
22000	1286	91	0.	+	0	-2.44000+	5	17	16
22000	1286	102	0.	+	0	8.14000+	6	395	390
22000	1286	103	0.	+	0	-3.21000+	6	8	8
22000	1286	107	0.	+	0	-2.03000+	6	6	6
						MAT TOTALS		3181	2849
42000	1287	1	0.	+	0	0.	+ 0	151	158
42000	1287	2	0.	+	0	0.	+ 0	25	23
42000	1287	4	0.	+	0	-9.19300+	5	19	16
42000	1287	16	0.	+	0	-7.80000+	6	16	16
42000	1287	17	0.	+	0	-1.48000+	7	7	7
42000	1287	91	0.	+	0	0.	+ 0	19	16
42000	1287	102	0.	+	0	7.25000+	6	121	272
42000	1287	251	0.	+	0	0.	+ 0	13	13
42000	1287	252	0.	+	0	0.	+ 0	13	13
42000	1287	253	0.	+	0	0.	+ 0	13	13
						MAT TOTALS		397	547
						TAPE TOTALS		28970	21994

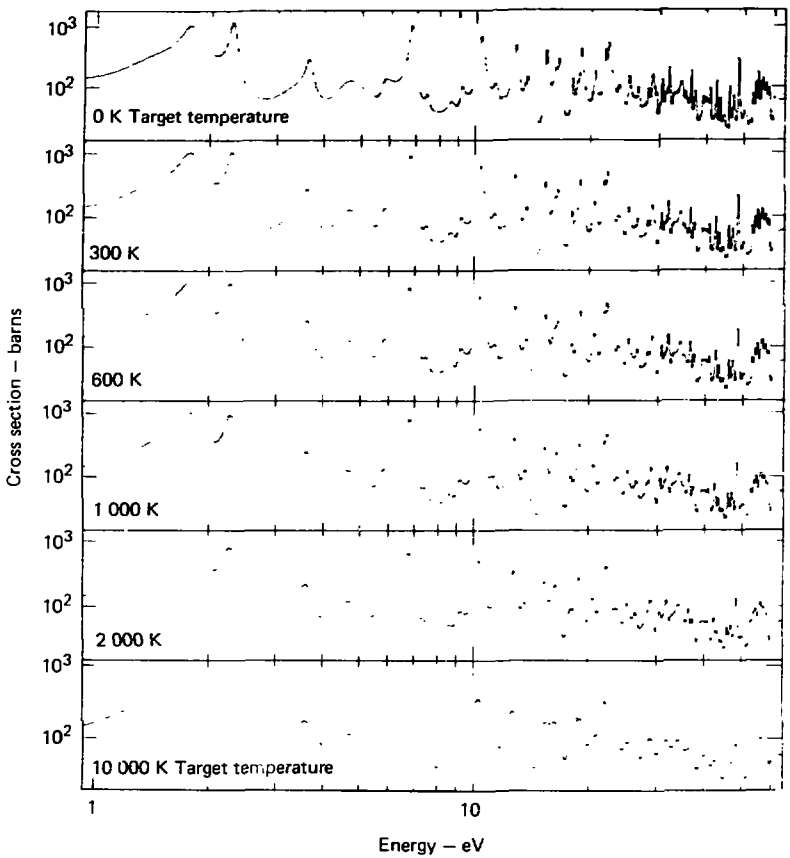


FIG. 2. Doppler broadening of the ^{233}U neutron total cross section to reactor-like temperatures (T = 300 K to 10 000 K).

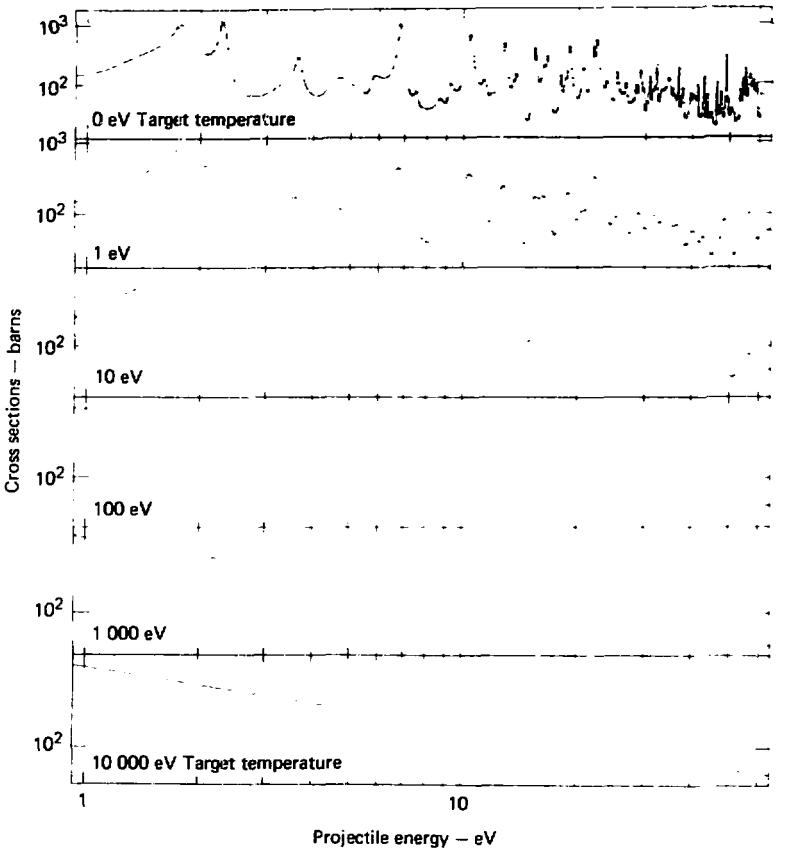


FIG. 3. Doppler broadening of the ^{233}U neutron total cross section to stellar or CTR-core temperatures (kT = 1 eV to 10 keV; T ≈ 1.2 × 10^4K to 1.2 ~ 10^8 K).

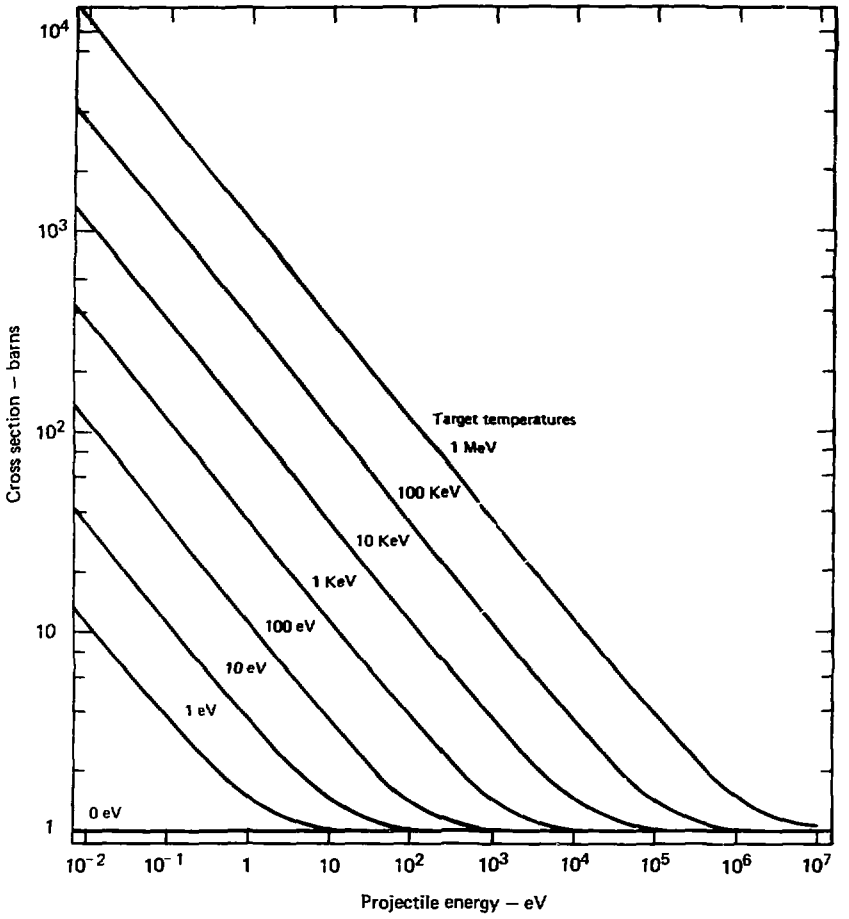


FIG. 4. Doppler broadening of an initially constant cross section to temperatures from 1 eV to 1 MeV. The results agree with theoretical predictions over the entire energy range.

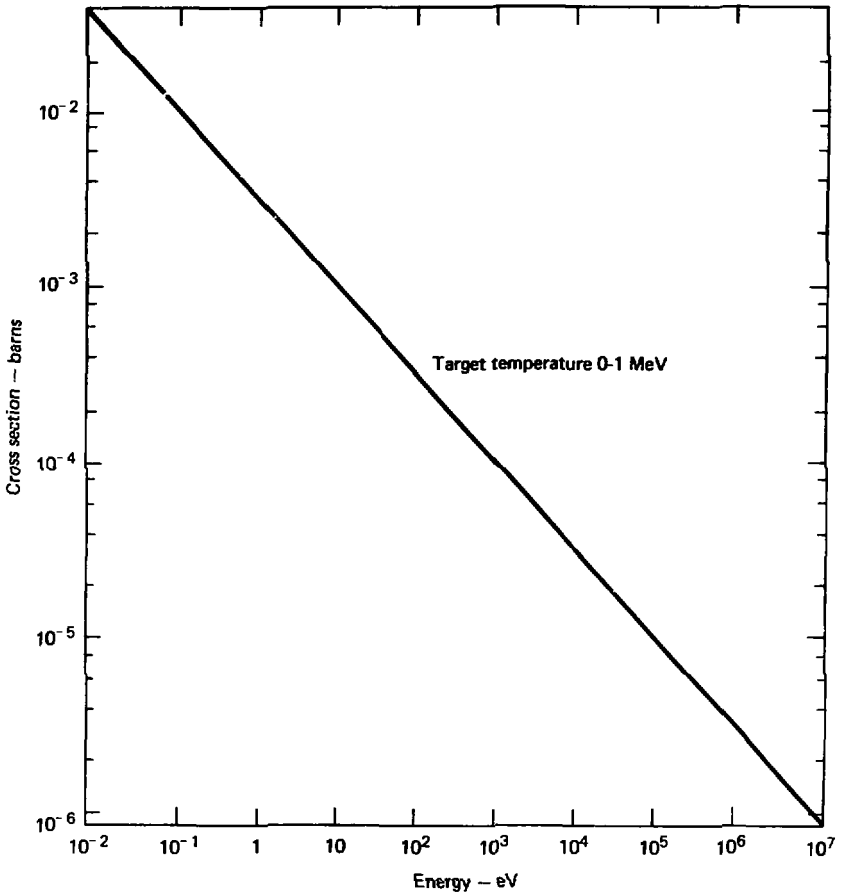
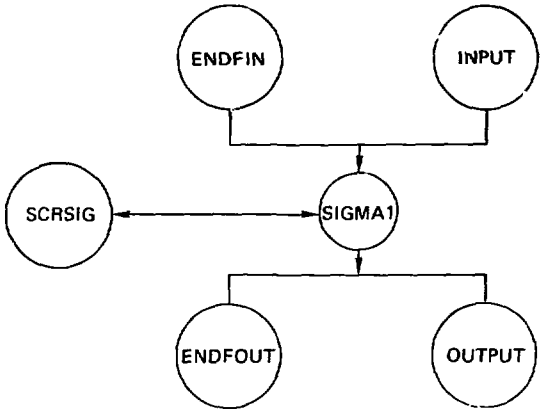


FIG. 5. Doppler broadening of a 1/v cross section. The result should be temperature-independent: to the scale of the figure, it is. There is some temperature dependence, but only for temperatures well above 100 keV, and only for extremely low projectile energies.

After these files are read from photostore INSIGMA1 should be renamed INPUT and edited to select the options required.

The program is small enough (28 000 words) to run at a low priority during the day.

The program will automatically use the disk filenames described below:



The program is designed to be compiled using either the CHAT compiler (for the CDC-7600) or the CIVIC compiler (for the CRAY-1).

CONVERSION TO OTHER INSTALLATIONS

This revision of the code is designed for use either on a LLL CDC-7600 or CRAY-1, or for export to any other installation that uses Fortran IV. Most of the coding is in standard Fortran. When an instruction takes different forms for the CDC-7600 or CRAY-1, it is present in three different forms--one for each of the LLL computers and one in standard Fortran. Each card in the group of three is inserted as a comment card and is labelled "CDC-7600," "CRAY-1," or "EXPORT" (this last label designates any machine using standard Fortran).

To use the code on any given computer activate the appropriate instruction in each set by eliminating the comment-card identifier "C" and the label, and leave the other two instructions in the set as inactive comment cards.

In particular see the following subroutines, which contain machine-dependent coding:

DROPIT — At LLL this subroutine creates a copy of the loaded program, which is then executed; the original program is not affected. In Fortran IV the subroutine does nothing and simply returns.

IBLOCK — This routine does the scratch I/O; in Fortran IV this is equivalent to binary I/O. Operation of SIGMA1 can be greatly improved by using the most efficient scratch I/O available at your installation.

IOFILE — Opens, closes, creates, and destroys disk files. In Fortran IV the subroutine simply returns.

This use of subroutines for I/O will be maintained in future versions of this code. Therefore it is recommended that, instead of replacing the calls to these subroutines, you supply equivalent subroutines for your computer. Your versions of DROPIT, IBLOCK, and IOFILE will be compatible with all future versions of this code and this will minimize your maintenance problem. Note that these same routines are also used by LINEAR,[2] RECENT,[7] and GROUPIE,[8] and, once converted, they can be used in all four programs.

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1978 AND 1979 EDITIONS

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*LLL 1980/5