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(ENDF - 269)

REFERENCE MANUAL FOR ENDF THERMAL NEUTRON SCATTERING DATA

by

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Introduction to Revised Edition

At the suggestion of Don Mathews (GA), the Reference Manual for ENDF Thermal Neutron Scattering Data has been reissued by the National Nuclear Data Center.

This edition (ENDF-269) contains additional and revised moderator information, an expanded discussion of the GASKET Code; and other updates provided by Don Mathews.

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CONTENTS

A. GENERALITIES AND COMPUTER CODES

A. 1 INTRODUCTION

This document is intended to serve as a general reference of information concerning the thermal neutron scattering law data submitted by Gulf General Atomic to the Evaluated Nuclear Data File (ENDF)[1] set up by the Neutron Cross Section Center at the Brookhaven National Laboratory. The data submitted to ENDF refers both to inelastic and elastic scattering. The inelastic scattering data, generally calculated in the incoherent approximation, is stored in the form of the scattering law $S(\alpha, \beta)$ related to the double differential cross section by the expression

$$\frac{d^2\sigma}{dEd\Omega} = \frac{a^2}{T}\sqrt{\frac{E}{E_o}}\, e^{-\beta/2}\, S(\alpha, \beta)$$

where

$$\alpha = \frac{K^2}{2MT} \quad \text{and} \quad \beta = \frac{E-E_o}{T}$$

and where E_o, E denote the initial and final neutron energies, K is the momentum exchange, a the bound scattering length of the scatterer and T its temperature.

The elastic scattering data, either coherent or incoherent is stored in the form of the Legendre moments P_0 through P_5.

The report is divided into two parts. Part A includes information on the ENDF system (Section A. 2) and a concise description of the computer codes used to generate the scattering data (Section A. 3). This description is not intended to replace the more complete discussion given in the corresponding references, which are listed in Section A. 4, but it permits an understanding of the source data as tabulated on the input cards to each code. These codes have all been written in FORTRAN and are available through the Argonne Code Center.

Part B contains the data corresponding to the different moderators. These data are included in a loose leaf format similar to the Gulf General Atomic Spectrum Book[2] to facilitate revisions and updating. The information corresponding to each moderator is given in six sections as follows: (1) A description of the model underlying the calculation, with enough physical content to satisfy the casual user plus all pertinent references; (2) following the description of those models which include a continuum of vibrational modes, is a graphical illustration of the corresponding frequency spectra; (3. 1) through (3. n) listings of the card input to all the codes used to generate the ENDF data for the moderator under consideration; (4) plots of the scattering law for several temperatures; (5) tabulated values of various integral quantities of the scattering law; and (6) miscellaneous information concerning the data and some quantities directly derived from the model such as the Debye-Waller integrals and effective temperatures. Comments as to the adequacy of the model and comparison with available measurements will also be included. For the convenience of easy updating pagination is by section in Part A and by moderator (alphabetically) in Part B. An index of the moderators currently included precedes the material of Part B.

A.2 THE ENDF SYSTEM

A.2.1 EVALUATED NUCLEAR DATA FILE (ENDF)

The Evaluated Nuclear Data File, developed by H. Honeck, is divided into two parts, ENDF/A and ENDF/B.

Specifications for ENDF/A are described in Ref. 1. The File presently contains UKAEA, KAPL, and GA data. Additions are made whenever significant data are received in the ENDF/A format.

Specifications for ENDF/B are contained in Ref. 3. ENDF/B is a cooperative effort among U.S. Laboratories organized by the USAEC Division of Reactor Development and Technology and coordinated by the Cross Section Evaluation Center at BNL. It is the objective of the participants (the Cross Section Evaluation Working Group) to assemble a library of recent evaluations for materials of interest to reactor designers. The materials presently included in the system are listed in Table 1 together with the Laboratory responsible for the selection of data. New materials will be added in the future.

Table 2 summarizes the characteristics of the Evaluated Nuclear Data Files A and B.

A.2.2 AVAILABILITY OF ENDF DATA

ENDF material is available to U.S. users from the National Neutron Cross Section Center (NNCSC) at BNL and to ENEA countries from the Neutron Data Compilation Centre at Saclay. Others can receive data from BNL provided bilaterial agreements exist for the exchange of neutron data or USAEC approval can be obtained.

A.2.3 TESTING OF ENDF/B DATA

The ENDF/B Library was assembled to increase the amount of

cross section data in a single format available to the reactor designer. Due to the tight schedule for completing the File, the data may contain errors and may not include the most recent evaluations. An iterative philosophy is used concerning ENDF/B. Periodically (perhaps annually) the File will be revised as errors become known and new data becomes available. For some materials, several revisions, or several years, may be necessary before ENDF/B will constitute a good set of data. In the meantime, the completeness of the File suggests that it can be used as a reference set of data for reactor calculations.

Table 1

ENDF/B DATA

Material	MAT	Laboratory	Material	MAT	Laboratory	Material	MAT	Laboratory
H-1	1001	BN	Zr-92	1079		Au-197	1037	BN
H_2O*	1002	GA	Zr-94	1080	BAPL-KAPL	Th-232	1038	BW
D-2	1003	BN	Zr-96	1081		Pa-233	1040	BAPL
D_2O*	1004	GA	ZrH*	1023	GA	U-233	1041	GA-ORNL
Li-6	1005	LASL	Nb	1024	GA	U-233 F.P.	1042	
Li-7	1006	LASL	Mo	1025	ANL	U-233 F.P.	1066	BW
Be	1007	GA	Xe-135	1026	BN	U-233 F.P.	1067	
Be-metal*	1064	GA	Sm-149	1027	BN	U-234	1043	GA
BeO*	1008	GA	Eu-151	1028	BN	U-235	1044	KAPL
B-10	1009	ORNL	Eu-153	1029	BN	U-235 F.P.	1045	
C	1010	KAPL	Gd	1030	ANL	U-235 F.P.	1068	BW
Graphite*	1065	GA	Dy-164	1031	BN	U-235 F.P.	1069	
CH_2*	1011	GA	Lu-175	1032	BN	U-236	1046	GA
N-14	1012	ORNL	Lu-176	1033	BN	U-238	1047	BW
O-16	1013	KAPL	Hf-174	1082		Np-237	1048	ID
Na	1059	APDA	Hf-176	1072		Pu-238	1050	AI
Mg	1014	ANL	Hf-177	1073		Pu-239	1051	GE
Al-27	1015	ORNL	Hf-178	1074	BAPL-KAPL	Pu-239 F.P.	1052	
Ti	1016	ANL	Hf-179	1075		Pu-239 F.P.	1070	BW
V	1017	ANL	Hf-180	1076		Pu-239 F.P.	1071	
Cr	1018	WAPD	Ta-181	1035	GE	Pu-240	1053	APDA
Mn-55	1019	BNL	W-182	1060		Pu-241	1054	GA
Fe	1020	WAPD	W-183	1061		Pu-242	1055	AI
Ni	1021	WAPD	W-184	1062	GE	Am-241	1056	ID
Zr-90	1077		W-186	1063		Am-243	1057	ID
Zr-91	1078	BAPL-KAPL				Cm-244	1058	AI

*Thermal data only

Table 2

CHARACTERISTICS OF THE DATA FILES

	ENDF/A	ENDF/B
Basic Storage Unit	Evaluated point cross section data covering a particular energy range for one reaction type and one material. Highly flexible format.	All evaluated point data for one material needed for a reactor calculation. Simple format.
Type of Data Included	All reaction types for all incident and final particle types.	Data for neutron-induced reactions required for reactor calculations.
Ordering of Data	Data stored in the order received by the ENDF center.	Ordered by material number, data type, and reaction type.
Selection and Revision of Data	No selection is made. All data is accepted and added to the master files. Hence many alternate evaluations occur.	One complete set of data for a material will be selected and stored. These data will be updated at regular intervals.
Main Usage	Storage of partial evaluations and alternate or older evaluations used as building blocks to generate complete evaluations.	Complete sets of evaluated point data used as direct input to reactor codes or codes to compute multi-group sets.

A.3 CODES

A.3.1 GASKET

GASKET is a unified code which calculates the inelastic scattering law for any material---solid, liquid, or gas. The calculation is performed in the incoherent approximation. This is generally a good approximation, since even for coherent scattering most of the interference scattering is elastic.

The scattering law $S(\alpha, \beta)$, as is well known, is defined by

$$\sigma(E_o \to E,\theta) = \frac{\sigma_b}{4\pi} \sqrt{\frac{E}{E_o}}\, e^{-\beta/2}\, S(\alpha,\beta) \qquad (1)$$

where $S(\alpha, \beta)$ is an explicit function of only two variables α and β defined as

$$\alpha = \frac{k^2}{2MT} \quad , \quad \beta = \frac{\varepsilon}{T} \qquad (2)$$

κ and ε being the neutron momentum and energy exchanges, M the atomic mass of the main scatterer, T the temperature, and σ_b the bound atom scattering cross section.*

One of the drawbacks of most of the previous codes (excepting the English program LEAP) was that they ignored this explicit dependence of S on only two variables and calculated $\sigma(E_0 \to E,\theta)$ for each set of values of E_0, E and θ of

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*We shall use a system of units in which Boltzmann's constant k_B and the neutron mass are unity.

a given energy and angular mesh. Instead, GASKET calculates S at points of a two-dimensional α, β mesh. From this two-dimensional array of S-values it is then easy to obtain the double differential cross section and the P_n scattering kernels by interpolation and integration in α- β space. This last step is actually performed by an auxiliary code called FLANGE.

The advantage of this two-step scheme is twofold: First, the number of S-values to be calculated is considerably reduced. Typically, for H_2O a mesh of 80 x 80 (α, β) points gives very satisfactory results in the energy range 0-2 eV. The minimum number of points in E_0, E, θ space required for an equivalent accuracy would be of the order of 80 x 80 x 15. For moderators with a lower cutoff frequency the savings would be even more impressive.

The second important advantage is that it takes very little time to recalculate $\sigma(E_0 - E,\theta)$ for different angular and energy meshes, since most of the computing time is spent in obtaining $S(\alpha, \beta)$, which has to be computed only once. Furthermore, the scattering law shows most of its structure at low β values, while it is rather smooth for large β's (i.e., for $\beta >> \omega_{max}$ where ω_{max} is the cutoff frequency of the material in question). This permits one to use a very fine β-mesh near the origin and a gradually coarser mesh as β increases. Clearly, such a fine mesh for small energy exchange at all initial energies between, say 0 and 2 eV, would require a hopelessly large total number of points if $\sigma(E_0 - E,\theta)$ were calculated at each angle-energy mesh point as in previous codes.

The keystone of GASKET is the use of numerical methods for evaluating Fourier transforms. For most scattering systems occurring in practice the Fourier transform $\chi(\alpha, t)$ of the scattering law can be expressed in a relatively simple analytical form. GASKET evaluates this so-called intermediate scattering function and does the Fourier inversion numerically. Using conventional numerical integration schemes, one runs into the difficulty of rapidly oscillating integrands at large values of β. This problem, however, is avoided by approximating χ by a piecewise linear function and integrating analytically over each linear segment. Due to detailed balance, the scattering law $S(\alpha, \beta)$ is an even function of β; hence its Fourier transform

$$\chi_{sym}(\alpha,t) = \int_{-\infty}^{\infty} e^{-i\varepsilon t} S(\alpha,\beta)\, d\varepsilon \tag{3}$$

is an even function of t. Although it would seem convenient to take advantage of this symmetry, it turns out that due to numerical problems arising for large values of β it is necessary to work with the nonsymmetric form defined by

$$\chi(\alpha,t) = \int_{-\infty}^{\infty} e^{-i\varepsilon t} \mathcal{S}(\alpha,\beta)\, d\varepsilon \tag{4}$$

where $\mathcal{S}(\alpha, \beta) = e^{-\beta/2} S(\alpha, \beta)$.

A relatively small number of dynamical modes are sufficient for characterizing the scattering from practically any material. The different

dynamical modes which can be handled by GASKET are the following:

1. Free translation (low density monoatomic gas)
2. Diffusive or Brownian motion
3. Harmonic isotropic vibrations with continuous
4. Harmonic anisotropic vibrations with continuous frequency spectrum
5. Harmonic isotropic vibrations with discrete frequency spectrum comprising up to 2 oscillators.

Any one or all of these modes may be present simultaneously, the only exception being that Modes 1 and 2 are mutually exclusive. At present the code is operational for all modes except Mode 4 (anisotropic vibrations).

A common feature of all the listed modes, excepting anisotropic vibrations, is that their intermediate scattering function is exponential in α:

$$\chi_i = e^{\alpha G_i(t)} \tag{5}$$

When more than one mode contributes to the scattering, the resulting χ - function is the product of the partial χ-functions which are then combined in the simple form

$$\chi = \exp\left[\alpha \sum_i w_i G_i(t)\right] \tag{6}$$

where the w_i's are weight factors normalized to one.

$$\sum_i w_i = 1 \tag{7}$$

In order to use the code properly, it is convenient to have an idea of how it works. The simplest way of explaining this is by means of an example. A convenient example is H_2O because it is one of the most general cases. Three dynamical modes contribute to the scattering law of H_2O computed for the ENDF:

1. Free translation of H_2O molecule: $w_1 = \frac{1}{18}$
2. Hindered rotations characterized by a continuous frequency spectrum: $w_3 = \frac{4}{9}$
3. Internal vibrations with two discrete frequencies: $w_5 = \frac{1}{2}$.

Hence, the intermediate scattering function has the form

$$\chi = \chi_1 \chi_3 \chi_5 \tag{8}$$

The code splits $\chi_{1,3}$ into two parts

$$\chi_{13}(t) = \chi_1(t)\left[\chi_3(t)-\chi_3(\infty)\right] + \chi_1(t)\chi_3(\infty) \tag{9}$$

where $\chi_3(\infty) = D$ is the so-called Debye-Waller factor. Thus the second term of the preceding expression describes the zero-phonon or quasi-elastic scattering. Its Fourier transform $S_{13}^{(2)}$ is done analytically. This separation of the asymptotic value of χ_3 considerably improves the convergence of the Fourier transform of the first term, which is done

numerically by evaluating the integral

$$S_{13}^{(1)} = \frac{e^{\beta/2} D}{\pi} \int_0^\infty dt \left[Q(t) \cos \lambda t + R(t) \sin \lambda t \right] \tag{10}$$

with

$$\lambda = (\beta + w_1 \alpha) T \tag{11}$$

Finally, the Fourier transform of the complete intermediate scattering function $\chi_{13}\ \chi_5$ is obtained by convolution with the two discrete oscillators of Mode 5

$$S(\alpha,\beta) = \int S_{13}\ (\alpha,\omega-\beta)\ S_5(\omega)\ d\omega \tag{12}$$

This convolution is done recursively and by interpolation for $S_{13}^{(1)}$ and analytically as a double sum for $S_{13}^{(2)}$. The printed output of GASKET gives the total $S(\alpha, \beta)$ as well as the components $S^{(1)}$ and $S^{(2)}$. The punched output is optional.

When the code is used for the first time for a new material, it is necessary to establish a convenient time mesh and time cutoff for the Fourier integrals. For this purpose, it is possible to print out the functions Q(t) and R(t). A rule of thumb for a first trial is

$$t_{max} > 20\ \pi / \omega_{min}$$

and (13)

$$\Delta t < \frac{2\pi}{5\ \omega_{max}}$$

where ω_{min} is the lowest peak frequency and ω_{max} is the cutoff of the frequency spectrum.

In addition, the α and β meshes must be carefully chosen. A fine β mesh is especially important for $\beta<\omega_{max}/T$ since in this region and for low α, the scattering law shows most of its structure. A fine α mesh for small α's is important in the case of non-solid moderators because of the singular behavior of the scattering law at $\alpha = 0$. The code allows for either an arbitrary input α,β mesh or else a regular mesh which is spaced arithmetically for small α,β values and logarithmically beyond limiting values specified by input.

Other important input numbers are the maximum number of phonons to be retained in the convolution with the discrete oscillators. A good estimate is

$$N_i \geq T\ \beta_{max}/\omega$$

Finally, it is worth mentioning that the code has the option of evaluating χ_3 in the short time collision approximation for α or β larger than two input numbers α_{sw} and β_{sw} ($\alpha_{sw} = \beta_{sw} = 100$ if left blank). This considerably speeds up the calculation, since in this case no time integrals have to be performed. Of course it is clear that when $w_3 = w_5 = 0$, the scattering law is calculated analytically over the whole α,β interval.

The following pages give the input instructions for GASKET.

INPUT FOR GASKET

Item	Columns	Format	Code Symbol	Report Symbol	Description
1	1-72	12A6	HØL		Title Card
2	1-5	I5	NT		Number of time points. If NT > 0, NT values of T will be read. If NT < 0, |NT| sets of ΔT and Tmax will be read. (Note 1)
	6-10	I5	NP		Number of α values (NP ≤ 80)
	11-15	I5	NE		Number of β values (NE ≤ 150)
	16-20	I5	NDAM		Damping option (Note 2)
	21-25	I5	NGPRT		G function print option. NGPRT = 0 to omit, = 1 to print.
	26-30	I5	NCP		Q and R function print option. NCP = 0 to omit, = 1 to print.
	31-35	I5	NMESH		Mesh choice option. NMESH = 0 to read α and β meshes, = 1 to calculate meshes using subroutine MESH, = -1 to read the α mesh and calculate the β mesh.
	36-40	I5	NREST		Restart indicator. NREST = 0 for a new problem = the number of the α value at which to begin for a restart problem. (Note 3)
	41-45	I5	NCVP		Convolution print option. NCVP = 0 to omit, = 1 to print.
	46-50	I5	NSEP		Separate S_1, S_2, output option. NSEP = 0 to punch combined $S_1 + S_2$, = 1 to punch $S_1 + S_2$, S_1, and S_2.
	51-56	I5	IPG		Precalculated H and F option. IPG = 0 to calculate H and F functions (GC and GS in the code) from an input frequency spectrum, = 1 to read already calculated values.
3	1-5	I5	JS3		Number of points in distributed frequency spectrum. If JS3 > 0, values of the frequencies will be read. If JS3 < 0, the maximum frequency is read and |JS3| evenly spaced values are calculated. (JS3 ≤ 100)

Item	Columns	Format	Code Symbol	Report Symbol	Description
	6-10	I5	JS4		Number of points in anisotropic part of the frequency spectrum. JS4 < 0 as for JS3. (JS4 ≦ 100)
	14-15	I5	JS5		Number of discrete oscillators. (JS5 ≦ 2 if $W_1 \neq 0$, JS5 ≦ 20 otherwise)
4	1-50	5E10	W1-W5		Weight of Mode 1-5. (not necessarily normalized)
5	1-50	5E10	T1-T5		Temperature of Mode 1-5. (eV)
	51-60	E10	TEMP	T	Over-all temperature for all modes. If left blank or 0, TEMP = max(T1, ..., T5).
6	1-10	E10	AM	M	Mass of scatterer. (amu) (The code divides this value by the neutron mass.)
	11-20	E10	DC	d	Diffusion constant.
	21-30	E10	BETSW	β_{sw}	β value above which short collision time (SCT) approximation is used, if $\alpha \geq$ ALPSW. BETSW = 100 if left blank.
	31-40	E10	ALPSW	α_{sw}	α value above which SCT approximation is used for all β. (ALPSW = 100 if left blank)
	41-50	E10	CRIT 1		Criterion used in recursive convolution of S_1 with a delta line. (CRIT1 = 0.001 if left blank)
	51-60	E10	CRIT 2		Criterion used in analytical convolution of S_2 with delta lines. (CRIT2 = 0.001 if left blank)
	61-70	E10	CRIT 3		Criterion for truncating time integrals. (CRIT3 = 0.00001 if left blank) (Note 4)

Item	Columns	Format	Code Symbol	Report Symbol	Description
		If JS3 = 0, Skip Cards 7 and 8 If IPG ≠ 0, Skip Cards 7 and 8			
7	1-70	7E10	X3	ω	If JS3 > 0, JS3 values of the frequency are read (eV). If JS3 < 0, X3(|JS3|) is read, and X3(I) = (I-1)X3(|JS3|)/|JS3|, I=1, . . . , |JS3|.
		If JS3 < 0 and X3(|JS3|) < 0, Skip Card 8 (Note 5)			
8	1-70	7E10	Q3	$f(\omega)$	Distributed frequency spectrum, Mode 3. (Unnormalized)
		If JS4 = 0, Skip Cards 9 and 10			
9	1-70	7E10	X4	ω	As in Cards 7 and 8 for Mode 3.
10	1-70	7E10	Q4	$f(\omega)$	
		If JS5 = 0, Skip Cards 11-13			
11	1-70	7E10	X5	ω_k	Frequencies of delta lines, Mode 5. (eV) ($\omega_1 < \omega_2 < \ldots < \omega_{JS5}$)
12	1-70	7E10	Q5	a_k	Weights of delta lines, Mode 5.
13	1-70	7I10	NPHØN		Maximum number of phonon terms calculated for the corresponding delta lines. NPHØN ≤ 20 for each line.
		If NMESH = 0, Skip Card 14			
14	1-10	E10	EMAX	E_{max}	Maximum energy of mesh chosen. (eV)
	11-20	E10	DALPHA	$\Delta\alpha$	α interval. (α_1 = DALPHA, α_2 = 2·DALPHA, . . . , α = ALPHAC)
	21-30	E10	ALPHAC	α_c	α value at which mesh spacing begins increasing geometrically.

Item	Columns	Format	Code Symbol	Report Symbol	Description
	31-40	E10	DBETA	$\Delta\beta$	β interval. ($\beta_1 = 0$, β_2 = DBETA, β_3 = 2 DBETA, . . . , β = BETAC)
	41-50	E10	BETAC	β_c	β value at which mesh spacing begins increasing geometrically.
		If NMESH > 0, Skip Cards 15 and 16			
15	1-70	7E10	ALPHA	α	α mesh
		If NMESH < 0, Skip Card 16			
16	1-70	7E10	BETA	β	β mesh ($\beta \geq 0$)
		If IPG = 0, Skip Cards 17-19			
17	1-10	E10	TBAR	$\overline{T}$	Effective temperature for Mode 3 (eV).
18	1-80	8E10	T	t	Integration time values (sec).
19	1-80	8E10	GS, GC	H, F	Values of the pre-calculated GS and GC functions, in the order (GS(I), GC(I), I=1, NT).
		If NT < 0, Skip Card 20			
20	1-70	7E10	T	t	Integration time points (eV^{-1})
		If NT > 0, Skip Card 21			
21	1-10	E10	DT	Δt	Δt (eV^{-1}) for time mesh.
	11-20	E10	TMAX		t max (eV^{-1}) (|NT| sets, see Note 1)
22	1-10	I10	ID		Numeric identification for S(α, β) deck.

Item	Columns	Format	Code Symbol	Report Symbol	Description
	11-20	I10	NPT		$S(\alpha, \beta)$ output option. NPT = 0 to punch on cards, NPT = 1 to write a binary output tape, NPT = 2 to do both.
	21-30	E10	SIGF	σ_f	Free atom cross section. (barns)
	31-40	E10	EPS		Significance Criterion for $S(\alpha, \beta)$ output. (Note 6, Note 7) |
		If NREST ≧ 0, Skip Card 23			
23					$S(\alpha, \beta)$ deck in ENDF/A format. (Note 8) |

Note 1. If $|NT1| < 0$, t starts at 0 and increases by Δt_1 until $t \geqq t_{max_1}$, then by Δt_2 up to $TMAX_2$, and so on up to $TMAX_{|NT|}$.

Note 2. If NDAM = 0, Parts 1 and 2 of S will be calculated if $W1 \neq 0$. If NDAM = 1 only S1 will be calculated, and the Mode 1 contribution (free gas) is only used to damp the Q and R functions.

Note 3. A tape containing $S(\alpha, \beta)$ for $\alpha = \alpha(1), \ldots, \alpha$ (NREST-1) must have been saved.

Note 4. Time integrals are cut off at t i if $\max(\sum_{j=i}^{i+19} Q_j, \sum_{j=i}^{i+19} R_j)/Q_1 \leqq CRIT3$.

Note 5. If $JS3 < 0$ and $X3(|JS3|) < 0$, a Debye spectrum, $f(\omega_3) = \omega_3^2$, will be calculated.

Note 6. If $S(\alpha, \beta) \times e^{\beta/2} < EPS \cdot \text{Max}\,(S(\alpha, \beta) \times e^{\beta/2})$, this (α, β) point is not punched. $EPS = 10^{-6}$ is an adequate choice.

Note 7. If Card 22 is blank, punching and error map printout are skipped and code returns to Card 23 for next input. |

Note 8. If $NREST < 0$, a previously calculated $S(\alpha, \beta)$ deck is read and all α points from $|NREST|$ on are re-calculated. |

A. 3. 2 GAKER[5]

The original version of GAKER was coded to compute the double differential scattering cross section for Nelkin's discrete oscillator model.[6] This model allows for free translations, a hindered rotational oscillator and several vibrational oscillators. The treatment of each oscillator depends on the initial neutron energy E and some input switching criteria E_c. In general, for $E_{cn} < E < E_{cn+1}$ oscillator n is treated exactly, oscillator n + 1 is treated with a two-term phonon expansion, oscillators 1, 2... n - 1 are treated in the short collision approximation and oscillators n + 2, n + 3... are treated in the elastic limit.* Each oscillator has a frequency ω with weight 1/M. The sum of the reciprocal masses must be normalized to 1.

The double differential cross section is related to the scattering law by:

$$\sigma(E_o \rightarrow E, \Omega) = \frac{\sigma_b}{4\pi}\sqrt{\frac{E}{E_o}}\, e^{-\beta/2}\, S(\alpha, \beta) .$$

The original GAKER was coded to read in a set of energies and scattering angles and to compute the double differential cross section and its first three Legendre moments. A modified version computes a set of α and β values and calculates $S(\alpha, \beta)$. In this modified version the switching depends on β rather than on the initial energy E. This is also an option in the original code. The input for the modified version of GAKER follows.

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*In its present version GAKER allows for a maximum of four oscillators.

INPUT FOR GAKER

Card	Col	Format	Code Symbol	Description
1	1-72	12A6	HOLREC	Comments
2	1-5	I5	ID	An identification number (negative)
	6-10	I5	NR	Number of vibrational osc.
	11-15	I5	IBX	Number of β mesh points
	16-20	I5	IZX	Number of α mesh points
3	1-10	E10.5	T	Temperature (T^{o} ev/.0253)
	11-20	E10.5	EC1	First Switching Criterion (ev/.0253)
3	21-30	E10.5	EC2	Second Switching Criterion (ev/.0253)
	31-40	E10.5	SIGF	Free atom scattering cross section (barns)
	41-50	E10.5	EPS	Punching Criterion ($\sim 10^{-6}$)
	51-60	E10.5	EMAX	Max. Energy Considered (ev)
	61-70	E10.5	AMASS	Scatterer mass (AMU)
4	1-10	E10.5	RT	Temperature (ev)
	11-20	E10.5	MT	Translational Mass
	21-30	E10.5	MR	Rotational Mass
	31-40	E10.5	WR	Rotational Frequency (ev)
5	1-10	E10.5	MV1	Mass of First Vibrator
	11-20	E10.5	W1	Frequency First Vibrator (ev)

Card	Col	Format	Code Symbol	Description
	21-30	E10.5	MV2	Mass of 2nd Vibrator
	31-40	E10.5	W2	Frequency of 2nd Vibrator (ev)
	41-50	E10.5	MV3	Mass of 3rd Vibrator
	51-60	E10.5	W3	Frequency of 3rd Vibrator (ev)
6	1-10	E10.5	EMAX	This card same as for GASKET Card 14
	11-20	E10.5	DALPHA	
	21-30	E10.5	ALPHAC	
	31-40	E10.5	DBETA	
	41-50	E10.5	BETAC	

A. 3. 3 HEXSCAT[7]

The HEXSCAT code calculates the Legendre moments P_o through P_5 of the coherent elastic neutron scattering cross section for a polycrystalline scatterer with hexagonal structure. These moments rather than the angle dependent elastic cross section are put on the ENDF/B tape. In order to recover the angular dependence of the elastic scattering one must use FLANGE II which gives the corresponding expansion in spherical harmonics.

The version of HEXSCAT used for computing the tabulated ENDF/B data is slightly different from the one described in the reference. While the original version computes group averages, the modified code gives point values of the elastic cross section. The energy points are calculated for E < EXACT and read in for E > EXACT (EXACT being an input quantity). The calculated energy points are evenly spaced between Bragg peaks with two points in the immediate vicinity of each peak, one just below and the other just above the peak energy. The small energy difference between the points adjacent to a peak and the actual Bragg energy is an input number called ESEP in the code (see input instructions following below).

INPUT FOR MODIFIED HEXSCAT

Card	Col	Format	Code Symbol	Description
1	1-80	13A6, A2	HOL	Comments
2	1-10	E10.5	SCOH	Coherent Scattering Cross Section (barns)
	11-20	E10.5	A	Magnitude of base plane lattice vector (cm)
	21-30	E10.5	C	Magnitude of lattice vector out of base plane (cm)
	31-40	E10.5	AMASC	Scatterer mass (AMU)
	41-50	E10.5	EXACT	For ENDF data code computes energy mesh for E < EXACT and reads in higher E (Ev), see EIN

Card	Col	Format	Code Symbol	Description
2 (cont)	51-60	I10	ID	ENDF/B ID number
	61-70	E10.5	ZA	ENDF/B mass number identification
	71-80	E10.5	AWR	ENDF/B mass value (neutron mass units)
3	1-5	I5	NES	Total number of energy points read in - see EIN
	6-10	I5	NTS	Number of Temperatures
	11-15	I5	NAV	Ignored for ENDF version
	16-20	I5	NXAV	Number of energy points computed between peaks
	21-25	I5	IP	Must be nonzero for this version
	26-30	I5	NCOS	Ignored for ENDF version
	31-35	I5	NPCH	$\neq 0$ to punch cards for ENDF/B
	36-40	I5	NFORM	Code contains an expression which is unique for each material 1 = Be,2 = BeO,3 = C
	41-50	E10.5	ESEP	Absolute value of smallest energy difference (eV), between calculated mesh points and Bragg peaks
4	1-70	7E10.5	EIN	Energies: $E_1 = E_{min}$, E_2 = EXACT; E_3, $E_4 \ldots E_{NES}$ are input energies (eV) for E > EXACT
5	1-70	7E10.5	WAL 2	Debye-Waller Integral/AMSC; NTS values
6	1-70	7E10.5	TMP	Temperatures, NTS values.

A.3.4 ZREND

This code calculates Legendre moments of the incoherent elastic cross section and was written explicitly to compute the cross section of hydrogen as bound in ZrH_x for ENDF/B. The Legendre moments are:

$$\sigma_n(E) = \frac{\sigma_b}{2} \int_{-1}^{1} P_n(\mu) \exp\left[-\frac{2EW}{A}(1-\mu)\right] d\mu, \quad n = 0, 1, \ldots 5 ,$$

where W is the Debye-Waller integral and A the atomic mass.

For high energies the moments are calculated recursively. For low energies the recursive calculation of the integrals blows up numerically and it is necessary to expand the exponential. Although the expansion is good for all energies the code has incorporated the feature of switching to the recursive method for $\frac{2EW}{A} > E_{switch}$.

INPUT FOR ZREND

Card	Col	Format	Code Symbol	Description
1	1-80	13A6,A2	COM	Comments
2	1-5	I5	NT	Number of temperatures
	6-10	I5	NE	Number of energies
	11-20	E10.5	SB	Bound atom cross section
	21-30	E10.5	SWITCH	E_{switch}
	31-40	E10.5	EPS	Criterion for expansion termination
	41-45	I5	NPCH	NPCH $\neq$ 0 for punching of $\sigma_n(E)$
3	1-70	7E10.5	T	Temperature ^{o}K; NT values
4	1-70	7E10.5	WP	W/A (eV^{-1}); NT values
5	1-70	7E10.5	E	Energies; NE values (eV)

A.4 REFERNCES FOR SECTIONS A.1, A.2, AND A.3

1. H. Honeck, Evaluated Nuclear Data File Description and Specifications. BNL 8381 (June 1964).

2. Theoretical and Experimental Neutron Spectra, General Atomic Report GA-5319 (May 1964).

3. H. Honeck, ENDF/B Specifications for an Evaluated Nuclear Data File for Reactor Applications, BNL 50066 (May 1966).

4. J. U. Koppel et al., A Unified Code for Thermal Neutron Scattering, General Atomic Report GA-7417 (Rev.) (March 10, 1967).

5. Integral Neutron Thermalization Annual Summary Report, p. 155, General Atomic Report GA-5798 (Oct. 15, 1964).

6. M. S. Nelkin, Scattering of Slow Neutrons by Water, Phys. Rev. 119, 741 (1960).

7. HEXSCAT: Coherent Elastic Scattering of Neutrons by Hexagonal Lattices, Y. D. Naliboff and J. U. Koppel, General Atomic Report GA-6026 (Dec. 15, 1964).

B. MODERATORS

MODERATOR INDEX (12/16/68)

Moderator	Page	Date Submitted to ENDF	Distinguishing Characteristic of Data
Be	Be - 1.1	4/66	Central force model
BeO	BeO - 1.1	9/66	Debye frequency spectrum
BeO	BeO - 1.1 (Rev. -12/31/69)	9/68	Shell model
C	C - 1.1	4/66	Central force model
$(CH_2)_n$	$(CH_2)_n$ - 1.1	9/66	Discrete oscillators model
$(CH_2)_n$	$(CH_2)_n$ - 1.1 (Rev. -12/31/69)	6/69	Model of noninteracting infinite chains of CH_2 radicals
C_6H_6	C_6H_6 - 1.1	3/68	Normal mode calculation of frequency spectra
D_2O	D_2O - 1.1	8/66	Torsional frequency band plus discrete oscillators
H_2O	H_2O - 1.1	4/66	Torsional frequency band plus discrete oscillators
UC	UC - 1.1	6/69	Central force model
UO_2	UO_2 - 1.1	9/68	Shell model
Z_rH_n	Z_rH_n - 1.1	8/66	Debye acoustical band plus Gaussian optical band about 0.13705
Z_rH_n	Z_rH_n - 1.1 (Rev. -12/31/69)	3/68	Central force model

BERYLLIUM

1. Physics

Using the incoherent and isotropic approximations, one finds that the scattering cross section for thermal neutrons depends solely upon the phonon spectrum of the lattice vibrations. Thus the inelastic scattering or the scattering kernel is determined once one computes the phonon spectrum. The force constants of the beryllium lattice dynamics have been measured by R. E. Schmunk, et al.[1] upon the assumption that the forces in beryllium are central and extend out to fifth nearest neighbors. These force constants are measured in the sense that the calculated dispersion curves were fit by a least squares method to the experimental ones. Using this force model the phonon spectrum was calculated by the root sampling method. The computed phonon spectrum gives good agreement with the measured specific heat.

The elastic scattering cross section was computed from the known lattice structure (hexagonal close-packed). Both infinite medium and angular-dependent spectral comparisons show that the scattering kernel computed by the above method gives good agreement with experiment.

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[1] R. E. Schmunk, R. M. Brugger, P. D. Randolph, and K. A. Strong, Phys. Rev. 128 (1962) 562.

2. Frequency Spectrum for Be