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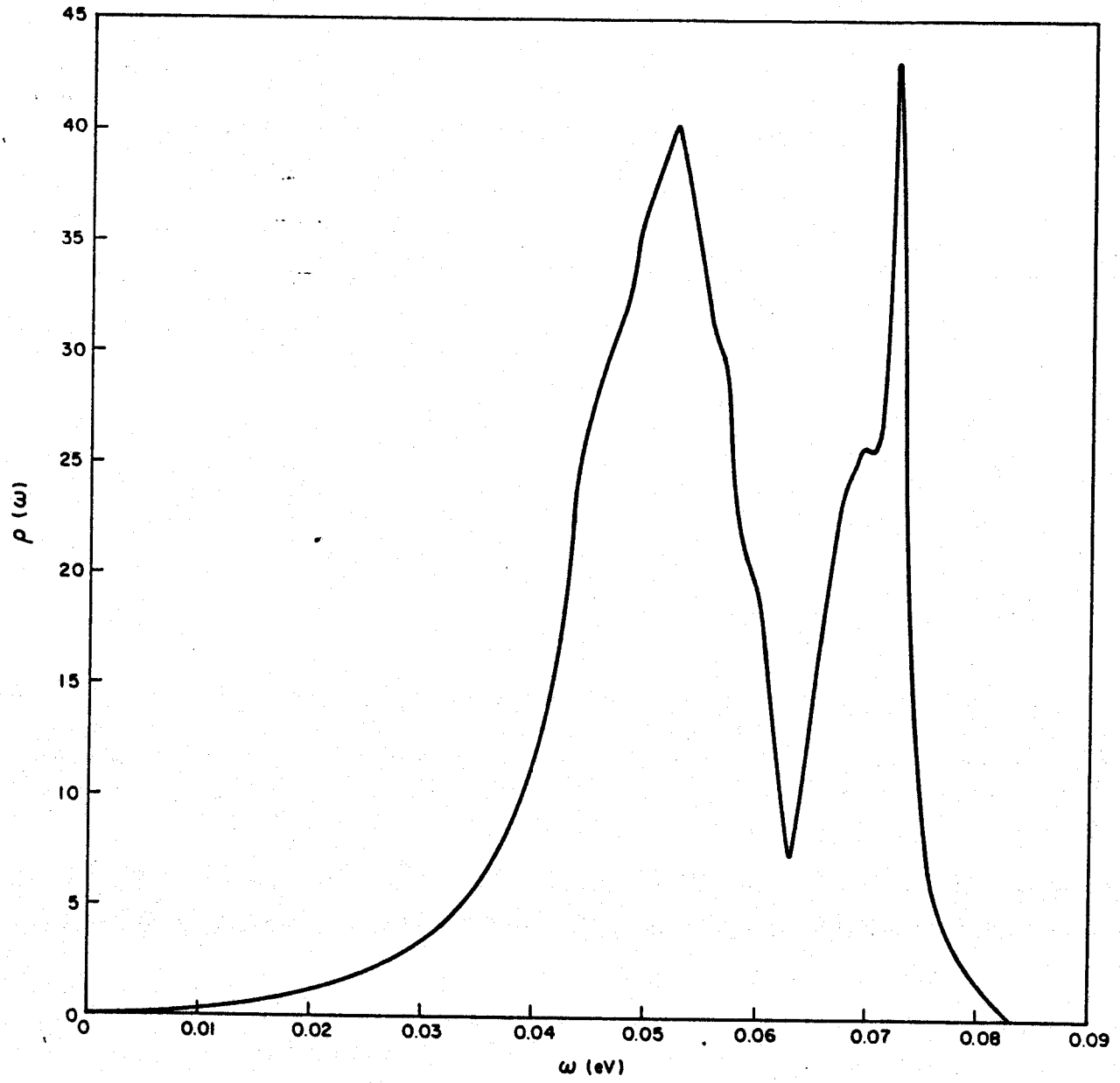
[1] R. E. Schmunk, R. M. Brugger, P. D. Randolph, and K. A. Strong, Phys. Rev. 128 (1962) 562.

2. Frequency Spectrum for Be



3.1 GASKET Input for Be at 296°K

The code GASKET is discussed in Section A. 3. The data tabulated below follows the format of the code input instructions also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6,A2	COM Be at 296°K
2	11I5	NT -8 NP 50 NE 80 NDAM 1 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 -54 JS4 0 JS5 0
4	5E10	W1 .002 W2 0.0 W3 1.0 W4 0.0 W5 0.0
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 0.0 T5 0.0
6	7E10	AM 9.01 DC 0.0 BETSW 15.0 ALPSW 15.0 CRIT1 0.0
		CRIT2 0.0 CRIT3 0.0
7	7E10	X3 .082948

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
8	7E10	Q3 .00312 .025 .06 .115 .17 .235
		.308 .39 .475 .595 .775 1.052
		1.1482 1.6233 1.5653 1.7423 2.4289 2.8072
		3.2863 3.7577 4.4397 5.4924 6.3315 7.6421
		9.5339 12.1016 15.0553 22.0154 26.6382 29.3387
		32.6036 35.777 37.6536 40.3845 37.1196 32.39
		29.8269 21.2831 18.9488 13.0186 7.33848 12.5075
		18.9031 23.5564 25.6923 25.5855 43.0544 17.8656
		6.81975 3.98963 2.99184 1.6843 .65772 0.0
9	Cards 9 and 10 are not needed	
10		
11	7E10	X5
12	7E10	Q5
13	7I10	NPHON
14	5E10	EMAX 1.0 DALPHA .25 ALPHAC 3.0 DBETA .15 BETAC 4.0
15, 16, 17, 18, 19 and 20 are not needed		
21	2E10	DT .025 TMAX .1
		.05 1.0
		.125 10.0
		.25 20.0
		.5 100.0
		1.0 150.0
		3.0 200.0
		10.0 4000.0
22	2I10 2E10	ID 24 NPT 0 SIGF 6.10 EPS .000001
23	Card 23 is not needed	

3.2 HEXSCAT Input for Be

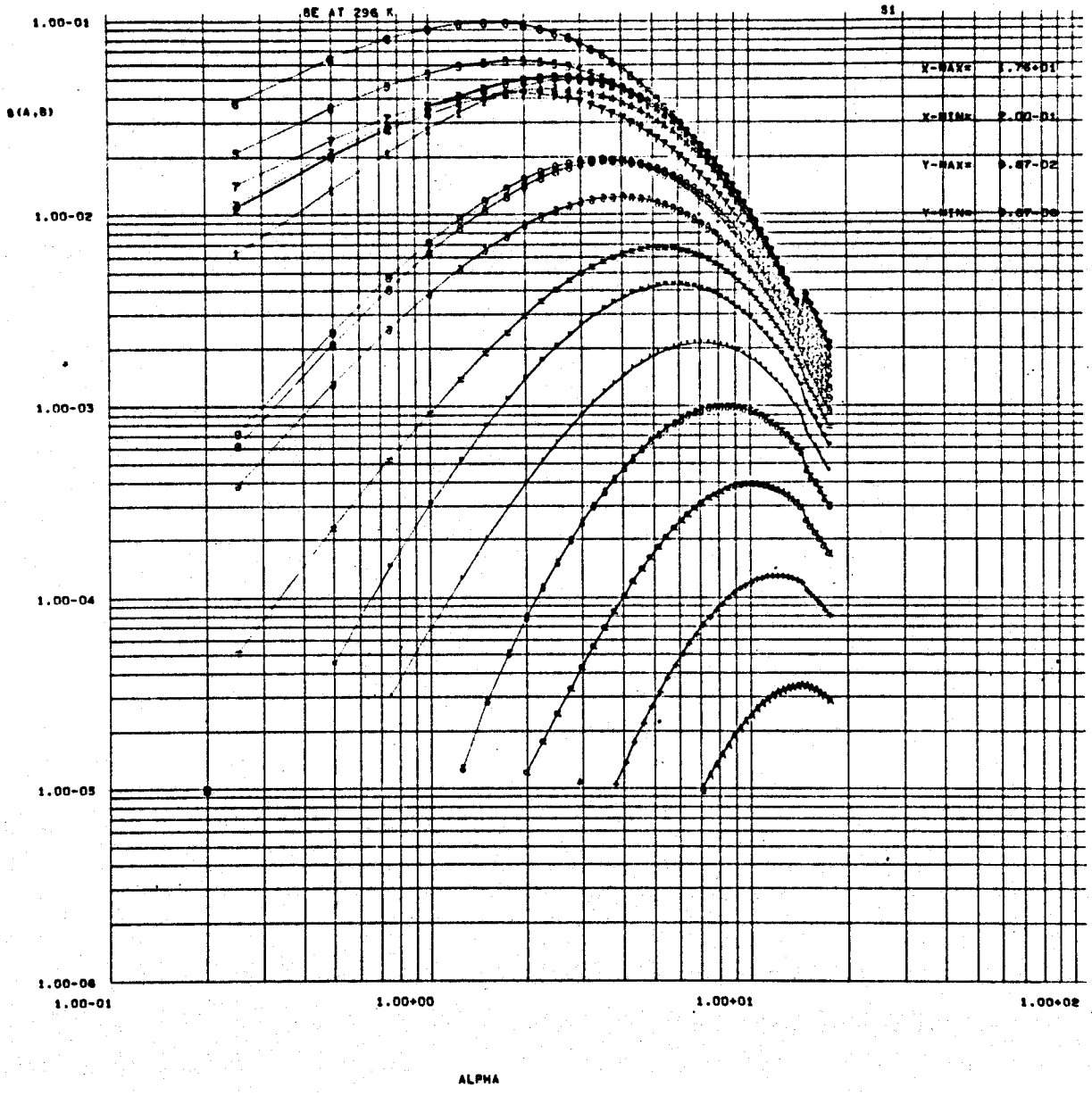
The code HEXSCAT is discussed in Section A. 3. The data tabulated below follows the format of the code input instruction also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required for the calculation.

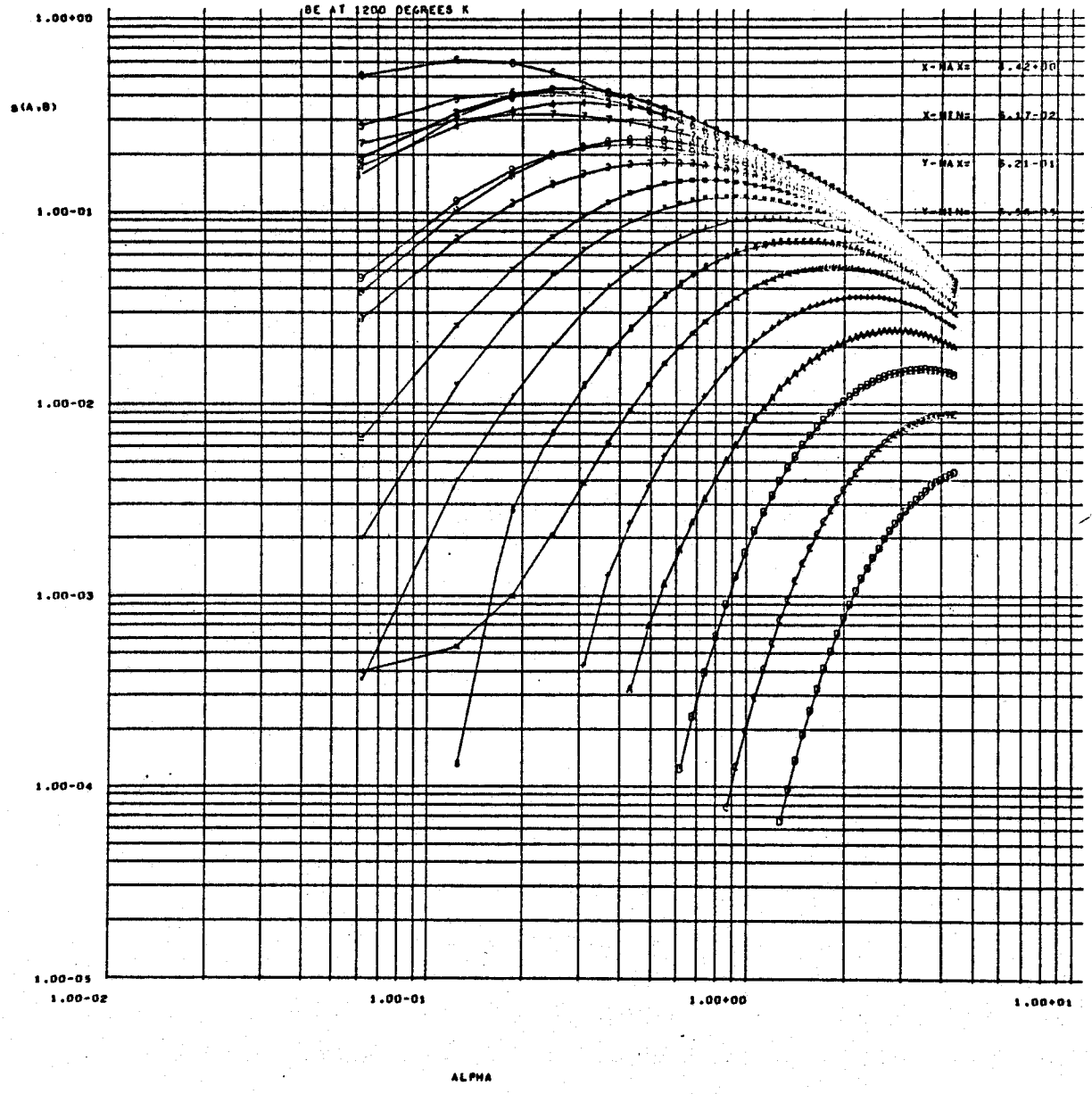
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6,A2	HOL HEXSCAT for ENDF Be
2	5E10,	SCOH 7.53 A 2.2856-8 C 3.5832-8 AMASC 9.01 EXACT .0625515
	1I10,	ID 1064 ZA 4009. AWR
3	8I5,	NES 32 NTS 8 NAV 0 NXAV 2 IP 1
	1E10	NCOS 0 NPCH 1 NFORM 1 ESEP 1.0001
4	7E10	EIN .00521943 .0625515 .06256401 .06262687 .06263940
		.06899716 .06901096 .06943835 .06945224 .07245131
		.07246580 .07298931 .07300391 .07634664 .07636191
		.07768249 .07803603 .08 .09 .092
		.099 .120 .130 .170 .220
		.270 .325 .400 .475 .575
		.800 1.0
5	7E10	WAL2 3.16663 3.88842 4.62944 5.40517 6.19880
		7.0042 8.63665 10.2865
6	7E10	TMP 296.0 400.0 500.0 600.0 700.0
		800.0 1000.0 1200.0

4. Plots of Scattering Law

β Values for Multicurve Plots

CURVE	INDEX	β(296K)	β(1200K)
1	1	0.00	0.00
2	2	.15	.037
3	3	.30	.074
4	4	.90	.222
5	5	1.50	.370
6	6	2.10	.518
7	7	2.70	.666
8	8	3.30	.814
9	9	3.90	.962
10	∂	4.55	1.12
11	=	5.33	1.31
12	"	6.27	1.55
13	'	7.42	1.83
14	δ	8.81	2.17
15	α	10.49	2.59
16	+	12.52	3.09
17	A	14.99	3.70
18	B	17.97	4.43
19	C	21.58	5.32
20	D	25.96	6.40


BE AT 296 K.
S1
X-MAX= 1.76+01
X-MIN= 2.00-01
Y-MAX= 9.67-02
Y-MIN= 9.67-06
S(A,B)
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-06
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA


BE AT 1200 DEGREES K
1.00+00
S(A,B)
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-02
1.00-01
1.00+00
1.00+01
ALPHA

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR BERYLLIUM AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00522	2.09751	-.81057	43	.02448	6.98328	-.18083
2	.00560	1.97670	-.69936	44	.02548	6.73219	-.13790
3	.00599	1.87109	-.60405	45	.02549	6.88446	-.15695
4	.00637	1.77846	-.52160	46	.02607	6.74354	-.13301
5	.00637	3.34561	-.74685	47	.02666	6.60905	-.11024
6	.00652	3.27802	-.71002	48	.02725	6.48062	-.08857
7	.00666	3.21390	-.67484	49	.02725	6.68300	-.11617
8	.00681	3.15248	-.64132	50	.02816	6.48772	-.08337
9	.00681	9.49546	-.88119	51	.02908	6.30518	-.05289
10	.00840	7.76248	-.53288	52	.02999	6.13351	-.02450
11	.01000	6.58706	-.29863	53	.03000	6.13242	-.02432
12	.01159	5.73626	-.13183	54	.03023	6.09011	-.01734
13	.01159	6.63154	-.24923	55	.03047	6.04850	-.01048
14	.01251	6.17464	-.16392	56	.03070	6.00757	-.00375
15	.01342	5.78029	-.09097	57	.03071	6.16935	-.02991
16	.01433	5.43726	-.02803	58	.03221	5.91556	.01193
17	.01434	5.43625	-.02784	59	.03371	5.68657	.04938
18	.01478	5.28684	-.00058	60	.03521	5.47933	.08294
19	.01522	5.14714	.02493	61	.03522	5.85388	.01353
20	.01566	5.01602	.04881	62	.03565	5.79242	.02379
21	.01566	6.09893	-.13779	63	.03609	5.73249	.03374
22	.01619	5.91501	-.10365	64	.03653	5.67358	.04343
23	.01672	5.74261	-.07188	65	.03654	5.78905	.02257
24	.01725	5.58028	-.04225	66	.03707	5.71869	.03424
25	.01725	5.57927	-.04207	67	.03760	5.65074	.04549
26	.01802	5.36105	-.00263	68	.03812	5.58510	.05635
27	.01879	5.16105	.03324	69	.03813	6.22625	-.05257
28	.01955	4.97695	.06596	70	.03869	6.14976	-.03939
29	.01956	6.08442	-.12842	71	.03925	6.07595	-.02668
30	.02000	5.96103	-.10577	72	.03981	6.00471	-.01440
31	.02044	5.84321	-.08419	73	.03982	6.00371	-.01423
32	.02088	5.73055	-.06362	74	.04026	5.94974	-.00493
33	.02088	5.89413	-.08963	75	.04070	5.89725	.00411
34	.02126	5.79755	-.07196	76	.04114	5.84618	.01290
35	.02164	5.70463	-.05498	77	.04115	6.21271	-.04692
36	.02203	5.61504	-.03867	78	.04173	6.14158	-.03442
37	.02203	6.81143	-.20774	79	.04232	6.07298	-.02237
38	.02218	6.77031	-.20037	80	.04290	6.00684	-.01073
39	.02232	6.72975	-.19309	81	.04291	6.17455	-.03762
40	.02247	6.68973	-.18592	82	.04362	6.09510	-.02351
41	.02247	7.55533	-.27923	83	.04433	6.01978	-.01000
42	.02348	7.25669	-.22776	84	.04503	5.94842	.00294

DATA FOR BERYLLIUM AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
85	.04504	6.17647	-.03412	127	.06238	5.89727	.03961
86	.04548	6.13152	-.02587	128	.06255	5.88823	.04133
87	.04592	6.08769	-.01784	129	.06256	5.92485	.03490
88	.04636	6.04493	-.01001	130	.06263	5.92159	.03552
89	.04637	6.11589	-.02149	131	.06264	5.99527	.02280
90	.04657	6.09629	-.01789	132	.06900	5.73915	.07209
91	.04677	6.07692	-.01433	133	.06901	5.85711	.05048
92	.04697	6.05777	-.01082	134	.06944	5.83988	.05381
93	.04698	6.19667	-.03300	135	.06945	6.01438	.02322
94	.04751	6.14598	-.02363	136	.07245	5.89457	.04694
95	.04803	6.09678	-.01455	137	.07247	5.99939	.02864
96	.04856	6.04902	-.00575	138	.07299	5.97920	.03266
97	.04857	6.04816	-.00559	139	.07300	6.08213	.01519
98	.04934	5.98148	.00667	140	.07635	6.00640	.03204
99	.05010	5.91762	.01839	141	.07636	6.14487	.00878
100	.05087	5.85645	.02958	142	.07768	6.09715	.01853
101	.05088	6.20969	-.02904	143	.07804	6.08481	.02103
102	.05170	6.14123	-.01614	144	.08000	6.04036	.03071
103	.05252	6.07582	-.00384	145	.08900	6.06915	.03295
104	.05334	6.01429	.00783	146	.10100	6.00351	.04658
105	.05335	6.22647	-.02653	147	.11300	5.97446	.05569
106	.05406	6.17402	-.01627	148	.12500	6.05891	.04620
107	.05476	6.12339	-.00641	149	.13700	6.02034	.05572
108	.05547	6.07453	.00307	150	.15200	6.03409	.05416
109	.05548	6.07378	.00321	151	.16800	6.05452	.05385
110	.05610	6.03253	.01117	152	.18400	6.02036	.05989
111	.05672	5.99253	.01885	153	.20000	6.03187	.06039
112	.05733	5.95374	.02627	154	.22400	6.04859	.06292
113	.05734	5.98329	.02121	155	.24800	6.05396	.06327
114	.05846	5.91556	.03413	156	.27200	6.06504	.06393
115	.05957	5.85144	.04624	157	.29600	6.06304	.06468
116	.06069	5.79076	.05760	158	.32500	6.05560	.06456
117	.06070	5.90991	.03626	159	.35500	6.05836	.06454
118	.06090	5.89896	.03835	160	.38500	6.06277	.06630
119	.06110	5.88812	.04041	161	.41500	6.06751	.06677
120	.06130	5.87739	.04245	162	.44500	6.06934	.06726
121	.06132	5.87674	.04257	163	.47500	6.07004	.06765
122	.06155	5.86442	.04491	164	.50500	6.07035	.06810
123	.06178	5.85223	.04721	165	.53500	6.07008	.06860
124	.06201	5.84019	.04949	166	.56500	6.06981	.06910
125	.06203	5.91557	.03610	167	.59500	6.06818	.06956
126	.06220	5.90638	.03786	168	.62500	6.06670	.06999

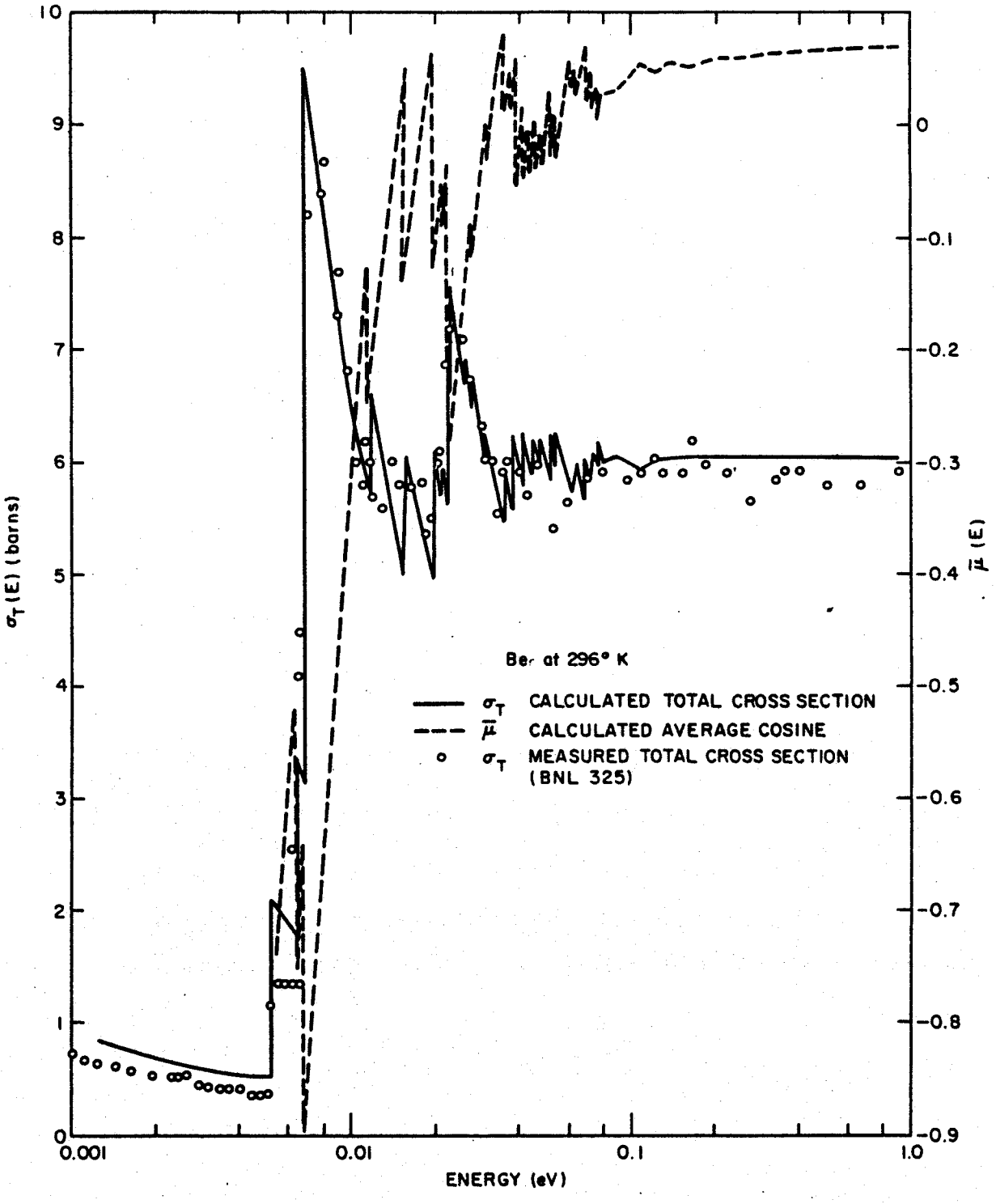
DATA FOR BERYLLIUM AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
169	.65500	6.06555	.07036	174	.80500	6.06679	.07070
170	.68500	6.06476	.07064	175	.85500	6.06962	.07025
171	.71500	6.06444	.07081	176	.90500	6.06623	.06921
172	.74500	6.06463	.07087	177	.95500	5.99581	.06371
173	.77500	6.06551	.07083				

THE ELASTIC CONTRIBUTION TO THE TOTAL CROSS SECTION WAS CALCULATED AT ALL OF THE TABULATED ENERGIES.THE INELASTIC CONTRIBUTION WAS CALCULATED ON A COARSER MESH AND WAS INTERPOLATED TO GIVE THE VALUES AT THE TABULATED ENERGIES.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV


Be at 296° K
σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
σ_T MEASURED TOTAL CROSS SECTION (BNL 325)
σ_T(E) (barns)
$\bar{\mu}$ (E)
ENERGY (eV)
0.001
0.01
0.1
1.0
0
1
2
3
4
5
6
7
8
9
10
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
-0.8
-0.9

6. Miscellaneous Notes on Beryllium

For temperatures other than 296°K the switching criteria for short collision and the α,β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral, effective temperature and ID numbers of the scattering law data on file.

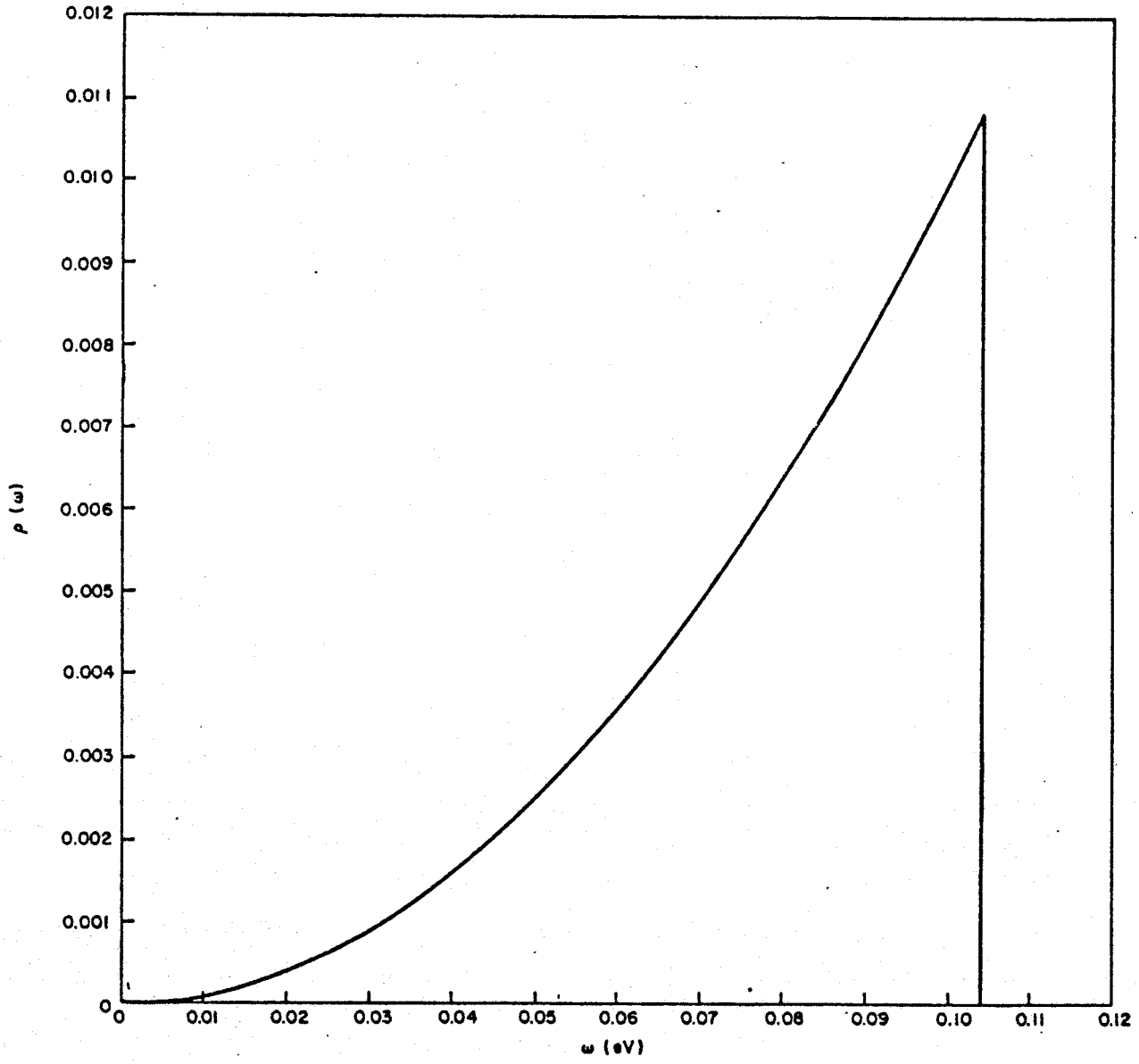
T(°K)	Debye Waller Integral (eV^{-1})	$\bar{T}$(°K)	ENDF ID No.
296	28.531	405.64	GA 0024
400	34.997	484.22	GA 0029
500	41.714	568.53	GA 0030
600	48.704	657.66	GA 0031
700	55.855	749.69	GA 0032
800	63.112	843.63	GA 0033
1000	77.822	1035.0	GA 0042
1200	92.688	1229.3	GA 0043

BERYLLIUM OXIDE

1. Physics

Beryllium oxide is a crystal formed by two interpenetrating lattices with hexagonal close packed structure, one corresponding to the Be atoms, the other to the O atoms. There are four atoms in a unit cell. The crystal has some properties of an ionic crystal and other properties of a crystal with covalent bonding. It is probably less than fifty percent ionic. While more sophisticated models for BeO have been tried, a scattering model has been made up based on the assumption of complete isotropy of the crystal. While such an assumption is of course unjustified, the resulting scattering kernel does predict neutron spectra in fair agreement with experiment. A Debye frequency spectrum was used assuming a Debye temperature of 1200°K and an average atomic mass of 12.5. The scattering law was then calculated with the code GASKET. Elastic coherent scattering for BeO has been calculated by means of HEXSCAT using the known lattice structure, and assuming a common Debye-Waller factor for both the oxygen and the beryllium atoms.

2. Debye Frequency Spectrum for BeO



CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
8	7E10	Q3
9	Cards 9 and 10 are not needed	
10		
11	7E10	X5
12	7E10	Q5
13	7I10	NPHON
14	5E10	EMAX 1.0 DALPHA .25 ALPHAC 3.0 DBETA .15 BETAC 4.0
15, 16, 17, 18, 19 and 20 are not needed		
21	2E10	DT .6 TMAX 3.0
		1.2 7.5
		1.8 30.0
		3.0 120.0
		6.0 600.0
		8.0 1500.0
		12.0 5000.0
22	2I10 2E10	ID 57 NPT 0 SIGF 9.86 EPS .000001
23	Card 23 is not needed	

3.1 GASKET Input for BeO at 296°K

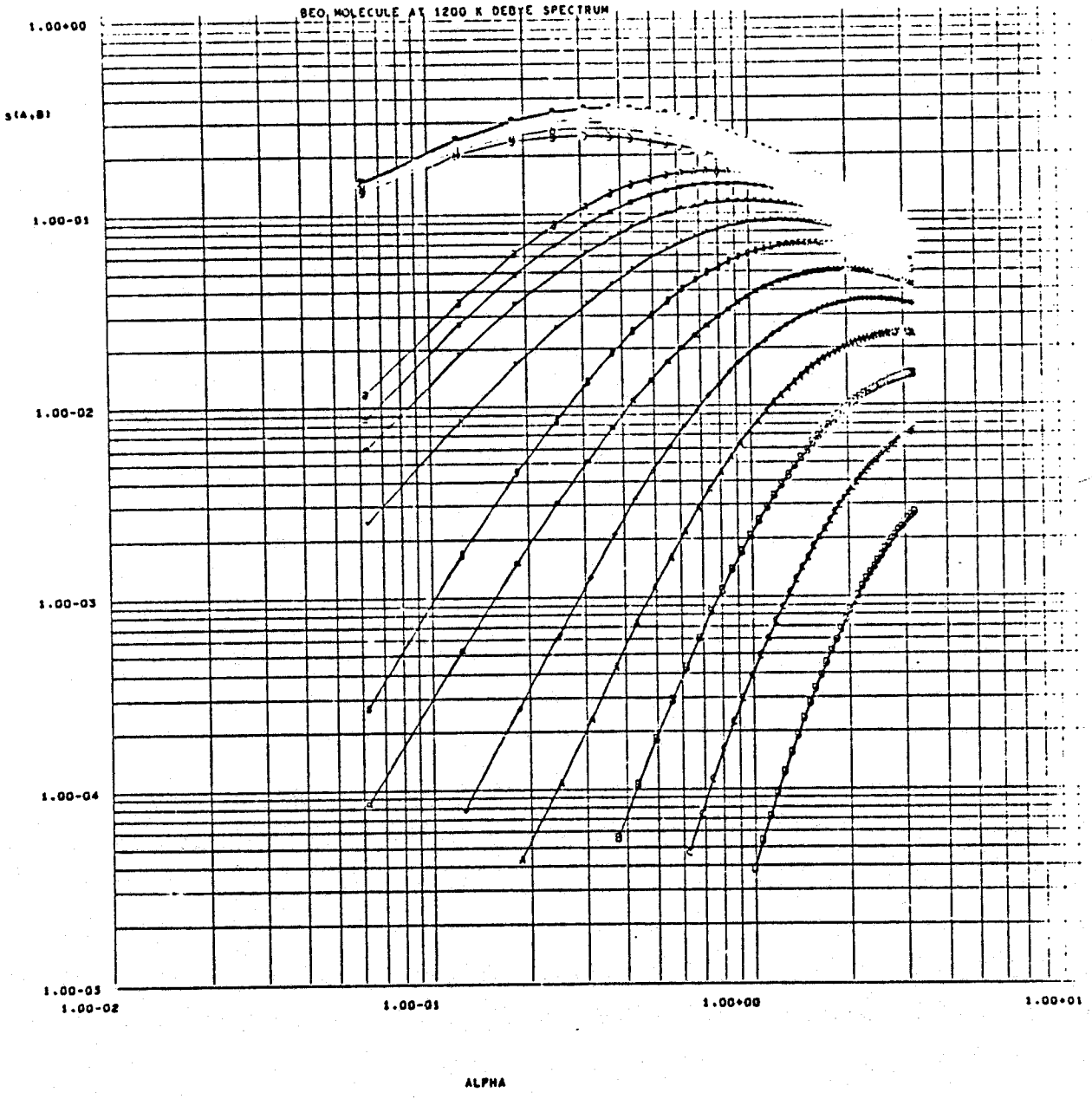
The code GASKET is discussed in Section A. 3. The data tabulated below follows the format of the code input instructions also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

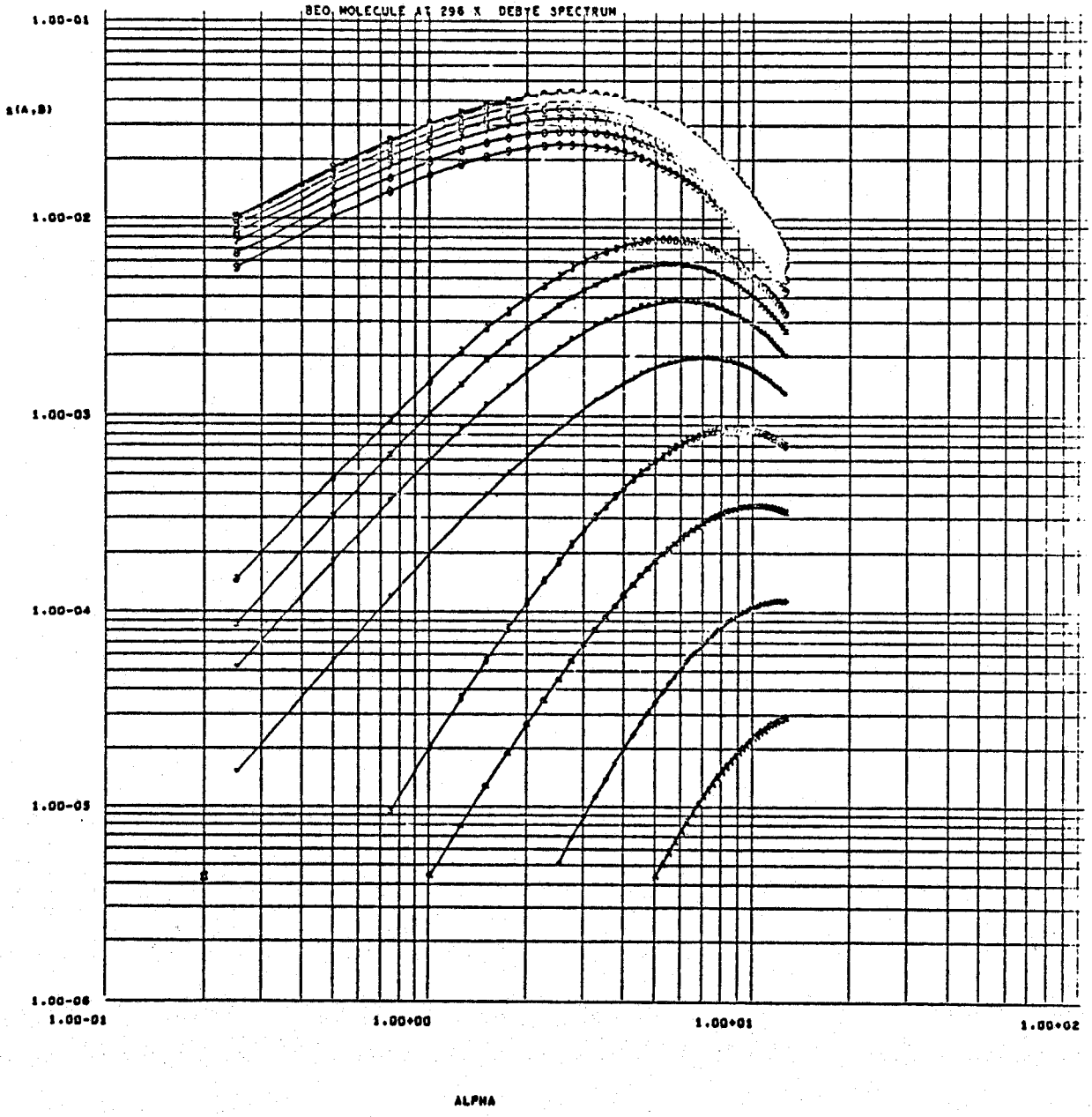
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6,A2	COM BeO Molecule at 296 K Debye Spectrum
2	11I5	NT -7 NP 50 NE 80 NDAM 1 NGPRT 0
		NCP 1 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 -80 JS4 0 JS5 0
4	5E10	W1 .001 W2 0.0 W3 1.00 W4 0.0 W5 0.0
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 0.0 T5 0.0
6	7E10	AM 12.5 DC 0.0 BETSW 0.0 ALPSW 0.0 CRIT1 0.0
		CRIT2 0.0 CRIT3 0.0
7	7E10	X3 -.104

3.2 HEXSCAT Input for BeO

The code HEXSCAT is discussed in Section A. 3. The data tabulated below follows the format of the code input instruction also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES				
1	13A6,A2	HOL HEXSCAT FOR ENDF BeO				
2	5E10,	SCOH 1.0	A 2.695-8	C 4.39-8	AMASC 12.5	EXACT .05
	1I10,	ID 1008	ZA 200.0	AWR		
3	8I5,	NES 22	NTS 8	NAV 0	NXAV 2	IP 1
	1E10	NCOS 0	NPCH 1	NFORM 2	ESEP 1.0001	
4	7E10	EIN 3.754475-3	.05	.05280088	.05281143	.05834735
		.05835902	.06442	.07132077	.07548925	.07826468
		.08325706	.09662996	.120	.130	.150
		.200	.260	.300	.425	.600
		.800	1.0			
5	7E10	WAL2 1.5862	1.8857	2.2048	2.5423	2.8913
		3.2480	3.9761	4.7161		
6	7E10	TMP 296.0	400.0	500.0	600.0	700.0
		800.0	1000.0	1200.0		

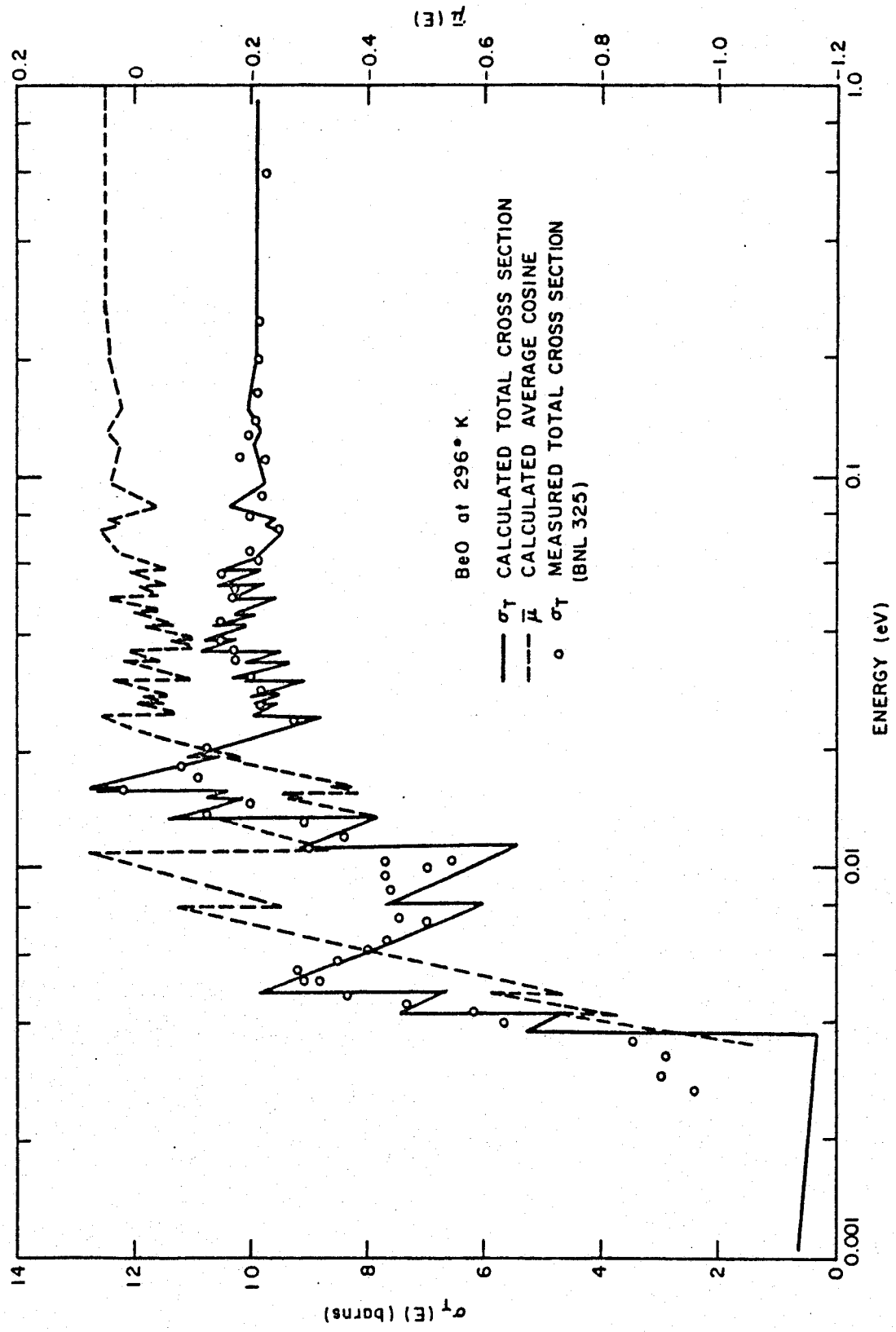

BEO MOLECULE AT 1200 K DEBYE SPECTRUM
1.00+00
S(A,B)
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-02
1.00-01
1.00+00
1.00+01
ALPHA


BEO, MOLECULE AT 296 K DEBYE SPECTRUM
1.00-01
S(A,B)
1.00-02
1.00-03
1.00-04
1.00-05
1.00-06
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA

4. Plots of Scattering Law

β Values for Multicurve Plots

CURVE	INDEX	β(296K)	β(1200K)
1	1	0.00	0.00
2	2	.15	.037
3	3	.30	.074
4	4	.90	.222
5	5	1.50	.370
6	6	2.10	.518
7	7	2.70	.666
8	8	3.30	.814
9	9	3.90	.962
10	∂	4.55	1.12
11	=	5.33	1.31
12	"	6.27	1.55
13	'	7.42	1.83
14	δ	8.80	2.17
15	α	10.48	2.58
16	+	12.51	3.08
17	A	14.97	3.69
18	B	17.94	4.42
19	C	21.54	5.31
20	D	25.89	6.39


BeO at 296° K
σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
o σ_T MEASURED TOTAL CROSS SECTION (BNL 325)
σ_T (E) (barns)
$\bar{\mu}$ (E)
ENERGY (eV)
0.001
0.01
0.1
1.0
0
2
4
6
8
10
12
14
0.2
0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2

DATA FOR BEO AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
169	.15000	10.05074	.02403	182	.53500	9.91824	.05159
170	.20000	9.92318	.04164	183	.56500	9.91450	.05200
171	.22400	9.95194	.04047	184	.59500	9.91411	.05201
172	.24800	9.91640	.04615	185	.62500	9.90988	.05242
173	.27200	9.90056	.04891	186	.65500	9.90721	.05265
174	.29600	9.92454	.04667	187	.68500	9.90546	.05278
175	.32500	9.94923	.04532	188	.71500	9.90319	.05296
176	.35500	9.89624	.04818	189	.74500	9.89990	.05323
177	.38500	9.88955	.04906	190	.77500	9.89934	.05322
178	.41500	9.92673	.05026	191	.80500	9.89678	.05340
179	.44500	9.92932	.05027	192	.85500	9.89179	.05359
180	.47500	9.91775	.05152	193	.90500	9.87097	.05375
181	.50500	9.92022	.05134	194	.95500	9.75098	.05210

THE ELASTIC CONTRIBUTION TO THE TOTAL CROSS SECTION WAS CALCULATED AT ALL OF THE TABULATED ENERGIES. THE INELASTIC CONTRIBUTION WAS CALCULATED ON A COARSER MESH AND WAS INTERPOLATED TO GIVE THE VALUES AT THE TABULATED ENERGIES.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV

DATA FOR BEO AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
85	.03053	10.35084	-.08681	127	.04331	10.30692	-.04423
86	.03101	10.19729	-.07060	128	.04333	10.30174	-.04370
87	.03150	10.04870	-.05494	129	.04334	10.29986	-.04351
88	.03199	9.90482	-.03979	130	.04391	10.17877	-.03107
89	.03200	9.90973	-.04025	131	.04448	10.06091	-.01900
90	.03259	9.74026	-.02244	132	.04504	9.94621	-.00727
91	.03319	9.57710	-.00532	133	.04505	10.31045	-.04235
92	.03378	9.41996	.01113	134	.04540	10.23837	-.03495
93	.03379	10.02387	-.04983	135	.04575	10.16750	-.02769
94	.03414	9.92763	-.03970	136	.04611	10.09778	-.02054
95	.03449	9.83343	-.02980	137	.04611	10.09597	-.02036
96	.03484	9.74122	-.02012	138	.04701	9.92332	-.00270
97	.03485	9.73940	-.01993	139	.04790	9.75770	.01419
98	.03518	9.65600	-.01118	140	.04880	9.59872	.03036
99	.03550	9.57420	-.00261	141	.04881	9.75546	.01379
100	.03582	9.49395	.00578	142	.04897	9.72718	.01668
101	.03583	10.89890	-.12394	143	.04913	9.69908	.01954
102	.03648	10.71741	-.10495	144	.04929	9.67118	.02239
103	.03713	10.54256	-.08667	145	.04930	9.98703	-.00997
104	.03779	10.37404	-.06908	146	.04935	9.97754	-.00900
105	.03779	10.37213	-.06888	147	.04940	9.96808	-.00803
106	.03787	10.35236	-.06682	148	.04946	9.95863	-.00706
107	.03795	10.33268	-.06477	149	.04947	10.27246	-.03740
108	.03803	10.31309	-.06273	150	.04960	10.24832	-.03491
109	.03804	10.81480	-.10621	151	.04973	10.22434	-.03244
110	.03809	10.80070	-.10474	152	.04986	10.20048	-.02998
111	.03814	10.78663	-.10328	153	.04987	10.34845	-.04384
112	.03820	10.77261	-.10182	154	.04991	10.34042	-.04301
113	.03820	10.85389	-.10851	155	.04996	10.33239	-.04218
114	.03932	10.56949	-.07901	156	.05000	10.32440	-.04136
115	.04043	10.30156	-.05129	157	.05280	9.85173	.00735
116	.04154	10.04881	-.02522	158	.05281	10.55524	-.05982
117	.04155	10.59007	-.07505	159	.05835	9.93095	.00822
118	.04168	10.55889	-.07184	160	.05836	10.51516	-.04782
119	.04182	10.52793	-.06864	161	.06442	9.83257	.02325
120	.04195	10.49718	-.06547	162	.07132	9.45374	.05939
121	.04196	10.60123	-.07462	163	.07549	9.77650	.02233
122	.04239	10.50244	-.06444	164	.07826	9.58484	.04278
123	.04282	10.40577	-.05448	165	.08326	10.41946	-.03688
124	.04325	10.31118	-.04475	166	.09663	9.76302	.04043
125	.04326	10.31730	-.04530	167	.12000	9.98707	.02629
126	.04328	10.31212	-.04477	168	.13000	9.83537	.04412

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR BEO AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00375	5.31846	-.94536	43	.01668	12.25262	-.31802
2	.00392	5.10697	-.86620	44	.01698	12.04307	-.29532
3	.00408	4.91227	-.79358	45	.01698	12.05358	-.29582
4	.00424	4.73243	-.72673	46	.01774	11.55216	-.24166
5	.00424	7.52647	-.82825	47	.01850	11.09249	-.19208
6	.00443	7.21405	-.75142	48	.01926	10.66988	-.14654
7	.00462	6.92740	-.68102	49	.01926	11.06179	-.17675
8	.00481	6.66337	-.61631	50	.01975	10.79782	-.14857
9	.00482	9.99211	-.74420	51	.02024	10.54680	-.12182
10	.00588	8.23086	-.43509	52	.02073	10.30772	-.09637
11	.00694	7.00908	-.22240	53	.02073	10.31971	-.09739
12	.00800	6.11249	-.06782	54	.02076	10.30754	-.09610
13	.00800	7.69343	-.25976	55	.02078	10.29545	-.09481
14	.00852	7.24260	-.18618	56	.02081	10.28334	-.09352
15	.00903	6.84450	-.12131	57	.02081	10.28135	-.09331
16	.00955	6.48924	-.06377	58	.02206	9.72273	-.03410
17	.00955	6.48799	-.06357	59	.02331	9.22509	.01841
18	.01012	6.13763	-.00723	60	.02456	8.77934	.06520
19	.01069	5.82482	.04277	61	.02457	10.10913	-.07506
20	.01126	5.54380	.08739	62	.02514	9.89120	-.05189
21	.01126	9.17810	-.34384	63	.02571	9.68334	-.02982
22	.01162	8.90768	-.30411	64	.02628	9.48470	-.00877
23	.01197	8.65326	-.26679	65	.02628	9.94616	-.05479
24	.01232	8.41363	-.23168	66	.02636	9.91712	-.05171
25	.01232	8.41204	-.23145	67	.02644	9.88830	-.04865
26	.01265	8.20277	-.20083	68	.02652	9.85962	-.04561
27	.01298	8.00415	-.17181	69	.02653	9.85776	-.04541
28	.01330	7.81552	-.14426	70	.02680	9.76407	-.03549
29	.01331	11.40469	-.41380	71	.02707	9.67229	-.02577
30	.01388	10.94919	-.35687	72	.02734	9.58236	-.01626
31	.01444	10.52996	-.30456	73	.02734	10.00675	-.05801
32	.01501	10.14276	-.25632	74	.02764	9.90461	-.04720
33	.01502	10.71709	-.29612	75	.02794	9.80470	-.03664
34	.01518	10.60607	-.28260	76	.02824	9.70700	-.02632
35	.01534	10.49741	-.26937	77	.02824	9.73859	-.02947
36	.01551	10.39104	-.25644	78	.02892	9.52322	-.00676
37	.01551	12.62341	-.38795	79	.02960	9.31788	.01482
38	.01570	12.47532	-.37151	80	.03028	9.12206	.03535
39	.01589	12.33085	-.35549	81	.03028	10.05828	-.06110
40	.01608	12.18979	-.33986	82	.03036	10.03379	-.05851
41	.01608	12.69528	-.36603	83	.03044	10.00944	-.05593
42	.01638	12.46993	-.34158	84	.03052	9.98525	-.05337

6. Miscellaneous Notes on Beryllium Oxide

For temperatures other than 296°K the switching criteria for short collision and the α,β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral, effective temperature and ID numbers of the scattering law data on file.

T(°K)	Debye Waller Integral (eV^{-1})	$\bar{T}$(°K)	ENDF ID No.
296	19.827	504.37	GA 0057
400	23.571	565.00	GA 0058
500	27.560	636.40	GA 0059
600	31.779	715.83	GA 0060
700	36.141	800.43	GA 0061
800	40.600	888.55	GA 0062
1000	49.701	1071.5	GA 0063
1200	58.951	1259.9	GA 0064

BERYLLIUM OXIDE

1. Physics

The scattering law of BeO has been calculated using the incoherent isotropic approximation.

Beryllium oxide consists of two interpenetrating hexagonal close-packed structures with four atoms per unit cell.

The lattice dynamics[1] has been developed on the basis of a shell model, whose parameters have been chosen in such a way to give the best agreement to the elastic constants data and to the measured Raman frequencies.

Only the negative ions (oxygen) have been assumed to be polarizable. The effective charge on the ions has been taken to be 1.1 electron units, as derived from the Szigeti relation. The negative charge on the shell of each oxygen ion has been taken as equal to 1.2 electron units. The isotropic elastic force constant connecting shell and core of the negative ions has been taken as equal to 3×10^5 dyn/cm. The long range forces have been computed using the Ewald method.

Short range repulsive forces are acting among first and second neighbors. These interactions take place between the positive ions and the shells of the negative ions. Introduction of the second neighbors interaction was found necessary in order to fit the preliminary dispersion relations measured by neutron scattering.[2]

The frequency spectra weighted by the squares of the amplitude vectors have been computed separately for beryllium and oxygen and have been used to calculate the relative scattering laws using the code GASKET.

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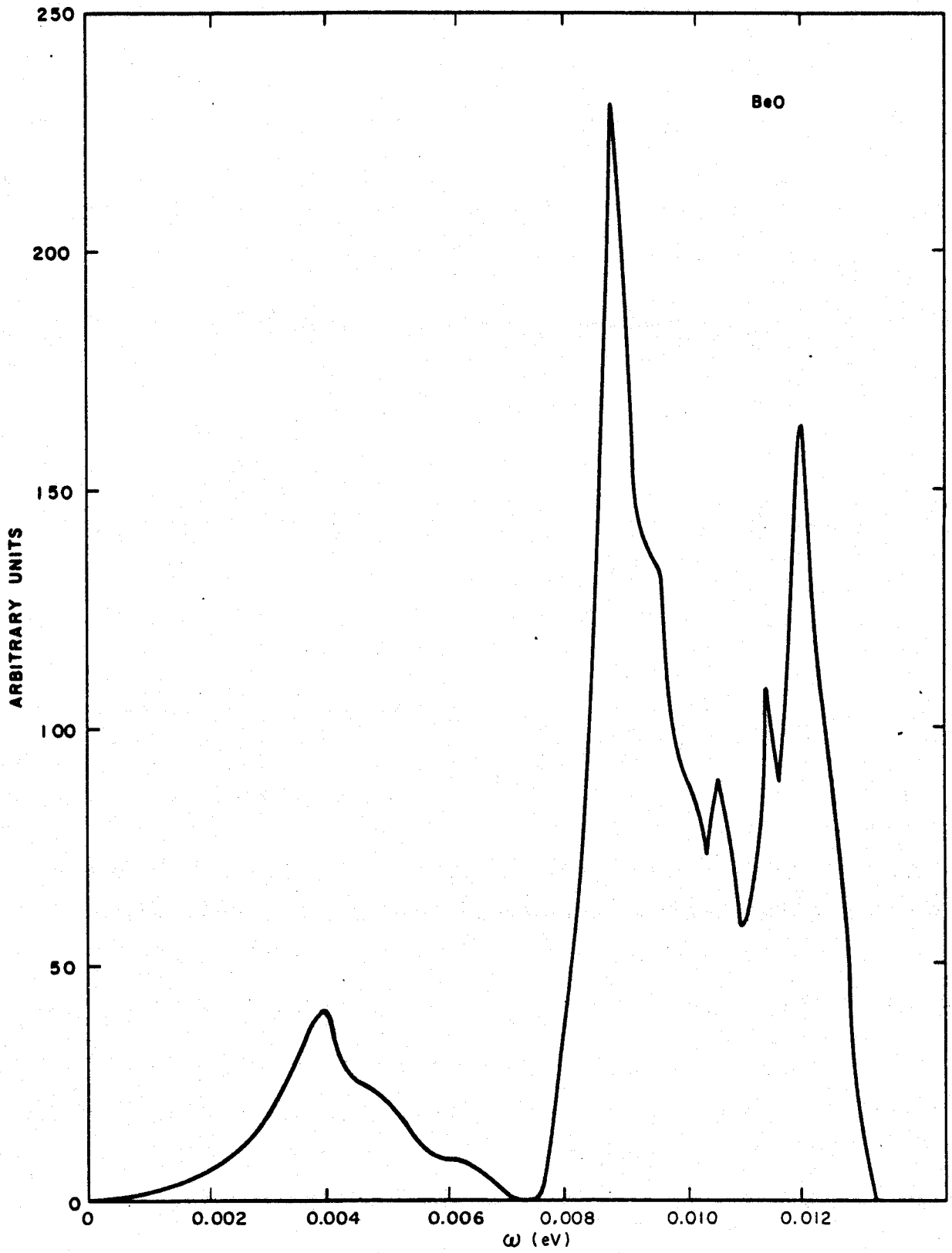
[1] G. Borgonovi, "Lattice Dynamics and Neutron Scattering of BeO," USAEC Report GA-8758, Gulf General Atomic Incorporated (1968).

[2] R. M. Brugger, K. A. Strong and J. M. Carpenter, J. Phys. Chem. Solids, 28, 249 (1967).

The two scattering laws have been combined and the total scattering law is referred to the beryllium atom.

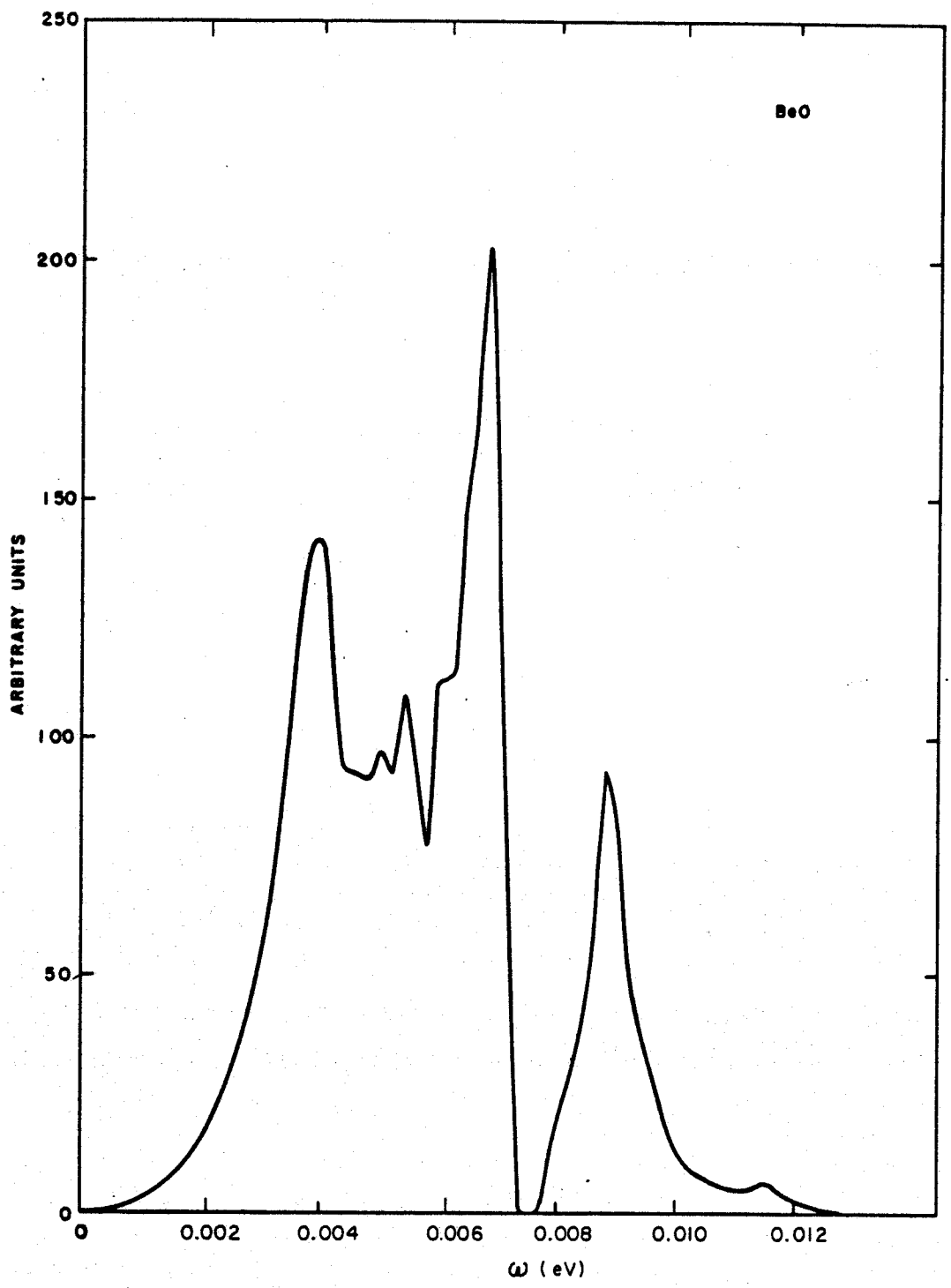
The elastic part of the scattering law has been calculated by the code HEXSCAT using the average of the Debye-Waller factors for beryllium and oxygen.

2. Weighted Frequency Spectrum for Be in BeO



BeO-2.1
(Rev.-12/31/69)

Weighted Frequency Spectrum for Oxygen in BeO



3.1 GASKET Input for Be(BeO) at 296°K

The code GASKET is discussed in Section A.3.1. The data tabulated below follows the format of the code input instructions also given in Section A.3.1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Be in BeO at 296 degrees K.
2	11I5	NT -5 NP 50 NE 80 NDAM 1 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 -83 JS4 0 JS5 0
4	5E10	W1 0.001 W2 0.0 W3 1.0 W4 . W5
5	6E10	T1 0.0255 T2 0.0 T3 0.0255 T4 T5
6	7E10	AM 9.013 DC 0.0 BETSW 40.0 ALPSW 20.0 CRIT1
		CRIT2 CRIT3
		X3 0.1371

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES						
8	7E10	Q3	0.3	0.7	0.9	1.0	1.2	1.6
			2.0	2.2	3.0	3.5	4.5	5.5
			6.8	8.0	9.2	10.9	12.9	15.5
			18.6	22.0	26.0	30.5	35.0	39.0
			40.0	34.0	28.0	26.0	24.4	23.0
			21.3	19.8	17.0	14.1	12.0	10.0
			9.0	9.0	8.5	7.5	6.0	4.6
			3.1	1.6	0.5	0.0	0.0	4.0
			15.0	38.0	52.0	70.0	105.0	165.0
			230.0	200.0	170.0	145.0	136.0	134.0
			112.0	96.0	89.0	84.0	75.0	87.0
			81.0	66.0	59.0	68.0	105.0	95.0
			97.0	135.0	163.0	130.0	111.0	92.0
			67.0	45.0	19.0	7.0	0.0	
9	Cards 9 and 10 are not needed							
10								
11	7E10	X5						
12	7E10	Q5						
13	7I10	NPHON						
14	5E10	EMAX 1.0 DALPHA 0.25 ALPHAC 2.95 DBETA 0.15 BETAC 4.0						
15, 16, 17, 18, 19 and 20 are not needed								
21	2E10	DT	0.15	TMAX	6.0			
			0.40		60.0			
			3.0		300.0			
			6.0		2500.0			
			10.0		5500.0			
22	2I10							
	2E10	ID 150 NPT 0 SIGF 6.09 EPS 1.0E-6						
23	Card 23 is not needed							

3.1.a GASKET Input for O(BeO)

The code GASKET is discussed in Section A.3.1. The data tabulated below follows the format of the code input instructions also given in Section A.3.1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Oxygen in BeO at 296 degrees K.
2	11I5	NT -5 NP 50 NE 80 NDAM 1 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 -83 JS4 0 JS5 0
4	5E10	W1 0.001 W2 0.0 W3 1.0 W4 W5
5	6E10	T1 0.0255 T2 0.0 T3 0.0255 T4 T5
6	7E10	AM 16.0 DC 0.0 BETSW 40.0 ALPSW 20.0 CRIT1
		CRIT2 CRIT3
		X3 0.1371

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES						
8	7E10	Q3	0.40	0.80	1.0	1.4	2.0	2.5
			3.5	4.8	6.2	8.9	11.0	14.0
			17.2	21.5	26.5	34.0	40.0	46.0
			58.0	60.0	93.0	110.0	129.0	141.0
			142.0	125.0	101.0	93.0	92.0	91.0
			95.0	95.0	98.0	108.0	93.0	78.0
			98.0	112.0	115.0	145.0	160.0	190.0
			190.0	120.0	43.0	0.0	0.0	1.0
			9.0	19.0	26.0	35.0	48.0	66.0
			92.0	82.0	56.0	44.0	35.0	29.0
			21.0	15.0	11.5	9.0	8.0	7.0
			6.0	5.2	4.5	5.0	5.9	6.0
			5.0	4.0	2.5	1.8	1.0	0.50
			0.50	0.20	0.0	0.0	0.0	
9	Cards 9 and 10 are not needed							
10								
11	7E10	X5						
12	7E10	Q5						
13	7I10	NPHON						
14	5E10	EMAX 1.0 DALPHA .1483 ALPHAC 1.618 DBETA 0.15 BETAC 4.0						
15, 16, 17, 18, 19 and 20 are not needed								
21	2E10	DT 0.15 TMAX 6.0						
			0.40	60.0				
			3.0	300.0				
			6.0	2500.0				
			10.0	5500.0				
22	2I10							
	2E10	ID 160 NPT 0 SIGF 3.76 EPS 1.0E-6						
23	Card 23 is not needed							

3.2 HEXSCAT Input for BeO

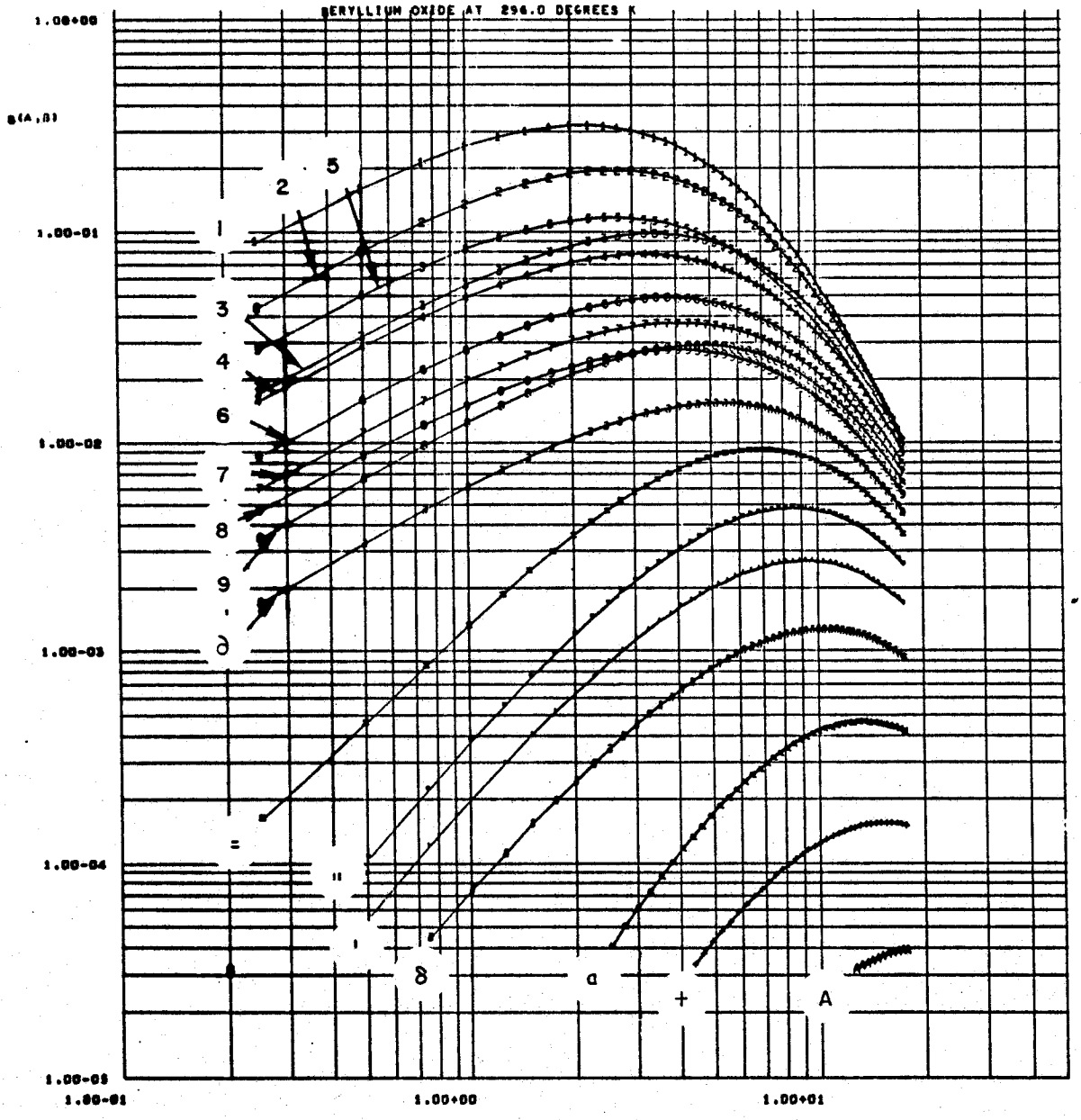
The code HEXSCAT is discussed in Section A. 3. 1. The data tabulated below follows the format of the code input instruction also given in Section A. 3. 1. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

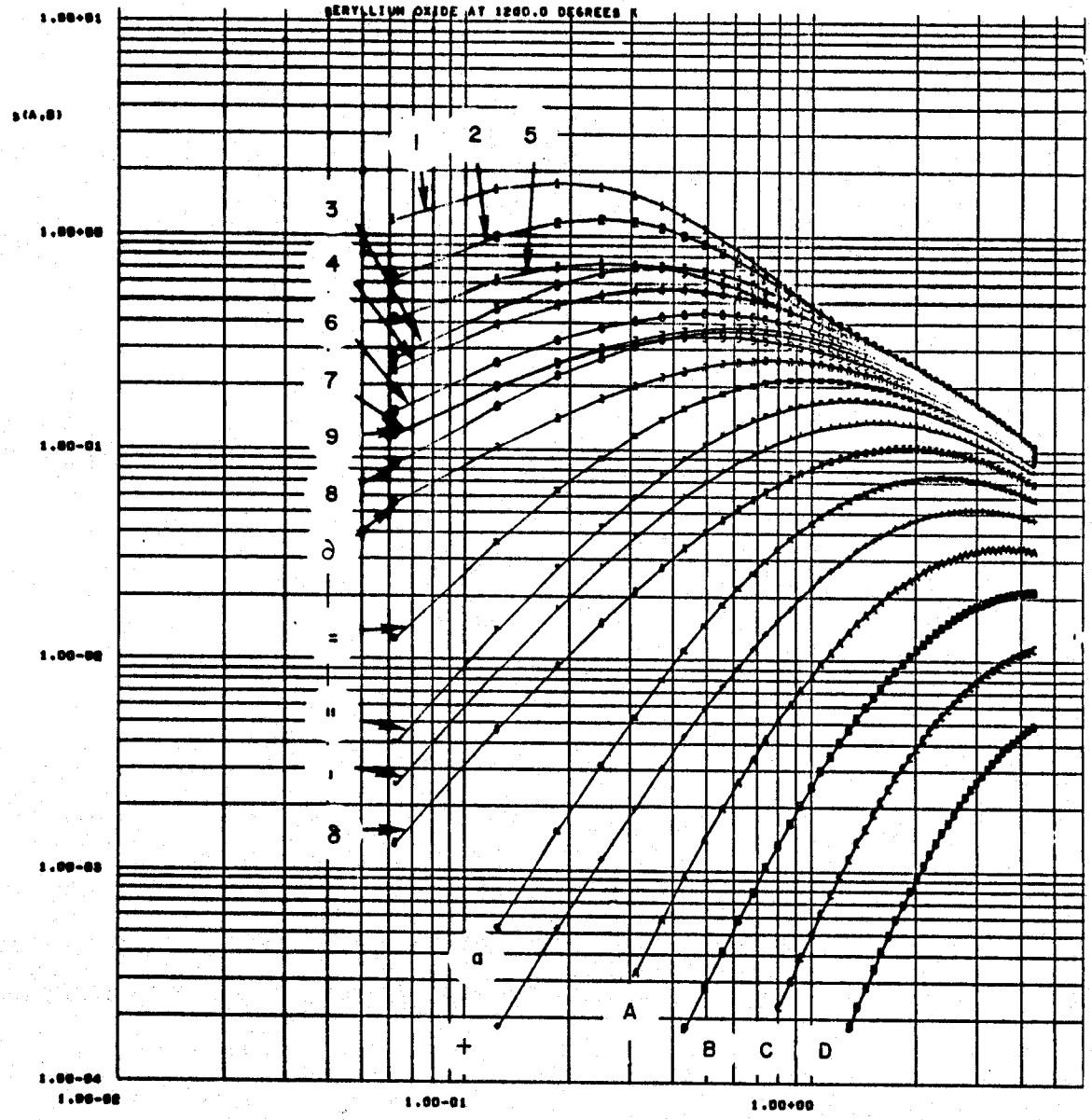
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES				
1	13A6, A2	HOL HEXSCAT for Borgonuuis shell model BeO				
2	5E10,	SCOH 1.0	A 2.695-8	C 4.39-8	AMASC 12.5	EXACT 0.05
	1I10,	ID 1108	ZA 200.0	AWR 24.7967		
3	8I5,	NES 22	NTS 8	NAV 0	NXAV 2	IP 1
	1E10	NCOS 0	NPCH 1	NFORM 2	ESEP 1.0001	
		EIN 3.754475-3	0.05	0.05280088	0.05281143	0.05834735
		0.05835902	0.06442	0.07132077	0.07548925	0.07826468
		0.08325706	0.09662996	0.120	0.130	0.150
		0.200	0.260	0.300	0.425	0.600
		0.800	1.0			
5	7E10	WAL2 2.153	2.6374	3.1348	3.6513	4.1798
		4.7164	5.8052	6.9068		
6	7E10	TMP 296.0	400.0	500.0	600.0	700.0
		800.0	1000.0	1200.0		

4. Plots of Scattering Law for BeO

BETA VALUES FOR MULTICURVE PLOT

Curve	Index	$\beta(296^{\circ}K)$	$\beta(1200^{\circ}K)$
1	1	0.00	0.0
2	2	0.150	0.036992
3	3	0.300	0.073984
4	4	0.900	0.22195
5	5	1.500	0.36992
6	6	2.100	0.51789
7	7	2.700	0.66586
8	8	3.300	0.81382
9	9	3.900	0.96179
10	∂	4.5456	1.1210
11	=	5.3273	1.3138
12	''	6.2738	1.5472
13	'	7.4199	1.8299
14	δ	8.8078	2.1721
15	α	10.488	2.5866
16	+	12.523	3.0884
17	A	14.987	3.6961
18	B	17.971	4.4319
19	C	21.584	5.3229
20	D	25.959	6.4017


BERYLLIUM OXIDE AT 296.0 DEGREES K
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-01
1.00+00
1.00+01
ALPHA
1
2
3
4
5
6
7
8
9
A


BERYLLIUM OXIDE AT 1200.0 DEGREES K
S(A,B)
1.00+01
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
ALPHA
1
2
5
3
4
6
7
9
8
A
B
C
D

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR BEO AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00375	5.34854	-.93566	43	.01668	12.10421	-.31304
2	.00392	5.13975	-.85719	44	.01698	11.90140	-.29073
3	.00408	4.94760	-.78526	45	.01698	11.91149	-.29121
4	.00424	4.77019	-.71911	46	.01774	11.42582	-.23802
5	.00424	7.53724	-.82232	47	.01850	10.98152	-.18942
6	.00443	7.22863	-.74601	48	.01926	10.57438	-.14496
7	.00462	6.94564	-.67615	49	.01926	10.94937	-.17415
8	.00481	6.68506	-.61198	50	.01975	10.69584	-.14663
9	.00482	9.97754	-.74009	51	.02024	10.45472	-.12053
10	.00588	8.23866	-.43523	52	.02073	10.22513	-.09577
11	.00694	7.03230	-.22300	53	.02073	10.23653	-.09674
12	.00800	6.15092	-.07111	54	.02076	10.22486	-.09548
13	.00800	7.70320	-.25866	55	.02078	10.21323	-.09423
14	.00852	7.26100	-.18625	56	.02081	10.20162	-.09298
15	.00903	6.87030	-.12262	57	.02081	10.19973	-.09278
16	.00955	6.52228	-.06635	58	.02206	9.66122	-.03529
17	.00955	6.52107	-.06615	59	.02331	9.18252	.01544
18	.01012	6.17897	-.01129	60	.02456	8.75515	.06038
19	.01069	5.87357	.03719	61	.02457	10.01224	-.07289
20	.01126	5.59856	.08028	62	.02514	9.80437	-.05055
21	.01126	9.14039	-.33895	63	.02571	9.60666	-.02933
22	.01162	8.87597	-.29989	64	.02628	9.41793	-.00915
23	.01197	8.62756	-.26324	65	.02628	9.85243	-.05288
24	.01232	8.39379	-.22880	66	.02636	9.82489	-.04992
25	.01232	8.39221	-.22857	67	.02644	9.79752	-.04698
26	.01265	8.18833	-.19858	68	.02652	9.77032	-.04406
27	.01298	7.99509	-.17019	69	.02653	9.76855	-.04387
28	.01330	7.81264	-.14329	70	.02680	9.67970	-.03435
29	.01331	11.29419	-.40761	71	.02707	9.59270	-.02505
30	.01368	10.85325	-.35150	72	.02734	9.50750	-.01595
31	.01445	10.44731	-.30004	73	.02734	9.90612	-.05557
32	.01501	10.07233	-.25267	74	.02764	9.80945	-.04521
33	.01502	10.62726	-.29164	75	.02794	9.71495	-.03510
34	.01518	10.51954	-.27836	76	.02824	9.62256	-.02523
35	.01534	10.41414	-.26538	77	.02824	9.65217	-.02821
36	.01551	10.31097	-.25269	78	.02892	9.44876	-.00654
37	.01551	12.46553	-.38187	79	.02960	9.25473	.01400
38	.01570	12.32211	-.36569	80	.03028	9.06999	.03348
39	.01589	12.18214	-.34992	81	.03028	9.94355	-.05740
40	.01608	12.04556	-.33453	82	.03036	9.92050	-.05492
41	.01608	12.53271	-.36029	83	.03044	9.89758	-.05247
42	.01638	12.31451	-.33622	84	.03052	9.87479	-.05002

DATA FOR BEO AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
85	.03053	10.21571	-.08173	127	.04331	10.16478	-.03934
86	.03101	10.07140	-.06624	128	.04333	10.16009	-.03884
87	.03150	9.93190	-.05131	129	.04334	10.15840	-.03866
88	.03199	9.79700	-.03690	130	.04391	10.04904	-.02712
89	.03200	9.80155	-.03733	131	.04448	9.94332	-.01595
90	.03259	9.64290	-.02042	132	.04504	9.84066	-.00514
91	.03319	9.49046	-.00423	133	.04505	10.16924	-.03730
92	.03376	9.34390	.01130	134	.04540	10.10476	-.03046
93	.03379	9.90289	-.04583	135	.04576	10.04136	-.02376
94	.03414	9.81330	-.03624	136	.04611	9.97905	-.01718
95	.03449	9.72571	-.02688	137	.04611	9.97742	-.01701
96	.03464	9.64007	-.01774	138	.04701	9.82322	-.00081
97	.03465	9.63839	-.01756	139	.04790	9.67545	.01462
98	.03510	9.56102	-.00932	140	.04880	9.53377	.02931
99	.03550	9.48521	-.00126	141	.04881	9.67397	.01438
100	.03582	9.41093	.00662	142	.04897	9.64877	.01701
101	.03583	10.70532	-.11516	143	.04913	9.62375	.01961
102	.03648	10.53817	-.09712	144	.04929	9.59892	.02219
103	.03713	10.37759	-.07982	145	.04930	9.88108	-.00702
104	.03779	10.22305	-.06321	146	.04935	9.87264	-.00614
105	.03779	10.22129	-.06302	147	.04940	9.86421	-.00525
106	.03787	10.20319	-.06106	148	.04946	9.85581	-.00437
107	.03795	10.18516	-.05915	149	.04947	10.13606	-.03190
108	.03803	10.16722	-.05722	150	.04960	10.11458	-.02962
109	.03804	10.02713	-.09602	151	.04973	10.09322	-.02736
110	.03809	10.01421	-.09664	152	.04986	10.07199	-.02511
111	.03814	10.00133	-.09525	153	.04987	10.20401	-.03772
112	.03820	10.58849	-.09388	154	.04991	10.19687	-.03696
113	.03820	10.66299	-.10017	155	.04996	10.18973	-.03620
114	.03932	10.40297	-.07235	156	.05000	10.18261	-.03545
115	.04043	10.15867	-.04630	157	.05280	9.76254	.00885
116	.04154	9.92886	-.02196	158	.05281	10.38598	-.05174
117	.04155	10.42104	-.06817	159	.05835	9.82993	.00989
118	.04160	10.39274	-.06515	160	.05836	10.34113	-.04005
119	.04162	10.36464	-.06216	161	.06442	9.73668	.02367
120	.04195	10.33674	-.05919	162	.07132	9.40065	.05574
121	.04196	10.43127	-.06770	163	.07549	9.66037	.02481
122	.04239	10.34172	-.05818	164	.07826	9.48388	.04272
123	.04282	10.25419	-.04889	165	.08326	10.14446	-.02422
124	.04325	10.16861	-.03983	166	.09663	9.56344	.04310
125	.04326	10.17417	-.04033	167	.12000	9.69701	.03481
126	.04328	10.16947	-.03984	168	.13000	9.60319	.04890

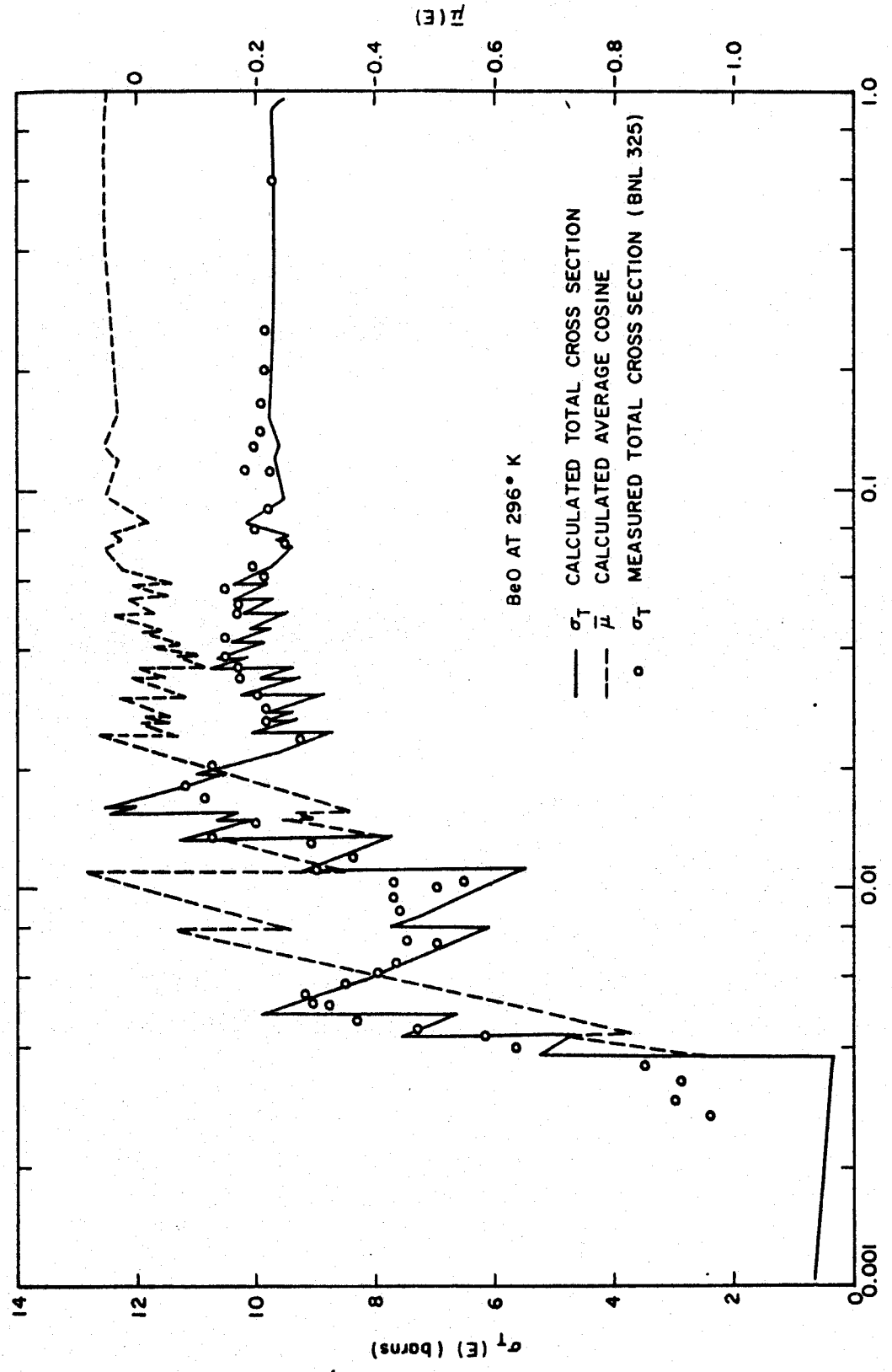
DATA FOR BEO AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
169	.15000	9.74734	.03483	183	.64500	9.77491	.05556
170	.38500	9.71551	.05368	184	.66500	9.77725	.05560
171	.40500	9.74522	.05470	185	.68500	9.77883	.05569
172	.42500	9.74804	.05393	186	.70500	9.78061	.05577
173	.44500	9.74973	.05450	187	.72500	9.78226	.05585
174	.46500	9.75211	.05479	188	.74500	9.78363	.05594
175	.48500	9.75543	.05489	189	.76500	9.78542	.05598
176	.50500	9.76004	.05489	190	.78500	9.78675	.05607
177	.52500	9.76261	.05493	191	.80500	9.78795	.05614
178	.54500	9.76420	.05512	192	.85500	9.78938	.05634
179	.56500	9.76622	.05523	193	.88500	9.78474	.05645
180	.58500	9.76874	.05530	194	.91500	9.76238	.05625
181	.60500	9.77062	.05541	195	.94500	9.71484	.05591
182	.62500	9.77299	.05546	196	.97500	9.53559	.05150

THE ELASTIC CONTRIBUTION TO THE TOTAL CROSS SECTION WAS CALCULATED AT ALL OF THE TABULATED ENERGIES. THE INELASTIC CONTRIBUTION WAS CALCULATED ON A COARSER MESH AND WAS INTERPOLATED TO GIVE THE VALUES AT THE TABULATED ENERGIES.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV


BeO AT 296° K
σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
σ_T MEASURED TOTAL CROSS SECTION (BNL 325)
σ_T (E) (barns)
$\bar{\mu}$(E)
ENERGY (eV)
0.001
0.01
0.1
1.0
0
2
4
6
8
10
12
14
-0.2
-0.4
-0.6
-0.8
-1.0

6. Miscellaneous Notes on Beryllium Oxide

For temperatures other than 296°K the switching criteria for short collision and the α, β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye-Waller integral and effective temperature of the scattering law data on file.

T(°K)	Debye-Waller Integral (eV^{-1}) for Beryllium	$\overline{T}$(°K) for Beryllium	Debye-Waller Integral (eV^{-1}) for Oxygen	$\overline{T}$(°K) for Oxygen
296	19.339	596.4	34.568	427.8
400	23.191	643.9	43.227	502.8
500	27.200	704.6	52.031	584.3
600	31.4021	775.3	61.096	671.3
700	35.7334	852.9	70.321	761.6
800	40.152	935.4	79.649	854.2
1000	49.161	1109.8	98.497	1043.7
1200	58.312	1292.3	117.50	1236.6

GRAPHITE

1. Physics

The scattering law data for graphite has been computed assuming that the incoherent and isotropic approximations are valid, so that the scattering depends solely upon the phonon spectrum of the lattice vibrations. The force model used to compute the phonon spectrum[1] contains four force constants. One force constant is used to describe a nearest neighbor central force which binds two hexagonal planes together, another describes a bond-bending force in a hexagonal plane, the third is for bond-stretching between nearest neighbors in the plane, and the fourth corresponds to a restoring force against bending of the hexagonal plane. The force constants have been evaluated numerically in this model by performing a very precise fit to the high and low temperature specific heat, and to the compressibility of reactor grade graphite. Calculations of neutron spectra using the phonon spectrum based on the above calculation gives excellent agreement when compared with experiment. The elastic scattering was evaluated using HEXSCAT and the known lattice structure of graphite.

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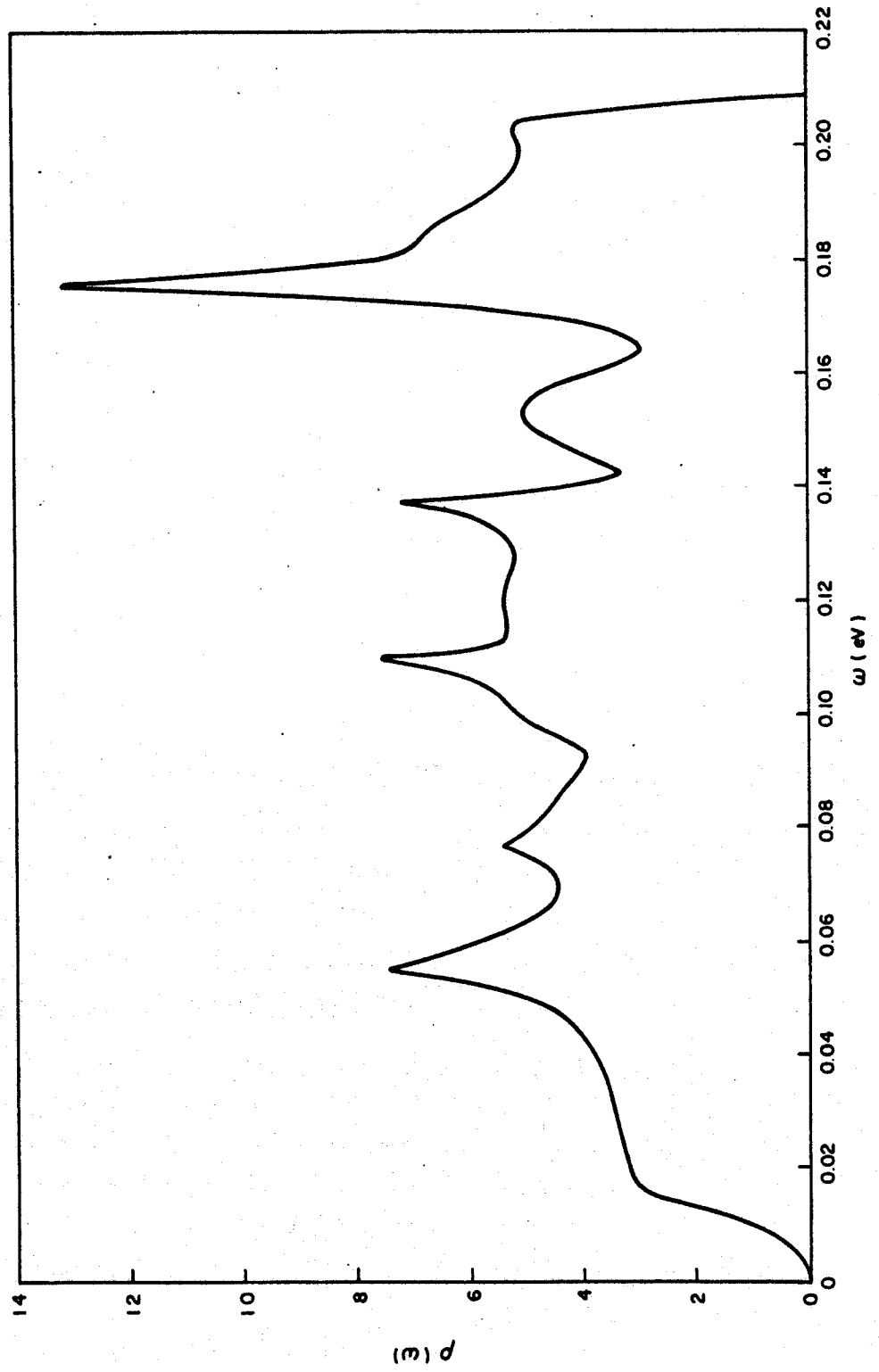
[1] Nukleonik Band 1, 295, (1965). (J. A. Young, N. F. Wikner & D. E. Parks)
J. Chem. Phys. 42, 357, (1965). (J. A. Young & J. U. Koppel)

2. Frequency Spectrum for Graphite



3.1 GASKET Input for Graphite at 296°K

The code GASKET is discussed in Section A. 3. The data tabulated below follows the format of the code input instructions also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6,A2	COM carbon at 296 K
2	11I5	NT -9 NP 40 NE 80 NDAM 1 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 -38 JS4 0 JS5 0
4	5E10	W1 .001 W2 0.0 W3 1.0 W4 0.0 W5 0.0
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 0.0 T5 0.0
6	7E10	AM 12.011 DC 0.0 BETSW 30.0 ALPSW 30.0 CRIT1 0.0
		CRIT2 0.0 CRIT3 0.0
7	7E10	X3 .20842

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES						
8	7E10	Q3	.346613	1.4135	3.03321	3.25901	3.38468	3.48269
			3.76397	4.05025	4.84696	7.35744	5.88224	4.63255
			4.48287	5.80642	4.63802	4.28503	3.92079	4.91352
			5.53836	7.51076	5.31651	5.40525	5.20376	5.3276
			7.17251	3.31813	4.50126	5.04663	4.2089	2.91985
			4.65109	13.1324	7.25016	6.5662	5.47181	5.06137
			5.19813	.457086				
9	Cards 9 and 10 are not needed							
11	7E10	X5						
12	7E10	Q5						
13	7I10	NPHON						
14	5E10	EMAX 1.0	DALPHA .25	ALPHAC 2.0	DBETA .1	BETAC 4.0		
15, 16, 17, 18, 19 and 20 are not needed								
21	2E10	DT	TMAX					
		.001	.01					
		.01	.1					
		.1	3.0					
		.25	6.0					
		.5	9.0					
		1.0	22.0					
		2.0	24.0					
		4.0	100.0					
		6.0	3000.0					
22	2I10							
	2E10	ID 34	NPT 0	SIGF 4.71	EPS .000001			
23	Card 23 is not needed							

3.2 HEXSCAT Input for Graphite

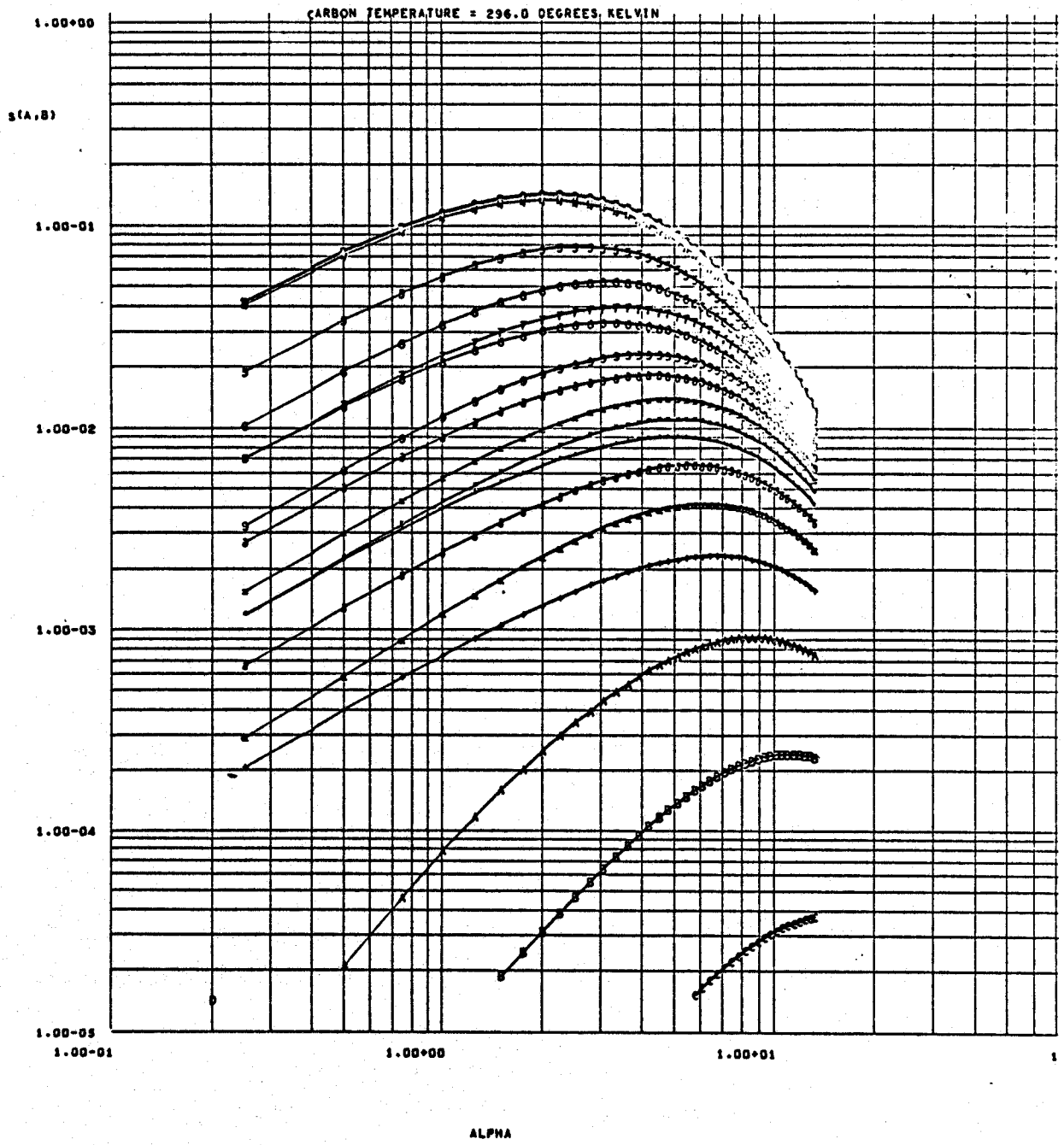
The code HEXSCAT is discussed in Section A. 3. The data tabulated below follows the format of the code input instruction also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

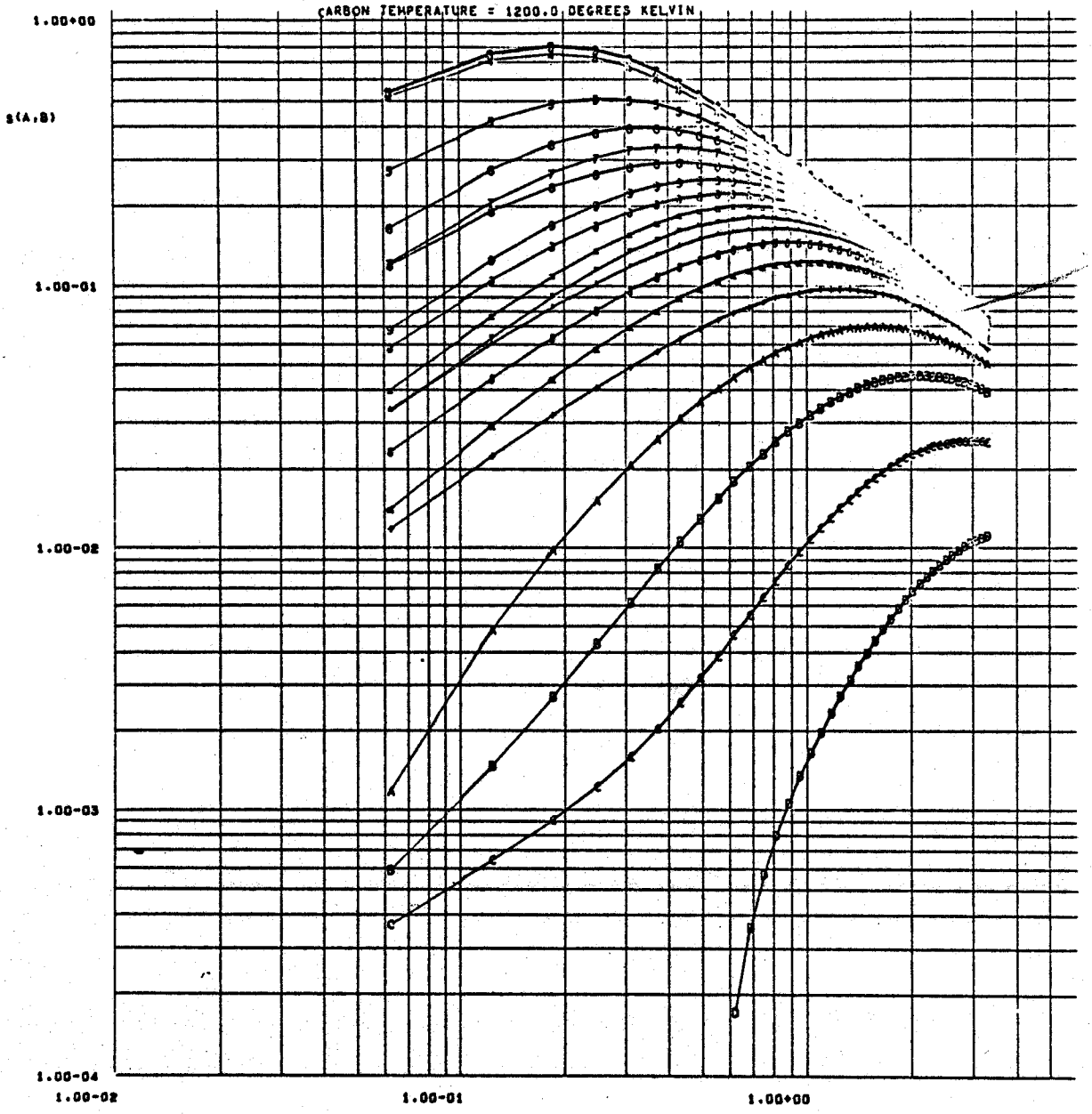
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
1	13A6,A2	HOL	HEXSCAT for ENDF carbon				
2	5E10,	SCOH	5.50	A 2.4573-8	C 6.700-8	AMASC 12.011	EXACT .04
	1I10,2E10	ID	1065	ZA 6000.0	AWR		
3	8I5,	NES	42	NTS 10	NAV 0	NXAV 2	IP 1
	1E10	NCOS	0	NPCH 1	NFORM 3	ESEP 1.0001	
4	7E10	EIN	1.822378-3	.04	.04037961	.0403876	.04063488
			.04064301	.0424569	.04246539	.04269718	.04270571
			.04299249	.04300109	.04555034	.04555945	.04792294
			.04793252	.05149859	.05392457	.05704441	.05909530
			.05910712	.05915034	.05916216	.06146790	.06148019
			.06978710	.07059208	.07302051	.07592887	.08101
			.09663674	.11	.15	.19	.25
			.32	.40	.50	.60	.75
			.90	1.0			
5	7E10	WAL2	2.1997	2.7448	3.2912	3.8510	4.4210
			4.9969	6.1624	7.3387	9.6287	11.992
6	7E10	TMP	296.0	400.0	500.0	600.0	700.0
			800.0	1000.0	1200.0	1600.0	2000.0

4. Plots of Scattering Law

β Values for Multicurve Plots

CURVE	INDEX	β (296K)	β (1200K)
1	1	0.00	0.00
2	2	.10	.025
3	3	.20	.049
4	4	.60	.148
5	5	1.00	.247
6	6	1.40	.345
7	7	1.80	.444
8	8	2.20	.543
9	9	2.60	.641
10	∂	3.00	.740
11	=	3.40	.838
12	"	3.80	.937
13	'	4.21	1.038
14	δ	4.76	1.175
15	α	5.56	1.372
16	+	6.72	1.657
17	A	8.38	2.067
18	B	10.79	2.660
19	C	14.25	3.514
20	D	19.25	4.748


CARBON TEMPERATURE = 296.0 DEGREES KELVIN
1.00+00
S(A,B)
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-01
1.00+00
1.00+01
1
ALPHA


CARBON TEMPERATURE = 1200.0 DEGREES KELVIN
1.00+00
S(A,B)
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
ALPHA

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR GRAPHITE AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00182	7.64834	-.97243	43	.01491	3.90989	.00688
2	.00258	5.44835	-.40168	44	.01537	3.80491	.03313
3	.00334	4.24816	-.09517	45	.01537	5.40999	-.27359
4	.00410	3.49297	.09385	46	.01555	5.35240	-.25969
5	.00410	3.49230	.09402	47	.01573	5.29618	-.24614
6	.00424	3.38405	.12071	48	.01590	5.24126	-.23292
7	.00438	3.28267	.14560	49	.01591	5.52492	-.27223
8	.00451	3.18756	.16883	50	.01607	5.47237	-.25982
9	.00452	3.53391	.05396	51	.01623	5.42092	-.24769
10	.00467	3.42510	.08193	52	.01640	5.37053	-.23581
11	.00482	3.32314	.10801	53	.01640	5.61010	-.26837
12	.00497	3.22742	.13236	54	.01682	5.48151	-.23856
13	.00497	5.02176	-.27283	55	.01723	5.35934	-.21030
14	.00543	4.61610	-.17032	56	.01764	5.24309	-.18346
15	.00588	4.27360	-.08432	57	.01765	5.24213	-.18324
16	.00634	3.98065	-.01131	58	.01779	5.20488	-.17465
17	.00634	4.39051	-.10372	59	.01792	5.16822	-.16621
18	.00665	4.19120	-.05427	60	.01806	5.13214	-.15790
19	.00697	4.01021	-.00957	61	.01806	5.16963	-.16395
20	.00729	3.84512	.03099	62	.01821	5.13040	-.15494
21	.00729	4.72471	-.16119	63	.01836	5.09186	-.14610
22	.00773	4.46711	-.09823	64	.01852	5.05394	-.13740
23	.00817	4.23772	-.04245	65	.01852	5.27439	-.17342
24	.00861	4.03220	.00722	66	.01897	5.15867	-.14713
25	.00862	4.79308	-.15284	67	.01943	5.04868	-.12219
26	.00954	4.35224	-.04741	68	.01988	4.94395	-.09851
27	.01046	3.99064	.03816	69	.01989	5.00858	-.11011
28	.01139	3.68904	.10862	70	.02020	4.93771	-.09415
29	.01139	3.68835	.10878	71	.02052	4.86912	-.07873
30	.01153	3.64768	.11820	72	.02083	4.80271	-.06384
31	.01167	3.60799	.12736	73	.02084	5.77090	-.22095
32	.01180	3.56926	.13629	74	.02086	5.76450	-.21955
33	.01181	3.72248	.08941	75	.02089	5.75811	-.21816
34	.01239	3.56202	.12709	76	.02091	5.75174	-.21677
35	.01297	3.41646	.16092	77	.02092	5.81086	-.22465
36	.01354	3.28395	.19138	78	.02133	5.70767	-.20223
37	.01355	4.26938	-.08392	79	.02175	5.60861	-.18075
38	.01370	4.22597	-.07289	80	.02216	5.51339	-.16015
39	.01385	4.18354	-.06213	81	.02216	5.67609	-.18417
40	.01400	4.14203	-.05161	82	.02222	5.66405	-.18158
41	.01400	4.14127	-.05142	83	.02227	5.65206	-.17901
42	.01446	4.02180	-.02125	84	.02232	5.64010	-.17644

DATA FOR GRAPHITE AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
85	.02232	5.63909	-.17623	127	.03420	4.92054	-.01292
86	.02319	5.44763	-.13521	128	.03446	4.88932	-.00642
87	.02406	5.27074	-.09751	129	.03446	4.91373	-.01136
88	.02493	5.10691	-.06278	130	.03488	4.86518	-.00127
89	.02494	5.10600	-.06259	131	.03529	4.81787	.00853
90	.02507	5.08132	-.05737	132	.03570	4.77178	.01805
91	.02521	5.05696	-.05223	133	.03571	4.91292	-.01122
92	.02535	5.03288	-.04715	134	.03576	4.90712	-.01001
93	.02535	5.07534	-.05510	135	.03581	4.90133	-.00880
94	.02585	4.98987	-.03710	136	.03586	4.89556	-.00760
95	.02634	4.90779	-.01988	137	.03587	4.89474	-.00743
96	.02683	4.82895	-.00341	138	.03621	4.85662	.00050
97	.02684	4.94596	-.02700	139	.03655	4.81930	.00823
98	.02761	4.82571	-.00186	140	.03690	4.78273	.01579
99	.02838	4.71249	.02164	141	.03690	4.78195	.01595
100	.02915	4.60573	.04363	142	.03757	4.71306	.03012
101	.02916	4.69557	.02364	143	.03823	4.64682	.04366
102	.02925	4.68234	.02638	144	.03889	4.58312	.05659
103	.02935	4.66921	.02909	145	.03890	4.62284	.04749
104	.02945	4.65617	.03179	146	.03927	4.58832	.05450
105	.02945	4.75553	.01020	147	.03963	4.55453	.06134
106	.02962	4.73315	.01486	148	.04000	4.52143	.06801
107	.02978	4.71101	.01946	149	.04038	4.48787	.07474
108	.02994	4.68915	.02400	150	.04039	4.54376	.06149
109	.02995	5.20704	-.07790	151	.04063	4.52195	.06589
110	.03050	5.12565	-.06064	152	.04064	4.67044	.03197
111	.03105	5.04737	-.04411	153	.04246	4.56562	.05248
112	.03160	4.97206	-.02827	154	.04247	4.83981	-.00718
113	.03161	5.00067	-.03382	155	.04270	4.81901	-.00278
114	.03176	4.98059	-.02960	156	.04271	5.09026	-.05593
115	.03191	4.96073	-.02544	157	.04299	5.06308	-.05008
116	.03206	4.94107	-.02132	158	.04300	5.16296	-.06844
117	.03207	5.11253	-.05414	159	.04555	4.93285	-.01915
118	.03252	5.05181	-.04136	160	.04556	4.97219	-.02690
119	.03297	4.99291	-.02900	161	.04792	4.79568	.01040
120	.03343	4.93577	-.01705	162	.04793	5.01332	-.03348
121	.03343	4.98823	-.02739	163	.05150	4.78590	.01526
122	.03351	4.97846	-.02534	164	.05392	4.62761	.04797
123	.03359	4.96875	-.02331	165	.05704	4.93436	-.01817
124	.03367	4.95908	-.02129	166	.05910	4.82089	.00618
125	.03367	4.98456	-.02629	167	.05911	4.96463	-.02295
126	.03394	4.95228	-.01954	168	.05915	4.96205	-.02239

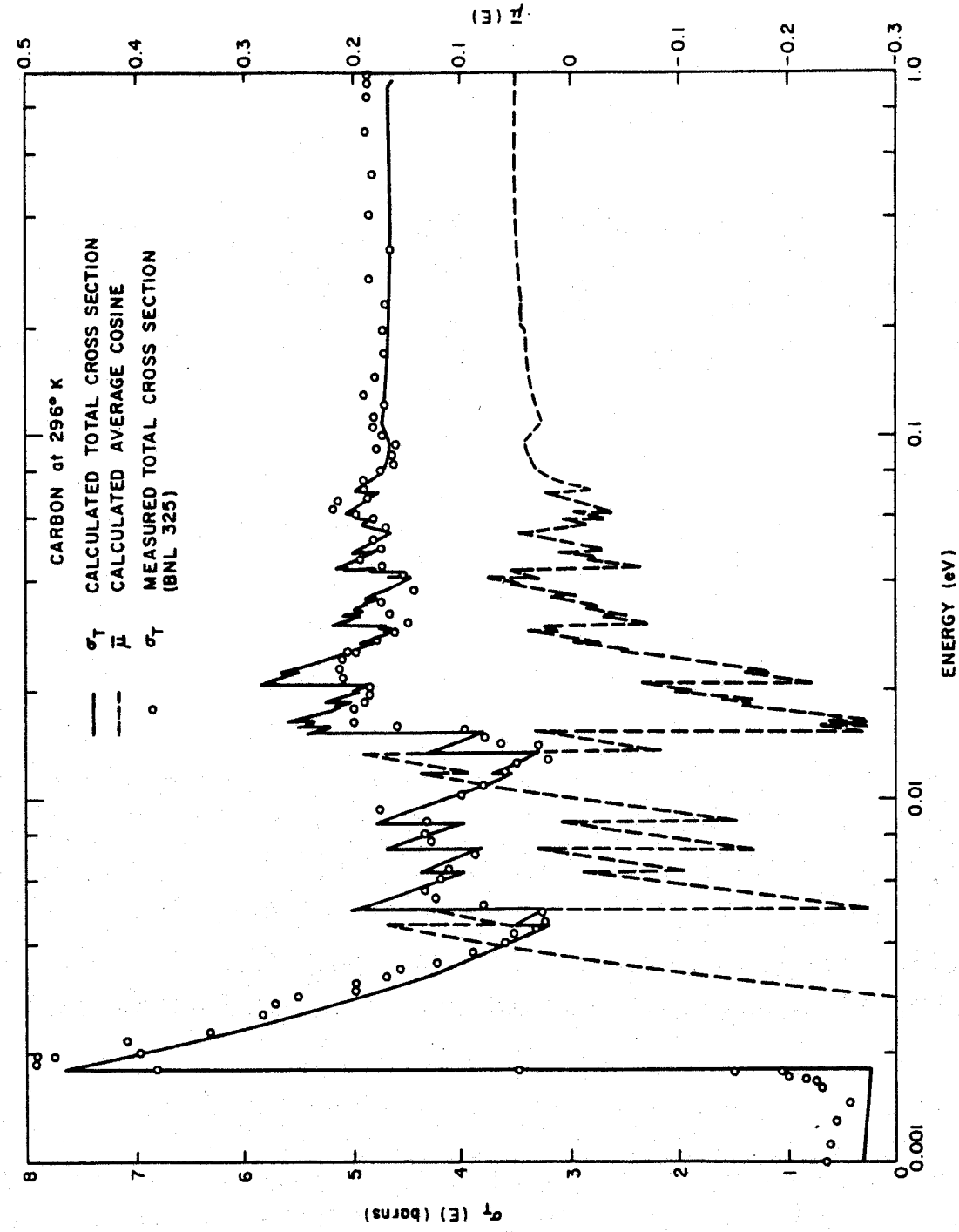
DATA FOR GRAPHITE AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
169	.05916	5.01539	-.03278	188	.38500	4.68239	.04906
170	.06147	4.94147	-.01546	189	.41500	4.68589	.04939
171	.06148	5.07408	-.04119	190	.44500	4.68729	.04940
172	.06979	4.77967	.02365	191	.47500	4.68802	.04985
173	.07059	4.98958	-.01909	192	.50500	4.69016	.05005
174	.07302	4.90137	.00019	193	.53500	4.69117	.05026
175	.07593	4.81484	.01883	194	.56500	4.69090	.05062
176	.08101	4.73567	.03471	195	.59500	4.69144	.05084
177	.09664	4.66335	.04515	196	.62500	4.69286	.05104
178	.11000	4.74872	.02675	197	.65500	4.69441	.05120
179	.15000	4.68711	.04064	198	.68500	4.69523	.05132
180	.19000	4.68832	.04176	199	.71500	4.69620	.05142
181	.20000	4.68662	.04359	200	.74500	4.69704	.05153
182	.22400	4.68899	.04484	201	.77500	4.69789	.05164
183	.24800	4.68608	.04637	202	.80500	4.69813	.05174
184	.27200	4.67786	.04855	203	.85500	4.69798	.05201
185	.29600	4.68374	.04782	204	.90500	4.69124	.05233
186	.32500	4.68236	.04801	205	.95500	4.64078	.05211
187	.35500	4.67689	.04928				

THE ELASTIC CONTRIBUTION TO THE TOTAL CROSS SECTION WAS CALCULATED AT ALL OF THE TABULATED ENERGIES. THE INELASTIC CONTRIBUTION WAS CALCULATED ON A COARSER MESH AND WAS INTERPOLATED TO GIVE THE VALUES AT THE TABULATED ENERGIES.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV


CARBON at 296° K
σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
σ_T MEASURED TOTAL CROSS SECTION (BNL 325)
σ_T (E) (barns)
$\bar{\mu}$ (E)
ENERGY (eV)
0.001
0.01
0.1
1.0

6. Miscellaneous Notes on Graphite

For temperatures other than 296°K the switching criteria for short collision and the α, βmesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral, effective temperature and ID numbers of the scattering law data on file.

T(°K)	Debye Waller Integral (eV^{-1})	$\bar{T}$(°K)	ENDF ID No.
296	26.421	713.39	GA 0034
400	32.968	754.68	GA 0035
500	39.531	806.67	GA 0036
600	46.255	868.38	GA 0037
700	53.101	937.64	GA 0038
800	60.018	1012.7	GA 0039
1000	74.016	1174.9	GA 0040
1200	88.145	1348.2	GA 0041
1600	115.65	1712.9	GA 0090
2000	144.03	2091.0	GA 0091

POLYETHYLENE

1. Physics

The frequency spectrum used for calculating the scattering law of polyethylene is based on a model of infinite chains proposed by Lin and Koenig.[1] The phase difference of the vibrations of corresponding atoms in two neighboring CH_2 groups of the same chain is a different function of frequency for each one of the nine different modes. From Lin and Koenig's calculated phase vs frequency curves a weighted frequency distribution was obtained by estimating the relative vibrational amplitudes from approximate physical arguments.[2] This frequency spectrum was then lumped into 5 discrete lines with frequencies and weights given by the following table:

Frequencies (eV)	Weights
0	.07144
.089	.07746
.14	.23200
.174	.30960
.360	.30960

The scattering law for this model was then calculated with the modified version of GAKER described in Section A.3.2. Only scattering by hydrogen is included in the tabulated data. Scattering by the carbon atoms should be taken into account by adding to the data the properly weighted $S(\alpha, \beta)$ for a free gas of mass 12.011. It is important to recall, however, that the α values for the carbon must be 1.008/12.011 times the α values

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[1] Tung Po Lin and J.L. Koenig, J. Mol. Spectra. 9, 228 (1962)

[2] J.U. Koppel and J.A. Young, Nucl. Sci. Eng. 21, 257 (1965)

for the hydrogen data in order to correspond to the same neutron momentum transfer K.

3.1 GAKER Input for $H(CH_2)$ at 296°K

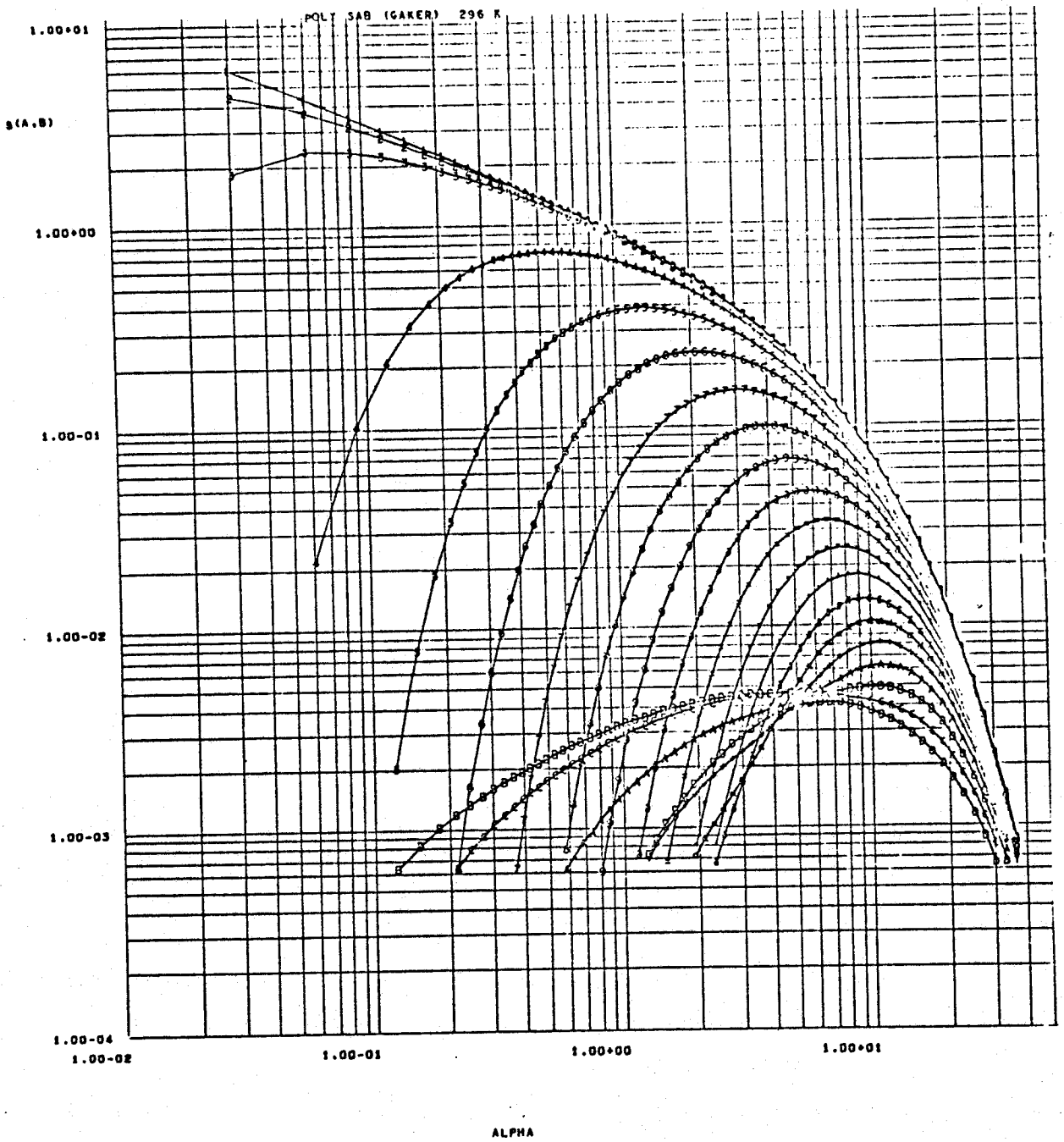
The code GAKER is discussed in Section A. 3. The data tabulated below follows the format of the code input instruction also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

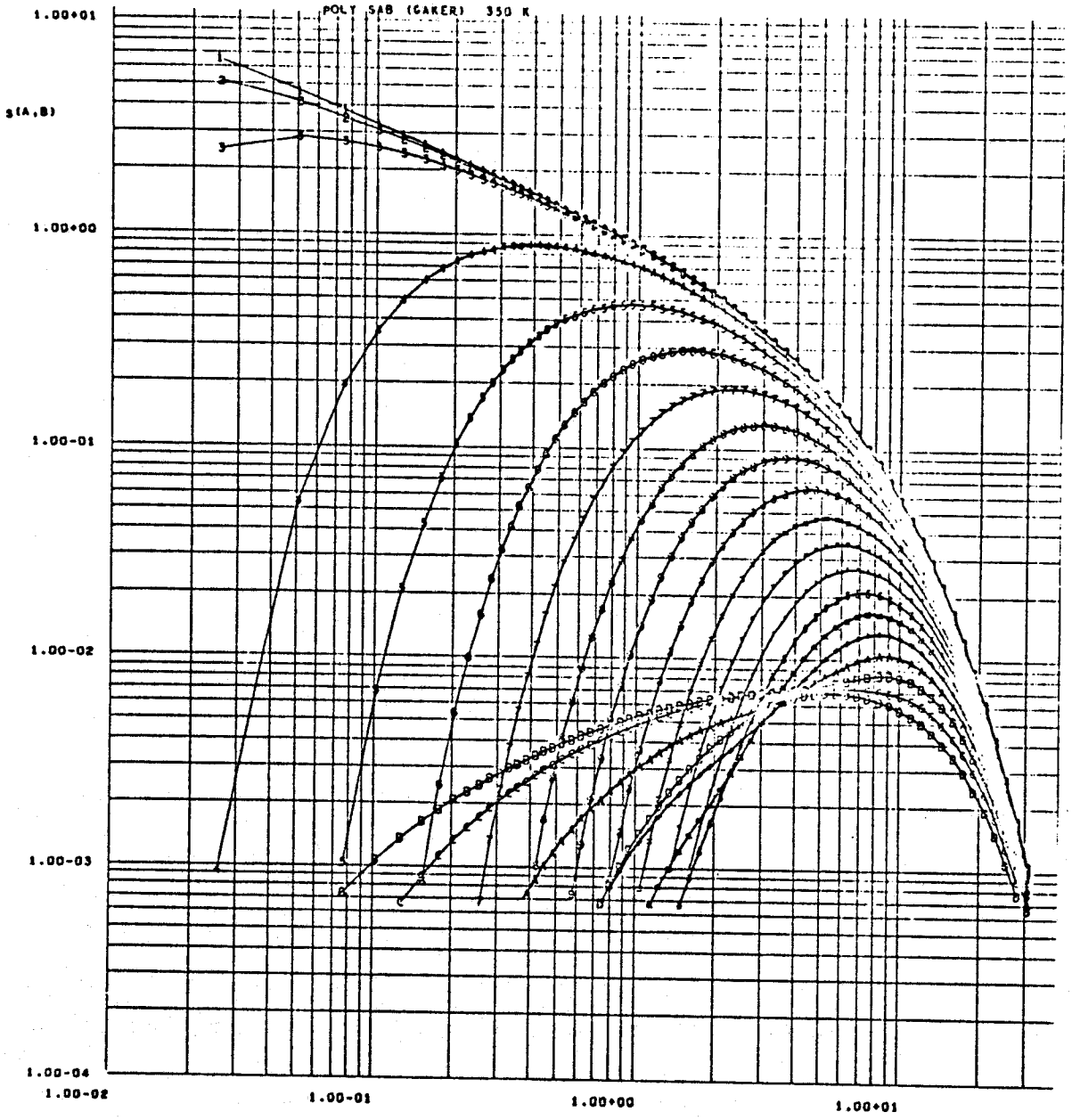
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	12A6	HOLREC Poly S(α,β) (Gaker) 296 K
2	4I5	ID -72 NR 3 IBX 120 IZX 80
3	7E10	T 1.0079 EC1 6.66667 EC2 12.941 SIGF 20.36 EPS 1.0-6
		EMAX 1.0 AMASS1.008
4	4E10	RT .0255 MT 14.0 MR 12.92 WR .089
5	6E10	MV1 4.31 W1 .14 MV2 3.23 W2 .174 MV3 3.23
		W3 .36
6	5E10	EMAX 1.0 DALPHA .03 ALPHAC .4 DBETA .05 BETAC 2.5

4. Plots of Scattering Law

β Values for Multicurve Plots

CURVE	INDEX	β(296K)	β(350K)
1	1	0.0	0.0
2	2	.050	.0422
3	3	.100	.0845
4	4	.300	.254
5	5	.500	.423
6	6	.700	.592
7	7	.900	.761
8	8	1.10	.930
9	9	1.30	1.10
10	∂	1.50	1.27
11	=	1.70	1.44
12	"	1.90	1.61
13	'	2.10	1.78
14	δ	2.30	1.94
15	α	2.50	2.11
16	+	2.72	2.30
17	A	2.99	2.52
18	B	3.32	2.81
19	C	3.74	3.16
20	D	4.26	3.60


POLY SAB (GAKER) 296 K
1.00+01
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
1.00+01
ALPHA


POLY SAB (GAKER) 350 K
1.00+01
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
1.00+01
ALPHA

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

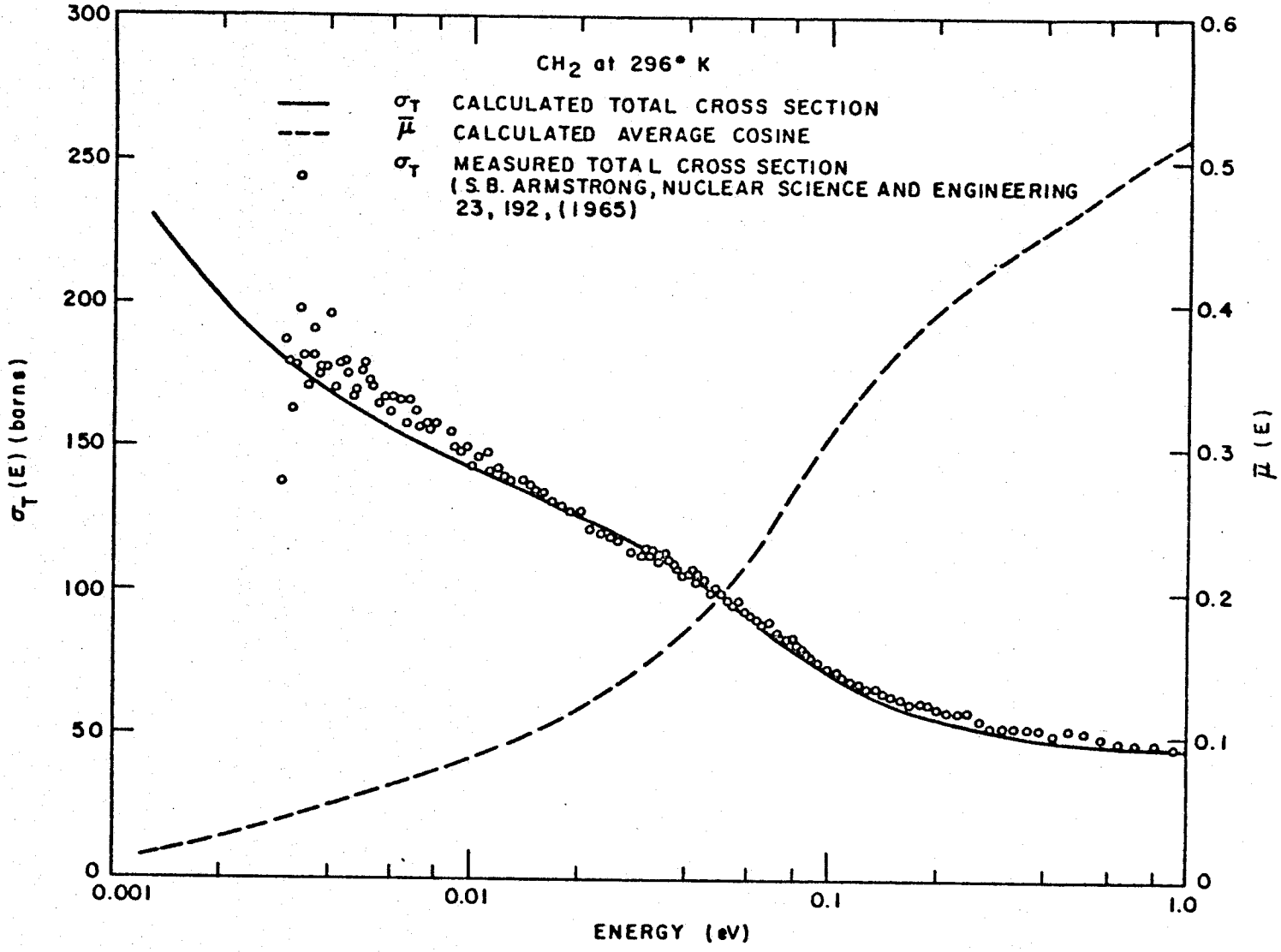
DATA FOR CH2 AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00025	446.54392	.00667	31	.12500	65.02025	.34152
2	.00075	280.08626	.01213	32	.13700	62.61880	.35342
3	.00125	232.25255	.01871	33	.15200	60.46828	.36653
4	.00175	208.58762	.02570	34	.16300	58.64099	.37843
5	.00225	193.98197	.03194	35	.18400	57.37348	.38804
6	.00275	184.07432	.03775	36	.20000	56.52137	.39595
7	.00325	177.09810	.04419	37	.22400	55.56429	.40577
8	.00375	171.19353	.04783	38	.24800	54.60317	.41418
9	.00450	164.92848	.05489	39	.27200	53.52354	.42159
10	.00550	158.59541	.06205	40	.29600	52.37512	.42801
11	.00650	153.80270	.06807	41	.32500	51.13421	.43569
12	.00750	150.01179	.07344	42	.35500	50.29617	.44127
13	.00850	146.95942	.07872	43	.38500	49.67909	.44610
14	.00950	144.20914	.08296	44	.41500	49.20479	.45125
15	.01100	140.61216	.08864	45	.44500	48.82713	.45643
16	.01300	136.55705	.09528	46	.47500	48.56203	.46173
17	.01500	133.16476	.10208	47	.50500	48.30338	.46662
18	.01700	130.11618	.10841	48	.53500	48.09713	.47129
19	.01900	127.32214	.11448	49	.56500	47.92123	.47571
20	.02100	124.73655	.12034	50	.59500	47.77162	.47986
21	.02500	119.99739	.13157	51	.62500	47.64028	.48372
22	.02900	115.64337	.14191	52	.65500	47.52317	.48737
23	.03600	109.05349	.16157	53	.68500	47.42226	.49075
24	.04400	102.25808	.18225	54	.71500	47.32754	.49395
25	.05300	95.55511	.20556	55	.74500	47.24099	.49700
26	.06500	87.76438	.23455	56	.77500	47.16058	.49982
27	.07700	81.26656	.26160	57	.80500	47.08432	.50252
28	.08900	75.94984	.28597	58	.85500	46.96680	.50669
29	.10100	71.61403	.30760	59	.90500	46.84759	.51043
30	.11300	68.00980	.32622	60	.95500	46.65063	.51329

THE TOTAL CROSS SECTION INCLUDES A CONSTANT SCATTERING CROSS SECTION OF 4.71 BARNS (SIG0) FOR THE CARBON ATOM. ALSO FOR THE CARBON, SIG1 = .666*SIG0/MASS WAS USED TO CALCULATE THE AVERAGE COSINE OF THE SCATTERING ANGLE.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV


CH_2 at 296° K
σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
σ_T MEASURED TOTAL CROSS SECTION
(S.B. ARMSTRONG, NUCLEAR SCIENCE AND ENGINEERING 23, 192, (1965)
σ_T (E) (barns)
$\bar{\mu}$ (E)
ENERGY (eV)
300
250
200
150
100
50
0
0.6
0.5
0.4
0.3
0.2
0.1
0
0.001
0.01
0.1
1.0

6. Miscellaneous Notes on Polyethylene

For temperatures other than 296°K the switching criteria for the treatment of the different oscillator and the α,β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperatures, effective temperature and ENDF ID numbers of the scattering law data on file

$T^{\circ}K$	$\overline{T}(^{\circ}K)$	ENDF ID No.
296	1222.	GA 0072
350	1239.	GA 0073

POLYETHYLENE

1. Physics

The scattering kernel of polyethylene has been calculated on the basis of a model of noninteracting infinite chains of CH_2 radicals originally developed by Lin and Koenig.[1] The lattice dynamics of polyethylene shows that nine branches of the dispersion relation are present, the frequency in each branch being a function of the phase difference of the vibration of corresponding atoms in neighboring CH_2 units. For some normal modes the ratio of the amplitude of the hydrogen atom vibrations to the amplitude of the carbon atom vibrations also depends strongly on the phase difference.

The neutron scattering has been computed from the weighted frequency spectrum, which has been calculated exactly for the hydrogen atoms using the computed frequencies and amplitude vectors.[2] The weighted frequency spectrum was first calculated in histogram form; two modifications were then made. The low frequency part of the histogram ($\omega < 0.02$ eV) was replaced by a Debye spectrum having the same area. Furthermore, to avoid numerical difficulties, the histogram was replaced by Gaussian functions of area equal to the area under each step and centered at the center of each interval in the histogram.

The inelastic scattering law was calculated using the code GASKET and the distributed weighted frequency spectrum for hydrogen. The incoherent elastic scattering cross section for hydrogen was obtained by the code ZREND. The contribution of the carbon atoms was taken into account by adding the scattering from a free gas of mass 12.011.

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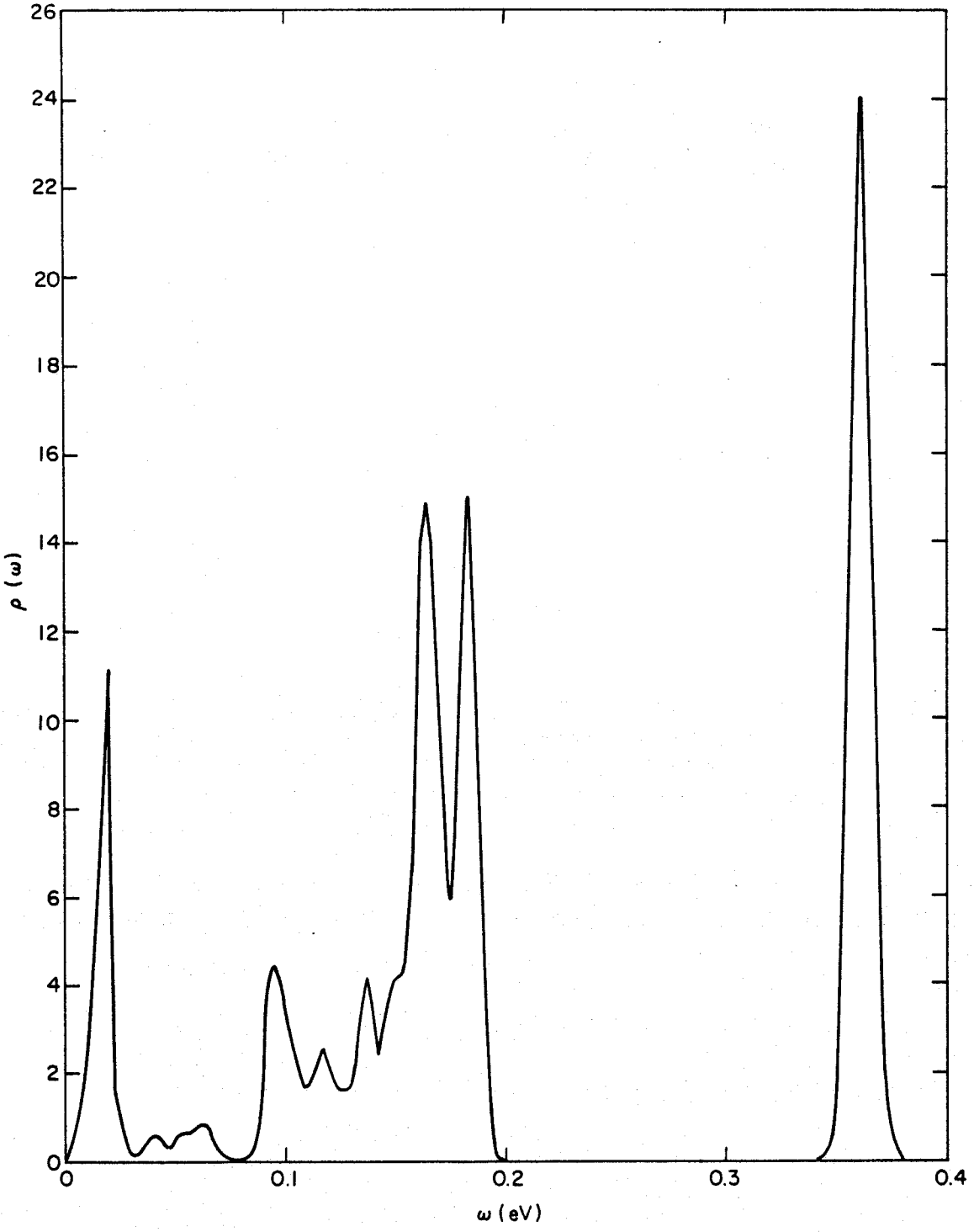
[1] T. P. Lin and J. L. Koenig, J. Molec. Spectra, 9, 228 (1962).

[2] D. Sprevak and J. U. Koppel, Nucleonik, 12, 87 (1969).

2.1 Frequency Spectrum for Hydrogen Bound in CH_2



3.1 GASKET Input for $H(CH_2)$

The code GASKET is discussed in Section A. 3. 1. The data tabulated below follows the format of the code input instructions also given in Section A. 3. 1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Hydrogen in CH_2 at 296 degrees K.
2	11I5	NT -5 NP 80 NE 80 NDAM 1 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 95 JS4 JS5
4	5E10	W1 .015 W2 0.0 W3 1.0 W4 W5
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 T5
6	7E10	AM 1.008 DC 0.0 BETSW 100.0 ALPSW 100.0 CRIT1
		CRIT2 CRIT3
		X3. .001239 .002478 .004957 .007435 .009914 .01239
		.01487 .01735 .01983 .02231 .02478 .02726
		.02974 .03222 .03470 .03718 .03965 .04213
		.04461 .04709 .04957 .05205 .05452 .0570
		.05948 .06196 .06444 .06692 .06940 .07187
		.07435 .07683 .07931 .08179 .08427 .08674
		.08922 .09170 .09418 .09660 .09914 .1016
		.1041 .1066 .1090 .1115 .1140 .1165
		.1190 .1214 .1239 .1264 .1289 .1314
		.1338 .1363 .1388 .1413 .1437 .1462
		.1487 .1512 .1537 .1561 .1586 .1611
		.1636 .1661 .1685 .1710 .1735 .1760
		.1784 .1809 .1834 .1859 .1884 .1908
		.1933 .1958 .1983 .3445 .3470 .3495
		.3519 .3544 .3569 .3594 .3618 .3643
		.3668 .3693 .3718 .3742 .3767

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
8	7E10	Q3. 003977 .015911 .063644 .14320 .254602 .398338
		.578936 .813588 1.11421 .142664 .123003 .0746544
		.0363266. 0178047. 0225532. 0381478. 0519083. 0538862
		.0370908. 0257432. 0412777. 0618430. 0643644. 0632159
		.072237 .07962 .06942 .04917 .02643 .008721
		.001547 .000142 .000068 .001319 .01442 .08034
		.23387 .38590 .43887 .42335 .36435 .29421
		.22868 .18341 .16967 .18547 .22267 .24696
		.22229 .18532 .16542 .16025 .16723 .22006
		.33729 .40786 .32494 .23689 .28456 .37861
		.41046 .41102 .43877 .60685 .99469 1.3731
		1.4766 1.3670 1.0876 .78606 .59386 .65628
		1.0720 1.4847 1.5015 1.2084 .69678 .23548
		.04206 .003843 .000178 .01371 .05987 .20453
		.54649 1.1421 1.8668 2.3868 2.3868 1.8668
		1.1421 .54649 .20453 .05987 .01371
9	Cards 9 and 10 are not needed	
10		
11	7E10	X5
12	7E10	Q5
13	7I10	NPHON
14	5E10	EMAX 1.5 DALPHA 0.01 ALPHAC 0.06 DBETA 0.08 BETAC 2.5
15, 16, 17, 18, 19 and 20 are not needed		
21	2E10	DT .20 TMAX 6.0
		.60 18.0
		1.5 168.0
		4.0 1368.0
		6.5 4618.0
22	2I10	
	2E10	ID 210 NPT 0 SIGF 20.36 EPS 1.0E-6
23	Card 23 is not needed	

3.2 ZREND Input for $H(CH_2)$

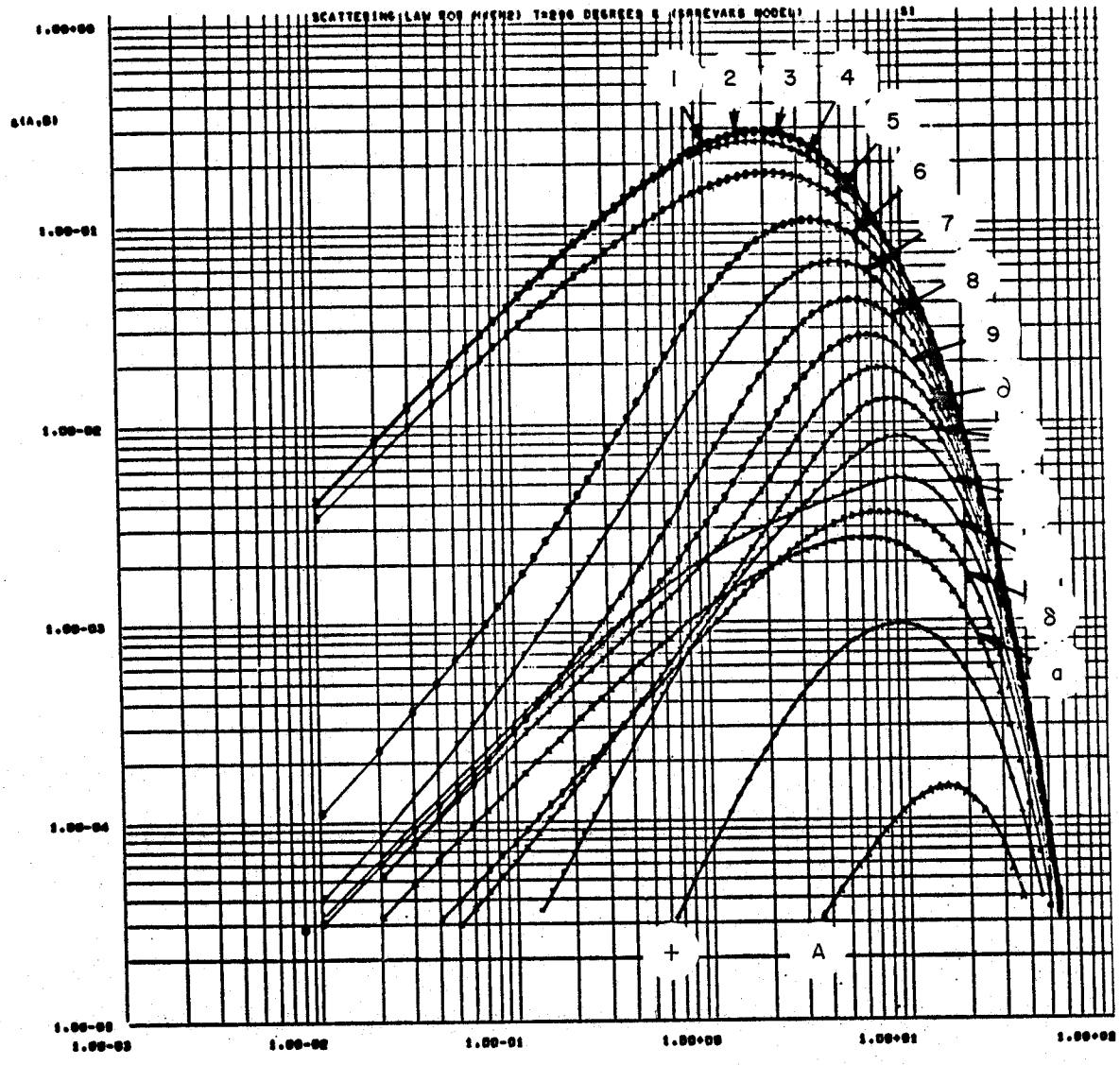
The code ZREND is discussed in Section A.3.1. The data tabulated below follows the format of the code input instruction also given in Section A.3.1. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

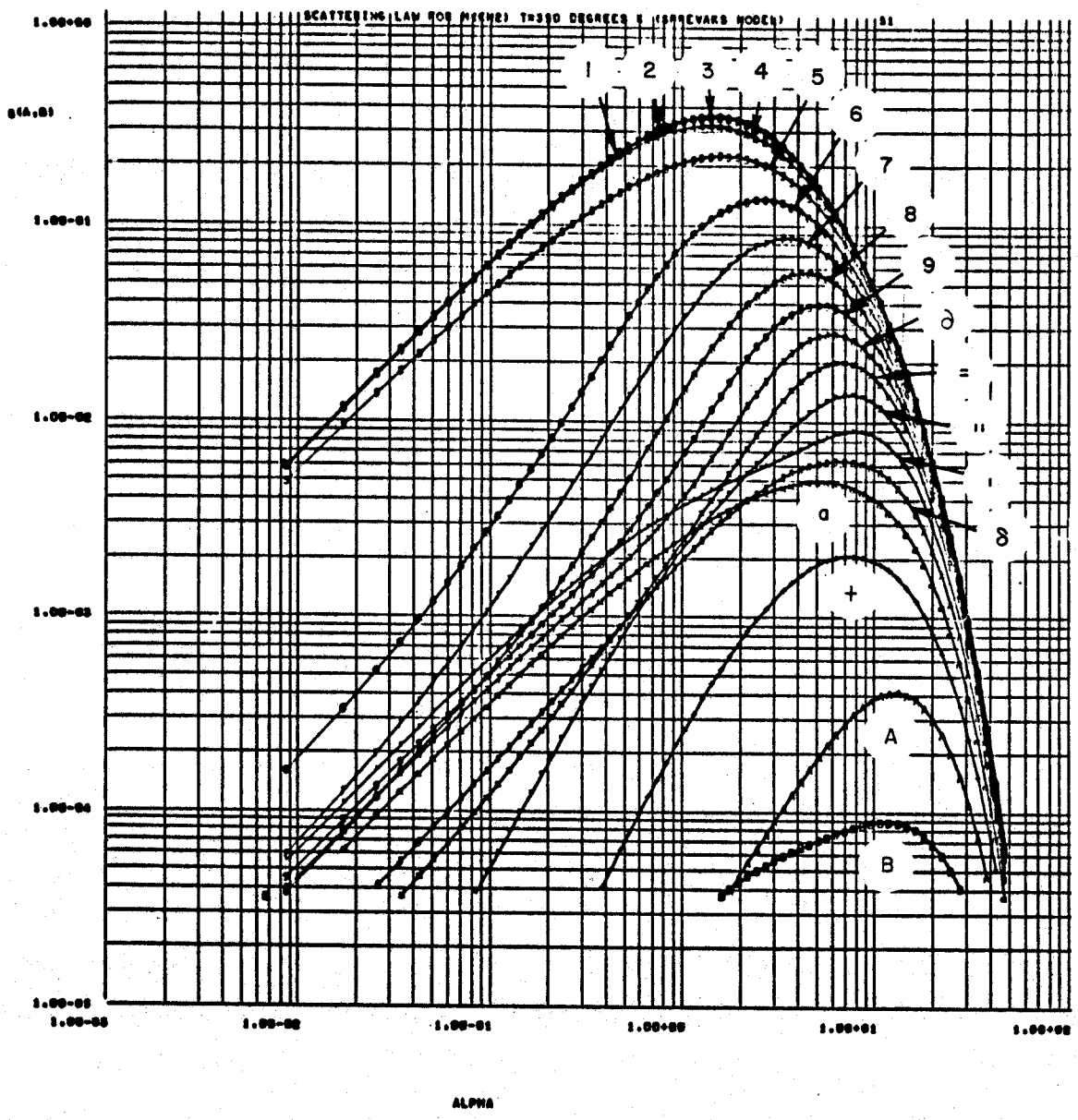
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Incoherent elastic scattering for $H(CH_2)$
2	2I5	NT 2 NE 117 SB 162.88 SWITCH 7.0 EPS 1.0-8
	3E10, I5	NPCH 1
3	7E10	T 296.0 350
4	7E10	WP 34.957 40.282
5	7E10	E .0005 .00053 .00056 .00060 .00064 .00068
		.00072 .00076 .00080 .00085 .00090 .00095
		.0010 .0011 .0012 .0013 .00145 .00160
		.00175 .00190 .00210 .00230 .00250 .00270
		.00290 .00310 .00330 .00350 .00380 .00410
		.00440 .00470 .0050 .0053 .0056 .0060
		.0064 .0068 .0072 .0076 .0080 .0085
		.0090 .0095 .010 .011 .012 .013
		.0145 .0160 .0175 .019 .0210 .0230
		.0250 .0270 .0290 .031 .033 .035
		.038 .041 .044 .047 .05 .053
		.056 .06 .064 .068 .072 .076
		.080 .085 .090 .095 .100 .110
		.120 .130 .145 .160 .175 .190
		.210 .230 .250 .270 .290 .310
		.330 .350 .380 .410 .440 .470
		.500 .530 .560 .600 .640 .680
		.720 .760 .800 .850 .900 .950
		1.000

4. Plots of Scattering Law for $H(CH_2)$

BETA VALUES FOR MULTICURVE PLOT

CURVE	INDEX	$\beta(296^{\circ}K)$	$\beta(350^{\circ}K)$
1	1	0.00	0.00
2	2	8.00 - 02	6.7646 - 02
3	3	1.60 - 01	1.3529 - 01
4	4	4.80 - 01	4.0588 - 01
5	5	8.00 - 01	6.7646 - 01
6	6	1.12 + 00	9.4704 - 01
7	7	1.44 + 00	1.2176 + 00
8	8	1.76 + 00	1.4882 + 00
9	9	2.08 + 00	1.7588 + 00
10	∂	2.40 + 00	2.0294 + 00
11	=	2.7425 + 00	2.3190 + 00
12	"	3.2183 + 00	2.7213 + 00
13	'	3.8924 + 00	3.2913 + 00
14	δ	4.8474 + 00	4.0989 + 00
15	a	6.2005 + 00	5.2430 + 00
16	+	8.1174 + 00	6.8639 + 00
17	A	1.0833 + 01	9.1604 + 00
18	B	1.4681 + 01	1.2414 + 01
19	C	2.0133 + 01	1.7024 + 01
20	D	2.7856 + 01	2.3554 + 01


1
2
3
4
5
6
7
8
9
ALPHA


SCATTERING LAW FOR MSCHE) T=300 DEGREES K (SAVEVARS MODEL)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-06
1.00-02
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA
1
2
3
4
5
6
7
8
9
∂
=
=
δ
a
+
A
B

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

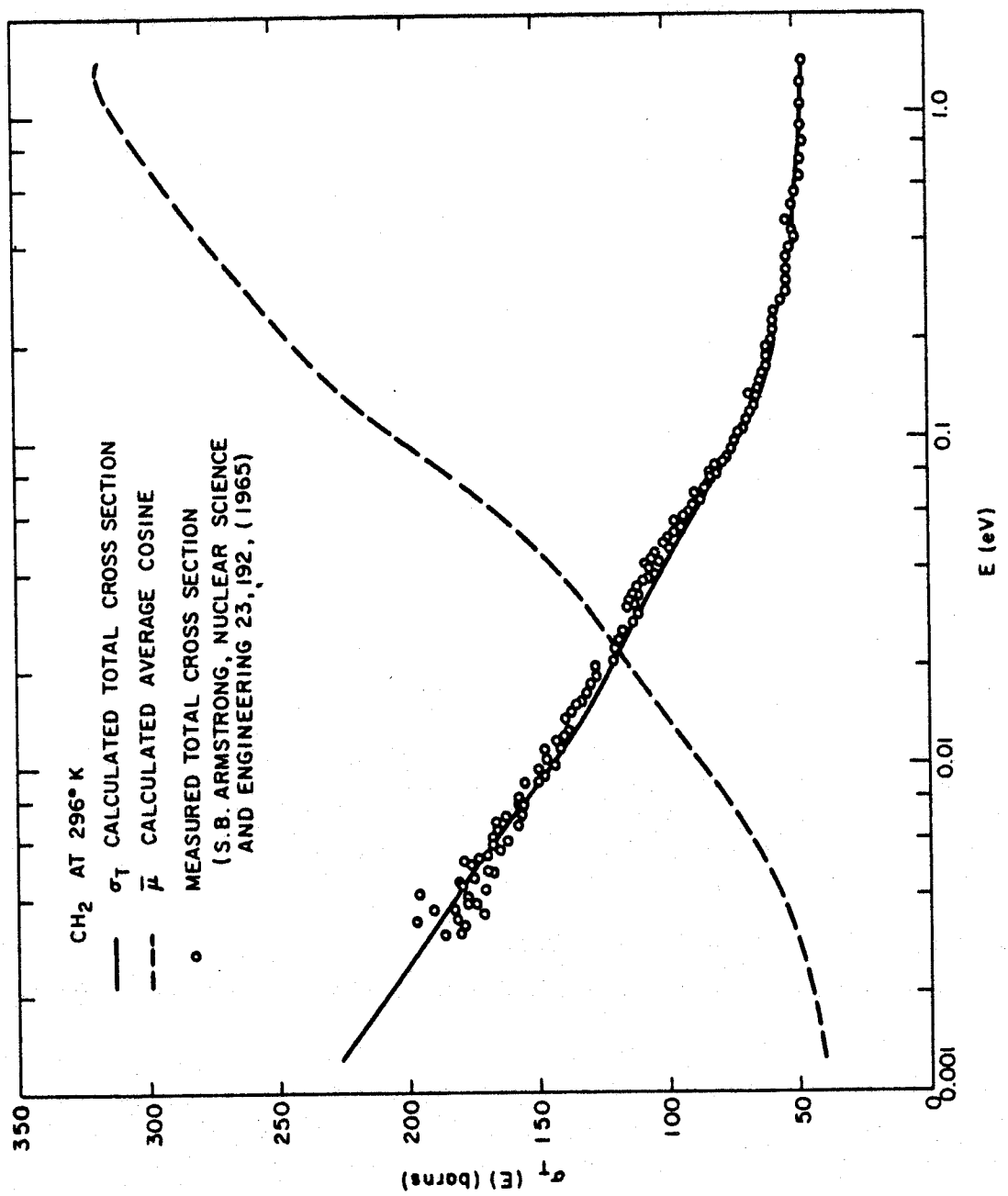
DATA FOR CH2 AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00025	311.33799	-.02495	34	.16800	60.14879	.36960
2	.00075	248.51643	-.02424	35	.18400	59.20434	.37728
3	.00125	226.74058	-.01957	36	.20000	58.57376	.38426
4	.00175	213.72123	-.01386	37	.22400	57.69464	.39431
5	.00225	204.33345	-.00779	38	.24800	56.58626	.40420
6	.00275	196.84912	-.00161	39	.27200	55.32418	.41377
7	.00325	190.39548	.00453	40	.29600	54.09652	.42272
8	.00375	184.84702	.01064	41	.32500	52.87445	.43231
9	.00450	177.75911	.01962	42	.35500	51.95551	.44005
10	.00550	169.59134	.03097	43	.38500	51.41874	.44683
11	.00650	162.81603	.04178	44	.41500	51.06172	.45325
12	.00750	156.85456	.05178	45	.44500	50.70884	.45955
13	.00850	151.75335	.06117	46	.47500	50.32440	.46544
14	.00950	147.21072	.06979	47	.50500	49.94807	.47086
15	.01100	141.44128	.08150	48	.53500	49.62847	.47572
16	.01300	135.20263	.09494	49	.56500	49.38096	.48019
17	.01500	130.27690	.10626	50	.59500	49.18140	.48434
18	.01700	126.33695	.11598	51	.62500	49.00008	.48828
19	.01900	123.09931	.12458	52	.65500	48.82160	.49196
20	.02100	120.33445	.13239	53	.68500	48.64081	.49538
21	.02500	115.57965	.14636	54	.71500	48.47474	.49858
22	.02900	111.40648	.15872	55	.74500	48.32658	.50160
23	.03600	105.11385	.17801	56	.77500	48.19965	.50439
24	.04400	99.09542	.19768	57	.80500	48.08537	.50703
25	.05300	93.27185	.21819	58	.85500	47.90923	.51108
26	.06500	86.61940	.24334	59	.90500	47.75075	.51475
27	.07700	80.97450	.26647	60	.95500	47.61439	.51806
28	.08900	76.16830	.28721	61	1.00500	47.49697	.52107
29	.10100	72.15747	.30580	62	1.10500	47.30117	.52622
30	.11300	68.82245	.32220	63	1.20500	47.14741	.53046
31	.12500	66.06128	.33639	64	1.30500	47.02555	.53409
32	.13700	63.80556	.34821	65	1.40500	46.91265	.53717
33	.15200	61.66796	.36001	66	1.50500	45.81654	.53142

THE TOTAL CROSS SECTION INCLUDES A CONSTANT SCATTERING CROSS SECTION OF 4.71 BARNS (SIG0) FOR THE CARBON ATOM. ALSO FOR THE CARBON, SIG1 = .666*SIG0/MASS WAS USED TO CALCULATE THE AVERAGE COSINE OF THE SCATTERING ANGLE.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.5 EV


CH_2 AT 296° K
σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
MEASURED TOTAL CROSS SECTION
(S.B. ARMSTRONG, NUCLEAR SCIENCE AND ENGINEERING 23, 192, (1965)
σ_T (E) (barns)
E (eV)
350
300
250
200
150
100
50
0
0.001
0.01
0.1
1.0

6. Miscellaneous Notes on CH_2

For temperatures other than 296°K the switching criteria for short collision and the α, β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral and effective temperature of the scattering law data on file.

T(°K)	Debye-Waller Integral (eV^{-1})	$\overline{T}$(°K)
296	34.957	1204.4
350	40.282	1215.1

BENZENE

1. Physics

The benzene molecule C_6H_6 has a hexagonal planar structure with symmetry D_{6h}. Two parameters describe the geometry of the molecule, namely the distance between two nearest carbon atoms, 1.39 Å, and the distance between a carbon and the nearest hydrogen, 1.08 Å.

The following assumptions have been made in order to describe the atomic motions in the benzene molecules:[1]

1. There is no interaction between vibrational and rotational states of the molecule.

2. The hindered rotations which describe the interactions of molecules in the liquid are replaced by translations of the whole molecule with an effective mass. The effective translational masses associated with the hydrogen and carbon atoms are 20.94 and 42.2 respectively (in atomic units).

Continuous frequency distributions weighted by the amplitudes of the polarization vectors have been obtained for the hydrogen and for the carbon atoms. Details of the normal mode calculation from which the frequency spectra were obtained are given in Ref. 2. The cluster of frequencies closely spaced around 0.38 eV was lumped into a single oscillator. The inelastic scattering laws for hydrogen and carbon in C_6H_6 were calculated from these weighted distributions by the code GASKET. The two scattering laws were then combined with the final value being referred to hydrogen as a primary scatterer.

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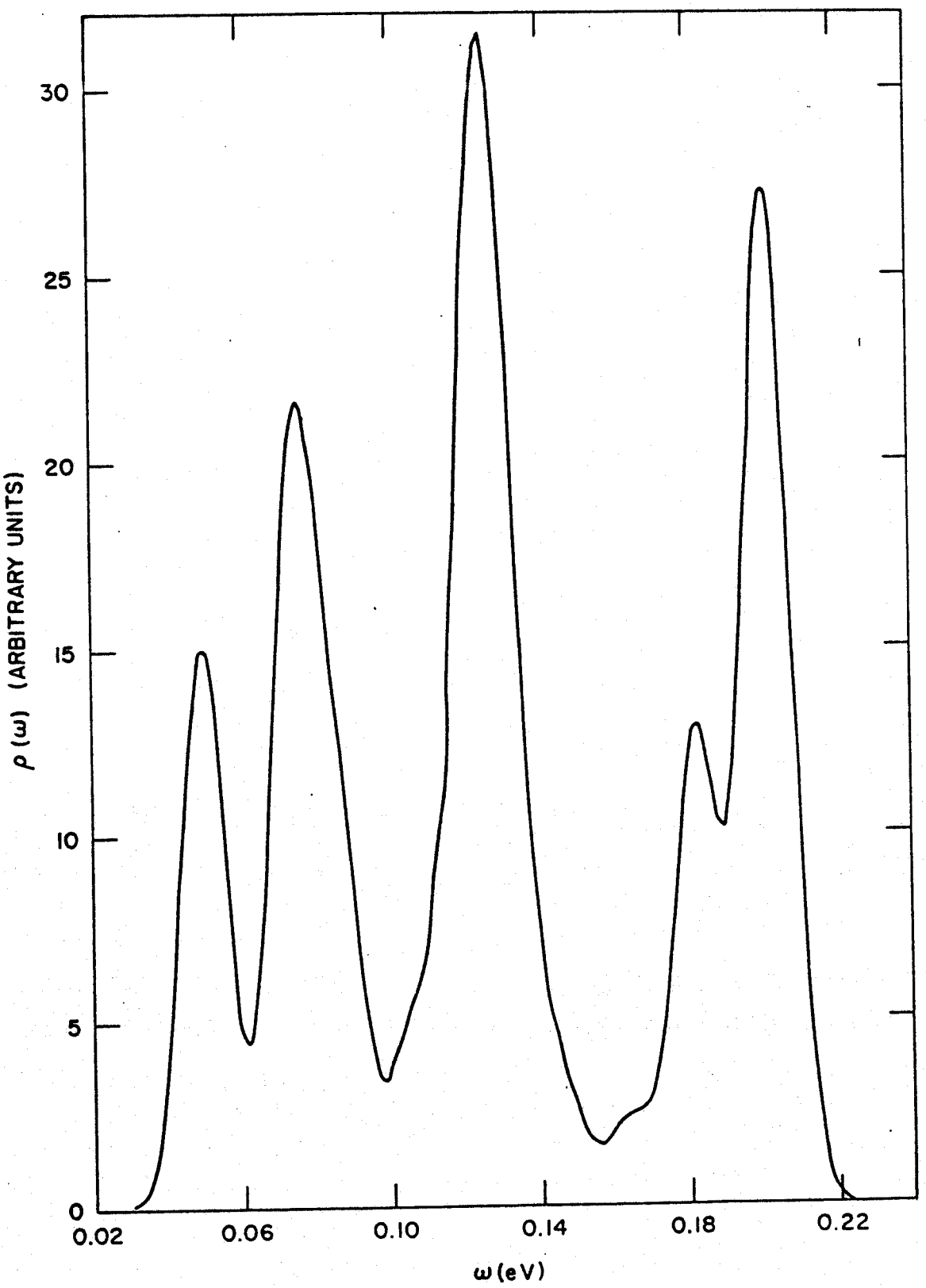
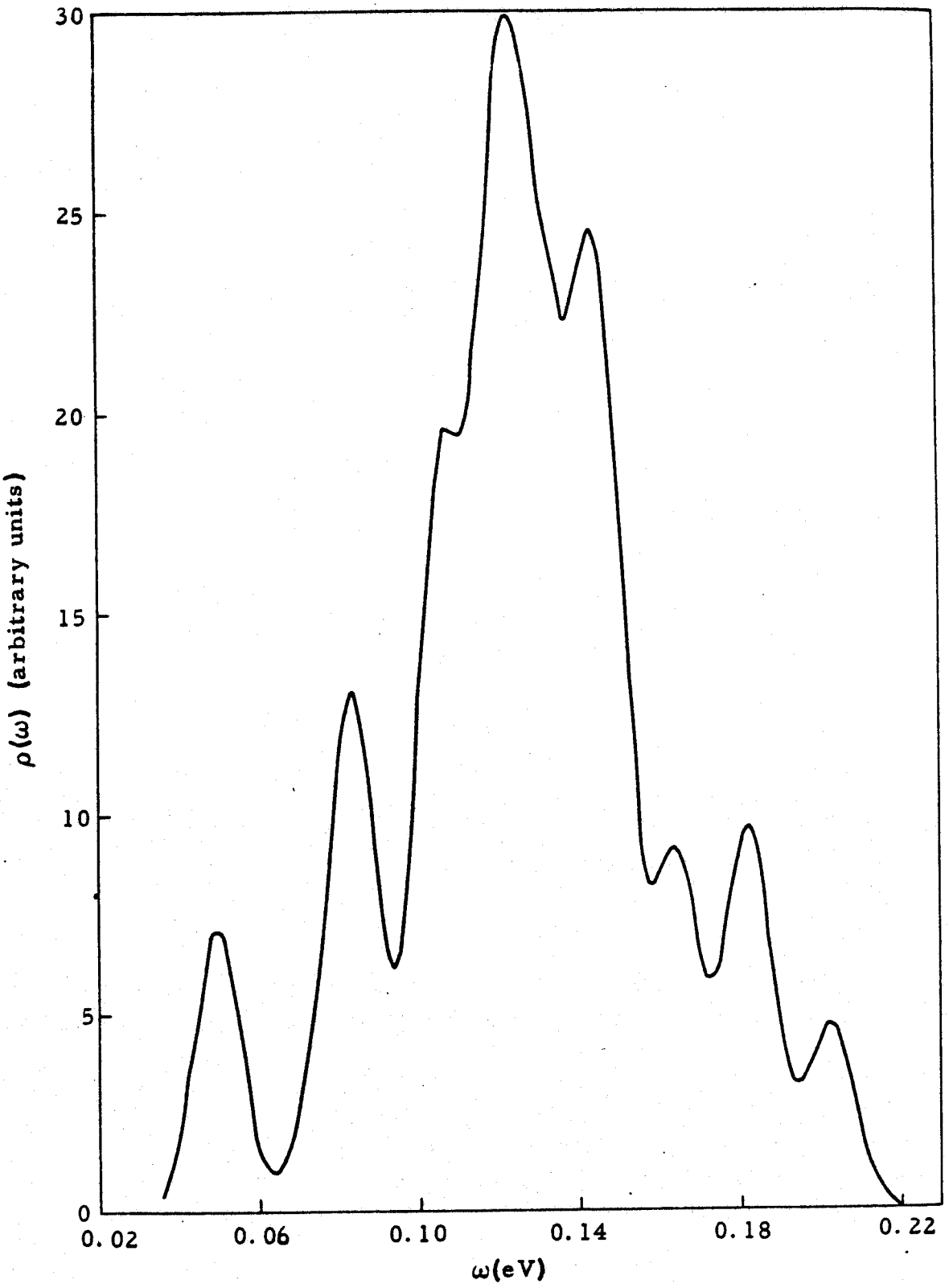
(1) D. Sprevak, G. M. Borgonovi, J. M. Neill and G. W. Carriveau, Nukleonik, 11, 233 (1968).

(2) D. Sprevak, G. M. Borgonovi, G. W. Carriveau and J. M. Neill, "Neutron Thermalization in Benzene," USAEC Report GA-8185, General Dynamics Corporation, General Atomic Division, August 1967.



Vibrational spectrum of the carbon atoms used to calculate benzene kernel. (The set of frequencies about 0.38 eV are now shown.)

C_6H_6 - 2.1



Vibrational spectrum of the hydrogen atoms used to calculate benzene kernel. (The set of frequencies about 0.38 eV are not shown.)

3.1 GASKET Input for $H(C_6H_6)$

The code GASKET is discussed in Section A. 3. 1. The data tabulated below follows the format of the code input instructions also given in Section A. 3. 1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Sprevak's $H(C_6H_6)$ at 296 degrees K.
2	11I5	NT -5 NP 80 NE 80 NDAM 0 NGPRT 0 NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0 IPG 0
3	3I5	JS3 84 JS4 0 JS5 1
4	5E10	W1.04775436W2. 0.0 W3.65331978W4 0.0 W5. 29892586
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 0.0 T5 .0255
6	7E10	AM 1.008 DC 0.0 BETSW 100.0 ALPSW 100.0 CRIT1 CRIT2 CRIT3
		X3.0210766 .0272756 .0334746 .0359542 .0384338 .0409134 .0433930 .0458726 .0483522 .0508318 .0533114 .0557910 .0582706 .0607502 .0632298 .0657094 .0681890 .0706686 .0731482 .0756278 .0781074 .080587 .0830666 .0855462 .0880258 .0905054 .092985 .0954646 .0979442 .10042 .102903 .105383 .107863 .110342 .112822 .114062 .115301 .116541 .117781 .119021 .120261 .1215 .12274 .12522 .127699 .130179 .132659 .135138 .137618 .140097 .142577 .145057 .147536 .150016 .152495 .154975 .157455 .159934 .162414 .164893 .167373 .169853 .172332 .174812 .177291 .179771 .182251 .18473 .18721 .189689 .192169 .194649 .197128 .199608 .202087 .204567 .207047 .209526 .212006 .214485 .216965 .219445 .221924 .225644

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
8	7E10	Q3 .657-4 .0557572 .162635 .46492 1.12039 2.27607
		3.89790 5.62736 6.84881 7.02751 6.08244 4.4523
		2.79484 1.61186 1.09722 1.22166 1.88249 3.00571
		4.59136 6.66954 9.11053 11.4021 12.712 12.3825
		10.5085 8.05225 6.37598 6.56681 8.92219 12.7375
		16.5438 18.9239 19.5314 19.4166 20.1650 21.1560
		22.5272 24.1431 25.8155 27.3473 28.5736 29.3896
		29.7608 29.3247 27.8637 26.0197 24.2628 23.0276
		22.7183 23.3652 24.2650 24.1488 22.0091 17.9748
		13.3792 9.87602 8.34718 8.45035 9.02810 8.98379
		8.00031 6.64683 5.86717 6.25846 7.62610 9.07965
		9.60776 8.75109 6.87802 4.87321 3.54396 3.20771
		3.64891 4.33341 4.70823 4.46195 3.63710 2.53857
		1.51375 .769813 .333320 .122689 .0383350 .491124-2
9	Cards 9 and 10 are not needed	
10		
11	7E10	X5
12	7E10	Q5
13	7I10	NPHON
14	5E10	EMAX DALPHA ALPHAC DBETA BETAC
15, 16, 17, 18, 19 and 20 are not needed		
21	2E10	DT TMAX
22	2I10	
	2E10	ID NPT SIGF EPS
23	Card 23 is not needed	

3.2 GASKET Input for $C(C_6H_6)$

The code GASKET is discussed in Section A.3.1. The data tabulated below follows the format of the code input instructions also given in Section A.3.1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

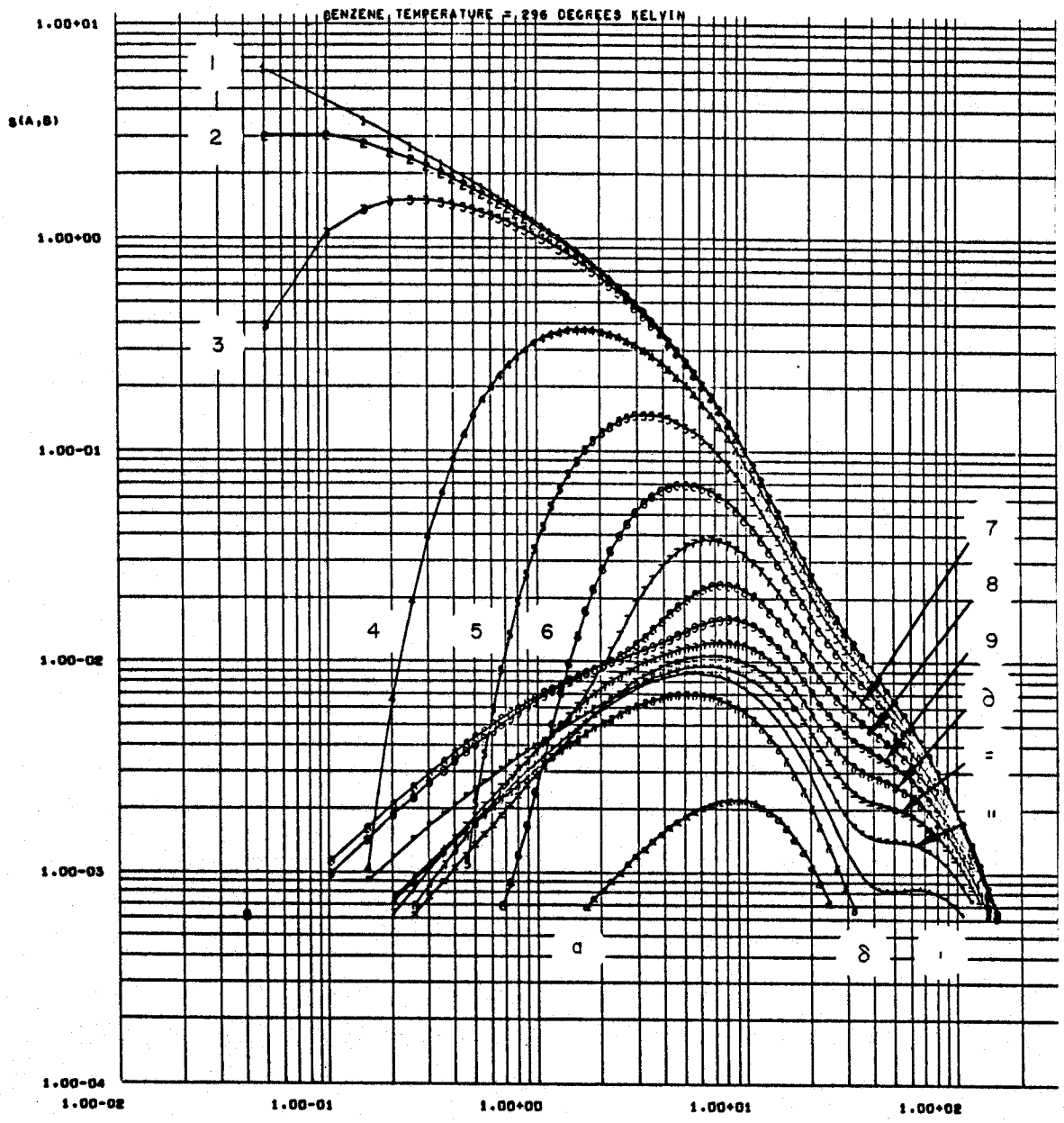
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Sprevak's $C(C_6H_6)$ at 296 degrees K.
2	11I5	NT -5 NP 80 NE 80 NDAM 0 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 86 JS4 0 JS5 1
4	5E10	W1 .2848568 W2 0.0 W3 .6799013 W4 0.0 W5 .03524188
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 0.0 T5 .0255
6	7E10	AM 12.011 DC ____ BETSW ____ ALPSW ____ CRIT1 ____
		CRIT2 ____ CRIT3 ____
		X3 .0210766 .024796 .0272756 .0297552 .0322348 .0359542
		.0384338 .0409134 .0433930 .0458726 .0483522 .050831
		.0533114 .0557910 .0582706 .0607502 .0632298 .0657094
		.0681890 .0706686 .0731482 .0756278 .0781074 .0805870
		.0830666 .0855462 .0880258 .0905054 .0929850 .0954646
		.0979442 .100424 .102903 .105383 .107863 .110342
		.112822 .115301 .117781 .120261 .122740 .125220
		.127699 .130179 .132659 .135138 .136378 .138858
		.141337 .143817 .146296 .148776 .151256 .153735
		.156215 .158694 .161174 .163654 .166133 .168613
		.171092 .173572 .176052 .178531 .181011 .183590
		.185970 .188540 .190929 .193409 .195888 .198368
		.200848 .202087 .204567 .207047 .209526 .212006
		.214485 .216965 .219445 .221924 .224404 .226883
		.229363 .231843 ____ ____ ____ ____
		____ ____ ____ ____ ____ ____
		____ ____ ____ ____ ____ ____

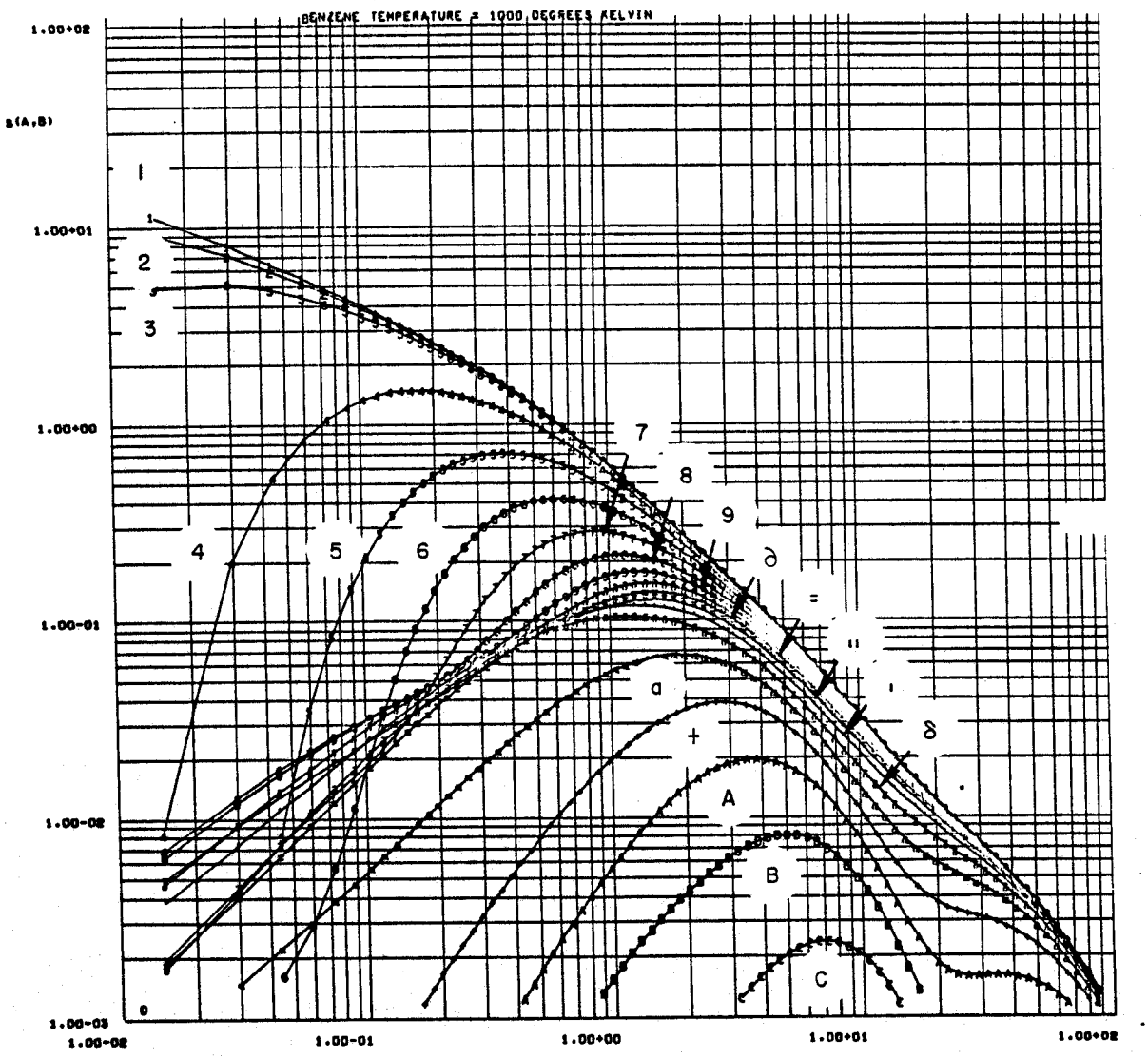
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
8	7E10	Q3 .0001394 .002276 .0118288 .0518248 .191408 .986323
		2.37689 4.82867 8.26939 11.9386 14.5310 14.9158
		12.9363 9.57165 6.34166 4.55398 4.94717 7.64850
		12.08790 16.9292 20.4759 21.6053 20.4665 18.1607
		15.6907 13.2922 10.7283 7.98262 5.50871 3.89351
		3.40532 3.83098 4.65451 5.43735 6.18629 7.45024
		10.0043 14.2772 19.8946 25.6449 29.9190 31.4131
		29.7227 25.4886 20.0272 14.7016 12.3965 8.76491
		6.37869 4.87859 3.83559 2.97089 2.24017 1.76195
		1.64964 1.86803 2.21706 2.46529 2.55559 2.73752
		3.49435 5.23719 7.89931 10.7300 12.59360 12.7343
		11.4726 10.2140 10.6759 13.8067 19.0333 24.3230
		27.1901 27.1773 24.1861 18.4339 12.0354 6.73345
		3.22796 1.32526 .465514 .139718 .0357764 .00780317
		.0014474 .000228
9	Cards 9 and 10 are not needed	
10		
11	7E10	X5 .3798541
12	7E10	Q5 1.0
13	7I10	NPHON 5
14	5E10	EMAX 2.0 DALPHA .0041967 ALPHAC .041967 DBETA .08 BETAC 2.5
15, 16, 17, 18, 19 and 20 are not needed		
21	2E10	DT .1 TMAX 6.0
		.2 16.0
		.4 68.0
		1.0 272.0
		2.0 1072.0
22	2I10	
	2E10	ID 96 NPT 0 SIGF 4.71 EPS 1.0-6
23	Card 23 is not needed	

4. Plots of Scattering Law for C_6H_6

BETA VALUES FOR MULTICURVE PLOT

CURVE	INDEX	$\beta(296^{\circ}K)$	$\beta(1000^{\circ}K)$
1	1	0.00	0.0
2	2	0.0800	0.0237
3	3	0.160	0.0474
4	4	0.480	0.1421
5	5	0.800	0.2368
6	6	1.120	0.3315
7	7	1.440	0.4262
8	8	1.760	0.5209
9	9	2.080	0.6156
10	∂	2.400	0.7103
11	=	2.745	0.8123
12	"	3.239	0.9586
13	'	3.963	1.173
14	δ	5.022	1.486
15	a	6.573	1.945
16	+	8.843	2.615
17	A	12.168	3.601
18	B	17.035	5.042
19	C	24.162	7.151
20	D	34.600	10.239


BENZENE, TEMPERATURE = 296 DEGREES KELVIN
S(A,B)
1.00+01
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
1.00+01
1.00+02
1
2
3
4
5
6
7
8
9
∂
=
"
α
δ
ι


ALPHA
BENZENE TEMPERATURE = 1000 DEGREES KELVIN
S(A,B)
1.00+02
1.00+01
1.00+00
1.00-01
1.00-02
1.00-03
1.00-02
1.00-01
1.00+00
1.00+01
1.00+02
1
2
3
4
5
6
7
8
9
∂
=
δ
a
+
A
B
C

5. INTEGRAL DATA

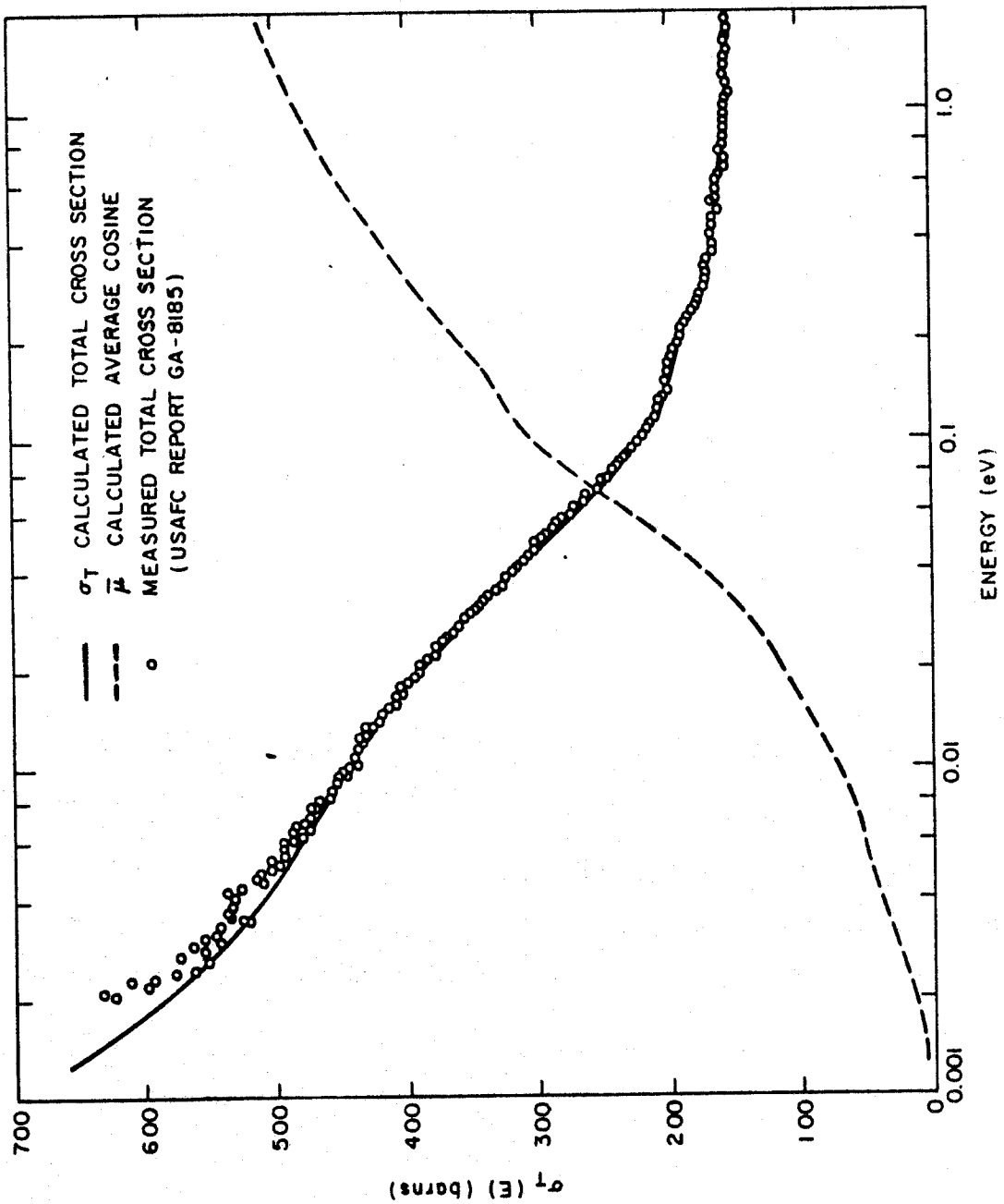
TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR C_6H_6 AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00025	1201.02400	-.00728	37	.22400	185.33761	.36956
2	.00075	779.53856	-.00495	38	.24800	181.47426	.37903
3	.00125	661.71517	.00264	39	.27200	178.33136	.38690
4	.00175	603.79501	.01029	40	.29600	175.42882	.39294
5	.00225	570.66467	.01766	41	.32500	172.49613	.40036
6	.00275	548.08026	.02424	42	.35500	169.76371	.40719
7	.00325	530.38136	.02998	43	.38500	167.67158	.41332
8	.00375	516.23259	.03472	44	.41500	166.14968	.41899
9	.00450	502.16706	.04212	45	.44500	164.88797	.42455
10	.00550	485.68152	.04904	46	.47500	163.67643	.42966
11	.00650	474.08694	.05548	47	.50500	162.61503	.43431
12	.00750	463.12953	.06060	48	.53500	161.80374	.43861
13	.00850	453.97712	.06431	49	.56500	161.11257	.44270
14	.00950	445.93833	.06947	50	.59500	160.49148	.44651
15	.01100	437.00513	.07798	51	.62500	159.93048	.45009
16	.01300	425.54068	.08790	52	.65500	159.43954	.45346
17	.01500	414.30129	.09577	53	.68500	158.98866	.45652
18	.01700	403.79544	.10322	54	.71500	158.56784	.45947
19	.01900	393.93216	.11044	55	.74500	158.18708	.46220
20	.02100	384.61083	.11748	56	.77500	157.82635	.46478
21	.02500	367.23240	.13084	57	.80500	157.48566	.46723
22	.02900	350.44792	.14120	58	.85500	156.97461	.47097
23	.03600	326.94867	.16417	59	.90500	156.52364	.47438
24	.04400	303.96256	.18775	60	.95500	156.11275	.47752
25	.05300	282.47900	.21229	61	1.00500	155.74192	.48041
26	.06500	259.85552	.24169	62	1.10500	155.12044	.48551
27	.07700	241.67532	.26677	63	1.20500	154.60915	.48988
28	.08900	227.56727	.28733	64	1.30500	154.17801	.49367
29	.10100	217.02069	.30325	65	1.40500	153.80699	.49701
30	.11300	209.55520	.31481	66	1.50500	153.46608	.50003
31	.12500	204.61051	.32289	67	1.60500	153.16526	.50275
32	.13700	201.21646	.32804	68	1.70500	152.87450	.50530
33	.15200	198.54208	.33467	69	1.80500	152.59381	.50768
34	.16800	195.88807	.34213	70	1.90500	152.25318	.50995
35	.18400	192.93460	.35019	71	2.00500	148.06259	.50528
36	.20000	189.83155	.35829				

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	2.0 EV


σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
MEASURED TOTAL CROSS SECTION
(USAFC REPORT GA-8185)
σ_T (E) (barns)
ENERGY (eV)
700
600
500
400
300
200
100
0
0.001
0.01
0.1
1.0

6. Miscellaneous Notes on Benzene

For temperatures other than 296°K the switching criteria for short collision and the α, β mesh input for 296°K were multiplied by $\frac{296°K}{T°K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral and effective temperature of the scattering law data on file.

T(°K)	Debye Waller Integral (eV^{-1}) for Hydrogen	$\overline{T}$(°K) for Hydrogen	Debye Waller Integral (eV^{-1}) for Carbon	$\overline{T}$(°K) for Carbon
296	9.3536	1165.9	10.730	685.54
350	9.7064	1177.8	11.315	712.02
400	10.093	1191.4	11.927	738.97
450	10.530	1207.7	12.593	768.10
500	11.009	1226.0	13.304	799.22
600	12.070	1268.7	14.831	866.63
800	14.471	1373.4	18.165	1017.3
1000	17.096	1497.7	21.720	1182.3

D_2O

1. Physics

Whereas hydrogen is nearly a completely incoherent neutron scatterer, the scattering from deuterium is largely coherent. Although it would appear that due to this fact a treatment of D_2O analog to the one used for H_2O would be inadequate, calculations[1] have shown that because of a great deal of cancellation between inter and intra- molecular interference scattering, integral quantities like the total cross section or thermal neutron spectra can actually be predicted quite accurately with an incoherent model.

The scattering law for D_2O calculated for the ENDF using the code GASKET is based on a model quite similar to the one used for H_2O. The internal modes of vibration are represented by oscillators having the measured frequencies of 0.142 and .305 eV (approximately $1/\sqrt{2}$ times the corresponding frequencies for H_2O as expected from the mass ratio) and the weights 1/6 and 1/3 respectively. The torsional oscillations are represented by a broad band of frequencies extending from 0 up to 0.127 eV and peaking at about 0.05 eV as shown in the figure of Section 2.1. Their total weight is 9/20. This torsional band was taken from the work of Haywood[2] although here,as well as in the case of H_2O, the low frequency range of his spectrum was replaced by a parabola $c\omega^2$ smoothly joining the rest of the torsional band at about 0.025 eV. Haywood's original spectrum showed several peaks in this low frequency range, corresponding to translational vibrations of the D_2O molecule as a whole. These modes

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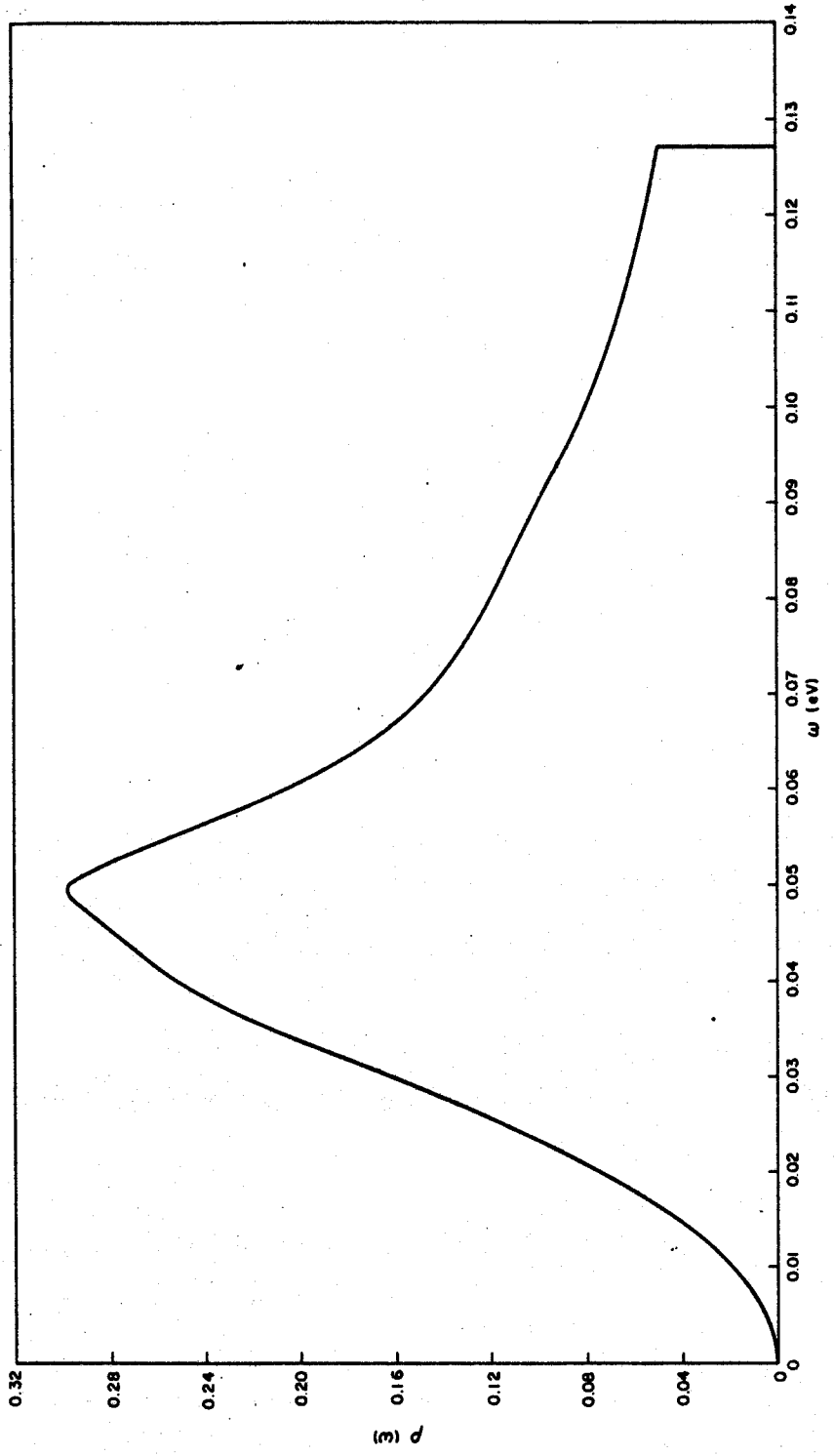
[1] J.U. Koppel and J.A. Young, Nukleonik, 7, 408 (1965).

[2] B.C. Haywood, Proceeding of the IAEA Symposium on Pulsed Neutron Research, Karlsruhe, Vol. 1, p. 434 (5/1965).

were replaced by free translations of mass 20 in order to avoid numerical difficulties.

The scattering by the oxygen atoms is not included in the tabulated scattering law data. It should be taken into account by adding to the data the properly weighted $S(\alpha, \beta)$ for a free gas of mass 16 recalling, however, that the α values for the oxygen must be 2.014/16 times those for the deuterium in order to correspond to the same neutron momentum transfer K.

2. Torsional Frequency Spectrum for D_2O



3.1 GASKET Input for D_2O at 296°K

The code GASKET is discussed in Section A. 3. The data tabulated below follows the format of the code input instructions also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

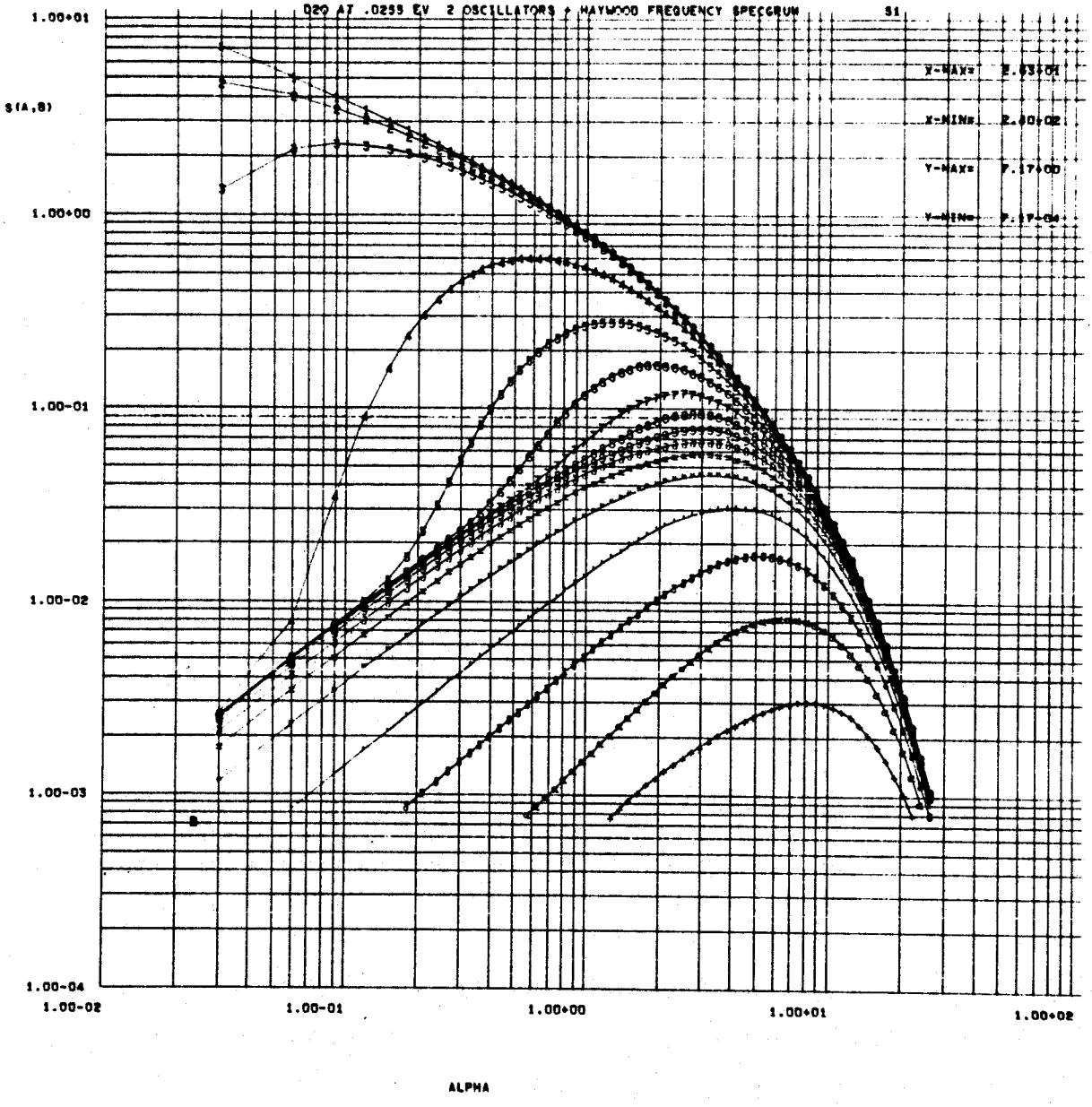
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6,A2	COM D_2O - 2 OSC. + Haywood Freq. Spectrum
2	11I5	NT -6 NP 80 NE 80 NDAM 0 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 -51 JS4 0 JS5 2
4	5E10	W1 .05 W2 0.0 W3 .45 W4 0.0 W5 .5
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 0.0 T5 .0255
6	7E10	AM 2.014 DC 0.0 BETSW 50.0 ALPSW 50.0 CRIT1 0.0
		CRIT2 0.0 CRIT3 1.0-7
7	7E10	X3 .129642

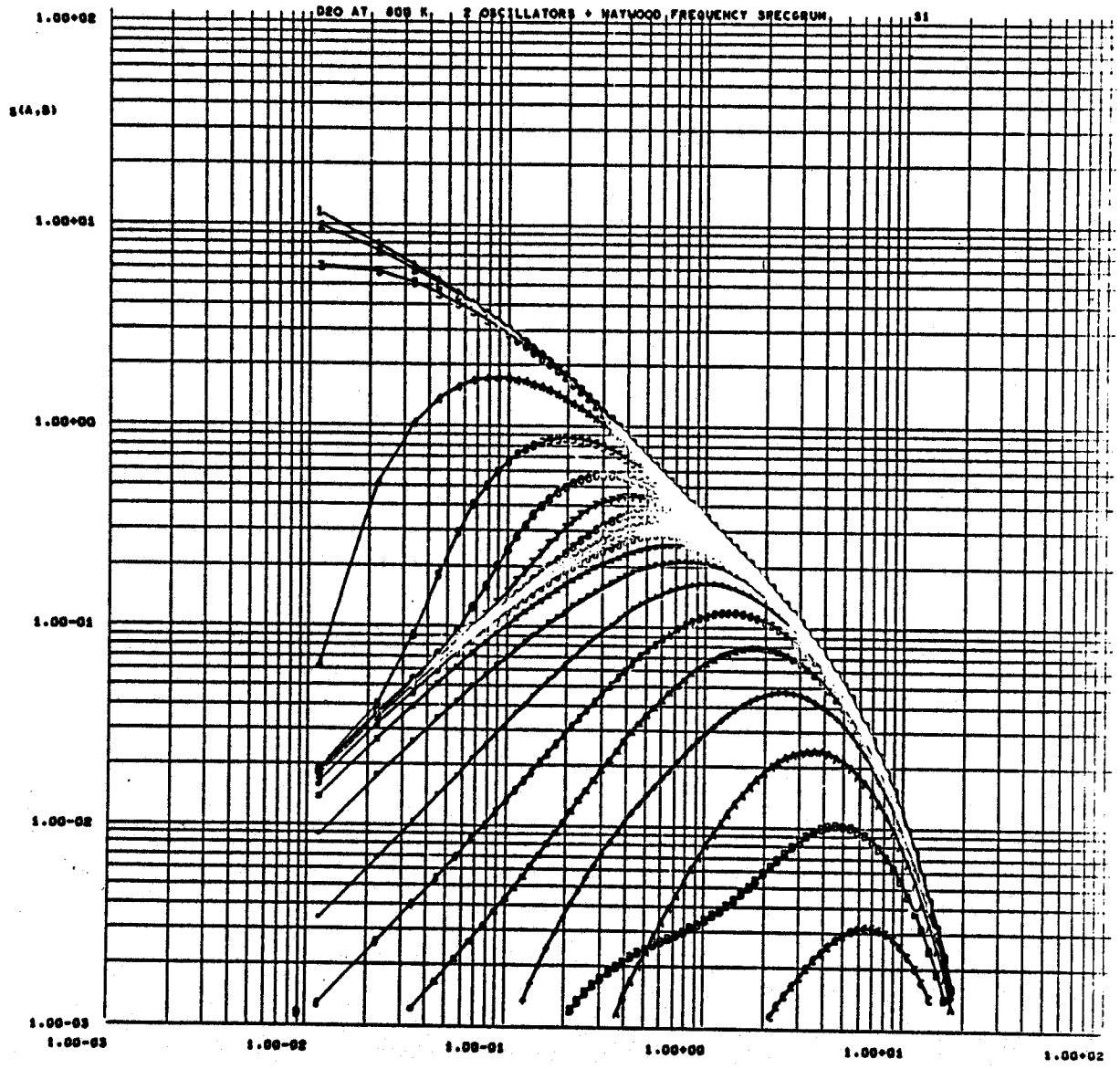
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES						
8	7E10	Q3	.0012	.0048	.0108	.0192	.03	.0432
			.0588	.0768	.0972	.12	.142	.17
			.195	.217	.24	.256	.27	.282
			.294	.291	.271	.245	.22	.20
			.178	.166	.153	.143	.135	.128
			.122	.118	.112	.106	.101	.098
			.092	.086	.081	.076	.074	.070
			.066	.064	.060	.058	.055	.053
			.051	.049	0.0			
9	Cards 9 and 10 are not needed							
10								
11	7E10	X5	.14235	.30504				
12	7E10	Q5	.3333333	.6666667				
13	7I10	NPHON	14	7				
14	5E10	EMAX	1.5	DALPHA	.03	ALPHAC	.3	DBETA .05 BETAC 1.5
15, 16, 17, 18, 19 and 20 are not needed								
21	2E10	DT	.1	TMAX	2.0			
			.25		10.0			
			.5		30.0			
			.75		100.0			
			5.0		500.0			
			10.0		2000.0			
22	2I10 2E10	ID	51	NPT	0	SIGF	3.37	EPS .000001
23	Card 23 is not needed							

4. Plots of Scattering Law

β Values for Multicurve Plots

CURVE	INDEX	β(296K)	β(800K)
1	1	0.00	0.00
2	2	.05	.0185
3	3	.10	.0370
4	4	.30	.111
5	5	.50	.185
6	6	.70	.259
7	7	.90	.333
8	8	1.10	.407
9	9	1.30	.481
10	∂	1.50	.555
11	=	1.73	.649
12	"	2.08	.788
13	'	2.59	.990
14	δ	3.34	1.29
15	α	4.46	1.72
16	+	6.12	2.36
17	A	8.57	3.29
18	B	12.20	4.65
19	C	17.57	6.64
20	D	25.51	9.56


D2O AT .0253 EV 2 OSCILLATORS + HAYWOOD FREQUENCY SPECTRUM
S(A,B)
1.00+01
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA


D2O AT 600 K, 2 OSCILLATORS + HATWOOD FREQUENCY SPECTRUM, S1
S(A,B)
1.00+02
1.00+01
1.00+00
1.00-01
1.00-02
1.00-03
1.00-03
1.00-02
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

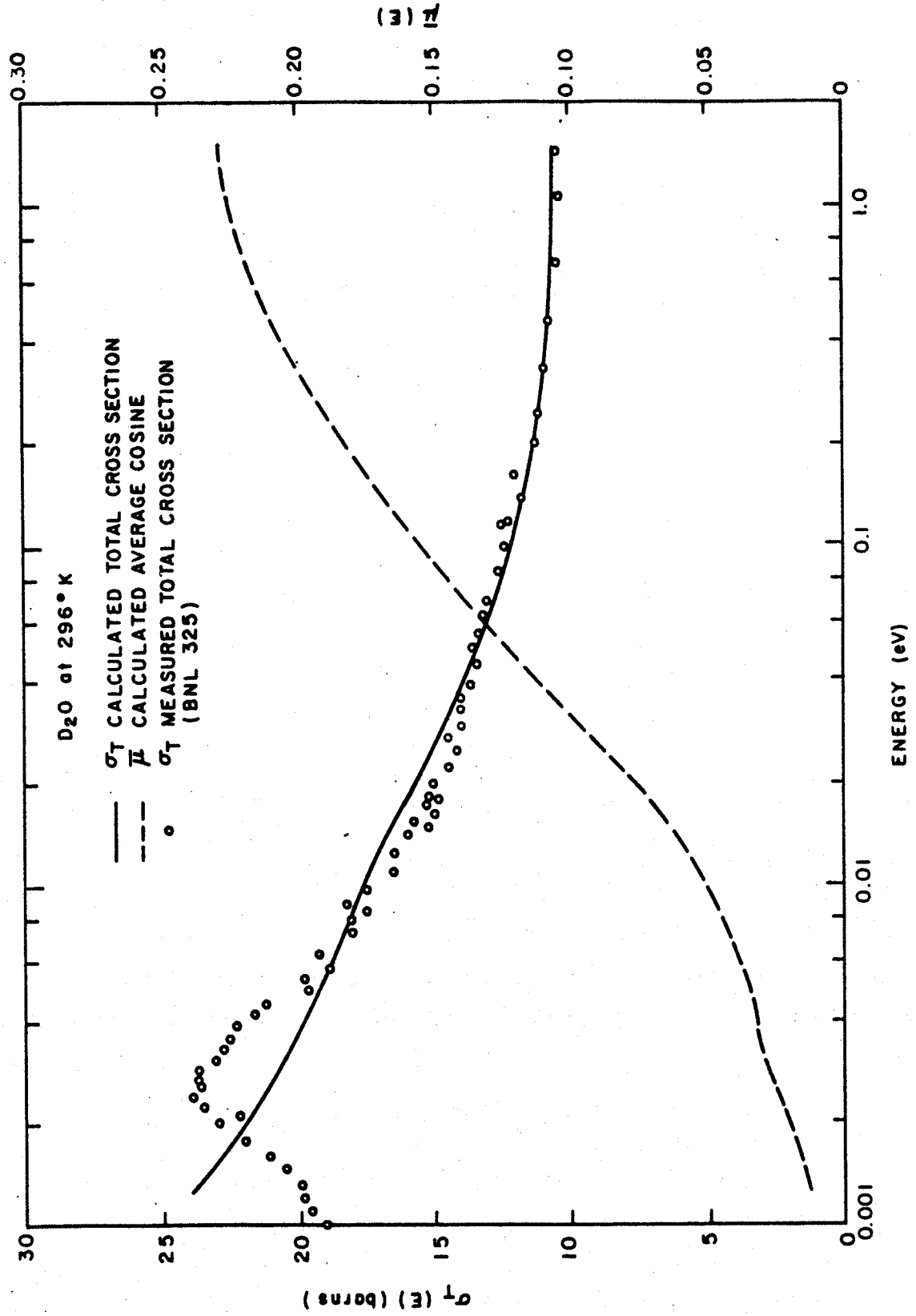
DATA FOR D2O AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00025	38.07525	.00066	34	.16800	11.59936	.17545
2	.00075	27.05134	.00570	35	.18400	11.50014	.17907
3	.00125	24.04814	.01321	36	.20000	11.40593	.18226
4	.00175	22.59090	.01931	37	.22400	11.27391	.18649
5	.00225	21.65168	.02357	38	.24800	11.15229	.19016
6	.00275	21.00219	.02638	39	.27200	11.04408	.19332
7	.00325	20.58357	.03124	40	.29600	10.95047	.19558
8	.00375	20.10239	.03082	41	.32500	10.88406	.19893
9	.00450	19.65958	.03502	42	.35500	10.84085	.20199
10	.00550	19.14117	.03805	43	.38500	10.81264	.20477
11	.00650	18.71781	.04077	44	.41500	10.79063	.20717
12	.00750	18.36669	.04357	45	.44500	10.77122	.20914
13	.00850	18.08219	.04698	46	.47500	10.75521	.21085
14	.00950	17.79570	.04941	47	.50500	10.74121	.21235
15	.01100	17.40920	.05333	48	.53500	10.72780	.21366
16	.01300	16.95268	.05792	49	.56500	10.71359	.21477
17	.01500	16.58219	.06387	50	.59500	10.69999	.21577
18	.01700	16.24372	.06957	51	.62500	10.68798	.21670
19	.01900	15.93826	.07499	52	.65500	10.67638	.21752
20	.02100	15.65841	.08006	53	.68500	10.66618	.21827
21	.02500	15.16453	.08892	54	.71500	10.65697	.21898
22	.02900	14.73386	.09520	55	.74500	10.64897	.21962
23	.03600	14.19817	.10819	56	.77500	10.64177	.22020
24	.04400	13.71790	.11768	57	.80500	10.63516	.22075
25	.05300	13.34724	.12669	58	.85500	10.62516	.22154
26	.06500	12.97677	.13503	59	.90500	10.61595	.22226
27	.07700	12.69793	.14290	60	.95500	10.60715	.22292
28	.08900	12.46789	.14963	61	1.00500	10.59875	.22351
29	.10100	12.27206	.15539	62	1.10500	10.58274	.22458
30	.11300	12.10244	.16033	63	1.20500	10.56753	.22553
31	.12500	11.95361	.16447	64	1.30500	10.55353	.22632
32	.13700	11.81880	.16718	65	1.40500	10.53852	.22683
33	.15200	11.70738	.17160	66	1.50500	10.37632	.21750

THE TOTAL CROSS SECTION INCLUDES A CONSTANT SCATTERING CROSS SECTION OF 3.76 BARNS (SIG0) FOR THE OXYGEN ATOM. ALSO FOR THE OXYGEN, SIG1 = .666*SIG0/MASS WAS USED TO CALCULATE THE AVERAGE COSINE OF THE SCATTERING ANGLE.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.5 EV


D_2O at 296° K
σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
σ_T MEASURED TOTAL CROSS SECTION (BNL 325)
σ_T (E) (barns)
$\bar{\mu}$ (E)
ENERGY (eV)
30
25
20
15
10
5
0
0.30
0.25
0.20
0.15
0.10
0.05
0
0.001
0.01
0.1
1.0

6. Miscellaneous Notes on D_2O

For temperatures other than 296°K the switching criteria for short collision and the α,β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral, effective temperature and ID numbers of the scattering law data on file.

T(°K)	Debye-Waller Integral (eV^{-1})	$\overline{T}$(°K)	ENDF ID No.
296	39.867	940.91	GA 0051
350	45.263	961.62	GA 0052
400	50.418	982.93	GA 0053
450	55.684	1006.1	GA 0054
500	61.033	1030.9	GA 0055
600	71.905	1085.1	GA 0056
800	94.068	1209.0	GA 0094
1000	116.52	1350.0	GA 0095

H_2O

1. Physics

The first realistic model for describing the scattering of thermal neutrons by hydrogen bound in H_2O was given by Nelkin.[1] In this model the scattering units are freely recoiling H_2O molecules. Each molecule can undergo torsional harmonic oscillations (hindered rotations) as a whole with a single frequency of 0.06 eV, as well as internal vibrations with frequencies of 0.205 and 0.48 eV. The effective masses attributed to these dynamical modes by Nelkin are respectively 2.32, 5.85 and 2.92.

The scattering law for H_2O calculated for the ENDF with the code GASKET is based on a model which retains the essential features of the Nelkin model but which replaces the single torsional oscillator by a broad band of distributed modes. This torsional frequency spectrum is shown in Section 2.1. Between 0.04 and 0.165 eV it was taken from the work of Haywood and Thorson,[2] but below 0.04 eV it was smoothly joined to a parabola $c\omega^2$. The original spectrum given by Haywood and Thorson showed several peaks in this low frequency range, corresponding to translational vibrations of the H_2O molecule as a whole. These modes were replaced by free translations of mass 18 in order to avoid numerical difficulties. The discrete internal modes of vibration of the H_2O molecule were taken over from the Nelkin model with slightly readjusted masses, namely 6 for the 0.205 eV mode and 3 for the 0.48 eV oscillator. The torsional band was then normalized to 4/9 in order to give the proper

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[1] M.S. Nelkin, Phys. Rev. 119, 741 (1960).

over-all normalization to one of the sum of all inverse masses.[2] The scattering by the oxygen atoms is not included in the tabulated scattering law data. It should be taken into account by adding to the data the properly weighted $S(\alpha, \beta)$ for a free gas of mass 16. It is important to note, however that the α values for the oxygen must be 1.008/16 times the α values for the hydrogen data, in order to correspond to the same neutron momentum transfer κ.

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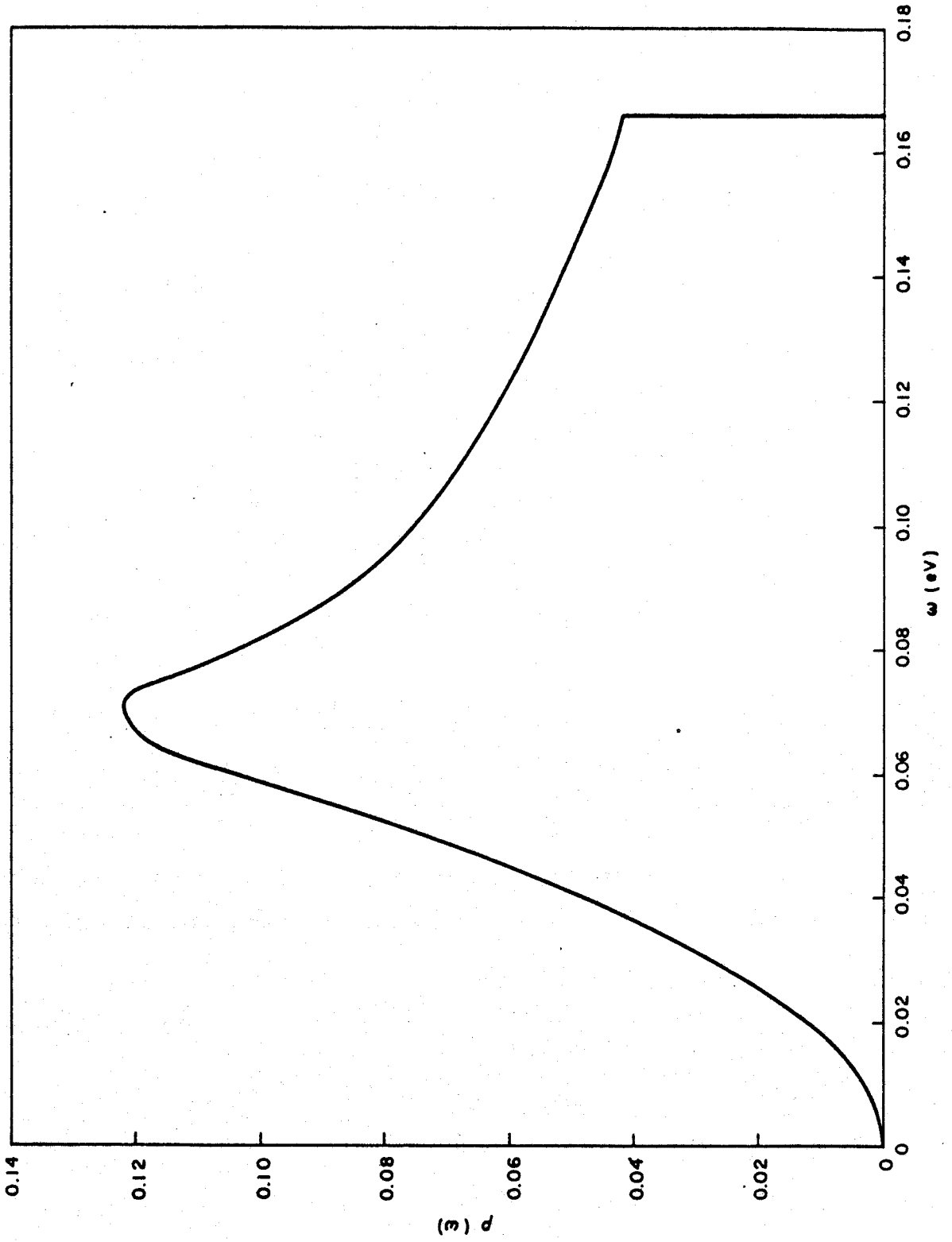
[2] B. C. Haywood and J. M. Thorson, Proc. Conf. on Neutron Thermalization, Brookhaven (4, 1962). Also see J. U. Koppel, Proc. ANS Conf. on Reactor Physics in the Resonance the Thermal Ref. on (S. Diego, 2/1966), The M.I.T. Press 1966.

2. Torsional Frequency Spectrum for $H(H_2O)$



H_2O - 2.1

3.1 GASKET Input for H_2O at 296°K

The code GASKET is discussed in Section A. 3. The data tabulated below follows the format of the code input instructions also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

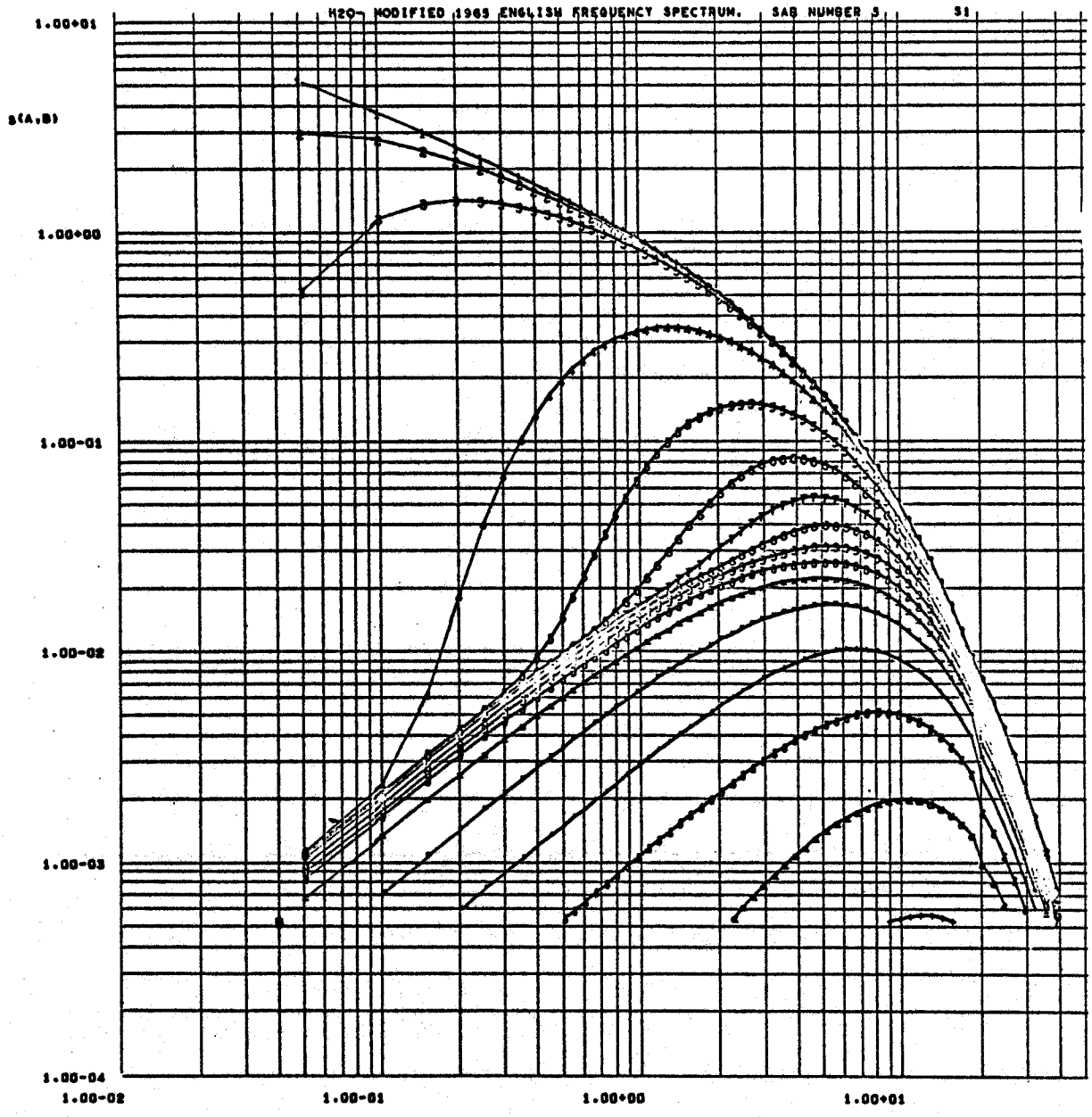
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6,A2	COM H_2O - Modified 1965 English Freq Spectrum
2	11I5	NT -5 NP 80 NE 80 NDAM 0 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 29 JS4 0 JS5 2
4	5E10	W1 .0555556 W2 0.0 W3 .4444444 W4 0.0 W5 .50
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 0.0 T5 .0255
6	7E10	AM 1.008 DC 0.0 BETSW 20.0 ALPSW 20.0 CRIT1
		CRIT2 CRIT3
7	7E10	X3 .006375 .01275 .019125 .0255 .031875 .03825
		.044625 .0510 .057375 .06375 .0663 .06885
		.0714 .07395 .0765 .082875 .08925 .095625
		.102 .108375 .11475 .121125 .1275 .133875
		.14025 .146625 .153 .159375 .16575

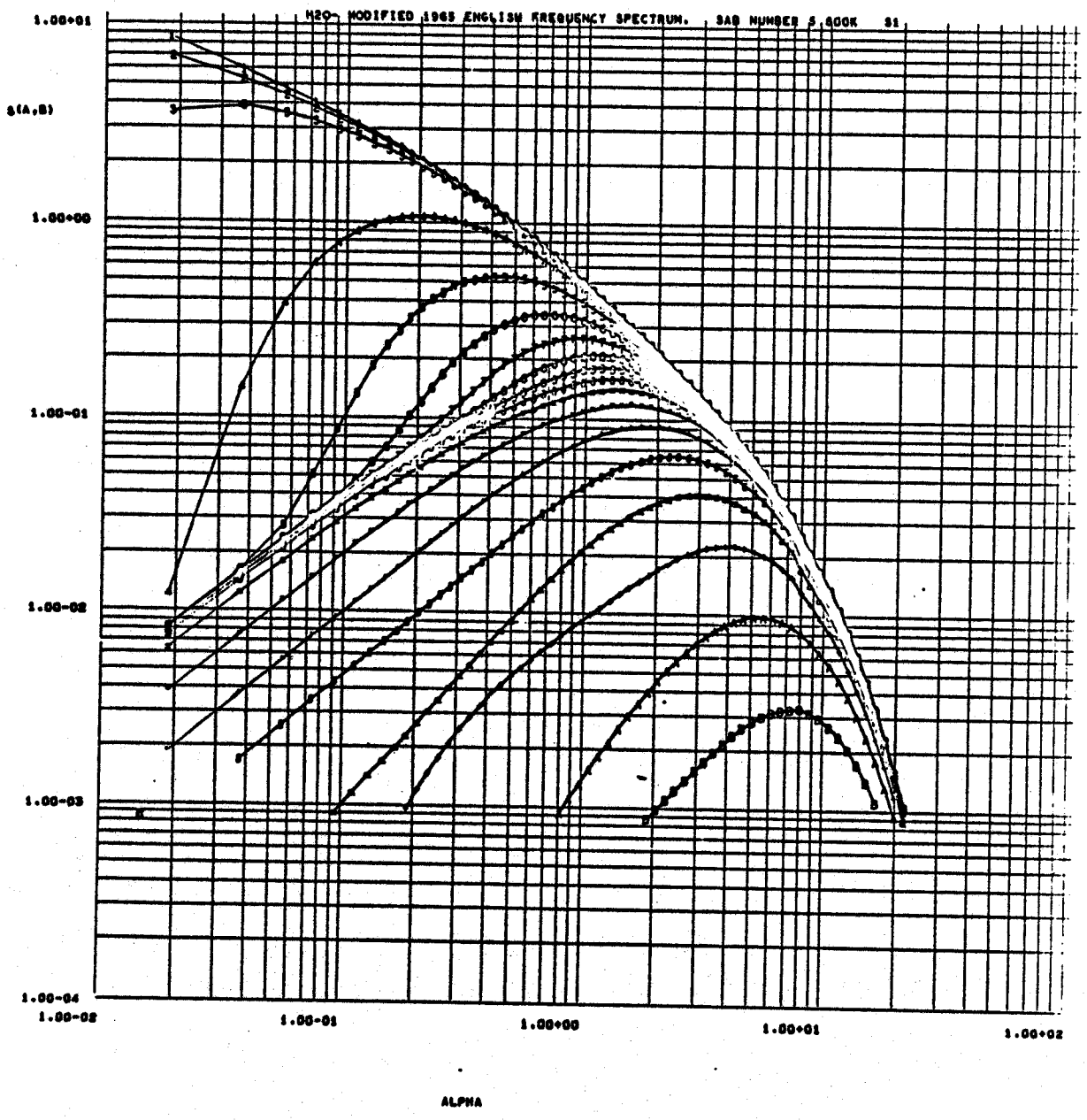
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
8	7E10	Q3 .00125	.005	.01125	.02	.03125	.045
		.059	.075	.095	.115	.1197	.1214
		.1218	.1195	.1125	.0975	.0871	.0791
		.0735	.0688	.065	.061	.0571	.054
		.0515	.0488	.0459	.0431	.042	
9	Cards 9 and 10 are not needed						
10							
11	7E10	X5 .205	.48				
12	7E10	Q5 .3333333	.6666667				
13	7I10	NPHON 10	5				
14	5E10	EMAX 2.0	DALPHA .05	ALPHAC .5	DBETA .08	BETAC 2.5	
15, 16, 17, 18, 19 and 20 are not needed							
21	2E10	DT .1	TMAX 2.0				
		.2	5.0				
		.5	20.0				
		1.0	100.0				
		2.0	600.0				
22	2I10						
	2E10	ID 1	NPT 0	SIGF 20.36	EPS .000001		
23	Card 23 is not needed						

4. Plots of Scattering Law

β Values for Multicurve Plots

CURVE	INDEX	β(296K)	β(800K)
1	1	0.00	0.00
2	2	.08	.0296
3	3	.16	.0592
4	4	.48	.1776
5	5	.80	.296
6	6	1.12	.414
7	7	1.44	.533
8	8	1.76	.651
9	9	2.08	.765
10	∂	2.40	.888
11	=	2.75	1.02
12	"	3.24	1.20
13	'	3.96	1.47
14	δ	5.02	1.86
15	α	6.57	2.43
16	+	8.84	3.27
17	A	12.17	4.50
18	B	17.04	6.30
19	C	24.16	8.94
20	D	34.60	12.80


H2O- MODIFIED 1965 ENGLISH FREQUENCY SPECTRUM. SAB NUMBER 5 S1
1.00+01
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
1.00+01
ALPHA


H2O- MODIFIED 1965 ENGLISH FREQUENCY SPECTRUM. SAB NUMBER 5.600K 31
S(A,B)
1.00+01
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

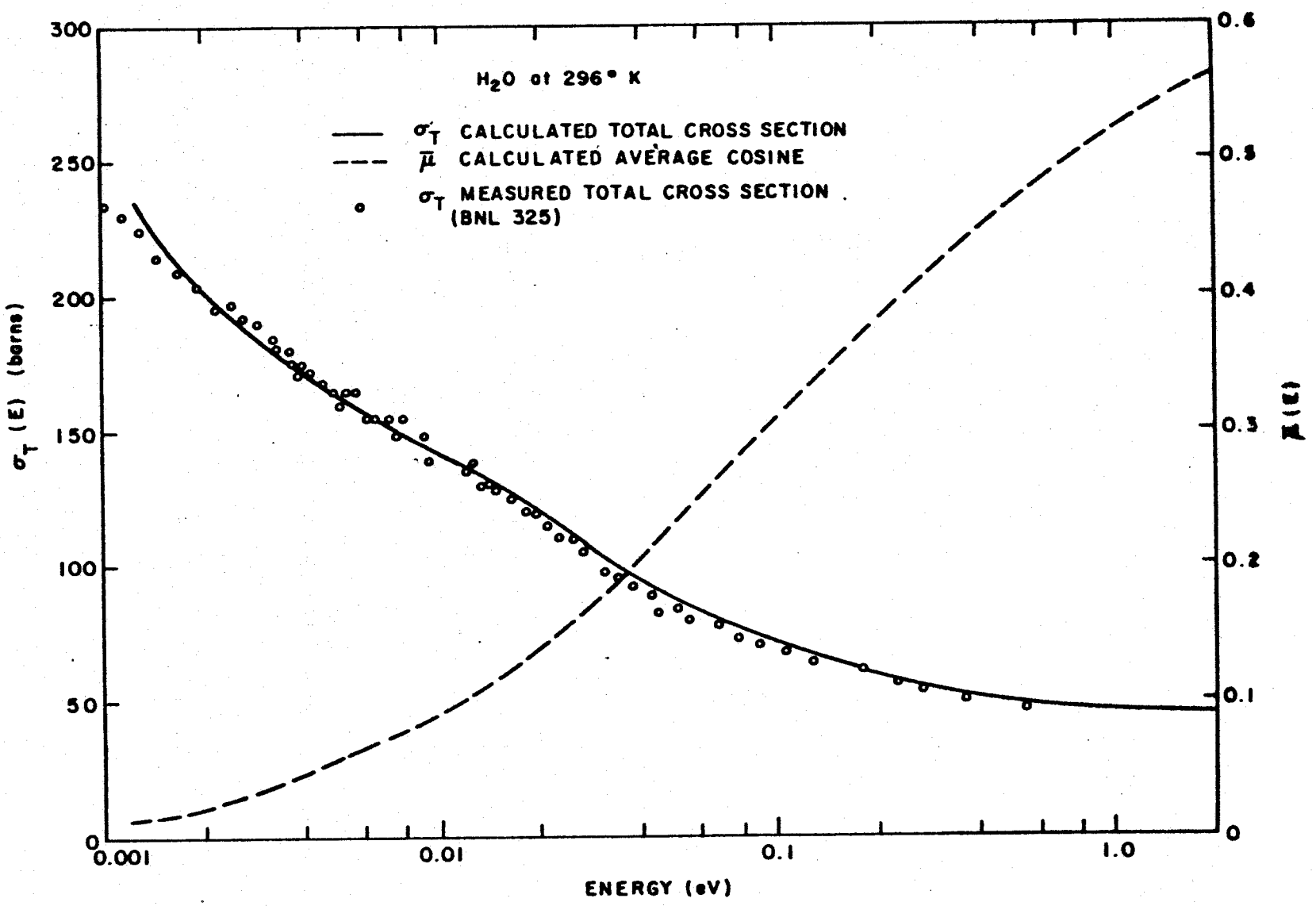
DATA FOR H2O AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00025	446.61971	-.00062	37	.22400	58.70315	.39348
2	.00075	282.53653	.00300	38	.24800	57.47408	.40517
3	.00125	235.44726	.01043	39	.27200	56.36451	.41506
4	.00175	211.74469	.01803	40	.29600	55.31012	.42290
5	.00225	197.61657	.02566	41	.32500	54.23526	.43161
6	.00275	187.82400	.03261	42	.35500	53.22526	.43916
7	.00325	180.28262	.03899	43	.38500	52.31221	.44591
8	.00375	174.26069	.04444	44	.41500	51.47195	.45179
9	.00450	167.82642	.05282	45	.44500	50.71632	.45715
10	.00550	160.71212	.06131	46	.47500	50.06524	.46199
11	.00650	155.49000	.06921	47	.50500	49.51662	.46655
12	.00750	150.82354	.07573	48	.53500	49.05239	.47094
13	.00850	146.91556	.08100	49	.56500	48.66251	.47526
14	.00950	143.49759	.08727	50	.59500	48.33092	.47953
15	.01100	139.45900	.09716	51	.62500	48.04959	.48369
16	.01300	134.57830	.10883	52	.65500	47.80850	.48774
17	.01500	130.06634	.11841	53	.68500	47.60161	.49161
18	.01700	125.98003	.12736	54	.71500	47.42690	.49522
19	.01900	122.25222	.13588	55	.74500	47.27436	.49870
20	.02100	118.81882	.14404	56	.77500	47.13997	.50197
21	.02500	112.66597	.15921	57	.80500	47.01971	.50507
22	.02900	107.04419	.17109	58	.85500	46.84422	.50992
23	.03600	99.47064	.19467	59	.90500	46.69502	.51431
24	.04400	92.58750	.21742	60	.95500	46.56007	.51831
25	.05300	86.63676	.23902	61	1.00500	46.43735	.52199
26	.06500	81.00226	.26240	62	1.10500	46.21047	.52849
27	.07700	76.98061	.28097	63	1.20500	46.00821	.53404
28	.08900	73.96602	.29640	64	1.30500	45.82845	.53893
29	.10100	71.53633	.30968	65	1.40500	45.67310	.54336
30	.11300	69.47619	.32143	66	1.50500	45.54009	.54743
31	.12500	67.68473	.33177	67	1.60500	45.42736	.55109
32	.13700	66.05334	.34024	68	1.70500	45.32688	.55445
33	.15200	64.35290	.35069	69	1.80500	45.23461	.55750
34	.16800	62.76767	.36123	70	1.90500	45.13252	.56038
35	.18400	61.37622	.37122	71	2.00500	44.19259	.55834
36	.20000	60.17616	.38052				

THE TOTAL CROSS SECTION INCLUDES A CONSTANT SCATTERING CROSS SECTION OF 3.76 BARNS (SIGO) FOR THE OXYGEN ATOM. ALSO FOR THE OXYGEN, SIG1 = .666*SIGO/MASS WAS USED TO CALCULATE THE AVERAGE COSINE OF THE SCATTERING ANGLE.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	2.0 EV


H_2O at 296° K
σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
σ_T MEASURED TOTAL CROSS SECTION (BNL 325)
σ_T (E) (barns)
$\bar{\mu}$ (E)
ENERGY (eV)
300
250
200
150
100
50
0
0.6
0.5
0.4
0.3
0.2
0.1
0
0.001
0.01
0.1
1.0

6. Miscellaneous Notes on H_2O

For temperatures other than 296°K the switching criteria for short collision and the α,β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input of the room temperature problem to do higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral, effective temperature and ID numbers of the scattering law data on file.

T(°K)	Debye Waller Integral (ev^{-1})	$\overline{T}$(°K)	ENDF ID No.
296	19.68	1396.8	GA 0001
350	21.62	1411.6	GA 0002
400	23.54	1427.4	GA 0003
450	25.54	1444.9	GA 0005
500	27.60	1464.1	GA 0006
600	31.88	1506.8	GA 0007
800	40.78	1605.8	GA 0092
1000	49.94	1719.8	GA 0093

URANIUM CARBIDE

1. Physics

The scattering laws for uranium and carbon in uranium carbide (UC) have been computed in the inelastic incoherent approximation by GASKET, using squared-amplitude weighted frequency distributions obtained from a central force lattice dynamical model.[1] Contributions from coherent elastic scattering by U and by C were computed[2] from the lattice structure. UC has a cubic structure of the NaCℓ type with a lattice constant of 4.9554 ± 0.003 Å. The central force model is based on three force constants, including next-nearest-neighbor interactions. The uranium-carbon force constant was adjusted to give a peak in the normal mode frequency distribution at about 0.045 eV in accordance with neutron data.[3] The carbon-carbon force constant was selected to give a reasonable width to this peak. Finally, the uranium-uranium force constant was chosen to make possible a good fit to specific heat data. Details of the work are given in a Gulf General Atomic report.[1] The frequency distributions are shown in Fig. 1.

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(1) E. L. Slaggie, "Central Force Lattice Dynamical Model for Uranium Carbide," USAEC Report GA-8675, Gulf General Atomic Incorporated, December 23, 1968.

(2) E. L. Slaggie, et al., "Integral Neutron Thermalization, Annual Summary Report, October 1, 1968 through September 30, 1969," USAEC Report GA-9753, Gulf General Atomic Incorporated (1969).

(3) S. N. Purohit, et al., "Inelastic Neutron Scattering in Metal Hydrides, UC and UO_2, and Applications of the Scattering Law," Proceedings of the IAEA Symposium on Neutron Thermalization, held July 1967 at the University of Michigan.

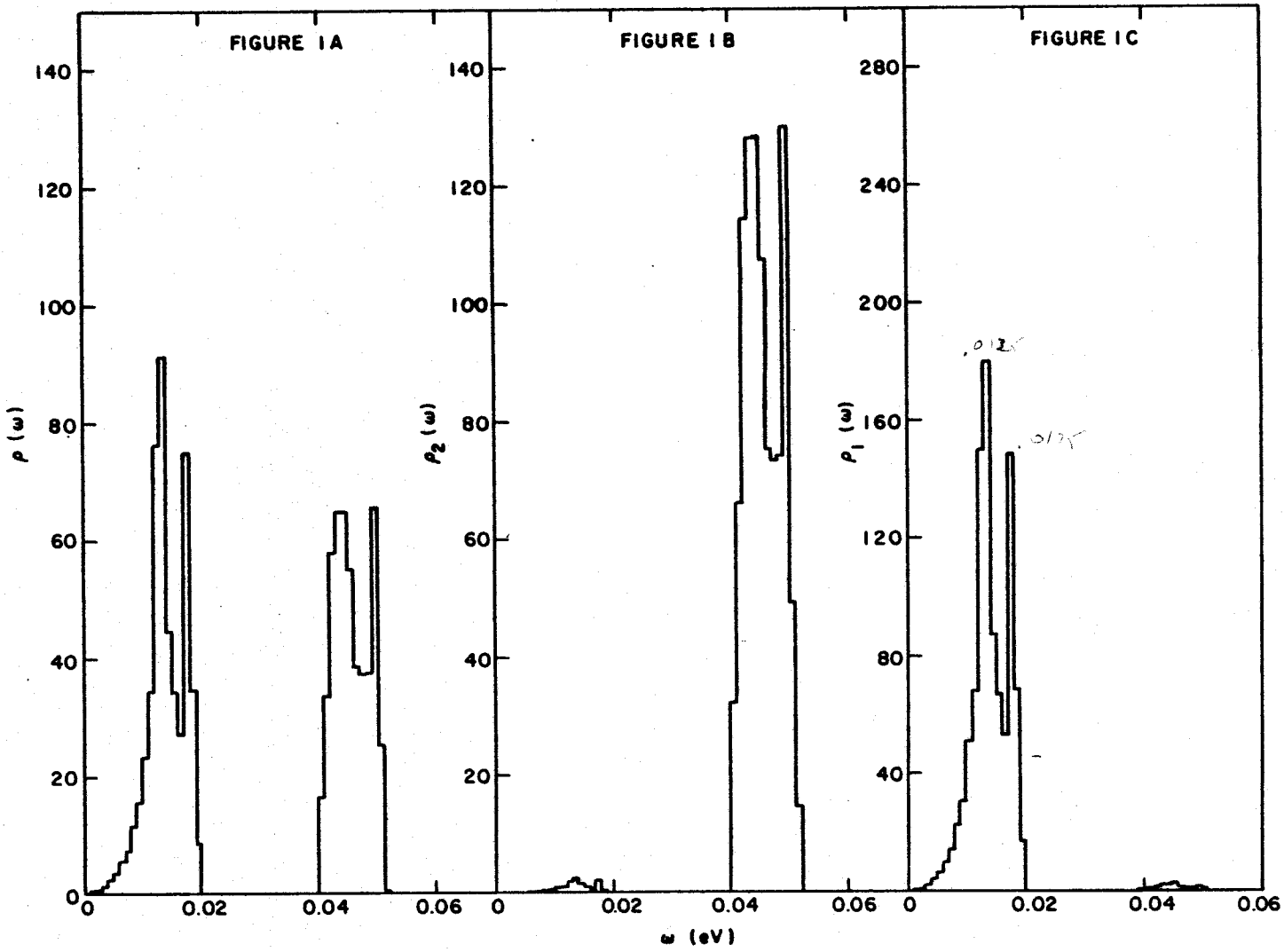


Figure 1A. Histogram representation of the normalized frequency distribution obtained from the central force mode for UC.

Figure 1B. Weighted frequency distribution for C in UC.

Figure 1C. Weighted frequency distribution for U in UC.

3.1 GASKET Input for U(UC)

The code GASKET is discussed in Section A.3.1. The data tabulated below follows the format of the code input instructions also given in Section A.3.1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Slaggie's U(UC) 296 degrees K.
2	11I5	NT -12 NP 50 NE 80 NDAM 1 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 37 JS4 JS5
4	5E10	W1 .001 W2 0.0 W3 1.0 W4 W5
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 T5
6	7E10	AM 238.0 DC BETSW ALPSW CRIT1
		CRIT2 CRIT3
		X3 .0005 .00150 .0025 .0035 .0045 .0055
		.0065 .0075 .0085 .0095 .0105 .0115
		.0125 .0135 .0145 .0155 .0165 .0175
		.0185 .0195 .0205 .0215 .0385 .0395
		.0405 .0415 .0425 .0435 .0445 .0455
		.0465 .0475 .0485 .0495 .0505 .0515
		.0525

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
8	7E10	Q3 .05191	.4848	1.3866	2.2571	4.7959	7.2844
		10.907	14.096	22.763	30.514	45.190	68.004
		150.84	180.33	87.874	67.360	53.466	148.94
		69.034	17.370	0.0	0.0	0.0	0.0
		1.1144	1.3690	1.5624	2.1094	2.3142	2.4207
		1.6425	1.2849	.8022	1.7380	.6595	.03506
		0.0					
9	Cards 9 and 10 are not needed						
10							
11	7E10	X5					
12	7E10	Q5					
13	7I10	NPHON					
14	5E10	EMAX 1.0 DALPHA .0075690 ALPHAC .10092 DBETA .05 BETAC 1.96					
15, 16, 17, 18, 19 and 20 are not needed							
21	2E10	DT .25	TMAX 1.0				
		1.0	20.0				
		1.25	100.0				
		175.0	152.5				
		2.5	200.0				
		3.0	500.0				
		5.0	1720.0				
		20.0	3000.0				
		25.0	4000.0	50.0	9500.0		
		30.0	7000.0	100.0	25000.0		
22	2I10						
	2E10	ID 190	NPT 0.0	SIGF 8.4	EPS 1.0-06		
23	Card 23 is not needed						

3.2 GASKET Input for C(UC)

The code GASKET is discussed in Section A.3.1. The data tabulated below follows the format of the code input instructions also given in Section A.3.1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

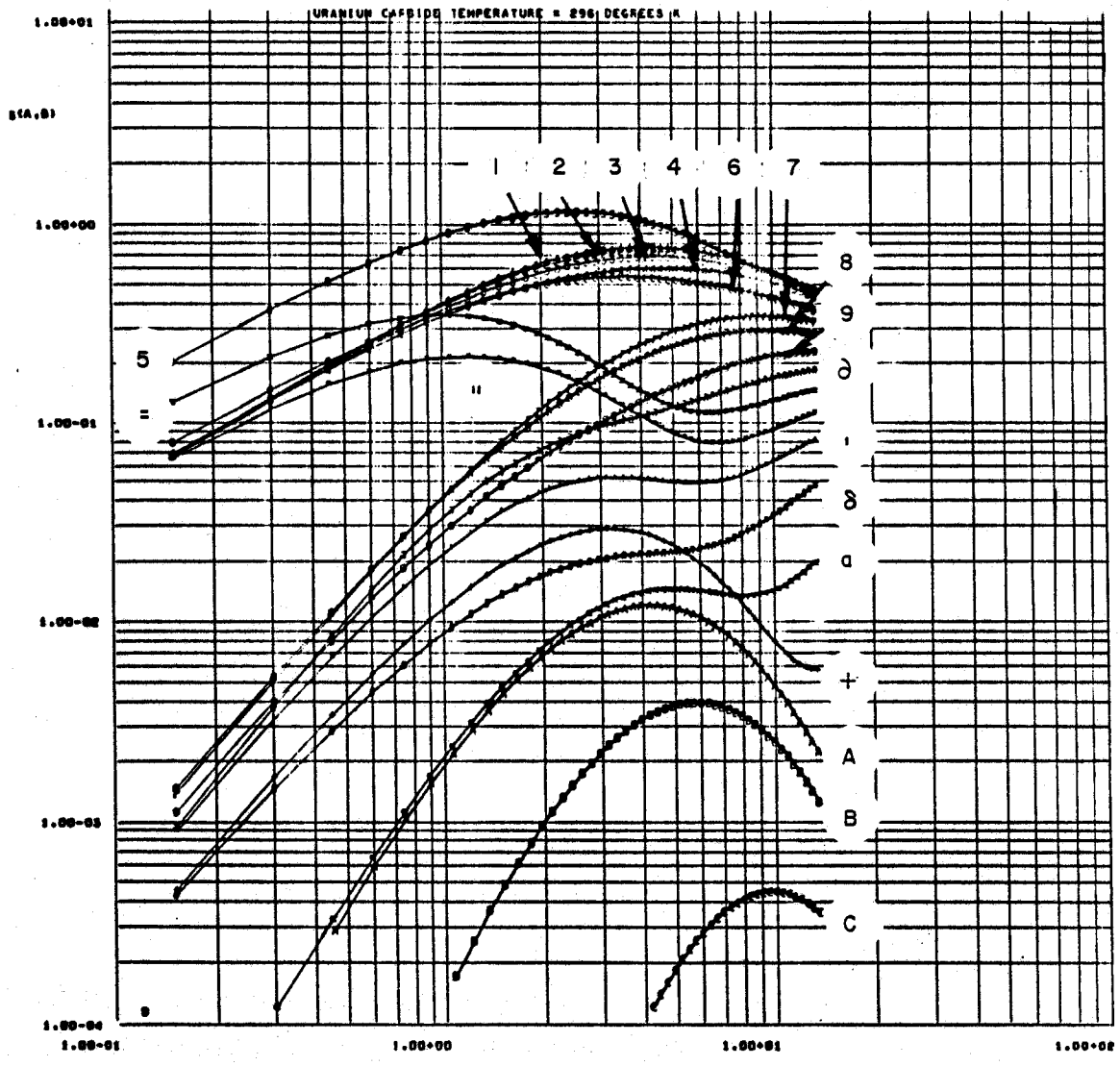
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Slaggie's C(UC) 296 degrees K.
2	11I5	NT -10 NP 50 NE 80 NDAM 1 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 37 JS4 JS5
4	5E10	W1 .001 W2 0.0 W3 1.0 W4 W5
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 T5
6	7E10	AM 12.011DC BETSW ALPSW CRIT1
		CRIT2 CRIT3 1.0-08
		X3 .0005 .00150 .0025 .0035 .0045 .0055
		.0065 .0075 .0085 .0095 .0105 .0115
		.0125 .0135 .0145 .0155 .0165 .0175
		.0185 .0195 .0205 .0215 .0385 .0395
		.0405 .0415 .0425 .0435 .0445 .0455
		.0465 .0475 .0485 .0495 .0505 .0515
		.0525

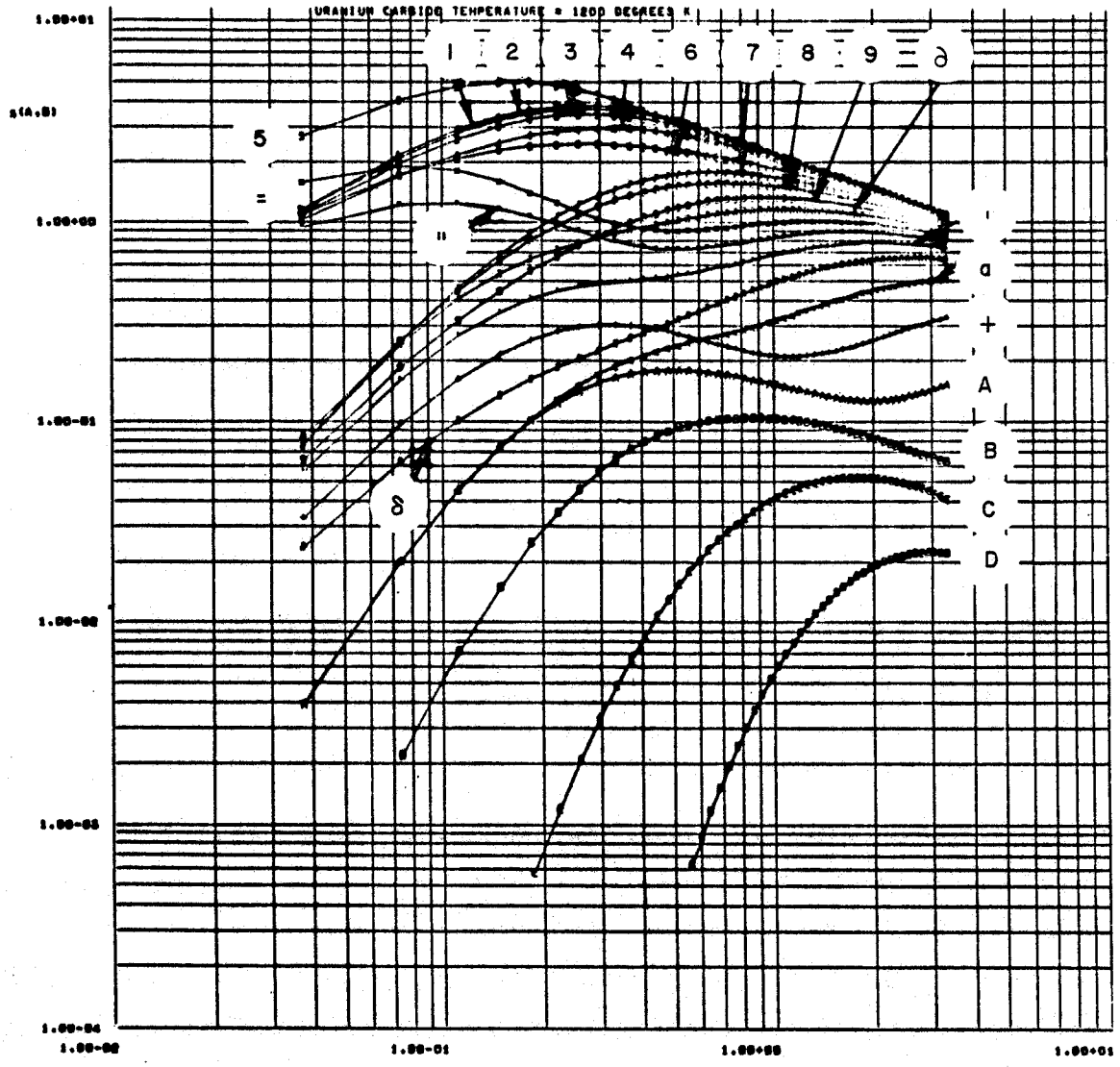
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
8	7E10	Q3 .002615 .02408 .06747 .10583 .22072 .31326
		.43465 .51740 .75688 .89469 1.1229 1.3203
		2.0546 2.9250 1.4443 1.1647 .66306 2.1415
		.79890 .079342 0.0 0.0 0.0 0.0
		32.606 66.574 114.73 128.14 128.37 107.84
		75.715 73.565 74.047 130.26 49.616 1.4920
		0.0
9	Cards 9 and 10 are not needed	
10		
11	7E10	X5
12	7E10	Q5
13	7I10	NPHON
14	5E10	EMAX 1.0 DALPHA .15 ALPHAC 2.0 DBETA .05 BETAC 1.96
15, 16, 17, 18, 19 and 20 are not needed		
21	2E10	DT .05 TMAX .1
		.10 1.0
		.25 20.0
		.50 150.0
		1.25 200.0
		2.5 700.0
		5.0 1000.0
		10.0 3000.0
		15.0 4000.0
		25.0 6000.0
22	2I10	
	2E10	ID 180 NPT 0 SIGF 4.71 EPS 1.0-06
23	Card 23 is not needed	

4. Plots of Scattering Law for UC

BETA VALUES FOR MULTICURVE PLOT

CURVE	INDEX	$\beta(296^{\circ}K)$	$\beta(1200^{\circ}K)$
1	1	0.00	0.0
2	2	5.00 - 2	1.233 - 2
3	3	1.00 - 1	2.4660 - 2
4	4	3.00 - 1	7.3980 - 2
5	5	5.00 - 1	1.2330 - 1
6	6	7.00 - 1	1.7262 - 1
7	7	9.00 - 1	2.2194 - 1
8	8	1.10 + 0	2.7126 - 1
9	9	1.30 + 0	3.2058 - 1
10	∂	1.50 + 0	3.6990 - 1
11	=	1.70 + 0	4.1922 - 1
12	"	1.90 + 0	4.6854 - 1
13	'	2.1187 + 0	5.2248 - 1
14	δ	2.4545 + 0	6.0527 - 1
15	a	2.9827 + 0	7.3554 - 1
16	+	3.8140 + 0	9.4053 - 1
17	A	5.1220 + 0	1.2631 + 0
18	B	7.1801 + 0	1.7706 + 0
19	C	1.0419 + 1	2.5693 + 0
20	D	1.5515 + 1	3.8259 + 0


URANIUM CARBIDE TEMPERATURE = 296 DEGREES K
1.00+01
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA
1
2
3
4
6
7
5
8
9
∂
δ
a
+
A
B
C


URANIUM CARBIDE TEMPERATURE = 1200 DEGREES K
1.00+01
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
1.00+01
1 2 3 4 6 7 8 9 ∂
5
=
II
δ
a
+
A
B
C
D
ALPHA

UC - 4.3

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR UC AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00250	25.49961	-.50606	43	.02833	19.56984	.02296
2	.00277	24.26205	-.41269	44	.02918	19.16881	.04639
3	.00304	23.16827	-.33304	45	.02918	19.26581	.03801
4	.00333	22.14040	-.27921	46	.02946	19.13709	.04542
5	.00333	35.36693	-.95030	47	.02973	19.00869	.05269
6	.00432	29.63622	-.51702	48	.03001	18.88262	.05983
7	.00543	25.42991	-.22032	49	.03001	20.79962	-.08797
8	.00667	22.23774	-.01040	50	.03110	20.26027	-.05477
9	.00667	31.30532	-.55953	51	.03222	19.74792	-.02371
10	.00746	28.82214	-.39804	52	.03335	19.26140	.00533
11	.00829	26.72125	-.26160	53	.03335	20.53140	-.08694
12	.00917	24.91032	-.14647	54	.03417	20.16654	-.06433
13	.00917	25.12126	-.16104	55	.03500	19.81334	-.04272
14	.00944	24.60662	-.12946	56	.03585	19.47278	-.02208
15	.00972	24.09851	-.09938	57	.03585	19.51078	-.02494
16	.01000	23.60544	-.07068	58	.03613	19.39770	-.01831
17	.01000	26.79644	-.27408	59	.03640	19.28241	-.01167
18	.01106	24.83514	-.15813	60	.03668	19.16788	-.00513
19	.01217	23.08604	-.05833	61	.03668	20.23688	-.08183
20	.01334	21.63161	.02659	62	.03778	19.77786	-.05453
21	.01334	23.13961	-.09662	63	.03889	19.34751	-.02874
22	.01415	22.22055	-.03901	64	.04002	18.94327	-.00446
23	.01498	21.35176	.01289	65	.04002	19.24627	-.02744
24	.01584	20.50125	.06063	66	.04084	18.96453	-.01020
25	.01584	20.60425	.05062	67	.04168	18.69741	.00624
26	.01612	20.34785	.06492	68	.04252	18.44294	.02188
27	.01639	20.09771	.07877	69	.04252	18.50491	.01679
28	.01667	19.85420	.09219	70	.04279	18.42511	.02177
29	.01667	24.03850	-.22135	71	.04307	18.34600	.02667
30	.01775	22.91898	-.15213	72	.04335	18.26762	.03148
31	.01886	21.90347	-.08966	73	.04335	19.05062	-.02978
32	.02001	20.99339	-.03301	74	.04445	18.76281	-.00995
33	.02001	24.08039	-.22633	75	.04556	18.51993	.00800
34	.02083	23.36309	-.18104	76	.04669	18.28502	.02476
35	.02166	22.65183	-.13888	77	.04669	19.64502	-.07482
36	.02251	21.97626	-.09935	78	.04751	19.45585	-.06036
37	.02251	22.06526	-.10505	79	.04835	19.27041	-.04654
38	.02386	21.09628	-.04824	80	.04919	19.08857	-.03332
39	.02525	20.23224	.00284	81	.04919	19.16857	-.03896
40	.02668	19.47213	.04815	82	.05056	18.88215	-.01861
41	.02668	20.41513	-.02829	83	.05195	18.60348	.00034
42	.02750	19.98380	-.00189	84	.05336	18.32364	.01816

DATA FOR UC AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
85	.05336	18.45462	.00803	127	.08670	17.98723	-.01897
86	.05418	18.27821	.01839	128	.09004	17.70731	-.00151
87	.05502	18.10704	.02834	129	.09004	17.93811	-.01811
88	.05586	17.94112	.03789	130	.09671	17.41421	.01550
89	.05586	17.96411	.03602	131	.09671	17.85364	-.01655
90	.05613	17.91044	.03908	132	.10004	17.59487	.00023
91	.05641	17.85691	.04210	133	.10004	17.86527	-.01909
92	.05669	17.80450	.04508	134	.11005	17.14921	.01578
93	.05669	18.73350	-.02629	135	.11005	17.36421	-.00019
94	.05779	18.51428	-.01270	136	.11338	17.14493	.01267
95	.05890	18.30211	.00022	137	.11338	17.34463	-.00207
96	.06003	18.09908	.01249	138	.11672	17.21898	.00807
97	.06003	18.72000	-.03327	139	.11672	17.40478	-.00548
98	.06085	18.56721	-.02363	140	.12672	17.10507	.01234
99	.06169	18.41952	-.01433	141	.12672	17.33127	-.00414
100	.06253	18.27492	-.00537	142	.13673	16.52153	.02240
101	.06253	18.32292	-.00887	143	.13673	16.76863	.00363
102	.06280	18.27627	-.00597	144	.14006	16.39852	.01628
103	.06308	18.22974	-.00311	145	.14006	16.51432	.00739
104	.06336	18.18334	-.00028	146	.15006	15.81775	.02630
105	.06336	18.55434	-.02730	147	.15007	15.96169	.01477
106	.06446	18.37175	-.01570	148	.16285	15.63813	.03288
107	.06557	18.20059	-.00475	149	.17118	15.70539	.02379
108	.06669	18.03831	.00560	150	.17591	15.48341	.02801
109	.06670	18.37132	-.01895	151	.18258	15.30891	.02222
110	.06752	18.25212	-.01112	152	.18675	15.27042	.02661
111	.06836	18.13397	-.00356	153	.19119	15.34195	.02278
112	.06920	18.01984	.00374	154	.20000	15.20270	.02735
113	.06920	18.07384	-.00030	155	.25000	14.90251	.02534
114	.06947	18.03640	.00207	156	.30000	14.63930	.02663
115	.06975	17.99897	.00442	157	.35000	14.42104	.02540
116	.07003	17.96153	.00674	158	.40000	14.31933	.02352
117	.07003	18.56255	-.03663	159	.45000	14.24787	.02090
118	.07113	18.40952	-.02649	160	.50000	14.16819	.01972
119	.07224	18.26045	-.01677	161	.55000	14.11693	.01794
120	.07336	18.11528	-.00748	162	.60000	14.07333	.01657
121	.07336	18.38728	-.02693	163	.65000	14.04072	.01516
122	.08003	17.60115	.02090	164	.70000	14.01274	.01406
123	.08003	17.82615	.00388	165	.75000	13.98909	.01312
124	.08337	17.50301	.02208	166	.80000	13.96798	.01240
125	.08337	17.76042	.00266	167	.85000	13.94927	.01178
126	.08670	17.42253	.02278	168	.90000	13.92481	.01114

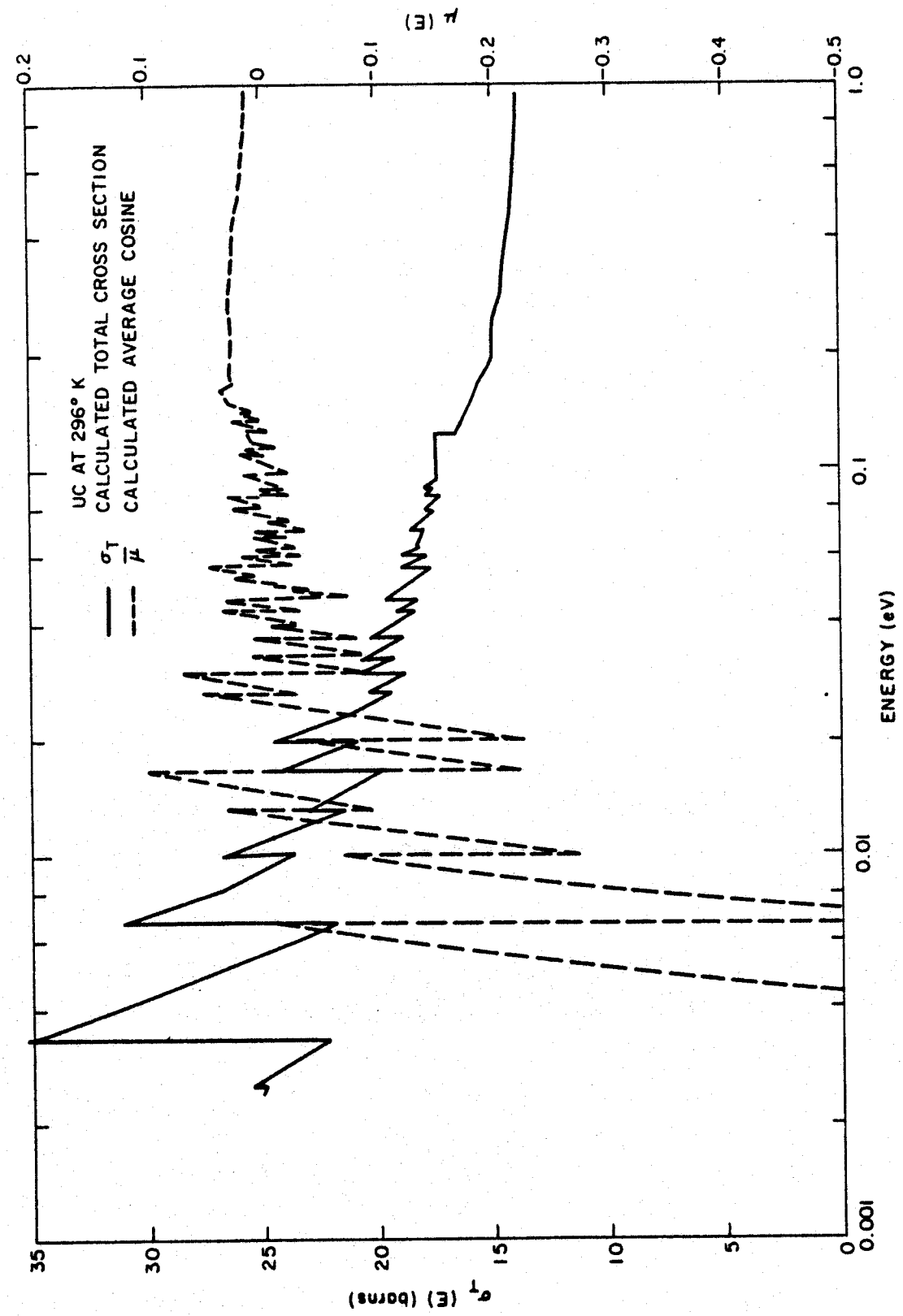
DATA FOR UC AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
169	.95000	13.81523	.01192	170	1.00000	12.67302	.02508

THE ELASTIC CONTRIBUTION TO THE TOTAL CROSS SECTION WAS CALCULATED AT ALL OF THE TABULATED ENERGIES.THE INELASTIC CONTRIBUTION WAS CALCULATED ON A COARSER MESH AND WAS INTERPOLATED TO GIVE THE VALUES AT THE TABULATED ENERGIES.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV


UC AT 296° K
CALCULATED TOTAL CROSS SECTION
CALCULATED AVERAGE COSINE
ENERGY (eV)
σT (E) (barns)
μ (E)

UC - 5.4

6. Miscellaneous Notes on Uranium Carbide

For temperatures other than 296°K the switching criteria for short collision and the α, β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral and effective temperature of the scattering law data on file.

T(°K)	Debye Waller Integral (eV^{-1}) for Uranium	$\overline{T}$(°K) for Uranium	Debye Waller Integral (eV^{-1}) for Carbon	$\overline{T}$(°K) for Carbon
296	362.72	304.79	39.558	369.78
400	486.29	406.58	49.766	455.89
500	605.69	505.28	60.128	545.17
600	725.41	604.40	70.778	637.84
700	845.32	703.78	81.599	732.56
800	965.34	803.30	92.527	828.55
1000	1205.6	1002.6	114.58	1022.9
1200	1446.0	1202.2	136.80	1219.2

URANIUM DIOXIDE

1. Physics

The scattering laws for uranium and oxygen in uranium dioxide (UO_2) have been calculated in the inelastic incoherent approximation by GASKET, using weighted phonon frequency distributions obtained from a lattice dynamical model. Coherent elastic scattering by U and O was calculated[1] from the known lattice structure, which is similar to CaF_2 (fluorite). The lattice dynamical model is that developed by Dolling, Cowley, and Woods[2] to fit dispersion curve measurements. In addition to short-range core-core forces, the model includes shell-core, shell-shell, and long-range Coulomb interactions. Weighted frequency distributions were calculated from a dynamical matrix based on this model. A review of the work by Dolling, et al. is given in a Gulf General Atomic report.[3]

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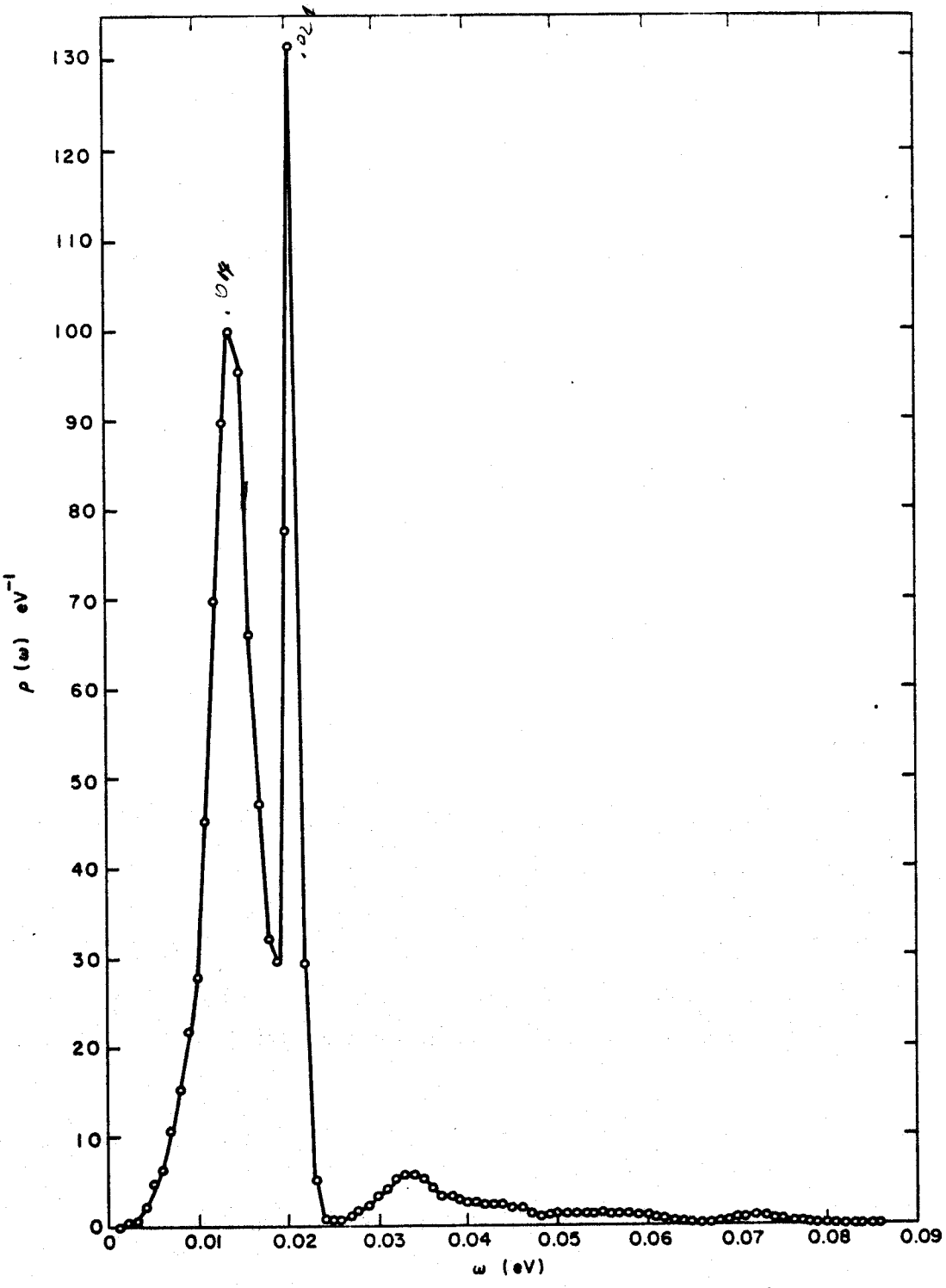
(1) E. L. Slaggie, et al., "Integral Neutron Thermalization, Annual Summary Report, October 1, 1968 through September 30, 1969," USAEC Report GA-9753, Gulf General Atomic Incorporated (1969).

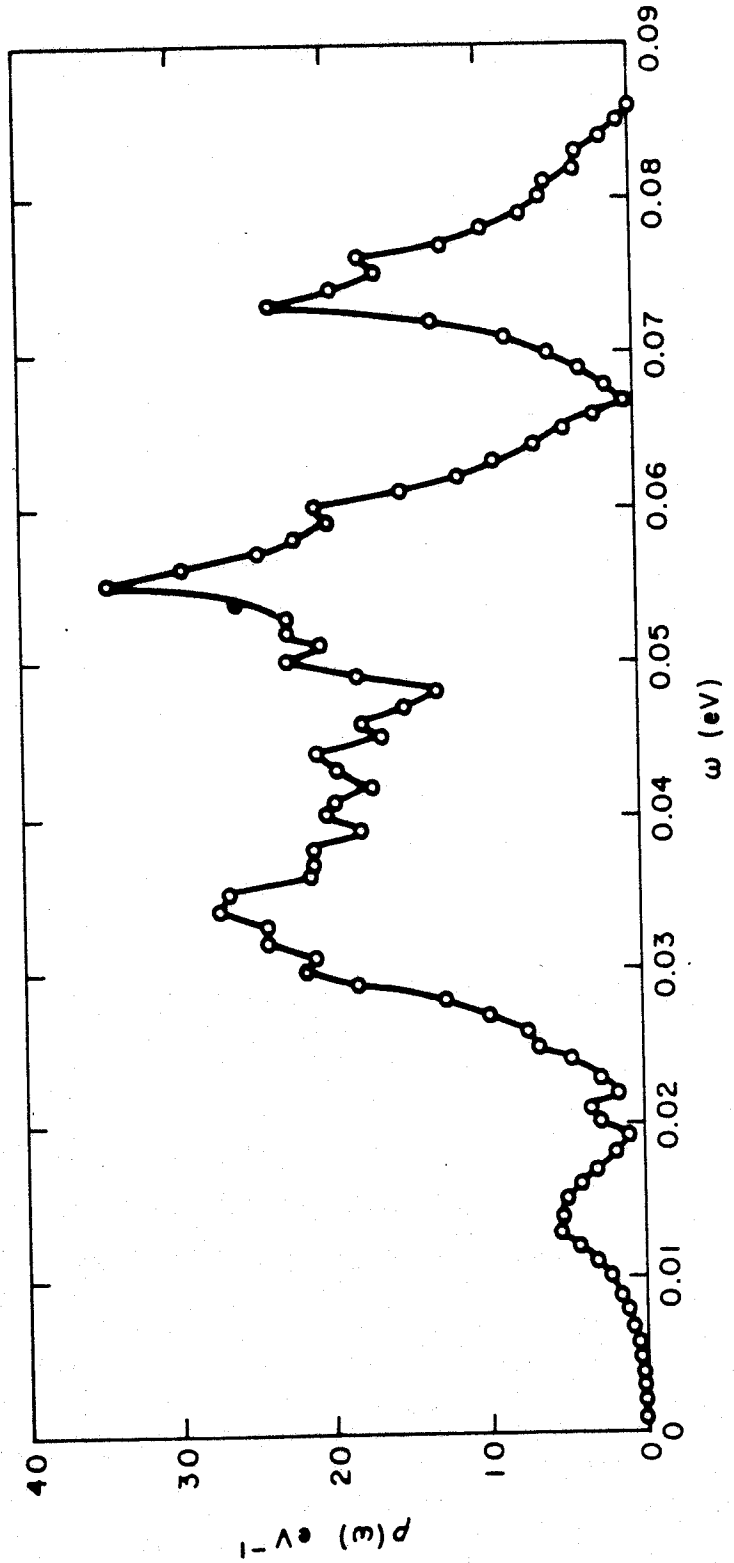
(2) G. Dolling, R. A. Cowley, and A. D. B. Woods, Can. J. Phys. 43, 1397 (1965).

(3) J. A. Young, "Neutron Scattering from Uranium Dioxide," USAEC Report GA-8760, Gulf General Atomic Incorporated, July 10, 1968.

2. Weighted Frequency Spectrum of Uranium in UO_2



3. Weighted Frequency Spectrum of Oxygen in UO_2



3.1 GASKET Input for $U(UO_2)$ at 296°K

The code GASKET is discussed in Section A.3.1. The data tabulated below follows the format of the code input instructions also given in Section A.3.1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM U in UO_2 at 296°K. FCC model.
2	11I5	NT -12 NP 50 NE 80 NDAM 1 NGPRT 0 NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0 IPG 0
3	3I5	JS3 -86 JS4 _____ JS5 _____
4	5E10	W1 .0001 W2 0.0 W3 1.0 W4 _____ W5 _____
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 _____ T5 _____
6	7E10	AM 238.03 DC _____ BETSW _____ ALPSW _____ CRIT1 _____ CRIT2 _____ CRIT3 _____
		X3 .086

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
8	7E10	Q3 0.0	.46260	1.0831	2.4514	4.9159	6.4420
		10.649	15.442	21.982	27.892	45.230	69.832
		89.965	99.874	95.651	66.029	47.279	32.150
		29.643	77.690	127.91	29.401	5.2336	.70288
		.63442	.64183	.99599	1.5331	2.3095	3.4823
		4.2186	5.2855	5.8177	5.9447	5.4349	4.1625
		3.4041	3.3047	2.8288	2.6629	2.6025	2.3100
		2.3287	2.4506	1.9019	2.0120	1.3254	.88542
		1.1558	1.3608	1.2867	1.3258	1.2356	1.2501
		1.2354	1.3677	1.2846	1.2589	1.1108	1.0409
		.76018	.58347	.45129	.31670	.21204	.13266
		.23744	.40970	.63213	.74042	.82127	.84773
		.80319	.56653	.39261	.27048	.18194	.13979
		.070214	.054065	.037417	.021232	.012110	.0036441
		.0004299	0.0				
9	Cards 9 and 10 are not needed						
10							
11	7E10	X5					
12	7E10	Q5					
13	7I10	NPHON					
14	5E10	EMAX 1.0 DALPHA .010083 ALPHAC .134437 DBETA .10 BETAC 2.95					
15, 16, 17, 18, 19 and 20 are not needed							
21	2E10	DT .05	TMAX .1				
		.10	1.0				
		.25	20.0				
		.50	100.0				
		1.25	150.0				
		2.5	200.0				
		3.0	500.0				
		5.0	1000.0				
		10.0	3000.0		25.0	7000.0	
		15.0	4000.0		40.0	9500.0	
22	2I10						
	2E10	ID 130	NPT 0	SIGF 8.4	EPS 1.0E-6		
23	Card 23 is not needed						

3.2 GASKET Input for $O(UO_2)$

The code GASKET is discussed in Section A.3.1. The data tabulated below follows the format of the code input instructions also given in Section A.3.1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

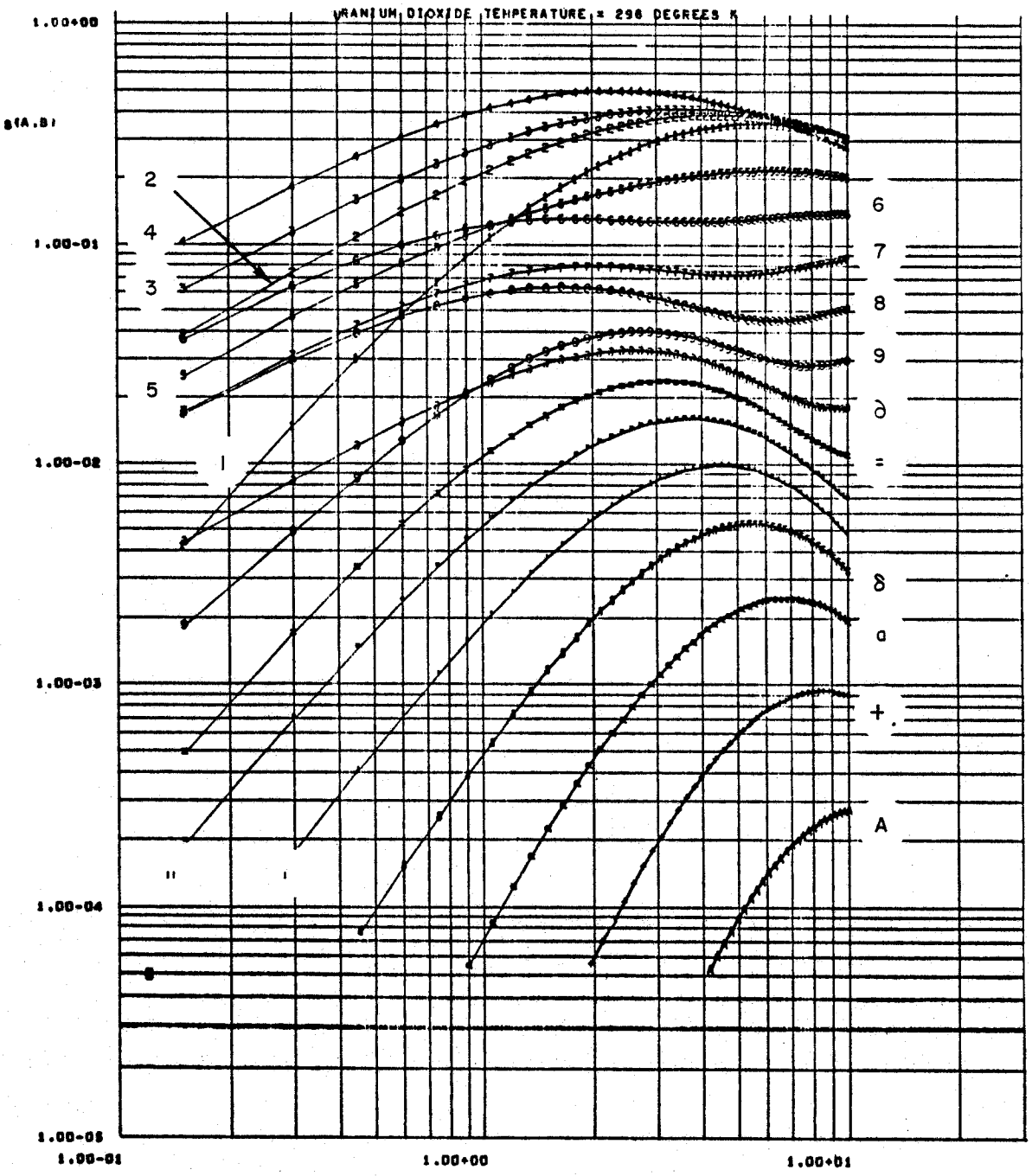
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM O in UO_2 at 296°K. FCC model.
2	11I5	NT -12 NP 50 NE 80 NDAM 1 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 -86 JS4 JS5
4	5E10	W1 .0001 W2 0.0 W3 1.0 W4 W5
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 T5
6	7E10	AM 16.0 DC BETSW ALPSW CRIT1
		CRIT2 CRIT3
		X3 .086

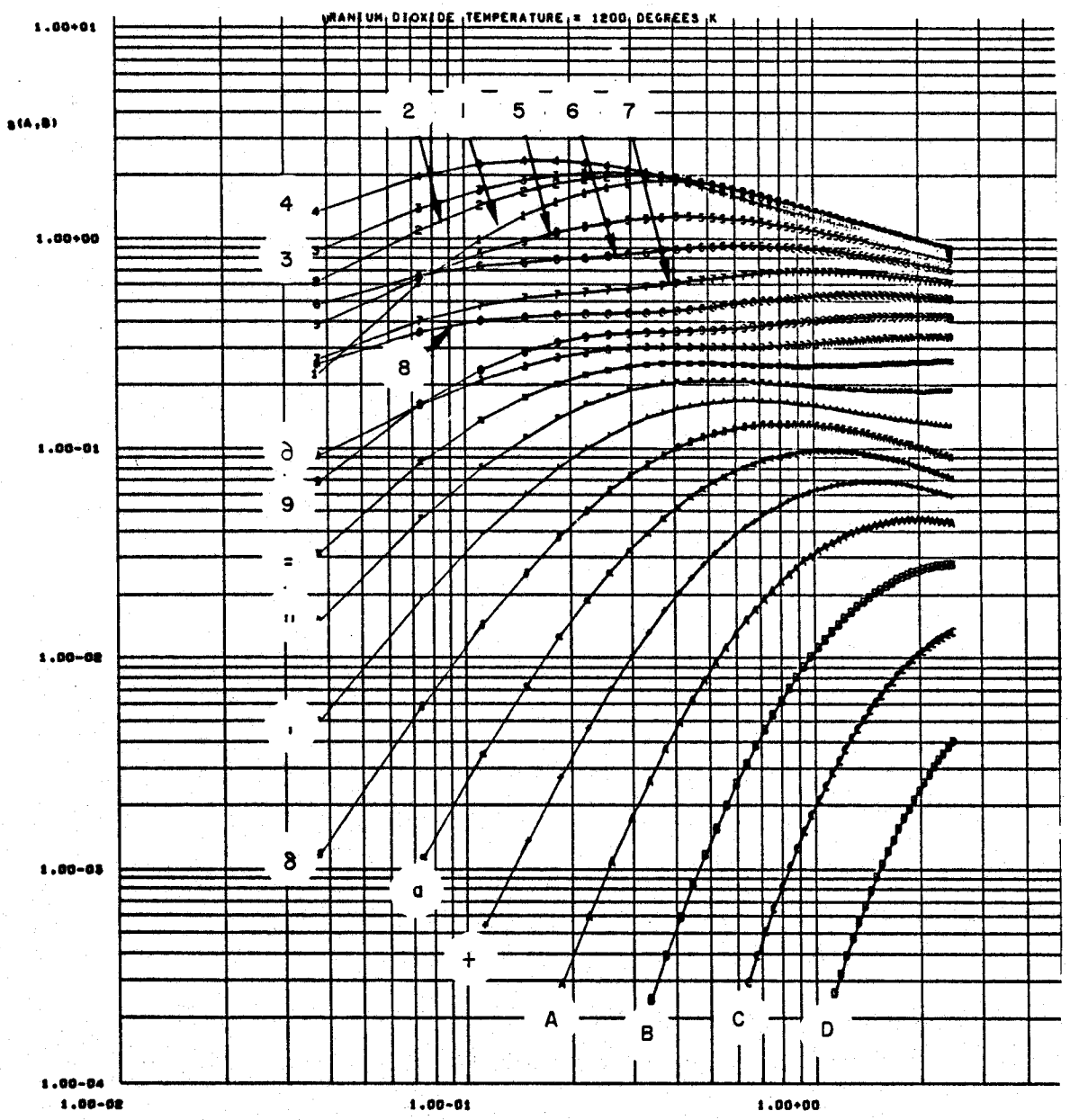
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES						
8	7E10	Q3	0.0	.031386	.074139	.16980	.34950	.46484
			.78298	1.1367	1.6674	2.0450	3.2024	4.3883
			5.3794	5.3587	5.0484	4.1062	3.0644	1.8615
			.94784	2.2904	2.9726	1.7011	2.8011	4.7463
			6.9724	7.5104	10.067	12.680	18.547	21.186
			21.040	24.496	24.452	27.417	26.769	21.396
			21.258	21.168	18.205	20.086	19.911	17.479
			19.859	20.873	16.838	18.154	15.296	13.225
			18.467	22.937	20.815	23.003	22.950	26.210
			34.566	29.607	24.674	22.470	20.377	20.659
			15.430	11.726	9.3296	6.6387	4.5238	2.6508
			.98949	2.0034	3.7310	5.5813	8.2498	13.318
			23.807	19.566	16.969	17.868	12.518	9.9532
			7.1559	6.0066	5.5223	3.8312	3.6634	1.9191
			.83710	0.0				
9	Cards 9 and 10 are not needed							
10								
11	7E10	X5						
12	7E10	Q5						
13	7I10	NPHON						
14	5E10	EMAX 1.0 DALPHA .15 ALPHAC 2.0 DBETA .10 BETAC 2.95						
15, 16, 17, 18, 19 and 20 are not needed								
21	2E10	DT .05 TMAX .10						
			.10	1.0				
			.25	20.0				
			.50	100.0				
			1.25	150.0				
			2.5	200.0				
			3.0	500.0				
			5.0	1000.0				
			10.0	3000.0		25.0	7000.0	
			15.0	4000.0		40.0	9500.0	
22	2I10 2E10	ID 140 NPT 0 SIGF 3.76 EPS 1.0E-6						
23	Card 23 is not needed							

4. Plots of Scattering Law for UO_2

BETA VALUES FOR MULTICURVE PLOT

CURVE	INDEX	$\beta(296^{\circ}K)$	$\beta(1200^{\circ}K)$
1	1	0.00	0.0
2	2	0.100	0.024661
3	3	0.200	0.049322
4	4	0.600	0.14797
5	5	1.00	0.24661
6	6	1.400	0.34525
7	7	1.800	0.44390
8	8	2.200	0.54254
9	9	2.600	0.64119
10	∂	3.00	0.73983
11	=	3.4716	0.85614
12	"	4.083	1.0069
13	'	4.8753	1.2023
14	δ	5.9024	1.4556
15	a	7.2336	1.7839
16	+	8.9590	2.2094
17	A	1.1195 + 01	2.7609
18	B	1.4094 + 01	3.4758
19	C	1.7852 + 01	4.4024
20	D	2.2722 + 01	5.6034


URANIUM DIOXIDE TEMPERATURE = 298 DEGREES K
1.00+00
S(A,B)
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-01
1.00+00
1.00+01
ALPHA
2
4
3
5
1
6
7
8
9
∂
=
δ
a
+
A


URANIUM DIOXIDE TEMPERATURE = 1200 DEGREES K
1.00+01
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-02
1.00-01
1.00+00
ALPHA
2 1 5 6 7
4
3
8
9
A
B
C
D

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR UO_2 AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00205	36.53458	-.92603	43	.02326	23.71562	-.05480
2	.00227	34.35072	-.74815	44	.02396	23.19428	-.02755
3	.00250	32.40761	-.59599	45	.02396	24.38127	-.09752
4	.00274	30.66762	-.46519	46	.02418	24.20632	-.08820
5	.00274	31.19432	-.50111	47	.02441	24.03379	-.07903
6	.00355	26.69415	-.18629	48	.02464	23.86357	-.07002
7	.00446	23.32185	.02201	49	.02464	23.90557	-.07249
8	.00548	20.70736	.16247	50	.02554	23.26979	-.03893
9	.00548	36.90198	-.76091	51	.02645	22.66688	-.00751
10	.00612	33.91461	-.57752	52	.02738	22.09404	.02191
11	.00681	31.33138	-.42278	53	.02738	24.47704	-.12056
12	.00753	29.08568	-.29118	54	.02805	24.02636	-.09626
13	.00753	32.72368	-.42956	55	.02874	23.59116	-.07301
14	.00775	31.99914	-.38918	56	.02943	23.16774	-.05070
15	.00798	31.30305	-.35065	57	.02943	23.59274	-.07516
16	.00821	30.63251	-.31387	58	.02966	23.45398	-.06786
17	.00821	30.74431	-.31631	59	.02989	23.31659	-.06066
18	.00906	28.49743	-.19708	60	.03012	23.18157	-.05357
19	.01000	26.53574	-.09354	61	.03012	23.20157	-.05473
20	.01095	24.81246	-.00473	62	.03102	22.69037	-.02803
21	.01095	27.53746	-.17577	63	.03193	22.20405	-.00280
22	.01162	26.33733	-.11210	64	.03285	21.74143	.02101
23	.01230	25.23030	-.05423	65	.03285	22.31643	-.01673
24	.01300	24.21089	-.00161	66	.03353	21.98382	.00064
25	.01300	25.77289	-.10515	67	.03422	21.66327	.01729
26	.01323	25.44174	-.08753	68	.03491	21.35371	.03324
27	.01346	25.11916	-.07041	69	.03491	21.99466	-.00959
28	.01369	24.80410	-.05377	70	.03513	21.89173	-.00415
29	.01369	24.93510	-.06213	71	.03536	21.79010	.00121
30	.01457	23.80079	-.00297	72	.03559	21.68878	.00650
31	.01549	22.76070	.05019	73	.03559	21.70078	.00572
32	.01643	21.80538	.09791	74	.03649	21.32868	.02552
33	.01643	27.45638	-.24827	75	.03741	20.97710	.04409
34	.01710	26.61854	-.20181	76	.03833	20.63931	.06164
35	.01776	25.83186	-.15839	77	.03833	23.25131	-.10142
36	.01848	25.08598	-.11775	78	.03901	22.96811	-.08516
37	.01848	26.28398	-.17885	79	.03969	22.69229	-.06949
38	.01959	25.12803	-.11671	80	.04038	22.42284	-.05438
39	.02073	24.06143	-.06038	81	.04038	23.17584	-.09600
40	.02190	23.08193	-.00941	82	.04151	22.73517	-.07116
41	.02190	24.82993	-.11389	83	.04265	22.31314	-.04770
42	.02258	24.26007	-.08355	84	.04380	21.90651	-.02555

DATA FOR UO2 AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
85	.04381	22.16149	-.04075	127	.06456	20.46604	.01495
86	.04448	21.92255	-.02803	128	.06571	20.24123	.02640
87	.04517	21.68845	-.01569	129	.06571	20.70023	-.00316
88	.04586	21.45955	-.00375	130	.06639	20.56492	.00386
89	.04586	21.66155	-.01636	131	.06707	20.43118	.01070
90	.04609	21.58694	-.01244	132	.06776	20.30098	.01737
91	.04631	21.51346	-.00856	133	.06776	20.60498	-.00209
92	.04654	21.43913	-.00472	134	.06799	20.56204	.00018
93	.04654	21.44813	-.00526	135	.06822	20.51816	.00243
94	.04745	21.16538	.00942	136	.06845	20.47534	.00465
95	.04836	20.89262	.02347	137	.06845	20.47634	.00463
96	.04928	20.62786	.03689	138	.06935	20.30865	.01325
97	.04928	21.84986	-.04060	139	.07026	20.14590	.02157
98	.04996	21.64557	-.02956	140	.07118	19.98709	.02961
99	.05064	21.44635	-.01887	141	.07118	21.15309	-.04279
100	.05133	21.25217	-.00850	142	.07186	21.02705	-.03589
101	.05133	21.63916	-.03217	143	.07255	20.90453	-.02915
102	.05156	21.57471	-.02868	144	.07324	20.78350	-.02258
103	.05179	21.51036	-.02522	145	.07324	21.04750	-.03818
104	.05202	21.44713	-.02179	146	.07346	21.00693	-.03596
105	.05202	21.45013	-.02194	147	.07369	20.96741	-.03376
106	.05292	21.20443	-.00880	148	.07392	20.92696	-.03158
107	.05384	20.97547	.00367	149	.07392	20.92796	-.03159
108	.05476	20.75268	.01561	150	.07550	20.66104	-.01705
109	.05476	21.41568	-.02597	151	.08213	19.84346	.02513
110	.05544	21.24825	-.01670	152	.08213	20.41546	-.01112
111	.05612	21.08400	-.00771	153	.08966	19.71877	.02360
112	.05681	20.92289	.00102	154	.08966	20.01878	.00430
113	.05681	21.34089	-.02474	155	.09309	19.63104	.02479
114	.05704	21.28687	-.02176	156	.09309	20.06204	-.00276
115	.05727	21.23287	-.01881	157	.09856	19.63290	.01846
116	.05749	21.17988	-.01588	158	.09856	19.86992	.00338
117	.05749	21.18186	-.01605	159	.10404	19.44108	.02431
118	.05840	20.97499	-.00478	160	.10404	19.94108	-.00741
119	.05931	20.77328	.00606	161	.10609	19.74705	.00309
120	.06023	20.57671	.01649	162	.10609	19.91905	-.00764
121	.06023	21.12472	-.01802	163	.11499	19.34816	.02102
122	.06091	20.97604	-.00997	164	.11499	19.61016	.00430
123	.06160	20.83142	-.00214	165	.11704	19.44890	.01281
124	.06229	20.68783	.00548	166	.11704	19.62590	.00164
125	.06229	20.92383	-.00934	167	.12594	19.39700	.01548
126	.06342	20.69244	.00308	168	.12594	19.60600	.00236

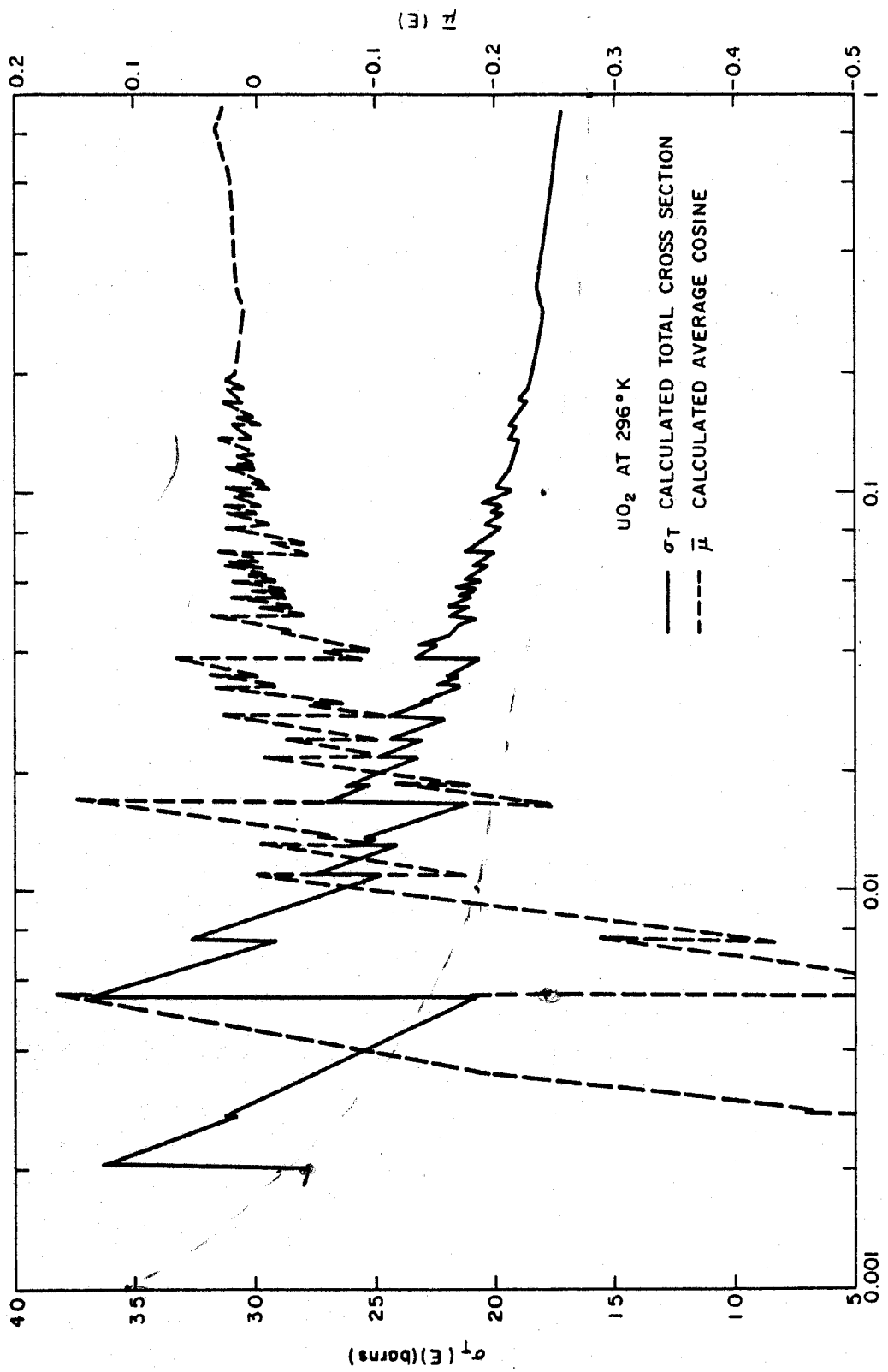
DATA FOR UO2 AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
169	.13689	19.03232	.02612	182	.19918	18.43967	.02206
170	.13689	19.32832	.00721	183	.24000	18.23501	.01961
171	.14784	19.14285	.01925	184	.28500	17.91529	.02108
172	.14784	19.41785	.00197	185	.32000	18.25172	.01632
173	.15332	19.10020	.01249	186	.36000	18.15018	.01859
174	.15332	19.22520	.00465	187	.41000	18.00830	.01891
175	.16130	18.82168	.01478	188	.46000	17.89775	.01952
176	.16975	18.57770	.02680	189	.51000	17.80177	.02003
177	.16975	18.76590	.01458	190	.60000	17.65328	.02097
178	.18070	18.54101	.02338	191	.70000	17.51905	.02185
179	.18070	18.69831	.01322	192	.80000	17.40802	.02251
180	.18275	18.62212	.01688	193	.90000	17.30783	.02301
181	.18825	18.53339	.01955	194	1.00000	15.79234	.03105

THE ELASTIC CONTRIBUTION TO THE TOTAL CROSS SECTION WAS CALCULATED AT ALL OF THE TABULATED ENERGIES. THE INELASTIC CONTRIBUTION WAS CALCULATED ON A COARSER MESH AND WAS INTERPOLATED TO GIVE THE VALUES AT THE TABULATED ENERGIES.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV


$\bar{\mu}$ (E)
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
UO_2 AT 296°K
σ_T CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
ENERGY (eV)
0.001
0.01
0.1
1
σ_T (E)(barns)
40
35
30
25
20
15
10
5

6. Miscellaneous Notes on Uranium Dioxide

For temperatures other than 296°K the switching criteria for short collision and the α, β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral and effective temperature of the scattering law data on file.

T(°K)	Debye Waller Integral (eV^{-1}) for Uranium	$\overline{T}$(°K) for Uranium	Debye Waller Integral (eV^{-1}) for Oxygen	$\overline{T}$(°K) for Oxygen
296	277.87	311.1	48.294	387.2
400	371.63	411.4	61.635	470.0
500	462.38	509.1	74.987	557.0
600	553.44	607.6	88.618	647.9
700	644.69	706.6	102.42	741.3
800	736.05	805.7	116.32	836.3
1000	918.98	1004.6	144.33	1029.1
1200	1102.1	1203.8	172.50	1224.4

ZIRCONIUM HYDRIDE

1. Physics

The crystal structure of gamma phase zirconium hydride is a face-centered cubic lattice of Zr atoms with interstitial H atoms forming a second cube of side a/2 centered inside the Zr cube of side a. In this arrangement each H atom is at the center of a tetrahedron formed by four Zr atoms. Because of the large mass ratio of Zr to H (91:1) one would expect to find in the frequency spectrum of zirconium hydride a rather narrow optical band corresponding to the proton oscillating isotropically in the potential set up by its practically stationary nearest Zr neighbors. Such an optical band centered at 0.137 eV is actually observed in neutron scattering experiments, but its width of about 15%[1] exceeds by far the one associated with the simple model of a proton harmonically bound in a spherically symmetric potential due to nearest neighbors of mass 91. The most likely cause for this broadening is the coupling between H atoms. Neutron scattering experiments further show that in addition to the optical band just mentioned the frequency spectrum of zirconium hydride has an acoustical band extending up to about .02 eV. Without further details of the lattice dynamics and since in the acoustical modes the H atoms essentially move together with their Zr neighbors, it is reasonable to assign a weight between 1/90 and 1/360 to these modes in a scattering law calculation. Of these two extreme weights, experimental evidence[2] seems to favor the smaller one.

The data stored on the ENDF were actually calculated with a phonon spectrum[2] consisting of a Debye spectrum with cut off at 0.02 eV and

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[1] W. L. Whittemore, USAEC Report GA-6583 (1965).

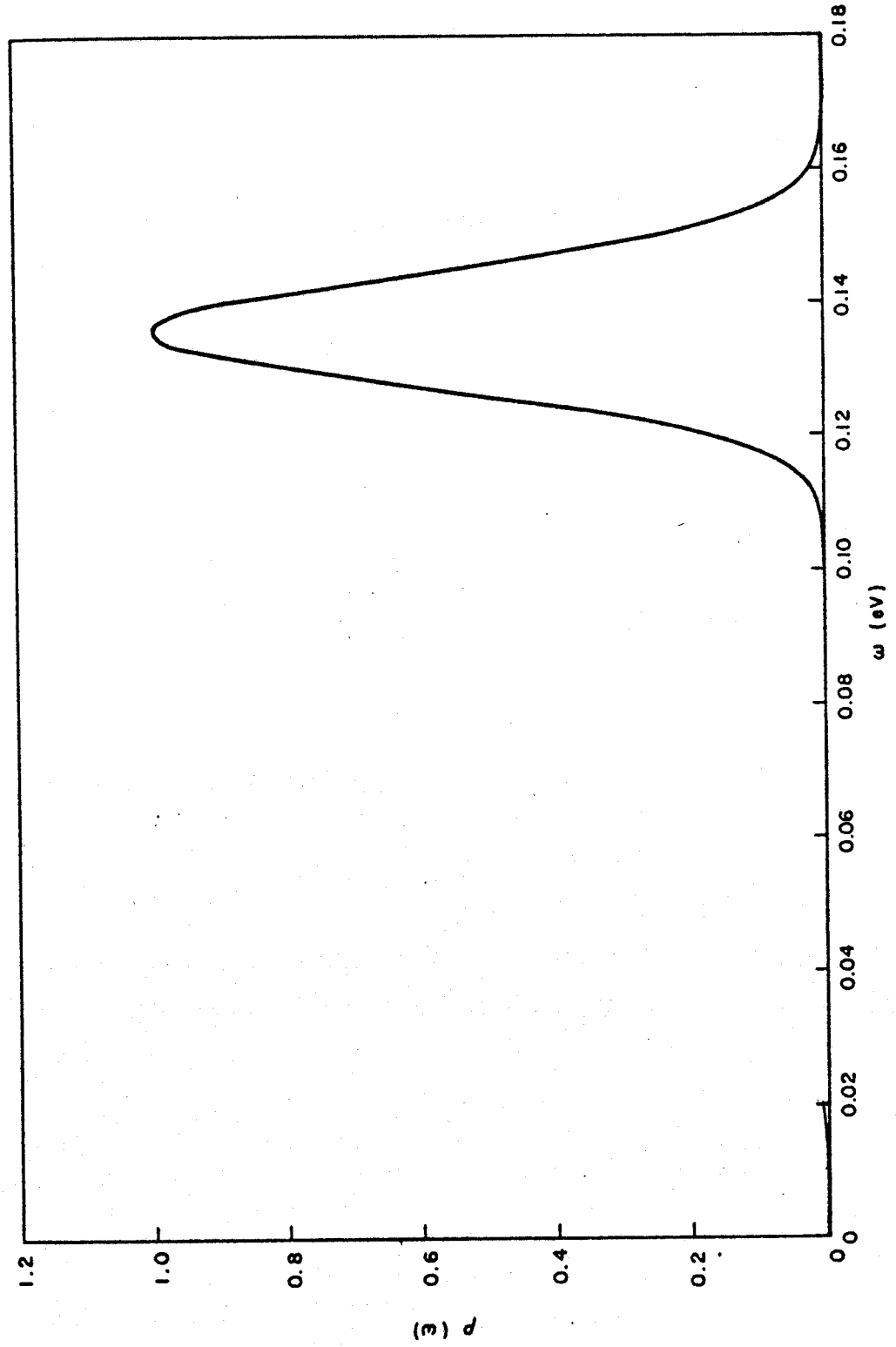
[2] J. C. Young et al., Nucl. Sci. Eng., 19, 230 (1964).

weight 1/360, plus a Gaussian centered at 0.137 eV and having a width of 0.02 eV at half maximum. The scattering law calculations were done with the code GASKET and do not include scattering by the Zr atoms.

Since H is essentially an incoherent scatterer, the Legendre moments of the elastic scattering cross section were obtained with the code ZREND.

It is not advisable to calculate the Zr contribution to the scattering law as free gas of mass 91 since this rather large mass would lead to numerical difficulties. It is preferable to consider the scattering from Zr atoms as elastic in the laboratory system.

2. Weighted Frequency Spectrum for H(ZrH)



3.1 GASKET Input for H(ZrH) at 296°K

The code GASKET is discussed in Section A. 3. The data tabulated below follows the format of the code input instructions also given in Section A. 3. The code symbols used below are defined on the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6,A2	COM Mass 360 H(ZRH) at 296°K
2	11I5	NT -5 NP 40 NE 150 NDAM 1 NGPRT 0
		NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 -84 JS4 0 JS5 0
4	5E10	W1 .00005 W2 0.0 W3 .99995 W4 0.0 W5 0.0
5	6E10	P1 .0255 P2 0.0 P3 .0255 P4 0.0 P5 0.0
6	7E10	AM 1.008 DC 0.0 BMIN 60.0 AMAX 60.0 CRIT1 0.0
		CRIT2 0.0 CRIT3 1.0-7
	7E10	X3 .168

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES						
8	7E10	Q3	.000085	.000352	.0008	.00142	.00222	.003188
			.00434	.00567	.007182	.008865	0.0	0.0
			0.0	0.0	0.0	0.0	0.0	0.0
			0.0	0.0	0.0	0.0	0.0	0.0
			0.0	0.0	0.0	0.0	0.0	0.0
			0.0	0.0	0.0	0.0	0.0	0.0
			0.0	0.0	0.0	0.0	0.0	0.0
			0.0	0.0	0.0	0.0	0.0	0.0
			0.0	0.0	0.0	0.0	.00195	.00437
			.00923	.01845	.03492	.06313	.10584	.16956
			.25702	.36861	.500	.64171	.77917	.89503
			.97265	1.0	.97265	.89503	.77917	.64171
			.500	.36861	.25702	.16956	.10584	.06313
			.03492	.01845	.00923	.00437	.00195	0.0
9	Cards 9 and 10 are not needed							
10								
11	7E10	X5						
12	7E10	Q5						
13	7I10	NPHON						
14	5E10	EMAX 1.0	DALPHA .5	ALPHAC 5.0	DBETA .25	BETAC 30.0		
15, 16, 17, 18, 19 and 20 are not needed								
21	2E10	DT .05	TMAX 6.0					
		.4	18.0					
		.4	60.0					
		3.0	300.0					
		6.0	3100.0					
22	2I10 2E10	ID 20	NPT 0	SIGF 20.36	EPS .000001			
23	Card 23 is not needed							

3.2 ZREND Input for H(ZrH)

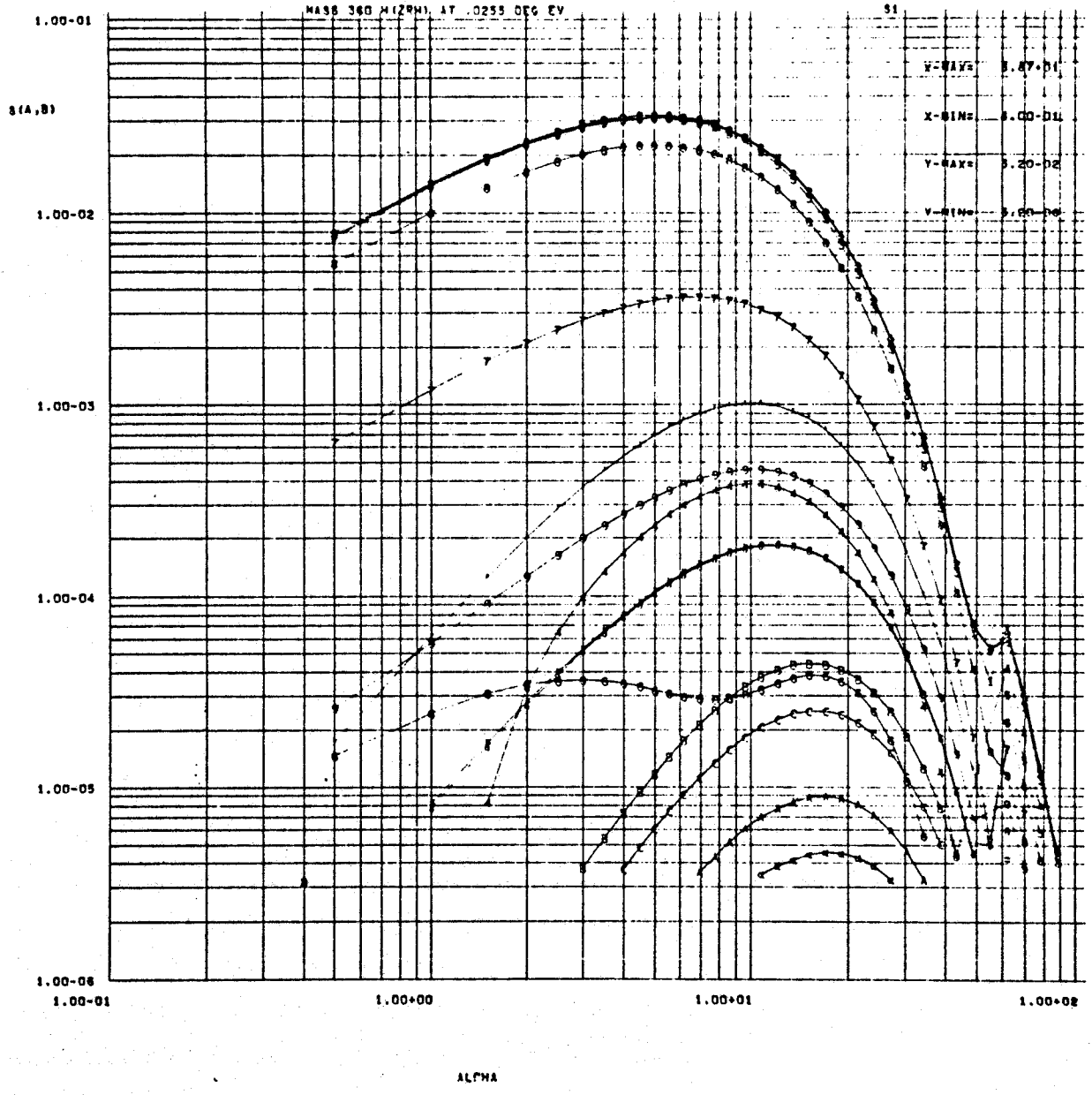
The code ZREND is discussed in Section A. 3. The data tabulated below follows the format of the code input instruction also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in the calculation.

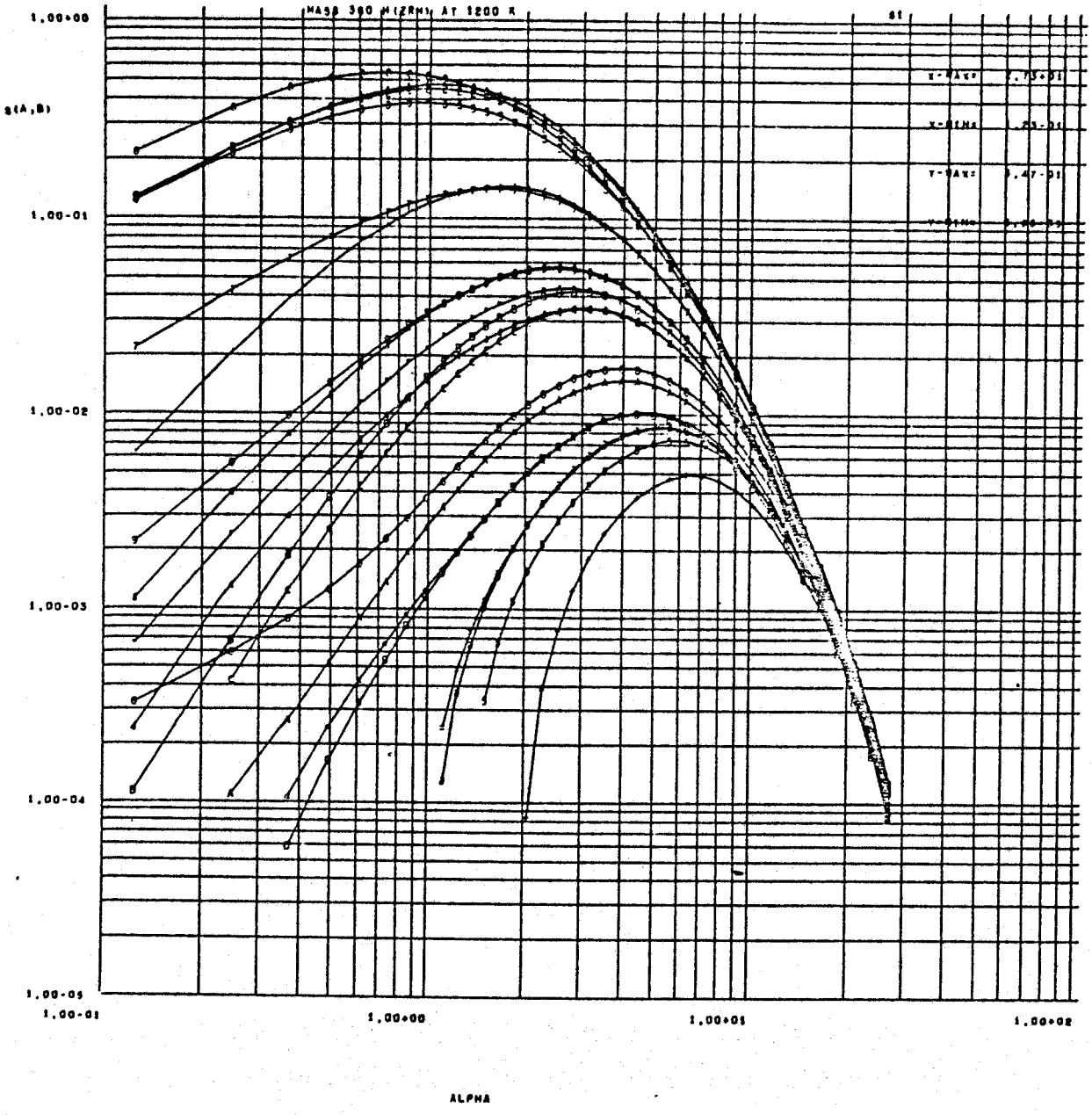
CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
1	13A6,A2	COM	ZREND FOR H(ZRH)				
2	2I5,	NT	8	NE	109	GB	81.44
	3E10,	NPCH	1				
	I5						
3	7E10	T	296.0	400.0	500.0	600.0	700.0	800.0
			1000.0	1200.0				
4	7E10	WP	8.5607	9.171	9.9143	10.783	11.745	12.778
			14.988	17.324				
5	7E10	E	.0005	.00053	.00056	.00060	.00064	.00068
			.00072	.00076	.00080	.00085	.00090	.00095
			.0010	.0011	.0012	.0013	.00145	.00160
			.00175	.00190	.00210	.00230	.00250	.00270
			.00290	.00310	.00330	.00350	.00380	.00410
			.00440	.00470	.0050	.0053	.0056	.0060
			.0064	.0068	.0072	.0076	.0080	.0085
			.0090	.0095	.010	.011	.012	.013
			.0145	.0160	.0175	.019	.0210	.0230
			.0250	.0270	.0290	.031	.033	.035
			.038	.041	.044	.047	.05	.053
			.056	.06	.064	.068	.072	.076
			.080	.085	.090	.095	.100	.110
			.120	.130	.145	.160	.175	.190
			.210	.230	.250	.270	.290	.310
			.330	.350	.380	.410	.440	.470
			.500	.530	.560	.600	.640	.680
			.720	.760	.800	.850	.900	.950
			1.000					

4. Plots of Scattering Law

β Values for Multicurve Plots

CURVE	INDEX	β(296K)	β(1200K)
1	1	0.00	0.00
2	2	.25	.062
3	3	.50	.123
4	4	1.50	.367
5	5	2.50	.617
6	6	3.50	.863
7	7	4.50	1.110
8	8	5.50	1.36
9	9	6.50	1.60
10	∂	7.50	1.85
11	=	8.50	2.10
12	"	9.50	2.34
13	'	10.50	2.59
14	δ	11.5	2.84
15	α	12.5	3.08
16	+	13.5	3.33
17	A	14.5	3.58
18	B	15.5	3.82
19	C	16.5	4.07
20	D	17.5	4.32


MASS 360 H(ZRH) AT .0255 DEG EV
S1
Y-MAX= 3.20-02
X-MIN= 1.00-01
S(A,B)
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-06
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA


MASS 390 H(ZRH) AT 1200 K
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

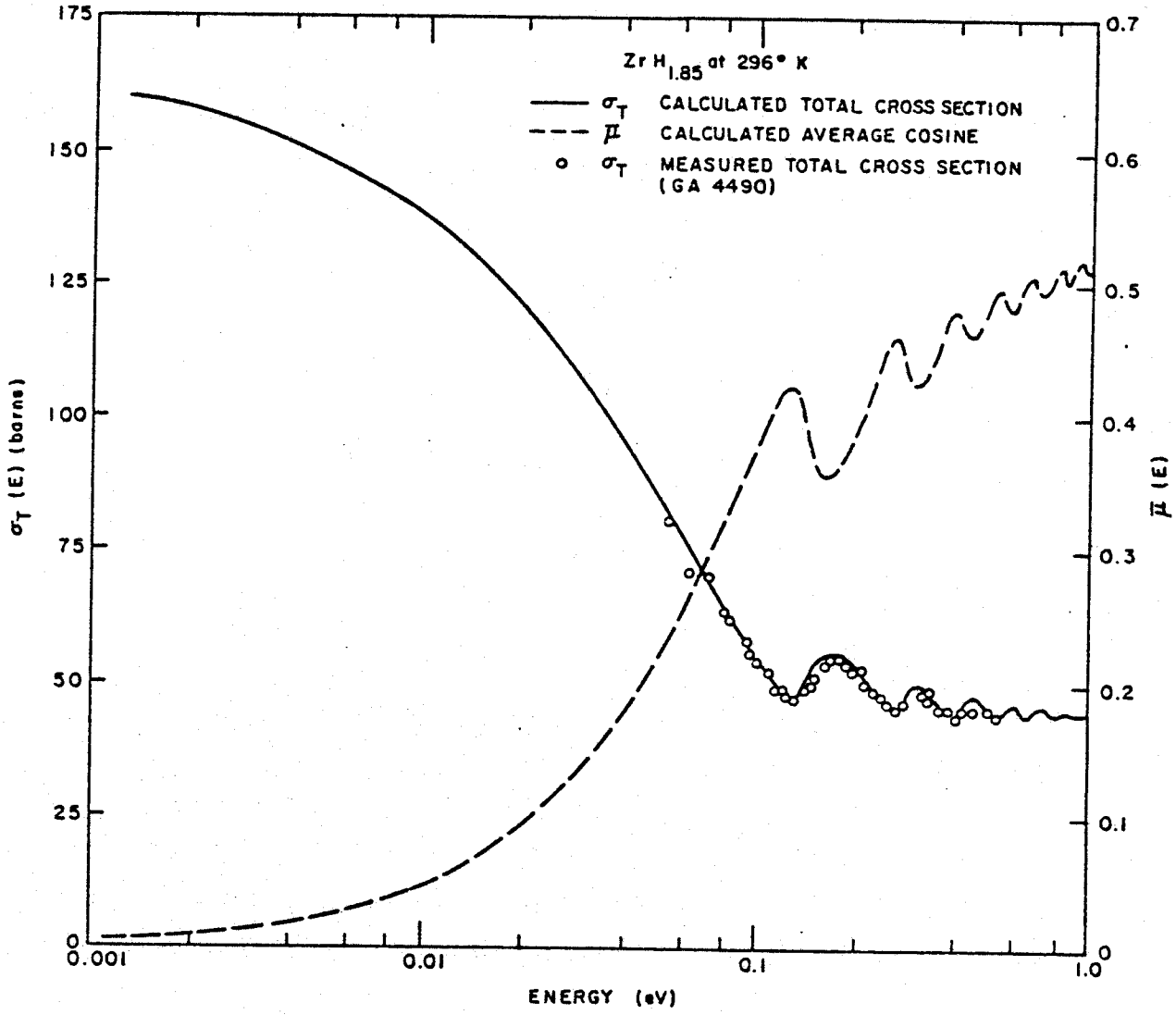
DATA FOR ZRH1.85 AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00025	173.69401	-.00123	43	.20000	52.91084	.39349
2	.00075	164.76159	.00195	44	.22400	49.46343	.42751
3	.00125	161.24719	.00448	45	.23200	47.95893	.43912
4	.00175	158.89221	.00698	46	.24000	47.27613	.44893
5	.00225	156.94430	.00955	47	.24800	46.32303	.45735
6	.00275	155.23716	.01211	48	.25600	45.40488	.46218
7	.00325	153.70253	.01464	49	.26400	45.77454	.46007
8	.00375	152.28257	.01713	50	.27200	46.67061	.45146
9	.00450	150.19403	.02094	51	.28000	47.66315	.44011
10	.00550	147.64045	.02596	52	.28800	48.81646	.43101
11	.00650	145.23604	.03096	53	.29600	49.58642	.42611
12	.00750	142.96808	.03592	54	.32500	49.53006	.43417
13	.00850	140.79476	.04086	55	.34500	48.16903	.44964
14	.00950	138.71328	.04576	56	.36500	46.57628	.46874
15	.01100	135.65881	.05309	57	.38500	45.14169	.48237
16	.01300	131.97168	.06244	58	.40500	45.61195	.47937
17	.01500	128.26519	.07208	59	.42500	46.91637	.46389
18	.01700	125.01956	.08108	60	.44500	47.85453	.46049
19	.01900	121.69225	.09041	61	.46500	47.48804	.46664
20	.02100	118.76694	.09905	62	.48500	46.61854	.47828
21	.02500	113.02615	.11663	63	.50500	45.49342	.49133
22	.02900	107.68299	.13398	64	.52500	44.86209	.49843
23	.03600	99.21736	.16371	65	.54500	45.34126	.49318
24	.04400	90.77676	.19641	66	.56500	46.31597	.48370
25	.05300	82.71070	.23127	67	.58500	46.73503	.48156
26	.06500	73.61620	.27485	68	.60500	46.45404	.48672
27	.07700	66.25242	.31418	69	.62500	45.75065	.49583
28	.08900	60.02175	.35031	70	.64500	44.99706	.50487
29	.09500	57.29667	.36696	71	.66500	44.72291	.50779
30	.10100	54.80363	.38265	72	.68500	45.20826	.50248
31	.10700	52.53138	.39726	73	.70500	45.88040	.49623
32	.11300	50.49899	.41037	74	.72500	46.09465	.49553
33	.11900	48.81115	.42072	75	.74500	45.82612	.50006
34	.12500	47.96196	.42427	76	.76500	45.26464	.50702
35	.13100	48.03683	.41765	77	.78500	44.76290	.51302
36	.13700	49.68011	.40033	78	.80500	44.67181	.51416
37	.15200	54.62310	.36212	79	.85500	45.67630	.50477
38	.16000	55.74407	.35725	80	.88500	45.39037	.50906
39	.16800	55.84918	.35926	81	.91500	44.70159	.51846
40	.17600	55.48195	.36501	82	.94500	44.60417	.51990
41	.18400	54.64420	.37366	83	.97500	45.16930	.51340
42	.19200	54.03148	.38263				

THE TOTAL CROSS SECTION INCLUDES A CONSTANT SCATTERING CROSS SECTION OF 6.2 BARNS (SIG0) FOR THE ZIRCONIUM. ALSO FOR THE ZIRC, SIG1 = .666*SIG0/MASS WAS USED TO CALCULATE THE AVERAGE COSINE OF THE SCATTERING ANGLE.

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV


Zr H1.85 at 296° K
σT CALCULATED TOTAL CROSS SECTION
μ̄ CALCULATED AVERAGE COSINE
σT MEASURED TOTAL CROSS SECTION (GA 4490)
σT (E) (barns)
μ̄ (E)
ENERGY (eV)
175
150
125
100
75
50
25
0
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.001
0.01
0.1
1.0

6. Miscellaneous Notes on Zirconium Hydride

For temperatures other than 296°K the switching criteria for short collision and the α,β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral, effective temperature and ID numbers of the scattering law data on file.

T(°K)	Debye Waller Integral (eV^{-1})	$\overline{T}$(°K)	ENDF ID No.
296	8.5607	795.48	GA 0020
400	9.1710	819.43	GA 0065
500	9.9143	858.80	GA 0066
600	10.783	911.35	GA 0067
700	11.745	973.92	GA 0068
800	12.778	1043.9	GA 0069
1000	14.988	1199.4	GA 0070
1200	17.324	1368.2	GA 0071

ZIRCONIUM HYDRIDE

1. Physics

The scattering laws for zirconium and for hydrogen in zirconium hydride were calculated by GASKET from squared-amplitude weighted frequency spectra obtained from a central force lattice dynamical model. This model approximated the slightly tetragonal lattice structure of ZrH_2 by a face-centered-cubic lattice. Four force constants - μ, γ, ν, and δ - were introduced describing respectively the interaction of a zirconium atom with its nearest neighbors (8H atoms) and the next nearest neighbors (12 Zr atoms) and the interaction of a hydrogen atom with its next nearest neighbors (6 H atoms) and its third nearest neighbors (12 H atoms). Eigenvalues and eigenvectors of the dynamical matrix were calculated and a phonon frequency spectrum obtained by means of root sampling techniques. In addition, weighted frequency spectra for use in neutron scattering calculations were obtained by appropriate use of the dynamical matrix eigenvectors.[1] These spectra are illustrated in Figs. 1, 2 and 3.

The final values of the force constants were obtained by fitting both specific heat and neutron data. The position of an optical peak - observed by neutron scattering techniques to be centered roughly around 0.14 eV - determines the constant μ, while the over-all width and shape of this peak determine ν and δ, respectively. Existing neutron data are not sufficiently precise to confirm the structure predicted in the optical peak by the central force model. Specific heat data were used to determine the force constant γ, which primarily determines the upper limit on the phonon energies associated with acoustic modes.

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[1] E. L. Slaggie, "Central Force Lattice Dynamical Model for Zirconium Hydride," General Atomic Report GA-8132, July 29, 1967.

In the plots for the scattering law some discontinuities are fairly prominent at high values of α. These discontinuities are associated with the switch to the short collision time approximation and are of no practical significance in this case because of the small values of the scattering law in the region of the discontinuities.

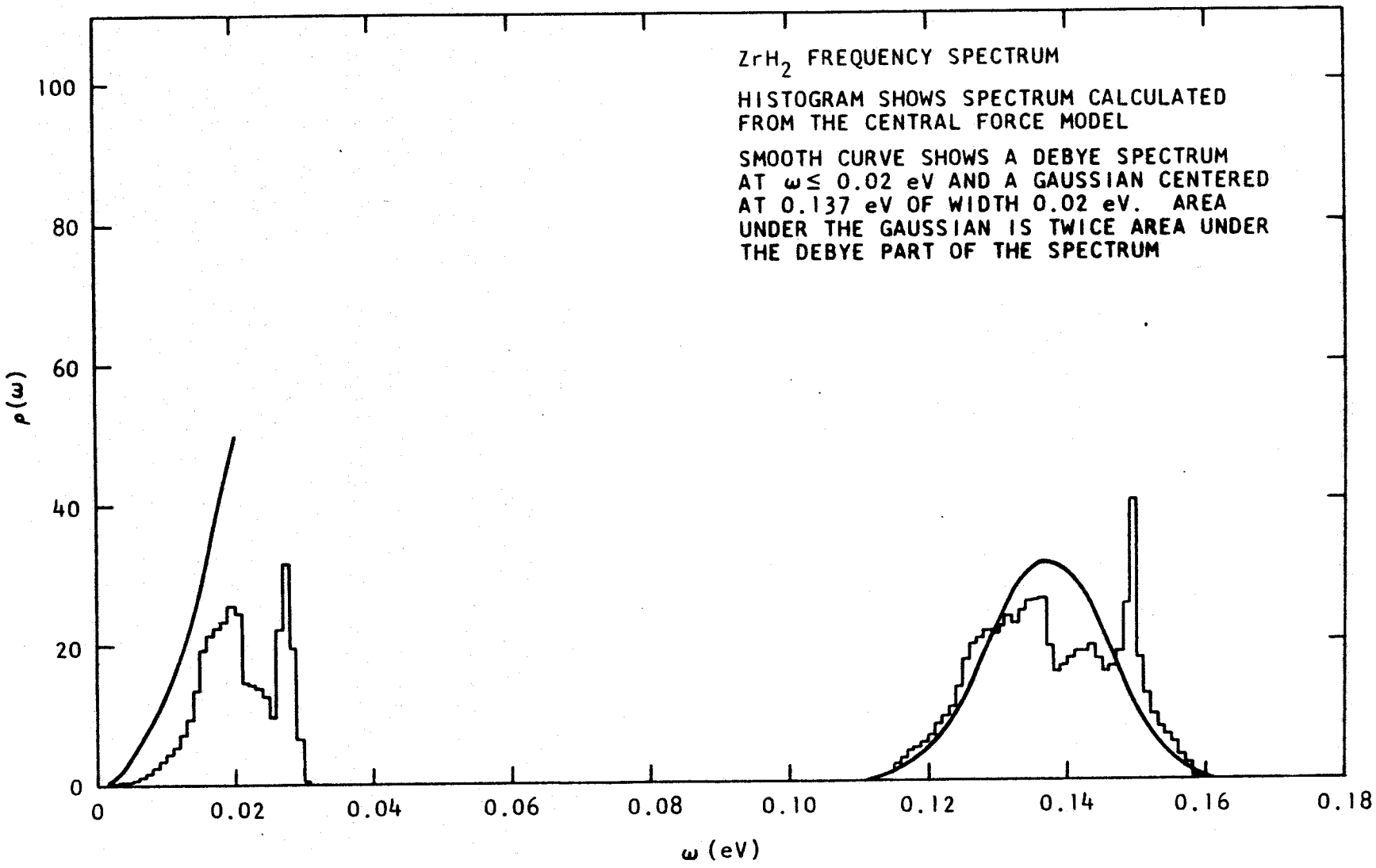


Fig. 1. ZrH_2 frequency spectrum calculated from the central force model. The smooth curve shows a Debye spectrum for $\omega \leq 0.02$ eV and a Gaussian of width 0.02 eV centered at 0.137 eV.

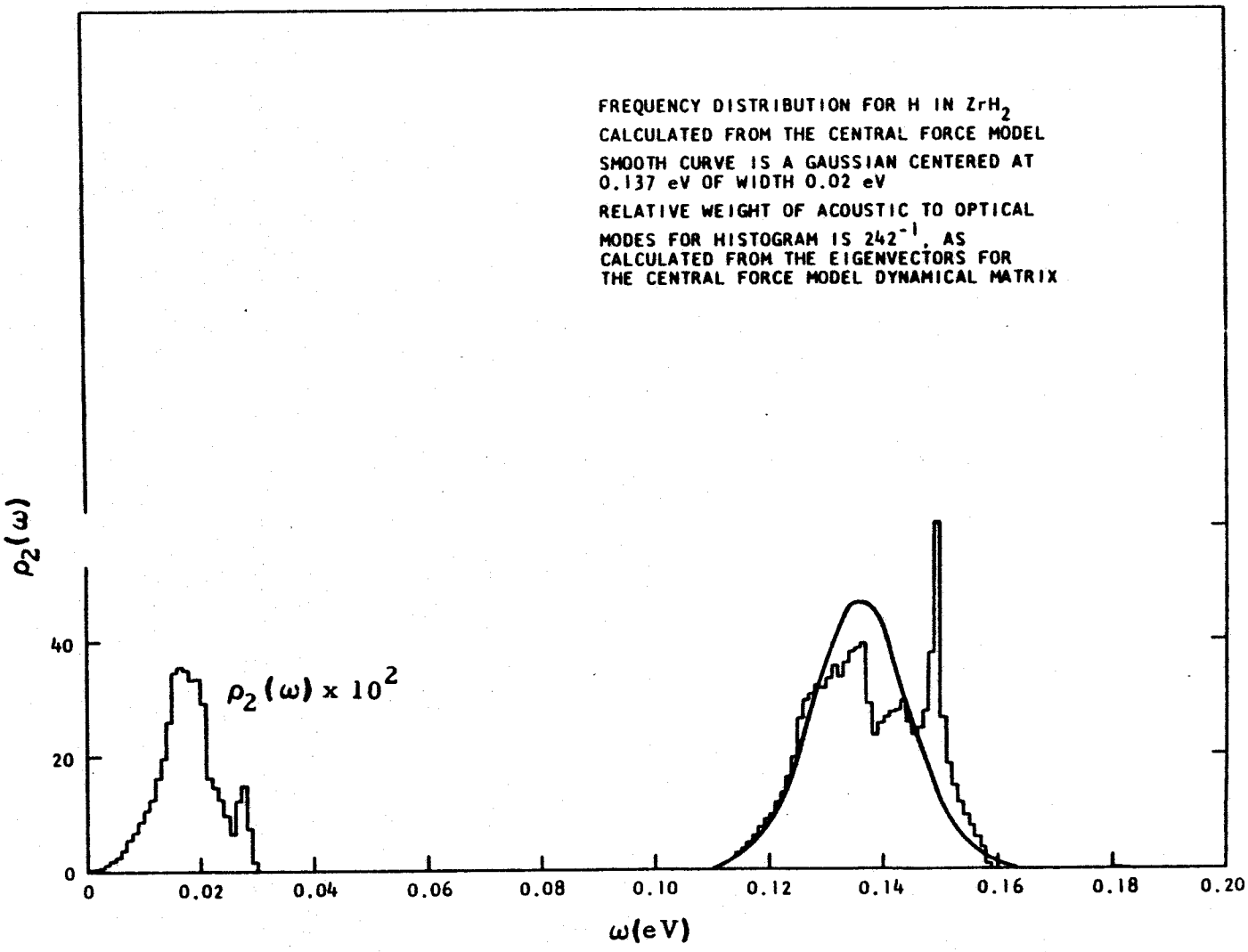


Fig. 2. Weighted frequency spectrum for H in ZrH_2 calculated from the central force model. Acoustic modes are shown multiplied by a factor 10^2.

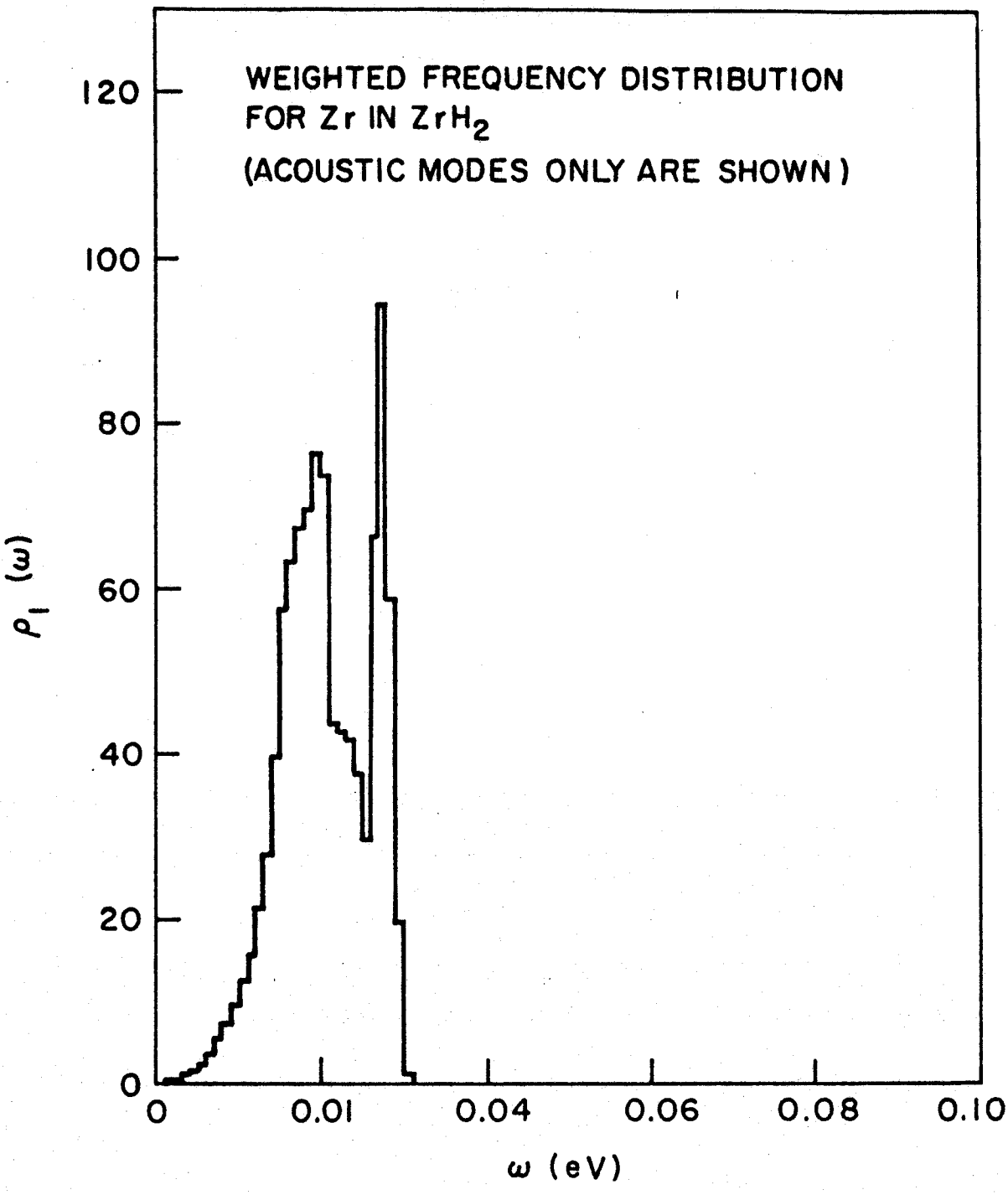


Fig. 3. Weighted frequency spectrum $\rho_1(\omega)$ for Zr in ZrH_2 calculated from the central force model.

3.1 GASKET Input for H(ZrH)

The code GASKET is discussed in Section A.3.1. The data tabulated below follows the format of the code input instructions also given in Section A.3.1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Slaggie's H(ZrH) at 296 degrees K.
2	11I5	NT -5 NP 40 NE 150 NDAM 1 NGPRT 0
		NCP 0 NMESH 0 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 80 JS4 JS5
4	5E10	W1 .00005 W2 0.0 W3 .99995 W4 W5
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 T5
6	7E10	AM 1.008 DC 0.0 BETSW 60.0 ALPSW 60.0 CRIT1
		CRIT2 CRIT3 1.0-5

X3

.001	.002	.003	.004	.005	.006
.007	.008	.009	.010	.011	.012
.013	.014	.015	.016	.017	.018
.019	.020	.021	.022	.023	.024
.025	.026	.027	.028	.029	.030
.031	.032	.113	.119	.115	.116
.117	.118	.119	.120	.121	.122
.123	.124	.125	.126	.127	.128
.129	.130	.131	.132	.133	.134
.135	.136	.137	.138	.139	.140
.141	.142	.143	.144	.145	.146
.147	.148	.149	.150	.151	.152
.153	.154	.155	.156	.157	.158
.159	.160				

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
8	7E10	Q3 8.75-04	3.5-03	8.0-03	.015	.0235	.0340
		.046	.061	.078	.094	.116	.144
		.1606	.1969	.2606	.3479	.3559	.3500
		.3322	.3328	.2911	.1617	.1431	.1248
		.09738	.06067	.1221	.1495	.07219	.01443
		1.0-04	0.0	0.0	.0499	2.010	3.560
		4.790	5.995	7.250	8.550	9.640	11.91
		13.52	16.04	19.79	26.10	29.39	30.82
		32.21	31.75	33.14	35.65	33.34	36.27
		38.18	38.75	39.48	28.99	23.29	25.18
		26.59	27.86	27.89	29.44	25.86	23.33
		24.66	27.51	37.94	60.77	26.66	18.54
		14.51	11.48	9.53	7.53	5.449	3.838
		8.497	0.0				
9	Cards 9 and 10 are not needed						
10							
11	7E10	X5					
12	7E10	Q5					
13	7I10	NPHON					
14	5E10	EMAX	DALPHA	ALPHAC	DBETA	BETAC	
15	7E10	ALPHA .5	1.0	1.5	2.0	2.5	3.0
		3.5	4.0	4.5	5.0	5.5635	6.1986
		6.9143	7.7209	8.6299	9.6544	10.809	12.110
		13.577	15.229	17.092	19.191	21.557	24.223
		27.228	30.615	34.431	38.732	47.580	49.043
		55.200	62.138	69.958	78.771	88.704	99.897
		112.51	126.73	142.75	160.81		

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
16	7E10.5	BETA 0.0	.078431	.15686	.23529	.31373	.39216
		.47059	.50980	.54902	.58824	.62745	.66667
		.70588	.74510	.78431	.82353	.86275	.94118
		1.0196	1.0980	1.1765	1.2549	1.3333	1.4510
		1.5686	1.6863	1.8039	1.92160	2.0392	2.1569
		2.2745	2.3922	2.5098	2.8627	3.1765	3.4902
		3.8431	4.1176	4.4314	4.5490	4.6275	4.7059
		4.7843	4.8627	4.9412	5.0196	5.098	5.1765
		5.2549	5.2941	5.3333	5.3725	5.4118	5.4902
		5.5686	5.6471	5.7255	5.7647	5.8039	5.8431
		5.8824	5.9216	5.9608	6.0392	6.1176	6.1961
		6.2745	6.8627	7.4510	8.0392	9.0196	9.3333
		9.6471	9.9608	10.275	10.588	10.667	10.745
		10.824	10.980	11.137	11.294	11.451	11.529
		11.608	11.686	11.765	11.843	11.922	12.235
		12.549	12.941	13.529	14.118	14.706	15.294
		15.647	15.882	16.118	16.353	16.588	16.824
		17.059	17.294	17.529	17.765	18.039	18.353
		18.824	19.608	20.392	20.784	21.176	21.569
		21.961	22.353	22.745	23.137	23.529	24.314
		25.098	25.490	25.882	26.275	26.667	27.059
		27.451	27.843	28.235	28.627	29.020	29.412
		30.000	30.588	30.980	31.373	31.765	32.157
		32.549	32.941	33.333	33.725	34.118	34.510
		35.294	36.078	36.863	37.647	38.431	39.216

17, 18, 19 and 20 are not needed

21	2E10	DT .15	TMAX 6.0	
		.40	60.0	
		3.0	300.0	
		6.0	2500.0	
		12.0	4100.0	
22	2I10			
	2E10	ID 104	NPT 0	SIGF 20.36 EPS 1.0-6
23	Card 23 is not needed			

3.2 GASKET Input for Zr(ZrH)

The code GASKET is discussed in Section A.3.1. The data tabulated below follows the format of the code input instructions also given in Section A.3.1. The code symbols used below are defined on the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES
1	13A6, A2	COM Slaggie's Zr(ZrH) at 296°K.
2	11I5	NT -5 NP 40 NE 118 NDAM 1 NGPRT 0
		NCP 0 NMESH 0 NREST 0 NCVP 0 NSEP 0
		IPG 0
3	3I5	JS3 80 JS4 JS5
4	5E10	W1 .005 W2 0.0 W3 1.0 W4 W5
5	6E10	T1 .0255 T2 0.0 T3 .0255 T4 T5
6	7E10	AM 91.22 DC 0.0 BETSW 60.0 ALPSW .66346 CRIT1
		CRIT2 CRIT3 1.0-5

X3

.001	.002	.003	.004	.005	.006
.007	.008	.009	.010	.011	.012
.013	.014	.015	.016	.017	.018
.019	.020	.021	.022	.023	.024
.025	.026	.027	.028	.029	.030
.031	.032	.113	.114	.115	.116
.117	.118	.119	.120	.121	.122
.123	.124	.125	.126	.127	.128
.129	.130	.131	.132	.133	.134
.135	.136	.137	.138	.139	.140
.141	.142	.143	.144	.145	.146
.147	.148	.149	.150	.151	.152
.153	.154	.155	.156	.157	.158
.159	.160				

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
8	7E10	Q3 .08	.32	.70	1.40	2.15	3.10
		4.50	6.30	8.40	11.0	14.2	16.4
		21.3	27.97	39.79	57.36	63.10	67.14
		69.42	76.32	73.70	43.53	42.53	41.67
		37.72	29.24	66.07	94.47	58.62	19.57
		1.031	0.0	0.0	.00218	.0828	.1340
		.1650	.1860	.2050	.2150	.2170	.2360
		.2340	.239	.242	.235	.223	.221
		.214	.198	.189	.170	.206	.207
		.202	.193	.197	.200	.212	.225
		.243	.253	.253	.262	.228	.195
		.194	.204	.263	.390	.170	.108
		.0775	.0592	.0406	.0235	.0112	.00424
		.000266	0.0				
9	Cards 9 and 10 are not needed						
10							
11	7E10	X5					
12	7E10	Q5					
13	7I10	NPHON					
14	5E10	EMAX	DALPHA	ALPHAC	DBETA	BETAC	
15	7E10	ALPHA .0055251	.011050	.016575	.02210	.027626	.033151
		.038676	.044201	.049726	.055251	.061478	.068496
		.076404	.085318	.095362	.10668	.11944	.13382
		.15003	.16828	.18887	.21206	.23821	.26767
		.30088	.33830	.38047	.42800	.48157	.54194
		.60997	.68664	.77305	.87044	.98020	1.1039
		1.2433	1.4004	1.5774	1.7770		

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
16	7E10	BETA 0.0	.098039	.19608	.29412	.39216	.43137
		.47059	.50980	.54902	.58824	.62745	.66667
		.70588	.74510	.78431	.82353	.86275	.90196
		.94118	.98039	1.0196	1.0588	1.0980	1.1373
		1.1765	1.2157	1.2549	1.3333	1.4118	1.4902
		1.5686	1.6471	1.7255	1.8039	1.8824	1.9608
		2.0392	2.1176	2.1961	2.2745	2.3529	2.4314
		2.5098	2.5882	2.7451	2.9020	3.0588	3.2157
		3.3725	3.5294	3.6863	3.8431	3.9216	4.3137
		4.7059	5.0980	5.4902	5.8824	6.2745	6.6667
		7.0588	7.4510	7.84310	8.2353	8.6275	9.0196
		9.4118	9.8039	10.196	10.588	10.980	11.373
		11.765	12.157	12.549	12.941	13.333	13.725
		14.118	14.510	14.902	15.294	15.686	16.078
		16.471	16.863	17.255	17.647	18.039	18.431
		18.824	19.216	19.608	20.392	21.176	21.961
		22.745	23.529	24.314	25.098	25.882	26.667
		27.451	28.235	29.020	29.804	30.588	31.373
		32.157	32.941	33.725	34.510	35.294	36.078
		36.863	37.647	38.431	39.216		

17, 18, 19 and 20 are not needed

21	2E10	DT .60	TMAX 6.0	
		1.0	60.0	
		4.0	300.0	
		6.0	1000.0	
		12.0	4500.0	
22	2I10			
	2E10	ID 112	NPT 0	SIGF 6.2 EPS 1.0-6
23	Card 23 is not needed			

3.3 ZREND Input for Zr(ZrH)

The code ZREND is discussed in Section A. 3. 1. The data tabulated below follows the format of the code input instruction also given in Section A. 3. 1. The code symbols used below are defined in the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO	FORMAT	CODE SYMBOLS AND VALUES					
1	13A6, A2	COM Slaggie's incoherent elastic for zirconium					
2	2I5,	NT 8	NE 109	SB 6.3366	SWITCH 10.0	EPS 1.0-15	
	3E10,	NPCH 1					
	I5						
3	7E10	T 296.0	400.0	500.0	600.0	700.0	800.0
		1000.0	1200.0				
4	7E10	WP 1.9957	2.6546	3.2946	3.9380	4.5835	5.2302
		6.5260	7.8236				
5	7E10	E .0005	.00053	.00056	.00060	.00064	.00068
		.00072	.00076	.00080	.00085	.00090	.00095
		.0010	.0011	.0012	.0013	.00145	.00160
		.00175	.00190	.00210	.00230	.00250	.00270
		.00290	.00310	.00330	.00350	.00380	.00410
		.00440	.00470	.0050	.0053	.0056	.0060
		.0064	.0068	.0072	.0076	.0080	.0085
		.0090	.0095	.010	.011	.012	.013
		.0145	.0160	.0175	.019	.0210	.0230
		.0250	.0270	.0290	.031	.033	.035
		.038	.041	.044	.047	.05	.053
		.056	.06	.064	.068	.072	.076
		.080	.085	.090	.095	.100	.110
		.120	.130	.145	.160	.175	.190
		.210	.230	.250	.270	.290	.310
		.330	.350	.380	.410	.440	.470
		.500	.530	.560	.600	.640	.680
		.720	.760	.800	.850	.900	.950
		1.000					

3.4 ZREND Input for H(ZrH)

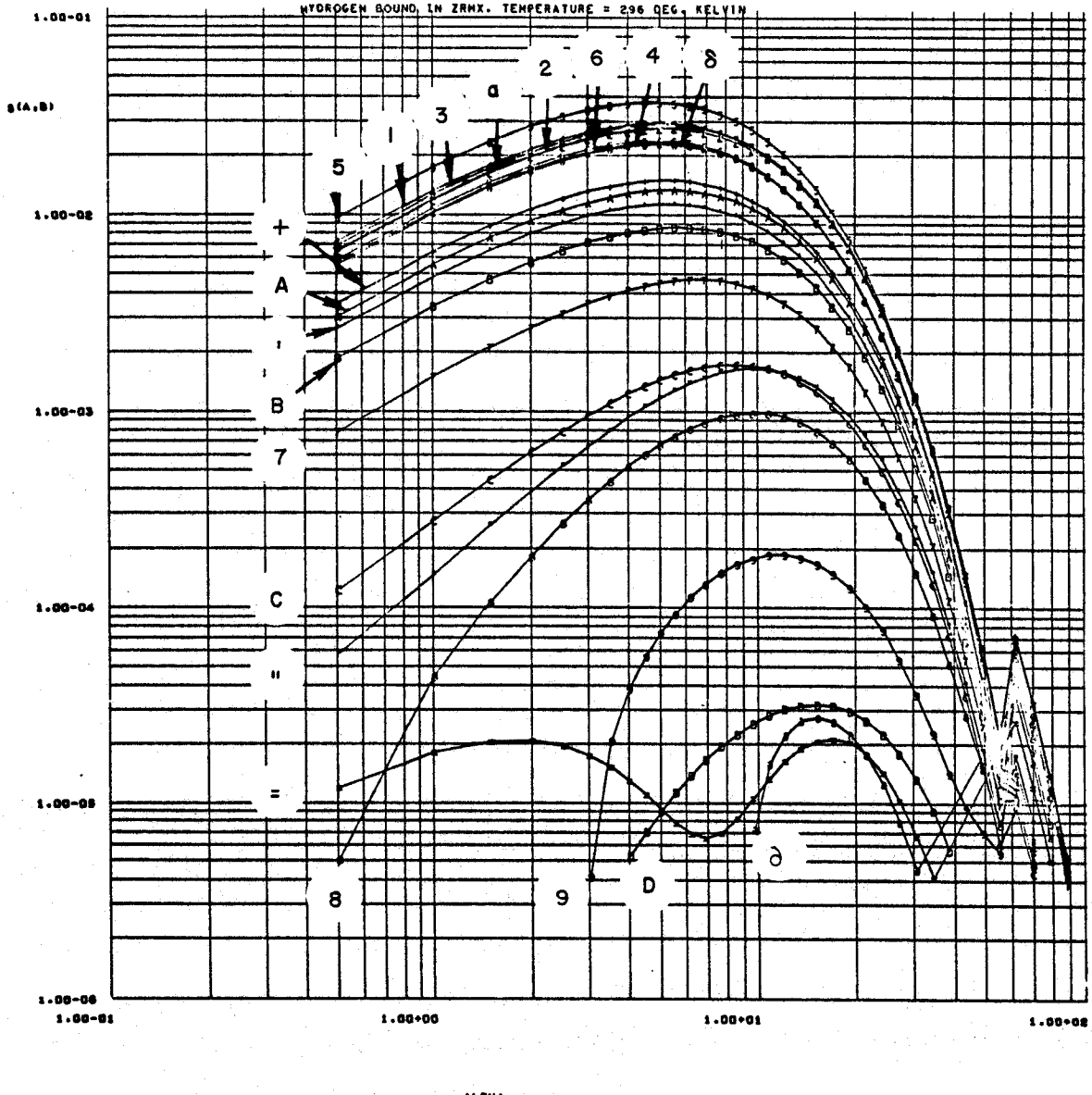
The code ZREND is discussed in Section A.3.1. The data tabulated below follows the format of the code input instruction also given in Section A.3.1. The code symbols used below are defined in the code input section. If no value is entered for a symbol then that datum was not required.

CARD NO.	FORMAT	CODE SYMBOLS AND VALUES					
1	13A6, A2	COM Slaggie's incoherent elastic for hydrogen					
2	2I5,	NT 8	NE 109	SB 81.44	SWITCH 10.0	EPS 1.0-15	
	3E10,	NPCH 1					
	I5						
3	7E10	T 296.0	400.0	500.0	600.0	700.0	800.0
		1000.0	1200.0				
4	7E10	WP 8.4795	9.0854	9.8196	10.676	11.625	12.643
		14.822	17.125				
5	7E10	E .0005	.00053	.00056	.00060	.00064	.00068
		.00072	.00076	.00080	.00085	.00090	.00095
		.0010	.0011	.0012	.0013	.00145	.00160
		.00175	.00190	.00210	.00230	.00250	.00270
		.00290	.00310	.00330	.00350	.00380	.00410
		.00440	.00470	.0050	.0053	.0056	.0060
		.0064	.0068	.0072	.0076	.0080	.0085
		.0090	.0095	.010	.011	.012	.013
		.0145	.0160	.0175	.019	.0210	.0230
		.0250	.0270	.0290	.031	.033	.035
		.038	.041	.044	.047	.05	.053
		.056	.06	.064	.068	.072	.076
		.080	.085	.090	.095	.100	.110
		.120	.130	.145	.160	.175	.190
		.210	.230	.250	.270	.290	.310
		.330	.350	.380	.410	.440	.470
		.500	.530	.560	.600	.640	.680
		.720	.760	.800	.850	.900	.950
		1.000					

4. Plots of Scattering Law

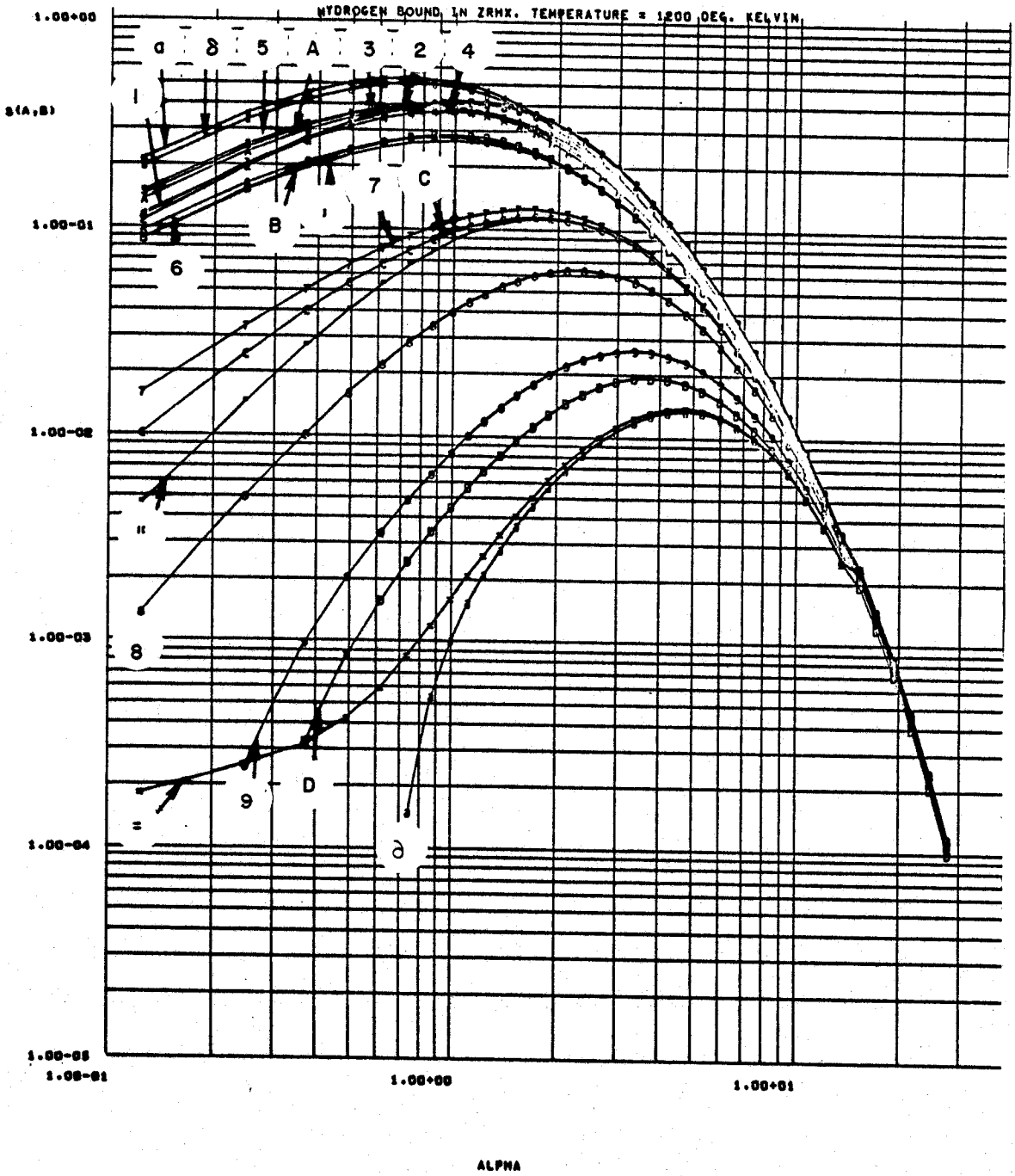
BETA VALUES FOR MULTICURVE PLOT

CURVE	INDEX	$\beta(296^{\circ}K)$	$\beta(1200^{\circ}K)$
1	1	0.00	0.0
2	2	7.843 - 02	1.934 - 02
3	3	1.569 - 01	3.868 - 02
4	4	4.706 - 01	1.161 - 01
5	5	6.275 - 01	1.547 - 01
6	6	7.843 - 01	1.934 - 01
7	7	1.030 + 00	2.515 - 01
8	8	1.333	3.288 - 01
9	9	1.804	4.449 - 01
10	∂	2.275	5.609 - 01
11	=	3.177	7.834 - 01
12	"	4.431	1.093
13	'	4.784	1.180
14	δ	5.098	1.257
15	a	5.333	1.315
16	+	5.569	1.373
17	A	5.804	1.431
18	B	5.961	1.470
19	C	6.275	1.547
20	D	9.020	2.224



ZrH_n - 4.2

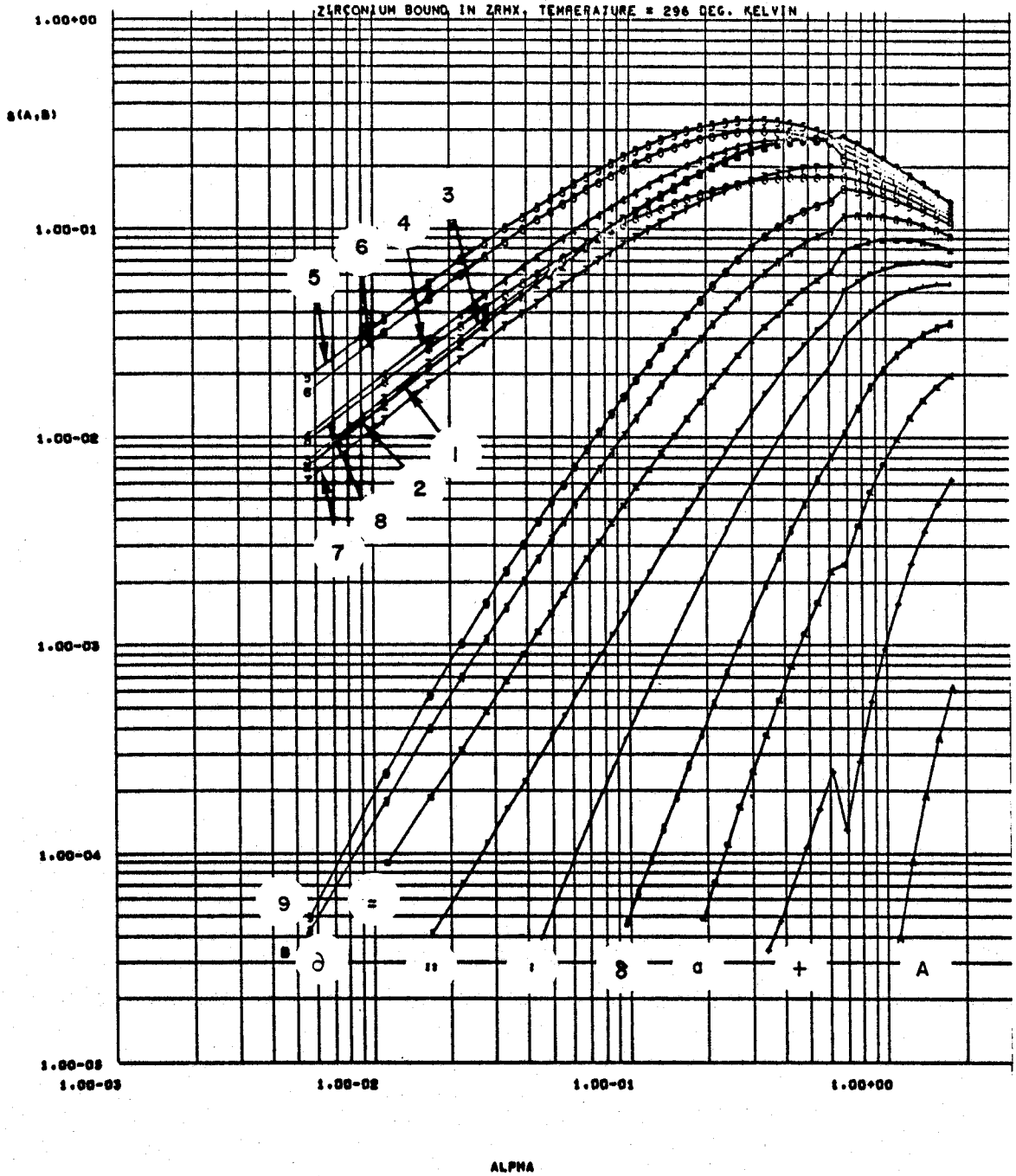
(Rev.-12/31/69)

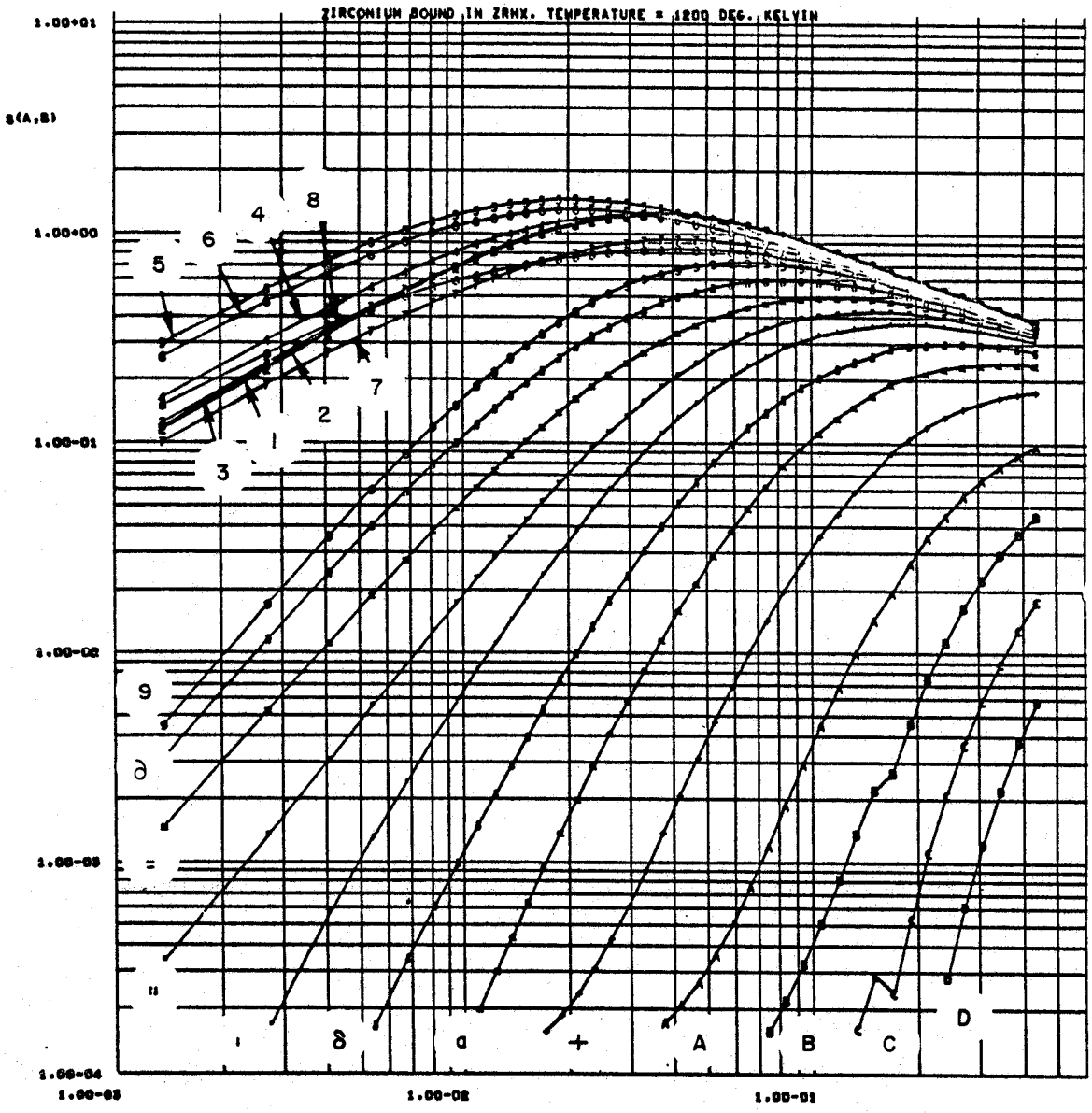

HYDROGEN BOUND IN ZRHX. TEMPERATURE = 1200 DEG. KELVIN
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-01
1.00+00
1.00+01
ALPHA

4. Plots of Scattering Law

BETA VALUES FOR MULTICURVE PLOT

CURVE	INDEX	$\beta(296^{\circ}K)$	$\beta(1200^{\circ}K)$
1	1	0.00	0.0
2	2	0.09804	0.02418
3	3	0.1961	0.04836
4	4	0.4706	0.1161
5	5	0.6275	0.1547
6	6	0.7843	0.1934
7	7	0.9412	0.2321
8	8	1.0980	0.2708
9	9	1.2549	0.3095
10	∂	1.5686	0.3868
11	=	1.8824	0.4642
12	"	2.1961	0.5416
13	'	2.5098	0.6190
14	δ	3.0588	0.7544
15	a	3.6863	0.9091
16	+	4.7059	1.1605
17	A	6.2745	1.5474
18	B	7.8431	1.9342
19	C	9.4118	2.3211
20	D	10.980	2.7078


ZIRCONIUM BOUND IN ZRHX, TEMPERATURE = 296 DEG. KELVIN
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-03
1.00-02
1.00-01
1.00+00
ALPHA
1
2
3
4
5
6
7
8
9


ZIRCONIUM BOUND IN ZRHX. TEMPERATURE = 1200 DEG. KELVIN
1.00+01
S(A,B)
1.00+00
1.00-01
1.00-02
1.00-03
1.00-04
1.00-03
1.00-02
1.00-01
ALPHA
1
2
3
4
5
6
7
8
9
δ
+
A
B
C
D

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR H IN ZRHX AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00025	89.90548	-.00197	43	.20000	25.41035	.43939
2	.00075	85.41316	.00143	44	.22400	23.56416	.48092
3	.00125	83.61810	.00404	45	.23200	23.67109	.49220
4	.00175	82.37898	.00670	46	.24000	22.74336	.50636
5	.00225	81.35449	.00934	47	.24800	21.85869	.52014
6	.00275	80.43537	.01195	48	.25600	22.18505	.52594
7	.00325	79.58997	.01455	49	.26400	21.76768	.52693
8	.00375	78.80482	.01715	50	.27200	21.74898	.52139
9	.00450	77.70758	.02107	51	.28000	22.96554	.51064
10	.00550	76.33323	.02632	52	.28800	23.44512	.49968
11	.00650	75.06864	.03154	53	.29600	23.56458	.49025
12	.00750	73.89089	.03669	54	.32500	23.96857	.49257
13	.00850	72.75033	.04183	55	.34500	22.87262	.50855
14	.00950	71.61374	.04704	56	.36500	22.49780	.53315
15	.01100	70.00706	.05460	57	.38500	21.30778	.55096
16	.01300	67.91289	.06470	58	.40500	21.55567	.55638
17	.01500	66.03109	.07459	59	.42500	21.77270	.53920
18	.01700	64.21587	.08443	60	.44500	22.52294	.52985
19	.01900	62.49634	.09403	61	.46500	22.88714	.53672
20	.02100	60.82376	.10353	62	.48500	22.50560	.54915
21	.02900	57.81927	.12210	63	.50500	21.92601	.56453
22	.02900	54.91148	.14068	64	.52500	21.49945	.57636
23	.03600	50.47814	.17214	65	.54500	21.45326	.57610
24	.04400	45.99742	.20757	66	.56500	21.84903	.56610
25	.05300	41.60040	.24643	67	.58500	22.18953	.55902
26	.06500	36.73023	.29580	68	.60500	22.19169	.56110
27	.07700	32.64858	.34259	69	.62500	21.91059	.57000
28	.08900	29.28834	.38629	70	.64500	21.53142	.58080
29	.09500	27.80668	.40694	71	.66500	21.26547	.58779
30	.10100	26.45179	.42675	72	.68500	21.31009	.58602
31	.10700	25.23214	.44550	73	.70500	21.58474	.57894
32	.11300	24.11972	.46297	74	.72500	21.80291	.57440
33	.11900	23.18157	.47735	75	.74500	21.78217	.57609
34	.12500	22.67095	.48322	76	.76500	21.57610	.58271
35	.13100	22.79364	.47524	77	.78500	21.30236	.59043
36	.13700	23.54648	.45613	78	.80500	21.14562	.59516
37	.15200	25.99740	.41136	79	.85500	21.51144	.58649
38	.16000	26.94315	.39964	80	.88500	21.56027	.58621
39	.16800	27.18711	.39881	81	.91500	21.29038	.59546
40	.17600	27.08507	.40454	82	.94500	21.07619	.60238
41	.18400	26.51098	.41500	83	.97500	21.19917	.59854
42	.19200	25.99781	.42631				

THE FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV

5. INTEGRAL DATA

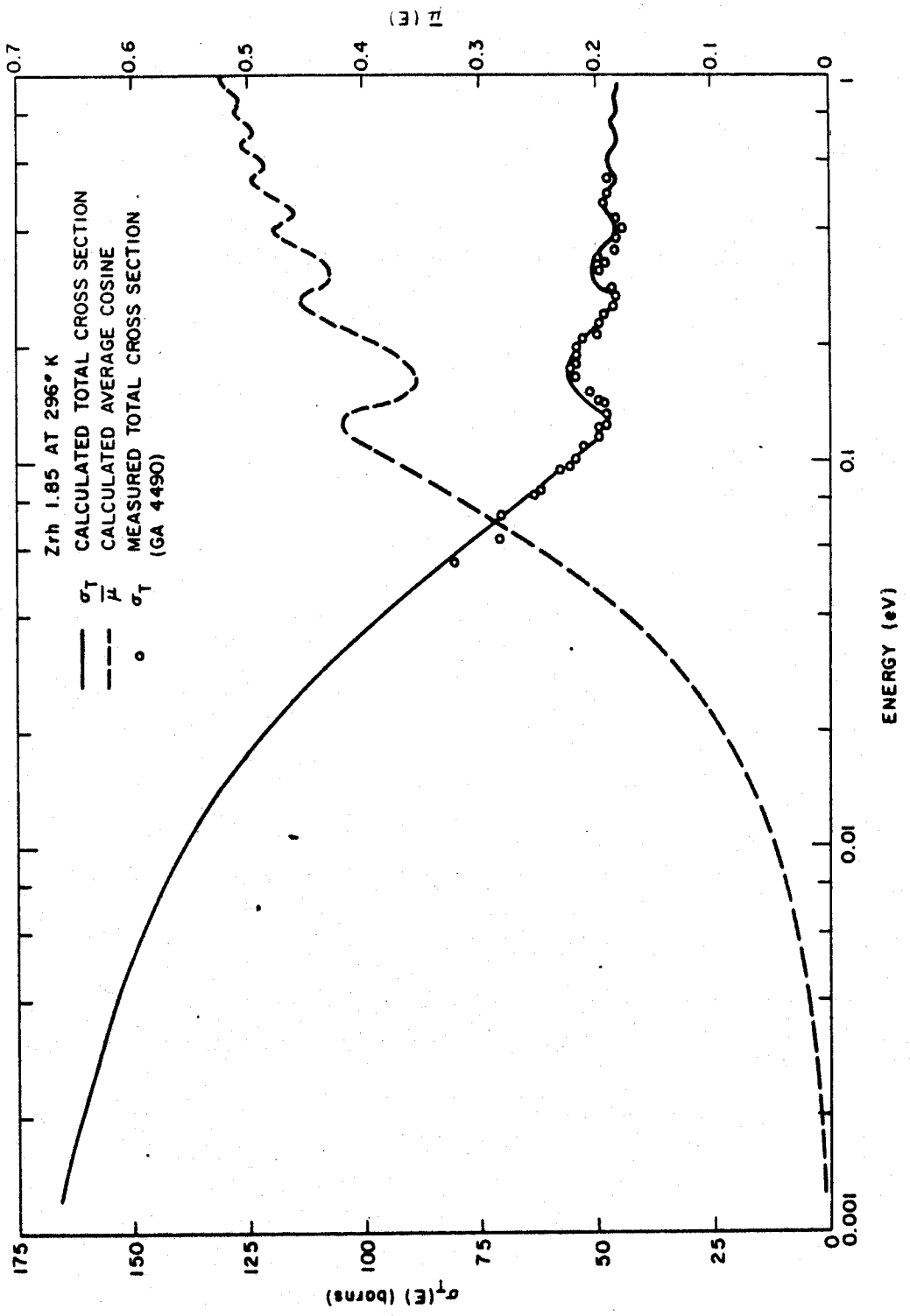
TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR ZR IN ZRHX AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00025	8.66627	-.01632	43	.20000	6.19278	.00984
2	.00075	7.68620	-.00635	44	.22400	6.18743	.00945
3	.00125	7.38165	-.00531	45	.23200	6.18612	.00931
4	.00175	7.21862	-.00502	46	.24000	6.18488	.00917
5	.00225	7.11269	-.00446	47	.24800	6.18370	.00904
6	.00275	7.03610	-.00403	48	.25600	6.18197	.00892
7	.00325	6.97962	-.00371	49	.26400	6.18042	.00882
8	.00375	6.93486	-.00344	50	.27200	6.17926	.00872
9	.00450	6.87102	-.00278	51	.28000	6.18619	.00842
10	.00550	6.79523	-.00168	52	.28800	6.28015	.00869
11	.00650	6.74561	-.00095	53	.29600	6.25926	.00849
12	.00750	6.71292	-.00055	54	.32500	6.38601	.00970
13	.00850	6.67560	.00016	55	.34500	6.32578	.00829
14	.00950	6.62947	.00131	56	.36500	6.31661	.00864
15	.01100	6.60235	.00176	57	.38500	6.31383	.00869
16	.01300	6.54735	.00323	58	.40500	6.31395	.00833
17	.01500	6.51775	.00391	59	.42500	6.31635	.00769
18	.01700	6.47672	.00518	60	.44500	6.31748	.00734
19	.01900	6.46143	.00554	61	.46500	6.31634	.00735
20	.02100	6.43391	.00638	62	.48500	6.31439	.00752
21	.02500	6.43064	.00599	63	.50500	6.31163	.00781
22	.02900	6.38246	.00749	64	.52500	6.30830	.00816
23	.03600	6.38426	.00658	65	.54500	6.30488	.00852
24	.04400	6.37524	.00635	66	.56500	6.30107	.00892
25	.05300	6.33238	.00743	67	.58500	6.29711	.00933
26	.06500	6.31315	.00762	68	.60500	6.29316	.00971
27	.07700	6.29098	.00796	69	.62500	6.28922	.01008
28	.08900	6.25814	.00868	70	.64500	6.28527	.01045
29	.09500	6.25300	.00867	71	.66500	6.28136	.01080
30	.10100	6.24862	.00864	72	.68500	6.27761	.01110
31	.10700	6.24506	.00857	73	.70500	6.27398	.01139
32	.11300	6.22549	.00902	74	.72500	6.27034	.01167
33	.11900	6.22141	.00903	75	.74500	6.26677	.01193
34	.12500	6.29081	.00696	76	.76500	6.26355	.01214
35	.13100	6.25738	.00810	77	.78500	6.26038	.01234
36	.13700	6.20674	.00882	78	.80500	6.25718	.01253
37	.15200	6.30571	.00743	79	.85500	6.24986	.01292
38	.16000	6.32325	.00694	80	.88500	6.24540	.01315
39	.16800	6.22104	.00945	81	.91500	6.23497	.01388
40	.17600	6.19942	.01020	82	.94500	6.17619	.01736
41	.18400	6.19583	.01014	83	.97500	5.83199	.02532
42	.19200	6.19423	.01000				

The FINAL ENERGY INTERVALS USED FOR INTEGRATION OF THE INELASTIC DATA ARE GIVEN BELOW.

	DELTA E	UP TO
1	.0005	.004 EV
2	.001	.01 EV
3	.002	.03 EV
4	.004	.05 EV
5	.006	.14 EV
6	.008	.30 EV
7	.01	1.0 EV



ZrH_n - 5.5

(Rev. -12/31/69)

6. Miscellaneous Notes on Zirconium Hydride

For temperatures other than 296°K the switching criteria for short collision and the α, β mesh input for 296°K were multiplied by $\frac{296^{\circ}K}{T^{\circ}K}$. The only other changes made in the input for higher temperatures were for obvious items: T, ID number and comments.

Tabulated below are the temperature, Debye Waller integral and effective temperature of the scattering law data on file.

T(°K)	Debye Waller Integral (eV^{-1}) for Hydrogen	$\overline{T}$(°K) for Hydrogen	Debye Waller Integral (eV^{-1}) for Zirconium	$\overline{T}$(°K) for Zirconium
296	8.4795	806.79	182.05	317.27
400	9.0854	829.98	242.15	416.25
500	9.8196	868.44	300.53	513.22
600	10.676	920.08	359.23	611.12
700	11.625	981.82	418.11	709.60
800	12.643	1051.1	477.10	808.43
1000	14.822	1205.4	595.30	1006.8
1200	17.125	1373.4	713.67	1205.7