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# REFERENCE MANUAL FOR ENDF THERMAL NEUTRON SCATTERING DATA

by

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## DISCLAIMER

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# 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 or will soon be 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[4]

The code GASKET was designed to calculate the neutron scattering law in the incoherent approximation for the following dynamical modes of motion of the scatterer.

1. Free translation (gas)
2. Diffusive or Brownian motion
3. Harmonic isotropic vibrations with continuous frequency spectrum.
4. Harmonic anisotropic vibrations with continuous frequency spectrum.
5. Harmonic isotropic vibrations with discrete frequency spectrum.

The general approach of the code is to treat separately all possible dynamical modes of motion and to combine their relative contribution by means of appropriate weighting factors $W_i$. At present the coding is complete for modes 1, 2, 3, and 5 only.

The code GASKET calculates the scattering law $S(\alpha, \beta)$ by numerical Fourier transformation of the intermediate scattering function $\chi(\alpha, t)$ defined as:

$$\chi(\alpha, t) = \int_{-\infty}^{\infty} e^{-i\beta Tt} S(\alpha, \beta) d\beta .$$

For each one of the listed dynamical modes (with exception of mode 4) $\chi$ has the form

$$\chi_i(\alpha, t) = \exp\left[\alpha G_i(t)\right] ,$$

where $G_i(t)$ is the time correlation function for the mode i. The $\chi$-function for a certain combination of modes then is simply

$$\chi(\alpha, t) = \exp\left[\alpha \sum_i W_i G_i(t)\right] .$$

All combinations are permitted with the exception that modes 1 and 2 are mutually exclusive.

The combination of vibrational modes with either free translation or diffusion leads to quasi-elastic scattering when no phonons are excited or absorbed. For the sake of fast convergence this zero phonon term is treated separately by the code when the vibrations have a distributed frequency spectrum (Mode 3 or 4). This quasi-elastic contribution to the scattering law is called $S^{(2)}$ in the code as opposed to $S^{(1)}$ which includes the contribution from all one or multiphonon processes.

In order to accelerate the calculations for large energy or momentum exchange the code has the capability to evaluate the scattering law in the short collision approximation for the distributed vibrational frequency spectrum when $\alpha$ or $\beta$ are larger than two given input numbers. The discrete modes, however, are always treated exactly since their frequency is generally much higher than the distributed band.

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 $\alpha$ values (NP ≤ 80) |
| | 11-15 | I5 | NE | | Number of $\beta$ 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 $\alpha$ and $\beta$ meshes, = 1 to calculate meshes using subroutine MESH, = -1 to read the $\alpha$ mesh and calculate the $\beta$ mesh. |
| | 36-40 | I5 | NREST | | Restart indicator. NREST = 0 for a new problem = the number of the $\alpha$ 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 | $\beta_{sw}$ | $\beta$ value above which short collision time (SCT) approximation is used, if $\alpha \geq$ ALPSW. BETSW = 100 if left blank. |
| | 31-40 | E10 | ALPSW | $\alpha_{sw}$ | $\alpha$ value above which SCT approximation is used for all $\beta$. (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<br>If IPG ≠ 0, Skip Cards 7 and 8 | | | |
| 7 | 1-70 | 7E10 | X3 | $\omega$ | If JS3 > 0, JS3 values of the frequency are read (eV).<br>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 | $\omega$ | 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 | $\omega_k$ | 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 | $\Delta\alpha$ | $\alpha$ interval. ($\alpha_1$ = DALPHA, $\alpha_2$ = 2·DALPHA, . . . , $\alpha$ = ALPHAC) |
| | 21-30 | E10 | ALPHAC | $\alpha_c$ | $\alpha$ value at which mesh spacing begins increasing geometrically. |

| Item | Columns | Format | Code Symbol | Report Symbol | Description |
|---|---|---|---|---|---|
| | 31-40 | E10 | DBETA | $\Delta\beta$ | $\beta$ interval. ($\beta_1 = 0$, $\beta_2$ = DBETA, $\beta_3$ = 2 DBETA, . . . , $\beta$ = BETAC) |
| | 41-50 | E10 | BETAC | $\beta_c$ | $\beta$ value at which mesh spacing begins increasing geometrically. |
| | | If NMESH > 0, Skip Cards 15 and 16 | | | |
| 15 | 1-70 | 7E10 | ALPHA | $\alpha$ | $\alpha$ mesh |
| | | If NMESH < 0, Skip Card 16 | | | |
| 16 | 1-70 | 7E10 | BETA | $\beta$ | $\beta$ 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 | $\Delta t$ | $\Delta t$ ($eV^{-1}$) 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($\alpha$, $\beta$) 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 | $\sigma_f$ | 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 $\Delta t_1$ until $t \geq t_{max_1}$, then by $\Delta t_2$ 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 $\max(\sum_{j=i}^{i+19} Q_j, \sum_{j=i}^{i+19} R_j)/Q_1 \leq$ 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 $(\alpha, \beta)$ 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 $\alpha$ points from |NREST| on are recalculated. |

## 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 $\omega$ 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 $\alpha$ and $\beta$ values and calculates $S(\alpha, \beta)$. In this modified version the switching depends on $\beta$ 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 $\beta$ mesh points |
| | 16-20 | I5 | IZX | Number of $\alpha$ 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; $E_3$, $E_4 \cdots E_{NES}$ 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).

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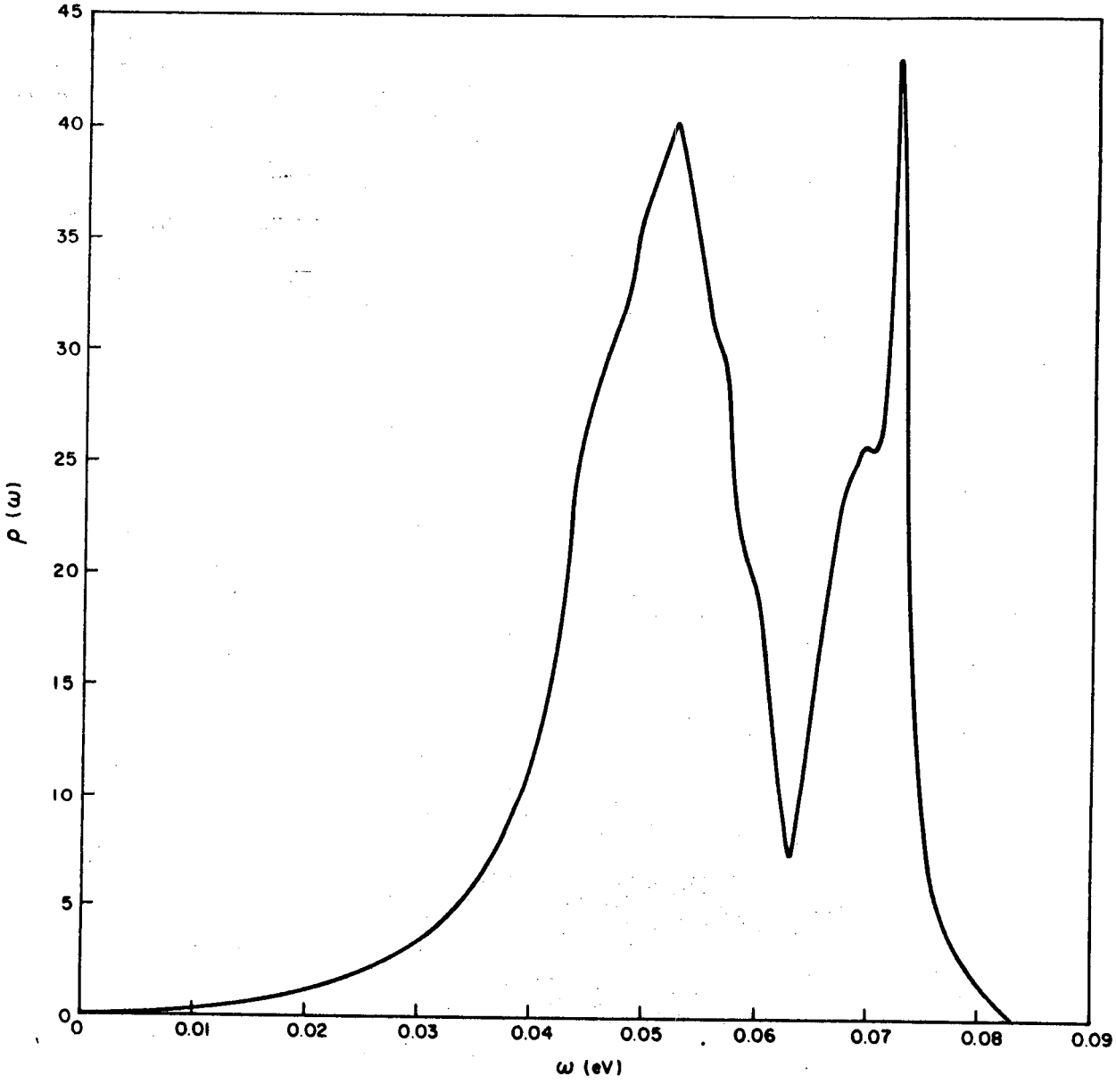
[1] R. E. Schmunk, R. M. Brugger, P. D. Randolph, and K. A. Strong, Phys. Rev. 128 (1962) 562.

## 2. 1. 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

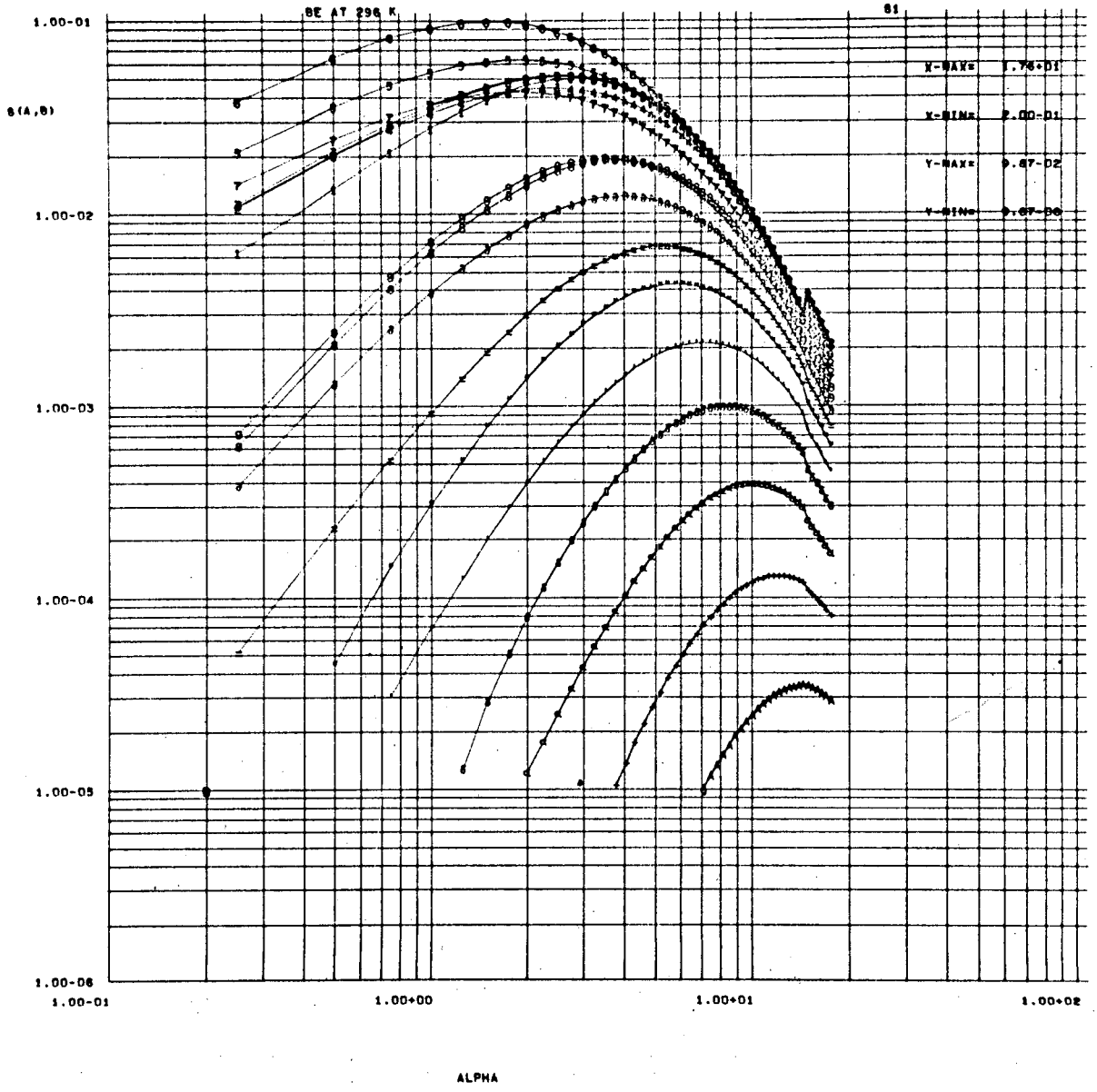
The code HEXSCAT is discussed in Section A. 3. The data tabulated below follows the format of the code input instruction also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required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

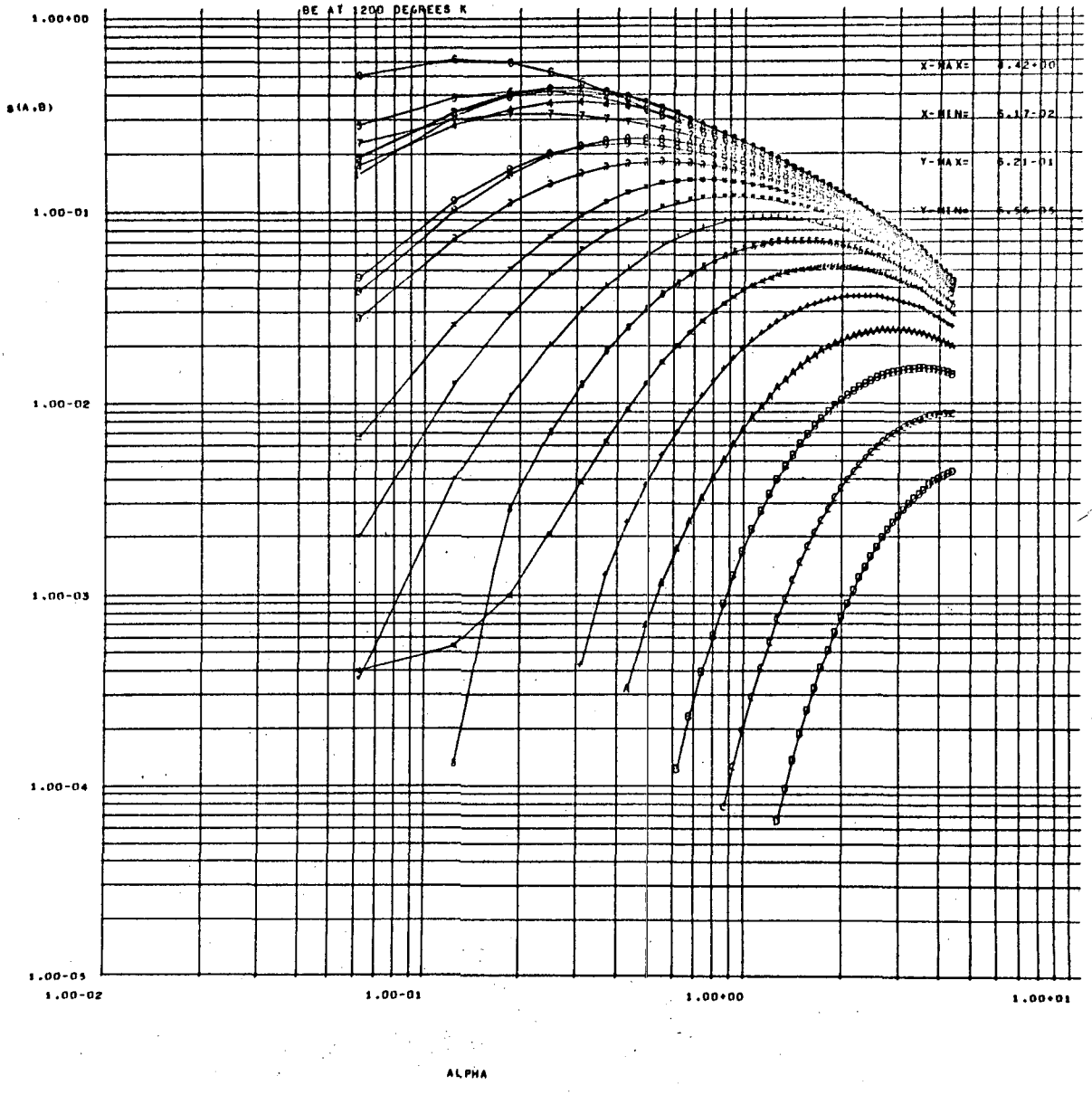
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES | | | | |
|---|---|---|---|---|---|---|
| 1 | 13A6,A2 | HOL HEXSCAT for ENDF Be | | | | |
| 2 | 5E10, | SCOH 7.53 | A 2.2856-8 | C 3.5832-8 | AMASC 9.01 | EXACT .0625515 |
| | 1I10, | ID 1064 | ZA 4009. | AWR | | |
| 3 | 8I5, | NES 32 | NTS 8 | NAV 0 | NXAV 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
S(A,B)
1.00+00
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
X-MAX= 8.42+00
X-MIN= 5.17-02
Y-MAX= 6.21-01
Y-MIN= 5.56-05

## 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 | 6.00213 | .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 |

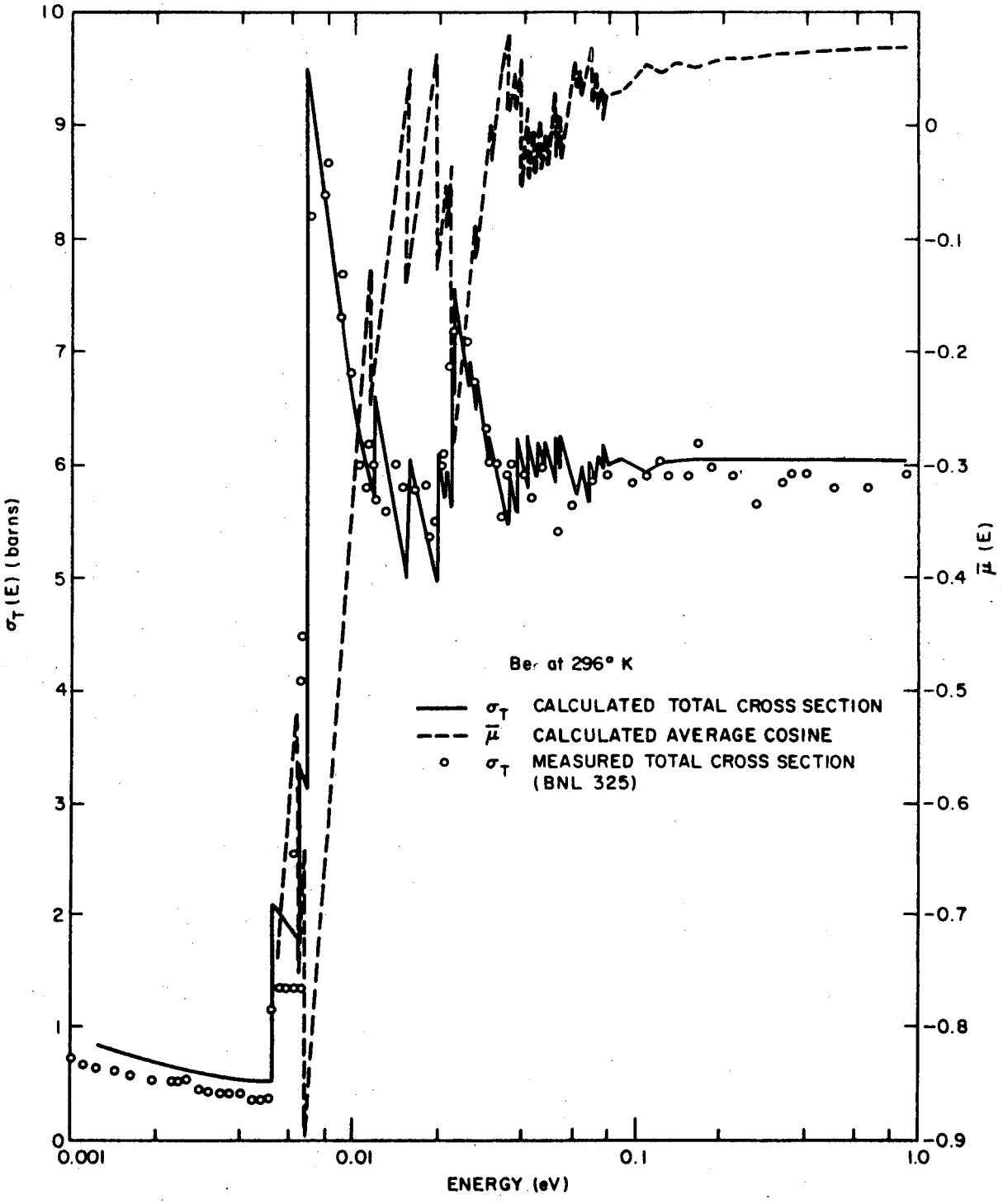
DATA FOR BERYLLIUM AT 296 DEGREES K.

| | 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
$\sigma_T$ CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
$\sigma_T$ MEASURED TOTAL CROSS SECTION (BNL 325)
$\sigma_T$(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
-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 $\alpha,\beta$ 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

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 $3 \times 10^5$ 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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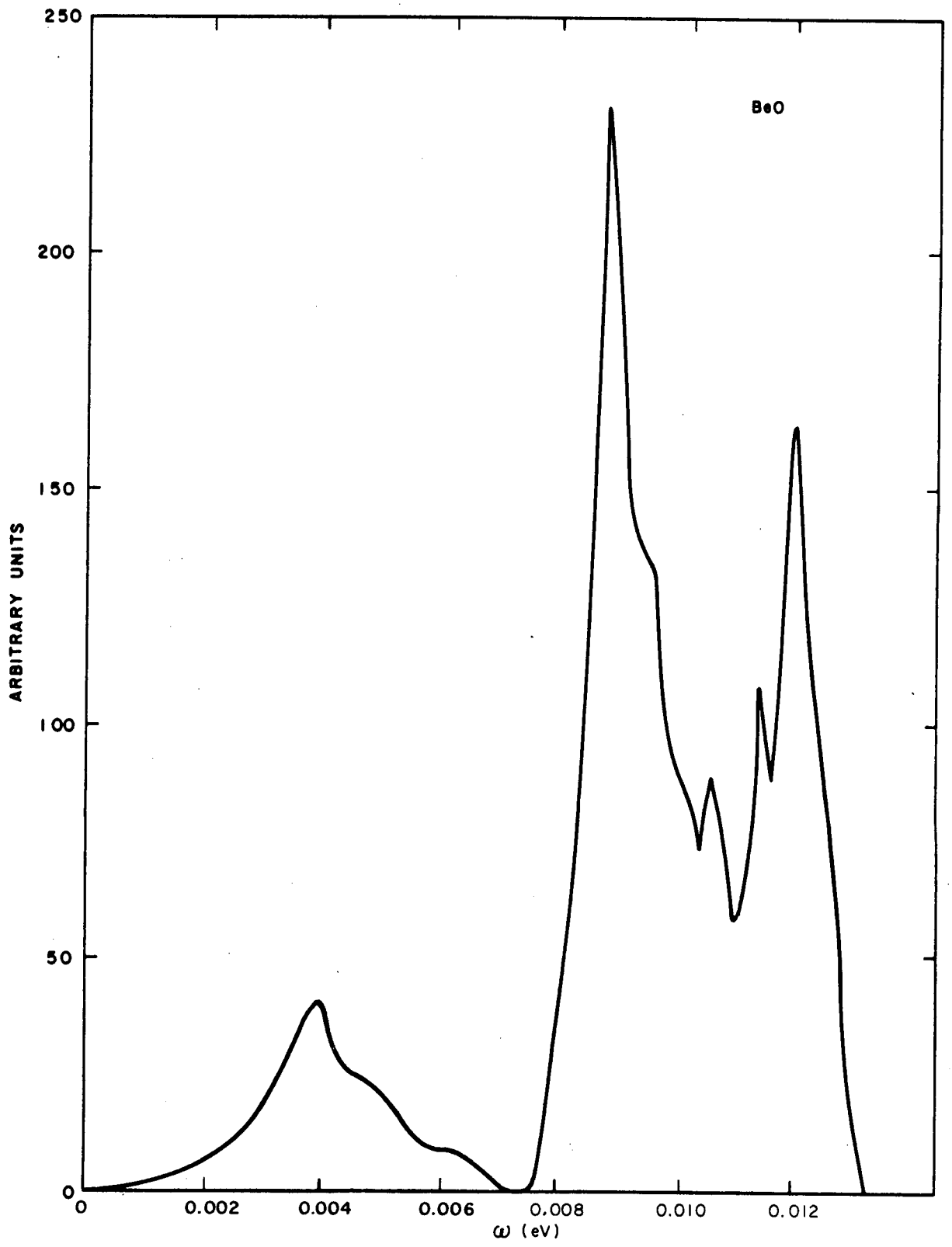
[1] G. Borgonovi, "Lattice Dynamics and Neutron Scattering of BeO," USAEC Report GA-8758, Gulf General Atomic Incorporated (1968).

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

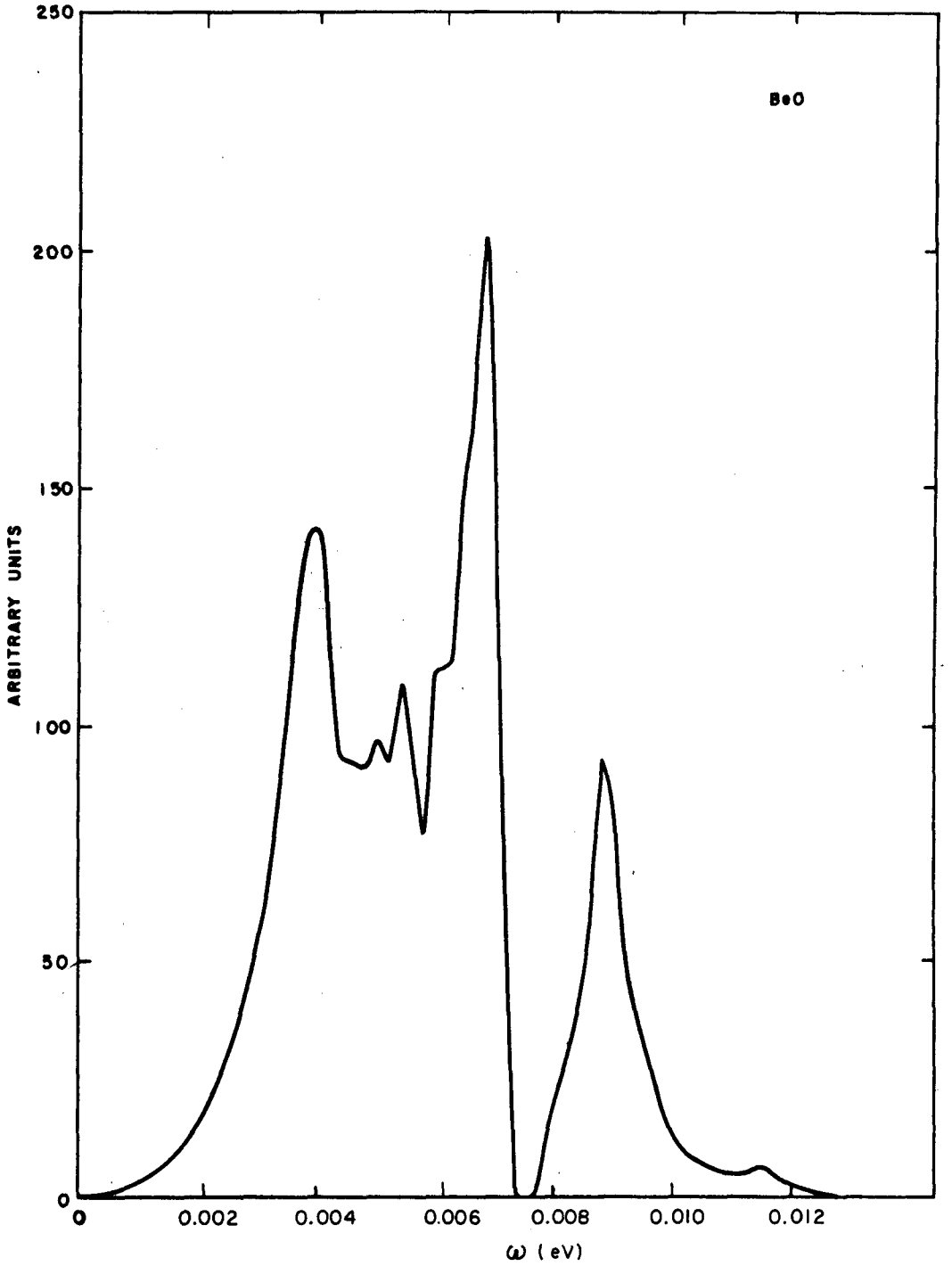
The two scattering laws have been combined and the total scattering law is referred to the beryllium atom.

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



## 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 .14083 ALPHAC 1.6618 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

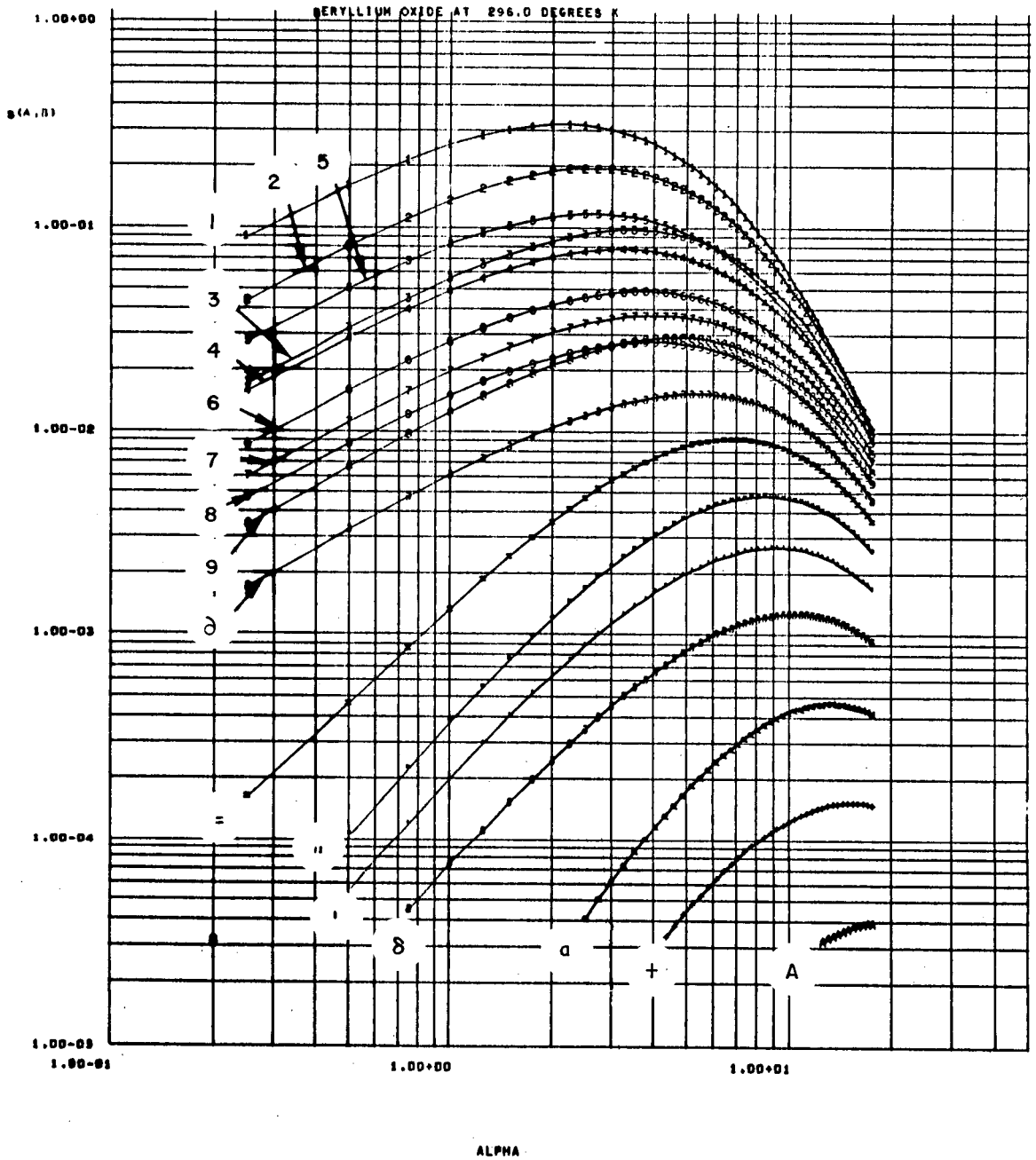
The code HEXSCAT is discussed in Section A. 3. 1. The data tabulated below follows the format of the code input instruction also given in Section A. 3. 1. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required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

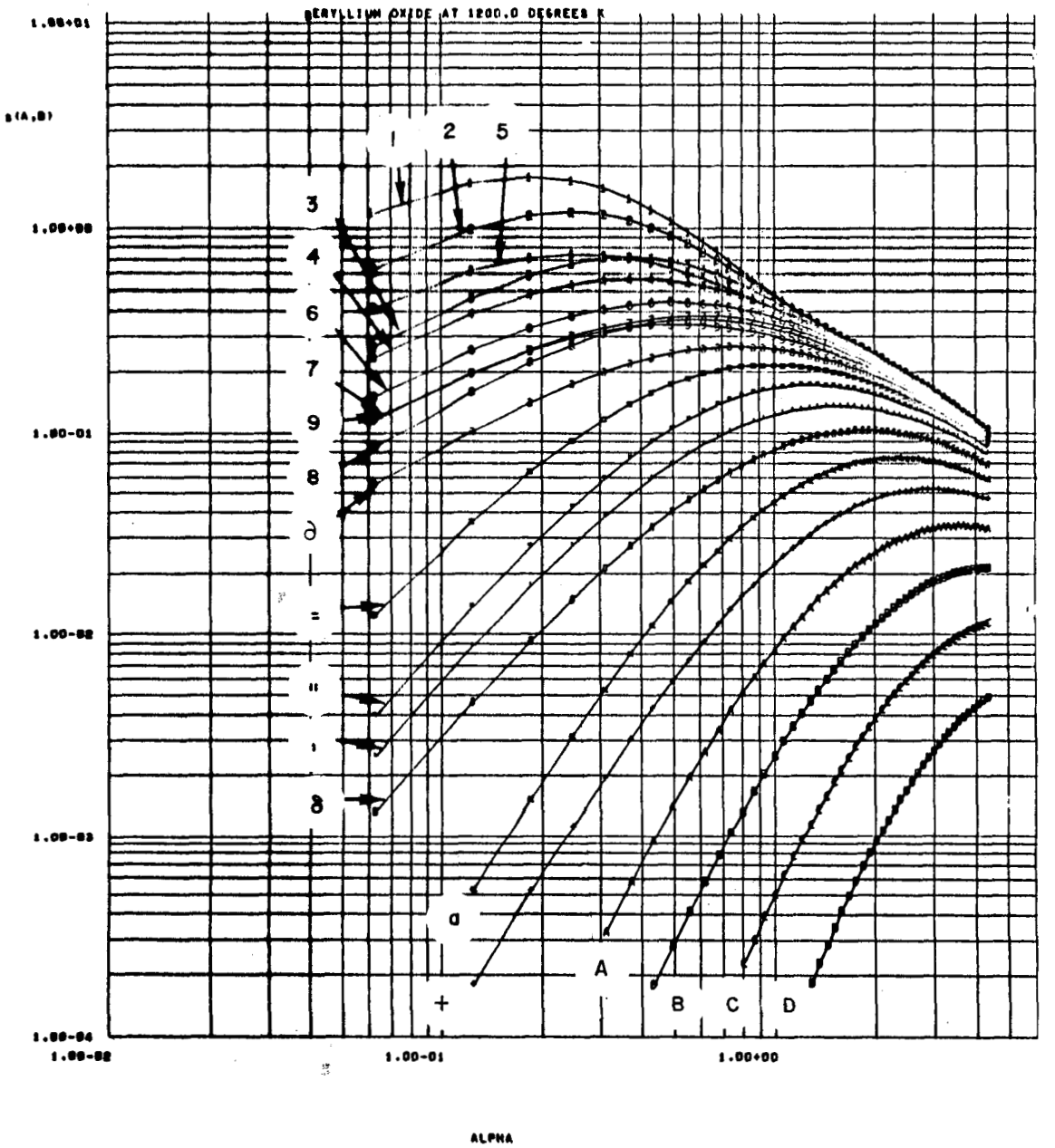
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES |
|---|---|---|
| 1 | 13A6, A2 | HOL HEXSCAT for Borgonuuis shell model BeO |
| 2 | 5E10, | SCOH 1.0 A 2.695-8 C 4.39-8 AMASC 1.0 EXACT 0.05 |
| | 1I10, | ID 1108 ZA 200.0 AWR 24.7967 |
| 3 | 8I5, | NES 22 NTS 8 NAV 0 NXAV 2 IP 1 |
| | 1E10 | NCOS 0 NPCH 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
0
=
"
'
δ
α
+
A


BERYLLIUM OXIDE AT 1200.0 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
1
2
5
3
4
6
7
9
8
0
=
"
'
8
a
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 | -.14490 |
| 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 | .00586 | 8.23806 | -.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 | .01388 | 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 | 12.04550 | -.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 | 9.34396 | .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 | .03485 | 9.63839 | -.01756 | 139 | .04790 | 9.67545 | .01462 |
| 98 | .03516 | 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 | 10.62713 | -.09802 | 151 | .04973 | 10.09322 | -.02736 |
| 110 | .03809 | 10.61421 | -.09664 | 152 | .04986 | 10.07199 | -.02511 |
| 111 | .03814 | 10.60133 | -.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 | .04182 | 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 | .04326 | 10.16947 | -.03984 | 168 | .13000 | 9.60319 | .04890 |

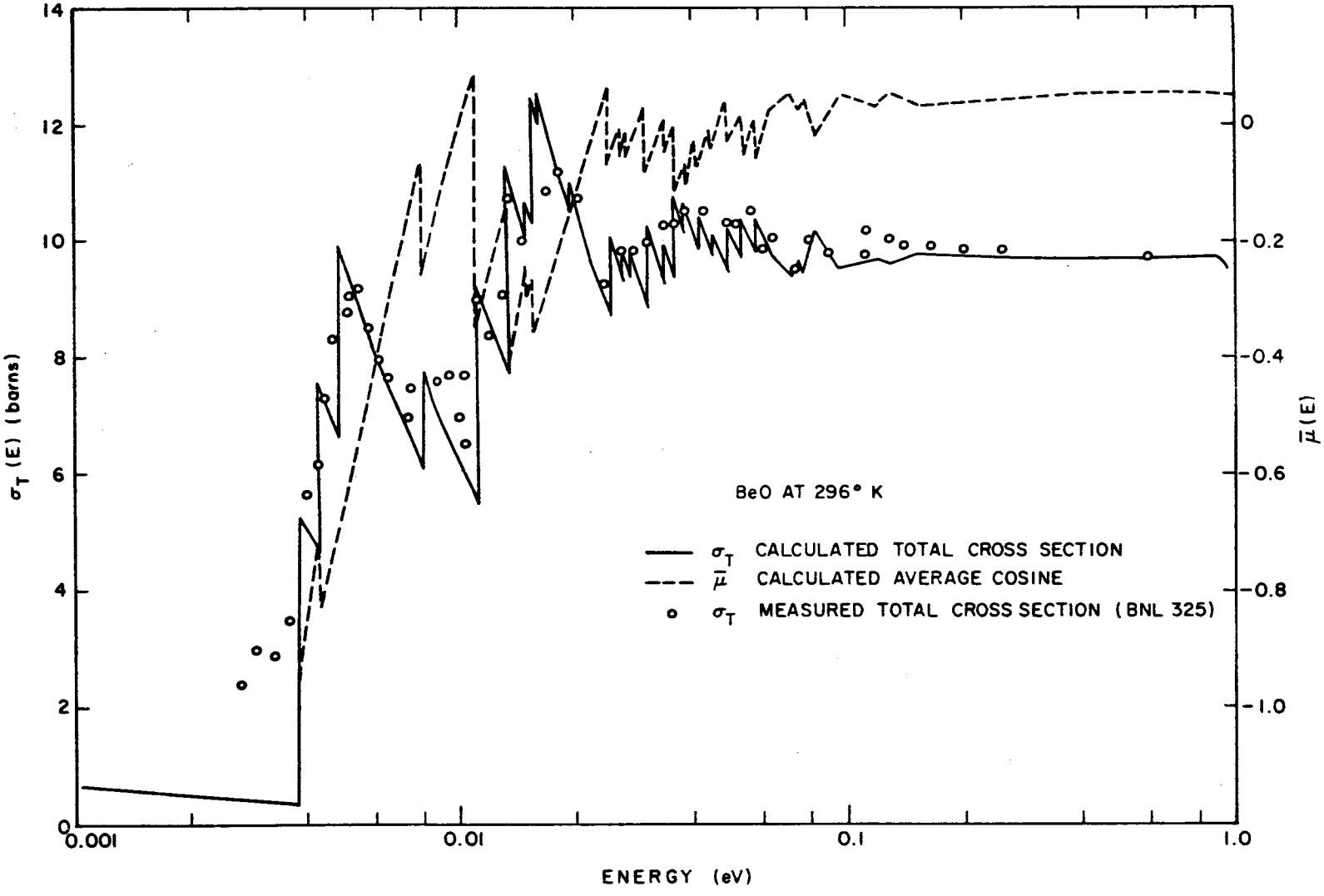
DATA FOR BEO AT 296 DEGREES K.

| | 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 |


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

## 6. Miscellaneous Notes on Beryllium Oxide

For temperatures other than 296°K the switching criteria for short collision and the $\alpha, \beta$ 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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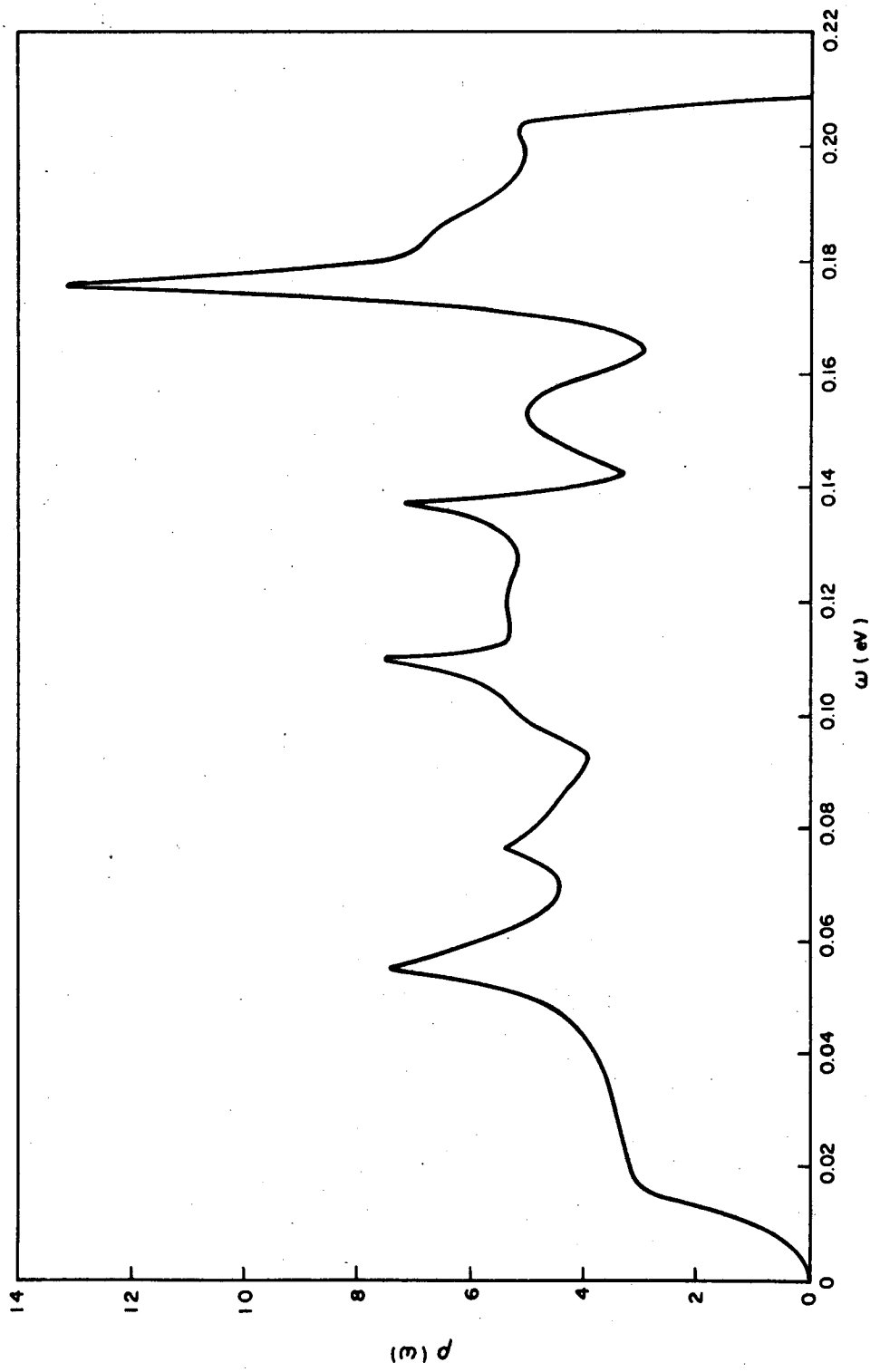
[1] Nukleonik Band 1, 295, (1965).

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 | | | | | | | |
| 10 | | | | | | | | |
| 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 | .001 | TMAX | .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

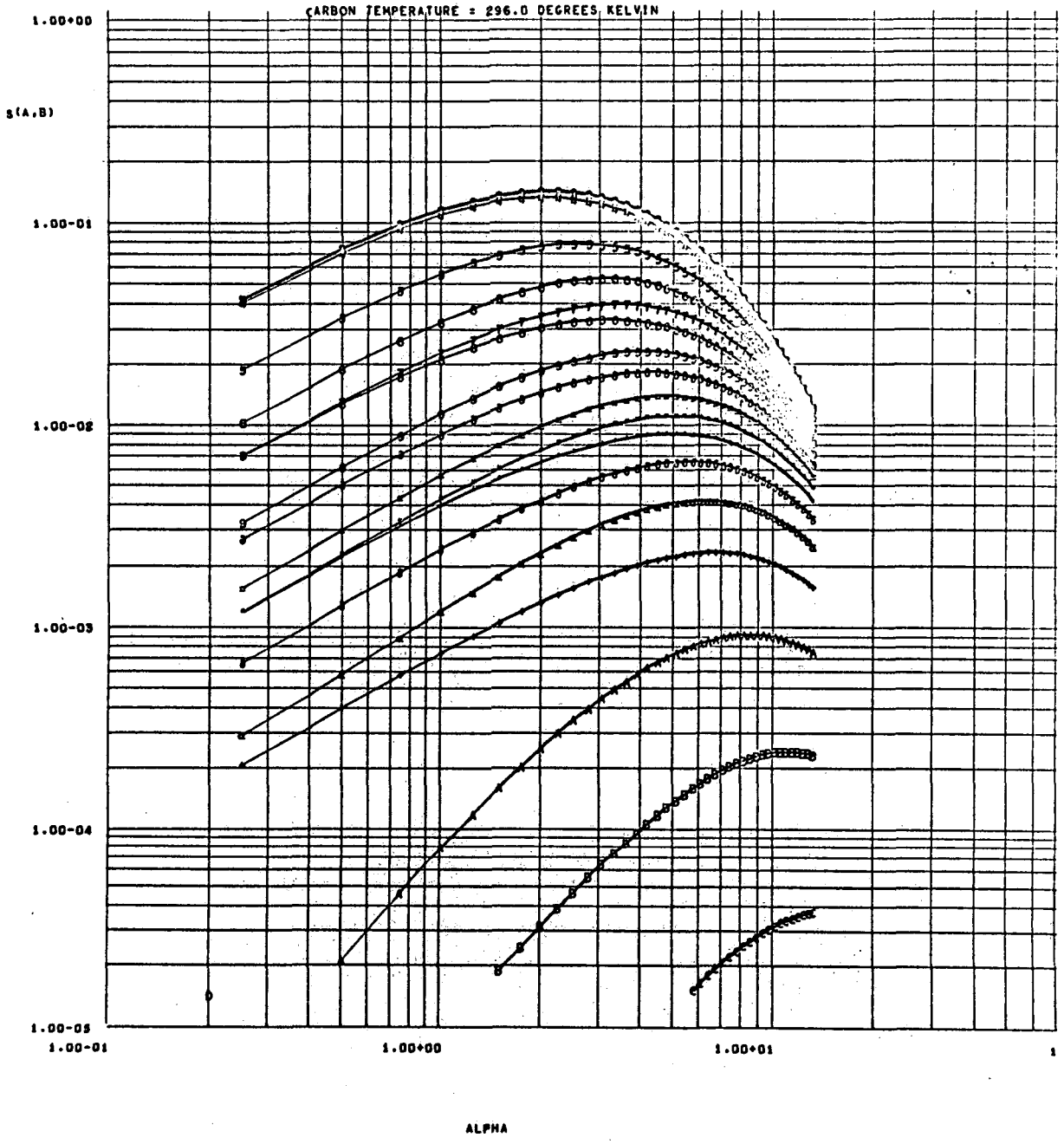
The code HEXSCAT is discussed in Section A. 3. The data tabulated below follows the format of the code input instruction also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required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

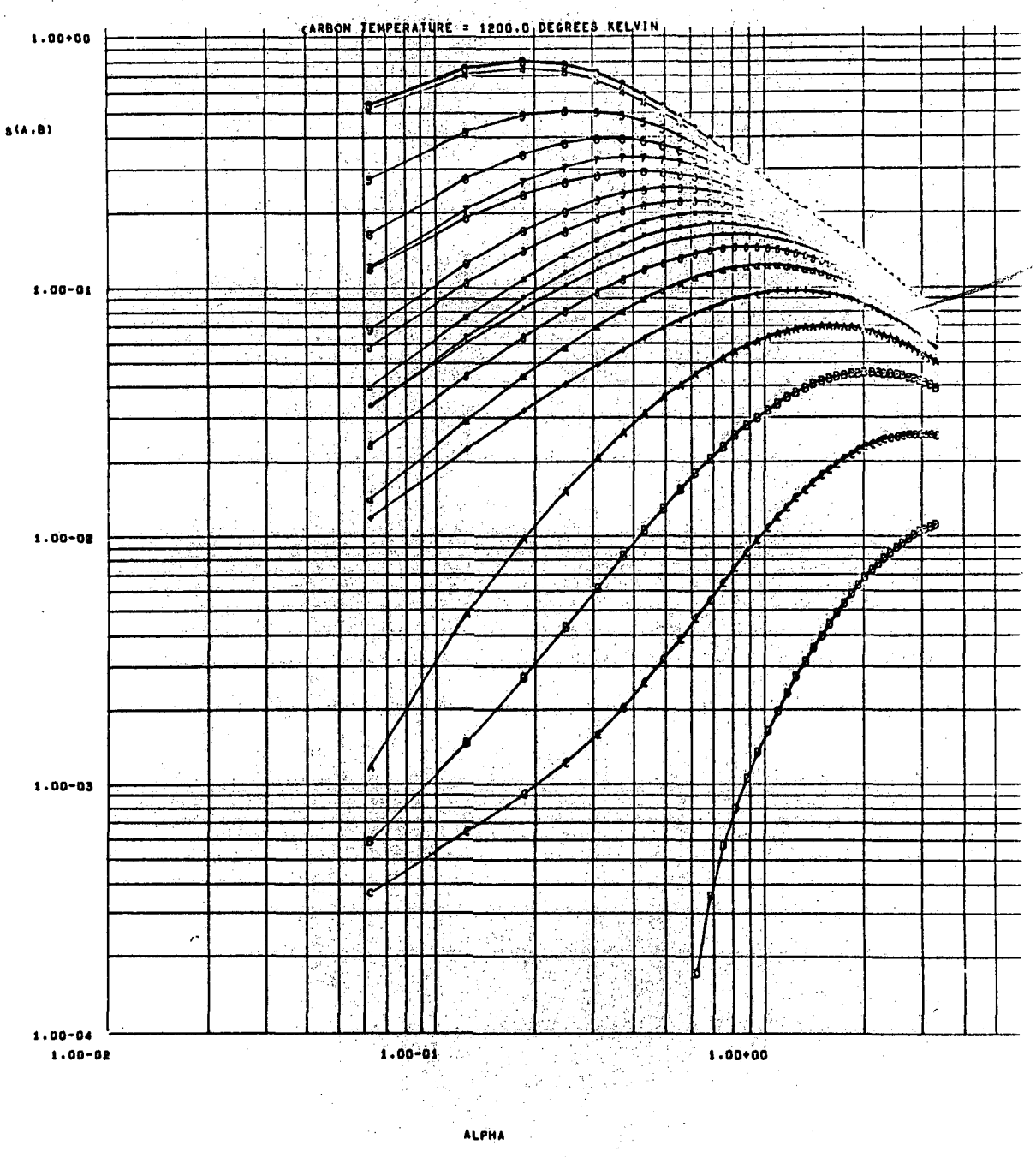
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES | | | | |
|---|---|---|---|---|---|---|
| 1 | 13A6,A2 | HOL HEXSCAT for ENDF carbon | | | | |
| 2 | 5E10, | SCOH 5.50 | A 2.4573-8 | C 6.700-8 | AMASC 12.011 | EXACT .04 |
| | 1I10,2E10 | ID 1065 | ZA 6000.0 | AWR | | |
| 3 | 8I5, | NES 42 | NTS 10 | NAV 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 | .08101450 |
| | | .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 |

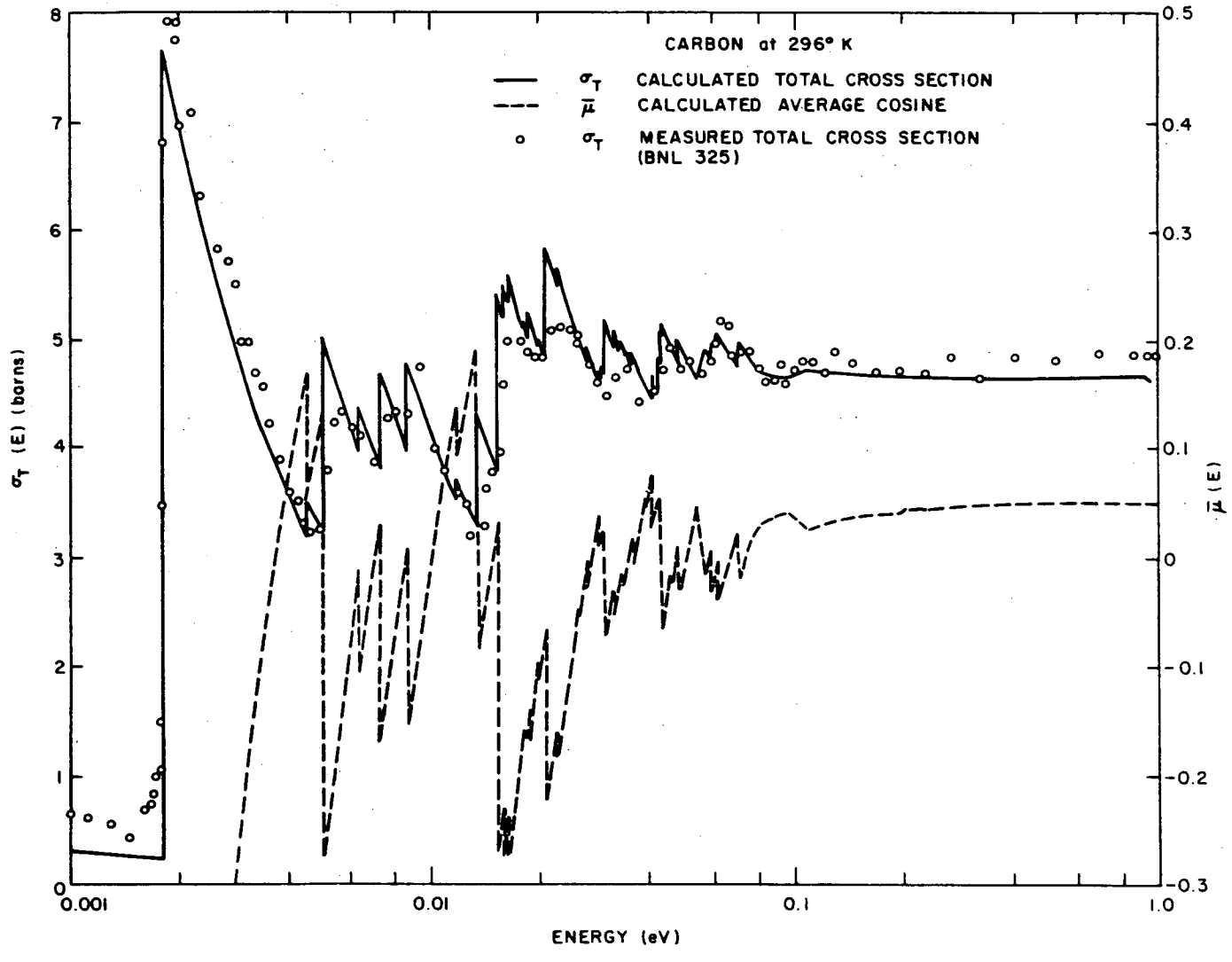
DATA FOR GRAPHITE AT 296 DEGREES K.

| | 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 | 4.68238 | .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
$\sigma_T$ CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
$\sigma_T$ MEASURED TOTAL CROSS SECTION (BNL 325)
$\sigma_T$ (E) (barns)
$\bar{\mu}$ (E)
ENERGY (eV)
0.001
0.01
0.1
1.0
0
1
2
3
4
5
6
7
8
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5

## 6. Miscellaneous Notes on Graphite

For temperatures other than 296°K the switching criteria for short collision and the $\alpha, \beta$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 | 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 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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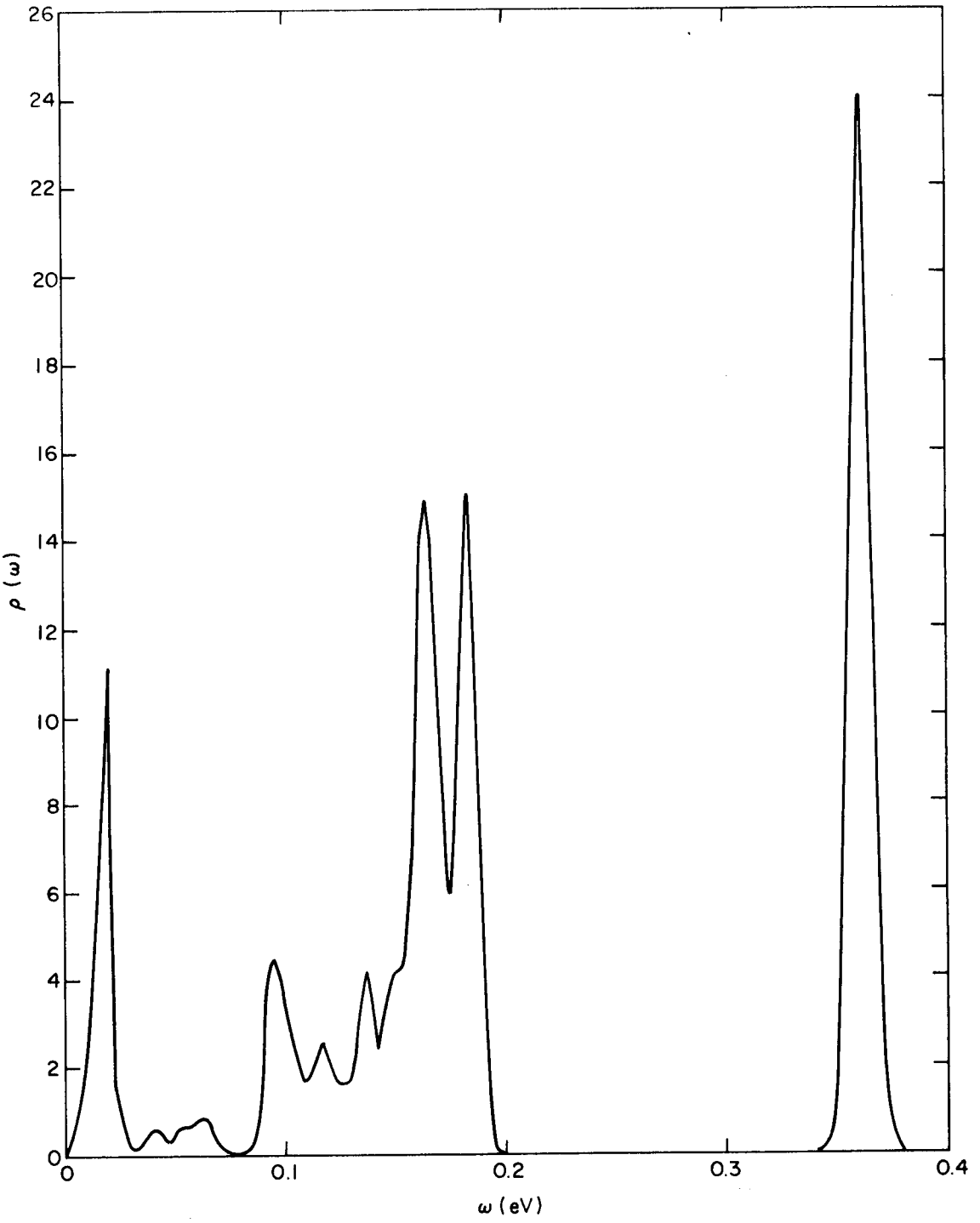
[1] T. P. Lin and J. L. Koenig, J. Molec. Spectra, 9, 228 (1962).

[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 | | | | | |

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

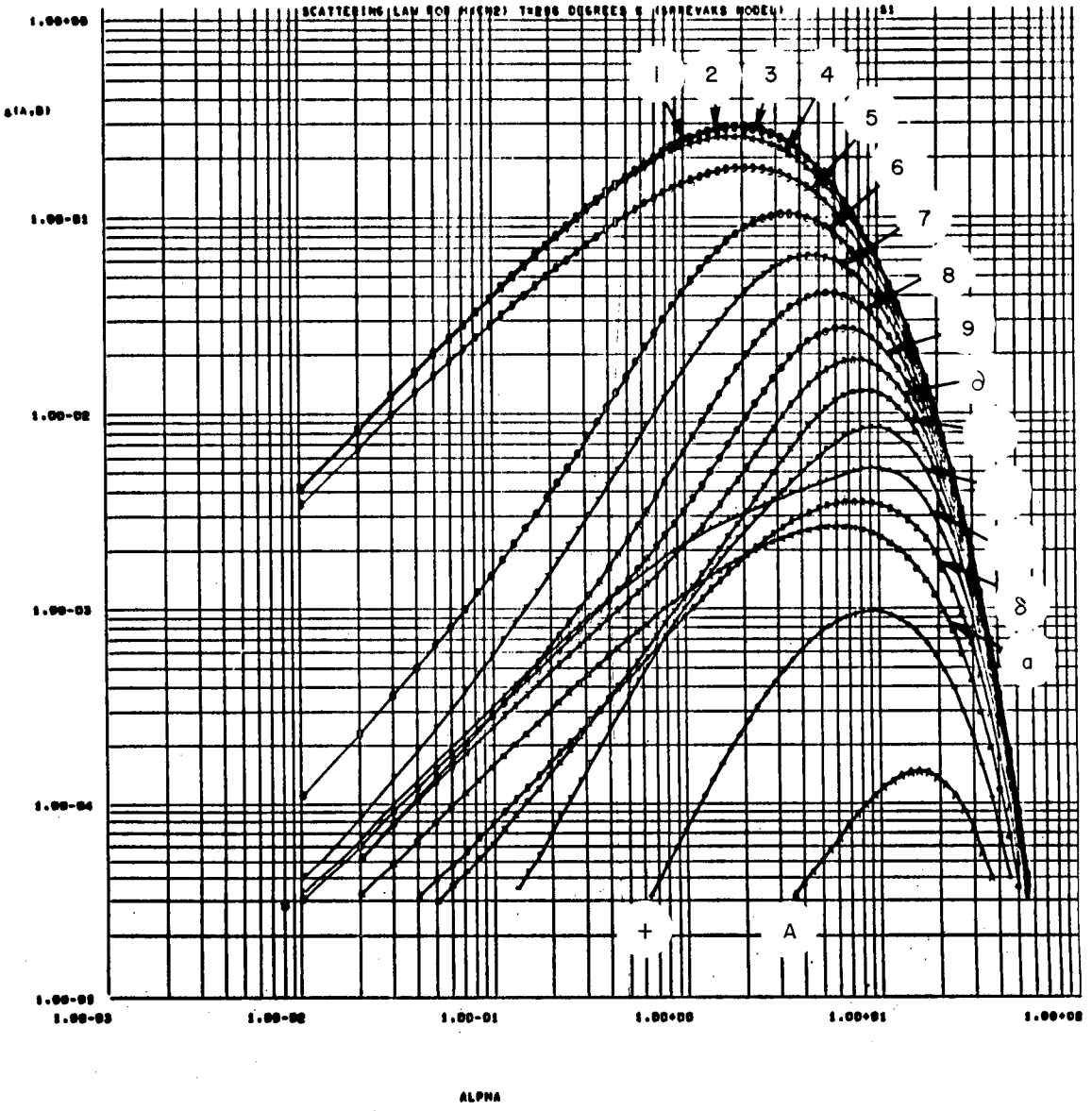
The code GAKER is discussed in Section A. 3. The data tabulated below follows the format of the code input instruction also given in Section A. 3. The code symbols used below are defined in the code input section. If no value is entered for a symbol the corresponding input quantity was not required in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

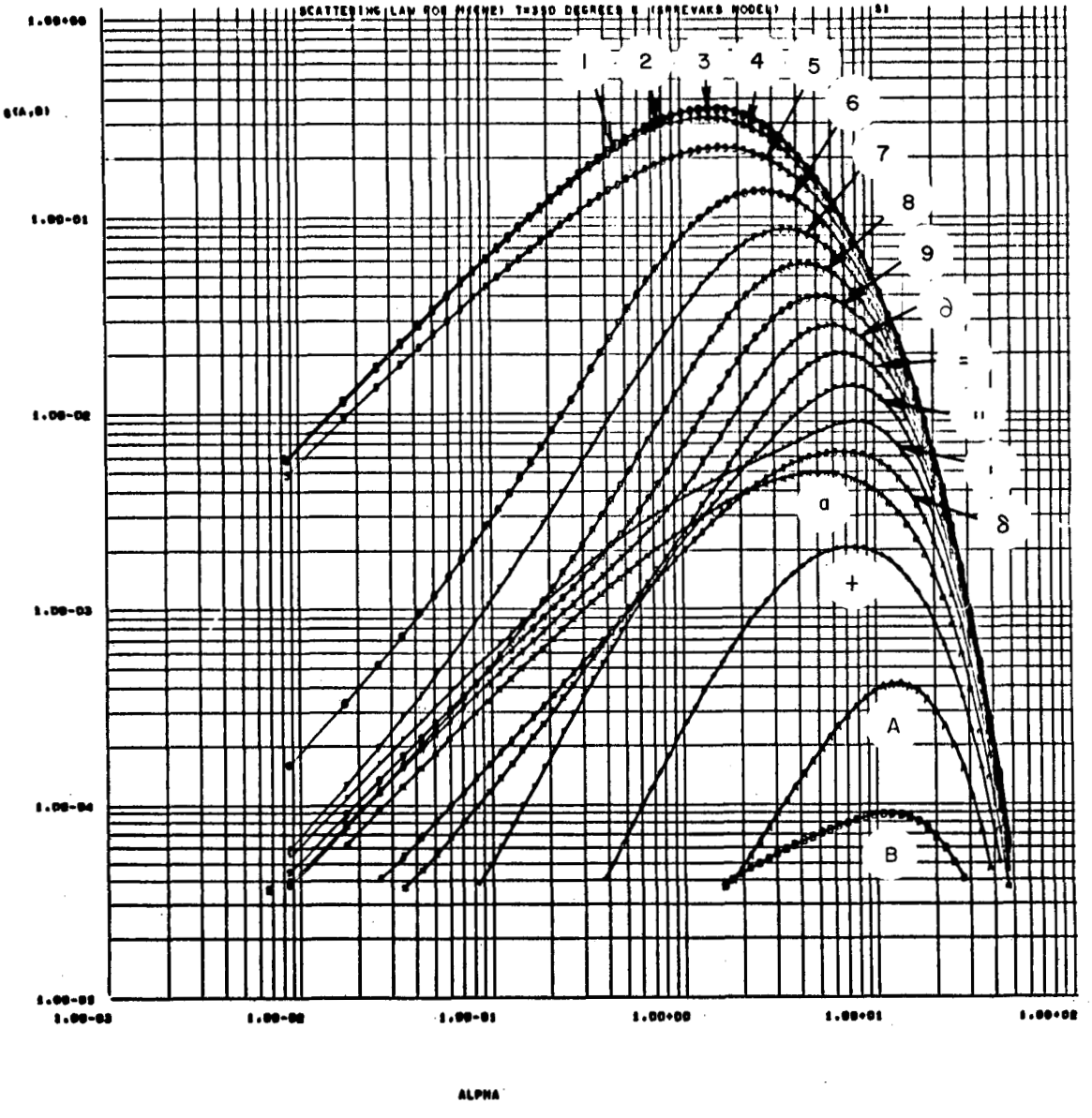
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES |
|---|---|---|
| 1 | 12A6 | HOLREC Poly S(α,β) (Gaker) 296 K |
| 2 | 4I5 | ID -72 NR 3 IBX 120 IZX 80 |
| 3 | 7E10 | T 1.0079 EC1 6.66667 EC2 12.941 SIGF 20.36 EPS 1.0-6 |
| | | EMAX 1.0 AMASS1.008 |
| 4 | 4E10 | RT .0255 MT 14.0 MR 12.92 WR .089 |
| 5 | 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 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 |


1.00+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
1.00+01
1.00+02
ALPHA
1
2
3
4
5
6
7
8
9
∂
δ
a
+
A


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
1.00+01
1.00+02
ALPHA
1
2
3
4
5
6
7
8
9
∂
=
a
δ
+
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).

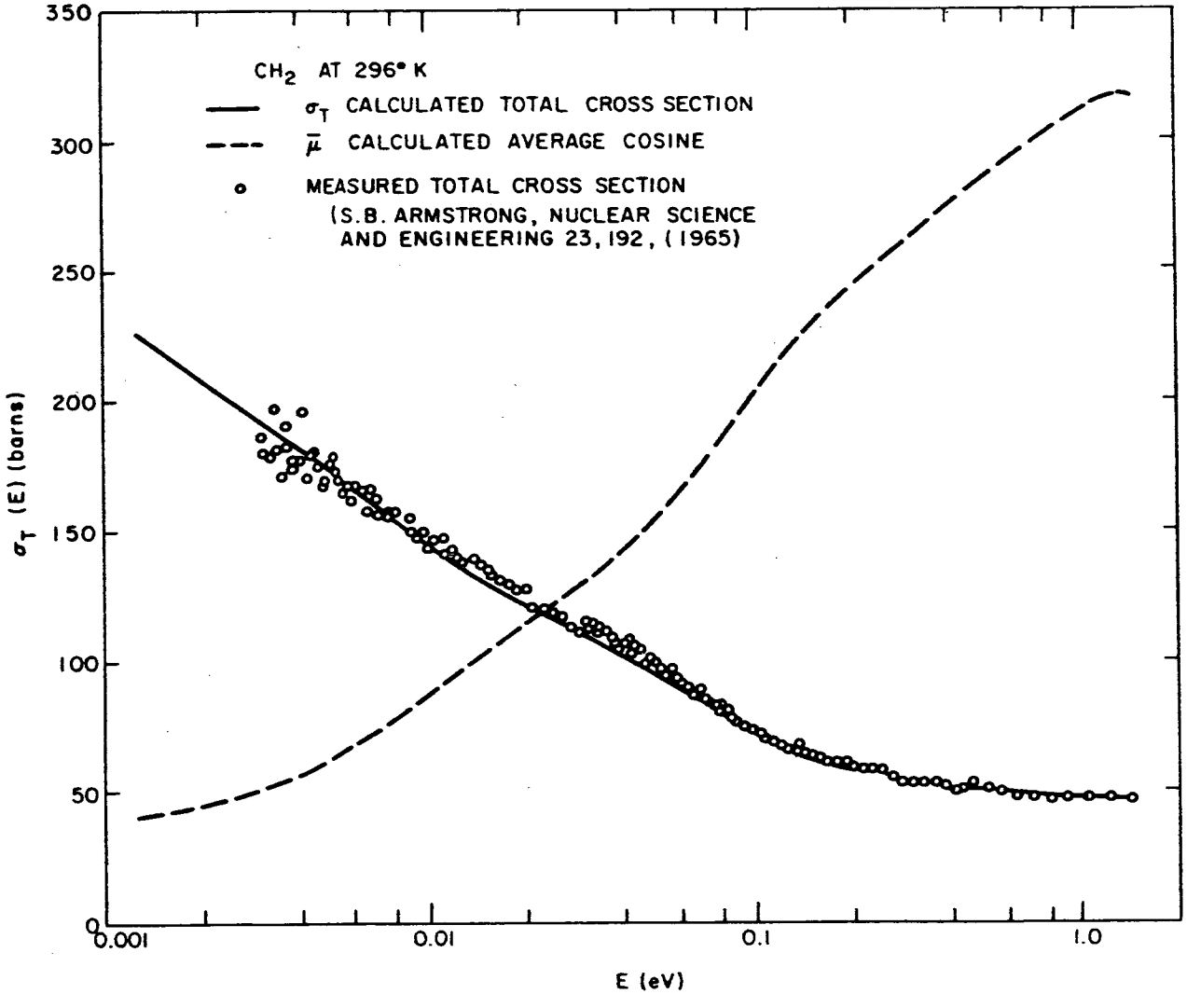
DATA FOR $CH_2$ AT 296 DEGREES K.

| | 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 | -.01586 | 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 | 184.84762 | .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 | .49198 |
| 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 (SIGO) FOR THE CARBON ATOM. ALSO FOR THE CARBON, 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 | 1.5 EV |


CH2 AT 296° K
σT CALCULATED TOTAL CROSS SECTION
μ̄ CALCULATED AVERAGE COSINE
MEASURED TOTAL CROSS SECTION
(S.B. ARMSTRONG, NUCLEAR SCIENCE AND ENGINEERING 23, 192, (1965)
σT (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 $\alpha, \beta$ 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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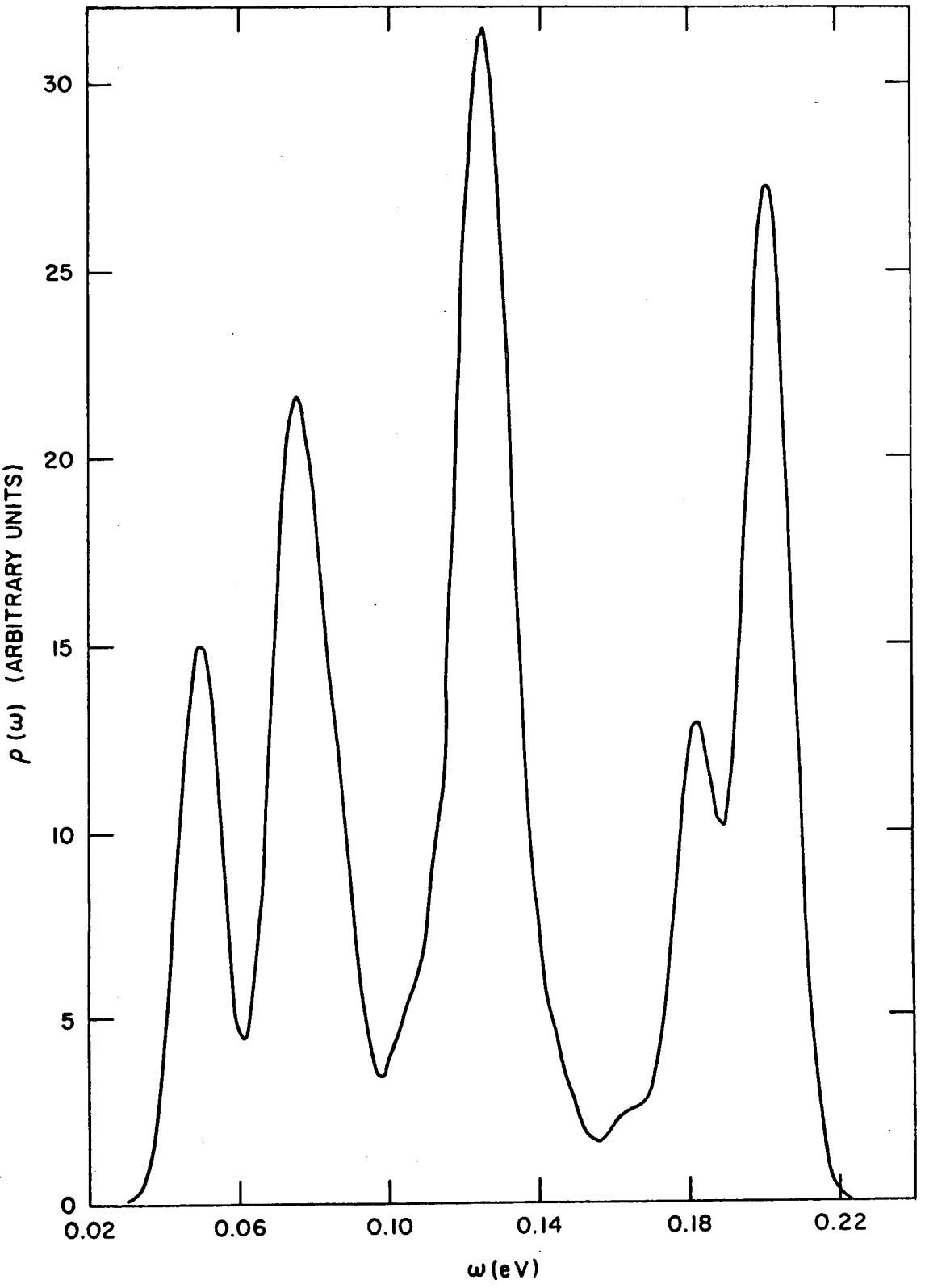
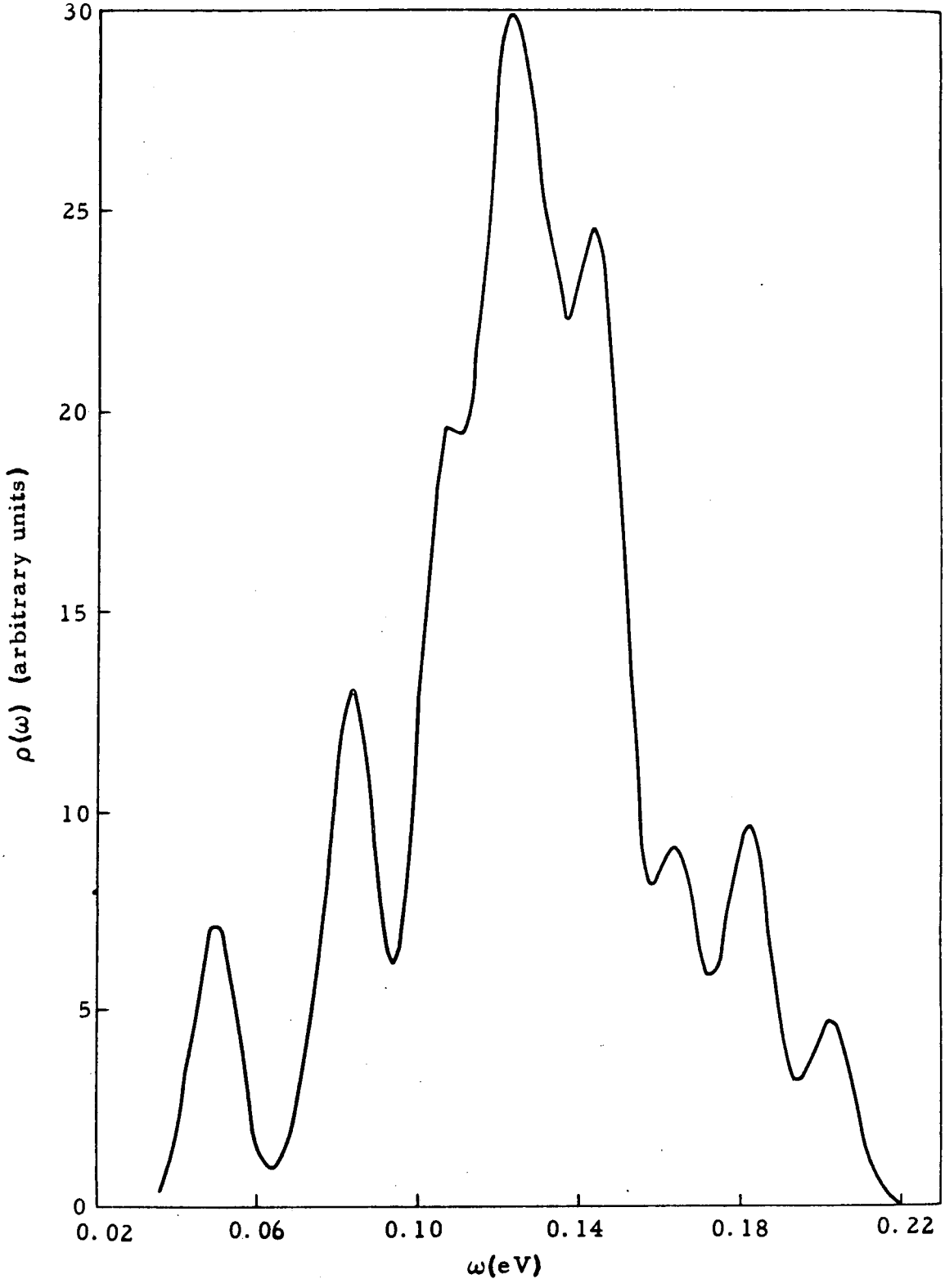
[1] D. Sprevak, G. M. Borgonovi, J. M. Neill and G. W. Carriveau, Nukleonik, 11, 233 (1968).

[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.)




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 | W1.0477543 W2. 0.0 W3.65331978 W4 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.

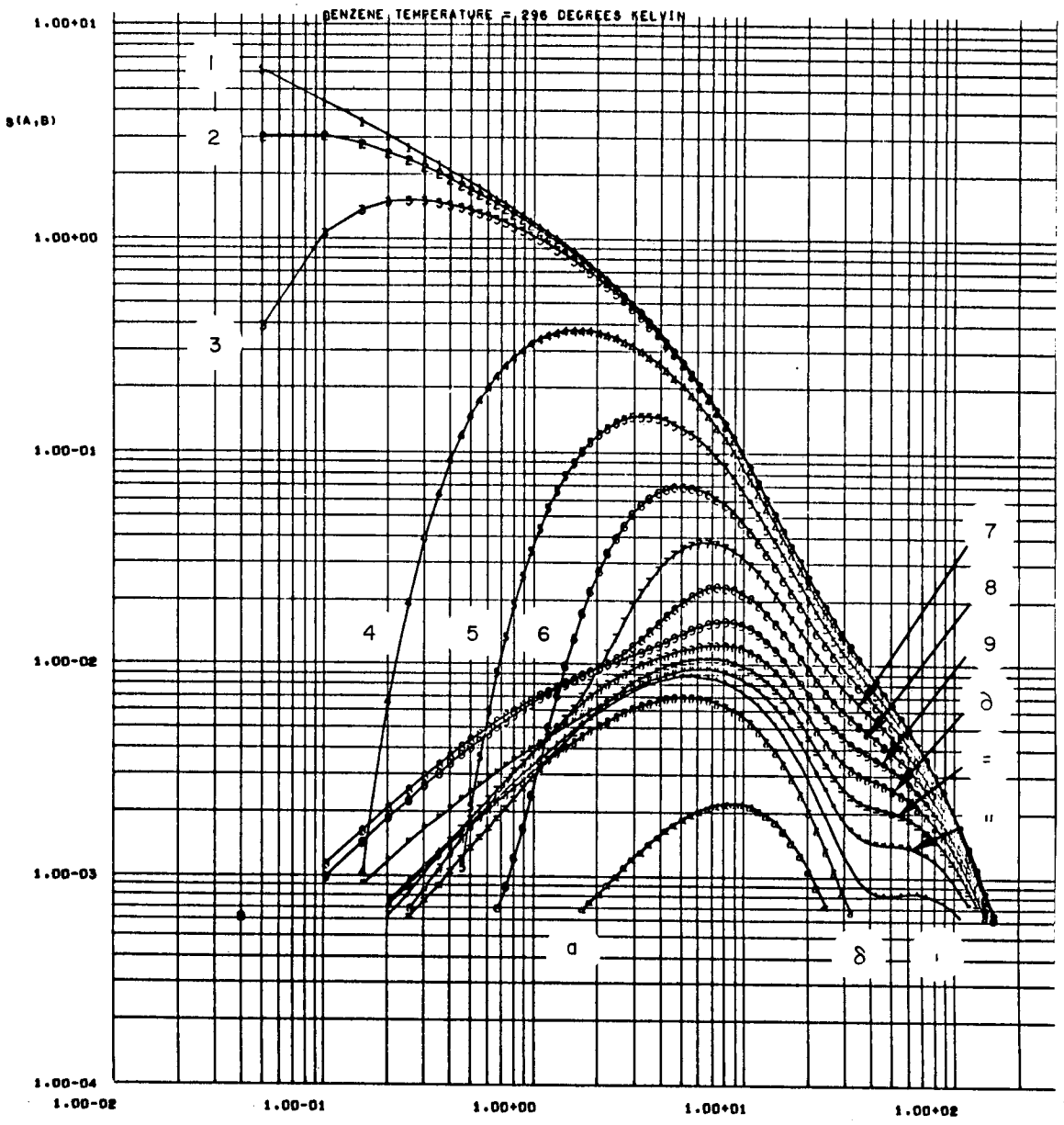
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES |
|---|---|---|
| 1 | 13A6, A2 | COM Sprevak's $C(C_6H_6)$ at 296 degrees K. |
| 2 | 11I5 | NT -5 NP 80 NE 80 NDAM 0 NGPRT 0 |
| | | NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0 |
| | | IPG 0 |
| 3 | 3I5 | JS3 86 JS4 0 JS5 1 |
| 4 | 5E10 | W1.2848568 W2 0.0 W3.6799013 W4 0.0 W5 .03524188 |
| 5 | 6E10 | T1 .0255 T2 0.0 T3 .0255 T4 0.0 T5 .0255 |
| 6 | 7E10 | AM 12.011DC BETSW ALPSW CRIT1 |
| | | CRIT2 CRIT3 |
| | | X3. .0210766 .024796 .0272756 .0297552 .0322348 .0359542 |
| | | .0384338 .0409134 .0433930 .0458726 .0483522 .0508318 |
| | | .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 |

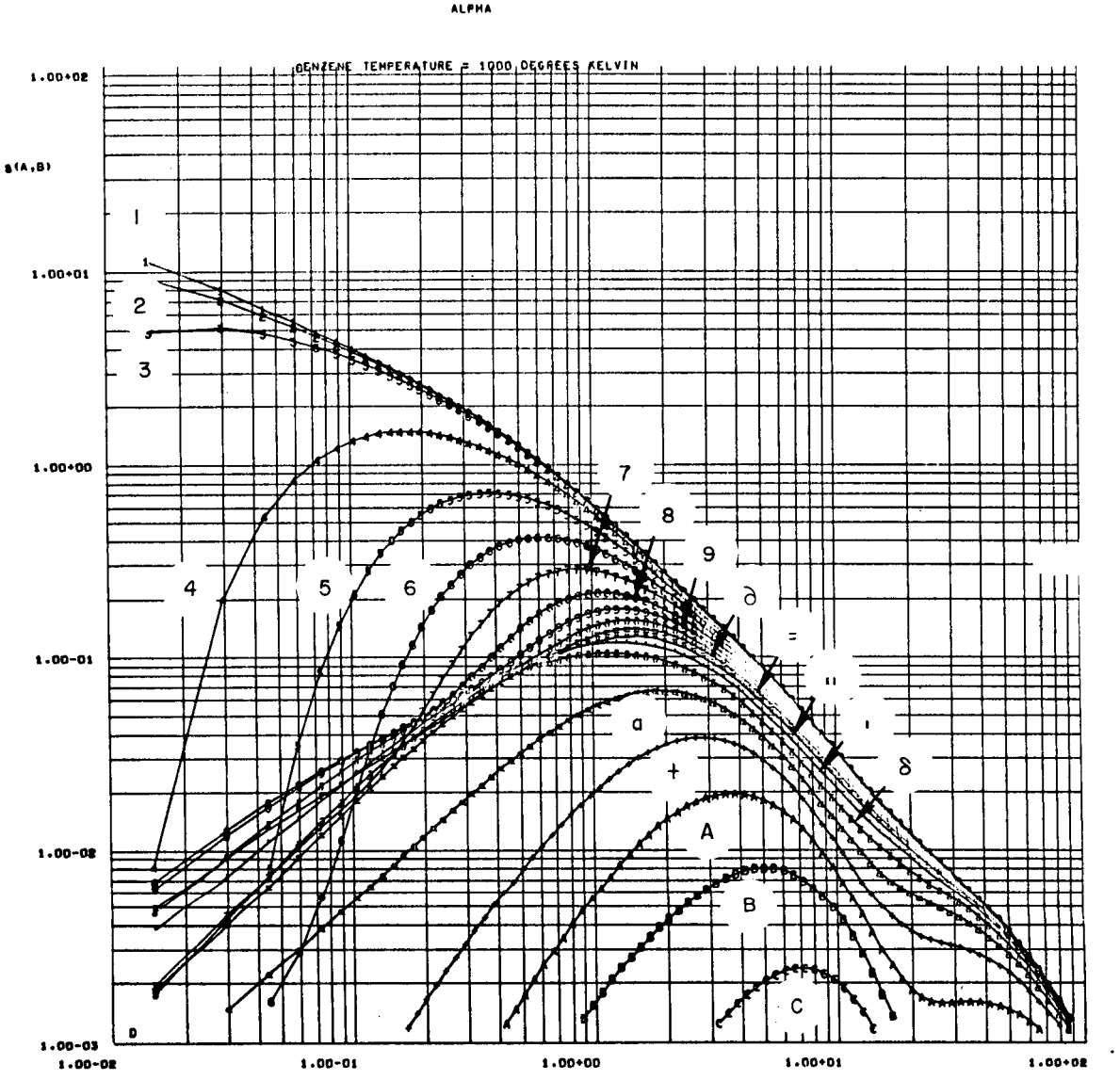
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES |
|---|---|---|
| 8 | 7E10 | Q3 .0001394 .002276 .0118288 .0518248 .191408 .986323 |
| | | 2.37689 4.82867 8.26939 11.9386 14.5310 14.9158 |
| | | 12.9363 9.57165 6.34166 4.55398 4.94717 7.64850 |
| | | 12.08790 16.9292 20.4759 21.6053 20.4665 18.1607 |
| | | 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


ALPHA
BENZENE TEMPERATURE = 1000 DEGREES KELVIN
1.00+02
S(A,B)
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
D

## 5. INTEGRAL DATA

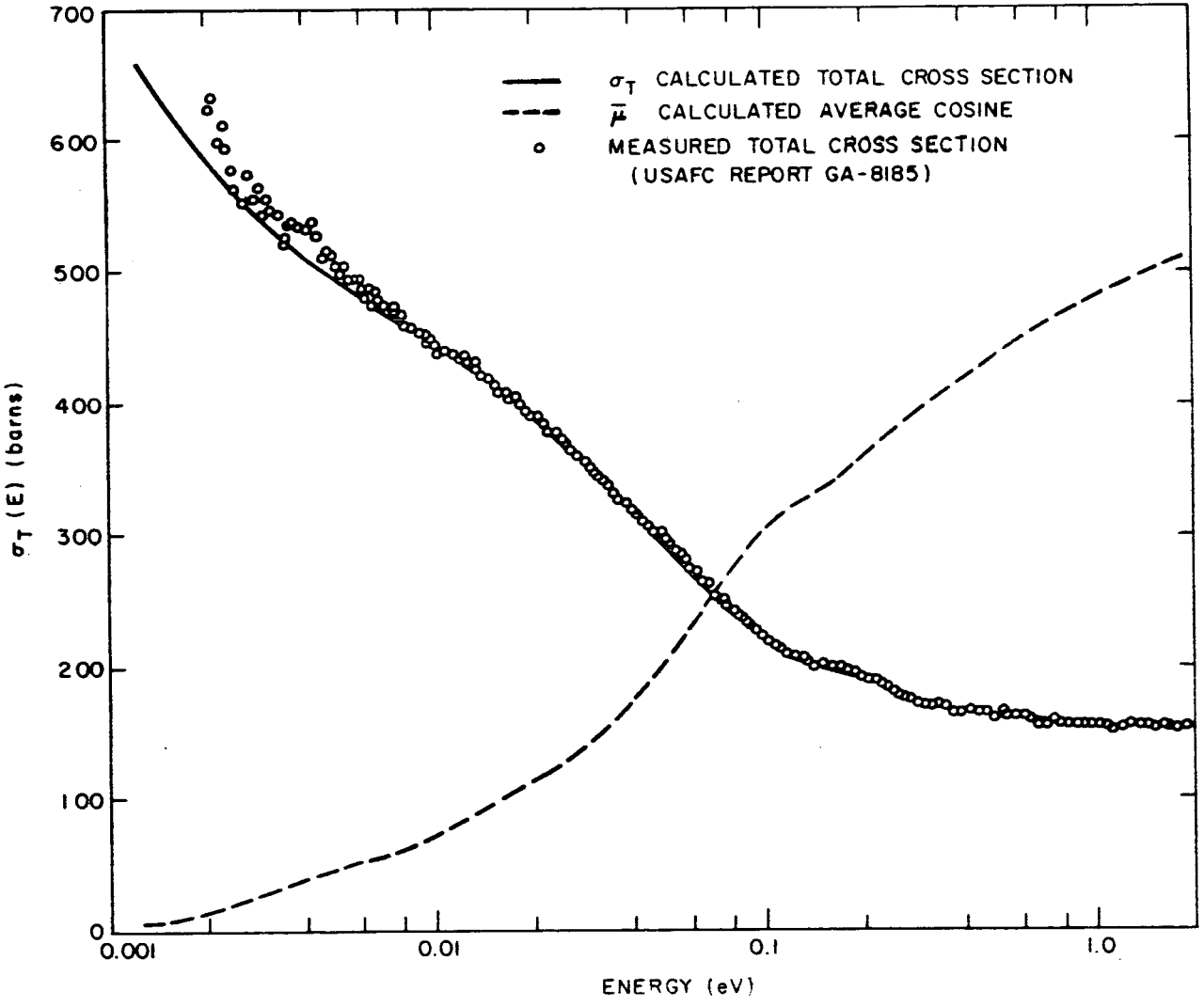
TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR $C_6H_6$ 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 |


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

## 6. Miscellaneous Notes on Benzene

For temperatures other than 296°K the switching criteria for short collision and the $\alpha, \beta$ 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 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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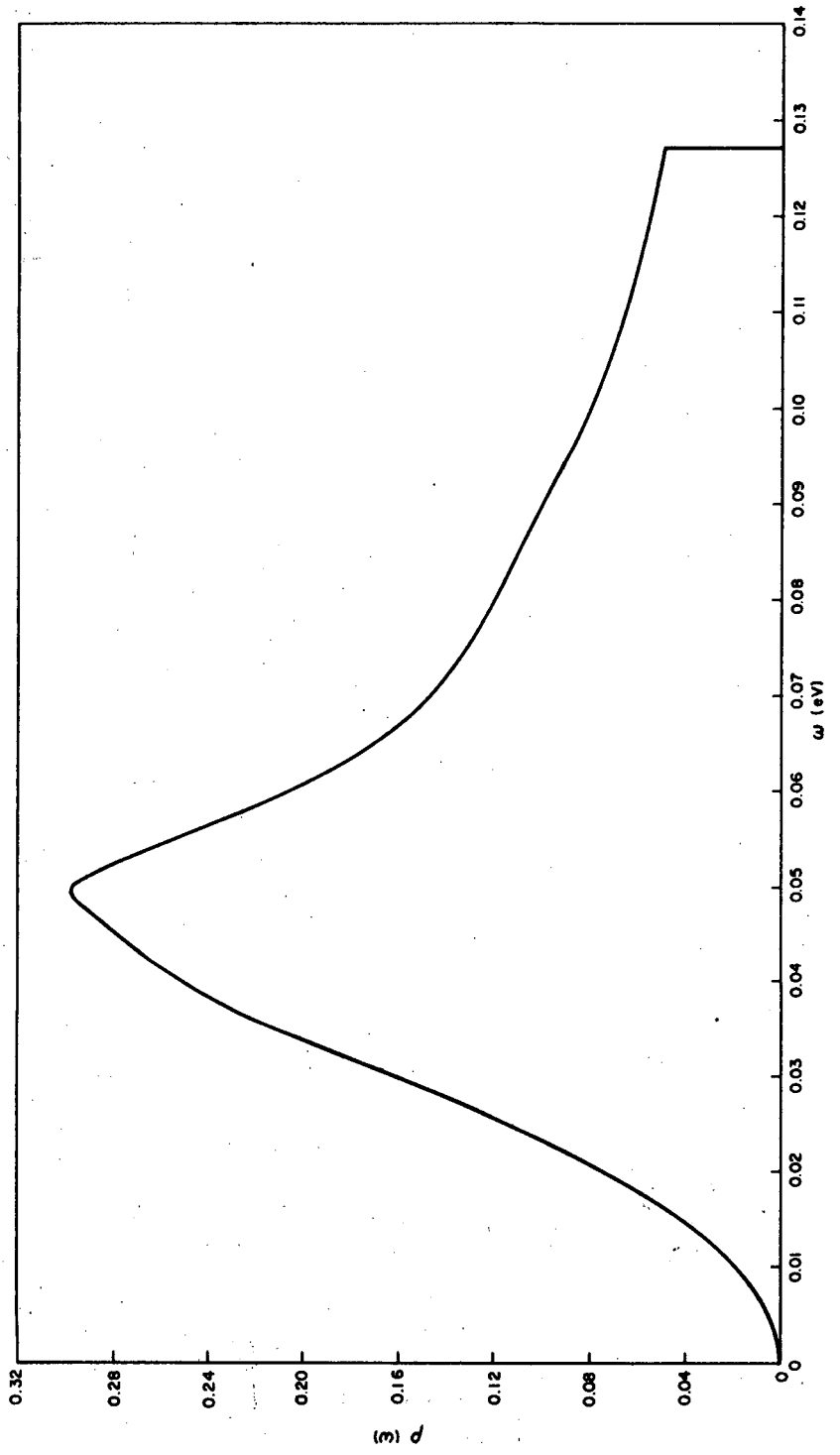
(1) J.U. Koppel and J.A. Young, Nukleonik, 7, 408 (1965).

(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 $\alpha$ 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.

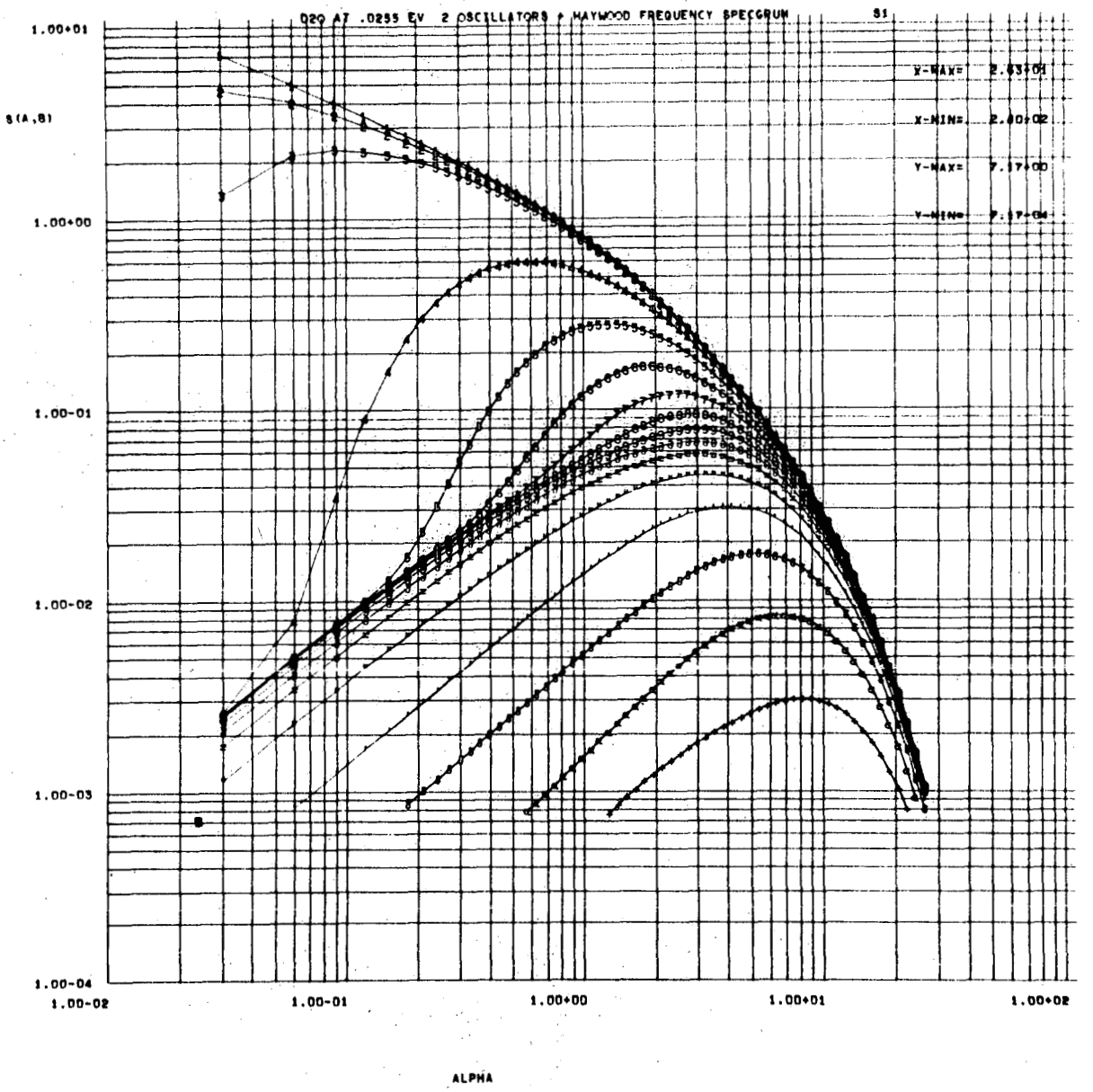
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES |
|---|---|---|
| 1 | 13A6,A2 | COM $D_2O$ - 2 OSC. + Haywood Freq. Spectrum |
| 2 | 11I5 | NT -6 NP 80 NE 80 NDAM 0 NGPRT 0 |
| | | NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0 |
| | | IPG 0 |
| 3 | 3I5 | JS3 -51 JS4 0 JS5 2 |
| 4 | 5E10 | W1 .05 W2 0.0 W3 .45 W4 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 |

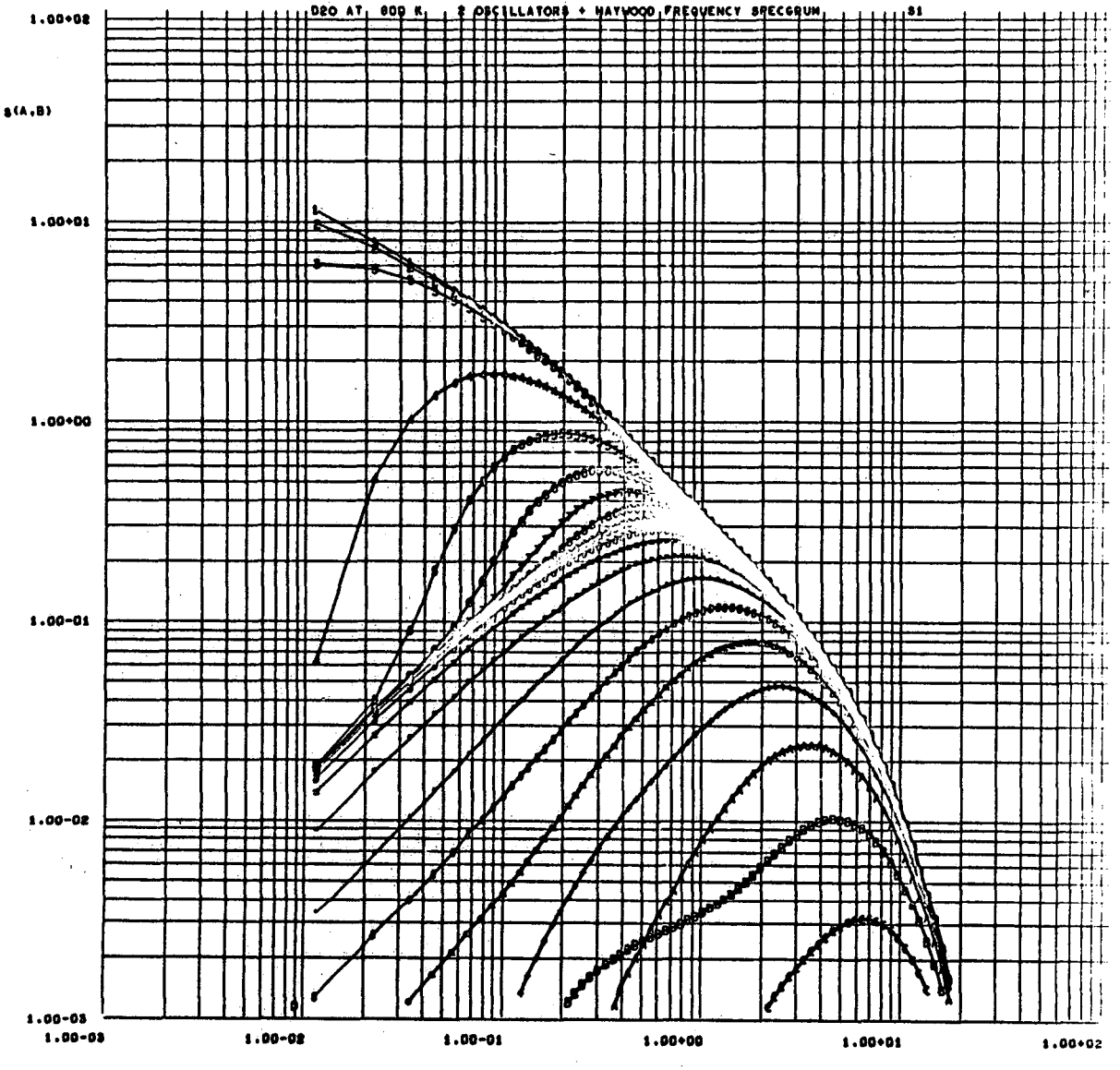
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES |
|---|---|---|
| 8 | 7E10 | Q3 .0012 .0048 .0108 .0192 .03 .0432 |
| | | .0588 .0768 .0972 .12 .142 .17 |
| | | .195 .217 .24 .256 .27 .282 |
| | | .294 .291 .271 .245 .22 .20 |
| | | .178 .166 .153 .143 .135 .128 |
| | | .122 .118 .112 .106 .101 .098 |
| | | .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<br>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 .0255 EV 2 OSCILLATORS + HAYWOOD FREQUENCY SPECTRUM
S1
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
X-MAX= 2.03+01
X-MIN= 2.00+02
Y-MAX= 7.17+00
Y-MIN= 7.17-04


D2O AT 600 K, 2 OSCILLATORS + HAYWOOD FREQUENCY SPECTRUM
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).

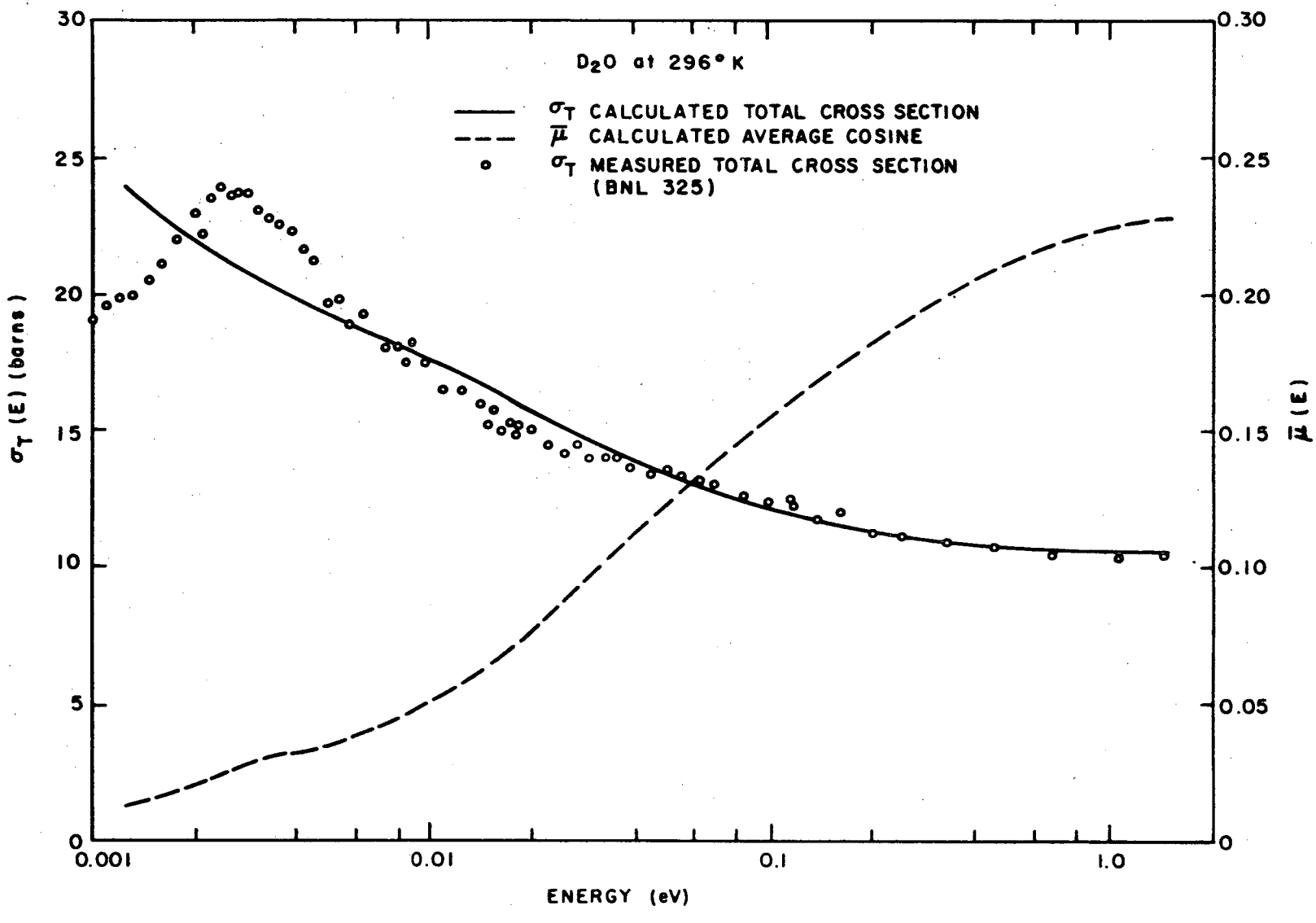
DATA FOR D2O AT 296 DEGREES K.

| | 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 |


D2O at 296° K
σT CALCULATED TOTAL CROSS SECTION
μ̄ CALCULATED AVERAGE COSINE
σT MEASURED TOTAL CROSS SECTION
(BNL 325)
σT (E) (barns)
μ̄ (E)
ENERGY (eV)
0.001
0.01
0.1
1.0
0
5
10
15
20
25
30
0.05
0.10
0.15
0.20
0.25
0.30

## 6. Miscellaneous Notes on $D_2O$

For temperatures other than 296°K the switching criteria for short collision and the $\alpha,\beta$ 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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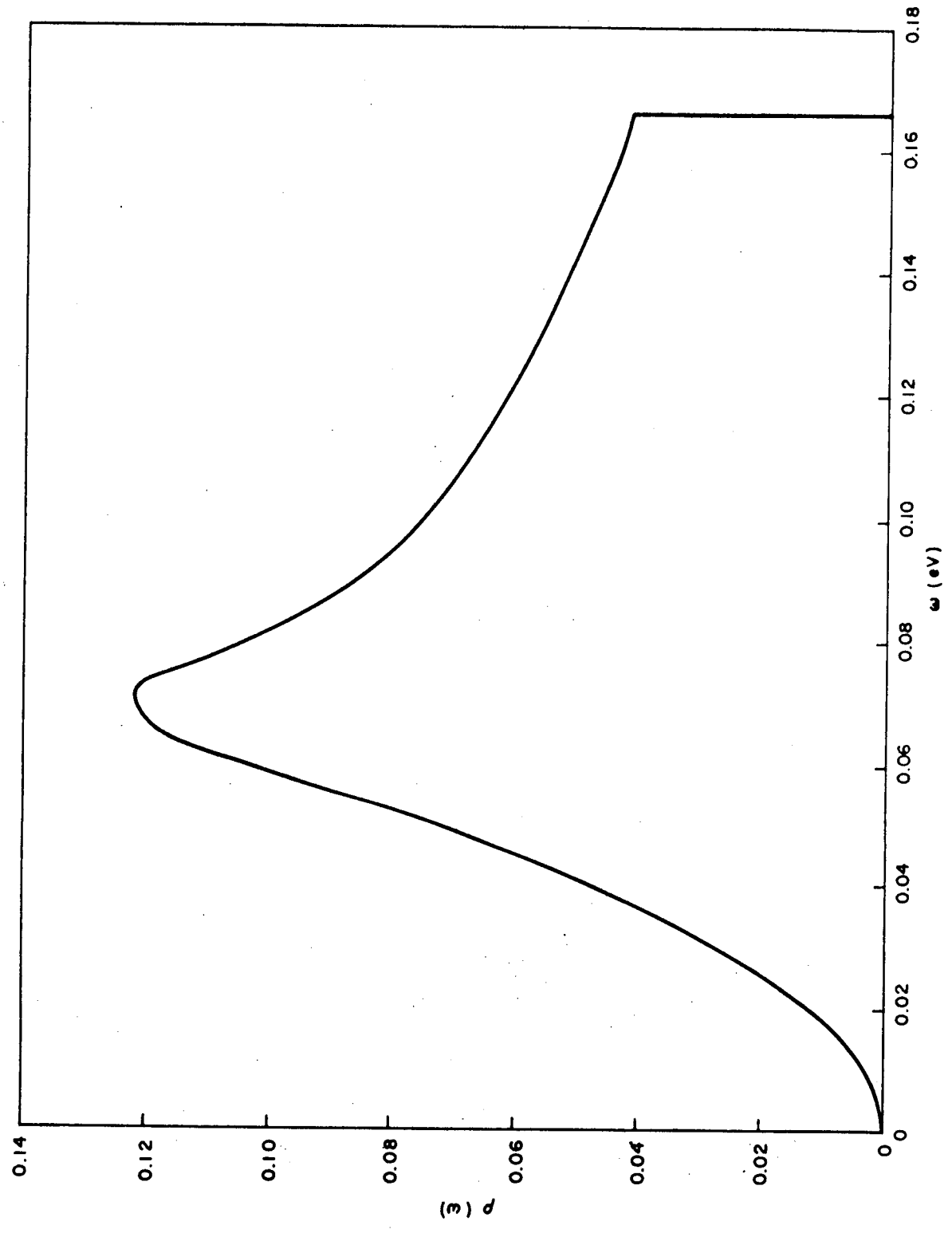
[1] M.S. Nelkin, Phys. Rev. 119, 741 (1960).

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 $\alpha$ values for the oxygen must be 1.008/16 times the $\alpha$ values for the hydrogen data, in order to correspond to the same neutron momentum transfer $\kappa$.

---

[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 $H(H_2O)$



## 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.

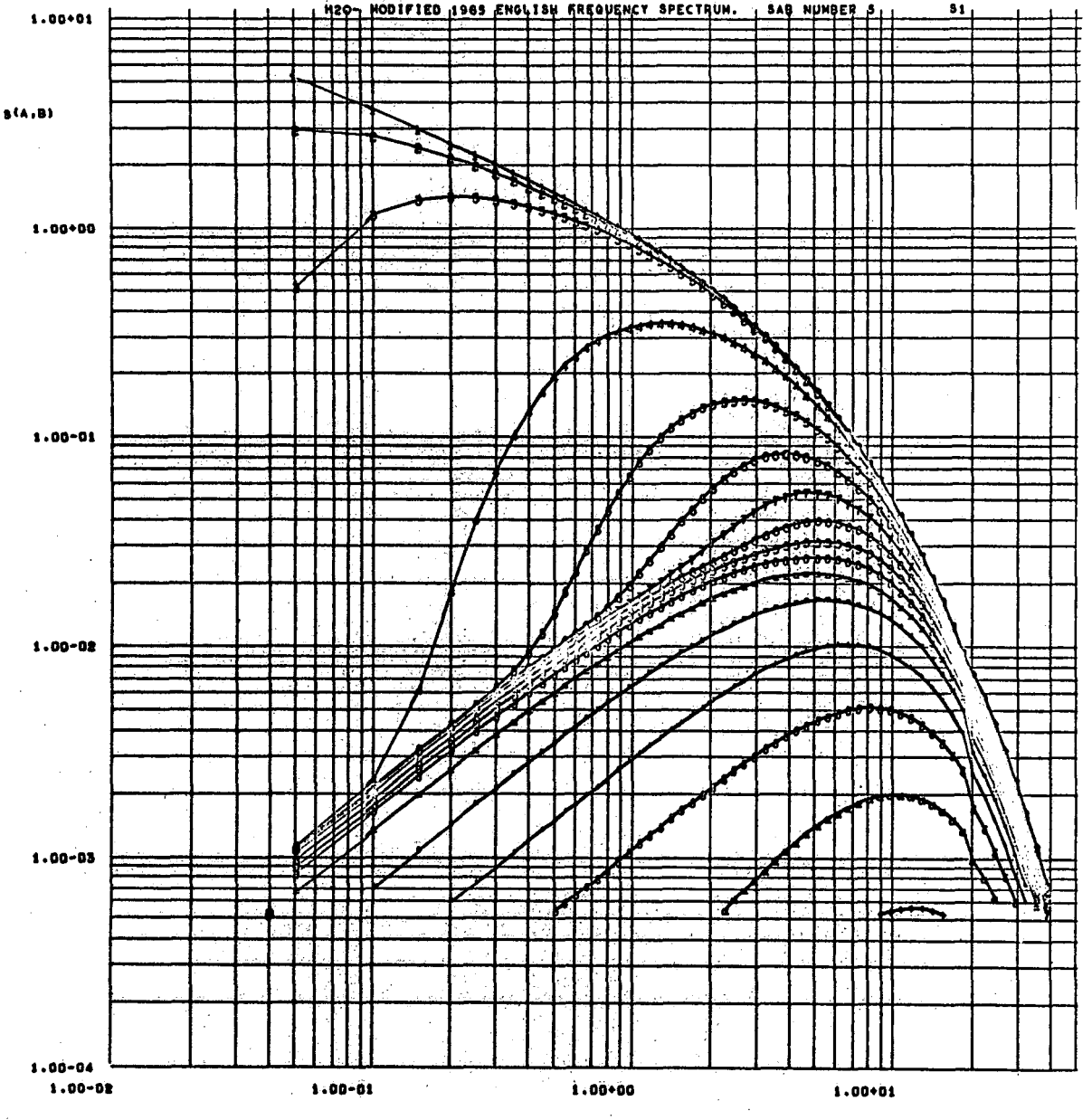
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES |
|---|---|---|
| 1 | 13A6,A2 | COM $H_2O$ - Modified 1965 English Freq Spectrum |
| 2 | 11I5 | NT -5 NP 80 NE 80 NDAM 0 NGPRT 0 |
| | | NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0 |
| | | IPG 0 |
| 3 | 3I5 | JS3 29 JS4 0 JS5 2 |
| 4 | 5E10 | W1 .0555556 W2 0.0 W3 .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 |

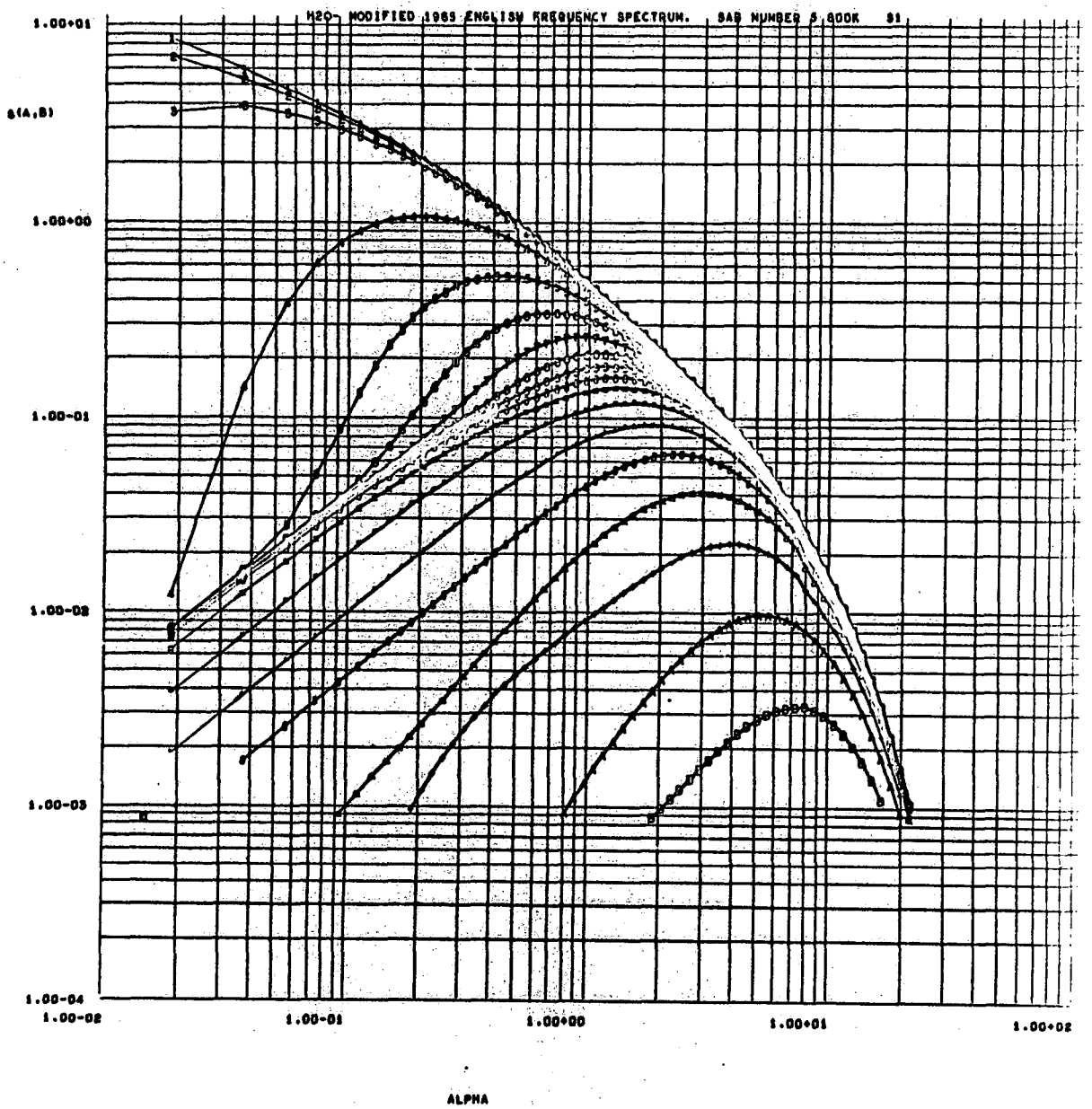
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES |
|---|---|---|
| 8 | 7E10.0 | Q3 .00125 .005 .01125 .02 .03125 .045 |
| | | .059 .075 .095 .115 .1197 .1214 |
| | | .1218 .1195 .1125 .0975 .0871 .0791 |
| | | .0735 .0688 .065 .061 .0571 .054 |
| | | .0515 .0488 .0459 .0431 .042 |
| 9 | Cards 9 and 10 are 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 1963 ENGLISH FREQUENCY SPECTRUM. SAB NUMBER 5 51
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
ALPHA


H2O - MODIFIED 1985 ENGLISH FREQUENCY SPECTRUM. SAB NUMBER 5 BOOK 91
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
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).

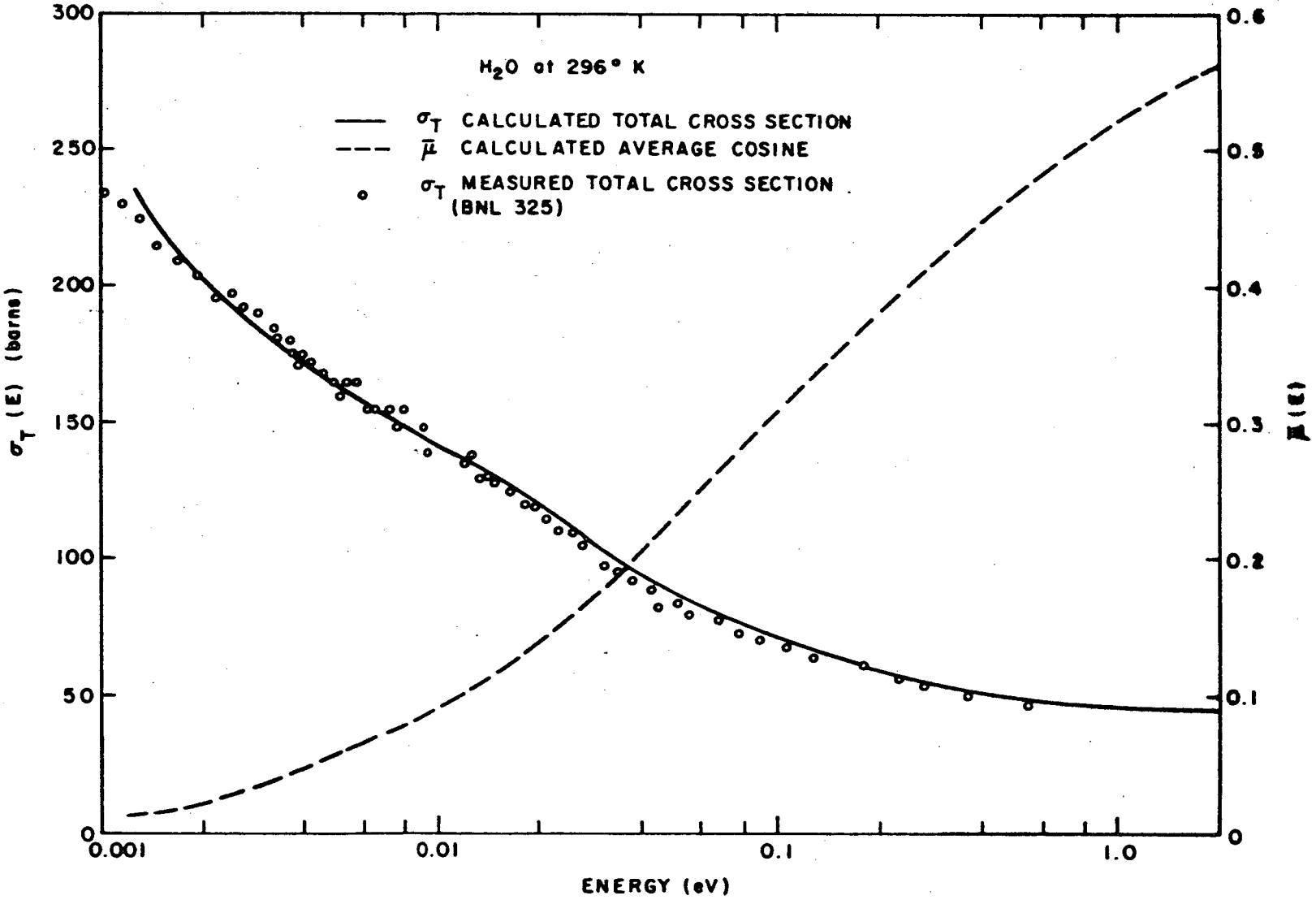
DATA FOR H2O AT 296 DEGREES K.

| | 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 (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 | 2.0 EV |


$H_2O$ at 296° K
$\sigma_T$ CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
$\sigma_T$ MEASURED TOTAL CROSS SECTION (BNL 325)
$\sigma_T$ (E) (barns)
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 $\alpha,\beta$ 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 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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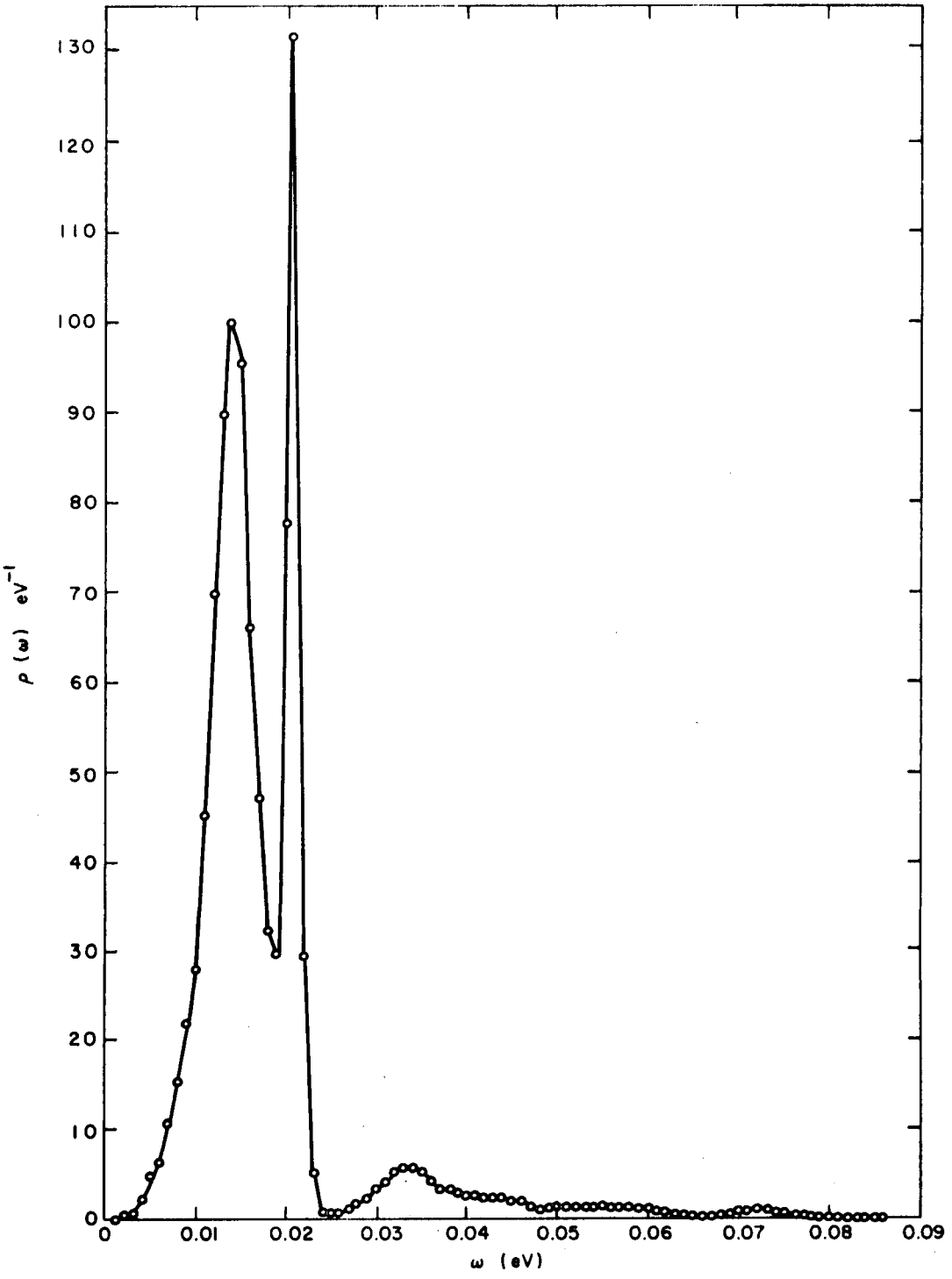
(1) E. L. Slaggie, et al., "Integral Neutron Thermalization, Annual Summary Report, October 1, 1968 through September 30, 1969," USAEC Report GA-9753, Gulf General Atomic Incorporated (1969).

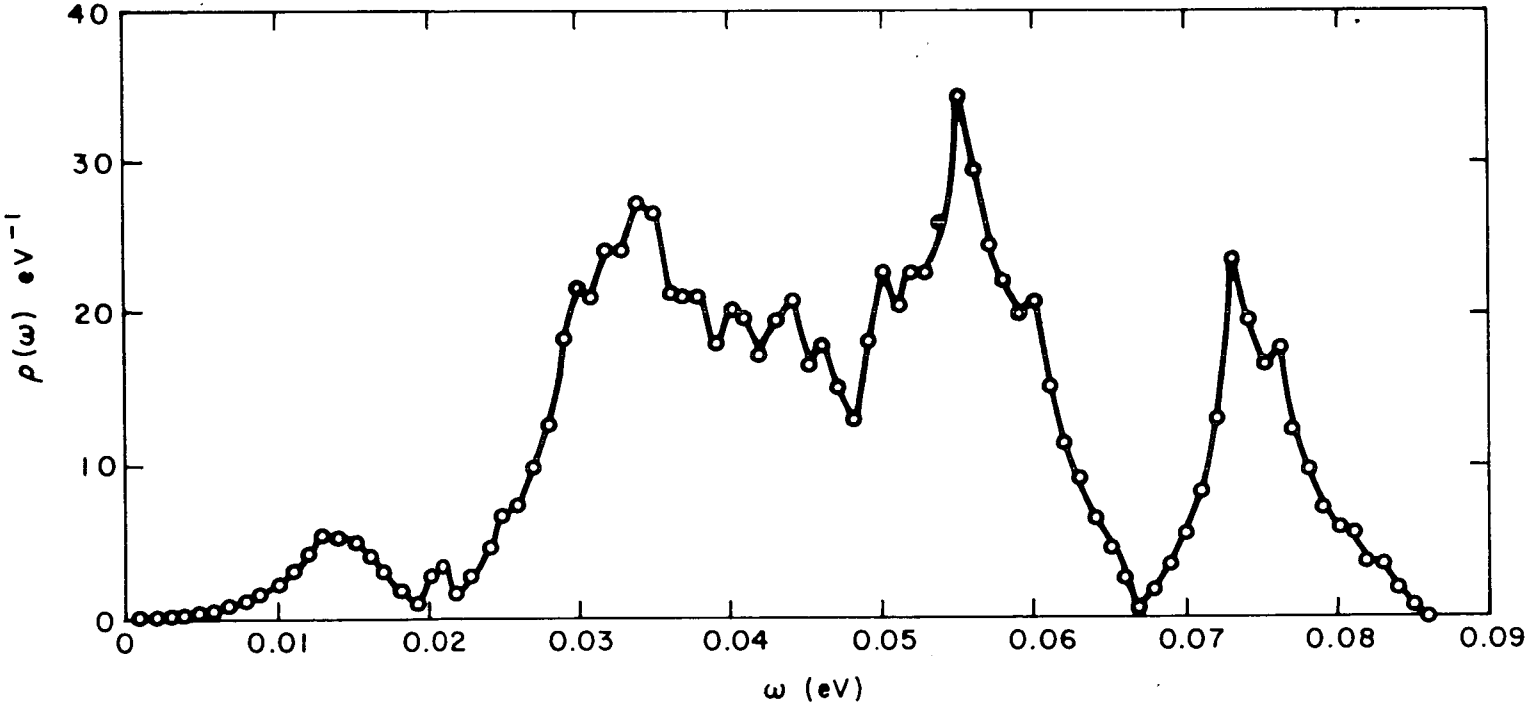
(2) G. Dolling, R. A. Cowley, and A. D. B. Woods, Can. J. Phys. 43, 1397 (1965).

(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<br>NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0<br>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<br>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.

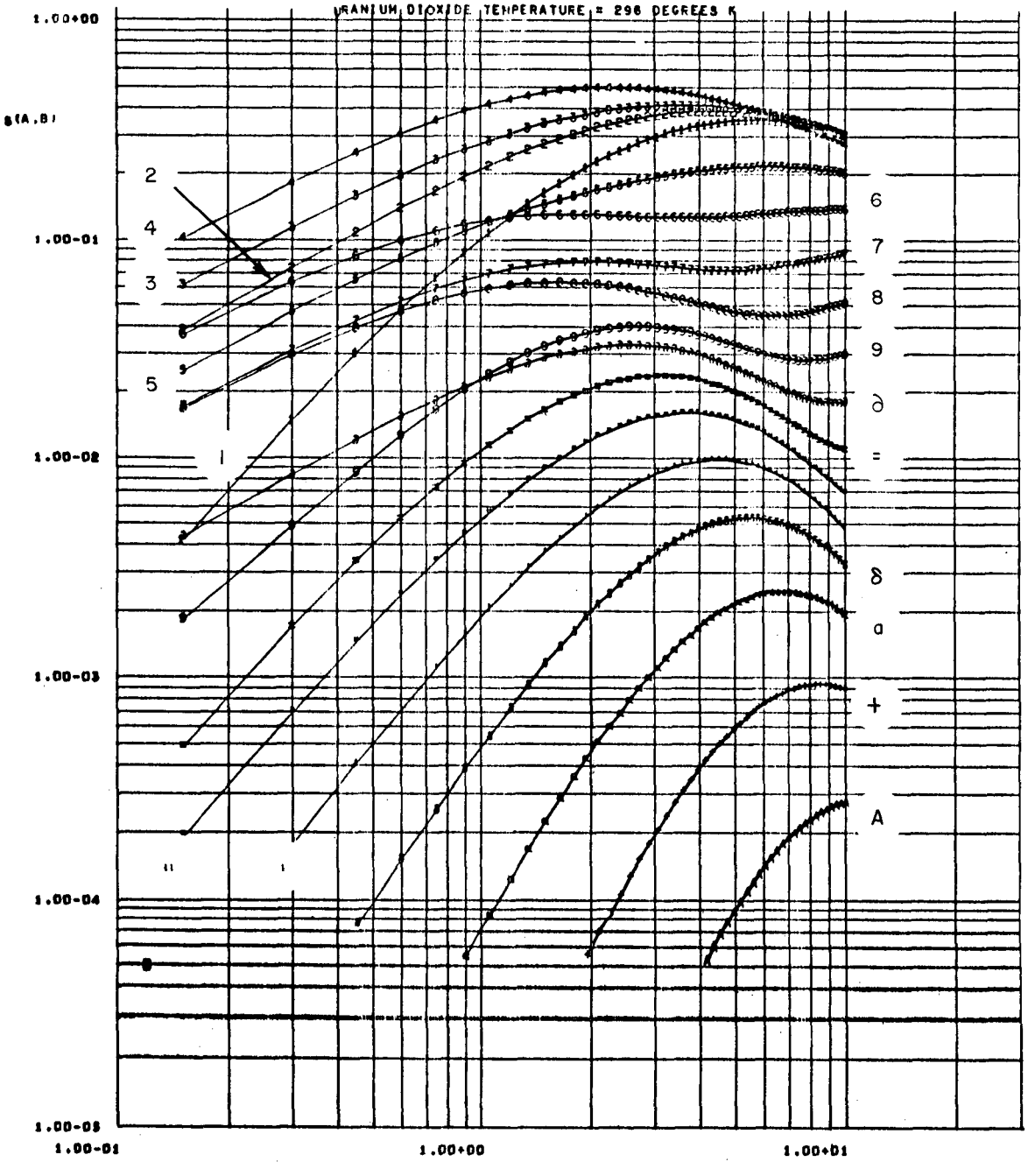
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES |
|---|---|---|
| 1 | 13A6, A2 | COM O in $UO_2$ at 296°K. FCC model. |
| 2 | 11I5 | NT -12 NP 50 NE 80 NDAM 1 NGPRT 0 |
| | | NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0 |
| | | IPG 0 |
| 3 | 3I5 | JS3 -86 JS4 JS5 |
| 4 | 5E10 | W1 .0001 W2 0.0 W3 1.0 W4 W5 |
|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

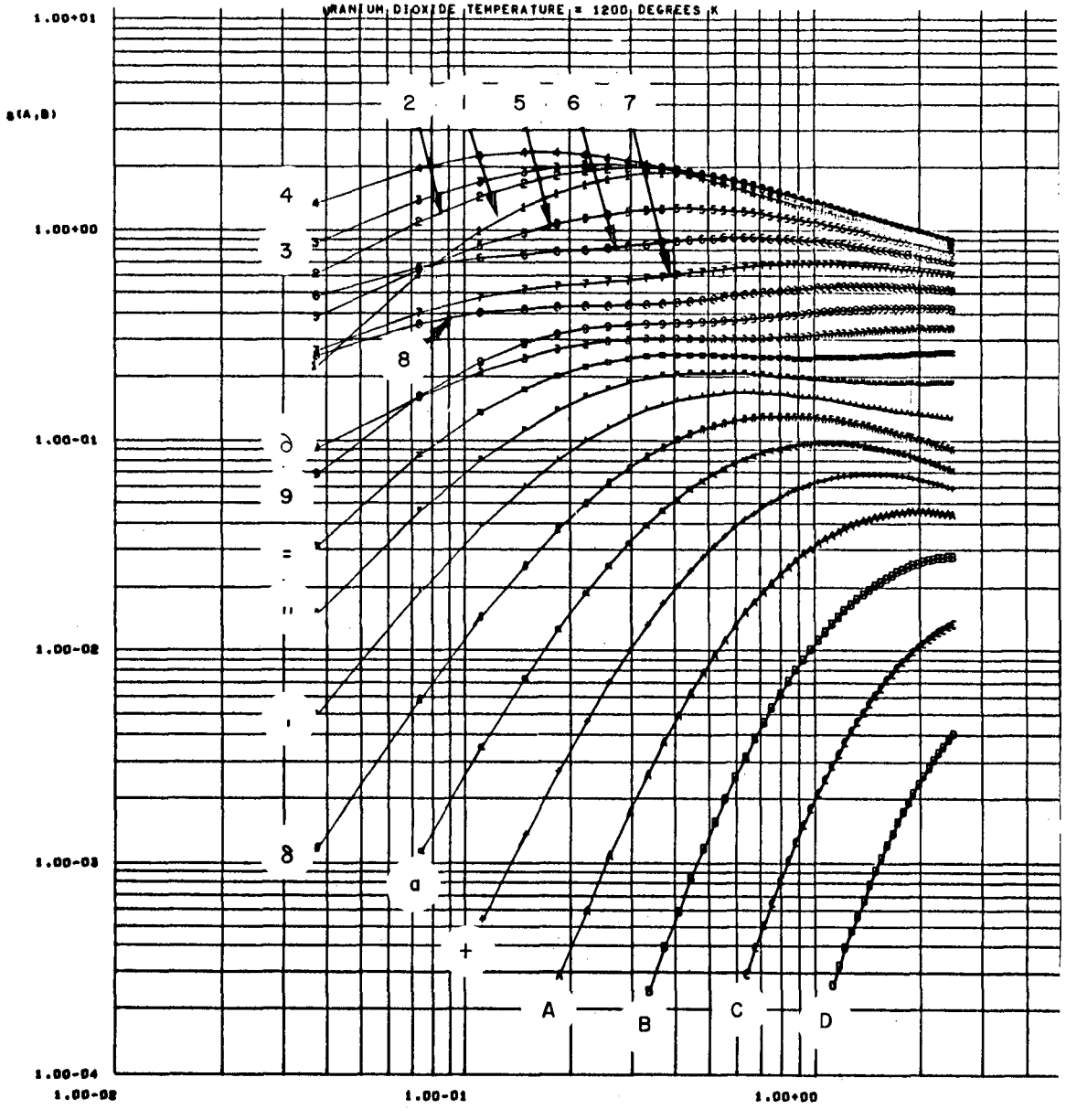
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 8 | 7E10 | Q3 | 0.0 | .031386 | .074139 | .16980 | .34950 | .46484 |
| | | | .78298 | 1.1367 | 1.6674 | 2.0450 | 3.2024 | 4.3883 |
| | | | 5.3794 | 5.3587 | 5.0484 | 4.1062 | 3.0644 | 1.8615 |
| | | | .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
1
2
3
4
5
6
7
8
9
∂
=
δ
a
+
A


URANIUM DIOXIDE 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
S(A,B)
ALPHA
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 | -.74615 | 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 | -.42950 | 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 | -.31831 | 59 | .02989 | 23.31659 | -.06066 |
| 18 | .00906 | 28.49743 | -.19708 | 60 | .03012 | 23.18157 | -.05357 |
| 19 | .01000 | 26.53574 | -.09554 | 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 | .00066 |
| 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 | -.05436 |
| 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 | -.02866 | 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 |

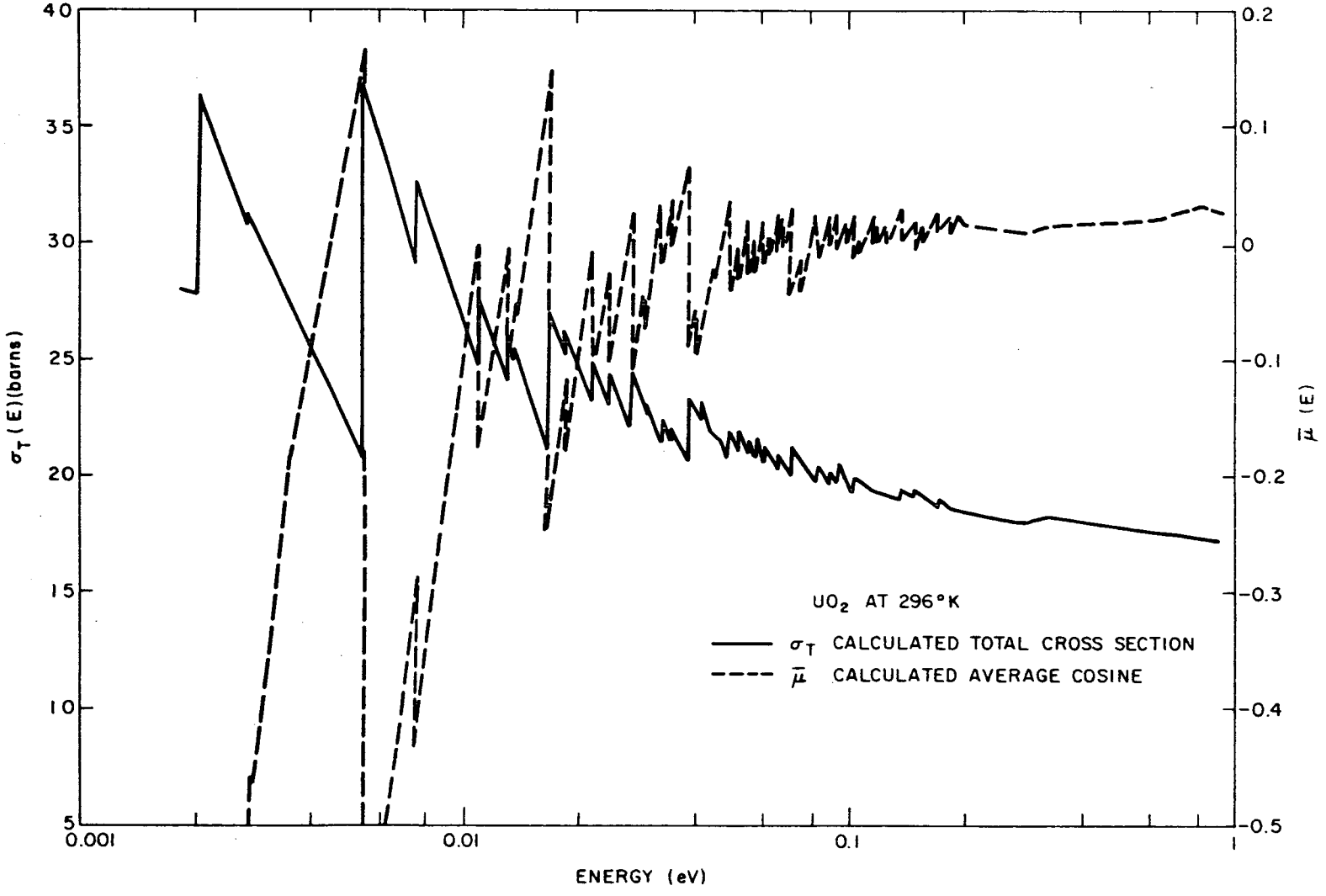
DATA FOR UO2 AT 296 DEGREES K.

| | 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 | .18823 | 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 |


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

## 6. Miscellaneous Notes on Uranium Dioxide

For temperatures other than 296°K the switching criteria for short collision and the $\alpha, \beta$ 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 |

## 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.

---

(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.

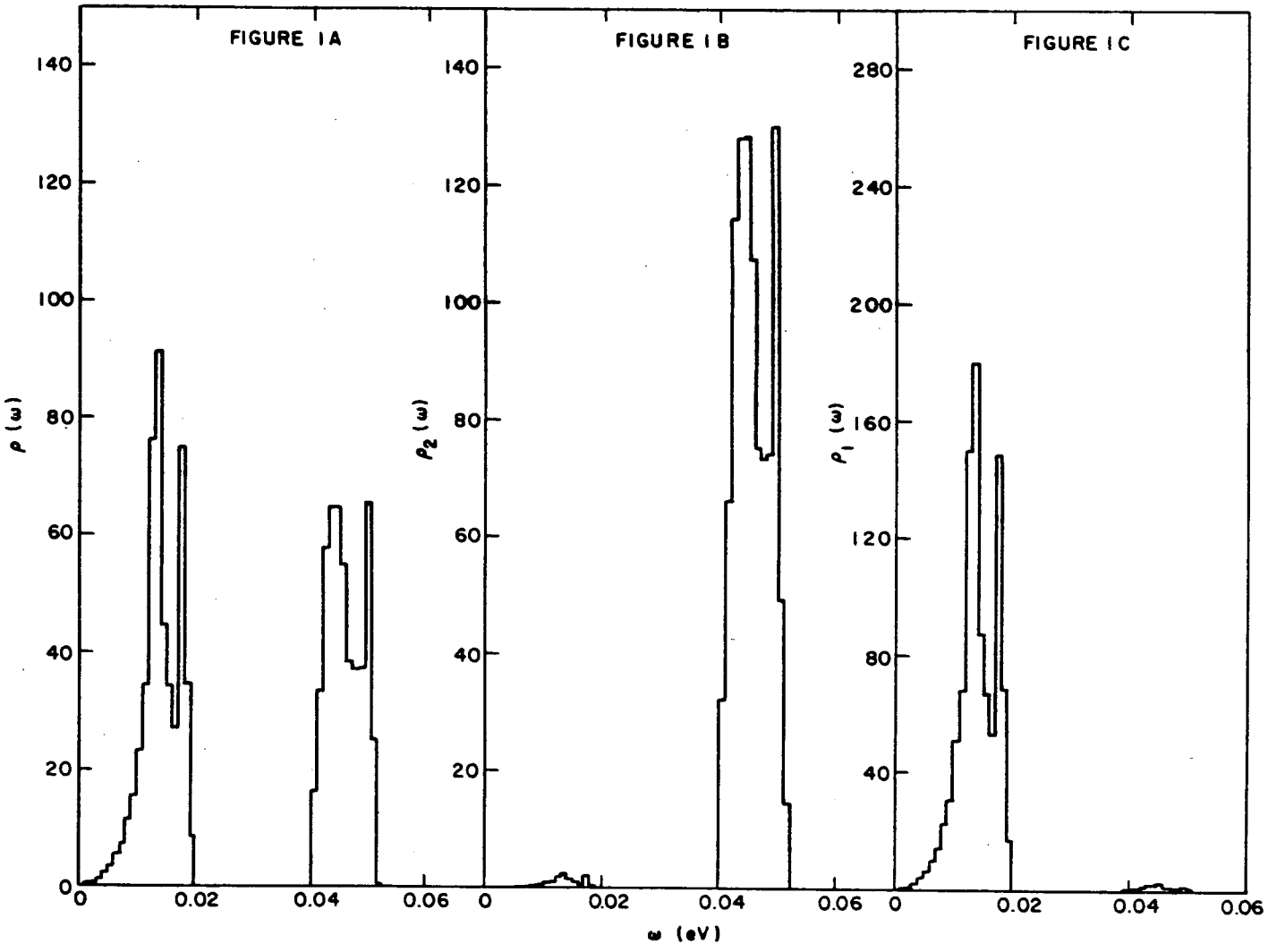



Figure 1A. Histogram representation of the normalized frequency distribution obtained from the central force mode for UC.

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<br>NCP 0 NMESH 1 NREST 0 NCVP 0 NSEP 0<br>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 12.011 DC BETSW ALPSW CRIT1<br>CRIT2 CRIT3 1.0-08 |

X3

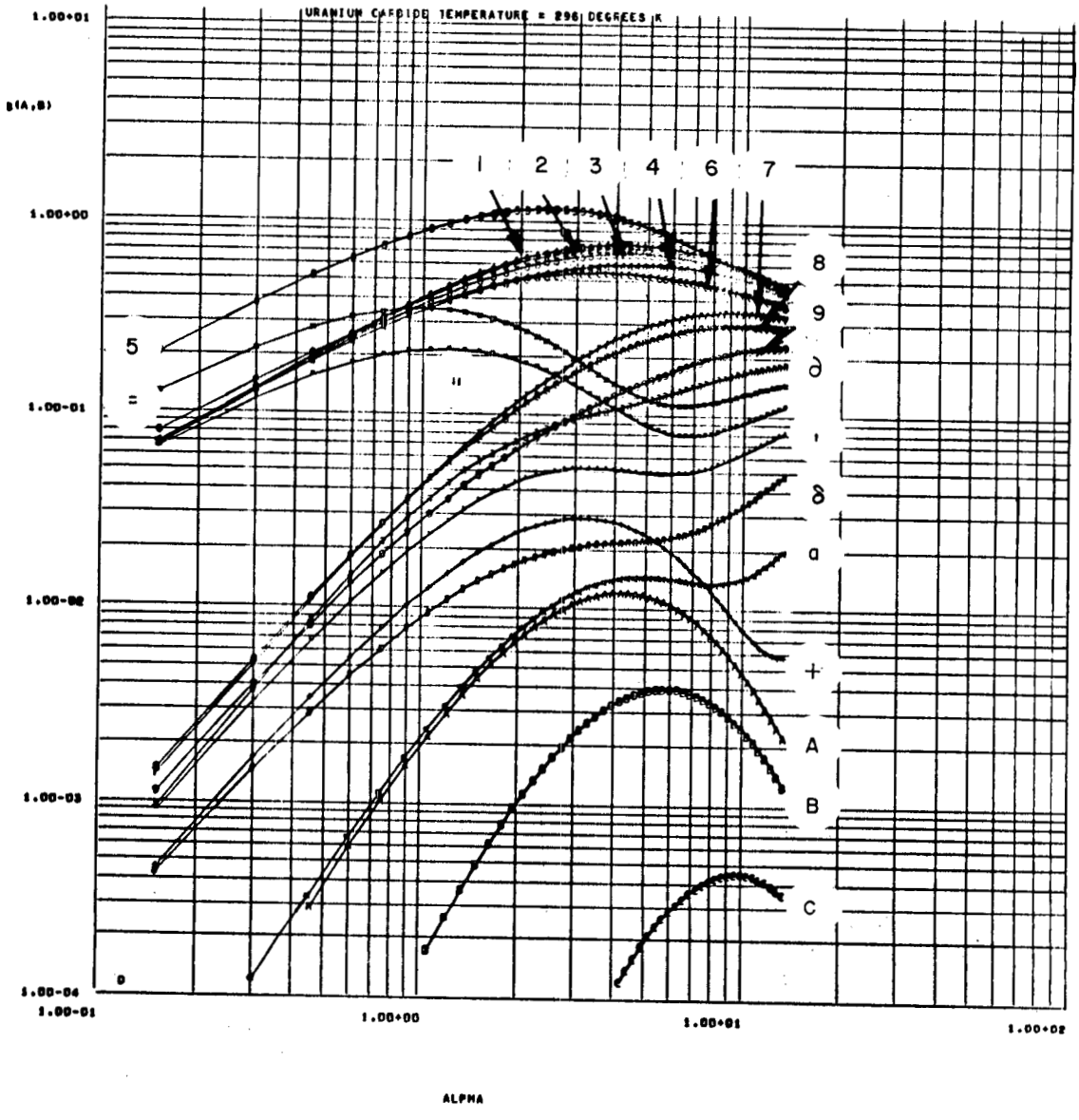
| | | | | | |
|---|---|---|---|---|---|
| .0005 | .00150 | .0025 | .0035 | .0045 | .0055 |
| .0065 | .0075 | .0085 | .0095 | .0105 | .0115 |
| .0125 | .0135 | .0145 | .0155 | .0165 | .0175 |
| .0185 | .0195 | .0205 | .0215 | .0385 | .0395 |
| .0405 | .0415 | .0425 | .0435 | .0445 | .0455 |
| .0465 | .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 | | | | | | | |

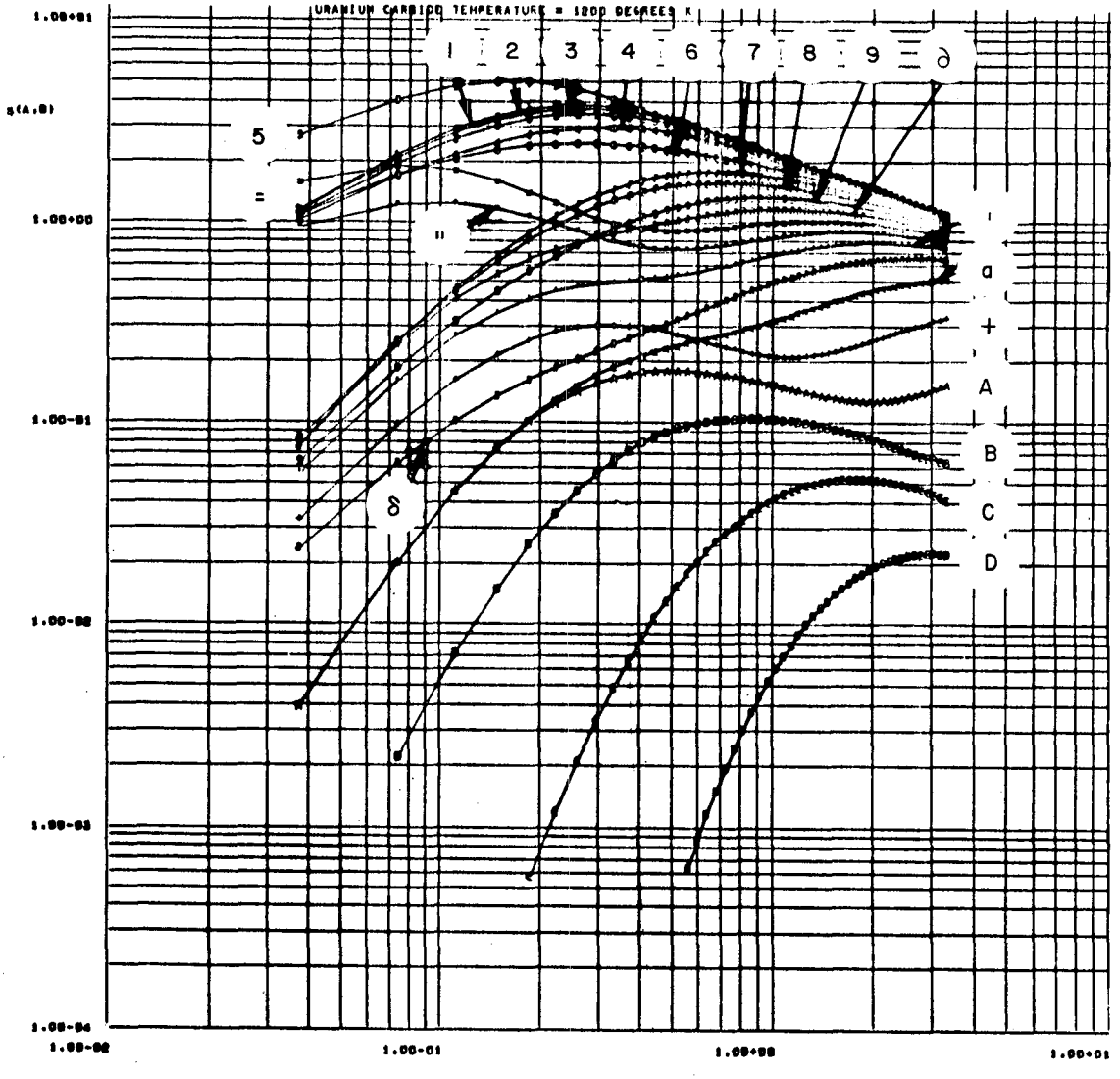
## 4. Plots of Scattering Law for UC

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
S(A,B)
1.00+01
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
0

UC - 4.2


URANIUM CARBIDE 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
1.00+01
ALPHA
1 2 3 4 6 7 8 9 ∂
5
=
II
δ
a
+
A
B
C
D

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 |

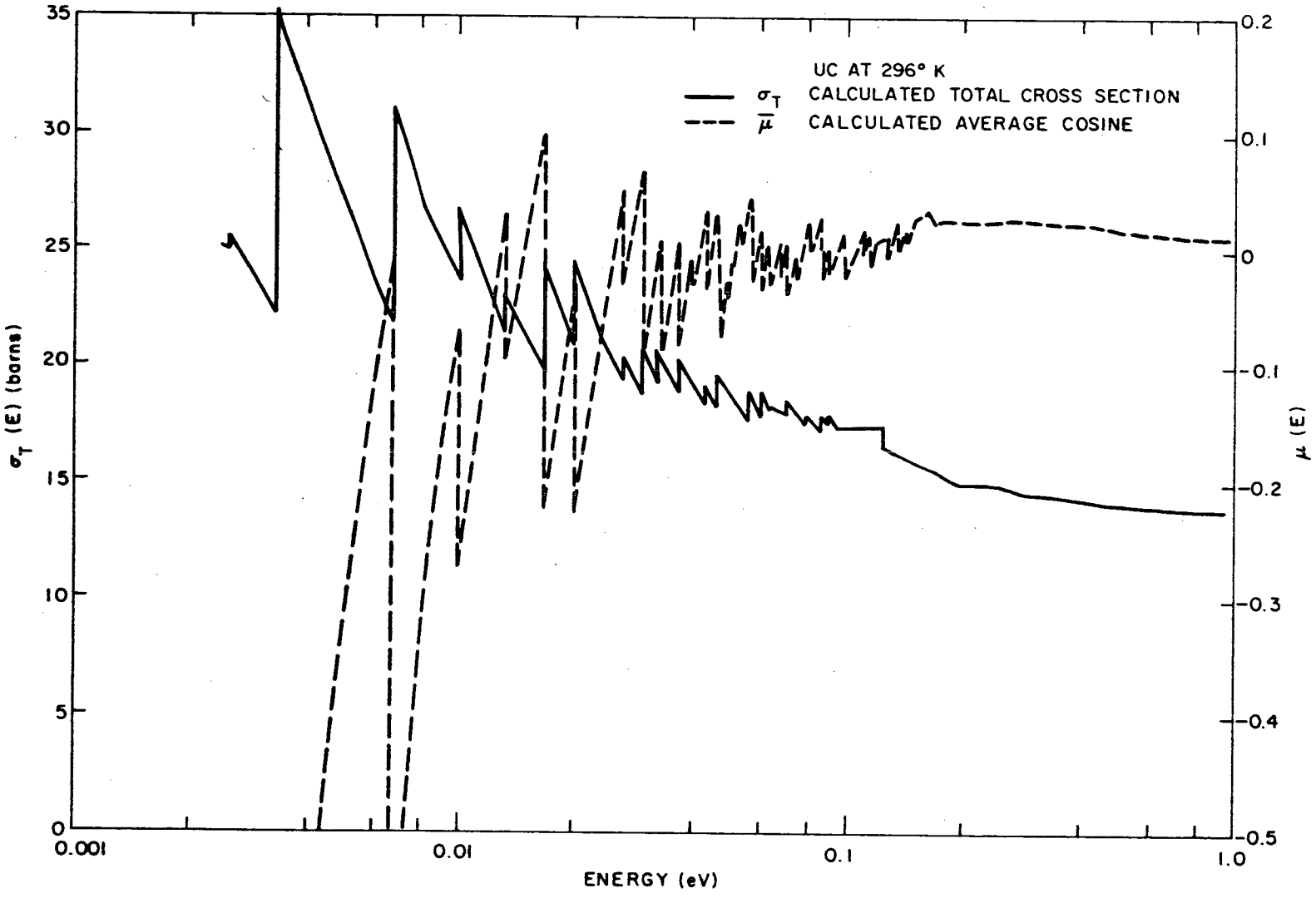
DATA FOR UC AT 296 DEGREES K.

| | 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
$\sigma_T$ CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
$\sigma_T$ (E) (barns)
$\mu$ (E)
ENERGY (eV)
0.001
0.01
0.1
1.0
0
5
10
15
20
25
30
35
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5

## 6. Miscellaneous Notes on Uranium Carbide

For temperatures other than 296°K the switching criteria for short collision and the $\alpha, \beta$ 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 |

## 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 - $\mu$, $\gamma$, $\nu$, and $\delta$ - 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 $\mu$, while the over-all width and shape of this peak determine $\nu$ and $\delta$, 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 $\gamma$, 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 $\alpha$. 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.

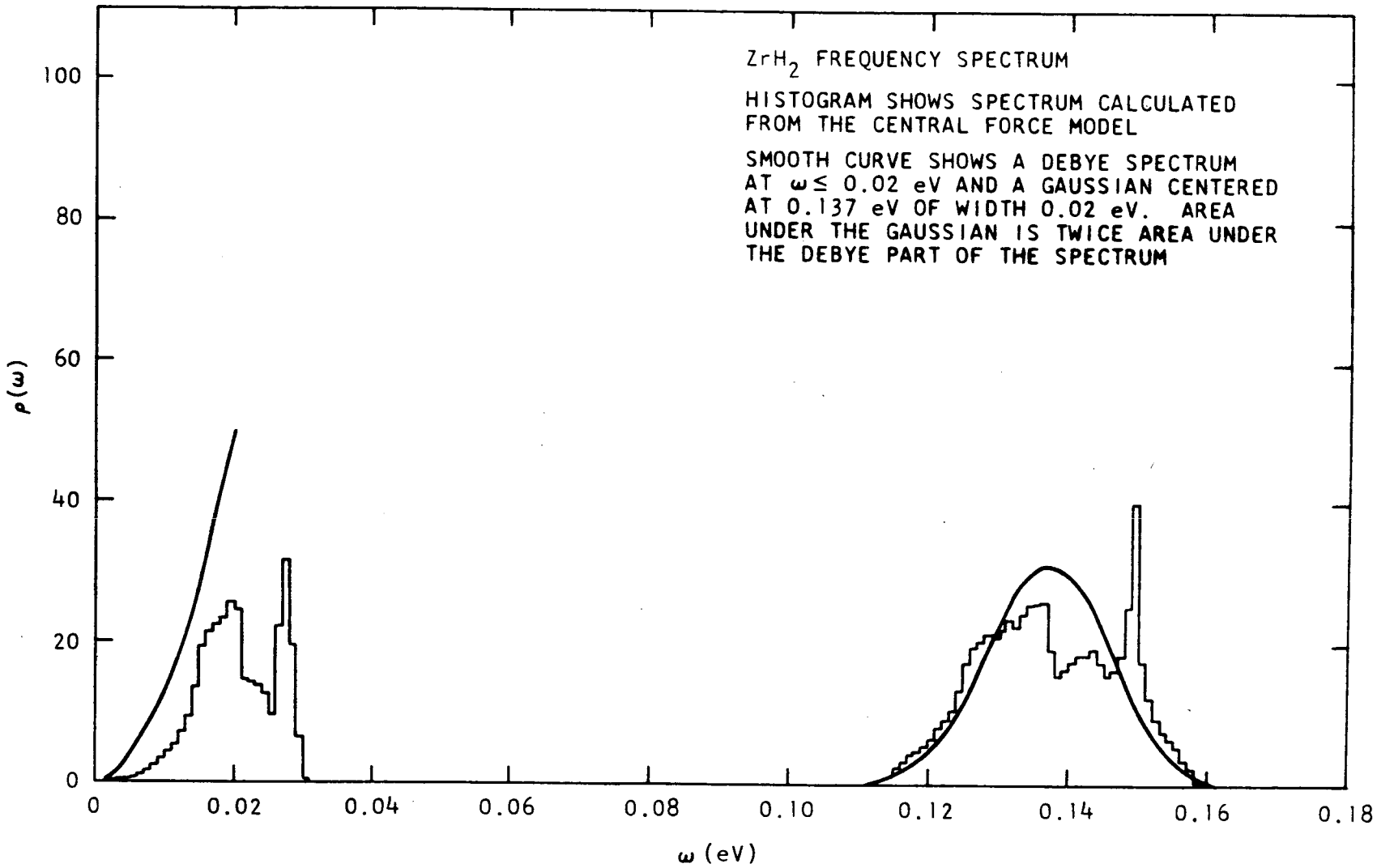



Fig. 1. $ZrH_2$ frequency spectrum calculated from the central force model. The smooth curve shows a Debye spectrum for $\omega \leq 0.02$ eV and a Gaussian of width 0.02 eV centered at 0.137 eV.

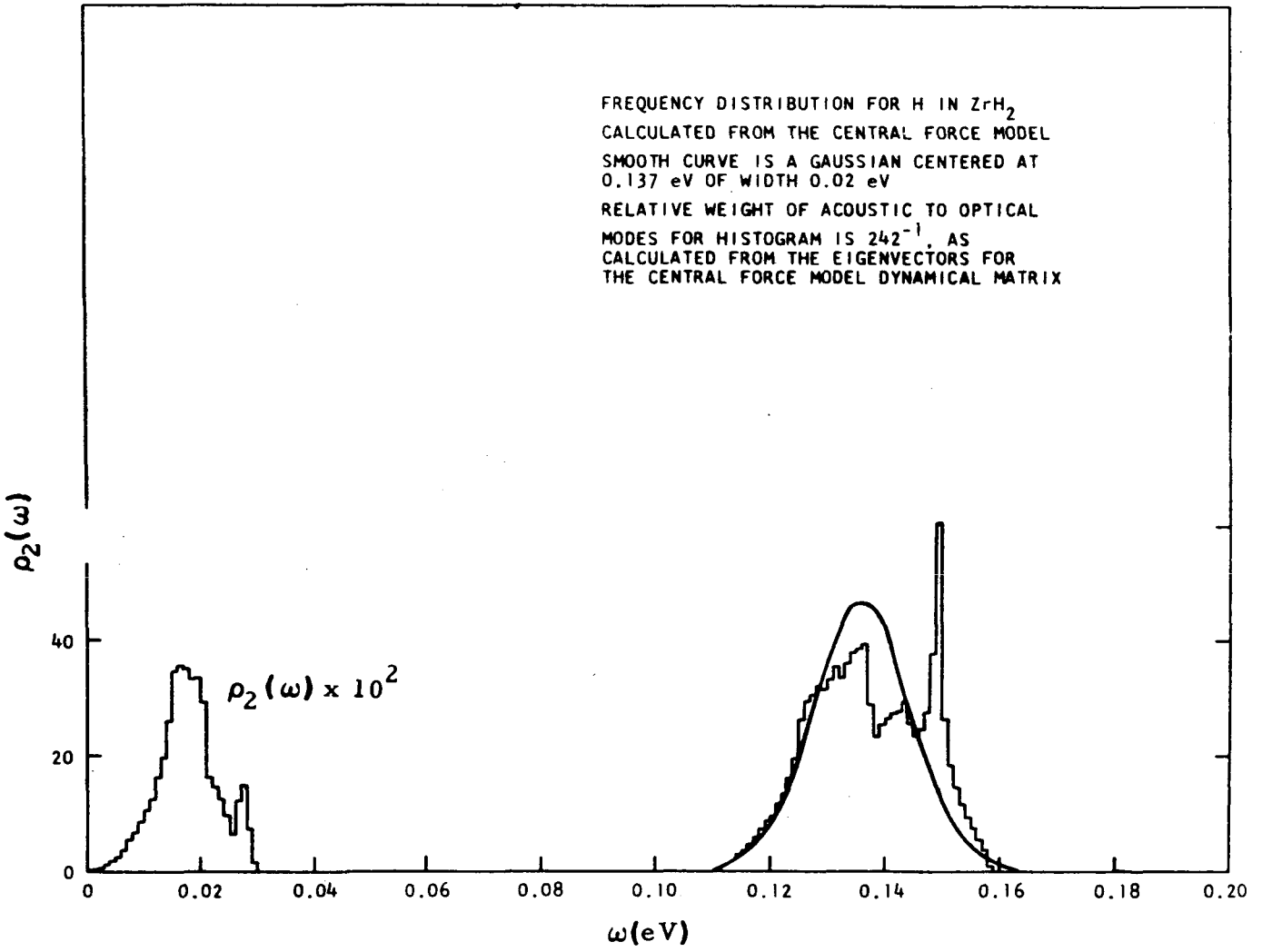



Fig. 2. Weighted frequency spectrum for H in $ZrH_2$ calculated from the central force model. Acoustic modes are shown multiplied by a factor $10^2$.

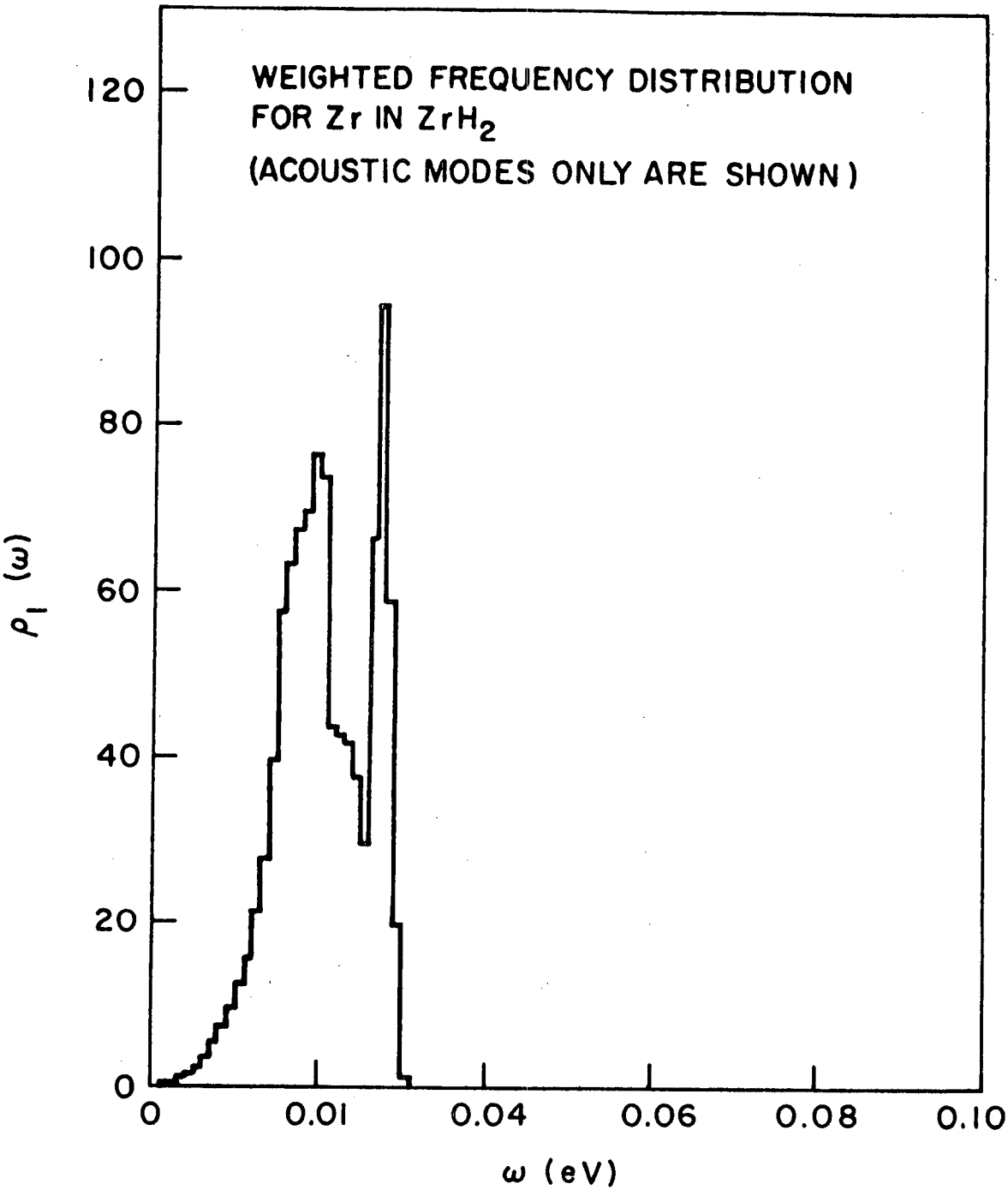



Fig. 3. Weighted frequency spectrum $\rho_1(\omega)$ for Zr in $ZrH_2$ calculated from the central force model.

## 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 | 1.011050 | .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)

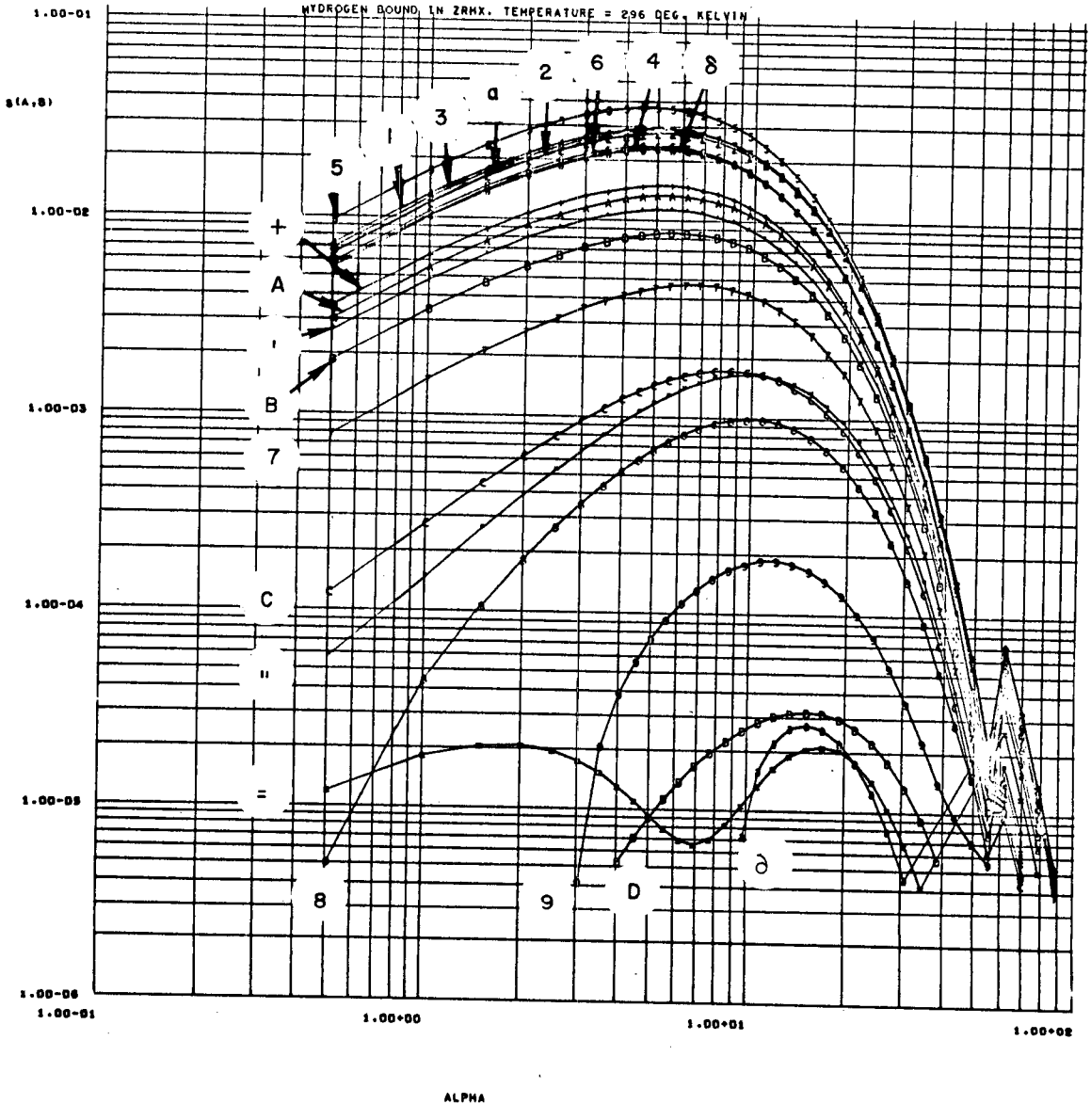
The code ZREND is discussed in Section A. 3. 1. The data tabulated below follows the format of the code input instruction also given in Section A. 3. 1. The code symbols used below are defined in the code input section. If no value is entered for a symbol then that datum was not required.

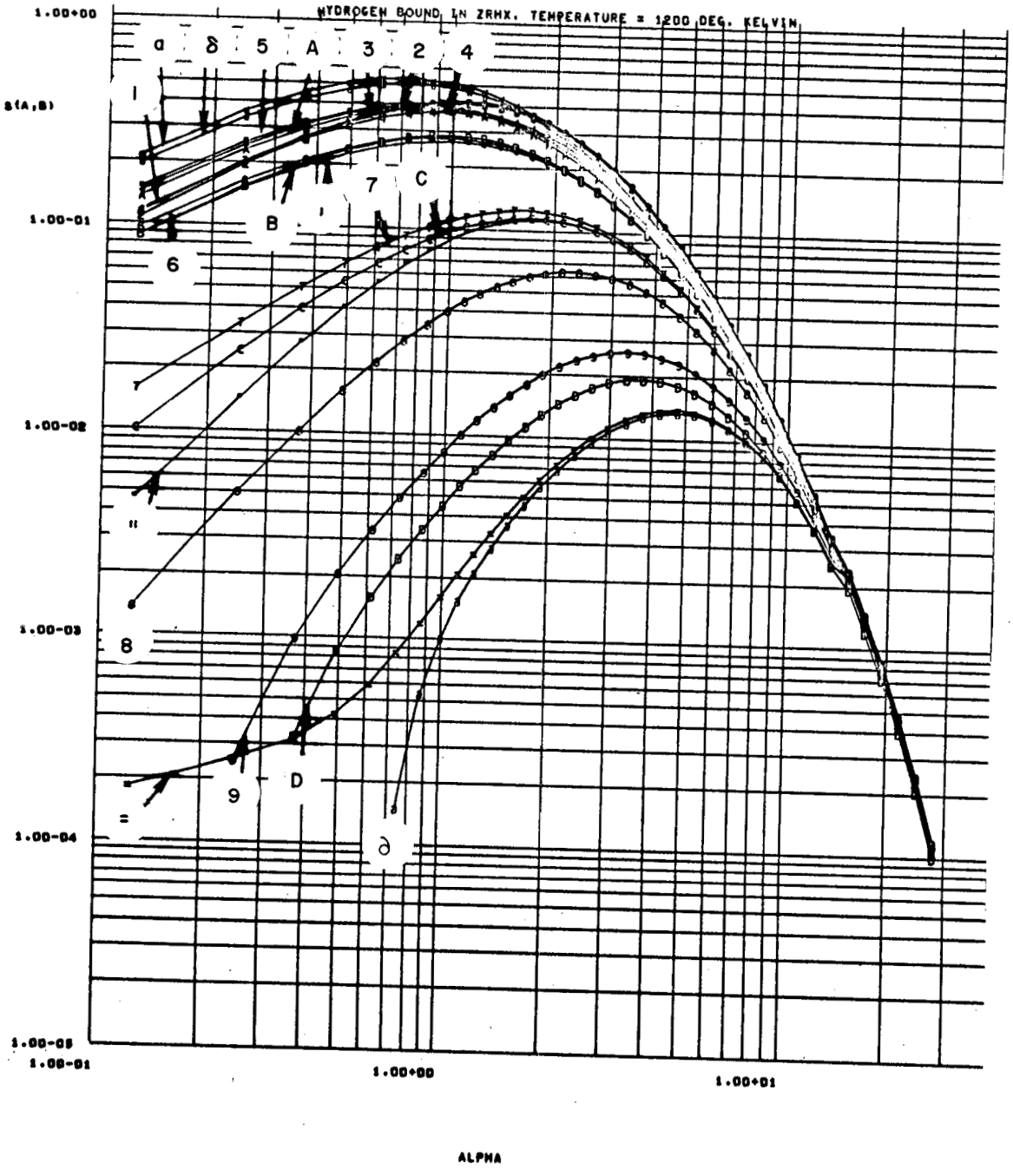
| CARD NO. | FORMAT | CODE SYMBOLS AND VALUES | | | | | |
|---|---|---|---|---|---|---|---|
| 1 | 13A6, A2 | COM Slaggie's incoherent elastic for hydrogen | | | | | |
| 2 | 2I5, | NT 8 | NE 109 | SB 81.44 | SWITCH 10.0 | EPS 1.0-15 | |
| | 3E10, | NPCH 1 | | | | | |
| | I5 | | | | | | |
| 3 | 7E10 | 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 |

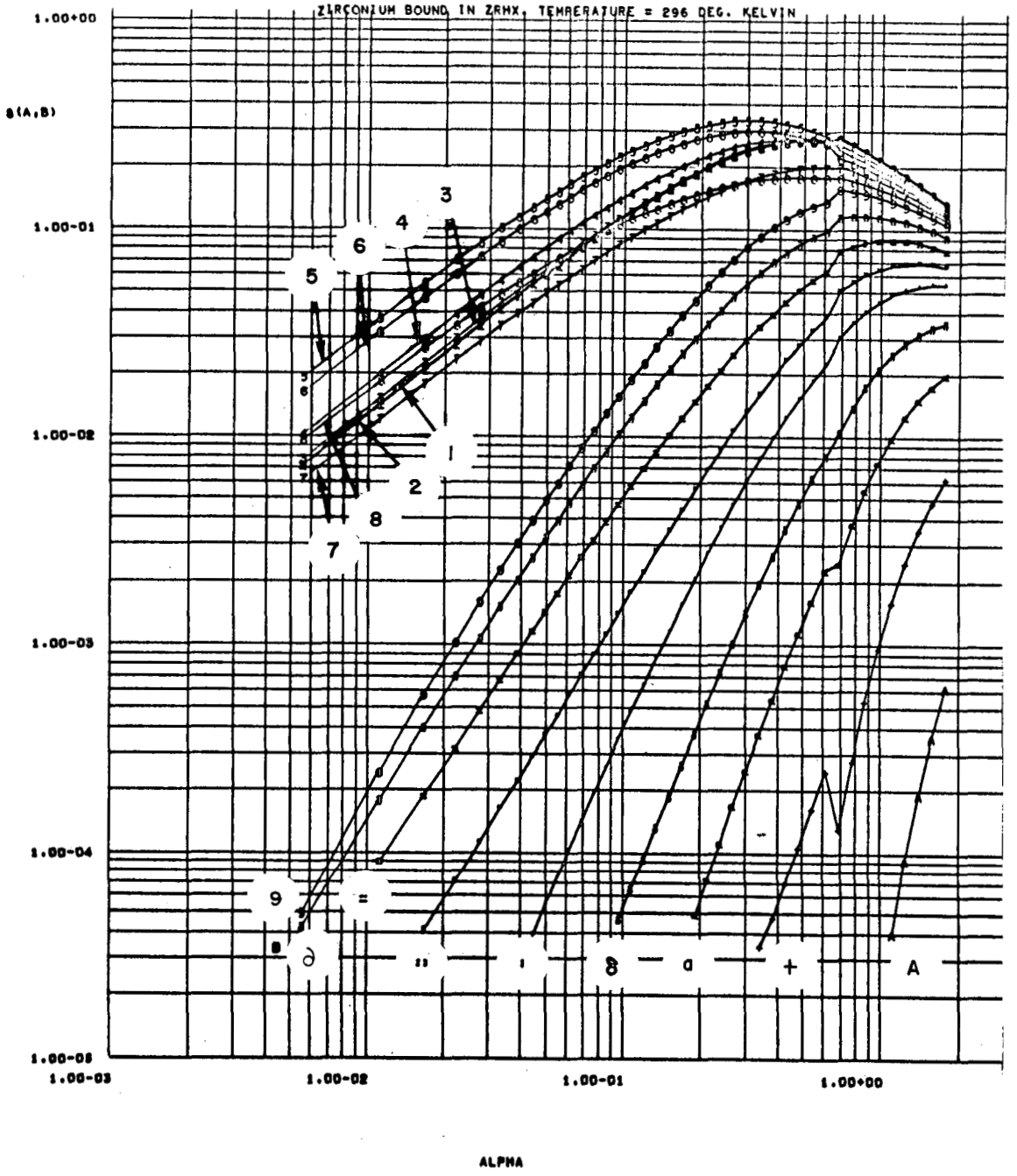

HYDROGEN BOUND IN ZRHX. TEMPERATURE = 296 DEG. KELVIN
S(A,B)
1.00-01
1.00-02
1.00-03
1.00-04
1.00-05
1.00-06
1.00-01
1.00+00
1.00+01
1.00+02
ALPHA
1
2
3
4
5
6
7
8
9
A
B
C
D


HYDROGEN BOUND IN ZRHX, TEMPERATURE = 1200 DEG. KELVIN
S(A,B)
ALPHA
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
a δ 5 A 3 2 4
I
7 C
B
6
II
8
9 D
=
∂

4. Plots of Scattering Law

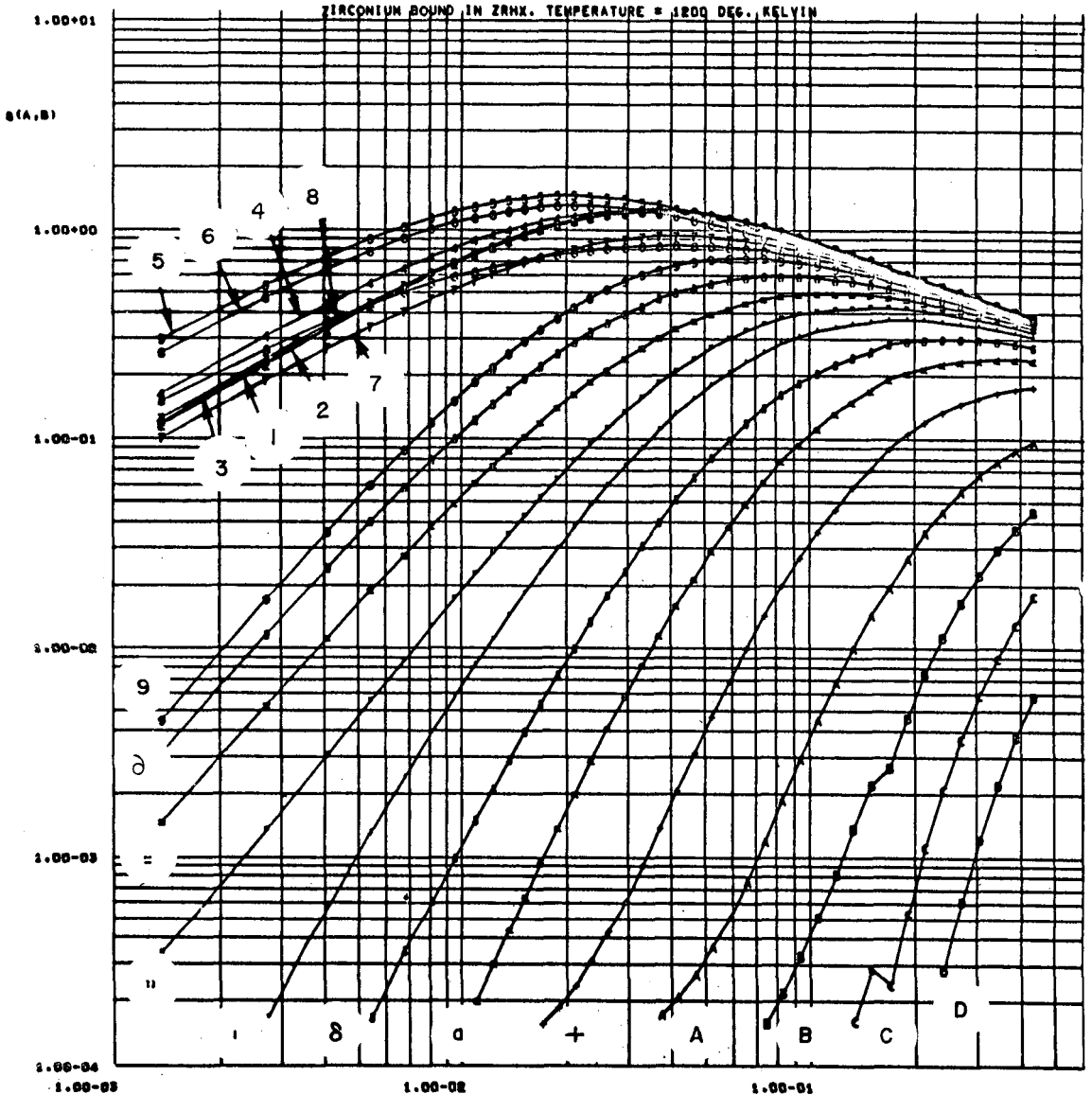
BETA VALUES FOR MULTICURVE PLOT

| 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 |




$ZrH_n$ - 4.5

(Rev. -12/31/69)


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
+
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

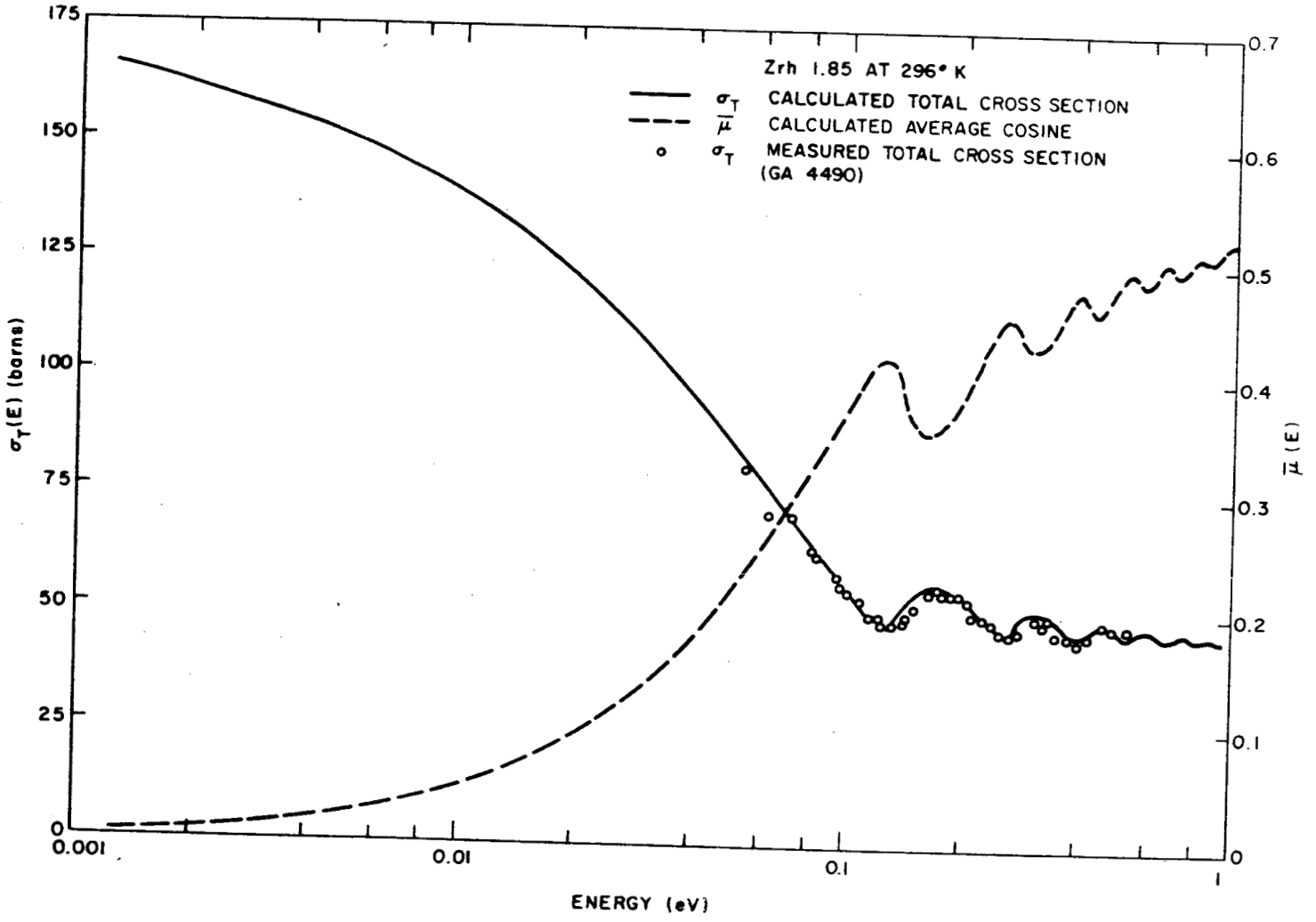
TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

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 | 6.38248 | .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 1.85 AT 296° K
$\sigma_T$ CALCULATED TOTAL CROSS SECTION
$\bar{\mu}$ CALCULATED AVERAGE COSINE
$\sigma_T$ MEASURED TOTAL CROSS SECTION (GA 4490)
$\sigma_T$(E) (barns)
$\bar{\mu}$ (E)
ENERGY (eV)
0.001
0.01
0.1
1
0
25
50
75
100
125
150
175
0.1
0.2
0.3
0.4
0.5
0.6
0.7

## 6. Miscellaneous Notes on Zirconium Hydride

For temperatures other than 296°K the switching criteria for short collision and the $\alpha, \beta$ 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 |