ERRATA

GA-7417

GASKET

A UNIFIED CODE FOR THERMAL
NEUTRON SCATTERING

by

J. U. Koppel, J. R. Triplett and Y. D. Naliboff

The following errata should be noted in GA-7417:

Page 30: Paragraph (9), second sentence should read,
For a new problem, NREST = 0.

Page 46: Item 9, comment under Description should read,
As in Cards 7 and 8 for Mode 3.

Page 49: Last paragraph, first sentence, next to last line
should read,output is also produced for S1,
S2 and S1 + S2.....

Pages 51-68:

These pages are out of order. They should appear
as follows: 51, 57, 58, 60, 59, 68, 63, 64, 62, 55,
54, 53, 52, 65, 66, 56, 67, 61.

Page 73: Second column, third line, add NP.

Page 74: Second column, third line, add NP in front of 40.

Columns labeled DT and TMAX should read

<u>0.001</u>	<u>0.01</u>
<u>0.01</u>	<u>0.1</u>
<u>0.1</u>	<u>3.0</u>
<u>0.25</u>	<u>6.0</u>
<u>0.5</u>	<u>9.0</u>
<u>1.0</u>	<u>22.0</u>
<u>2.0</u>	<u>24.0</u>
<u>4.0</u>	<u>100.0</u>
<u>6.0</u>	<u>3000.0</u>

Page 75: Second column, third line, add

NP in front of 40.

Frequency spectrum for ZrH has been omitted; it
will be added in the revised edition.

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DIVISION OF
GENERAL DYNAMICS

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J. U. Koppel, J. R. Triplett and Y. D. Naliboff

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CONTENTS

		<u>Page</u>
1.	INTRODUCTION.	1
2.	DYNAMICAL MODES	7
2.1	Free Gas	8
2.2	Diffusive Motion	8
2.3	Harmonic Vibration in Polycrystals: Isotropic Frequency Spectrum	10
2.4	Anisotropic Frequency Spectrum	12
2.5	Discrete Isotropic Frequency Spectrum	13
3.	COMBINATION OF MODES 1 AND 3	16
4.	COMBINATION OF MODES 2 AND 3	19
5.	COMBINATION OF DISCRETE MODES OF VIBRATION WITH ANY ADMIXTURE OF THE OTHER FOUR DYNAMICAL MODES	23
6.	APPROXIMATIONS MADE IN GASKET	25
6.1	Short Collision Approximation	25
6.2	Truncation of the Phonon Expansion for Mode 5	26
7.	PROGRAM DESCRIPTION	28
7.1	Main Program	28
7.2	Subroutines	34
7.3	Input Description	43
7.4	Output Description	49
	7.4.1 Printed Output.	49
	7.4.2 Punched Output	69
8.	SAMPLE PROBLEMS	71
8.1	Input	71
8.2	Machine Plots of $S(a, \beta)$	71
8.3	Discussion of Choice of Input Parameters	
	REFERENCES	

1. INTRODUCTION

With the advent of modern, fast, electronic computers it has become possible to construct and evaluate theoretical models which describe quite accurately the process of neutron scattering by matter. A large number of special programs tailored to the characteristics of the individual moderators occurring in reactor technology have been written in the past, and have been used quite successfully for predicting neutron spectra in reactors. This wide variety of computer programs, very often overlapping each other in their scopes, and each one requiring some specialized experience in order to yield sensible results, has made it highly desirable to develop a method of calculating scattering kernels by some unified technique which can be applied to all moderators. The outgrowth of this search for a unified method of calculating neutron scattering is the code GASKET which has already been used successfully for a large number of problems. It is well known that in the incoherent approximation the double differential scattering cross section can be expressed in the form

$$\sigma(E_0 \rightarrow E, \theta) = \frac{\sigma_b}{4\pi} \sqrt{\frac{E}{E_0}} e^{-\frac{\beta}{2}} S(\alpha, \beta) \quad (1.1)$$

where $S(\alpha, \beta)$ is an explicit function (usually called the scattering law^{*}) of only the two variables α and β defined as

^{*}Some authors define a nondimensional scattering law $S'(\alpha, \beta) = TS(\alpha, \beta)$.

$$\alpha = \frac{\kappa^2}{2MT}, \quad \beta = \frac{\epsilon}{T}$$

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

One of the drawbacks of most of the previous codes (excepting the English program LEAP)⁽¹⁾ was that they ignored this explicit dependence of S on only two variables and calculated $\sigma(E_0 \rightarrow E, \theta)$ for each set of values of E_0 , E and θ of a given energy and angular mesh. Instead, GASKET calculates S at points of a two-dimensional α, β mesh. From this two-dimensional array of S -values it is then easy to obtain the double differential cross section and the P_n scattering kernels by interpolation and integration in $\alpha - \beta$ space. This last step is actually performed by an auxiliary code called FLANGE.⁽²⁾

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

The second important advantage is that it takes very little time to recalculate $\sigma(E_0 \rightarrow E, \theta)$ for different angular and energy meshes since most of the computing time is spent in obtaining $S(\alpha, \beta)$, which has to be computed only once. Furthermore, the scattering law shows most of its structure at low β values, while it is rather smooth for large β 's (i.e., for $\beta \gg \omega_{\max}$ where $\omega_{\max}$ is the cut-off frequency of the material

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

in question). This permits one to use a very fine β -mesh near the origin and a gradually coarser mesh as β increases. Clearly, such a fine mesh for small energy exchange at all initial energies between, say 0 and 2 eV, would require a hopelessly large total number of points if $\sigma(E_0 \rightarrow E, \theta)$ were calculated at each angle-energy mesh point as in previous codes.

The keystone of the new approach is the use of numerical methods for evaluating Fourier transforms. For most scattering systems occurring in practice the Fourier transform $\chi(\alpha, t)$ of the scattering law can be expressed in a relatively simple analytical form. GASKET evaluates this so-called intermediate scattering function and does the Fourier inversion numerically. Using conventional numerical integration schemes, one runs into the difficulty of rapidly oscillating integrands at large values of β . This problem, however, is avoided by approximating χ by a piecewise linear function and integrating analytically over each linear segment. The details of this integration procedure are given in Section 7. Due to detailed balance, the scattering law $S(\alpha, \beta)$ is an even function of β . Hence its Fourier transform

$$\chi_{\text{sym}}(\alpha, t) = \int_{-\infty}^{\infty} e^{-i\epsilon t} S(\alpha, \beta) d\epsilon \quad (1.2)$$

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

$$\chi_{\text{n. sym}}(\alpha, t) = \int_{-\infty}^{\infty} e^{-i\epsilon t} \mathcal{L}(\alpha, \beta) d\epsilon \quad (1.3)$$

and

$$\mathcal{A}(\alpha, \beta) = e^{-\beta/2} S(\alpha, \beta) \quad (1.4)$$

A useful relation between the two forms of the intermediate scattering function is

$$\chi_{\text{sym}}(\alpha, t) = \chi_{\text{n.sym}}\left(\alpha, t + \frac{i}{2T}\right) \quad (1.5)$$

which can be obtained by analytical continuation of the Fourier transforms assuming that χ_{sym} is analytic in the domain $\left(-\infty < \text{Re}[t] < \infty, 0 \leq \text{Im}[t] \leq \frac{1}{2T}\right)^*$. The numerical Fourier inversion of Eq. (1.3) requires splitting $\chi_{\text{n.sym}}$ into even and odd parts which then have to be inverted separately. However, as a result of this slight complication it is possible to reach any practical value of β . Typically, for a cut-off energy of 1 eV and a temperature of 300°K the maximum required β is 40. For very large α and β the code also provides an option to calculate $S(\alpha, \beta)$ in Wick's short collision approximation.

The increase in computing time due to the split into even and odd components is largely compensated by the much faster convergence of the nonsymmetric time integrals. The reason for this can be found in the uncertainty principle relating the widths of two distributions which are Fourier transforms of each other. ⁽³⁾

As mentioned earlier, GASKET calculates the scattering law in the incoherent approximation. Coherent elastic scattering can be handled separately and added to the diagonal elements of the P_n scattering kernels. For hexagonal crystals, for instance, the coherent contribution is calculated with the code HEXSCAT. ⁽⁴⁾

* Eq. (1.5) leads to $\mathcal{A}(\alpha, \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\epsilon t} \chi_{\text{sym}}\left(\alpha, t - \frac{i}{2T}\right) dt$ only if the stated analyticity condition is satisfied, as it can easily be verified by contour integration.

As mentioned above it would be desirable to have a code which could be used for all common moderators. With this goal in mind provision has been made in GASKET for the following dynamical modes 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 (as applied for instance to graphite).
5. Harmonic isotropic vibrations with discrete frequency spectrum.

Any one or all of these modes may be present simultaneously. The treatment in GASKET of Modes 1 to 5 as well as their different combinations will be described in the following sections. The coding, however, has only been completed for combinations of Modes 1, 3 and 5.

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

$$\chi_i = \exp \left[\alpha G_i(t) \right] \quad (1.6)$$

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

$$\chi = \exp \left[\alpha \sum_i w_i G_i(t) \right] \quad (1.7)$$

where the w 's are weight factors normalized to 1:

$$\sum_i w_i = 1 \quad (1.8)$$

An important point to be mentioned is that for crystals $S(\alpha, \beta)$ has a δ -function singular contribution due to elastic scattering. This means that $\chi(\alpha, t)$ approaches a nonvanishing limit as t goes to infinity. It is necessary to subtract this constant part, which is essentially the Debye-Waller factor, in order to make the time integrals convergent. Even in the presence of diffusion or Doppler broadening of this zero-phonon term, as occurs in the case of liquid, it is convenient to calculate its contribution to $S(\alpha, \beta)$ independently in order to improve the time convergence. This will be discussed in Sections 3 and 4.

When only Modes 1 or 2 (i. e., free translations or diffusion) contribute, the scattering law is evaluated analytically. The time integration is used only if distributed vibrational modes are present, whereas the discrete modes are taken care of by a convolution of the $S(\alpha, \beta)$ for the continuum with all the discrete lines arising from the phonon expansion corresponding to each discrete oscillator. The details of this convolution procedure will be given in Section 5.

2. DYNAMICAL MODES

In the previous section we have introduced the intermediate scattering function χ . In this section the symbol $\chi_i(\alpha, t)$ shall always designate the nonsymmetric intermediate scattering function as defined by Eq. (1.3), corresponding to the dynamical mode i according to the order in which they are listed in Section 1.

All the χ_i should be consistent with the following conditions which correspond to Placzek's⁽⁵⁾ well known sum rules for $S(\alpha, \beta)$ and its first few moments:

$$\chi(\alpha, 0) = \lim_{t \rightarrow 0} \chi(\alpha, t) = 1 \quad (2.1)$$

$$\left[\frac{\partial \chi(\alpha, t)}{\partial t} \right]_{t=0} = i\alpha T \quad (2.2)$$

$$\left[\frac{\partial^2 \chi(\alpha, t)}{\partial t^2} \right]_{t=0} = -2\alpha T \bar{T} - (\alpha T)^2 \quad (2.3)$$

($\bar{T}$ is two-thirds of the mean kinetic energy of the scattering nuclei.) Furthermore the principle of detailed balance requires that $\chi\left(\alpha, t + \frac{i}{2T}\right)$ be an even real function of t (for real α).

Of all dynamical modes considered in Section 1, only the 4th (anisotropic vibration) requires an average over orientations of the scattering system. This case must be treated separately. All other modes have an exponential χ -function and can be combined according to Eq. (1.7). In the following we shall give the corresponding $G_i(t)$ as defined by Eq. (1.6) or

$$G_i(t) = \frac{1}{\alpha w_i} \log \chi_i(\alpha, t) \quad (2.4)$$

2.1 FREE GAS

According to Zemach and Glauber⁽⁶⁾

$$G_1(t) = iTt - T^2 t^2 \quad (2.5)$$

and

$$G_1(t + i/2T) = - \left(1/4 + T^2 t^2 \right) \quad (2.6)$$

The corresponding scattering law S_1 is easily evaluated as

$$S_1(\alpha, \beta) = \frac{1}{\sqrt{4\pi\alpha w_1 T^2}} \exp \left[- \frac{1}{4\alpha w_1} \left(\beta^2 + w_1^2 \alpha^2 \right) \right] \quad (2.7)$$

2.2 DIFFUSIVE MOTION

A completely rigorous treatment of the diffusive motion in liquids has not yet been given. For most practical cases it will be sufficient to use the approximate expression suggested by Egelstaff and Schofield⁽⁷⁾

$$G_2(t) = 2d \left(\sqrt{T^2 t^2 + c^2} - iTt - c \right) \quad (2.8)$$

or

$$G_2\left(t + \frac{i}{2T}\right) = 2d \left(\sqrt{T^2 t^2 + c^2 + 1/4} - c \right) \quad (2.9)$$

where d is the diffusion coefficient and c an adjustable parameter. Both are nondimensional with our system of units. The expression (2.8) has the correct asymptotic behavior for $t \rightarrow \infty$ corresponding to classical diffusion theory. It also satisfies detailed balance and condition (2.1). Condition (2.2), however, can only be satisfied if

$$\frac{d}{c} = 1 \quad (2.10)$$

Condition (2.3) cannot be met simultaneously with Eq. (2.2), but this is not a serious handicap.

The main reason for adopting a diffusive G -function of the form (2.8) is that its contribution to the scattering law can be obtained analytically, with the result

$$S_2(\alpha, \beta) = \frac{\exp(2w_2 d c \alpha) 2w_2 d (c^2 + 1/4)^{1/2} \alpha}{\pi T [\beta^2 (2w_2 d \alpha)^2]^{1/2}} K_1 \left\{ (c^2 + 1/4)^{1/2} [\beta^2 + (2w_2 d \alpha)^2]^{1/2} \right\} \quad (2.11)$$

Here $K_1(x)$ is the modified Bessel function of the second kind and first order. (8)

When the only nonvanishing weight is either w_1 or w_2 , the scattering law is obtained analytically from Eqs. (2.7) or (2.11) and no numerical integration is required. When discrete oscillators (Mode 5) are added, the convolution procedure described in Section 5 still provides an analytical expression for $S(\alpha, \beta)$. Furthermore, when Modes 1 or 2 are combined with continuous vibrational modes, Eqs. (2.7) and (2.11) will be used to give the zero-phonon term (see Sections 2 and 4). In fact, for small values of α , this term (which is a δ -function when $w_1 = w_2 = 0$) is a sharply peaked function of β so that it is extremely convenient to have it in analytical form.

2.3 HARMONIC VIBRATION IN POLYCRYSTALS: ISOTROPIC FREQUENCY SPECTRUM

The exact intermediate scattering function for the ℓ -th atom in the unit cell of a harmonic crystal is

$$\chi_3^{(\ell)}(\alpha, t) = \exp \left\{ \frac{w_3}{2NM_\ell} \sum_{\vec{k}, s} |\vec{\alpha} \cdot \vec{C}(\ell | \vec{k}_s)|^2 g[\omega_s(\vec{k}), t] \right\} \quad (2.12)$$

where

$$g(\omega, t) = \frac{1}{\omega} \left[\frac{e^{\omega/T}}{e^{\omega/T} - 1} (e^{i\omega t} - 1) + \frac{1}{e^{\omega/T} - 1} (e^{-i\omega t} - 1) \right] \quad (2.13)$$

N being the total number of unit cells, and $\vec{C}(\ell | \vec{k}_s)$ the polarization vector of the ℓ -th atom for a normal mode corresponding to the wave vector $\vec{k}$ and the branch s . For a Bravais lattice with cubic symmetry Eq. (2.12) takes the much simpler form

$$\chi_3(\alpha, t) = \exp [\alpha w_3 G_3(t)] \quad (2.14)$$

with

$$G_3(t) = \gamma(t) - \gamma(0) \quad (2.15)$$

and

$$\gamma(t) = T \int_{-\infty}^{\infty} \frac{f(|\omega|) e^{\omega/2T}}{2\omega \sinh \omega/2T} e^{i\omega t} d\omega \quad (2.16)$$

Here $f(\omega)$ is the frequency spectrum of the normal modes of vibration of the crystal, which is normalized to unity:

$$\int_0^{\infty} f(\omega) d\omega = 1$$

The quantity

$$D = \exp \left[-\alpha w_3 \gamma(0) \right] \quad (2.17)$$

is the so-called Debye-Waller factor. Separating the real and imaginary parts in Eq. (2.16) we get

$$\gamma(t) = T \int_0^{\infty} f(\omega) (\coth \omega/2T \cos \omega t + i \sin \omega t) d\omega/\omega \quad (2.18)$$

and furthermore

$$\gamma\left(t + \frac{i}{2T}\right) = T \int_0^{\infty} \frac{f(\omega) \cos \omega t}{\omega \sinh \omega/2T} d\omega \quad (2.19)$$

It is seen from Eqs. (2.14) - (2.16) that for the very special case of a cubic Bravais lattice, the crystal orientation has dropped out of the expression for χ , which therefore is completely determined by the frequency spectrum $f(\omega)$.

For a noncubic monoatomic but polycrystalline scatterer Eqs. (2.14) - (2.19) are still good approximations, since for polycrystals it is necessary to perform an average over orientation of the microcrystals. In fact one can derive these equations directly from Eq. (2.12)

by averaging in the exponent of its R. H. S. This approximate averaging procedure is generally satisfactory, since it gives the exact result in the limits $\kappa^2 \rightarrow 0$ and $\epsilon \rightarrow \infty$.

For a polyatomic crystal the simple frequency spectrum $f(\omega)$ is no longer sufficient to determine the χ -function. In this more general case it is seen from Eq. (2.12) that the frequency spectrum must be weighted by the factor $|C(\ell|k_s)|^2$. Within the approximation of the preceding paragraph, the χ -function can then be obtained by substituting this amplitude weighted frequency spectrum for $f(\omega)$ in Eq. (2.16) - (2.19).

The Fourier inversion of $\chi_3(\alpha, t)$ requires splitting this function into even and odd components. This is discussed in Section 3 for the more general case when $w_3 \neq 0$, $w_1 \neq 0$.

2.4 ANISOTROPIC FREQUENCY SPECTRUM

For extremely anisotropic crystals, the approximate averaging procedure used above might no longer be good enough. In some cases, as for example, graphite, it is possible to introduce an orientation-dependent frequency spectrum of the form

$$f(\omega) = f_{\parallel}(\omega)\cos^2\theta + f_{\perp}(\omega)(1-\cos^2\theta) \quad (2.20)$$

where θ is the angle between a preferred direction in the microcrystal (the normal to the basal planes in the case of graphite) and a fixed axis which is conveniently taken parallel to the momentum exchange $\vec{\kappa}$.

$f_{\perp}(\omega)$ and $f_{\parallel}(\omega)$ are the frequency spectra associated with modes having polarization vectors perpendicular or parallel to the preferred direction.

In this case we get

$$\chi_4(\alpha, t) = \int_0^1 d(\cos\theta) \exp \left\{ w_4 \alpha \left[G_{//}(t) \cos^2 \theta + G_{\perp}(t) (1 - \cos^2 \theta) \right] \right\} \quad (2.21)$$

or

$$\chi_4(\alpha, t) = \exp \left[\alpha w_4 G_{\perp}(t) \right] \int_0^1 d\mu \exp \left\{ -\alpha w_4 \left[G_{\perp}(t) - G_{//}(t) \right] \mu^2 \right\} \quad (2.22)$$

where $G_{\perp}(t)$ and $G_{//}(t)$ are given by Eqs. (2.15) and (2.16) with $f(\omega)$ replaced respectively by $f_{\perp}(\omega)$ and $f_{//}(\omega)$. Both $f_{\perp}(\omega)$ and $f_{//}(\omega)$ are normalized to unity.

The integral in Eq. (2.22) yields functions which are well known⁽⁸⁾

$$\int_0^1 d\mu e^{-x\mu^2} = 1/2 \sqrt{\frac{\pi}{x}} \operatorname{erf}(\sqrt{x}) \quad \text{for } x > 0 \quad (2.23)$$

$$= \Phi(1/2, 3/2, -x) = 1/2 \sqrt{\frac{\pi}{-x}} \operatorname{erf}(i\sqrt{-x}) \quad \text{for } x < 0$$

where Φ denotes a confluent hypergeometrical function.

2.5 DISCRETE ISOTROPIC FREQUENCY SPECTRUM

The frequency spectra of molecular crystals or liquids contains some rather sharp lines corresponding to internal vibrations of the molecules (for instance the bending and stretching modes of the H_2O molecule in water or the CH_2 radical in polyethylene). For these modes we can introduce the discrete frequency spectrum

$$f(\omega) = \sum_k a_k \delta(\omega - \omega_k) \quad (2.24)$$

with

$$\sum_k a_k = 1 \quad (2.25)$$

From the formulae of Section 2.3 we find at once the corresponding χ -function. Evaluated at $t + \frac{i}{2T}$ it is

$$\chi_5\left(\alpha, t + \frac{i}{2T}\right) = \prod_k \exp\left(-\alpha T w_5 \frac{a_k}{\omega_k} \coth \frac{\omega_k}{2T}\right) \cdot \exp\left(\alpha T w_5 \frac{a_k \cos \omega_k t}{\omega_k \sinh \frac{\omega_k}{2T}}\right) \quad (2.26)$$

Since

$$e^{x \cos \theta} = \sum_{n=-\infty}^{\infty} I_n(x) e^{-in\theta} = \sum_{n=-\infty}^{\infty} I_n(x) \cos n\theta \quad (2.27)$$

each term in (2.24) generates a phonon series

$$\chi_{5,k}\left(\alpha, t + \frac{i}{2T}\right) = \sum_{n=-\infty}^{\infty} C_k^{(n)}(\alpha) \cos(n\omega_k t) \quad (2.28)$$

where

$$C_k^{(n)}(\alpha) = I_n\left(\frac{\alpha T w_5 a_k}{\omega_k \sinh \frac{\omega_k}{2T}}\right) \exp\left(-\alpha T w_5 \frac{a_k}{\omega_k} \coth \frac{\omega_k}{2T}\right) \quad (2.29)$$

$I_n(x)$ being the modified Bessel function of the first kind and n -th order. The Fourier transform of Eq. (2.28) is

$$S_{5,k}(\alpha, \beta) = \sum_{n=-\infty}^{\infty} C_k^{(n)}(\alpha) \delta(T\beta - n\omega_k) \quad (2.30)$$

From this and the convolution theorem it is easy to obtain $S_5(\alpha, \beta)$, the complete Fourier transform of Eq. (2.26). Since discrete vibrational modes can only occur in combination with other dynamical modes, we shall come back to this point in Section 5.

3. COMBINATION OF MODES 1 AND 3

From the definition of the nonsymmetric scattering law $S(\alpha, \beta)$ according to (1.3) and (1.4) and recalling Eqs. (1.7), (2.5) and (2.15) - (2.18) we get for this case

$$\begin{aligned} \mathcal{S}(\alpha, \beta) = & \frac{D}{2\pi} \int_{-\infty}^{\infty} dt \exp \left[iTt(\beta + \alpha w_1) + i\alpha T w_3 \int_0^{\infty} f(\omega) \sin \omega t \frac{d\omega}{\omega} \right] \cdot \\ & \cdot \exp \left\{ -\alpha T \left[w_1 T t^2 - w_3 \int_0^{\infty} f(\omega) \coth \frac{\omega}{2T} \cos \omega t \frac{d\omega}{\omega} \right] \right\} \quad (3.1) \end{aligned}$$

Splitting the integrand into even and odd components we have

$$\begin{aligned} \mathcal{S}(\alpha, \beta) = & \frac{D}{\pi} \int_0^{\infty} dt \cos \left[(\beta + \alpha w_1) T t + \alpha T w_3 \int_0^{\infty} f(\omega) \sin \omega t \frac{d\omega}{\omega} \right] \cdot \\ & \cdot \exp \left\{ \alpha T \left[-w_1 T t^2 + w_3 \int_0^{\infty} f(\omega) \coth \frac{\omega}{2T} \cos \omega t \frac{d\omega}{\omega} \right] \right\} \quad (3.2) \end{aligned}$$

As mentioned in Section 1, it is convenient to separate from $\chi(\alpha, t)$ the term which corresponds to zero-phonon scattering (or elastic scattering in the limit when $w_1 = 0$)

$$\chi_1 \chi_3 = \chi_1 (\chi_3 - D) + \chi_1 D \quad (3.3)$$

Then, defining the odd and even functions

$$F(t) = w_3 T \int_0^{\infty} f(\omega) \sin \omega t \frac{d\omega}{\omega} \quad (3.4)$$

and

$$H(t) = w_3 T \int_0^{\infty} f(\omega) \coth \frac{\omega}{2T} \cos \omega t \frac{d\omega}{\omega} \quad (3.5)$$

we can rewrite Eq. (3.3) in the form

$$\begin{aligned} \mathcal{L}(\alpha, \beta) = & \frac{D}{\pi} \int_0^{\infty} dt \left\{ \cos \left[(\beta + \alpha w_1) T t + \alpha F(t) \right] \cdot \exp \left[-\alpha w_1 T^2 t^2 + \alpha H(t) \right] - \right. \\ & \left. - \cos \left[(\beta + \alpha w_1) T t \right] \exp \left(-\alpha w_1 T^2 t^2 \right) \right\} + \frac{D}{2\pi} \int_{-\infty}^{\infty} e^{i\beta T t} \chi_1(\alpha, t) dt \quad (3.6) \end{aligned}$$

or else

$$S(\alpha, \beta) = S^{(1)}(\alpha, \beta) + S^{(2)}(\alpha, \beta) \quad (3.7)$$

with

$$S^{(2)}(\alpha, \beta) = \frac{D}{\sqrt{4\pi\alpha w_1 T^2}} \exp \left[-\frac{1}{4\alpha w_1} (\beta^2 + w_1^2 \alpha^2) \right] \quad (3.8)$$

which follows from Eq. (2.7), and

$$S^{(1)}(\alpha, \beta) = \frac{e^{\beta/2} D}{\pi} \int_0^\infty dt [Q(t) \cos \lambda t - R(t) \sin \lambda t] \quad (3.9)$$

where

$$\lambda = (\beta + \alpha w_1) T \quad (3.10)$$

$$Q(t) = \left\{ \cos [\alpha F(t)] e^{\alpha H(t)} - 1 \right\} e^{-\alpha w_1 T^2 t^2} \quad (3.11)$$

$$R(t) = \sin [\alpha F(t)] e^{-\alpha w_1 T^2 t^2 + \alpha H(t)} \quad (3.12)$$

The numerical evaluation of the integral in Eq. (3.9) will be described in Section 8.

4. COMBINATION OF MODES 2 AND 3

This case will be treated in a manner quite similar to the preceding one. First, it is necessary to split $G_2(t)$, as given by Eq. (2.8), into even and odd components. With this purpose we rewrite the square root in Eq. (2.8) in the following form:

$$\begin{aligned}
 & + \sqrt{\tau^2 - i\tau + c^2} = + \sqrt[4]{(\tau^2 + c^2)^2 + \tau^2} e^{\frac{i}{2} \arg(\tau^2 + c^2 + i\tau)} \quad (c^2 > 0) \\
 & = \frac{1}{\sqrt{2}} \sqrt[4]{(\tau^2 + c^2)^2 + \tau^2} \left\{ \sqrt{1 + \cos \left[\arg(\tau^2 + c^2 - i\tau) \right]} \pm i \sqrt{1 - \cos \left[\arg(\tau^2 + c^2 - i\tau) \right]} \right\} \\
 & = \frac{1}{\sqrt{2}} \left\{ \sqrt{\sqrt{(\tau^2 + c^2)^2 + \tau^2} + \tau^2 + c^2} \pm i \sqrt{\sqrt{(\tau^2 + c^2)^2 + \tau^2} - \tau^2 - c^2} \right\} \quad (4.1)
 \end{aligned}$$

where τ stands for Tt . The minus sign applies when $\tau > 0$ and the plus sign when $\tau < 0$. This sign convention corresponds to staying consistently on the same branch of the square root. It is important to notice that $\sqrt{\tau^2 + c^2 - i\tau}$ has two branch points at

$$\tau_{1,2} = i \left(\frac{1}{2} \pm \sqrt{c^2 + \frac{1}{4}} \right) \quad (4.2)$$

Hence Eq. (1.5) applies for $c^2 > 0$.

From Eq. (4.1) and (2.8) we get

$$\chi_2(t) = e^{2\alpha w_2^{dc}} \exp \left\{ -\alpha w_2 \left[G_{2 \text{ even}}(t) + i G_{2 \text{ odd}}(t) \right] \right\} \quad (4.3)$$

where

$$G_{2 \text{ even}}(t) = d\sqrt{2} \sqrt{\sqrt{(T^2 t^2 + c^2)^2 + T^2 t^2} + T^2 t^2 + c^2} \quad (4.4)$$

and

$$G_{2 \text{ odd}}(t) = -\eta d\sqrt{2} \sqrt{\sqrt{(T^2 t^2 + c^2)^2 + T^2 t^2} - T^2 t^2 - c^2} \quad (4.5)$$

with

$$\left. \begin{aligned} \eta &= +1 \text{ for } t > 0 \\ \eta &= -1 \text{ for } t < 0 \end{aligned} \right\} \quad (4.6)$$

Thus we have factored χ_2 into a product of an even and an odd function of t . Now combining χ_2 with χ_3 as given by Eq. (2.14) we obtain

$$\chi(\alpha, t) = \exp \left\{ -\alpha w_2 \left[-2dc + G_{2 \text{ even}}(t) + i G_{2 \text{ odd}}(t) \right] + \alpha w_3 [\gamma(t) - \gamma(0)] \right\} \quad (4.7)$$

Recalling Eq. (2.18) and introducing the functions

$$\overline{H}(t) = -w_2 G_{2 \text{ even}}(t) + w_3 H(t) \quad (4.8)$$

$$\overline{F}(t) = -w_2 G_{2 \text{ odd}}(t) + w_3 F(t) \quad (4.9)$$

and

$$\overline{D} = \exp \left\{ \alpha \left[2 w_2 dc - w_3 \gamma(0) \right] \right\} \quad (4.10)$$

Eq. (4.7) can be rewritten in the more compact form

$$\chi(t) = \overline{D} \exp \left\{ \alpha \left[\overline{H}(t) + i \overline{F}(t) \right] \right\} \quad (4.11)$$

Notice that $\overline{H}(t)$ is even and $\overline{F}(t)$ is odd. This permits us to write the Fourier transform of Eq. (4.11) in the form

$$\mathcal{L}(\alpha, \beta) = \frac{\overline{D}}{\pi} \int_0^{\infty} \cos [\beta Tt + \alpha \overline{F}(t)] \exp [\alpha \overline{H}(t)] dt \quad (4.12)$$

Now for the same reason given in the preceding section, we want to separate from Eq. (4.12) the contribution due to the zero-phonon term. Hence we write

$$\begin{aligned} \mathcal{L}(\alpha, \beta) = & \frac{\overline{D}}{\pi} \int_0^{\infty} dt \left\{ \cos [\beta Tt + \alpha \overline{F}(t)] \exp [\alpha \overline{H}(t)] - \right. \\ & \left. - \cos [\beta Tt - \alpha w_2 G_{2 \text{ odd}}(t)] \exp [-\alpha w_2 G_{2 \text{ even}}(t)] \right\} + \\ & + \frac{\overline{D}}{\pi} \int_0^{\infty} dt \cos [\beta Tt - \alpha w_2 G_{2 \text{ odd}}(t)] \exp [-\alpha w_2 G_{2 \text{ even}}(t)] \end{aligned}$$

or else

$$S(\alpha, \beta) = S^{(1)}(\alpha, \beta) + S^{(2)}(\alpha, \beta)$$

with

$$\begin{aligned} S^{(2)}(\alpha, \beta) = & \exp \left\{ \alpha \left[2w_2 dc - w_3 \dot{\gamma}(0) \right] \right\} \frac{2 \alpha w_2 d \left(c^2 + \frac{1}{4} \right)^{1/2}}{T \pi \left[\beta^2 + (2 \alpha w_2 d)^2 \right]^{1/2}} \cdot \\ & \cdot K_1 \left\{ \left(c^2 + \frac{1}{4} \right)^{1/2} \left[\beta^2 + (2 \alpha w_2 d)^2 \right]^{1/2} \right\} \end{aligned}$$

which follows from Eq. (2.11), and

$$S^{(1)}(\alpha, \beta) = \frac{e^{\beta/2\overline{D}}}{\pi} \int_0^\infty dt [Q(t) \cos \beta Tt - R(t) \sin \beta Tt]$$

where

$$Q(t) = \cos [\alpha \overline{F}(t)] \exp [\alpha \overline{H}(t)] - \cos [\alpha w_2 G_{2 \text{ odd}}(t)] \exp [-\alpha w_2 G_{2 \text{ even}}(t)]$$

and

$$R(t) = \sin [\alpha \overline{F}(t)] \exp [\alpha \overline{H}(t)] + \sin [\alpha w_2 G_{2 \text{ odd}}(t)] \exp [-\alpha w_2 G_{2 \text{ even}}(t)]$$

The parallel with the preceding section is quite obvious.

5. COMBINATION OF DISCRETE MODES OF VIBRATION WITH ANY ADMIXTURE OF THE OTHER FOUR DYNAMICAL MODES

The discrete modes of oscillation are taken into account by convolving the scattering law obtained from the translational, diffusive and distributed vibrational modes, with the n -phonon terms corresponding to the different discrete oscillators. This convolution is done recursively for the part we have called $S^{(1)}$ in Sections 3 and 4, and analytically, as a multiple sum for $S^{(2)}$. For $S^{(1)}$ we write

$$S_k^{(1)}(\alpha, \beta) = \sum_{n=-N_k}^{N_k} C_k^{(n)}(\alpha) S_{k-1}^{(1)}\left(\alpha, \beta - n \frac{\omega_k}{T}\right) \quad (5.1)$$

where the coefficients $C_k^{(n)}(\alpha)$ were defined by Eq. (2.29). In the present section the symbol $S_k^{(i)}(\alpha, \beta)$ ($i = 1$ or 2) shall denote the scattering law ($S^{(1)}$ or $S^{(2)}$) computed including all contributions but the discrete oscillators of frequencies ω_{k+1} and higher. The limit N_k of the sum in Eq. (5.1) is the maximum number of phonons of frequency ω_k to be considered in the calculation of $S(\alpha, \beta)$; clearly it must be of the order

$$N_k \sim \frac{T\beta_{\max}}{\omega_k} \quad (5.2)$$

if $T\beta_{\max}$ is the maximum energy exchange for which a kernel is going to be evaluated.

The values of $S_{k-1}^{(1)}$ at the arguments $\beta T - n\omega_k$ required in Eq. (5.1) are determined by logarithmic interpolation between the values obtained for $S_{k-1}^{(1)}(\alpha, \beta)$ at the previous stage of recursion.

For $S^{(2)}$ the same recursive procedure could be used. However, since the unconvolved $S^{(2)}(\alpha, \beta)$ is calculated analytically, it is more convenient to write out $S^{(2)}$ explicitly as a multiple sum, which by repeated application of Eq. (5.1) must have the form:

$$S_k^{(2)}(\alpha, \beta) = \sum_{n_1=-N_1}^{N_1} \dots \sum_{n_k=-N_k}^{N_k} C_1^{(n_1)}(\alpha) \dots C_k^{(n_k)}(\alpha) S_o^{(2)}\left(\alpha, \beta - \sum_{i=1}^k n_i \omega_i / T\right) \quad (5.3)$$

In practice, the number of discrete oscillators hardly exceeds $k = 2$, so that for the time being this will be the maximum k allowed for. Each term in Eq. (5.3) is obtained analytically equating $S_o^{(2)}(\alpha, \beta)$ to the expression (3.8).

6. APPROXIMATIONS MADE IN GASKET

6.1 SHORT COLLISION APPROXIMATION

For large values of α and β it is convenient to make Wick's short collision approximation for the vibrational modes with continuous isotropic frequency spectrum (Mode 3). This approximation is obtained by expanding the corresponding G-function in powers of t and retaining terms up to t^2 . Then, if diffusive and anisotropic vibrational modes are absent ($w_2 = w_4 = 0$) one obtains the following analytical expression for the unconvolved scattering law (i. e., before convolving with the discrete modes):

$$e^{-\beta/2} S(\alpha, \beta) = \frac{e^{-\frac{\beta T}{2\bar{T}}}}{\sqrt{4\pi\alpha w T \bar{T}}} \exp \left[-\frac{T}{4\alpha w \bar{T}} (\beta^2 + w^2 \alpha^2) \right] \quad (6.1)$$

with

$$w\bar{T} = w_1 T + w_3 \bar{T}_3 \quad (6.2)$$

and

$$w = w_1 + w_3 \quad (6.3)$$

$\bar{T}_3$ is the effective temperature associated with the (isotropic) distributed modes of vibration:

$$\overline{T}_3 = 1/2 \int_0^{\infty} f(\omega) \omega \coth \frac{\omega}{2T} d\omega \quad (6.4)$$

Expression (6.1) is meant only for downscattering ($\beta < 0$). Upscattering should be calculated by detailed balance:

$$S(\alpha, \beta) = S(\alpha, -\beta)$$

Clearly Eq. (6.1) does not satisfy this relation, but this is not important for large values of $|\beta|$ where upscattering becomes very small. The short collision approximation for Mode 3 can save a considerable amount of computing time. It is used in GASKET when either $|\beta| > \beta_{sw}$ or $\alpha > \alpha_{sw}$, where β_{sw} and α_{sw} are two input numbers. When this approximation is used, the zero-phonon term which was called $S^{(2)}(\alpha, \beta)$ in Eq. (3.7) must be set equal to zero since all phonon terms are included in the approximate expression (6.1). Actually two cases must be considered. First, for $\alpha > \alpha_{sw}$ the quantity $S_k^{(2)}(\alpha, \beta)$ (see Eq. 5.3) must be set to zero for all β 's; second for $|\beta| > \beta_{sw}$ but $\alpha < \alpha_{sw}$, the quantity $S_o^{(2)}(\alpha, \beta - \sum_i n_i \omega_i / T)$ must be equated to zero whenever the argument $|\beta - \sum_i n_i \omega_i / T|$ exceeds β_{sw} .

6.2 TRUNCATION OF THE PHONON EXPANSION FOR MODE 5

Equation (5.3) has been programmed for a maximum of two discrete oscillators ($k = 2$). But not all the terms of Eq. (5.3) are actually calculated. The criterion for dropping small contributions is as follows: For each n_2 in the interval

$$-N_2 \leq n_2 \leq N_2$$

the exponential factor in

$$S_o^{(2)} \left[\alpha, \beta - (n_1 \omega_1 + n_2 \omega_2) / T \right]$$

is largest when the argument

$$\lambda \equiv \left| \beta - (n_1 \omega_1 + n_2 \omega_2) / T \right|$$

is minimum. Since this exponential factor gives the dominant behavior, terms are dropped for which

$$\exp \left(- \frac{\lambda^2}{4\alpha} \right) < \sigma \exp \left(- \frac{\lambda_{\min}^2}{4\alpha} \right)$$

where σ is a very small (input) number. This is the same as

$$\lambda^2 - \lambda_{\min}^2 > 4\alpha \log \sigma$$

As for the terms in $S^{(1)}$, the logarithmic interpolation is carried out only when the contributions are expected to be significant, as discussed in Section 7.2.10.

7. PROGRAM DESCRIPTION

7.1 MAIN PROGRAM*

The main program of GASKET controls the over-all flow of the calculation, using subroutines for most of the detailed calculation. This description of the main program follows the flow chart of Fig. 1. The numbers in parentheses refer to the box numbers on the flow chart.

The short collision time expression for $S(\alpha, \beta)$, as given by Formula 6.1, is included as an arithmetic function SCT at the beginning of the main program, with arguments α , β , T , $\bar{T}$ and W (weight).

(1) All input and preliminary calculations are performed by subroutine PREP.

(2) If $w_3 = 0$ (no distributed frequency spectrum), boxes 3, 4, and 5, which refer to Mode 3 only, are skipped.

(3) If $IPG \neq 0$ (precalculated t , $\bar{T}$, $F(t)$ and $H(t)$ available for input on cards), box 4 is skipped (this is a convenient option for polyatomic crystals like BeO).

(4) The integrals $F(t)$ and $H(t)$, Formulas 3.4 and 3.5, are calculated by the subroutine GTG (F and H are called GS and GC in the code itself). GTG also calculates $\bar{T}$ for Mode 3 according to Eq. 6.4.

(5) An effective temperature, $TBAR13$, for calculating $S(\alpha, \beta)$ for Modes 1 and 3 in short collision time, is evaluated. The Debye-Waller integral is obtained as $\frac{M}{w_3} H(t=0)$ (for output only).

* The coding of Modes 2 and 4 and their combination with the remaining ones has not yet been completed. Hence in this first version it will always be assumed that $w_2 = w_4 = 0$.

Fig. 1--Flow chart for GASKET

(6) IF JS5 = 0 (no discrete lines), box 7, which calculates the contribution to the total effective temperature from the discrete lines, is skipped.

(7, 8) An over-all effective temperature for Modes 1, 3, and 5 is calculated (for output only).

(9) The main loop over all α values covers the range IP = NREST to NP, the maximum number of α points. For a new problem, NREST = 1. For a restarted problem for which a scratch tape containing $S(\alpha, \beta)$ values for $\alpha(1), \dots, \alpha(N)$ has been saved, NREST = N + 1. One further option is available: to recalculate S values beyond some $\alpha(N)$ for an existing $S(\alpha, \beta)$ deck, NREST is input as $-(N + 1)$ along with the $S(\alpha, \beta)$ deck.

(10) The value of $S(\alpha, \beta)$ in short collision approximation, calculated for all β and the current $\alpha(IP)$, is placed in the arrays SC, S, and S1. The Debye-Waller factor is set to 1, and S2 is set to 0.*

(11) If $\alpha(IP)$ is greater than α_{sw} , the value of α beyond which $S(\alpha, \beta)$ for Modes 1 and 3 is to be calculated completely in the short collision approximation, control is transferred to the convolution section (Mode 5). Notice that when $w_3 = 0$, TBAR13 = T1 (box 1).

(12) If $\alpha < \alpha_{sw}$ and $w_3 = 0$ (no distributed frequency spectrum), S1 is set to 0 (box 16), and control transfers to box 19.

(13) The $w_3 \neq 0$ calculation begins with the Debye-Waller factor, DBW, given by Eq. 2.17, or $DBW = \exp \left[-\frac{\kappa^2}{2} H(0) \right]$.

(14) The functions Q(t) and R(t), Formulas 3.11 and 3.12, are evaluated for the entire set of t values.

*In the present section S1 and S2 denote the quantities which in earlier sections were called $S^{(1)}$ and $S^{(2)}$.

(15) A check is made (subroutine ENDPT) to find the largest t value needed for the main Fourier transformation (which takes $\sim 85\%$ of the calculating time) by examining the behavior of the $Q(t)$ and $R(t)$ functions. Sums of the absolute value of sets of 20 adjacent $Q(t)$ or $R(t)$ are compared to an input convergence criterion (CRIT3) multiplied by $Q(0)$, the largest value of $Q(t)$ and $R(t)$. This test has produced reasonable upper time integration limits for most moderators calculated so far (H_2O , D_2O , Be, C, CH_2 , etc.) except for ZrH. The convergence criterion for this particular moderator has to be made extremely small to include the significant areas of Q and R in the integration limits. *

(16, 17) The actual Fourier transformation is done by subroutine SCINT, for values of $\beta \leq \beta_{sw}$, the value of β above which $S1(\alpha, \beta)$ is calculated in short collision approximation. The subroutine SCINT calculates the nonsymmetric scattering law $S^{(1)}(\alpha, \beta)$, which for numerical reasons is better calculated for negative β -values (downscattering). Since by input $\beta \geq 0$, the sign of the β 's supplied to SCINT must be reversed. The resulting $S^{(1)}(\alpha, \beta)$ is then converted to the symmetric form $S1(\alpha, \beta)$ by dividing by $\exp \frac{|\beta|}{2}$. Any negative values of $S1(\alpha, \beta)$ (which can only be due to numerical error) are replaced by 0.

(18) $S1(\alpha, \beta)$ for $\beta > \beta_{sw}$ is set to the SCT value.

(19) IF $w_1 = 0$ or $NDAM \neq 0$, control is transferred to box 21.

* The explanation for this can be found in the following argument. For large α the absolute value of the functions $Q(t)$ and $R(t)$ (Eqs. 3.11 and 3.12) becomes very large for $H(t) > 0$ and very small for $H(t) < 0$ (actually in the latter case $Q(t) \sim -1$ and $R(t) \sim 0$). Hence in order to avoid stopping the calculation in the first region of negative $H(t)$ it is necessary to make $CRIT3 < 20/Q(0)$ which for large α is a very small number. Now ZrH, because of its frequency spectrum and because $M = 1$ (main scatterer is H) requires a larger α_{sw} and hence a smaller CRIT3 value, than any one of the other moderators considered so far.

(20) S2 is evaluated according to Eq. 3.8.

(21) Finally, the total scattering law is gotten by adding the distributed and free gas parts, $S(\alpha, \beta) = S1(\alpha, \beta) + S2(\alpha, \beta)$. However, if the free gas contribution has only been included as a device to speed up convergence of the Fourier transformation ($NDAM \neq 0$), $S(\alpha, \beta) = S1(\alpha, \beta)$ only.

(22) Output for the unconvolved scattering law is printed if $\alpha < \alpha_{sw}$.

(23) If there are no discrete lines ($JS5 = 0$), control is transferred to the end of the α loop. If $JS5 \neq 0$, provision is made for recursive convolution of $S1(\alpha, \beta)$, with up to 20 lines, and for analytical convolution of $S2(\alpha, \beta)$ with either one or two lines. More subroutines can be added for the analytic convolution of $S2(\alpha, \beta)$ with more than two lines if necessary.

(23a) The coefficients for convolution of discrete lines with the scattering law already obtained for Modes 1 and 3, are calculated according to Formula 2.29.

(24, 25) If $w_3 \neq 0$ the recursive convolution routine (RCØNV) is called for S1.

(26, 27, 28, 29) The one or two line analytic convolution routine (ACØN2 or ACØN1) is called for S2 if $w_1 \neq 0$ and $\alpha < \alpha_{sw}$. The analytic convolution routines do not add contributions to S2 from any $\beta > \beta_{sw}$, since for $\beta > \beta_{sw}$ $S1(\alpha, \beta)$ contains the full contribution to the scattering law. In order to combine Modes 1 and 5 (free gas and one or two discrete lines) when $w_3 = 0$, α_{sw} should be set to a larger value than the largest α to be calculated (otherwise the convolution routine would be bypassed for $\alpha > \alpha_{sw}$). Also β_{sw} should be larger than β_{max} .

(30) The total convolved scattering law is calculated for all β .

(31) Output for the convolved scattering law is printed (for all α).

(32) At the end of the α loop, $S(\alpha, \beta)$ is written on a scratch unit for later use by ERRMAP (which needs to have the entire $S(\alpha, \beta)$ array available in memory at once) or for restarting the calculation if the problem should run out of time or a machine error should occur. If a warning time subroutine is available the code checks to see if the warning period has started and terminates the calculation at the current α value if it has.

(33, 34) If time has not run out, the calculation is repeated until $\alpha = \alpha_{\max}$.

(35) Subroutine ERRMAP is called to produce punched and printed output for $S(\alpha, \beta)$ and an error map which estimates the errors made in interpolating logarithmically in either α or β .

The basic flow of the code is for the general case $w_1 \neq 0$, $w_3 \neq 0$, $w_5 \neq 0$. All other calculations bypass part of this basic structure.

For $w_1 \neq 0$, $w_3 \neq 0$, $w_5 = 0$ the program bypasses all boxes from 23a to 31.

For $w_1 \neq 0$, $w_3 = w_5 = 0$, using $\alpha_{\text{sw}} > \alpha_{\max}$ the program follows the path (given by block numbers) 10, 11, 12, 16, 19, 20, 21, 22, 23, 32, 33, 34 and 10. If $w_5 \neq 0$, the sequence is 10, 11, 12, 16, 19, 20, 21, 22, 23, 23a, 24, 26, 27, 28, 29, 30, 31, 32, 33, 34 and 10.

For $w_1 = 0$, $w_3 \neq 0$, $w_5 = 0$, the path is: 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 21, 22, 23, 32, 33, 34 and 10 for $\alpha < \alpha_{\text{sw}}$ and 10, 11, 23, 32, 33, 34 and 10 for $\alpha > \alpha_{\text{sw}}$. For $w_5 \neq 0$, the sequence is 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 21, 22, 23, 23a, 24, 25, 26, 28, 30, 31, 32, 33, 34 and 10 for $\alpha < \alpha_{\text{sw}}$ and 10, 11, 23, 23a, 24, 25, 26, 28, 30, 31, 32, 33, 34 and 10 for $\alpha > \alpha_{\text{sw}}$. It should be mentioned, however, that the case $w_1 = 0$, $w_5 \neq 0$ is unphysical and leads to singular scattering kernels. Hence it should be avoided.

7.2 SUBROUTINES

a. PREP. This subroutine reads input data and calculates initial constants. Several variables are modified by the code after being read: the SCT switching parameters, α_{sw} and β_{sw} , are set to 100 if they have been left blank in the input; the convergence criteria for recursive convolution, analytic convolution, and for truncating the time integrals are set to 10^{-3} , 10^{-3} , and 10^{-5} if input is 0. The mass in unified AMU is converted to neutron mass units by dividing by 1.0086654. The weights w_i are normalized to unit sum and so are the a_k (oscillator weights for the different lines of Mode 5).

In order to check the adequacy of the frequency mesh, the expression

$$Z(\omega_i) = \frac{f_3(\omega_i) e^{\omega_i/2T_3}}{2 \omega_i \sinh(\omega_i/2T_3)}$$

is calculated and printed. This also gives an easy check on $\frac{1}{\alpha} S(\alpha, \beta)$ for very small α where this quantity becomes proportional to $Z(T\beta)$.

Although physically the temperature should be the same for all modes, the code allows for different temperatures for each mode. An over-all temperature, TEMP, is chosen as the maximum of the temperatures of the various modes if not specified in the input.

Meshes for α and β are either calculated by subroutines MESH, read in completely, or the β mesh is calculated by MESH and the α mesh is read in. Values of $p^2/2 = \alpha \cdot M \cdot \text{TEMP}$, and $\epsilon = \beta \cdot \text{TEMP}$, are calculated for later use. The time mesh is either read in directly or a series of time intervals for calculating the mesh are read. Values of the expressions $e^{\beta/2}$,

$$w_5 a_k / \left[M \omega_k \sinh \left(\frac{\omega_k}{2T_5} \right) \right]$$

and

$$w_5 \alpha_k / \left[M \omega_k \tanh \left(\frac{\omega_k}{2T_5} \right) \right]$$

are then calculated (where k is the oscillator index).

b. ERRMAP. ERRMAP produces printed and punched output for $S(\alpha, \beta)$. The printed output includes an error map which gives an estimate of the error made when interpolating $S(\alpha, \beta)$ (linearly in the logarithm of $S(\alpha, \beta)$) between neighboring mesh points. This estimate is obtained by comparing the value of S at each mesh point with that calculated from the two adjacent α or β points.

$S(\beta)$ is written on a scratch unit for each α as it is calculated, to save memory space during the main calculation; the $S(\alpha, \beta)$ array is read back into memory by ERRMAP, which requires all values of $S(\alpha, \beta)$ for its calculations. $S(\alpha, \beta)$ is multiplied by the temperature, T , at this point to produce values consistent with the definitions used in FLANGE.

c. SPCH. SPCH punches $S(\alpha_I, \beta_J)$ for a fixed J and the range of I 's given in $ILT(J)$ and $IHT(J)$. A subroutine for this punching was written to allow for adequate labeling of the punched output without complicating the ERRMAP routine. The labeling, in Columns 73-80, consists of the β -value index, J , in Columns 73-76 and a card sequence number (for this β -value block) in Columns 77-80. For a fixed J , $ILT(J)$ and $IHT(J)$ are the lower and higher limits, respectively, of the Index I for which $S(\alpha_I, \beta_J)$ satisfies the significance criterion described in the input instructions (Note 6).

d. MESH. MESH is used as a simple method for generating α and β meshes from a few numbers. The maximum α and β values are determined from the input maximum energy, $E_{\max}$, moderator temperature T , and scatterer mass M

$$\beta_{\max} = E_{\max}/T, \quad \alpha_{\max} = 4 \beta_{\max}/M.$$

The input numbers $\Delta\beta$, β_c , $\Delta\alpha$ and α_c are used to generate uniform α and β meshes over the ranges

$$\alpha = \Delta\alpha, 2\Delta\alpha, \dots, \alpha_c,$$

$$\beta = 0, \Delta\beta, 2\Delta\beta, \dots, \beta_c.$$

The remainder of the α, β meshes are then filled out with geometrically increasing α and β intervals, arranged to reach $\alpha_{\max}$ and $\beta_{\max}$ with the number of values requested in the input.

e. GTG. GTG evaluates Eqs. 3.4 and 3.5 for $F(t)$ and $H(t)$. The distributed frequency spectrum for Mode 3 is first normalized multiplying by the factor R , defined as

$$\frac{1}{R} = \int_0^{\omega_{\max}} f(\omega) d\omega = \frac{1}{3} f_1 \omega_1 + \frac{1}{2} \sum_{s=2}^{NS} (\omega_s - \omega_{s-1}) (f_s + f_{s-1}),$$

where NS is the number of points tabulated in the $f(\omega)$ array, and $f(\omega)$ is assumed proportional to ω^2 in the interval $0 \leq \omega \leq \omega_1$. All the ω_s are assumed nonzero, and it is understood that $\omega_0 = 0$. For $t=0$, subroutine INTG is used to evaluate $F(0)$ and $H(0)$. For $t \neq 0$, subroutine FTRANS is used. Contributions from the interval $0 \leq \omega \leq \omega_1$ are calculated separately, using the ω^2 behavior of $f(\omega)$ explicitly.

f. FTRANS. This routine is used by GTG to evaluate the integrals appearing in Eqs. 3.4 and 3.5, namely:

$$\frac{1}{w_3 T} H(t) = \int_0^{\omega_{\max}} q(\omega) \cos \omega t d\omega$$

with

$$q(\omega) = \frac{f(\omega)}{\omega} \coth \frac{\omega}{2T}$$

and

$$\frac{1}{w_3 T} F(t) = \int_0^{\omega_{\max}} r(\omega) \sin \omega t d\omega$$

with

$$r(\omega) = \frac{f(\omega)}{\omega}$$

Since t can take rather large values, a straightforward trapezoidal integration would require too many meshpoints. However, if we take only the factors $q(\omega)$ and $r(\omega)$ of the integrand to be linear between meshpoints, the contribution from each interval can be obtained analytically. For the interval (ω_{s-1}, ω_s) the contributions to the two integrals are

$$\begin{aligned} H_s &= \frac{f(\omega_s)}{\omega_s} \coth (\omega_s / 2T) \left[\left(1 - \frac{\sin \theta_s}{\theta_s} \right) \sin \omega_s t + \left(\frac{1 - \cos \theta_s}{\theta_s} \right) \cos \omega_s t \right] \\ &- \frac{f(\omega_{s-1})}{\omega_{s-1}} \coth (\omega_{s-1} / 2T) \left[\left(1 - \frac{\sin \theta_s}{\theta_s} \right) \sin \omega_{s-1} t - \left(\frac{1 - \cos \theta_s}{\theta_s} \right) \cos \omega_{s-1} t \right] \end{aligned}$$

and

$$F_s = \frac{f(\omega_s)}{\omega_s} \left[\left(\frac{1 - \cos \theta_s}{\theta_s} \right) \sin \omega_s t - \left(1 - \frac{\sin \theta_s}{\theta_s} \right) \cos \omega_s t \right] \\ + \frac{f(\omega_{s-1})}{\omega_{s-1}} \left[\left(\frac{1 - \cos \theta_s}{\theta_s} \right) \sin \omega_{s-1} t + \left(\frac{1 - \sin \theta_s}{\theta_s} \right) \cos \omega_{s-1} t \right],$$

where

$$\theta_s = (\omega_s - \omega_{s-1}) t.$$

g. INTG. INTG is a trapezoidal integration routine for calculating the integral

$$I = \int_{x_1}^{x_N} f(x) dx, \quad N \geq 2$$

where $f(x)$ is assumed to be piecewise linear in each interval. The contribution of the interval (x_{s-1}, x_s) is

$$I_s = 1/2 (x_s - x_{s-1}) (f_s + f_{s-1}), \quad x_s \geq x_{s-1}.$$

h. SCINT. This routine is very similar to FTRANS and is used for evaluating the integral of Eq. 3.9

$$S(\lambda) = \int_0^{t_{\max}} dt [Q(t) \cos \lambda t - R(t) \sin \lambda t]$$

Adequate values for $t_{\max}$ will be discussed in Section 8.

For the special case $\lambda = 0$, the simple trapezoidal integration routine INTG is used. Otherwise using the same scheme as for FTRANS, the integral is calculated as a sum over contributions (corresponding to the interval t_{s-1}, t_s) of the form

$$S_s = Q_s \left(ST \cdot \sin t_s \lambda + CT \cdot \cos t_s \lambda \right) - Q_{s-1} \left(ST \cdot \sin t_{s-1} \lambda - CT \cdot \cos t_{s-1} \lambda \right) \\ - R_s \left(-ST \cdot \cos t_s \lambda + CT \cdot \sin t_s \lambda \right) + R_{s-1} \left(-ST \cdot \cos t_{s-1} \lambda - CT \cdot \sin t_{s-1} \lambda \right)$$

where

$$\left. \begin{aligned} ST &= \frac{1 - \sin \Delta}{\Delta} \\ CT &= \frac{1 - \cos \Delta}{\Delta} \end{aligned} \right\} \text{ for } \Delta = \lambda(t_s - t_{s-1}) > 0.005$$

or, to avoid loss of accuracy due to cancellation for small arguments Δ

$$\left. \begin{aligned} ST &= \frac{\Delta^2}{6} - \frac{\Delta^4}{120} \\ CT &= \frac{\Delta}{2} - \frac{\Delta^3}{24} \end{aligned} \right\} \text{ for } \Delta \leq 0.005$$

The nonsymmetric result of this routine is transformed back to the symmetric form by the main program immediately after it is calculated, dividing by the tabulated factor $\exp(\beta/2)$.

i. STERP and SNEAR. The recursive convolution of the scattering law corresponding to the continuous modes of vibration with the contribution from each one of the discrete modes requires values of $S1(\alpha, \beta)$ at arguments between β -meshpoints (see Eq. 5.1). The interpolation is

done linearly in the logarithm of S_1 by the subroutine STERP. This type of interpolation seems to be adequate for the various problems checked. Since the logarithmic interpolation is somewhat time consuming it is desirable to calculate only those terms of Eq. 5.1 which make a significant contribution to the sum. In order to discard the nonsignificant terms subroutine SNEAR makes a quick estimate of the interpolated S_1 by taking the average of its value at the two nearest β -mesh-point. The convolution subroutine (RCØNV) then decides whether or not to include this term in the sum. The β index is left available for STERP if the term is to be retained.

j. RCØNV. This subroutine performs the recursive convolution of S_1 as given by Eq. 5.1. The convolution is done no matter how the unconvolved S_1 was calculated, i.e., exactly by Eq. 3.9 ($\alpha < \alpha_{sw}$) or by the short collision approximation ($\alpha \geq \alpha_{sw}$).

A flow chart for RCØNV is given in Fig. 2. The sum in Eq. 5.1 is first done for $0 \leq n \leq N = \left[\frac{\epsilon(I)}{\omega_k} \right] + 1$, the range from which the principal contribution to $S_k^{(1)}$ is expected. The sum then ranges over the values $(-NPHØN(k) \leq n \leq -1)$ and $(N+1 \leq n \leq NPHØN(k))$, calculating contributions from terms for which $C_k^{(n)}(\alpha)$ are nonzero and for which the approximate contribution of the term to $S_k^{(1)}$, as calculated by SNEAR, satisfies a relative criterion. The symbol $[A]$ is used for the integral part of A .

k. ACØN1 and ACØN2. These are routines for the analytic convolution of $S_2(\alpha, \beta)$ for $\alpha < \alpha_{sw}$ and $\beta < \beta_{sw}$. ACØN1 is used for the convolution with a single discrete line, and ACØN2 for two lines. More routines may be added for a larger number of oscillators. The coding follows Eq. 5.3; a flow chart for ACØN2 is given (Fig. 3) to show the specific methods used. The coefficients $C_K^{(n)}$ are calculated in the main program. The function $SZ_2(x)$ is the expression for $S(\alpha, \beta)$ for a free gas (given in Eq. 2.7) at the current value of α .

Fig. 2--Flow chart for RCONV

$$SZ2(E) = 0 \sqrt{\frac{M}{2\pi\kappa^2 W_1 T_1}} \exp \left\{ -\frac{M}{2\kappa^2 W_1 T_1} \left[E^2 + \left(\frac{\kappa^2 W_1}{2M} \right)^2 \right] \right\}$$

Fig. 3--Flow chart for ACON2

1. BESSL. BESSL is a subroutine to calculate the $I_n(x)$ of Eq. 2.29 by a backward recursion technique available in the literature. ⁽⁹⁾

7.3 INPUT DESCRIPTION

The input to the code is described on the following pages. The column labeled "Report Symbol" lists the symbols used in the text that are different from the code symbols, which are the names actually used in the code.

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

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

<u>Item</u>	<u>Columns</u>	<u>Format</u>	<u>Code Symbol</u>	<u>Report Symbol</u>	<u>Description</u>
If JS3 = 0, Skip Cards 7 and 8 If IPG $\neq$ 0, Skip Cards 7 and 8					
7	1-70	7E10	X3	ω	If JS3 > 0, JS3 values of the frequency are read (eV). If JS3 < 0, X3(JS3) is read, and X3(I) = (I-1)X3(JS3)/ JS3 , I=1,..., JS3 .
If JS3 < 0 and X3(JS3) < 0, Skip Card 8 (Note 5)					
8	1-70	7E10	Q3	f(ω)	Distributed frequency spectrum, Mode 3. (Unnormalized)
If JS4 = 0, Skip Cards 9 and 10					
9	1-70	7E10	X4	ω	As in Cards 7 and 8 for Mode 4.
10	1-70	7E10	Q4	f(ω)	
If JS5 = 0, Skip Cards 11-13					
11	1-70	7E10	X5	ω_k	Frequencies of delta lines, Mode 5. (eV) ($\omega_1 < \omega_2 < \dots < \omega_{JS5}$)
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 $\leq$ 20 for each line.
If NMESH = 0, Skip Card 14					
14	1-10	E10	EMAX	$E_{\max}$	Maximum energy of mesh chosen. (eV)
	11-20	E10	DALPHA	$\Delta\alpha$	α interval. ($\alpha_1 = \text{DALPHA}$, $\alpha_2 = 2 \cdot \text{DALPHA}$, ..., $\alpha = \text{ALPHAC}$)
	21-30	E10	ALPHAC	α_c	α value at which mesh spacing begins increasing geometrically.

<u>Item</u>	<u>Columns</u>	<u>Format</u>	<u>Code Symbol</u>	<u>Report Symbol</u>	<u>Description</u>
	31-40	E10	DBETA	$\Delta\beta$	β interval. ($\beta_1 = 0$, $\beta_2 = \text{DBETA}$, $\beta_3 = 2 \text{ DBETA}$, ..., $\beta = \text{BETAC}$)
	41-50	E10	BETAC	β_c	β value at which mesh spacing begins increasing geometrically.
If NMESH > 0, Skip Cards 15 and 16					
15	1-70	7E10	ALPHA	α	α mesh
If NMESH < 0, Skip Card 16					
16	1-70	7E10	BETA	β	β mesh ($\beta \geq 0$)
If IPG = 0, Skip Cards 17-19					
17	1-10	E10	TBAR	$\bar{T}$	Effective temperature for Mode 3 (eV).
18	1-80	8E10	T	t	Integration time values (sec).
19	1-80	8E10	GS, GC	H, F	Values of the pre-calculated GS and GC functions, in the order (GS(I), GC(I), I=1, NT).
If NT < 0, Skip Card 20					
20	1-70	7E10	T	t	Integration time points (eV^{-1})
If NT > 0, Skip Card 21					
21	1-10	E10	DT	Δt	Δt (eV^{-1}) for time mesh.
	11-20	E10	TMAX		t max (eV^{-1}) ($ NT $ sets, see Note 1)
22	1-10	I10	ID		Numeric identification for S(α, β) deck.

<u>Item</u>	<u>Columns</u>	<u>Format</u>	<u>Code Symbol</u>	<u>Report Symbol</u>	<u>Description</u>
	11-20	I10	NPT		$S(\alpha, \beta)$ output option. NPT = 0 to punch on cards, NPT = 1 to write a binary output tape, NPT = 2 to do both.
	21-30	E10	SIGF	σ_f	Free atom cross section. (barns)
	31-40	E10	EPS		Significance Criterion for $S(\alpha, \beta)$ output. (Note 6)

If NREST $\geq$ 0, Skip Card 23

23

$S(\alpha, \beta)$ deck in ENDF/A format. (Note 7)

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

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

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

Note 4. Time integrals are cut off at t_i if $\max(\sum_{j=1}^{i+19} Q_j, \sum_{j=1}^{i+19} R_j)/Q_1 \leq CRIT3$.

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

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

Note 7. If NREST < 0, a previously calculated $S(\alpha, \beta)$ deck is read and all α points from $|NREST|$ on are re-calculated.

7.4 OUTPUT DESCRIPTION

7.4.1 Printed Output

The first section of output consists of the input data and a few calculated quantities: The values of $\kappa^2/2 = \alpha MT$ corresponding to each α , $\epsilon = \beta T$ for each β , the Debye-Waller integral $\gamma(0)$ (Eq. 2.16), the effective temperature for Mode 3 (Eq. 6.4) (if $w_3 \neq 0$), and the over-all effective temperature for Modes 1, 3 and 5 (if $w_3 \neq 0$).

If $NGPRT \neq 0$, the integrals F and H (Eqs. 3.4 and 3.5) are printed for each t value.

If $NCP \neq 0$ and $w_3 \neq 0$, the functions Q and R (Eqs. 3.11 and 3.12) are printed for each t value.

The main calculation evaluates the scattering law as a function of β for each α . For $\alpha < \alpha_{sw}$, each block of output is headed by the α values, the number of points used in the basic integration for S_1 (Eq. 3.9), and the Debye-Waller factor (Eq. 2.17). The rest of the block consists of β and the unconvolved values of S_1 , $S_1 e^{\beta/2}$, S_2 , $S_2 e^{\beta/2}$, S , $S e^{\beta/2}$ and a last column giving $S e^{\beta/2}$ in the short collision approximation. If $w_5 \neq 5$ each one of the preceding blocks is followed by another one giving the coefficients $C_k^{(n)}$ (Eq. 2.29) and then the convolved scattering law in the same format as the unconvolved data. For $\alpha > \alpha_{sw}$ only the convolved data is printed (if $w_5 \neq 0$). When $w_5 \neq 0$ there is no output for $\alpha > \alpha_{sw}$.

If a timing subroutine is available, the fraction of computation time used for calculating the Q and R functions, $T(CHI)$, for performing the S_1 integration, $T(S)$, for the recursive and analytic convolution with two discrete oscillators, $T(C\emptyset NV1)$ and $T(C\emptyset NV2)$ are printed.

The rest of the output relates to the total S ($S_1 + S_2$) if $NSEP = 0$, (the usual case) or is repeated for S_1 , S_2 , and $S_1 + S_2$ if $NSEP \neq 0$, in which case separate punched output also is produced for S_1 , S_2 and for use by later codes, giving $SP(\alpha, \beta) = TS(\alpha, \beta)$ (see footnote on page 2).

$SP(\alpha, \beta)$ is then printed as a function of α for each β but only for the range in which the significance criterion (described in the input) is satisfied.

Interpolation error maps for β interpolation for fixed α and for α interpolation for fixed β are printed last.

Sample output for H bound in H_2O at room temperature is given on the following pages.

H2O- MODIFIED 1965 ENGLISH FREQUENCY SPECTRUM. SAB NUMBER 5

NT= -5 NP= 2 NE= 80 NDAM= 0 NGPRT= 1 NCP= 1 NMESH= 1 NREST= -0 NCVP=-0 NSEP=-0 IPG=-0

JS3= 29 JS4= 0 JS5= 2

W1-W5= 5.555560-02 0.000000 4.444444-01 0.000000 5.000000-01

T1-T5= 2.550000-02 0.000000 2.550000-02 0.000000 2.550000-02

M= 1.000000+00 D= 0.000000

SCT FOR S.LT.U OR BETA.GT. 2.000000+01 OR ALPHA.GT. 2.000000+01

CRITERION FOR CONVOLUTION OF PART 1= 1.000000-03 CRITERION FOR CONVOLUTION OF PART 2= 1.000000-03

CRITERION FOR TRUNCATION OF TIME INTEGRALS= 1.000000-05

MODE 3

	OMEGA	RHO(OMEGA)	OPHON(OMEGA)
1	6.375000-03	1.250000-03	8.664337-01
2	1.275000-02	5.000000-03	9.966644-01
3	1.912500-02	1.125000-02	1.114856+00
4	2.350000-02	2.000000-02	1.240766+00
5	3.187500-02	3.125000-02	1.374070+00
6	3.825000-02	4.500000-02	1.514373+00
7	4.462500-02	5.900000-02	1.600202+00
8	5.100000-02	7.500000-02	1.700761+00
9	5.737500-02	9.500000-02	1.850852+00
10	6.375000-02	1.150000-01	1.965238+00
11	6.630000-02	1.197000-01	1.950294+00
12	6.885000-02	1.214000-01	1.890291+00
13	7.140000-02	1.218000-01	1.816334+00
14	7.395000-02	1.195000-01	1.710049+00
15	7.650000-02	1.125000-01	1.547641+00
16	8.287500-02	9.750000-02	1.223927+00
17	8.925000-02	8.710000-02	1.006298+00
18	9.562500-02	7.910000-02	8.471117-01
19	1.020000-01	7.350000-02	7.340325-01
20	1.083750-01	6.880000-02	6.440192-01
21	1.147500-01	6.500000-02	5.728122-01
22	1.211250-01	6.100000-02	5.080071-01
23	1.275000-01	5.710000-02	4.508811-01
24	1.338750-01	5.400000-02	4.054891-01
25	1.402500-01	5.150000-02	3.887082-01
26	1.466250-01	4.880000-02	3.338845-01
27	1.530000-01	4.590000-02	3.007455-01
28	1.593750-01	4.310000-02	2.709544-01
29	1.657500-01	4.200000-02	2.537752-01

ALPHA 2 = 1.000000-01 P**2/2= 2.528093-03
T, Q(T), R(T)

0.00	2.256-02	0.000	1.00-01	2.256-02	1.159-04	2.00-01	2.256-02	2.317-04	3.00-01	2.255-02	3.475-04
4.00-01	2.255-02	4.633-04	5.00-01	2.254-02	5.791-04	6.00-01	2.254-02	6.944-04	7.00-01	2.253-02	8.104-04
8.00-01	2.255-02	9.271-04	9.00-01	2.253-02	1.042-03	1.00+00	2.252-02	1.158-03	1.10+00	2.250-02	1.273-03
1.20+00	2.249-02	1.388-03	1.30+00	2.247-02	1.503-03	1.40+00	2.245-02	1.618-03	1.50+00	2.244-02	1.732-03
1.60+00	2.242-02	1.847-03	1.70+00	2.240-02	1.961-03	1.80+00	2.238-02	2.075-03	1.90+00	2.236-02	2.189-03
2.00+00	2.234-02	2.303-03	2.20+00	2.229-02	2.530-03	2.40+00	2.223-02	2.755-03	2.60+00	2.218-02	2.980-03
2.80+00	2.211-02	3.204-03	3.00+00	2.205-02	3.426-03	3.20+00	2.198-02	3.647-03	3.40+00	2.190-02	3.866-03
3.60+00	2.182-02	4.084-03	3.80+00	2.174-02	4.301-03	4.00+00	2.165-02	4.515-03	4.20+00	2.156-02	4.729-03
4.40+00	2.146-02	4.940-03	4.60+00	2.130-02	5.149-03	4.80+00	2.126-02	5.356-03	5.00+00	2.115-02	5.562-03
5.50+00	2.087-02	6.066-03	6.00+00	2.050-02	6.555-03	6.50+00	2.022-02	7.029-03	7.00+00	1.987-02	7.487-03
7.50+00	1.949-02	7.927-03	8.00+00	1.909-02	8.349-03	8.50+00	1.868-02	8.752-03	9.00+00	1.825-02	9.134-03
9.50+00	1.780-02	9.497-03	1.00+01	1.734-02	9.838-03	1.05+01	1.686-02	1.016-02	1.10+01	1.637-02	1.046-02
1.15+01	1.587-02	1.073-02	1.20+01	1.530-02	1.098-02	1.25+01	1.484-02	1.121-02	1.30+01	1.431-02	1.142-02
1.35+01	1.378-02	1.160-02	1.40+01	1.324-02	1.176-02	1.45+01	1.270-02	1.190-02	1.50+01	1.216-02	1.201-02
1.55+01	1.162-02	1.211-02	1.60+01	1.107-02	1.218-02	1.65+01	1.053-02	1.222-02	1.70+01	9.996-03	1.225-02
1.75+01	9.462-03	1.225-02	1.80+01	8.933-03	1.224-02	1.85+01	8.410-03	1.220-02	1.90+01	7.894-03	1.215-02
1.95+01	7.386-03	1.208-02	2.00+01	6.887-03	1.199-02	2.10+01	5.920-03	1.175-02	2.20+01	4.997-03	1.146-02
2.30+01	4.124-03	1.111-02	2.40+01	3.305-03	1.072-02	2.50+01	2.543-03	1.028-02	2.60+01	1.840-03	9.815-03
2.70+01	1.198-03	9.323-03	2.80+01	6.162-04	8.813-03	2.90+01	9.457-05	8.292-03	3.00+01	-3.684-04	7.766-03
3.10+01	-7.748-04	7.242-03	3.20+01	-1.127-03	6.724-03	3.30+01	-1.429-03	6.219-03	3.40+01	-1.684-03	5.729-03
3.50+01	-1.895-03	5.259-03	3.60+01	-2.060-03	4.810-03	3.70+01	-2.206-03	4.386-03	3.80+01	-2.315-03	3.988-03
3.90+01	-2.397-03	3.616-03	4.00+01	-2.457-03	3.270-03	4.10+01	-2.500-03	2.951-03	4.20+01	-2.529-03	2.656-03
4.30+01	-2.547-03	2.386-03	4.40+01	-2.550-03	2.138-03	4.50+01	-2.562-03	1.910-03	4.60+01	-2.564-03	1.699-03
4.70+01	-2.564-03	1.504-03	4.80+01	-2.562-03	1.323-03	4.90+01	-2.561-03	1.152-03	5.00+01	-2.560-03	9.891-04
5.10+01	-2.559-03	8.327-04	5.20+01	-2.557-03	6.807-04	5.30+01	-2.554-03	5.314-04	5.40+01	-2.549-03	3.833-04
5.50+01	-2.540-03	2.356-04	5.60+01	-2.525-03	9.738-05	5.70+01	-2.505-03	-6.161-05	5.80+01	-2.477-03	-2.114-04
5.90+01	-2.439-03	-3.617-04	6.00+01	-2.392-03	-5.118-04	6.10+01	-2.333-03	-6.609-04	6.20+01	-2.261-03	-8.077-04
6.30+01	-2.177-03	-9.511-04	6.40+01	-2.080-03	-1.099-03	6.50+01	-1.970-03	-1.221-03	6.60+01	-1.847-03	-1.345-03
6.70+01	-1.712-03	-1.458-03	6.80+01	-1.565-03	-1.560-03	6.90+01	-1.409-03	-1.650-03	7.00+01	-1.243-03	-1.725-03
7.10+01	-1.070-03	-1.784-03	7.20+01	-8.919-04	-1.828-03	7.30+01	-7.103-04	-1.854-03	7.40+01	-5.273-04	-1.863-03
7.50+01	-3.451-04	-1.855-03	7.60+01	-1.650-04	-1.830-03	7.70+01	8.489-06	-1.788-03	7.80+01	1.758-04	-1.731-03
7.90+01	3.341-04	-1.658-03	8.00+01	4.818-04	-1.572-03	8.10+01	6.174-04	-1.475-03	8.20+01	7.396-04	-1.367-03
8.30+01	8.473-04	-1.250-03	8.40+01	9.399-04	-1.127-03	8.50+01	1.017-03	-9.994-04	8.60+01	1.078-03	-8.693-04
8.70+01	1.123-03	-7.386-04	8.80+01	1.153-03	-6.093-04	8.90+01	1.169-03	-4.831-04	9.00+01	1.170-03	-3.617-04
9.10+01	1.159-03	-2.464-04	9.20+01	1.130-03	-1.387-04	9.30+01	1.104-03	-3.944-05	9.40+01	1.062-03	5.045-05
9.50+01	1.014-03	1.305-04	9.60+01	9.605-04	2.005-04	9.70+01	9.030-04	2.602-04	9.80+01	8.431-04	3.099-04
9.90+01	7.823-04	3.499-04	1.00+02	7.219-04	3.308-04	1.02+02	6.067-04	4.186-04	1.04+02	5.047-04	4.307-04
1.06+02	4.201-04	4.258-04	1.08+02	3.540-04	4.127-04	1.10+02	3.045-04	3.993-04	1.12+02	2.675-04	3.918-04
1.14+02	2.374-04	3.943-04	1.16+02	2.075-04	4.081-04	1.18+02	1.719-04	4.320-04	1.20+02	1.255-04	4.625-04
1.22+02	5.486-05	4.943-04	1.24+02	-1.102-05	5.212-04	1.26+02	-1.009-04	5.369-04	1.28+02	-2.011-04	5.356-04
1.30+02	-3.064-04	5.130-04	1.32+02	-4.099-04	4.667-04	1.34+02	-5.042-04	3.967-04	1.36+02	-5.822-04	3.052-04
1.38+02	-6.378-04	1.966-04	1.40+02	-6.664-04	7.721-05	1.42+02	-6.656-04	-4.576-05	1.44+02	-6.352-04	-1.645-04
1.46+02	-5.774-04	-2.714-04	1.48+02	-4.967-04	-3.602-04	1.50+02	-3.991-04	-4.260-04	1.52+02	-2.918-04	-4.658-04
1.54+02	-1.824-04	-4.791-04	1.56+02	-7.799-05	-4.675-04	1.58+02	1.496-05	-4.345-04	1.60+02	9.173-05	-3.853-04
1.62+02	1.494-04	-3.258-04	1.64+02	1.870-04	-2.625-04	1.66+02	2.057-04	-2.014-04	1.68+02	2.084-04	-1.475-04
1.70+02	1.991-04	-1.046-04	1.72+02	1.827-04	-7.477-05	1.74+02	1.643-04	-5.817-05	1.76+02	1.485-04	-5.341-05
1.78+02	1.390-04	-5.765-05	1.80+02	1.383-04	-6.704-05	1.82+02	1.473-04	-7.728-05	1.84+02	1.652-04	-8.407-05
1.86+02	1.900-04	-8.373-05	1.88+02	2.183-04	-7.356-05	1.90+02	2.463-04	-5.219-05	1.92+02	2.698-04	-1.972-05
1.94+02	2.847-04	2.231-05	1.96+02	2.879-04	7.107-05	1.98+02	2.774-04	1.228-04	2.00+02	2.524-04	1.732-04
2.02+02	2.136-04	2.178-04	2.04+02	1.632-04	2.528-04	2.06+02	1.044-04	2.750-04	2.08+02	4.142-05	2.825-04

50	6.120199+00	7.610490-04	1.623293-02	0.000000	0.000000	7.610490-04	1.623293-02	0.000000
51	6.563443+00	1.561679-04	4.157435-03	0.000000	0.000000	1.561679-04	4.157435-03	0.000000
52	7.050916+00	4.966772-06	1.687179-04	0.000000	0.000000	4.966772-06	1.687179-04	0.000000
53	7.587033+00	2.163358-06	9.607971-05	3.927476-11	1.744283-09	2.163397-06	9.608145-05	0.000000
54	8.176648+00	4.308697-06	2.569700-04	7.044151-04	4.201121-02	7.067238-04	4.226818-02	0.000000
55	8.825098+00	1.470964-06	1.213243-04	2.791676-27	2.302560-25	1.470964-06	1.213243-04	0.000000
56	9.538254+00	8.606470-07	1.013983-04	0.000000	0.000000	8.606470-07	1.013983-04	0.000000
57	1.032257+01	7.021547-07	1.224479-04	1.295327-18	2.258904-16	7.021547-07	1.224479-04	0.000000
58	1.118516+01	2.998274-07	8.048181-05	1.463696-16	3.928956-14	2.998274-07	8.048181-05	0.000000
59	1.213382+01	9.655766-08	4.164971-05	0.000000	0.000000	9.655766-08	4.164971-05	0.000000
60	1.317714+01	3.596675-08	2.613853-05	8.358740-27	6.074643-24	3.596675-08	2.613853-05	0.000000
61	1.432457+01	2.261981-08	2.917634-05	0.000000	0.000000	2.261981-08	2.917634-05	0.000000
62	1.558651+01	6.709279-09	1.626457-05	1.248943-17	3.027676-14	6.709279-09	1.626457-05	0.000000
63	1.697436+01	2.690562-09	1.305506-05	1.516095-39	7.356345-36	2.690562-09	1.305506-05	0.000000
64	1.850071+01	3.975542-09	4.137841-05	1.265685-09	1.317356-05	5.241227-09	5.455197-05	0.000000
65	2.017936+01	2.992977-09	7.211007-05	0.000000	0.000000	2.992977-09	7.211007-05	0.000000
66	2.202552+01	1.076232-09	6.526606-05	6.515948-31	3.951473-26	1.076232-09	6.526606-05	0.000000
67	2.405591+01	1.250334-10	2.092666-05	1.581383-13	2.646737-08	1.251915-10	2.095312-05	0.000000
68	2.628690+01	1.891594-13	9.669169-06	3.753986-23	1.918856-17	1.891594-13	9.669169-08	0.000000
69	2.874471+01	5.641120-14	9.844633-06	0.000000	0.000000	5.641120-14	9.844633-08	0.000000
70	3.144558+01	4.400706-15	2.963760-06	1.742641-38	1.173623-31	4.400706-15	2.963760-08	0.000000
71	3.441596+01	4.388356-16	1.305066-06	1.522896-24	4.528985-17	4.388356-16	1.305066-08	0.000000
72	3.768275+01	1.298725-16	1.977978-06	4.836780-13	7.366491-05	4.838079-13	7.368468-05	0.000000
73	4.127551+01	2.260237-17	2.075000-06	0.000000	0.000000	2.260237-17	2.075000-08	0.000000
74	4.522679+01	5.735845-21	3.797263-11	5.653500-26	3.742749-16	5.735901-21	3.797300-11	0.000000
75	4.957236+01	3.246324-22	1.887523-11	0.000000	0.000000	3.246324-22	1.897523-11	0.000000
76	5.435155+01	2.341486-24	1.485186-12	4.502017-38	2.855593-26	2.341486-24	1.485186-12	0.000000
77	5.960764+01	1.031549-24	9.059938-12	0.000000	0.000000	1.031549-24	9.059938-12	0.000000
78	6.538823+01	8.677360-29	1.371704-14	0.000000	0.000000	8.677360-29	1.371704-14	0.000000
79	7.174563+01	5.148887-31	1.954699-15	0.000000	0.000000	5.148887-31	1.954699-15	0.000000
80	7.373743+01	1.238695-32	1.550884-15	0.000000	0.000000	1.238695-32	1.550884-15	0.000000

ALPHA 1 = 5.000000-02

CONVOLVED

I	BETA	S1	S1*EXP(BETA/2)	S2	S2*EXP(BETA/2)	S	S*EXP(BETA/2)	SC7
1	0.000000	4.457161-02	4.457161-02	2.070261+02	2.070261+02	2.070707+02	2.070707+02	5.161419+01
2	8.000000-02	4.458013-02	4.639948-02	1.163782+02	1.211277+02	1.164228+02	1.211741+02	5.093986+01
3	1.600000-01	4.454587-02	4.825597-02	2.067338+01	2.239520+01	2.071793+01	2.244346+01	4.686902+01
4	2.400000-01	4.446297-02	5.013186-02	1.160498+00	1.308458+00	1.204961+00	1.358590+00	4.020254+01
5	3.200000-01	4.436302-02	5.206048-02	2.058594-02	2.415782-02	6.494895-02	7.621830-02	3.214849+01
6	4.000000-01	4.430879-02	5.411888-02	1.153958-04	1.409447-04	4.442419-02	5.425983-02	2.396664+01
7	4.800000-01	4.418169-02	5.616594-02	2.044100-07	2.598561-07	4.418190-02	5.616620-02	1.665686+01
8	5.600000-01	4.402300-02	5.824814-02	1.144215-10	1.513945-10	4.402300-02	5.824814-02	1.079242+01
9	6.400000-01	4.382599-02	6.035398-02	2.023984-14	2.787284-14	4.382599-02	6.035398-02	6.519040+00
10	7.200000-01	4.360716-02	6.250342-02	1.131355-18	1.621605-18	4.360716-02	6.250342-02	3.671031+00
11	8.000000-01	4.339110-02	6.473191-02	1.998406-23	2.981272-23	4.339110-02	6.473191-02	1.927223+00
12	8.800000-01	4.316867-02	6.702830-02	1.115481-28	1.732016-28	4.316867-02	6.702830-02	9.432254-01
13	9.600000-01	4.291369-02	6.935172-02	1.967585-34	3.179763-34	4.291369-02	6.935172-02	4.303664-01
14	1.040000+00	4.261937-02	7.168695-02	0.000000	0.000000	4.261937-02	7.168695-02	1.830631-01
15	1.120000+00	4.229910-02	7.405187-02	0.000000	0.000000	4.229910-02	7.405187-02	7.259431-02
16	1.200000+00	4.198034-02	7.649316-02	0.000000	0.000000	4.198034-02	7.649316-02	2.683761-02
17	1.280000+00	4.166947-02	7.902535-02	0.000000	0.000000	4.166947-02	7.902535-02	9.249638-03
18	1.360000+00	4.131524-02	8.155123-02	0.000000	0.000000	4.131524-02	8.155123-02	2.971973-03
19	1.440000+00	4.085617-02	8.393627-02	0.000000	0.000000	4.085617-02	8.393627-02	8.902351-04
20	1.520000+00	4.025270-02	8.607140-02	0.000000	0.000000	4.025270-02	8.607140-02	2.486016-04
21	1.600000+00	3.951182-02	8.793516-02	0.000000	0.000000	3.951182-02	8.793516-02	6.472061-05
22	1.680000+00	3.867949-02	8.959590-02	0.000000	0.000000	3.867949-02	8.959590-02	1.570800-05
23	1.760000+00	3.782777-02	9.119896-02	0.000000	0.000000	3.782777-02	9.119896-02	3.554174-06
24	1.840000+00	3.701943-02	9.289249-02	0.000000	0.000000	3.701943-02	9.289249-02	7.497141-07
25	1.920000+00	3.629960-02	9.480353-02	0.000000	0.000000	3.629960-02	9.480353-02	1.474322-07
26	2.000000+00	3.567954-02	9.698705-02	5.188928-37	1.410497-36	3.567954-02	9.698705-02	2.702890-08
27	2.080000+00	3.512846-02	9.938603-02	1.332450-32	3.769791-32	3.512846-02	9.938603-02	4.619595-09
28	2.160000+00	3.461256-02	1.019229-01	1.061210-28	3.183816-28	3.461256-02	1.019229-01	7.360700-10
29	2.240000+00	3.409221-02	1.044877-01	2.772443-25	8.497132-25	3.409221-02	1.044877-01	1.093387-10
30	2.320000+00	3.352084-02	1.069292-01	2.246513-22	7.166227-22	3.352084-02	1.069292-01	1.514147-11
31	2.400000+00	3.282197-02	1.089728-01	5.752451-20	1.909881-19	3.282197-02	1.089728-01	1.954797-12
32	2.480000+00	3.190530-02	1.102524-01	4.654637-18	1.608462-17	3.190530-02	1.102524-01	2.352744-13
33	2.560000+00	3.069176-02	1.103872-01	1.190180-16	4.280647-16	3.069176-02	1.103872-01	2.639899-14
34	2.647983+00	2.898670-02	1.089434-01	1.112061-15	4.179561-15	2.898670-02	1.089434-01	2.196001-15
35	2.744745+00	2.672965-02	1.054404-01	2.598746-15	1.025127-14	2.672965-02	1.054404-01	1.292323-16
36	2.851163+00	2.393803-02	9.958882-02	9.441763-16	3.928035-15	2.393803-02	9.958882-02	5.092042-18
37	2.968200+00	2.069995-02	9.130735-02	2.946151-17	1.299545-16	2.069995-02	9.130735-02	1.259006-19
38	3.096916+00	1.726498-02	8.121813-02	3.773988-20	1.775364-19	1.726498-02	8.121813-02	1.809440-21
39	3.238476+00	1.411060-02	7.124781-02	7.948045-25	4.013160-24	1.411060-02	7.124781-02	1.380880-23
40	3.394162+00	1.150761-02	6.280845-02	8.876821-32	4.844962-31	1.150761-02	6.280845-02	5.027514-26
41	3.565383+00	9.263575-03	5.519865-02	0.000000	0.000000	9.263575-03	5.519865-02	7.691121-29
42	3.753690+00	7.451831-03	4.858179-02	0.000000	0.000000	7.451831-03	4.858179-02	4.251848-32
43	3.960788+00	5.944439-03	4.307101-02	0.000000	0.000000	5.944439-03	4.307101-02	7.099854-36
44	4.188551+00	4.710013-03	3.824321-02	0.000000	0.000000	4.710013-03	3.824321-02	0.000000
45	4.439041+00	3.668620-03	3.376201-02	0.000000	0.000000	3.668620-03	3.376201-02	0.000000
46	4.714528+00	2.819819-03	2.978297-02	1.195653-33	1.262850-32	2.819819-03	2.978297-02	0.000000
47	5.017504+00	2.107853-03	2.590463-02	1.648128-23	2.025480-22	2.107853-03	2.590463-02	0.000000
48	5.350713+00	1.547833-03	2.247071-02	1.209211-20	1.755475-19	1.547833-03	2.247071-02	0.000000
49	5.717172+00	1.110277-03	1.935975-02	1.629987-27	2.842185-26	1.110277-03	1.935975-02	0.000000

50	6.120199+00	7.618362-04	1.624973-02	0.000000	0.000000	7.618362-04	1.624973-02	0.000000
51	6.563443+00	1.557112-04	4.145276-03	0.000000	0.000000	1.557112-04	4.145276-03	0.000000
52	7.050916+00	4.177554-06	1.419087-04	0.000000	0.000000	4.177554-06	1.419087-04	0.000000
53	7.587033+00	1.342314-06	5.961528-05	0.000000	0.000000	1.342314-06	5.961528-05	0.000000
54	8.176648+00	3.485631-06	2.078824-04	0.000000	0.000000	3.485631-06	2.078824-04	0.000000
55	8.825098+00	6.634535-07	5.472126-05	0.000000	0.000000	6.634535-07	5.472126-05	0.000000
56	9.538254+00	1.082969-07	1.275915-05	0.000000	0.000000	1.082969-07	1.275915-05	0.000000
57	1.032257+01	7.318258-08	1.276222-05	0.000000	0.000000	7.318258-08	1.276222-05	0.000000
58	1.118516+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
59	1.213382+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
60	1.317714+01	7.774136-10	5.649787-07	0.000000	0.000000	7.774136-10	5.649787-07	0.000000
61	1.432457+01	1.455350-08	1.877194-05	0.000000	0.000000	1.455350-08	1.877194-05	0.000000
62	1.558651+01	5.661792-09	1.372526-05	0.000000	0.000000	5.661792-09	1.372526-05	0.000000
63	1.697436+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
64	1.850071+01	7.601164-10	7.911477-06	0.000000	0.000000	7.601164-10	7.911477-06	0.000000
65	2.017936+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
66	2.202552+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
67	2.405591+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
68	2.628890+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
69	2.874471+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
70	3.144558+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
71	3.441596+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
72	3.768275+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
73	4.127551+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
74	4.522679+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
75	4.957236+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
76	5.435155+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
77	5.960764+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
78	6.538823+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
79	7.174563+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
80	7.373743+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

ANK(K,I)=	9.989633-01	1.860378-05	1.732299-10	1.075358-15	5.006623-21	1.864775-26	5.787978-32
	1.539857-37	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	

ANK(K,I)=	9.991150-01	7.232455-08	2.617737-15	6.316478-23	1.143103-30	1.654953-38	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	

50	6.120199+00	1.549751-03	3.305571-02	0.000000	0.000000	1.549751-03	3.305571-02	0.000000
51	6.563443+00	3.732471-04	9.936422-03	0.000000	0.000000	3.732471-04	9.936422-03	0.000000
52	7.050916+00	2.314747-05	7.863040-04	0.000000	0.000000	2.314747-05	7.863040-04	0.000000
53	7.587033+00	1.143852-05	5.080110-04	0.000000	0.000000	1.143852-05	5.080110-04	0.000000
54	8.176648+00	9.498607-06	5.664954-04	0.000000	0.000000	9.498607-06	5.664954-04	0.000000
55	8.825098+00	3.579507-06	2.952356-04	0.000000	0.000000	3.579507-06	2.952356-04	0.000000
56	9.538254+00	1.267061-06	1.492805-04	0.000000	0.000000	1.267061-06	1.492805-04	0.000000
57	1.032257+01	4.790771-07	8.354566-05	0.000000	0.000000	4.790771-07	8.354566-05	0.000000
58	1.118516+01	1.019609-07	2.736908-05	0.000000	0.000000	1.019609-07	2.736908-05	0.000000
59	1.213382+01	1.792510-08	7.731910-06	0.000000	0.000000	1.792510-08	7.731910-06	0.000000
60	1.317714+01	5.126942-09	3.725961-06	0.000000	0.000000	5.126942-09	3.725961-06	0.000000
61	1.432457+01	1.652382-08	2.131338-05	0.000000	0.000000	1.652382-08	2.131338-05	0.000000
62	1.558651+01	7.051833-09	1.709499-05	0.000000	0.000000	7.051833-09	1.709499-05	0.000000
63	1.697436+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
64	1.850071+01	1.367090-09	1.422900-05	0.000000	0.000000	1.367090-09	1.422900-05	0.000000
65	2.017936+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
66	2.202552+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
67	2.405591+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
68	2.628690+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
69	2.874471+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
70	3.144558+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
71	3.441596+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
72	3.768275+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
73	4.127551+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
74	4.522679+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
75	4.957236+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
76	5.435155+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
77	5.960764+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
78	6.538623+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
79	7.174563+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
80	7.873743+01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

ANK(K,I)=	9.979276-01	3.716898-05	6.922012-10	8.593948-15	8.002291-20	5.961094-25	3.700466-30
	1.968974-35	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	

ANK(K,I)=	9.982307-01	1.445211-07	1.046168-14	5.048710-22	1.827346-29	5.291161-37	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	

OSCILLATOR	ENERGY	WEIGHT	PHONONS
1	2.050000-01	3.333333-01	10
2	4.800000-01	6.666667-01	5

EMAX= .200000+01

ALPHA MESH, 2 POINTS, INTERVAL= .05000
 TRANSITION AT .50000 EXPANSION BY .00000

1	.05000	2	.10000
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BETA MESH, 80 POINTS, INTERVAL= .08000
 TRANSITION AT 2.50000 EXPANSION BY 1.09979

1	.00000	2	.08000	3	.16000	4	.24000	5	.32000	6	.40000	7	.48000
8	.56000	9	.64000	10	.72000	11	.80000	12	.88000	13	.96000	14	1.04000
15	1.12000	16	1.20000	17	1.28000	18	1.36000	19	1.44000	20	1.52000	21	1.60000
22	1.68000	23	1.76000	24	1.84000	25	1.92000	26	2.00000	27	2.08000	28	2.16000
29	2.24000	30	2.32000	31	2.40000	32	2.48000	33	2.56000	34	2.64798	35	2.74475
36	2.85116	37	2.96820	38	3.09692	39	3.23848	40	3.39416	41	3.56538	42	3.75369
43	3.96079	44	4.18855	45	4.43904	46	4.71453	47	5.01750	48	5.35071	49	5.71717
50	6.12020	51	6.56344	52	7.05092	53	7.58703	54	8.17665	55	8.82510	56	9.53825
57	10.32257	58	11.18516	59	12.13382	60	13.17714	61	14.32457	62	15.58651	63	16.97436
64	18.50071	65	20.17936	66	22.02552	67	24.05591	68	26.28890	69	28.74471	70	31.44558
71	34.41596	72	37.68275	73	41.27551	74	45.22679	75	49.57236	76	54.35155	77	59.60764
78	65.38823	79	71.74563	80	78.73743								

ALPHA, P**2/2

1	5.000000-02	1.264046-03	2	1.000000-01	2.528093-03
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BETA, EPS

1	0.000000	0.000000	2	8.000000-02	2.040000-03	3	1.600000-01	4.080000-03
4	2.400000-01	6.120000-03	5	3.200000-01	8.160000-03	6	4.000000-01	1.020000-02
7	4.800000-01	1.224000-02	8	5.600000-01	1.428000-02	9	6.400000-01	1.632000-02
10	7.200000-01	1.836000-02	11	8.000000-01	2.040000-02	12	8.800000-01	2.244000-02
13	9.600000-01	2.448000-02	14	1.040000+00	2.652000-02	15	1.120000+00	2.856000-02
16	1.200000+00	3.060000-02	17	1.280000+00	3.264000-02	18	1.360000+00	3.468000-02
19	1.440000+00	3.672000-02	20	1.520000+00	3.876000-02	21	1.600000+00	4.080000-02
22	1.680000+00	4.284000-02	23	1.760000+00	4.488000-02	24	1.840000+00	4.692000-02
25	1.920000+00	4.896000-02	26	2.000000+00	5.100000-02	27	2.080000+00	5.304000-02
28	2.160000+00	5.508000-02	29	2.240000+00	5.712000-02	30	2.320000+00	5.916000-02
31	2.400000+00	6.120000-02	32	2.480000+00	6.324000-02	33	2.560000+00	6.528000-02
34	2.647983+00	6.752356-02	35	2.744745+00	6.999100-02	36	2.851163+00	7.270466-02
37	2.968200+00	7.568911-02	38	3.096916+00	7.897137-02	39	3.239476+00	8.258115-02
40	3.394162+00	8.655114-02	41	3.565383+00	9.091728-02	42	3.753690+00	9.571910-02
43	3.960788+00	1.010001-01	44	4.188551+00	1.068080-01	45	4.439041+00	1.131956-01
46	4.714528+00	1.202205-01	47	5.017504+00	1.279463-01	48	5.350713+00	1.364432-01
49	5.717172+00	1.457879-01	50	6.120199+00	1.560651-01	51	6.563443+00	1.673678-01
52	7.050916+00	1.797984-01	53	7.587033+00	1.934693-01	54	8.176648+00	2.085045-01
55	8.325098+00	2.250400-01	56	9.538254+00	2.432255-01	57	1.032257+01	2.632256-01
58	1.118516+01	2.852216-01	59	1.213382+01	3.094124-01	60	1.317714+01	3.360171-01
61	1.432457+01	3.652766-01	62	1.558651+01	3.974559-01	63	1.697436+01	4.328462-01
64	1.850071+01	4.717680-01	65	2.017936+01	5.145737-01	66	2.202552+01	5.616508-01
67	2.405591+01	6.134256-01	68	2.628890+01	6.703669-01	69	2.874471+01	7.329901-01

70	3.144558+01	8.018623-01	71	3.441596+01	8.776070-01	72	3.768275+01	9.609100-01
73	4.127551+01	1.052526+00	74	4.522679+01	1.153283+00	75	4.957236+01	1.264095+00
76	5.435155+01	1.385965+00	77	5.960764+01	1.519995+00	78	6.538823+01	1.667400+00
79	7.174563+01	1.829514+00	80	7.873743+01	2.007804+00			

	DT	TMAX
1	1.000000-01	2.000000+00
2	2.000000-01	5.000000+00
3	5.000000-01	2.000000+01
4	1.000000+00	1.000000+02
5	2.000000+00	6.000000+02

DEBYE-WALLER INTEGRAL= 1.968378+01
TOTAL TBAR= 1.203628-01

TBAR (MODE 3)= 4.916647-02

T(CH)= 1.176505-01

G3(0)= 8.824152+00
1, T(I), G3C(I), G3S(I)

1	0.000000	8.824152+00	0.000000	2	1.000000-01	8.823930+00	4.481848-02
3	2.000000-01	8.823269+00	8.963273-02	4	3.000000-01	8.822167+00	1.344385-01
5	4.000000-01	8.820623+00	1.792316-01	6	5.000000-01	8.818639+00	2.240078-01
7	6.000000-01	8.816214+00	2.687629-01	8	7.000000-01	8.813350+00	3.134926-01
9	8.000000-01	8.820497+00	3.586382-01	10	9.000000-01	8.813885+00	4.032500-01
11	1.000000+00	8.809124+00	4.478512-01	12	1.100000+00	8.802428+00	4.923422-01
13	1.200000+00	8.797068+00	5.369147-01	14	1.300000+00	8.791122+00	5.813984-01
15	1.400000+00	8.784235+00	6.257702-01	16	1.500000+00	8.777453+00	6.701552-01
17	1.600000+00	8.770028+00	7.144140-01	18	1.700000+00	8.762769+00	7.586699-01
19	1.800000+00	8.754672+00	8.028387-01	20	1.900000+00	8.746675+00	8.469259-01
21	2.000000+00	8.739598+00	8.911297-01	22	2.200000+00	8.720134+00	9.788156-01
23	2.400000+00	8.699841+00	1.066230+00	24	2.600000+00	8.677754+00	1.153245+00
25	2.800000+00	8.654247+00	1.239828+00	26	3.000000+00	8.628877+00	1.325929+00
27	3.200000+00	8.601839+00	1.411538+00	28	3.400000+00	8.573173+00	1.496612+00
29	3.600000+00	8.542874+00	1.581131+00	30	3.800000+00	8.511042+00	1.665079+00
31	4.000000+00	8.477430+00	1.748359+00	32	4.200000+00	8.442380+00	1.831038+00
33	4.400000+00	8.405625+00	1.913008+00	34	4.600000+00	8.367467+00	1.994307+00
35	4.800000+00	8.327659+00	2.074822+00	36	5.000000+00	8.286326+00	2.154592+00
37	5.200000+00	8.176446+00	2.350477+00	38	6.000000+00	8.057510+00	2.540997+00
39	6.200000+00	7.929637+00	2.725681+00	40	7.000000+00	7.793281+00	2.904176+00
41	7.500000+00	7.648856+00	3.076131+00	42	8.000000+00	7.496718+00	3.241189+00
43	8.500000+00	7.337276+00	3.399031+00	44	9.000000+00	7.170964+00	3.549360+00
45	9.500000+00	6.998251+00	3.691923+00	46	1.000000+01	6.819577+00	3.826469+00
47	1.050000+01	6.635417+00	3.952801+00	48	1.100000+01	6.446279+00	4.070733+00
49	1.150000+01	6.252622+00	4.180100+00	50	1.200000+01	6.054953+00	4.280776+00
51	1.250000+01	5.853769+00	4.372667+00	52	1.300000+01	5.649583+00	4.455703+00
53	1.350000+01	5.442897+00	4.529847+00	54	1.400000+01	5.234200+00	4.595078+00
55	1.450000+01	5.023996+00	4.651408+00	56	1.500000+01	4.812801+00	4.699915+00
57	1.550000+01	4.601073+00	4.737631+00	58	1.600000+01	4.389306+00	4.767672+00
59	1.650000+01	4.177961+00	4.789151+00	60	1.700000+01	3.967502+00	4.802228+00
61	1.750000+01	3.758361+00	4.807056+00	62	1.800000+01	3.550984+00	4.803855+00

171	1.500000+02	-1.712421-01	-1.828332-01	172	1.520000+02	-1.254453-01	-2.003395-01
173	1.540000+02	-7.853163-02	-2.064966-01	174	1.560000+02	-3.362841-02	-2.019245-01
175	1.580000+02	6.529926-03	-1.880954-01	176	1.600000+02	3.983820-02	-1.671559-01
177	1.620000+02	6.498582-02	-1.416861-01	178	1.640000+02	8.153497-02	-1.144243-01
179	1.660000+02	8.990655-02	-8.798583-02	180	1.680000+02	9.127853-02	-6.460683-02
181	1.700000+02	8.740977-02	-4.593705-02	182	1.720000+02	8.041110-02	-3.290513-02
183	1.740000+02	7.248820-02	-2.566402-02	184	1.760000+02	6.568643-02	-2.362402-02
185	1.780000+02	6.166369-02	-2.556405-02	186	1.800000+02	6.151477-02	-2.980831-02
187	1.820000+02	6.566577-02	-3.444655-02	188	1.840000+02	7.384617-02	-3.757347-02
189	1.860000+02	8.514182-02	-3.752007-02	190	1.880000+02	9.811833-02	-3.305200-02
191	1.900000+02	1.110017-01	-2.351463-02	192	1.920000+02	1.218937-01	-8.909399-03
193	1.940000+02	1.289984-01	1.010507-02	194	1.960000+02	1.308346-01	3.228531-02
195	1.980000+02	1.264106-01	5.594029-02	196	2.000000+02	1.153436-01	7.911682-02
197	2.020000+02	9.791122-02	9.981256-02	198	2.040000+02	7.503006-02	1.161923-01
199	2.060000+02	4.816616-02	1.267848-01	200	2.080000+02	1.918608-02	1.306389-01
201	2.100000+02	-9.832885-03	1.274223-01	202	2.120000+02	-3.681329-02	1.174535-01
203	2.140000+02	-5.988581-02	1.016653-01	204	2.160000+02	-7.757261-02	8.150289-02
205	2.180000+02	-8.892766-02	5.877046-02	206	2.200000+02	-9.361824-02	3.544260-02
207	2.220000+02	-9.194169-02	1.346104-02	208	2.240000+02	-8.477538-02	-5.460792-03
209	2.260000+02	-7.346744-02	-2.000491-02	210	2.280000+02	-5.968059-02	-2.937075-02
211	2.300000+02	-4.520616-02	-3.333914-02	212	2.320000+02	-3.177100-02	-3.227287-02
213	2.340000+02	-2.085443-02	-2.705561-02	214	2.360000+02	-1.353824-02	-1.897594-02
215	2.380000+02	-1.040300-02	-9.571172-03	216	2.400000+02	-1.148198-02	-4.476142-04
217	2.420000+02	-1.627573-02	6.901676-03	218	2.440000+02	-2.382518-02	1.126325-02
219	2.460000+02	-3.283388-02	1.183457-02	220	2.480000+02	-4.182519-02	8.307643-03
221	2.500000+02	-4.931664-02	8.960242-04	222	2.520000+02	-5.399215-02	-9.696058-03
223	2.540000+02	-5.485362-02	-2.235906-04	224	2.560000+02	-5.133454-02	-3.570722-02
225	2.580000+02	-4.336586-02	-4.823662-04	226	2.600000+02	-3.138442-02	-5.849527-02
227	2.620000+02	-1.628702-02	-6.524537-02	228	2.640000+02	6.663513-04	-6.750137-02
229	2.660000+02	1.798867-02	-6.512820-02	230	2.680000+02	3.412562-02	-5.788979-02
231	2.700000+02	4.762164-02	-4.644326-02	232	2.720000+02	5.727465-02	-3.177975-02
233	2.740000+02	6.226224-02	-1.521886-02	234	2.760000+02	6.222630-02	1.731239-03
235	2.780000+02	5.730754-02	1.753261-02	236	2.800000+02	4.812651-02	3.077828-02
237	2.820000+02	3.571398-02	4.033727-02	238	2.840000+02	2.139839-02	4.546883-02
239	2.860000+02	6.663603-03	4.589362-02	240	2.880000+02	-7.008597-03	4.181530-02
241	2.900000+02	-1.629288-02	3.389048-02	242	2.920000+02	-2.615574-02	2.315079-02
243	2.940000+02	-2.995840-02	1.038678-02	244	2.960000+02	-2.951504-02	-1.494581-03
245	2.980000+02	-2.510243-02	-1.262165-02	246	3.000000+02	-1.741926-02	-2.130415-02
247	3.020000+02	-7.501438-03	-2.665691-02	248	3.040000+02	3.397834-03	-2.818879-02
249	3.060000+02	1.394899-02	-2.584753-02	250	3.080000+02	2.289325-02	-2.001648-02
251	3.100000+02	2.917943-02	-1.146424-02	252	3.120000+02	3.207610-02	-1.253213-03
253	3.140000+02	3.124730-02	9.382348-03	254	3.160000+02	2.678393-02	1.917522-02
255	3.180000+02	1.918828-02	2.696576-02	256	3.200000+02	9.313727-03	3.182879-02
257	3.220000+02	-1.733193-03	3.317350-02	258	3.240000+02	-1.271684-02	3.090541-02
259	3.260000+02	-2.240990-02	2.494458-02	260	3.280000+02	-2.972790-02	1.619845-02
261	3.300000+02	-3.384716-02	5.492618-03	262	3.320000+02	-3.429317-02	-6.032229-03
263	3.340000+02	-3.099017-02	-1.714581-02	264	3.360000+02	-2.426698-02	-2.666235-02
265	3.380000+02	-1.481918-02	-3.356868-02	266	3.400000+02	-3.631846-03	-3.713232-02
267	3.420000+02	8.128587-03	-3.697858-02	268	3.440000+02	1.924048-02	-3.312805-02
269	3.460000+02	2.855822-02	-2.599129-02	270	3.480000+02	3.513405-02	-1.632165-02
271	3.500000+02	3.831730-02	-5.131564-03	272	3.520000+02	3.782058-02	6.418063-03
273	3.540000+02	3.374649-02	1.714333-02	274	3.560000+02	2.657188-02	2.596357-02
275	3.580000+02	1.709226-02	3.201554-02	276	3.600000+02	6.332830-03	3.474253-02
277	3.620000+02	-4.564681-03	3.394956-02	278	3.640000+02	-1.446544-02	2.981904-02

63	1.850000+01	3.345768+00	4.792816+00	64	1.900000+01	3.143119+00	4.774190+00
65	1.950000+01	2.943410+00	4.748229+00	66	2.000000+01	2.747003+00	4.715203+00
67	2.100000+01	2.365417+00	4.629128+00	68	2.200000+01	2.000804+00	4.518448+00
69	2.300000+01	1.655251+00	4.385828+00	70	2.400000+01	1.330466+00	4.234063+00
71	2.500000+01	1.027773+00	4.066057+00	72	2.600000+01	7.481174-01	3.884711+00
73	2.700000+01	4.920615-01	3.692942+00	74	2.800000+01	2.598052-01	3.493596+00
75	2.900000+01	5.120427-02	3.289406+00	76	3.000000+01	-1.342065-01	3.082961+00
77	3.100000+01	-2.971883-01	2.876669+00	78	3.200000+01	-4.387553-01	2.672727+00
79	3.300000+01	-5.601444-01	2.473085+00	80	3.400000+01	-6.627752-01	2.279443+00
81	3.500000+01	-7.482105-01	2.093233+00	82	3.600000+01	-8.181074-01	1.915598+00
83	3.700000+01	-8.741855-01	1.747411+00	84	3.800000+01	-9.181833-01	1.589268+00
85	3.900000+01	-9.518185-01	1.441500+00	86	4.000000+01	-9.767561-01	1.304194+00
87	4.100000+01	-9.945683-01	1.177201+00	88	4.200000+01	-1.006719+00	1.060173+00
89	4.300000+01	-1.014529+00	9.525801-01	90	4.400000+01	-1.019161+00	8.537444-01
91	4.500000+01	-1.021609+00	7.628700-01	92	4.600000+01	-1.022683+00	6.790750-01
93	4.700000+01	-1.023004+00	6.014233-01	94	4.800000+01	-1.023015+00	5.289559-01
95	4.900000+01	-1.022975+00	4.607220-01	96	5.000000+01	-1.022972+00	3.958073-01
97	5.100000+01	-1.022944+00	3.333571-01	98	5.200000+01	-1.022688+00	2.726019-01
99	5.300000+01	-1.021377+00	2.128764-01	100	5.400000+01	-1.020096+00	1.536307-01
101	5.500000+01	-1.016850+00	9.444807-02	102	5.600000+01	-1.011601+00	3.504514-02
103	5.700000+01	-1.003785+00	-2.472089-02	104	5.800000+01	-9.928412-01	-8.485488-02
105	5.900000+01	-9.782329-01	-1.452280-01	106	6.000000+01	-9.594709-01	-2.055895-01
107	6.100000+01	-9.361317-01	-2.655732-01	108	6.200000+01	-9.078770-01	-3.247193-01
109	6.300000+01	-8.744662-01	-3.824856-01	110	6.400000+01	-8.357681-01	-4.382718-01
111	6.500000+01	-7.917679-01	-4.914333-01	112	6.600000+01	-7.425723-01	-5.413103-01
113	6.700000+01	-6.884096-01	-5.872425-01	114	6.800000+01	-6.296261-01	-6.285920-01
115	6.900000+01	-5.666310-01	-6.647640-01	116	7.000000+01	-5.001365-01	-6.952247-01
117	7.100000+01	-4.306453-01	-7.195167-01	118	7.200000+01	-3.589375-01	-7.372721-01
119	7.300000+01	-2.858037-01	-7.482267-01	120	7.400000+01	-2.120757-01	-7.522271-01
121	7.500000+01	-1.386109-01	-7.492351-01	122	7.600000+01	-6.626949-02	-7.393321-01
123	7.700000+01	4.101005-03	-7.227158-01	124	7.800000+01	7.168776-02	-6.996989-01
125	7.900000+01	1.357279-01	-6.707010-01	126	8.000000+01	1.955259-01	-6.362402-01
127	8.100000+01	2.504667-01	-5.969192-01	128	8.200000+01	3.000296-01	-5.534158-01
129	8.300000+01	3.437964-01	-5.064633-01	130	8.400000+01	3.814586-01	-4.568366-01
131	8.500000+01	4.128230-01	-4.053344-01	132	8.600000+01	4.378112-01	-3.527613-01
133	8.700000+01	4.564596-01	-2.999111-01	134	8.800000+01	4.689163-01	-2.475499-01
135	8.900000+01	4.754322-01	-1.964003-01	136	9.000000+01	4.763522-01	-1.471267-01
137	9.100000+01	4.721074-01	-1.003236-01	138	9.200000+01	4.631989-01	-5.650444-02
139	9.300000+01	4.501846-01	-1.609326-02	140	9.400000+01	4.336655-01	2.058098-02
141	9.500000+01	4.142697-01	5.328810-02	142	9.600000+01	3.926341-01	8.189709-02
143	9.700000+01	3.693918-01	1.063751-01	144	9.800000+01	3.451566-01	1.267835-01
145	9.900000+01	3.205087-01	1.432711-01	146	1.000000+02	2.959810-01	1.560662-01
147	1.020000+02	2.491270-01	1.718301-01	148	1.040000+02	2.075717-01	1.770809-01
149	1.060000+02	1.730604-01	1.753376-01	150	1.080000+02	1.460612-01	1.701994-01
151	1.100000+02	1.258576-01	1.649341-01	152	1.120000+02	1.107631-01	1.621277-01
153	1.140000+02	9.843067-02	1.634343-01	154	1.160000+02	8.621680-02	1.694413-01
155	1.180000+02	7.156069-02	1.796660-01	156	1.200000+02	5.233528-02	1.926722-01
157	1.220000+02	2.713326-02	2.062947-01	158	1.240000+02	-4.540274-03	2.179386-01
159	1.260000+02	-4.218787-02	2.249210-01	160	1.280000+02	-8.435615-02	2.248152-01
161	1.300000+02	-1.287827-01	2.157597-01	162	1.320000+02	-1.726350-01	1.966989-01
163	1.340000+02	-2.128102-01	1.675314-01	164	1.360000+02	-2.462666-01	1.291516-01
165	1.380000+02	-2.703456-01	8.338173-02	166	1.400000+02	-2.830539-01	3.280506-02
167	1.420000+02	-2.832729-01	-1.948123-02	168	1.440000+02	-2.708768-01	-7.016558-02
169	1.460000+02	-2.467477-01	-1.160406-01	170	1.480000+02	-2.126881-01	-1.543072-01

50	6.120199+00	1.546481-03	3.298595-02	8.294701-33	1.769233-31	1.546481-03	3.298595-02	0.000000
51	6.563443+00	3.747999-04	9.977759-03	0.000000	0.000000	3.747999-04	9.977759-03	0.000000
52	7.050916+00	2.621109-05	8.903734-04	4.385754-22	1.489811-20	2.621109-05	8.903734-04	0.000000
53	7.587033+00	1.465176-05	6.507184-04	5.427869-07	2.410642-05	1.519455-05	6.748248-04	0.000000
54	8.176648+00	1.274327-05	7.600066-04	2.298725-03	1.370956-01	2.311468-03	1.378556-01	0.000000
55	8.825098+00	6.764881-06	5.579635-04	4.576204-15	3.774426-13	6.764881-06	5.579635-04	0.000000
56	9.538254+00	4.234644-06	4.989103-04	0.000000	0.000000	4.234644-06	4.989103-04	0.000000
57	1.032257+01	2.962730-06	5.166669-04	5.304291-14	9.250088-12	2.962730-06	5.166669-04	0.000000
58	1.118516+01	1.296657-06	3.480580-04	5.638494-13	1.513525-10	1.296658-06	3.480581-04	0.000000
59	1.213382+01	4.035323-07	1.740618-04	0.000000	0.000000	4.035323-07	1.740618-04	0.000000
60	1.317714+01	1.461651-07	1.062242-04	5.592523-25	4.064318-22	1.461651-07	1.062242-04	0.000000
61	1.432457+01	5.134598-08	6.622901-05	5.729675-39	7.390466-36	5.134598-08	6.622901-05	0.000000
62	1.558651+01	1.162013-08	2.816942-05	1.868034-12	4.528470-09	1.162200-08	2.817394-05	0.000000
63	1.697436+01	1.075954-08	5.220710-05	2.058148-23	9.986481-20	1.075954-08	5.220710-05	0.000000
64	1.850071+01	1.412242-08	1.469896-04	1.921077-07	1.999504-03	2.062301-07	2.146493-03	0.000000
65	2.017936+01	1.183044-08	2.850320-04	0.000000	0.000000	1.183044-08	2.850320-04	0.000000
66	2.202552+01	4.295428-09	2.604881-04	8.736099-26	5.297842-21	4.295428-09	2.604881-04	0.000000
67	2.405591+01	5.016856-10	8.396638-05	1.047435-12	1.753077-07	5.027331-10	8.414169-05	0.000000
68	2.628890+01	2.421518-12	1.237796-06	2.855475-16	1.459619-10	2.421804-12	1.237942-06	0.000000
69	2.874471+01	5.150284-13	8.988049-07	1.553299-31	2.710748-25	5.150284-13	8.988049-07	0.000000
70	3.144558+01	3.630076-14	2.444761-07	1.500508-27	1.010553-20	3.630076-14	2.444761-07	0.000000
71	3.441596+01	1.371468-15	4.078651-08	3.510053-19	1.043865-11	1.371819-15	4.079695-08	0.000000
72	3.768275+01	9.914425-16	1.509982-07	1.428928-12	2.176279-04	1.429919-12	2.177789-04	0.000000
73	4.127551+01	1.805088-16	1.657153-07	0.000000	0.000000	1.805088-16	1.657153-07	0.000000
74	4.522679+01	1.548976-19	1.025458-09	4.216446-21	2.791385-11	1.591141-19	1.053372-09	0.000000
75	4.957236+01	5.467381-21	3.178921-10	0.000000	0.000000	5.467381-21	3.178921-10	0.000000
76	5.435155+01	3.865784-23	2.452036-11	2.296319-29	1.456537-17	3.865786-23	2.452037-11	0.000000
77	5.960764+01	1.645058-23	1.444830-10	2.182766-36	1.917091-23	1.645058-23	1.444830-10	0.000000
78	6.538823+01	3.221607-27	5.092670-13	2.261917-39	3.575607-25	3.221607-27	5.092670-13	0.000000
79	7.174563+01	6.435103-30	2.442992-14	0.000000	0.000000	6.435103-30	2.442992-14	0.000000
80	7.873743+01	3.955305-31	4.952164-14	0.000000	0.000000	3.955305-31	4.952164-14	0.000000

T(CH1)= 9.39612-03 T(S)= 7.76016-01 T(CONV1)= 1.00572-01 T(CONV2)= 1.14016-01

ALPHA= 5.000000-02

396

396

DEBYE-WALLER FACTOR=

9.889078-01

I	BETA	S1	S1*EXP(BETA/2)	S2	S2*EXP(BETA/2)	S	S*EXP(BETA/2)	SCT
1	0.000000	4.465739-02	4.465739-02	2.074246+02	2.074246+02	2.074692+02	2.074692+02	5.161419+01
2	8.000000-02	4.466593-02	4.648878-02	1.166022+02	1.213608+02	1.166469+02	1.214073+02	5.093986+01
3	1.600000-01	4.463161-02	4.834884-02	2.071317+01	2.243831+01	2.075780+01	2.248665+01	4.686902+01
4	2.400000-01	4.454854-02	5.022834-02	1.162731+00	1.310976+00	1.207280+00	1.361204+00	4.020254+01
5	3.200000-01	4.444840-02	5.216067-02	2.062555-02	2.420431-02	6.507395-02	7.636499-02	3.214849+01
6	4.000000-01	4.439407-02	5.422304-02	1.156178-04	1.412159-04	4.450969-02	5.436425-02	2.396664+01
7	4.800000-01	4.426672-02	5.627403-02	2.048034-07	2.603562-07	4.426693-02	5.627429-02	1.665686+01
8	5.600000-01	4.410772-02	5.836025-02	1.146417-10	1.516859-10	4.410772-02	5.836025-02	1.079242+01
9	6.400000-01	4.391033-02	6.047014-02	2.027879-14	2.792648-14	4.391033-02	6.047014-02	6.519040+00
10	7.200000-01	4.369108-02	6.262371-02	1.133533-18	1.624726-18	4.369108-02	6.262371-02	3.671031+00
11	8.000000-01	4.347460-02	6.485649-02	2.002252-23	2.987010-23	4.347460-02	6.485649-02	1.927223+00
12	8.800000-01	4.325175-02	6.715730-02	1.117628-28	1.735349-28	4.325175-02	6.715730-02	9.432254-01
13	9.600000-01	4.299628-02	6.948519-02	1.971371-34	3.185883-34	4.299628-02	6.948519-02	4.303664-01
14	1.040000+00	4.270139-02	7.182492-02	0.000000	0.000000	4.270139-02	7.182492-02	1.830631-01
15	1.120000+00	4.238051-02	7.419439-02	0.000000	0.000000	4.238051-02	7.419439-02	7.259431-02
16	1.200000+00	4.206113-02	7.664038-02	0.000000	0.000000	4.206113-02	7.664038-02	2.683761-02
17	1.280000+00	4.174967-02	7.917744-02	0.000000	0.000000	4.174967-02	7.917744-02	9.249638-03
18	1.360000+00	4.139475-02	8.170818-02	0.000000	0.000000	4.139475-02	8.170818-02	2.971973-03
19	1.440000+00	4.093480-02	8.409781-02	0.000000	0.000000	4.093480-02	8.409781-02	8.902351-04
20	1.520000+00	4.033017-02	8.623704-02	0.000000	0.000000	4.033017-02	8.623704-02	2.486016-04
21	1.600000+00	3.958786-02	8.810439-02	0.000000	0.000000	3.958786-02	8.810439-02	6.472061-05
22	1.680000+00	3.875393-02	8.976832-02	0.000000	0.000000	3.875393-02	8.976832-02	1.570800-05
23	1.760000+00	3.790057-02	9.137447-02	0.000000	0.000000	3.790057-02	9.137447-02	3.554174-06
24	1.840000+00	3.709066-02	9.307124-02	0.000000	0.000000	3.709066-02	9.307124-02	7.497141-07
25	1.920000+00	3.636945-02	9.498595-02	0.000000	0.000000	3.636945-02	9.498595-02	1.474322-07
26	2.000000+00	3.574819-02	9.717367-02	0.000000	0.000000	3.574819-02	9.717367-02	2.702890-08
27	2.080000+00	3.519605-02	9.957726-02	0.000000	0.000000	3.519605-02	9.957726-02	4.619595-09
28	2.160000+00	3.467915-02	1.021190-01	0.000000	0.000000	3.467915-02	1.021190-01	7.360700-10
29	2.240000+00	3.415780-02	1.046887-01	0.000000	0.000000	3.415780-02	1.046887-01	1.093387-10
30	2.320000+00	3.358533-02	1.071350-01	0.000000	0.000000	3.358533-02	1.071350-01	1.514147-11
31	2.400000+00	3.288512-02	1.091824-01	0.000000	0.000000	3.288512-02	1.091824-01	1.954797-12
32	2.480000+00	3.196668-02	1.104645-01	0.000000	0.000000	3.196668-02	1.104645-01	2.352744-13
33	2.560000+00	3.075081-02	1.105996-01	0.000000	0.000000	3.075081-02	1.105996-01	2.639899-14
34	2.647983+00	2.904245-02	1.091529-01	0.000000	0.000000	2.904245-02	1.091529-01	2.196001-15
35	2.744745+00	2.678106-02	1.056432-01	0.000000	0.000000	2.678106-02	1.056432-01	1.292323-16
36	2.851163+00	2.398406-02	9.978035-02	0.000000	0.000000	2.398406-02	9.978035-02	5.092042-18
37	2.968200+00	2.073975-02	9.148291-02	0.000000	0.000000	2.073975-02	9.148291-02	1.259006-19
38	3.096916+00	1.729817-02	8.137424-02	0.000000	0.000000	1.729817-02	8.137424-02	1.809440-21
39	3.238476+00	1.413770-02	7.138469-02	0.000000	0.000000	1.413770-02	7.138469-02	1.380880-23
40	3.394162+00	1.152970-02	6.292902-02	0.000000	0.000000	1.152970-02	6.292902-02	5.027514-26
41	3.565383+00	9.301375-03	5.530449-02	0.000000	0.000000	9.301375-03	5.530449-02	7.691121-29
42	3.753690+00	7.466093-03	4.877496-02	0.000000	0.000000	7.466093-03	4.877496-02	4.251848-32
43	3.960788+00	5.955781-03	4.315319-02	0.000000	0.000000	5.955781-03	4.315319-02	7.099854-36
44	4.188551+00	4.718953-03	3.831580-02	0.000000	0.000000	4.718953-03	3.831580-02	0.000000
45	4.439041+00	3.675514-03	3.382546-02	0.000000	0.000000	3.675514-03	3.382546-02	0.000000
46	4.714528+00	2.625011-03	2.983780-02	0.000000	0.000000	2.625011-03	2.983780-02	0.000000
47	5.017504+00	2.111551-03	2.595009-02	0.000000	0.000000	2.111551-03	2.595009-02	0.000000
48	5.350713+00	1.550289-03	2.250637-02	0.000000	0.000000	1.550289-03	2.250637-02	0.000000
49	5.717172+00	1.111789-03	1.938611-02	0.000000	0.000000	1.111789-03	1.938611-02	0.000000

ALPHA 1 = 5.000000-02 P**2/2= 1.264046-03
T, Q(T), R(T)

0.00	1.122-02	0.000	1.00-01	1.122-02	5.729-05	2.00-01	1.122-02	1.146-04	3.00-01	1.121-02	1.718-04
4.00-01	1.121-02	2.291-04	5.00-01	1.121-02	2.863-04	6.00-01	1.121-02	3.435-04	7.00-01	1.120-02	4.007-04
8.00-01	1.121-02	4.584-04	9.00-01	1.120-02	5.154-04	1.00+00	1.120-02	5.724-04	1.10+00	1.119-02	6.293-04
1.20+00	1.118-02	6.863-04	1.30+00	1.117-02	7.431-04	1.40+00	1.117-02	7.998-04	1.50+00	1.116-02	8.566-04
1.60+00	1.115-02	9.131-04	1.70+00	1.114-02	9.697-04	1.80+00	1.113-02	1.026-03	1.90+00	1.112-02	1.082-03
2.00+00	1.111-02	1.139-03	2.20+00	1.108-02	1.251-03	2.40+00	1.106-02	1.363-03	2.60+00	1.103-02	1.474-03
2.80+00	1.100-02	1.584-03	3.00+00	1.097-02	1.694-03	3.20+00	1.093-02	1.804-03	3.40+00	1.089-02	1.912-03
3.60+00	1.085-02	2.020-03	3.80+00	1.081-02	2.127-03	4.00+00	1.077-02	2.234-03	4.20+00	1.073-02	2.339-03
4.40+00	1.068-02	2.444-03	4.60+00	1.063-02	2.548-03	4.80+00	1.058-02	2.650-03	5.00+00	1.053-02	2.752-03
5.50+00	1.038-02	3.002-03	6.00+00	1.023-02	3.245-03	6.50+00	1.007-02	3.480-03	7.00+00	9.392-03	3.707-03
7.50+00	9.707-03	3.926-03	8.00+00	9.512-03	4.136-03	8.50+00	9.307-03	4.336-03	9.00+00	9.094-03	4.527-03
9.50+00	8.873-03	4.707-03	1.00+01	8.644-03	4.878-03	1.05+01	8.408-03	5.038-03	1.10+01	8.167-03	5.187-03
1.15+01	7.919-03	5.324-03	1.20+01	7.666-03	5.451-03	1.25+01	7.409-03	5.567-03	1.30+01	7.149-03	5.671-03
1.35+01	6.885-03	5.764-03	1.40+01	6.619-03	5.845-03	1.45+01	6.351-03	5.915-03	1.50+01	6.082-03	5.973-03
1.55+01	5.812-03	6.021-03	1.60+01	5.543-03	6.057-03	1.65+01	5.274-03	6.083-03	1.70+01	5.007-03	6.098-03
1.75+01	4.741-03	6.102-03	1.80+01	4.470-03	6.096-03	1.85+01	4.217-03	6.080-03	1.90+01	3.960-03	6.055-03
1.95+01	3.707-03	6.020-03	2.00+01	3.450-03	5.977-03	2.10+01	2.975-03	5.864-03	2.20+01	2.514-03	5.721-03
2.30+01	2.077-03	5.550-03	2.40+01	1.667-03	5.355-03	2.50+01	1.285-03	5.141-03	2.60+01	9.329-04	4.909-03
2.70+01	6.105-04	4.665-03	2.80+01	3.182-04	4.411-03	2.90+01	5.597-05	4.152-03	3.00+01	-1.769-04	3.890-03
3.10+01	-3.816-04	3.629-03	3.20+01	-5.591-04	3.370-03	3.30+01	-7.113-04	3.118-03	3.40+01	-8.398-04	2.873-03
3.50+01	-9.467-04	2.638-03	3.60+01	-1.034-03	2.413-03	3.70+01	-1.104-03	2.201-03	3.80+01	-1.159-03	2.001-03
3.90+01	-1.201-03	1.815-03	4.00+01	-1.232-03	1.642-03	4.10+01	-1.254-03	1.482-03	4.20+01	-1.269-03	1.334-03
4.30+01	-1.278-03	1.199-03	4.40+01	-1.284-03	1.074-03	4.50+01	-1.286-03	9.595-04	4.60+01	-1.287-03	8.540-04
4.70+01	-1.287-03	7.562-04	4.80+01	-1.287-03	6.650-04	4.90+01	-1.287-03	5.791-04	5.00+01	-1.287-03	4.974-04
5.10+01	-1.286-03	4.189-04	5.20+01	-1.286-03	3.425-04	5.30+01	-1.284-03	2.674-04	5.40+01	-1.282-03	1.929-04
5.50+01	-1.278-03	1.186-04	5.60+01	-1.271-03	4.399-05	5.70+01	-1.261-03	-3.103-05	5.80+01	-1.247-03	-1.065-04
5.90+01	-1.228-03	-1.622-04	6.00+01	-1.204-03	-2.579-04	6.10+01	-1.175-03	-3.331-04	6.20+01	-1.139-03	-4.072-04
6.30+01	-1.097-03	-4.795-04	6.40+01	-1.048-03	-5.493-04	6.50+01	-9.929-04	-6.159-04	6.60+01	-9.311-04	-6.782-04
6.70+01	-8.631-04	-7.357-04	6.80+01	-7.893-04	-7.873-04	6.90+01	-7.103-04	-8.325-04	7.00+01	-6.268-04	-8.705-04
7.10+01	-5.397-04	-9.008-04	7.20+01	-4.490-04	-9.228-04	7.30+01	-3.582-04	-9.364-04	7.40+01	-2.659-04	-9.412-04
7.50+01	-1.739-04	-9.373-04	7.60+01	-8.335-05	-9.248-04	7.70+01	4.703-06	-9.038-04	7.80+01	8.923-05	-8.749-04
7.90+01	1.693-04	-8.384-04	8.00+01	2.440-04	-7.952-04	8.10+01	3.126-04	-7.459-04	8.20+01	3.745-04	-6.914-04
8.30+01	4.291-04	-6.326-04	8.40+01	4.760-04	-5.704-04	8.50+01	5.150-04	-5.060-04	8.60+01	5.461-04	-4.402-04
8.70+01	5.692-04	-3.742-04	8.80+01	5.846-04	-3.088-04	8.90+01	5.926-04	-2.449-04	9.00+01	5.935-04	-1.834-04
9.10+01	5.880-04	-1.250-04	9.20+01	5.768-04	-7.038-05	9.30+01	5.604-04	-2.004-05	9.40+01	5.396-04	2.562-05
9.50+01	5.153-04	6.630-05	9.60+01	4.882-04	1.019-04	9.70+01	4.591-04	1.323-04	9.80+01	4.288-04	1.576-04
9.90+01	3.981-04	1.780-04	1.00+02	3.675-04	1.938-04	1.02+02	3.090-04	2.132-04	1.04+02	2.573-04	2.196-04
1.06+02	2.143-04	2.172-04	1.08+02	1.807-04	2.107-04	1.10+02	1.556-04	2.040-04	1.12+02	1.368-04	2.004-04
1.14+02	1.215-04	2.018-04	1.16+02	1.063-04	2.091-04	1.18+02	8.816-05	2.215-04	1.20+02	6.440-05	2.373-04
1.22+02	3.333-05	2.539-04	1.24+02	-5.638-06	2.679-04	1.26+02	-5.187-05	2.763-04	1.28+02	-1.036-04	2.759-04
1.30+02	-1.579-04	2.645-04	1.32+02	-2.115-04	2.409-04	1.34+02	-2.604-04	2.050-04	1.36+02	-3.010-04	1.578-04
1.38+02	-3.301-04	1.018-04	1.40+02	-3.453-04	4.001-05	1.42+02	-3.452-04	-2.374-05	1.44+02	-3.298-04	-8.540-05
1.46+02	-3.001-04	-1.411-04	1.48+02	-2.584-04	-1.874-04	1.50+02	-2.078-04	-2.219-04	1.52+02	-1.521-04	-2.428-04
1.54+02	-9.515-05	-2.501-04	1.56+02	-4.073-05	-2.443-04	1.58+02	7.849-06	-2.273-04	1.60+02	4.805-05	-2.018-04
1.62+02	7.832-05	-1.708-04	1.64+02	9.816-05	-1.378-04	1.66+02	1.081-04	-1.059-04	1.68+02	1.096-04	-7.762-05
1.70+02	1.049-04	-5.512-05	1.72+02	9.635-05	-3.943-05	1.74+02	8.675-05	-3.072-05	1.76+02	7.851-05	-2.824-05
1.78+02	7.361-05	-3.052-05	1.80+02	7.335-05	-3.554-05	1.82+02	7.818-05	-4.102-05	1.84+02	8.780-05	-4.468-05
1.86+02	1.011-04	-4.456-05	1.88+02	1.164-04	-3.920-05	1.90+02	1.315-04	-2.785-05	1.92+02	1.442-04	-1.054-05
1.94+02	1.523-04	1.194-05	1.96+02	1.543-04	3.808-05	1.98+02	1.489-04	6.589-05	2.00+02	1.356-04	9.305-05
2.02+02	1.149-04	1.172-04	2.04+02	8.795-05	1.362-04	2.06+02	5.637-05	1.484-04	2.08+02	2.239-05	1.527-04

2.10+02	-1.150-05	1.487-04	2.12+02	-4.292-05	1.369-04	2.14+02	-6.972-05	1.183-04	2.16+02	-9.014-05	9.469-05
2.18+02	-1.032-04	6.817-05	2.20+02	-1.084-04	4.105-05	2.22+02	-1.063-04	1.556-05	2.24+02	-9.788-05	-6.304-06
2.26+02	-8.489-05	-2.306-05	2.28+02	-6.860-05	-3.380-05	2.30+02	-5.194-05	-3.830-05	2.32+02	-3.645-05	-3.701-05
2.34+02	-2.389-05	-3.098-05	2.36+02	-1.540-05	-2.169-05	2.38+02	-1.188-05	-1.092-05	2.40+02	-1.309-05	-5.099-07
2.42+02	-1.851-05	7.848-06	2.44+02	-2.700-05	1.279-05	2.46+02	-3.722-05	1.341-05	2.48+02	-4.732-05	9.397-06
2.50+02	-5.569-05	1.012-06	2.52+02	-6.086-05	-1.093-05	2.54+02	-6.172-05	-2.515-05	2.56+02	-5.765-05	-4.009-05
2.58+02	-4.861-05	-5.406-05	2.60+02	-3.512-05	-6.544-05	2.62+02	-1.819-05	-7.285-05	2.64+02	7.358-07	-7.534-05
2.66+02	2.001-05	-7.245-05	2.68+02	3.789-05	-6.427-05	2.70+02	5.276-05	-5.147-05	2.72+02	6.333-05	-3.515-05
2.74+02	6.871-05	-1.680-05	2.76+02	6.854-05	1.907-06	2.78+02	6.300-05	1.928-05	2.80+02	5.279-05	3.377-05
2.82+02	3.910-05	4.417-05	2.84+02	2.330-05	4.968-05	2.86+02	7.263-06	5.004-05	2.88+02	-7.633-06	4.550-05
2.90+02	-1.987-05	3.680-05	2.92+02	-2.835-05	2.509-05	2.94+02	-3.240-05	1.177-05	2.96+02	-3.185-05	-1.613-06
2.98+02	-2.704-05	-1.359-05	3.00+02	-1.872-05	-2.289-05	3.02+02	-8.050-06	-2.858-05	3.04+02	3.632-06	-3.015-05
3.06+02	1.489-05	-2.759-05	3.08+02	2.430-05	-2.132-05	3.10+02	3.100-05	-1.218-05	3.12+02	3.401-05	-1.329-06
3.14+02	3.305-05	9.925-06	3.16+02	2.827-05	2.024-05	3.18+02	2.020-05	2.840-05	3.20+02	9.784-06	3.344-05
3.22+02	-1.829-06	3.477-05	3.24+02	-1.330-05	3.221-05	3.26+02	-2.339-05	2.602-05	3.28+02	-3.094-05	1.686-05
3.30+02	-3.515-05	5.703-06	3.32+02	-3.553-05	-6.248-06	3.34+02	-3.204-05	-1.772-05	3.36+02	-2.502-05	-2.748-05
3.38+02	-1.525-05	-3.452-05	3.40+02	-3.737-06	-3.809-05	3.42+02	8.312-06	-3.784-05	3.44+02	1.964-05	-3.382-05
3.46+02	2.907-05	-2.647-05	3.48+02	3.560-05	-1.658-05	3.50+02	3.882-05	-5.199-06	3.52+02	3.822-05	6.486-06
3.54+02	3.401-05	1.728-05	3.56+02	2.672-05	2.611-05	3.58+02	1.714-05	3.211-05	3.60+02	6.332-06	3.475-05
3.62+02	-4.563-06	3.387-05	3.64+02	-1.440-05	2.967-05	3.66+02	-2.220-05	2.271-05	3.68+02	-2.721-05	1.383-05
3.70+02	-2.901-05	4.050-06	3.72+02	-2.752-05	-5.536-06	3.74+02	-2.303-05	-1.388-05	3.76+02	-1.615-05	-2.011-05
3.78+02	-7.724-06	-2.358-05	3.80+02	1.220-06	-2.398-05	3.82+02	9.674-06	-2.134-05	3.84+02	1.665-05	-1.605-05
3.86+02	2.136-05	-8.737-06	3.88+02	2.330-05	-2.913-07	3.90+02	2.226-05	8.309-06	3.92+02	1.838-05	1.607-05
3.94+02	1.210-05	2.212-05	3.96+02	4.142-06	2.577-05	3.98+02	-4.612-06	2.660-05	4.00+02	-1.319-05	2.451-05
4.02+02	-2.067-05	1.974-05	4.04+02	-2.619-05	1.279-05	4.06+02	-2.919-05	4.417-06	4.08+02	-2.933-05	-4.489-06
4.10+02	-2.661-05	-1.298-05	4.12+02	-2.131-05	-2.015-05	4.14+02	-1.403-05	-2.526-05	4.16+02	-5.516-06	-2.779-05
4.18+02	3.315-06	-2.750-05	4.20+02	1.154-05	-2.445-05	4.22+02	1.832-05	-1.901-05	4.24+02	2.296-05	-1.177-05
4.26+02	2.503-05	-3.521-06	4.28+02	2.434-05	4.851-06	4.30+02	2.105-05	1.247-05	4.32+02	1.554-05	1.854-05
4.34+02	8.462-06	2.247-05	4.36+02	5.314-07	2.388-05	4.38+02	-7.229-06	2.267-05	4.40+02	-1.414-05	1.905-05
4.42+02	-1.942-05	1.345-05	4.44+02	-2.254-05	6.512-06	4.46+02	-2.323-05	-9.804-07	4.48+02	-2.145-05	-8.210-06
4.50+02	-1.745-05	-1.440-05	4.52+02	-1.170-05	-1.891-05	4.54+02	-4.878-06	-2.129-05	4.56+02	2.262-06	-2.133-05
4.58+02	8.937-06	-1.907-05	4.60+02	1.444-05	-1.483-05	4.62+02	1.817-05	-9.110-06	4.64+02	1.979-05	-2.577-06
4.66+02	1.915-05	4.023-06	4.68+02	1.637-05	9.953-06	4.70+02	1.181-05	1.456-05	4.72+02	6.019-06	1.734-05
4.74+02	-3.476-07	1.801-05	4.76+02	-6.532-06	1.651-05	4.78+02	-1.186-05	1.303-05	4.80+02	-1.573-05	7.975-06
4.82+02	-1.770-05	1.911-06	4.84+02	-1.755-05	-4.484-06	4.86+02	-1.531-05	-1.050-05	4.88+02	-1.120-05	-1.548-05
4.90+02	-5.688-06	-1.688-05	4.92+02	6.440-07	-2.033-05	4.94+02	7.115-06	-1.967-05	4.96+02	1.304-05	-1.698-05
4.98+02	1.780-05	-1.254-05	5.00+02	2.090-05	-6.837-06	5.02+02	2.201-05	-4.576-07	5.04+02	2.106-05	5.927-06
5.06+02	1.816-05	1.166-05	5.08+02	1.362-05	1.616-05	5.10+02	7.955-06	1.899-05	5.12+02	1.763-06	1.990-05
5.14+02	-4.318-06	1.884-05	5.16+02	-9.663-06	1.597-05	5.18+02	-1.373-05	1.164-05	5.20+02	-1.614-05	6.360-06
5.22+02	-1.669-05	7.157-07	5.24+02	-1.540-05	-4.674-06	5.26+02	-1.246-05	-9.232-06	5.28+02	-8.249-06	-1.240-05
5.30+02	-3.284-06	-1.411-05	5.32+02	1.360-06	-1.398-05	5.34+02	6.597-06	-1.213-05	5.36+02	1.040-05	-8.933-06
5.38+02	1.284-05	-4.474-06	5.40+02	1.360-05	4.317-07	5.42+02	1.278-05	5.318-06	5.44+02	1.031-05	9.630-06
5.46+02	6.540-06	1.288-05	5.48+02	1.397-06	1.471-05	5.50+02	-3.106-06	1.492-05	5.52+02	-7.924-06	1.347-05
5.54+02	-1.201-05	1.053-05	5.56+02	-1.490-05	6.422-06	5.58+02	-1.637-05	1.580-06	5.60+02	-1.619-05	-3.475-06
5.62+02	-1.439-05	-8.206-06	5.64+02	-1.117-05	-1.212-05	5.66+02	-6.892-06	-1.481-05	5.68+02	-2.005-06	-1.601-05
5.70+02	2.991-06	-1.561-05	5.72+02	7.559-06	-1.367-05	5.74+02	1.124-05	-1.043-05	5.76+02	1.368-05	-6.241-06
5.78+02	1.405-05	-1.563-06	5.80+02	1.407-05	3.107-06	5.82+02	1.206-05	7.280-06	5.84+02	8.861-06	1.053-05
5.86+02	4.856-05	1.254-05	5.88+02	4.860-07	1.313-05	5.90+02	-3.759-06	1.229-05	5.92+02	-7.422-06	1.012-05
5.94+02	-1.012-05	6.930-06	5.96+02	-1.150-05	3.089-06	5.98+02	-1.167-05	-9.587-07	6.00+02	-1.041-05	-4.755-06

2.10+02	-2.125-05	2.747-04	2.12+02	-7.915-05	2.524-04	2.14+02	-1.283-04	2.178-04	2.16+02	-1.657-04	1.741-04
2.18+02	-1.893-04	1.251-04	2.20+02	-1.987-04	7.521-05	2.22+02	-1.945-04	2.847-05	2.24+02	-1.798-04	-1.151-05
2.26+02	-1.544-04	-4.205-05	2.28+02	-1.250-04	-6.153-05	2.30+02	-9.441-05	-6.962-05	2.32+02	-6.614-05	-6.717-05
2.34+02	-4.327-05	-5.612-05	2.36+02	-2.800-05	-3.923-05	2.38+02	-2.145-05	-1.972-05	2.40+02	-2.359-05	-9.190-07
2.42+02	-3.331-05	1.412-05	2.44+02	-4.859-05	2.296-05	2.46+02	-6.671-05	2.404-05	2.48+02	-8.467-05	1.682-05
2.50+02	-9.948-05	1.807-06	2.52+02	-1.085-04	-1.948-05	2.54+02	-1.098-04	-4.477-05	2.56+02	-1.024-04	-7.123-05
2.58+02	-8.621-05	-9.587-05	2.60+02	-6.217-05	-1.158-04	2.62+02	-3.215-05	-1.287-04	2.64+02	1.286-05	-1.329-04
2.66+02	3.520-05	-1.275-04	2.68+02	6.654-05	-1.129-04	2.70+02	9.251-05	-9.024-05	2.72+02	1.108-04	-6.151-05
2.74+02	1.200-04	-2.934-05	2.76+02	1.195-04	3.324-06	2.78+02	1.096-04	3.353-05	2.80+02	9.166-05	5.963-05
2.82+02	6.774-05	7.652-05	2.84+02	4.042-05	8.590-05	2.86+02	1.253-05	8.634-05	2.88+02	-1.314-05	7.934-05
2.90+02	-3.413-05	6.323-05	2.92+02	-4.860-05	4.301-05	2.94+02	-5.543-05	2.014-05	2.96+02	-5.438-05	-2.753-06
2.98+02	-4.605-05	-2.315-05	3.00+02	-3.182-05	-3.891-05	3.02+02	-1.364-05	-4.847-05	3.04+02	6.147-06	-5.104-05
3.06+02	2.514-05	-4.659-05	3.08+02	4.100-05	-3.592-05	3.10+02	5.213-05	-2.049-05	3.12+02	5.705-05	-2.229-06
3.14+02	5.532-05	1.661-05	3.16+02	4.721-05	3.380-05	3.18+02	3.366-05	4.731-05	3.20+02	1.626-05	5.559-05
3.22+02	-3.023-06	5.767-05	3.24+02	-2.201-05	5.330-05	3.26+02	-3.860-05	4.295-05	3.28+02	-5.096-05	2.776-05
3.30+02	-5.774-05	9.369-06	3.32+02	-5.823-05	-1.024-05	3.34+02	-5.236-05	-2.897-05	3.36+02	-4.081-05	-4.483-05
3.38+02	-2.480-05	-5.617-05	3.40+02	-6.050-06	-6.183-05	3.42+02	1.347-05	-6.127-05	3.44+02	3.172-05	-5.462-05
3.46+02	4.685-05	-4.264-05	3.48+02	5.735-05	-2.664-05	3.50+02	6.223-05	-8.335-06	3.52+02	6.111-05	1.037-05
3.54+02	5.425-05	2.756-05	3.56+02	4.250-05	4.153-05	3.58+02	2.720-05	5.094-05	3.60+02	1.002-05	5.500-05
3.62+02	-7.193-06	5.346-05	3.64+02	-2.267-05	4.671-05	3.66+02	-3.480-05	3.566-05	3.68+02	-4.261-05	2.166-05
3.70+02	-4.530-05	6.324-06	3.72+02	-4.280-05	-8.624-06	3.74+02	-3.577-05	-2.157-05	3.76+02	-2.501-05	-3.115-05
3.78+02	-1.193-05	-3.642-05	3.80+02	1.890-06	-3.694-05	3.82+02	1.487-05	-3.290-05	3.84+02	2.551-05	-2.459-05
3.86+02	3.264-05	-1.335-05	3.88+02	3.550-05	-4.439-07	3.90+02	3.383-05	1.263-05	3.92+02	2.786-05	2.436-05
3.94+02	1.829-05	3.343-05	3.96+02	6.249-06	3.892-05	3.98+02	-6.928-06	3.996-05	4.00+02	-1.976-05	3.672-05
4.02+02	-3.085-05	2.949-05	4.04+02	-3.900-05	1.905-05	4.06+02	-4.333-05	6.558-06	4.08+02	-4.342-05	-6.646-06
4.10+02	-3.927-05	-1.915-05	4.12+02	-3.130-05	-2.965-05	4.14+02	-2.057-05	-3.707-05	4.16+02	-8.062-06	-4.066-05
4.18+02	4.843-06	-4.011-05	4.20+02	1.679-05	-3.557-05	4.22+02	2.656-05	-2.756-05	4.24+02	3.320-05	-1.701-05
4.26+02	3.606-05	-5.074-06	4.28+02	3.497-05	5.969-06	4.30+02	3.015-05	1.786-05	4.32+02	2.220-05	2.647-05
4.34+02	1.204-05	3.198-05	4.36+02	8.323-07	3.387-05	4.38+02	-1.022-05	3.207-05	4.40+02	-1.992-05	2.686-05
4.42+02	-2.728-05	1.890-05	4.44+02	-3.158-05	9.122-06	4.46+02	-3.243-05	-1.369-06	4.48+02	-2.985-05	-1.143-05
4.50+02	-2.420-05	-1.998-05	4.52+02	-1.610-05	-2.615-05	4.54+02	-6.723-06	-2.935-05	4.56+02	3.115-06	-2.930-05
4.58+02	1.224-05	-2.612-05	4.60+02	1.970-05	-2.024-05	4.62+02	2.472-05	-1.239-05	4.64+02	2.683-05	-3.494-06
4.66+02	2.583-05	5.436-06	4.68+02	2.205-05	1.340-05	4.70+02	1.585-05	1.954-05	4.72+02	8.049-06	2.319-05
4.74+02	-4.566-07	2.400-05	4.76+02	-8.676-06	2.193-05	4.78+02	-1.570-05	1.725-05	4.80+02	-2.074-05	1.052-05
4.82+02	-2.326-05	2.512-06	4.84+02	-2.290-05	-5.874-06	4.86+02	-1.997-05	-1.371-05	4.88+02	-1.457-05	-2.014-05
4.90+02	-7.374-06	-2.447-05	4.92+02	8.326-07	-2.626-05	4.94+02	9.164-06	-2.532-05	4.96+02	1.673-05	-2.179-05
4.98+02	2.275-05	-1.603-05	5.00+02	2.661-05	-8.795-06	5.02+02	2.793-05	-5.805-07	5.04+02	2.663-05	7.492-06
5.06+02	2.287-05	1.469-05	5.08+02	1.710-05	2.028-05	5.10+02	9.952-06	2.375-05	5.12+02	2.196-06	2.479-05
5.14+02	-5.359-06	2.338-05	5.16+02	-1.194-05	1.974-05	5.18+02	-1.690-05	1.434-05	5.20+02	-1.980-05	7.804-06
5.22+02	-2.040-05	8.750-07	5.24+02	-1.375-05	-5.692-06	5.26+02	-1.511-05	-1.120-05	5.28+02	-9.972-06	-1.509-05
5.30+02	3.954-06	-1.699-05	5.32+02	2.230-06	-1.676-05	5.34+02	7.886-06	-1.450-05	5.36+02	1.238-05	-1.051-05
5.38+02	1.523-05	-5.305-06	5.40+02	1.610-05	5.099-07	5.42+02	1.504-05	6.257-06	5.44+02	1.209-05	1.129-05
5.46+02	7.639-06	1.504-05	5.48+02	2.211-06	1.711-05	5.50+02	-3.597-06	1.727-05	5.52+02	-9.130-06	1.554-05
5.54+02	-1.379-05	1.210-05	5.56+02	-1.700-05	7.348-06	5.58+02	-1.866-05	1.801-06	5.60+02	-1.836-05	-3.044-06
5.62+02	-1.626-05	-9.277-06	5.64+02	-1.258-05	-1.364-05	5.66+02	-7.724-06	-1.660-05	5.68+02	-2.235-06	-1.787-05
5.70+02	3.327-05	-1.736-05	5.72+02	8.372-06	-1.514-05	5.74+02	1.240-05	-1.150-05	5.76+02	1.503-05	-6.856-06
5.78+02	1.602-05	-1.709-06	5.80+02	1.533-05	3.385-06	5.82+02	1.308-05	7.897-06	5.84+02	9.575-06	1.137-05
5.86+02	5.224-06	1.349-05	5.88+02	5.250-07	1.406-05	5.90+02	-4.004-06	1.309-05	5.92+02	-7.877-06	1.075-05
5.94+02	-1.070-05	7.327-06	5.96+02	-1.219-05	3.252-06	5.98+02	-1.223-05	-1.005-06	6.00+02	-1.087-05	-4.964-06

ALPHA= 1.000000-01

396

396

DEBYE-WALLER FACTOR=

9.779387-01

	BETA	S1	S1*EXP(BETA/2)	S2	S2*EXP(BETA/2)	S	S*EXP(BETA/2)	SCT
1	0.000000	8.848773-02	8.848773-02	1.449437+02	1.449437+02	1.450322+02	1.450322+02	3.637197+01
2	8.000000-02	8.848297-02	9.209403-02	1.086733+02	1.131083+02	1.087617+02	1.132004+02	3.653176+01
3	1.600000-01	8.841222-02	9.577581-02	4.580286+01	4.961764+01	4.589127+01	4.971342+01	3.542779+01
4	2.400000-01	8.825811-02	9.951074-02	1.085198+01	1.223557+01	1.094024+01	1.233509+01	3.317320+01
5	3.200000-01	8.807801-02	1.033605-01	1.445347+00	1.696130+00	1.533425+00	1.799491+00	2.999165+01
6	4.000000-01	8.796719-02	1.074434-01	1.082136-01	1.321724-01	1.961808-01	2.396157-01	2.618081+01
7	4.800000-01	8.768951-02	1.114752-01	4.554471-03	5.789867-03	9.224398-02	1.172651-01	2.206661+01
8	5.600000-01	8.737724-02	1.156114-01	1.077558-04	1.425749-04	8.748500-02	1.157540-01	1.795799+01
9	6.400000-01	8.700153-02	1.198122-01	1.433146-06	1.973625-06	8.700297-02	1.198142-01	1.411074+01
10	7.200000-01	8.657947-02	1.240969-01	1.071485-08	1.535791-08	8.657948-02	1.240969-01	1.070561+01
11	8.000000-01	8.614553-02	1.285140-01	4.503278-11	6.718101-11	8.614553-02	1.285140-01	7.842288+00
12	8.800000-01	8.568026-02	1.330363-01	1.063942-13	1.651991-13	8.568026-02	1.330363-01	5.546819+00
13	9.600000-01	8.516476-02	1.376326-01	1.413037-16	2.283572-16	8.516476-02	1.376326-01	3.788043+00
14	1.040000+00	8.460047-02	1.423003-01	1.054960-19	1.774472-19	8.460047-02	1.423003-01	2.497788+00
15	1.120000+00	8.397679-02	1.470158-01	4.427561-23	7.751209-23	8.397679-02	1.470158-01	1.590252+00
16	1.200000+00	8.334542-02	1.518653-01	1.044576-26	1.903342-26	8.334542-02	1.518653-01	9.775659-01
17	1.280000+00	8.269223-02	1.568242-01	1.385361-30	2.627311-30	8.269223-02	1.568242-01	5.802243-01
18	1.360000+00	8.193638-02	1.617324-01	1.032835-34	2.038690-34	8.193638-02	1.617324-01	3.325182-01
19	1.440000+00	8.099487-02	1.663986-01	0.000000	0.000000	8.099487-02	1.663986-01	1.839945-01
20	1.520000+00	7.980201-02	1.706387-01	0.000000	0.000000	7.980201-02	1.706387-01	9.843344-02
21	1.600000+00	7.836998-02	1.744156-01	0.000000	0.000000	7.836998-02	1.744156-01	5.070989-02
22	1.680000+00	7.677600-02	1.778414-01	0.000000	0.000000	7.677600-02	1.778414-01	2.525755-02
23	1.760000+00	7.514143-02	1.811584-01	0.000000	0.000000	7.514143-02	1.811584-01	1.214674-02
24	1.840000+00	7.357411-02	1.846188-01	0.000000	0.000000	7.357411-02	1.846188-01	5.640239-03
25	1.920000+00	7.215146-02	1.884377-01	0.000000	0.000000	7.215146-02	1.884377-01	2.528747-03
26	2.000000+00	7.090100-02	1.927289-01	0.000000	0.000000	7.090100-02	1.927289-01	1.094669-03
27	2.080000+00	6.977590-02	1.974111-01	0.000000	0.000000	6.977590-02	1.974111-01	4.575408-04
28	2.160000+00	6.871709-02	2.023498-01	0.000000	0.000000	6.871709-02	2.023498-01	1.846490-04
29	2.240000+00	6.764079-02	2.073091-01	0.000000	0.000000	6.764079-02	2.073091-01	7.195052-05
30	2.320000+00	6.644216-02	2.119460-01	0.000000	0.000000	6.644216-02	2.119460-01	2.707013-05
31	2.400000+00	6.497973-02	2.157403-01	0.000000	0.000000	6.497973-02	2.157403-01	9.833695-06
32	2.480000+00	6.309617-02	2.180429-01	0.000000	0.000000	6.309817-02	2.180429-01	3.449154-06
33	2.560000+00	6.067110-02	2.132121-01	0.000000	0.000000	6.067110-02	2.132121-01	1.168096-06
34	2.647963+00	5.732537-02	2.154512-01	0.000000	0.000000	5.732537-02	2.154512-01	3.409850-07
35	2.744745+00	5.292579-02	2.087763-01	0.000000	0.000000	5.292579-02	2.087763-01	8.382267-08
36	2.851163+00	4.747981-02	1.975292-01	0.000000	0.000000	4.747981-02	1.975292-01	1.688313-08
37	2.968200+00	4.117529-02	1.816240-01	0.000000	0.000000	4.117529-02	1.816240-01	2.697639-09
38	3.096916+00	3.450538-02	1.623206-01	0.000000	0.000000	3.450538-02	1.623206-01	3.291544-10
39	3.238476+00	2.628475-02	1.428166-01	0.000000	0.000000	2.828475-02	1.428166-01	2.931754-11
40	3.394162+00	2.303624-02	1.257316-01	0.000000	0.000000	2.303624-02	1.257316-01	1.807126-12
41	3.565383+00	1.860214-02	1.106054-01	0.000000	0.000000	1.860214-02	1.106054-01	7.235909-14
42	3.753690+00	1.493266-02	9.755301-02	0.000000	0.000000	1.493266-02	9.755301-02	1.745782-15
43	3.960788+00	1.191829-02	8.635515-02	0.000000	0.000000	1.191829-02	8.635515-02	2.320850-17
44	4.188551+00	9.441425-03	7.666017-02	0.000000	0.000000	9.441425-03	7.666017-02	1.528338-19
45	4.439041+00	7.371292-03	6.783740-02	0.000000	0.000000	7.371292-03	6.783740-02	4.391079-22
46	4.714528+00	5.660553-03	5.978684-02	0.000000	0.000000	5.660553-03	5.978684-02	4.730305-25
47	5.017504+00	4.234982-03	5.204617-02	0.000000	0.000000	4.234982-03	5.204617-02	1.594175-28
48	5.350713+00	3.118629-03	4.527477-02	0.000000	0.000000	3.118629-03	4.527477-02	1.353496-32
49	5.717172+00	2.244735-03	3.914113-02	0.000000	0.000000	2.244735-03	3.914113-02	0.000000

ALPHA 2 =

1.000000-01

CONVOLVED

I	BETA	S1	S1*EXP(BETA/2)	S2	S2*EXP(BETA/2)	S	S*EXP(BETA/2)	SCT
1	0.000000	8.814812-02	8.814812-02	1.443874+02	1.443874+02	1.444756+02	1.444756+02	3.637197+01
2	8.000000-02	8.814337-02	9.174057-02	1.082562+02	1.126742+02	1.083443+02	1.127659+02	3.653176+01
3	1.600000-01	8.807289-02	9.540823-02	4.562707+01	4.942721+01	4.571514+01	4.952262+01	3.542779+01
4	2.400000-01	8.791938-02	9.912882-02	1.081033+01	1.218861+01	1.089825+01	1.228774+01	3.317320+01
5	3.200000-01	8.773997-02	1.029638-01	1.439800+00	1.689621+00	1.527540+00	1.792584+00	2.999165+01
6	4.000000-01	8.762958-02	1.070310-01	1.077983-01	1.316651-01	1.954278-01	2.386961-01	2.618081+01
7	4.800000-01	8.735296-02	1.110474-01	4.536991-03	5.767646-03	9.188995-02	1.168150-01	2.206661+01
8	5.600000-01	8.704189-02	1.151677-01	1.073422-04	1.420277-04	8.714923-02	1.153097-01	1.795799+01
9	6.400000-01	8.666763-02	1.193524-01	1.427645-06	1.966050-06	8.666905-02	1.193544-01	1.411074+01
10	7.200000-01	8.624719-02	1.236206-01	1.067373-08	1.529897-08	8.624720-02	1.236206-01	1.070561+01
11	8.000000-01	8.581491-02	1.280208-01	4.485994-11	6.692317-11	8.581491-02	1.280208-01	7.842288+00
12	8.800000-01	8.535142-02	1.325258-01	1.059859-13	1.645650-13	8.535142-02	1.325258-01	5.546819+00
13	9.600000-01	8.483790-02	1.371044-01	1.407613-16	2.274808-16	8.483790-02	1.371044-01	3.788043+00
14	1.040000+00	8.427577-02	1.417542-01	1.050911-19	1.767661-19	8.427577-02	1.417542-01	2.497788+00
15	1.120000+00	8.365449-02	1.464516-01	4.410568-23	7.721460-23	8.365449-02	1.464516-01	1.590252+00
16	1.200000+00	8.302555-02	1.512824-01	1.040567-26	1.896037-26	8.302555-02	1.512824-01	9.775659-01
17	1.280000+00	8.237487-02	1.562224-01	1.380044-30	2.617228-30	8.237487-02	1.562224-01	5.802243-01
18	1.360000+00	8.162191-02	1.611117-01	1.028871-34	2.030865-34	8.162191-02	1.611117-01	3.325182-01
19	1.440000+00	8.088403-02	1.657599-01	0.000000	0.000000	8.088403-02	1.657599-01	1.839945-01
20	1.520000+00	7.949574-02	1.699838-01	0.000000	0.000000	7.949574-02	1.699838-01	9.830234-02
21	1.600000+00	7.806921-02	1.737462-01	0.000000	0.000000	7.806921-02	1.737462-01	5.070989-02
22	1.680000+00	7.648136-02	1.771589-01	9.791471-37	2.268064-36	7.648136-02	1.771589-01	2.525755-02
23	1.760000+00	7.485307-02	1.804632-01	1.571245-33	3.788115-33	7.485307-02	1.804632-01	1.214674-02
24	1.840000+00	7.329178-02	1.839103-01	1.417399-30	3.556665-30	7.329178-02	1.839103-01	5.640239-03
25	1.920000+00	7.167460-02	1.877146-01	7.187555-28	1.877171-27	7.167460-02	1.877146-01	2.528747-03
26	2.000000+00	7.062395-02	1.919894-01	2.048884-25	3.569444-25	7.062395-02	1.919894-01	1.094669-03
27	2.080000+00	6.950816-02	1.966537-01	3.283252-23	9.289032-23	6.950816-02	1.966537-01	4.575409-04
28	2.160000+00	6.845342-02	2.015734-01	2.957560-21	8.709065-21	6.845342-02	2.015734-01	1.846490-04
29	2.240000+00	6.738126-02	2.065137-01	1.497648-19	4.590074-19	6.738126-02	2.065137-01	7.195052-05
30	2.320000+00	6.618724-02	2.111329-01	4.263173-18	1.359924-17	6.618724-02	2.111329-01	2.707013-05
31	2.400000+00	6.473043-02	2.149126-01	6.821895-17	2.264949-16	6.473043-02	2.149126-01	9.833695-06
32	2.480000+00	6.285609-02	2.172063-01	6.136510-16	2.120541-15	6.285609-02	2.172063-01	3.449154-06
33	2.560000+00	6.043335-02	2.173750-01	3.103022-15	1.116045-14	6.043335-02	2.173750-01	1.168096-06
34	2.647983+00	5.710547-02	2.146248-01	9.485120-15	3.564881-14	5.710547-02	2.146248-01	3.409850-07
35	2.744745+00	5.272278-02	2.079755-01	1.449975-14	5.719714-14	5.272278-02	2.079755-01	8.382267-08
36	2.851163+00	4.729772-02	1.967716-01	8.739873-15	3.636029-14	4.729772-02	1.967716-01	1.688313-08
37	2.968200+00	4.101741-02	1.809276-01	1.543853-15	6.809929-15	4.101741-02	1.809276-01	2.697639-09
38	3.096916+00	3.457311-02	1.616984-01	5.525592-17	2.599355-16	3.457311-02	1.616984-01	3.291544-10
39	3.238476+00	2.817639-02	1.422694-01	2.535763-19	1.280368-18	2.817639-02	1.422694-01	2.931754-11
40	3.394162+00	2.294805-02	1.252503-01	8.474370-23	4.625305-22	2.294805-02	1.252503-01	1.807126-12
41	3.565383+00	1.853101-02	1.101824-01	1.026459-27	6.103162-27	1.853101-02	1.101824-01	7.235909-14
42	3.753690+00	1.487567-02	9.713068-02	1.909162-34	1.247229-33	1.487567-02	9.718068-02	1.745782-15
43	3.960788+00	1.187294-02	8.602656-02	0.000000	0.000000	1.187294-02	8.602656-02	2.320850-17
44	4.188551+00	9.405687-03	7.636999-02	0.000000	0.000000	9.405687-03	7.636999-02	1.528338-19
45	4.439041+00	7.343663-03	6.758314-02	9.250822-34	8.513456-33	7.343663-03	6.758314-02	4.391079-22
46	4.714528+00	5.639765-03	5.956727-02	4.900905-26	5.176342-25	5.639765-03	5.956727-02	4.730305-25
47	5.017504+00	4.220148-03	5.186386-02	5.753991-21	7.071415-20	4.220148-03	5.186386-02	1.594175-28
48	5.350713+00	3.108716-03	4.513087-02	1.558564-19	2.262650-18	3.108716-03	4.513087-02	1.353496-32
49	5.717172+00	2.238584-03	3.903387-02	5.722236-23	9.977782-22	2.238584-03	3.903387-02	0.000000

279	3.660000+02	-2.236352-02	2.288566-02	280	3.680000+02	-2.748782-02	1.397338-02
281	3.700000+02	-2.938148-02	4.102467-03	282	3.720000+02	-2.794650-02	-5.623929-03
283	3.740000+02	-2.344869-02	-1.414034-02	284	3.760000+02	-1.648343-02	-2.053408-02
285	3.780000+02	-7.905971-03	-2.414235-02	286	3.800000+02	1.265482-03	-2.462099-02
287	3.820000+02	9.963354-03	-2.197773-02	288	3.840000+02	1.718815-02	-1.656696-02
289	3.860000+02	2.211729-02	-9.046555-03	290	3.880000+02	2.419336-02	-3.024498-04
291	3.900000+02	2.318270-02	8.651211-03	292	3.920000+02	1.919780-02	1.678445-02
293	3.940000+02	1.268209-02	2.316483-02	294	3.960000+02	4.358637-03	2.705895-02
295	3.980000+02	-4.851351-03	2.801143-02	296	4.000000+02	-1.393061-02	2.589287-02
297	4.020000+02	-2.187770-02	2.091199-02	298	4.040000+02	-2.781630-02	1.359079-02
299	4.060000+02	-3.108996-02	4.705978-03	300	4.080000+02	-3.133231-02	-4.796981-03
301	4.100000+02	-2.850532-02	-1.390733-02	302	4.120000+02	-2.290156-02	-2.165887-02
303	4.140000+02	-1.511079-02	-2.723424-02	304	4.160000+02	-5.954487-03	-3.065213-02
305	4.180000+02	3.603931-03	-2.982857-02	306	4.200000+02	1.256389-02	-2.660539-02
307	4.220000+02	1.999516-02	-2.074355-02	308	4.240000+02	2.513749-02	-1.288180-02
309	4.260000+02	2.748042-02	-3.866120-03	310	4.280000+02	2.681613-02	5.342829-03
311	4.300000+02	2.325676-02	1.377374-02	312	4.320000+02	1.722929-02	2.054882-02
313	4.340000+02	9.407025-03	2.497695-02	314	4.360000+02	6.543849-04	2.662587-02
315	4.380000+02	-8.077988-03	2.536569-02	316	4.400000+02	-1.565423-02	2.137949-02
317	4.420000+02	-2.185368-02	1.513998-02	318	4.440000+02	-2.545791-02	7.355136-03
319	4.460000+02	-2.631512-02	-1.110908-03	320	4.480000+02	-2.437477-02	-9.333110-03
321	4.500000+02	-1.988948-02	-1.642630-02	322	4.520000+02	-1.338405-02	-2.164401-02
323	4.540000+02	-5.595293-03	-2.444122-02	324	4.560000+02	2.610523-03	-2.456400-02
325	4.580000+02	1.033341-02	-2.204113-02	326	4.600000+02	1.673799-02	-1.719440-02
327	4.620000+02	2.114404-02	-1.059699-02	328	4.640000+02	2.309923-02	-3.088165-03
329	4.660000+02	2.242619-02	4.711352-03	330	4.680000+02	1.923952-02	1.169470-02
331	4.700000+02	1.593061-02	1.716379-02	332	4.720000+02	7.122538-03	2.051390-02
333	4.740000+02	-4.000499-04	2.137859-02	334	4.760000+02	-7.777897-03	1.966820-02
335	4.780000+02	-1.417187-02	1.557842-02	336	4.800000+02	-1.385462-02	9.546292-03
337	4.820000+02	-2.128956-02	2.299824-03	338	4.840000+02	-2.118859-02	-5.416391-03
339	4.860000+02	-1.854223-02	-1.272940-02	340	4.880000+02	-1.361968-02	-1.883091-02
341	4.900000+02	-6.938248-03	-2.304488-02	342	4.920000+02	7.938766-04	-2.490025-02
343	4.940000+02	3.754394-03	-2.418094-02	344	4.960000+02	1.609885-02	-2.094807-02
345	4.980000+02	2.204703-02	-1.553200-02	346	5.000000+02	2.597146-02	-8.495226-03
347	5.020000+02	2.746165-02	-5.706194-04	348	5.040000+02	2.636726-02	7.418416-03
349	5.060000+02	2.281271-02	1.464699-02	350	5.080000+02	1.718177-02	2.037722-02
351	5.100000+02	1.007437-02	2.403669-02	352	5.120000+02	2.240554-03	2.527851-02
353	5.140000+02	-5.561353-03	2.401654-02	354	5.160000+02	-1.235325-02	2.043208-02
355	5.180000+02	-1.762271-02	1.495186-02	356	5.200000+02	-2.079650-02	8.199512-03
357	5.220000+02	-2.159382-02	9.262976-04	358	5.240000+02	-1.999424-02	-6.071369-03
359	5.260000+02	-1.623708-02	-1.203859-02	360	5.280000+02	-1.079255-02	-1.634336-02
361	5.300000+02	-4.308449-03	-1.854392-02	362	5.320000+02	2.462385-03	-1.843492-02
363	5.340000+02	8.744848-03	-1.606746-02	364	5.360000+02	1.382660-02	-1.174127-02
365	5.380000+02	1.713529-02	-5.969609-03	366	5.400000+02	1.829990-02	5.783392-04
367	5.420000+02	1.718992-02	7.151949-03	368	5.440000+02	1.392792-02	1.300179-02
369	5.460000+02	8.674543-03	1.746157-02	370	5.480000+02	2.567726-03	2.002053-02
371	5.500000+02	-4.239382-03	2.037837-02	372	5.520000+02	-1.065471-02	1.847702-02
373	5.540000+02	-1.652954-02	1.450577-02	374	5.560000+02	-2.063770-02	8.879702-03
375	5.580000+02	-2.272323-02	2.193503-03	376	5.600000+02	-2.254914-02	-4.843733-03
377	5.620000+02	-2.012214-02	-1.148585-02	378	5.640000+02	-1.569086-02	-1.770305-02
379	5.660000+02	-9.717601-03	-2.089471-02	380	5.680000+02	-2.828440-03	-2.267724-02
381	5.700000+02	4.257107-03	-2.220062-02	382	5.720000+02	1.080216-02	-1.952900-02
383	5.740000+02	1.613271-02	-1.495992-02	384	5.760000+02	1.970965-02	-8.989864-03
385	5.780000+02	2.118552-02	-2.260192-03	386	5.800000+02	2.044045-02	4.513441-03
387	5.820000+02	1.759319-02	1.061880-02	388	5.840000+02	1.298604-02	1.542371-02
389	5.860000+02	7.145942-03	1.844361-02	390	5.880000+02	7.258683-04	1.939252-02
391	5.900000+02	-5.567122-03	1.821219-02	392	5.920000+02	-1.164903-02	1.507616-02
393	5.940000+02	-1.513302-02	1.036895-02	394	5.960000+02	-1.739224-02	4.642161-03
395	5.980000+02	-1.760519-02	-1.446964-03	396	6.000000+02	-1.577790-02	-7.208217-03

7.4.2 Punched Output

The punched output in ENDF/A format is given on the following page.

<u>Item</u>	<u>Format</u>	<u>Variable</u>	<u>Description</u>
1	17A4, A2, 5X I5	(HØL(J), J=1, 18), ID	Comments and ID number
2	11HDCC2 [†]402, 11X 1H4, 5X 1H5, 1XI5	JX	Number of β points
3	6(1PE 11.4, 1X)	SIGF	Free atom scattering cross section (barns)
		EPSI	Maximum β value ($= E_{\max}/T$)
		A	Scatterer mass (neutron mass units)
		$E_{\max}$	Maximum energy (eV)
		ALAM	Debye-Waller integral
4	29HDCC1.....401.....3.....4.....0..I6, 13X 1PE 11.4	IX	Number of α values
		BETA (1)	First β value
5	6(1PE 11.4, 1X)	(ALPHA(I), I=1, IX)	α values
6	6(1PE 11.4, 1X)	(S(I, 1), I=1, IX)	$S(\alpha, \beta)$ for first β value
	Cards 7 and 8 are repeated for J=2, JX (remaining β values)		
7	29HDCC1.....401.....4.....4.....0, I6, I6, 7X 1PE 11.4	LDB	$LDB = IHT(J) - ILT(J) + 1$
		IL	$IL = ILT(J)$
		BETA(J)	J^{th} β value
8	6(1PE 11.4, 1X)	(S(I, J), I=1, JX)	$S(\alpha, \beta)$ for J^{th} β value
9	11HEND.....500		End-of-deck indicator

The arrays ILT(J) and IHT(J) contain values of the lower and upper limits of $S(\alpha, \beta)$, for the J^{th} β , which satisfy the significance criterion

$$S(\alpha_I, \beta_J) > EPS \cdot \max \left[S(\alpha, \beta) e^{\beta/2} \right].$$

[†] = space

8. SAMPLE PROBLEMS

Input for a few representative moderators is given in this section, along with computer produced plots of $S(\alpha, \beta)$ vs α for a range of β -values, and a discussion of the choices made for some of the more arbitrary input numbers.

8.1 INPUT

Tables 1, 2, 3 and 4 list the input data for some scattering law calculations made recently. The first two are for hydrogen bound in water at room temperature and a higher temperature, the third and fourth are for graphite and hydrogen bound in zirconium hydride at room temperature. Numbers not specified are taken to be zero. Table 2 (H_2O at 500°K) lists only those data that are different from Table 1.

8.2 MACHINE PLOTS OF $S(\alpha, \beta)$

A plotting program has been written to produce several types of machine plots (in the Stromberg-Carlson 4020 plotter) for each $S(\alpha, \beta)$ deck. Automated plotting of this sort is the only reliable way to scan the large amounts of data produced in a reasonable time. The plot given in Fig. 4 is of $S(\alpha, \beta)$ vs α for the β -values tabulated on the page facing the plot.

Table 1

13A6, A2 COMMENTS: H(H₂O) Modified Haywood Spectrum at room temperature

13I5	NT-5	7E10	X ₃	7E10	Q ₃	7E10	X ₅	.205, .45
	NP 80		.006375		.00125	7E10	Q ₅	1/3, 2/3
	NE 80		.01275		.005			
	NDAM		.019125		.01125	7E10	NPHON 10,	5
	NGPRT		.0255		.02	5E10	EMAX	2.0
	NCP		.031875		.03125		DALPHA	.05
	NMESH 1		.03825		.045		ALPHAC	.5
	NREST		.044625		.059		DBETA	.08
	NCVP		.051		.075		BETAC	2.5
	NSEP		.057375		.095			
	NAD 1		.00375		.115			
	NAD 2		.0663		.1197	2E10	DT	TMAX
	NAD 3		.06885		.1214		.1	2.
3I5	JS3	29	.0714		.1218		.2	5.
	JS4		.07395		.1195		.5	20.
	JS5	2	.0765		.1125		1.	100.
5E10	W1	.05555	.082875		.0975		2.	600.
	W2	0	.08925		.0871			
	W3	.4444	.095625		.0791			
	W4	0	.102		.0735			
	W5	.500	.108375		.0688			
6E10	T1	.0255	.11475		.065			
	T2		.121125		.061			
	T3	.0255	.1275		.0571	2I10,	ID	296
	T4		.133875		.054	3E10	NPT	0
	T5	.0255	.14025		.0515		SIGF	20.36
	TEMP		.146625		.0488		EPS	10 ⁻⁶
7E10	Am	1.00866	.153		.0459			
	DC		.159375		.0431			
	BETSW 20.		.16575		.042			
	ALPSW 20.							
	CRIT1							
	CRIT2							
	CRIT3							

Table 2

13A6, A2 COMMENTS: H(H₂O) Modified Haywood Spectrum at 500°K

13I5	NT	7E10	X ₃	7E10	Q ₃	7E10	X ₅		
						7E10	Q ₅		
	NE								
	NDAM					7E10	NPHON		
	NGPRT					5E10	EMAX	2.0	
	NCP						DALPHA	.029594	
	NMESH						ALPHAC	.29594	
	NREST						DBETA	.04735	
	NCVP						BETAC	1.47970	
	NSEP								
	NAD1								
	NAD2					2E10	DT	TMAX	
	NAD3								
3I5	JS3								
	JS4								
	JS5								
5E10	W1								
	W2								
	W3								
	W4								
	W5								
6E10	T1	.043082							
	T2								
	T3	.043082				2I10, ID 500			
	T4					3E10 NPT			
	T5	.043082				SIGF			
	TEMP					EPS			
7E10	Am								
	DC								
	BETSW 11.838								
	ALPSW 11.838								
	CRIT1								
	CRIT2								
	CRIT3								

Table 3

13A6, A2 COMMENTS: Graphite J. A. Young Spectrum at Room Temperature

1315	NT-9	7E10	X ₃	Q ₃	7E10	X ₅		
	40		<u>.20842</u>	<u>.346613</u>	<u>6.5662</u>	7E10	Q ₅	
	NE 80			<u>1.4135</u>	<u>5.47181</u>			
	NDAM 1			<u>3.03321</u>	<u>5.06137</u>	7E10	NPHON	
	NGPRT			<u>3.25901</u>	<u>5.19813</u>	5E10	EMAX	1.0
	NCP			<u>3.38468</u>	<u>.457086</u>		DALPHA	.25
	NMESH 1			<u>3.48269</u>			ALPHAC	2.
	NREST			<u>3.76397</u>			DBETA	.1
	NCVP			<u>4.05025</u>			BETAC	4.
	NSEP			<u>4.84696</u>				
	NAD1			<u>7.35744</u>				
	NAD2			<u>5.88224</u>		2E10	DT	TMAX
	NAD3			<u>4.63255</u>				
315	JS3 -38			<u>4.48287</u>				
	JS4			<u>5.80642</u>				
	JS5			<u>4.63802</u>				
5E10	W1	.001		<u>4.28503</u>				
	W2			<u>3.92079</u>				
	W3	1.0		<u>4.91352</u>				
	W4			<u>5.53836</u>				
	W5			<u>7.51076</u>				
6E10	T1	.0255		<u>5.31651</u>				
	T2			<u>5.40525</u>				
	T3	.0255		<u>5.20376</u>				
	T4			<u>5.3276</u>		2110, ID	34	
	T5			<u>7.17251</u>		3E10 NPT	0	
	TEMP			<u>3.31813</u>		SIGF	4.7	
7E10	Am	12.011		<u>4.50126</u>		EPS	10 ⁻⁶	
	DC			<u>5.04663</u>				
	BETSW 30.			<u>4.2089</u>				
	ALPSW 30.			<u>2.91985</u>				
	CRIT1			<u>4.65109</u>				
	CRIT2			<u>13.1324</u>				
	CRIT3			<u>7.25016</u>				

Table 4

13A6, A2 COMMENTS: H(ZrH) at room temperature

13I5	NT-5	7E10	X ₃	7E10	Q ₃	7E10	X ₅
	40		0.168			7E10	Q ₅
	NE 150						
	NDAM 1					7E10	NPHON
	NGPRT					5E10	EMAX 1.0
	NCP						DALPHA .5
	NMESH 1						ALPHAC 5.
	NREST						DBETA .25
	NCVP						BETAC 30.
	NSEP						
	NAD1						
	NAD2					2E10	DT TMAX
	NAD3						.3 6.
3I5	JS3 -84						.6 18.
	JS4						1.2 60.
	JS5						3. 300.
5E10	W1 5 x 10 ⁻⁵						6. 3100
	W2						
	W3 .99995						
	W4						
	W5						
6E10	T1 .0255						
	T2					2I10, ID	360
	T3 .0255					3E10	NPT 0
	T4						SIGF 20.36
	T5						EPS 10 ⁻⁶
	TEMP						
7E10	Am 1.00866						
	DC						
	BETSW 160.						
	ALPSW 160.						
	CRIT1						
	CRIT2						
	CRIT3						

H(H₂O) at 296°K

<u>Curve Index</u>	<u>Beta</u>
1	0.
2	.08
3	.16
4	.24
5	.48
6	.72
7	.96
8	1.2
9	1.44
∂	1.68
=	1.92
"	2.16
'	2.4
δ	2.65
α	2.97
+	3.39
A	3.96
B	4.72
C	5.72
D	7.06

Fig. 4-- $S(\alpha, \beta)$ for $H(H_2O)$ at $296^{\circ}K$

8.3 DISCUSSION OF CHOICE OF INPUT PARAMETERS

The basic physical model chosen is sufficient to specify most of the GASKET input. There are, however, still a few parameters which must be specified by the user. A few guidelines and suggestions for these parameters are given here.

For the present method of calculating S_1 for $w_3 \neq 0$, the following prescription has provided adequate time meshes:

$$t_{\max} \geq 20\pi/\theta_{\min}$$

$$\Delta t_{\max} < 2\pi/(5 \theta_{\max})$$

where $\theta_{\min}$ (in eV) is the lowest frequency point for Mode 3 at which there is significant structure, and $\theta_{\max}$ is the frequency cut off for Mode 3. The time mesh should start out with relatively small intervals, since most of the important structure occurs at small t , gradually increasing to $\Delta t_{\max}$. A reasonable choice for a first try is

Δt	up to
$\Delta t_{\max}/20$	$t_{\max}/200$
$\Delta t_{\max}/10$	$t_{\max}/80$
$\Delta t_{\max}/5$	$t_{\max}/20$
$\Delta t_{\max}/2$	$t_{\max}/5$
$\Delta t_{\max}$	$t_{\max}$,

The rationale for this scheme is that at large times $Q(t)$ and $R(t)$ show damped oscillation with a period determined by the lowest frequency structure in the distributed frequency spectrum. This choice of $t_{\max}$ covers about 10 full cycles of this longest wavelength behavior. The

smallest wavelength is determined by the cutoff frequency of the distributed frequency spectrum; the choice of $\Delta t_{\max}$ puts about five points per full cycle of the shortest wavelength behavior (at large t 's, where the amplitude of the oscillations are small). Of course these are not absolute rules, and in each case a careful check of the adequacy of the time mesh is necessary.

Choice of α_{sw} and β_{sw} , the values of α and β beyond which $S(\alpha, \beta)$ is calculated in short collision time approximation has been made empirically. Lacking detailed studies of the effect of the parameters on single- and double-differential quantities, conservative choices have been made so that a fairly smooth transition to SCT behavior is obtained for $e^{\beta/2} S(\alpha, \beta)$ which is proportional to the double-differential cross section (presumably the quantity most sensitive to choice of α_{sw} and β_{sw}).

The largest number of phonon terms calculated for each oscillator is given, conservatively, by the maximum energy for which $S(\alpha, \beta)$ is to be calculated, divided by the frequency of the oscillator.

A value of 10^{-6} for the significance criterion used to discard insignificant values of $e^{\beta/2} S(\alpha)$ for fixed β has been adequate for all moderators treated so far.

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