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GASKET
A UNIFIED CODE FOR THERMAL NEUTRON SCATTERING

by

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DISCLAIMER

The GASKET computer code is described herein as it existed on September 22. The code has been in continuous development for 2 years and in its presented form has been applied successfully by General Atomic to the kind of problems discussed later in this report. However, the development and improvement of the code are being continued, so that duplication of results (or even close agreement) between problems run with the code as published and the code as it existed either before or after this time is not necessarily to be expected.

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NOTICE

This document has been revised to incorporate corrections and additions to the original publication dated September 22, 1966.

The changes are indicated in the following manner:

1. Changed words, sentences, or paragraphs are underlined and flagged by a vertical line in the right margin.

2. Page numbers of revised pages have a single underline.

3. Underlined page numbers of pages that have not been revised indicate that the page has been relocated.

4. Page numbers of added pages have a double underline (as below).

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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

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

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 $S'(\alpha, \beta) = TS(\alpha, \beta)$.

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

$\varkappa$ 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 α - β 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 x 80 (α, β) points gives very satisfactory results in the energy range 0-2 eV. The minimum number of points in E_0, E, θ space required for an equivalent accuracy would be of the order of 80 x 80 x 15. For moderators with 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 ω_{max} is the cut-off frequency of the material

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*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

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

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

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

and

$$\mathscr{S}(\alpha, \beta) = e^{-\beta/2} S(\alpha, \beta) \qquad (1.4)$$

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

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

which can be obtained by analytical continuation of the Fourier transforms assuming that χ_{sym} is analytic in the domain $\left(-\infty < \mathrm{Re}[t] < \infty,\ 0 \leq \mathrm{Im}[t] \leq \frac{1}{2T}\right)^{*}$. The numerical Fourier inversion of Eq. (1.3) requires splitting $\chi_{n.sym}$ 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)]

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*Eq. (1.5) leads to $\mathscr{S}(\alpha, \beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\epsilon t}\chi_{sym}\left(\alpha, t - \frac{i}{2T}\right) dt$ 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 anistropic 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:

$$\chi_i = \exp\left[\alpha G_i(t)\right] \tag{1.6}$$

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

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

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

$$\sum_i w_i = 1 \tag{1.8}$$

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:

$$\chi(\alpha, 0) = \lim_{t \to 0} \chi(\alpha, t) = 1 \tag{2.1}$$

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

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

($\overline{T}$ 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 overorientations 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

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

2.1 FREE GAS

According to Zemach and Glauber[6]

$$G_1(t) = iTt - T^2t^2 \tag{2.5}$$

and

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

The corresponding scattering law S_1 is easily evaluated as

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

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]

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

or

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

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 $t \to \infty$ corresponding to classical diffusion theory. It also satisfies detailed balance and condition (2.1). Condition (2.2), however, can only be satisfied if

$$\frac{d}{c} = 1 \tag{2.10}$$

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

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

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

$$X_3^{(\ell)}(\alpha, t) = \exp\left\{\frac{w_3}{2NM_\ell} \sum_{\vec{k}, s} |\vec{\varkappa} \cdot \vec{C}\left(\ell \middle| \begin{matrix}\vec{k} \\ s\end{matrix}\right)|^2 \, g\left[\omega_s(\vec{k}), t\right]\right\} \tag{2.12}$$

where

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

N being the total number of unit cells, and $\vec{C}\left(\ell \middle| \begin{matrix}\vec{k} \\ s\end{matrix}\right)$ 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

$$X_3(\alpha, t) = \exp\left[\alpha w_3 G_3(t)\right] \tag{2.14}$$

with

$$G_3(t) = \gamma(t) - \gamma(0) \tag{2.15}$$

and

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

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

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

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

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

and furthermore

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

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 overorientation 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 $\varkappa^2 \to 0$ and $\epsilon \to \infty$.

For a polyatomic crystal the simple frequency spectrum $f(\omega)$ is no longer sufficient to determine the X-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 X-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 $X_3(\alpha, t)$ 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

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

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 $\vec{\varkappa}$. $f_{\perp}(\omega)$ 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

$$X_4(\alpha, t) = \int_0^1 d(\cos\theta) \exp\left\{w_4\alpha \left[G_{//}(t)\cos^2\theta + G_{\perp}(t)\left(1-\cos^2\theta\right)\right]\right\} \quad (2.21)$$

or

$$X_4(\alpha, t) = \exp\left[\alpha w_4 G_{\perp}(t)\right] \int_0^1 d\mu \exp\left\{-\alpha w_4\left[G_{\perp}(t)-G_{//}(t)\right]\mu^2\right\} \quad (2.22)$$

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]

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

$$= \Phi(1/2, 3/2, -x) = 1/2\sqrt{\frac{\pi}{-x}}\,\mathrm{erf}\,(i\sqrt{-x}) \text{ for } x<0 \quad (2.23)$$

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

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

with

$$\sum_k a_k = 1 \tag{2.25}$$

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

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

Since

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

each term in (2.24) generates a phonon series

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

where

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

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

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

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

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

$$\cdot \exp\left\{-\alpha T \left[w_1 T t^2 - w_3 \int_0^{\infty} f(\omega) \coth \frac{\omega}{2T} \cos \omega t \frac{d\omega}{\omega}\right]\right\} \quad (3.1)$$

Splitting the integrand into even and odd components we have

$$\mathcal{S}(\alpha, \beta) = \frac{D}{\pi} \int_0^{\infty} dt \cos\left[\left(\beta + \alpha w_1\right) Tt + \alpha T w_3 \int_0^{\infty} f(\omega) \sin \omega t \frac{d\omega}{\omega}\right] \cdot$$

$$\cdot \exp\left\{\alpha T \left[-w_1 T t^2 + w_3 \int_0^{\infty} f(\omega) \coth \frac{\omega}{2T} \cos \omega t \frac{d\omega}{\omega}\right]\right\} \quad (3.2)$$

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 $w_1 = 0$)

$$X_1 X_3 = X_1\left(X_3 - D\right) + X_1 D \tag{3.3}$$

Then, defining the odd and even functions

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

and

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

we can rewrite Eq. (3. 3) in the form

$$\mathcal{S}(\alpha, \beta) = \frac{D}{\pi} \int_0^\infty dt \left\{ \cos \left[\left(\beta + \alpha w_1\right) Tt + \alpha F(t)\right] \cdot \exp \left[-\alpha w_1 T^2 t^2 + \alpha H(t)\right] - \right.$$

$$\left. - \cos \left[\left(\beta + \alpha w_1\right) Tt\right] \exp \left(-\alpha w_1 T^2 t^2\right)\right\} + \frac{D}{2\pi} \int_{-\infty}^{\infty} e^{i\beta Tt} X_1(\alpha, t) dt \tag{3.6}$$

or else

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

with

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

which follows from Eq. (2.7), and

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

where

$$\lambda = \left(\beta + \alpha w_1\right) T \qquad (3.10)$$

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

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

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:

$$+\sqrt{\tau^2 - i\tau + c^2} = +\sqrt[4]{\left(\tau^2+t^2\right)^2+\tau^2}\; e^{\frac{i}{2}\arg(\tau^2+c^2+i\tau)} \qquad \left(c^2>0\right)$$

$$= \frac{1}{\sqrt{2}}\sqrt[4]{\left(\tau^2+c^2\right)^2+\tau^2}\left\{\sqrt{1+\cos\left[\arg\left(\tau^2+c^2-i\tau\right)\right]} \pm i\sqrt{1-\cos\left[\arg\left(\tau^2+t^2-i\tau\right)\right]}\right\}$$

$$= \frac{1}{\sqrt{2}}\left\{\sqrt{\sqrt{\left(\tau^2+c^2\right)^2+\tau^2}+\tau^2+c^2} \pm i\sqrt{\sqrt{\left(\tau^2+c^2\right)^2+\tau^2}-\tau^2-c^2}\right\} \tag{4.1}$$

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

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

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

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

$$X_2(t) = e^{2\alpha w_2 dc} \exp\left\{-\alpha w_2\left[G_{2\,\text{even}}(t) + i\,G_{2\,\text{odd}}(t)\right]\right\} \tag{4.3}$$

where

$$G_{2\ even}(t) = d\sqrt{2}\ \sqrt{\sqrt{\left(T^2t^2+c^2\right)^2 + T^2t^2} + T^2t^2 + c^2} \qquad (4.4)$$

and

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

with

$$\left.\begin{array}{l} \eta = +1 \text{ for } t > 0 \\ \eta = -1 \text{ for } t < 0 \end{array}\right\} \qquad (4.6)$$

Thus we have factored X_2 into a product of an even and an odd function of t. Now combining X_2 with X_3 as given by Eq. (2.14) we obtain

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

Recalling Eq. (2.18) and introducing the functions

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

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

and

$$\overline{D} = \exp\left\{\alpha\left[2\ w_2dc - w_3\ \gamma(0)\right]\right\} \qquad (4.10)$$

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

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

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

$$\mathcal{S}(\alpha, \beta) = \frac{\overline{D}}{\pi} \int_0^\infty \cos\left[\beta T t + \alpha \overline{F}(t)\right] \exp\left[\alpha \overline{H}(t)\right] dt \qquad (4.12)$$

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

$$\mathcal{S}(\alpha, \beta) = \frac{\overline{D}}{\pi} \int_0^\infty dt \left\{ \cos\left[\beta T t + \alpha \overline{F}(t)\right] \exp\left[\alpha \overline{H}(t)\right] - \right.$$

$$\left. - \cos\left[\beta T t - \alpha w_2 G_{2\ odd}(t)\right] \exp\left[-\alpha w_2 G_{2\ even}(t)\right] \right\} +$$

$$+ \frac{\overline{D}}{\pi} \int_0^\infty dt \cos\left[\beta T t - \alpha w_2 G_{2\ odd}(t)\right] \exp\left[-\alpha w_2 G_{2\ even}(t)\right]$$

or else

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

with

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

$$\cdot K_1\left\{\left(c^2 + \frac{1}{4}\right)^{1/2} \left[\beta^2 + \left(2\alpha w_2 d\right)^2\right]^{1/2}\right\}$$

which follows from Eq. (2.11), and

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

where

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

and

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

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

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

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

$$N_k \sim \frac{T\beta_{max}}{\omega_k} \tag{5.2}$$

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:

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

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):

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

with

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

and

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

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

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

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

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

is largest when the argument

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

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

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

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

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

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, $\overline{T}$ 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, $\overline{T}$, 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 $\overline{T}$ 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 $\underline{\frac{H(t=o)}{W_3 T}}$ (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 $w_2 = w_4 = 0$.

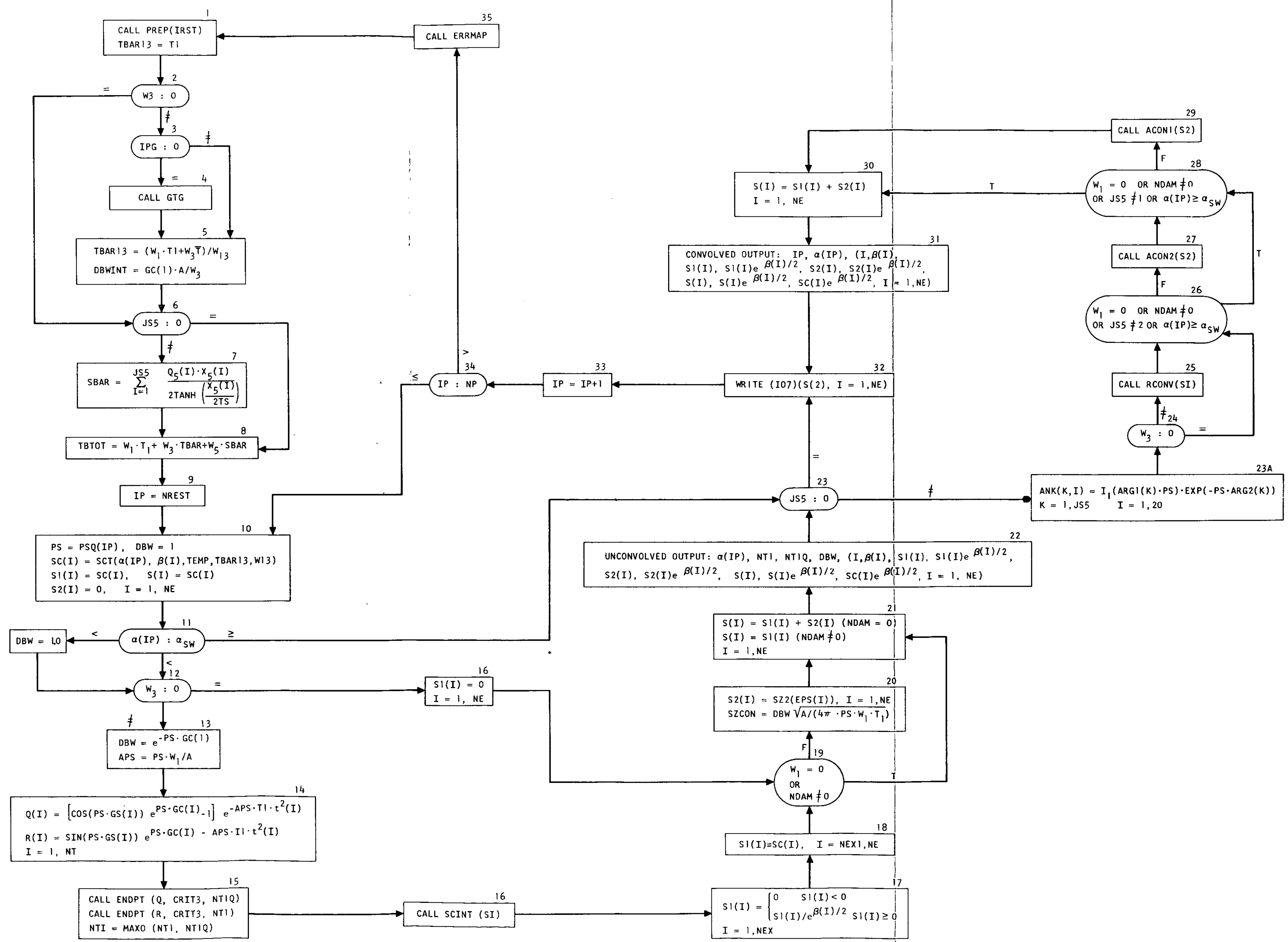

Fig. 1--Flow chart for GASKET

(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 = 0. For a restarted problem for which a scratch tape containing $S(\alpha, \beta)$ values for $\alpha(1), \ldots, \alpha(N)$ 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 $DBW = \exp\left[-\frac{\varkappa^2}{2} H(0)\right]$.

(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 ~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 $\beta \geq \beta_{sw}$, 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 $w1 \neq 0$, $w3 \neq 0$, $w5 \neq 0$. 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 $w1 \neq 0$, $w3 = w5 = 0$, using $\alpha_{sw} > \alpha_{max}$ the program follows the path (given by block numbers) 10, 11, 12, 16, 19, 20, 21, 22, 23, 32, 33, 34 and 10. If $w5 \neq 0$, 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 $w1 = 0$, $w3 \neq 0$, $w5 = 0$, the path is: 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 21, 22, 23, 32, 33, 34 and 10 for $\alpha < \alpha_{sw}$ and 10, 11, 23, 32, 33, 34 and 10 for $\alpha > \alpha_{sw}$. For $w5 \neq 0$, 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 $\alpha < \alpha_{sw}$ and 10, 11, 23, 23a, 24, 25, 26, 28, 30, 31, 32, 33, 34 and 10 for $\alpha > \alpha_{sw}$. 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

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

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

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

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

The remainder of the α, β meshes are then filled out with geometrically increasing α and β intervals, arranged to reach α_{max} and β_{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 $0 \le \omega \le \omega_1$. All the ω_s are assumed nonzero, and it is understood that $\omega_o = 0$. For t=o, subroutine INTG is used to evaluate F(0) and H(0). For t$\neq$o, subroutine FTRANS is used. Contributions from the interval $0 \le \omega \le \omega_1$ are calculated separately, using the ω^2 behavior of $f(\omega)$ explicitly.

f. <u>FTRANS.</u> 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

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

$$- \frac{f(\omega_{s-1})}{\omega_{s-1}} \coth (\omega_{s-1}/2T) \left[\left(1 - \frac{\sin \theta_s}{\theta_s}\right) \sin \omega_{s-1} t - \left(\frac{1 - \cos \theta_s}{\theta_s}\right) \cos \omega_{s-1} t \right]$$

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. <u>INTG</u>. INTG is a trapezoidal integration routine for calculating the integral

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

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

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

h. <u>SCINT</u>. 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

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

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

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

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. <u>STERP and SNEAR</u>. 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 S1 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 S1 by taking the average of its value at the two nearest β-meshpoint. 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. <u>RCØNV</u>. This subroutine performs the recursive convolution of S1 as given by Eq. 5.1. The convolution is done no matter how the unconvolved S1 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 ($-\mathrm{NPH\emptyset N}(k) \leq n \leq -1$) and ($N + 1 \leq n \leq \mathrm{NPH\emptyset N}(k)$), 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. <u>ACØN1 and ACØN2</u>. These are routines for the analytic convolution of $S2(\alpha, \beta)$ 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 SZ2(x) is the expression for $S(\alpha, \beta)$ for a free gas (given in Eq. 2.7) at the current value of α.

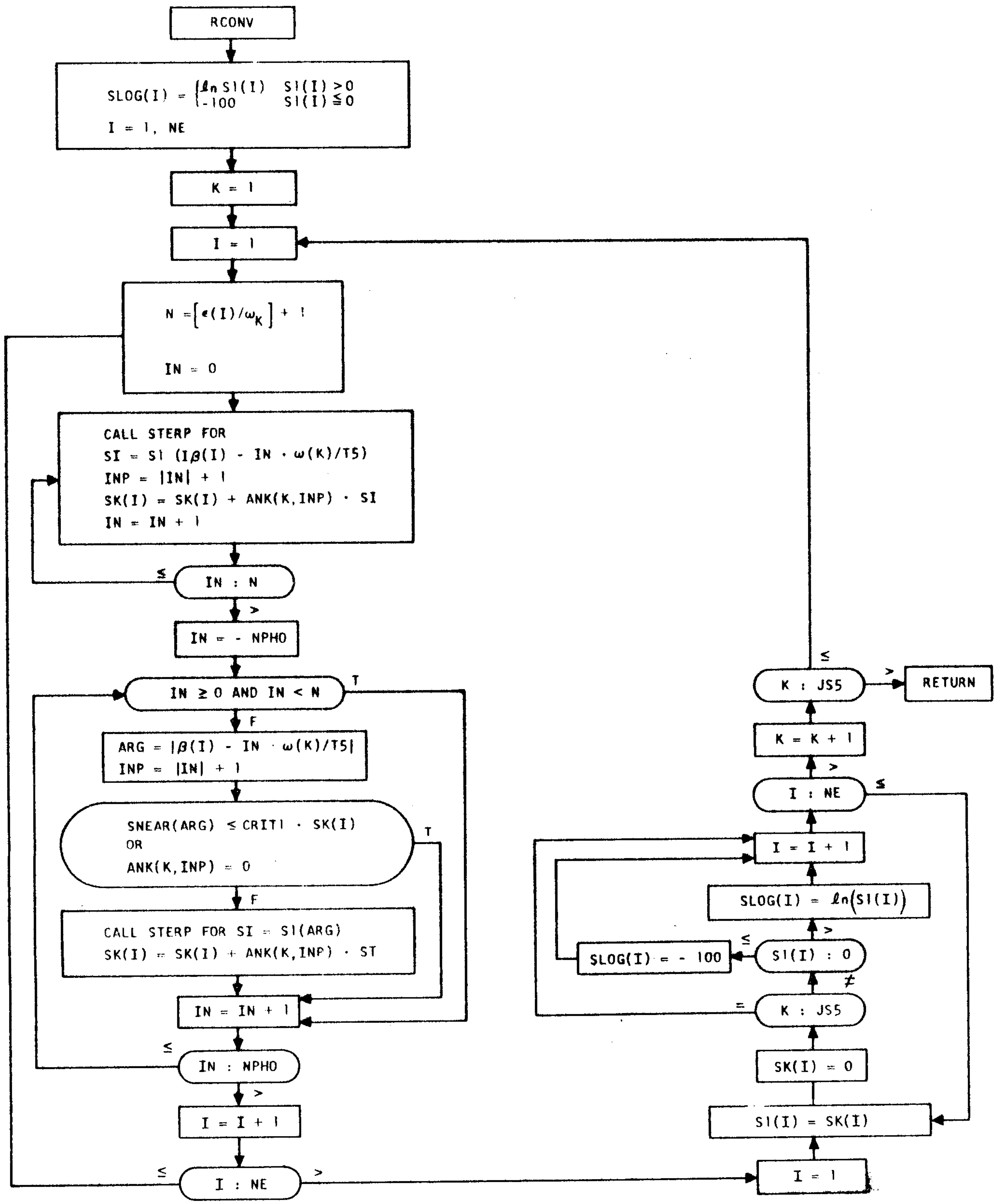

Fig. 2--Flow chart for RCONV

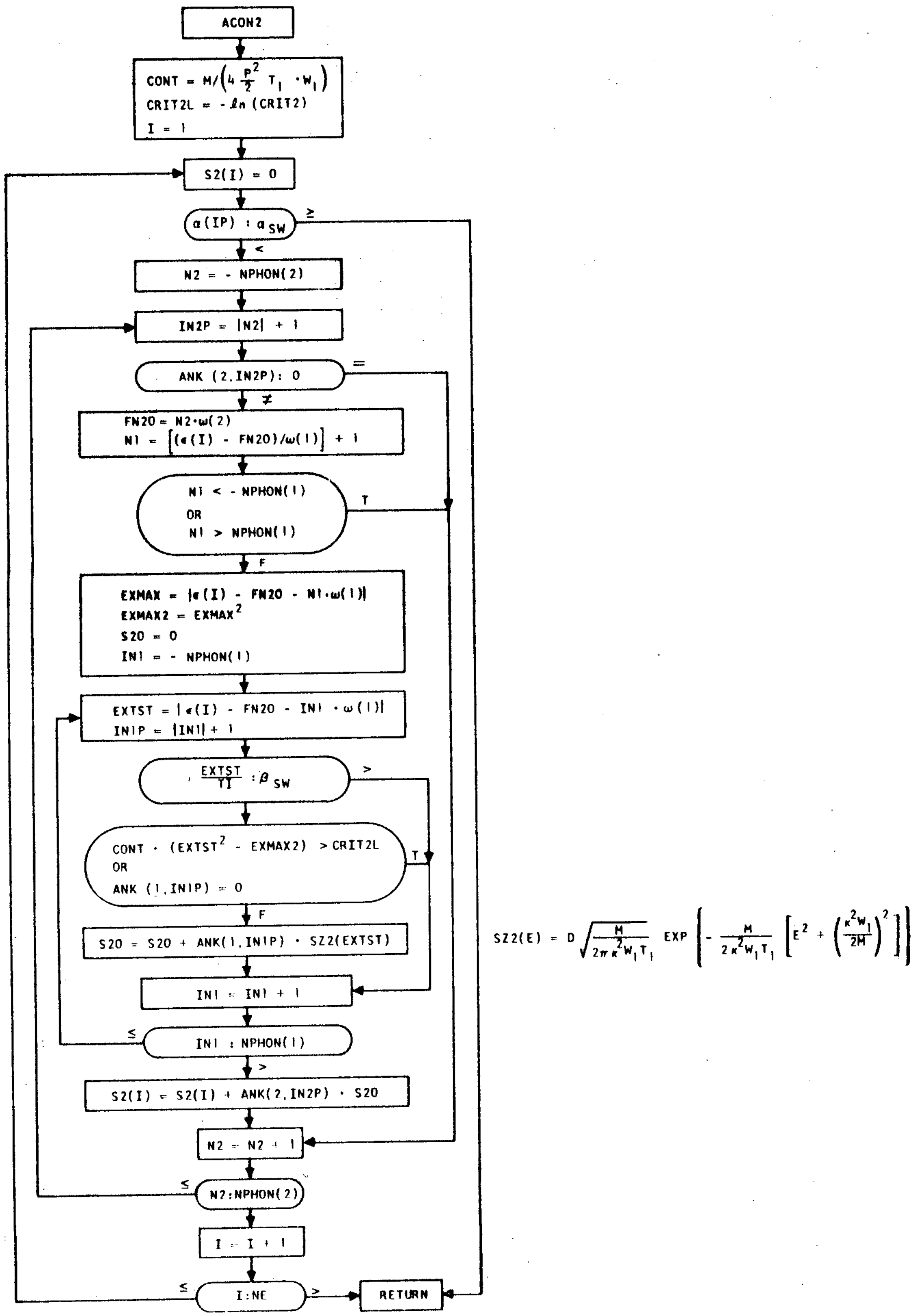

Fig. 3--Flow chart for ACON2

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.

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

Item	Columns	Format	Code Symbol	Report Symbol	Description
	6-10	I5	JS4		Number of points in anisotropic part of the frequency spectrum. JS4 < 0 as for JS3. (JS4 $\leqq$ 100)
	14-15	I5	JS5		Number of discrete oscillators. (JS5 $\leqq$ 2 if $W_1 \neq 0$, JS5 $\leqq$ 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 $\alpha \geqq$ ALPSW. BETSW = 100 if left blank.
	31-40	E10	ALPSW	α_{sw}	α value above which SCT approximation is used <u>for</u> <u>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)

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

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

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

Note 1. If $|NT1| < 0$, t starts at 0 and increases by Δt_1 until $t \geq t\ max_1$, 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 $\alpha = \alpha(1), \ldots, \alpha$ (NREST-1) must have been saved.

Note 4. Time integrals are cut off at t_i if $\max\left(\sum_{j=i}^{i+19} Q_j, \sum_{j=i}^{i+19} R_j\right)/Q_1 \leq$ 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 Card 22 is blank, punching and error map printout are skipped and code returns to Card 23 for next input.

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

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 $\varkappa^2/2 = \alpha MT$ 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 $w3 \neq 0$), and the over-all effective temperature for Modes 1, 3 and 5 (if $w3 \neq 0$).

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 $w3 \neq 0$, 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 S1 (Eq. 3.9), and the Debye-Waller factor (Eq. 2.17). The rest of the block consists of β and the unconvolved values of S1, $S1e^{\beta/2}$, S2, $S2e^{\beta/2}$, S, $Se^{\beta/2}$ and a last column giving $Se^{\beta/2}$ 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 S1 integration, T(S), for the recursive and analytic convolution with two discrete oscillators, T(CØNV1) and T(CØNV2), are printed.

The rest of the output relates to the total S (S1 + S2) if NSEP = 0, (the usual case) or is repeated for S1, S2, and S1 + S2 if NSEP $\neq$ 0, in which case separate punched output also is produced for S1, S2 and S1+S2 for use by later codes, giving $SP(\alpha, \beta) = TS(\alpha, \beta)$ (see footnote on page 2).

SP(α, β) 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.0 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	8.864337-01
2	1.275000-02	5.000000-03	9.966644-01
3	1.912500-02	1.125000-02	1.114856+00
4	2.550000-02	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	1.850652+00
10	6.375000-02	1.150000-01	1.965238+00
11	6.630000-02	1.197000-01	1.950284+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	6.830000-02	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	3.687082-01
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

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

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

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	3.238476+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	8.825098+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 TBAR (MODE 3)= 4.916647-02 T(CH)= 1.176505-01

TOTAL TBAR= 1.203628-01

G3(0)= 8.824152+00

I, 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	5.500000+00	8.176446+00	2.350477+00	38	6.000000+00	8.057510+00	2.540997+00
39	6.500000+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	4.698915+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

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	-1.021877+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	-5.666810-01	-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

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	1.274225-01	202	2.120000+02	-3.681329-02	1.174535-01
203	2.140000+02	-5.968581-02	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	-2.235906-02	224	2.560000+02	-5.133454-02	-3.570722-02
225	2.580000+02	-4.336586-02	-4.823662-02	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	-6.760137-02
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	-1.829288-02	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	3.080541-02
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

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	3.860000+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	-2.167770-02	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	-3.005213-02
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	-1.585423-02	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	-2.164061-02
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	-3.008165-03
329	4.660000+02	2.242619-02	4.711362-03	330	4.680000+02	1.923952-02	1.169470-02
331	4.700000+02	1.393061-02	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	1.956829-02
335	4.780000+02	-1.417187-02	1.557842-02	336	4.800000+02	-1.885462-02	9.566292-03
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	-1.893091-02
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	-5.501353-03	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	-1.703050-02
379	5.660000+02	-9.717801-03	-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	-1.952909-02
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	2.044046-02	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	-1.104903-02	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

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	9.892-03	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	4.476-03	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	3.456-03	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	3.119-03	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	-1.822-04	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	-4.496-04	-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	-5.636-06	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	-1.058-04	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	7.333-05	-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	-8.469-05	-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	-1.546-05	-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	-2.706-05	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	2.436-05	-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	3.566-05	-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	1.226-06	-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	7.976-06
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	6.446-07	-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	-6.249-06	-1.249-05
5.30+02	-3.284-06	-1.411-05	5.32+02	1.866-06	-1.398-05	5.34+02	6.597-06	-1.213-05	5.36+02	1.040-05	-8.833-06
5.38+02	1.284-05	-4.474-06	5.40+02	1.366-05	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	1.897-06	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	-1.493-05	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	1.465-05	-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	4.856-06	1.254-05	5.88+02	4.868-07	1.313-05	5.90+02	-3.759-06	1.228-05	5.92+02	-7.422-06	1.012-05
5.94+02	-1.012-05	6.930-06	5.96+02	-1.158-05	3.089-06	5.98+02	-1.167-05	-9.587-07	6.00+02	-1.041-05	-4.755-06

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	2.825011-03	2.983780-02	0.000000	0.000000	2.825011-03	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

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	7.873743+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	

ALPHA 1 = 5.000000-02 CONVOLVED

I	BETA	S1	S1*EXP(BETA/2)	S2	S2*EXP(BETA/2)	S	S*EXP(BETA/2)	SCT
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	1.081210-28	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	9.283575-03	5.519865-02	0.000000	0.000000	9.283575-03	5.519865-02	7.691121-29
42	3.753690+00	7.451831-03	4.868179-02	0.000000	0.000000	7.451831-03	4.868179-02	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	7.610490-04	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	7.087238-04	4.226818-02	0.000000
55	8.825098+00	1.470964-06	1.213243-04	2.791678-27	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	1.113516+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	9.669169-08	3.753886-23	1.918856-17	1.891594-13	9.669169-08	0.000000
69	2.874471+01	5.641120-14	9.844633-08	0.000000	0.000000	5.641120-14	9.844633-08	0.000000
70	3.144558+01	4.400706-15	2.963760-08	1.742641-38	1.173623-31	4.400706-15	2.963760-08	0.000000
71	3.441596+01	4.388356-16	1.305066-08	1.522896-24	4.528985-17	4.388356-16	1.305066-08	0.000000
72	3.768275+01	1.298725-16	1.977978-08	4.836780-13	7.366491-05	4.838079-13	7.368468-05	0.000000
73	4.127551+01	2.260237-17	2.075000-08	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	1.887523-11	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	7.873743+01	1.238695-32	1.550884-15	0.000000	0.000000	1.238695-32	1.550884-15	0.000000

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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	6.948-04	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	2.136-02	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	2.056-02	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	1.536-02	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	-2.065-03	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	-2.558-03	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	8.738-05	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	-1.089-03	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	-1.658-04	-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	1.136-03	-1.387-04	9.30+01	1.104-03	-3.949-05	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	3.808-04	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	6.486-05	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

2.10+02	-2.125-05	2.747-04	2.12+02	-7.916-05	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	-1.788-04	-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	1.286-06	-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
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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	4.106-05	-3.592-05	3.10+02	5.213-05	-2.048-05	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	-6.055-06	-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	-3.486-05	3.566-05	3.68+02	-4.261-05	2.166-05
3.70+02	-4.530-05	6.324-06	3.72+02	-4.286-05	-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	1.895-06	-3.694-05	3.82+02	1.467-05	-3.280-05	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	3.882-05	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	-3.136-05	-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	6.969-06	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	-1.618-05	-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	2.588-05	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	-2.296-05	-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	-8.705-06	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	6.750-07	5.24+02	-1.875-05	-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	2.235-06	-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	1.615-05	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	-1.706-05	7.348-06	5.58+02	-1.866-05	1.801-06	5.60+02	-1.836-05	-3.944-06
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	3.327-06	-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	5.256-07	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

I	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	8.807301-02	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	7.960201-02	1.706387-01	0.000000	0.000000	7.960201-02	1.706387-01	9.830234-02
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	4.575409-04
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	6.309817-02	2.180429-01	0.000000	0.000000	6.309817-02	2.180429-01	3.449154-06
33	2.560000+00	6.067110-02	2.182121-01	0.000000	0.000000	6.067110-02	2.182121-01	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	2.828475-02	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

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	2.628890+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	7.873743+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	

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	8.068403-02	1.657599-01	0.000000	0.000000	8.068403-02	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	7.187460-02	1.877146-01	7.187555-28	1.877171-27	7.187460-02	1.877146-01	2.528747-03
26	2.000000+00	7.062895-02	1.919894-01	2.048884-25	5.569444-25	7.062895-02	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	6.043835-02	2.173750-01	3.103022-15	1.116045-14	6.043835-02	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	3.437311-02	1.616984-01	5.525592-17	2.599355-16	3.437311-02	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	9.718068-02	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

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

S1+S2

```
ID=     1      SIGF=  2.036000+01      EPS=  1.000000-06

SP(ALPHA,BETA) FOR BETA    1=      .00000
    1  5.26030+00       2  3.68413+00

SP(ALPHA,BETA) FOR BETA    2=      .08000
    1  2.96876+00       2  2.76278+00

SP(ALPHA,BETA) FOR BETA    3=      .16000
    1  5.28307-01       2  1.16574+00

SP(ALPHA,BETA) FOR BETA    4=      .24000
    1  3.07265-02       2  2.77906-01

SP(ALPHA,BETA) FOR BETA    5=      .32000
    1  1.65620-03       2  3.89523-02

SP(ALPHA,BETA) FOR BETA    6=      .40000
    1  1.13263-03       2  4.98348-03

SP(ALPHA,BETA) FOR BETA    7=      .48000
    1  1.12635-03       2  2.34328-03

SP(ALPHA,BETA) FOR BETA    8=      .56000
    1  1.12268-03       2  2.22225-03

SP(ALPHA,BETA) FOR BETA    9=      .64000
    1  1.11755-03       2  2.20960-03

SP(ALPHA,BETA) FOR BETA   10=      .72000
    1  1.11197-03       2  2.19911-03

SP(ALPHA,BETA) FOR BETA   11=      .80000
    1  1.10646-03       2  2.18825-03

SP(ALPHA,BETA) FOR BETA   12=      .88000
    1  1.10083-03       2  2.17644-03

SP(ALPHA,BETA) FOR BETA   13=      .96000
    1  1.09425-03       2  2.16333-03

SP(ALPHA,BETA) FOR BETA   14=     1.04000
    1  1.08676-03       2  2.14903-03

SP(ALPHA,BETA) FOR BETA   15=     1.12000
    1  1.07854-03       2  2.13309-03

SP(ALPHA,BETA) FOR BETA   16=     1.20000
    1  1.07053-03       2  2.11708-03
```

```
SP(ALPHA,BETA) FOR BETA   17=     1.28000
    1  1.06255-03      2  2.10060-03

SP(ALPHA,BETA) FOR BETA   18=     1.36000
    1  1.05356-03      2  2.08136-03

SP(ALPHA,BETA) FOR BETA   19=     1.44000
    1  1.04182-03      2  2.05746-03

SP(ALPHA,BETA) FOR BETA   20=     1.52000
    1  1.02651-03      2  2.02719-03

SP(ALPHA,BETA) FOR BETA   21=     1.60000
    1  1.00757-03      2  1.99076-03

SP(ALPHA,BETA) FOR BETA   22=     1.68000
    1  9.88319-04      2  1.95025-03

SP(ALPHA,BETA) FOR BETA   23=     1.76000
    1  9.64600-04      2  1.90877-03

SP(ALPHA,BETA) FOR BETA   24=     1.84000
    1  9.44012-04      2  1.86886-03

SP(ALPHA,BETA) FOR BETA   25=     1.92000
    1  9.25650-04      2  1.83283-03

SP(ALPHA,BETA) FOR BETA   26=     2.00000
    1  9.09756-04      2  1.80087-03

SP(ALPHA,BETA) FOR BETA   27=     2.08000
    1  8.95718-04      2  1.77231-03

SP(ALPHA,BETA) FOR BETA   28=     2.16000
    1  8.82577-04      2  1.74544-03

SP(ALPHA,BETA) FOR BETA   29=     2.24000
    1  8.69347-04      2  1.71819-03

SP(ALPHA,BETA) FOR BETA   30=     2.32000
    1  8.54745-04      2  1.68768-03

SP(ALPHA,BETA) FOR BETA   31=     2.40000
    1  8.36913-04      2  1.65053-03

SP(ALPHA,BETA) FOR BETA   32=     2.48000
    1  8.13549-04      2  1.60275-03

SP(ALPHA,BETA) FOR BETA   33=     2.56000
    1  7.82604-04      2  1.54111-03

SP(ALPHA,BETA) FOR BETA   34=     2.64798
    1  7.39137-04      2  1.45614-03
```

```
SP(ALPHA,BETA) FOR BETA   35=    2.74475
    1  6.81588-04      2  1.34443-03

SP(ALPHA,BETA) FOR BETA   36=    2.85116
    1  6.10408-04      2  1.20604-03

SP(ALPHA,BETA) FOR BETA   37=    2.96820
    1  5.27829-04      2  1.04591-03

SP(ALPHA,BETA) FOR BETA   38=    3.09692
    1  4.40235-04      2  8.76471-04

SP(ALPHA,BETA) FOR BETA   39=    3.23848
    1  3.59807-04      2  7.18461-04

SP(ALPHA,BETA) FOR BETA   40=    3.39416
    1  2.93436-04      2  5.85153-04

SP(ALPHA,BETA) FOR BETA   41=    3.56538
    1  2.36725-04      2  4.72516-04

SP(ALPHA,BETA) FOR BETA   42=    3.75369
    1  1.90015-04      2  3.79326-04

SP(ALPHA,BETA) FOR BETA   43=    3.96079
    1  1.51582-04      2  3.02758-04

SP(ALPHA,BETA) FOR BETA   44=    4.18855
    1  1.20100-04      2  2.39835-04

SP(ALPHA,BETA) FOR BETA   45=    4.43904
    1  9.35457-05      2  1.87253-04

SP(ALPHA,BETA) FOR BETA   46=    4.71453
    1  7.19021-05      2  1.43812-04

SP(ALPHA,BETA) FOR BETA   47=    5.01750
    1  5.37480-05      2  1.07609-04

SP(ALPHA,BETA) FOR BETA   48=    5.35071
    1  3.94694-05      2  7.92688-05

SP(ALPHA,BETA) FOR BETA   49=    5.71717
    1  2.83105-05      2  5.70813-05

SP(ALPHA,BETA) FOR BETA   50=    6.12020
    1  1.94061-05      2  3.94337-05

SP(ALPHA,BETA) FOR BETA   51=    6.56344
    1  3.98201-06      2  9.55738-06

SP(ALPHA,BETA) FOR BETA   52=    7.05092
    2  6.67409-07
```

```
SP(ALPHA,BETA) FOR BETA   53=    7.58703
    2  3.66844-07

SP(ALPHA,BETA) FOR BETA   54=    8.17665
    1  1.60724-05      2  5.89422-05

SP(ALPHA,BETA) FOR BETA   55=    8.82510
    2  1.72269-07

SP(ALPHA,BETA) FOR BETA   56=    9.53825
    2  1.07915-07

SP(ALPHA,BETA) FOR BETA   57=   10.32257
    2  7.54582-08

SP(ALPHA,BETA) FOR BETA   58=   11.18516
    2  3.30474-08

SP(ALPHA,BETA) FOR BETA   64=   18.50071
    2  5.25843-09

SP(ALPHA,BETA) FOR BETA   65=   20.17936
    2  3.01676-10

SP(ALPHA,BETA) FOR BETA   66=   22.02552
    2  1.09527-10

SP(ALPHA,BETA) FOR BETA   72=   37.68275
    2  3.64629-14
```

INTERPOLATION ERROR MAP

I= 1 ALPHA= .05000

14.38	.53-00	3	13.98	.31-01	4	.95	.17-02	5	31.76	.11-02	6	4.68	.11-02	7
.03	.11-02	8	.02	.11-02	9	.01	.11-02	10	.00	.11-02	11	.00	.11-02	12
.01	.11-02	13	.01	.11-02	14	.01	.11-02	15	.00	.11-02	16	.00	.11-02	17
.01	.11-02	18	.03	.10-02	19	.04	.10-02	20	.05	.10-02	21	.03	.99-03	22
.01	.96-03	23	.01	.94-03	24	.02	.93-03	25	.03	.91-03	26	.02	.90-03	27
.01	.88-03	28	.00	.87-03	29	.02	.85-03	30	.05	.84-03	31	.09	.81-03	32
.13	.76-03	33	.19	.74-03	34	.24	.66-03	35	.28	.61-03	36	.31	.53-03	37
.28	.44-03	38	.03	.36-03	39	.24	.29-03	40	.12	.24-03	41	.21	.19-03	42
.21	.15-03	43	.21	.12-03	44	.08	.94-04	45	.15	.72-04	46	.02	.54-04	47
.15	.39-04	48	.10	.28-04	49	.16	.19-04	50	15.30	.40-05	51	22.36	.13-06	52
38.71	.55-07	53	87.99	.18-04	54									

I= 2 ALPHA= .10000

7.19	.12+01	3	7.14	.28-00	4	6.64	.39-01	5	1.14	.50-02	6	16.27	.23-02	7
8.77	.22-02	8	.59	.22-02	9	.01	.22-02	10	.00	.22-02	11	.01	.22-02	12
.01	.22-02	13	.01	.21-02	14	.01	.21-02	15	.00	.21-02	16	.00	.21-02	17
.02	.21-02	18	.03	.21-02	19	.04	.20-02	20	.04	.20-02	21	.03	.20-02	22
.01	.19-02	23	.00	.19-02	24	.02	.18-02	25	.02	.18-02	26	.02	.18-02	27
.01	.17-02	28	.01	.17-02	29	.03	.17-02	30	.05	.17-02	31	.09	.16-02	32
.12	.15-02	33	.18	.15-02	34	.23	.13-02	35	.27	.12-02	36	.30	.10-02	37
.26	.88-03	38	.06	.72-03	39	.18	.59-03	40	.16	.47-03	41	.20	.38-03	42
.21	.30-03	43	.20	.24-03	44	.11	.19-03	45	.11	.14-03	46	.00	.11-03	47
.17	.79-04	48	.10	.57-04	49	.11	.39-04	50	13.23	.96-05	51	14.44	.67-06	52
31.19	.39-06	53	73.67	.59-04	54									

7.4.2 Punched Output

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

Item	Format	Variable	Description
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 1PE11.4	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 1PE11.4	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

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

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† = 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 plots given in Figs. 4, 5, and 6 are of $S(\alpha, \beta)$ vs α for the β-values given in Tables 5, 6, and 7, respectively.

Table 1

13A6, A2 COMMENTS: $H(H_2O)$ Modified Haywood Spectrum at room temperature

			X_3	7E10	Q_3	
13I5	NT-5	7E10				
	NP 80		.006375		.00125	
	NE 80		.01275		.005	
	NDAM		.019125		.01125	
	NGPRT		.0255		.02	
	NCP		.031875		.03125	
	NMESH 1		.03825		.045	
	NREST		.044625		.059	
	NCVP		.051		.075	
	NSEP		.057375		.095	
	NAD 1		.00375		.115	
	NAD 2		.0663		.1197	
	NAD 3		.06885		.1214	
3I5	JS3	29	.0714		.1218	
	JS4		.07395		.1195	
	JS5	2	.0765		.1125	
5E10	W1	.05555	.082875		.0975	
	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	
	T4		.133875		.054	
	T5	.0255	.14025		.0515	
	TEMP		.146625		.0488	
7E10	Am	1.00866	.153		.0459	
	DC		.159375		.0431	
	BETSW	20.	.16575		.042	
	ALPSW	20.				
	CRIT1					
	CRIT2					
	CRIT3					

7E10	X_5	.205, .45
7E10	Q_5	1/3, 2/3
7E10	NPHON	10, 5
5E10	EMAX	2.0
	DALPHA	.05
	ALPHAC	.5
	DBETA	.08
	BETAC	2.5

2E10	DT	TMAX
	.1	2.
	.2	5.
	.5	20.
	1.	100.
	2.	600.

2I10,	ID	296
3E10	NPT	0
	SIGF	20.36
	EPS	10^{-6}

Table 2

13A6, A2 COMMENTS: $H(H_2O)$ Modified Haywood Spectrum at 500^oK

Format	Variable	Value	X_3	7E10	Q_3		Format	Variable	Value
13I5	NT	7E10					7E10	X_5	
	NP		______	______	______	______	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

13I5	NT-9	7E10	X_3		Q_3		7E10	X_5		
	NP	40	.20842		.346613	6.5662	7E10	Q_5		
	NE	80			1.4135	5.47181				
	NDAM	1			3.03321	5.06137	7E10	NPHON		
	NGPRT				3.25901	5.19813	5E10	EMAX	1.0	
	NCP				3.38468	.457086		DALPHA	.25	
	NMESH	1			3.48269			ALPHAC	2.	
	NREST				3.76397			DBETA	.1	
	NCVP				4.05025			BETAC	4.	
	NSEP				4.84696					
	NAD1				7.35744					
	NAD2				5.88224		2E10		DT	TMAX
	NAD3				4.63255				0.001	0.01
3I5	JS3	-38			4.48287				0.01	0.1
	JS4				5.80642				0.1	3.0
	JS5				4.63802				0.25	6.0
5E10	W1	.001			4.28503				0.5	9.0
	W2				3.92079				1.0	22.0
	W3	1.0			4.91352				2.0	24.0
	W4				5.53836				4.0	100.0
	W5				7.51076				6.0	3000.0
6E10	T1	.0255			5.31651					
	T2				5.40525					
	T3	.0255			5.20376					
	T4				5.3276		2I10,	ID	34	
	T5				7.17251		3E10	NPT	0	
	TEMP				3.31813			SIGF	4.7	
7E10	Am	12.011			4.50126			EPS	10^{-6}	
	DC				5.04663					
	BETSW	30.			4.2089					
	ALPSW	30.			2.91985					
	CRIT1				4.65109					
	CRIT2				13.1324					
	CRIT3				7.25016					

Table 4

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

Card	Parameter	Card	X_3	7E10	Q_3	
13I5	NT-5	7E10				
	NP 40		0.168		.00034	.36861
	NE 150				.00141	.25702
	NDAM 1				.0032	.16956
	NGPRT				.00568	.10584
	NCP				.00888	.06313
	NMESH 1				.01275	.03492
	NREST				.01736	.01845
	NCVP				.02268	.00923
	NSEP				.02873	.00437
	NAD1				.03546	.00195
	NAD2				(points 11	0.
	NAD3				thru 52=0)	
3I5	JS3 -84				.00195	
	JS4				.00437	
	JS5				.00923	
5E10	W1 5×10^{-5}				.01845	
	W2				.03492	
	W3 .99995				.06313	
	W4				.10584	
	W5				.16956	
6E10	T1 .0255				.25702	
	T2				.36861	
	T3 .0255				.5	
	T4				.64171	
	T5				.77917	
	TEMP				.89503	
7E10	Am 1.00866				.97265	
	DC				1.0	
	BETSW 160.				.97265	
	ALPSW 160.				.89503	
	CRIT1				.77917	
	CRIT2				.64171	
	CRIT3				.5	

Card	Parameter	Value
7E10	X_5	
7E10	Q_5	
7E10	NPHON	
5E10	EMAX	1.0
	DALPHA	.5
	ALPHAC	5.
	DBETA	.25
	BETAC	30.

Card	DT	TMAX
2E10		
	.3	6.
	.6	18.
	1.2	60.
	3.	300.
	6.	3100

Card	Parameter	Value
2I10,	ID	360
3E10	NPT	0
	SIGF	20.36
	EPS	10^{-6}

Table 5

$H(H_2O)$ at 296°K

Curve Index	Beta
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

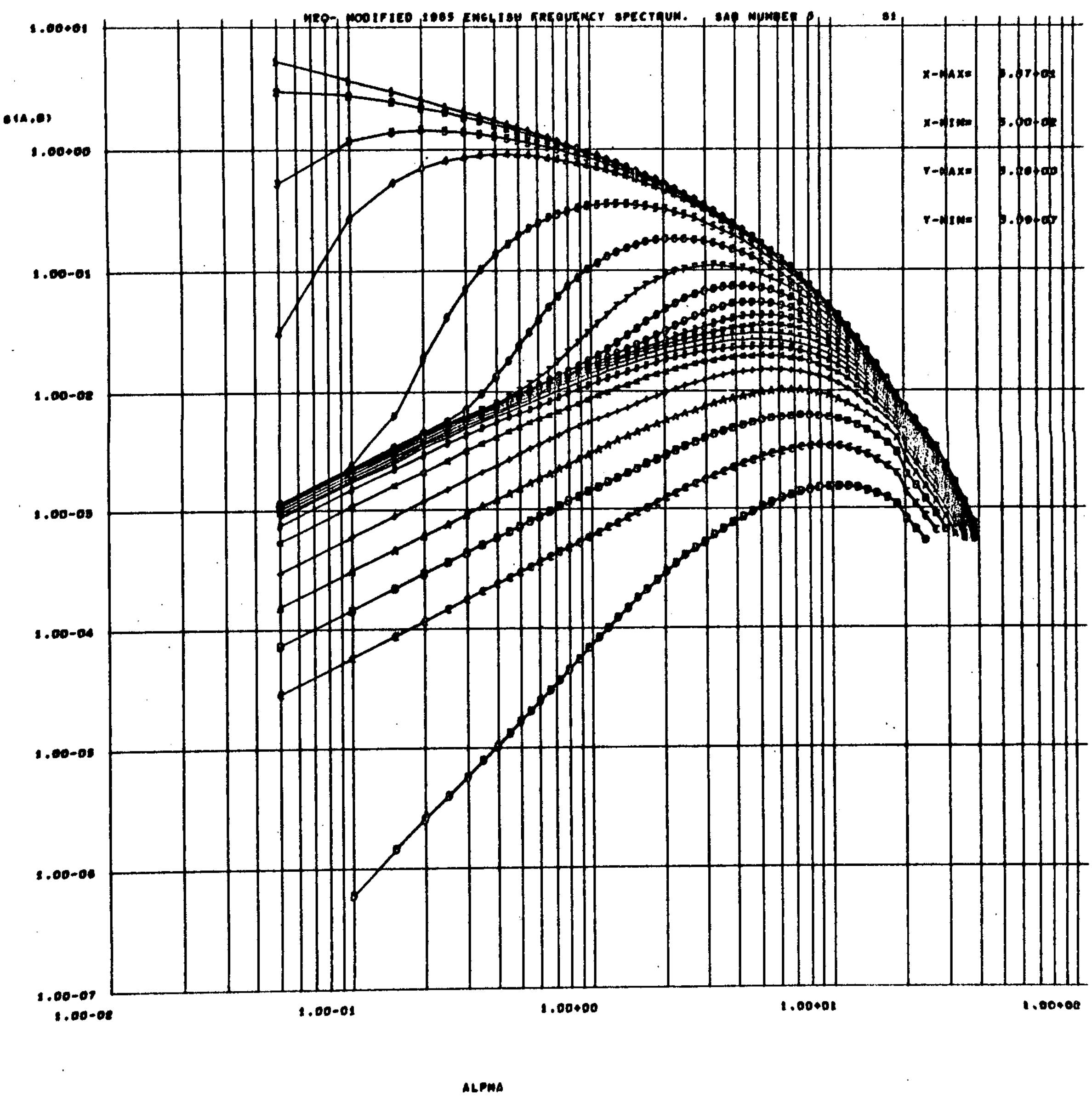

Fig. 4--$S(\alpha, \beta)$ for $H(H_2O)$ at 296°k

Table 6

CARBON AT 1000°K

Curve	Beta
1	0.
2	2.959400-02
3	5.918800-02
4	1.775600-01
5	2.959400-01
6	4.143200-01
7	5.326900-01
8	6.510700-01
9	7.694400-01
10	8.878200-01
11	1.006200 00
12	1.124600 00
13	1.245800 00
14	1.409800 00
15	1.646500 00
16	1.987900 00
17	2.480600 00
18	3.191600 00
19	4.217400 00
20	5.697600 00

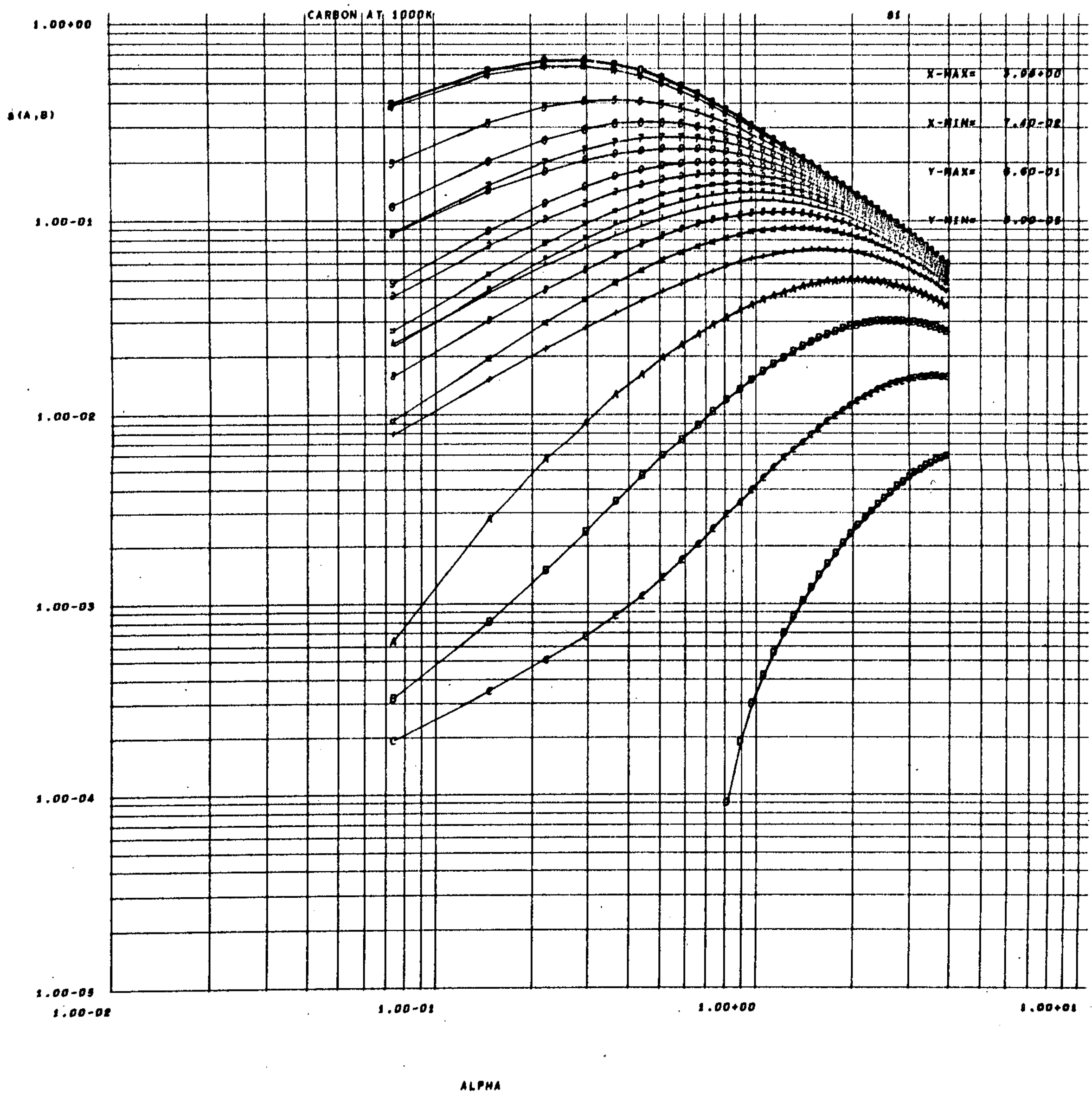

Fig. 5--S(α, β) for graphite at 1000°K

Table 7

MASS 360 H(ZrH) AT 1200°C

Curve	Beta
1	0.
2	5.025000-02
3	1.005000-01
4	3.015000-01
5	5.025000-01
6	7.035000-01
7	9.045000-01
8	1.105500 00
9	1.306500 00
10	1.507500 00
11	1.708500 00
12	1.909500 00
13	2.110500 00
14	2.311500 00
15	2.512500 00
16	2.713500 00
17	2.914500 00
18	3.115500 00
19	3.316500 00
20	3.517500 00

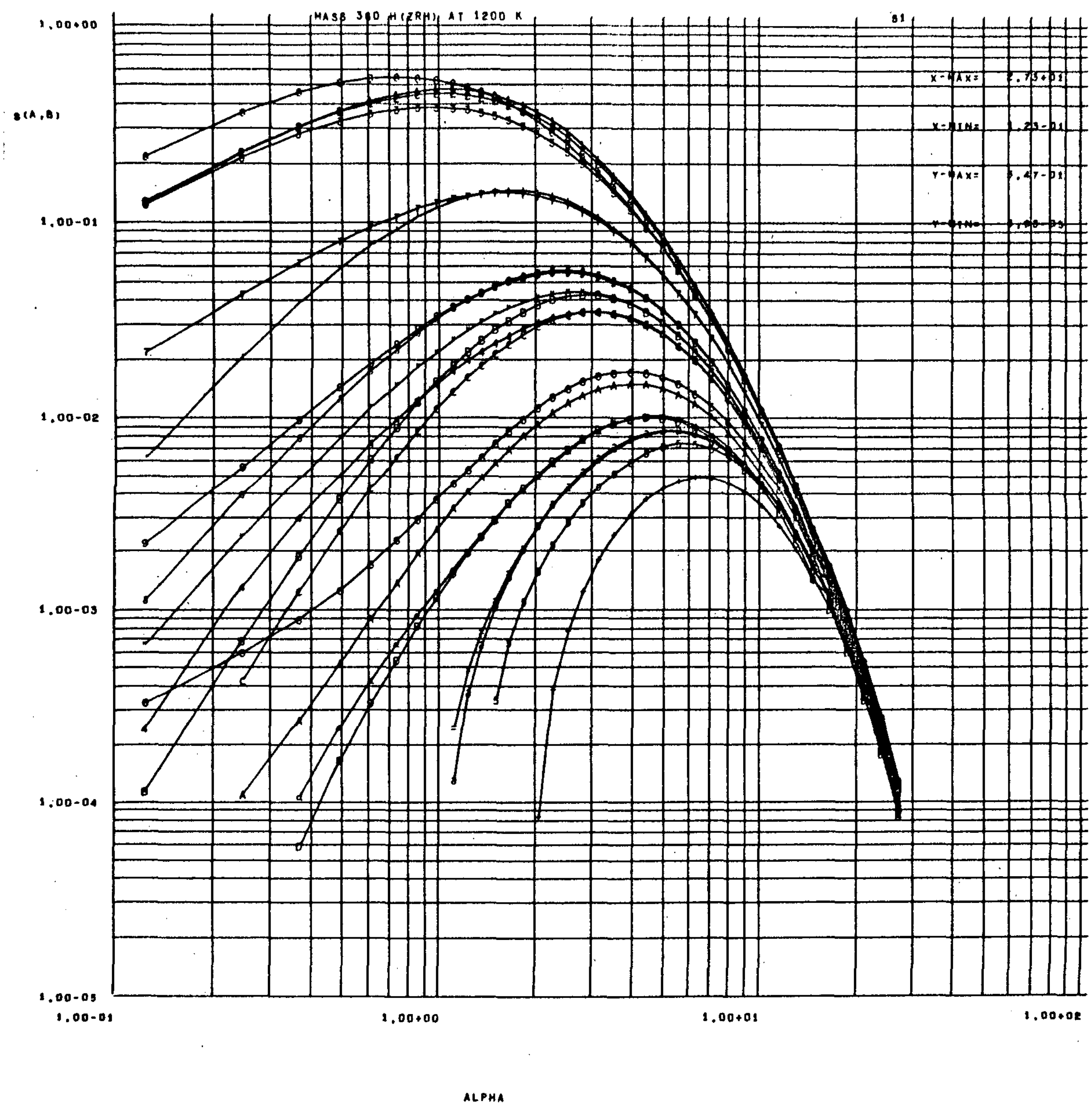

Fig. 6--$S(\alpha, \beta)$ for H(ZrH) at $1200^{\circ}K$

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 S1 for w3 $\neq 0$, the following prescription has provided adequate time meshes:

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

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

where θ_{min} (in eV) is the lowest frequency point for Mode 3 at which there is significant structure, and θ_{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 Δt_{max}. A reasonable choice for a first try is

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

FORTRAN LISTING OF THE GASKET PROGRAM

```
@I      FOR DATA/S1,DATA/S1,DATA/R1
        BLOCK DATA
        COMMON /IOCOM/IO5,IO6,IO7,IOPCH
        DATA IO5,IO6,IO7,IOPCH/5,6,9,0/
        END
```

```
@I    FOR GASKET/S1,GASKET/S1,GASKET/R1
      COMMON HOL(20),NT,NP,NE,NDAM,NGPRT,NCP,NMESH,NREST,NCVP,NSEP,
     1NSUMCV,JS3,JS4,JS5,W1,W2,W3,W4,W5,T1,T2,T3,T4,T5,TEMP,AM,DC,
     2BETSW,ALPSW,CRIT1,CRIT2,CRIT3,X3(100),Q3(100),X4(100),Q4(100),
     3X5(20),Q5(20),NPHON(20),ALPHA(100),BETA(150),EB2(150),PSQ(100),
     4EPS(150),T(1000),H(1000),R5(20),ANK(20,21),ARG1(20),ARG2(20),
     5BF(21),SK(150),S1(150),S2(150),S1EB(150),S2EB(150),SEB(150),S(150)
     6,SC(150),W12,R(1000),Q(1000),GS(1000),GC(1000),ZPHON(100),
     7EPSM(150),SCEB(150),IP,W13,TBAR13,NEX,NEX1,TSX,TCONV1,TCONV2,
     8TCHI,SZCON,PS,IPG,TBAR
C
      COMMON /STERPC/SLOG(150)
C
C     SYMBOLIC I/O ASSIGNMENTS
      COMMON /IOCOM/I05,I06,I07,IOPCH
C     IF IOPCH=0, THE PUNCH STATEMENT WILL BE USED
C     IF IOPCH.NE.0, PUNCHING WILL BE WRITTEN ON UNIT IOPCH
C
C     SHORT COLLISION TIME EXPRESSION FOR S(ALPHA,BETA)
      SCT(A,B,T,TB,W)=EXP(-T*(B**2+(A*W)**2)/(4.*A*W*TB)-0.5*B*(1.-
     1 T/TB))/SQRT(12.566371*A*W*T*TB)
C     ANALYTIC FREE GAS S(ALPHA,BETA) FOR MODE 5
      SZ2(E)=SZCON*EXP(-AM*(E**2+(PS*W1/AM)**2)/(4.*PS*T1*W1))
C
C
   10 CALL PREP(IRST)
C
C     DISTRIBUTED ISOTROPIC FREQUENCY SPECTRUM G FUNCTIONS
      IF(W3.EQ.0.0)WRITE(I07)(DDUM,I=1,2001)
      IF(W3.EQ.0.) GO TO 80
      CALL TICKER(TSTART)
      IF(NREST.NE.1 .AND. IRST.EQ.0) GO TO 30
      IF(IPG.EQ.0)CALL GTG(W3,T3,AM,X3,Q3,T,GC,GS,JS3,NT,TBAR)
      IF(IPG.EQ.0)WRITE(I07)GC,GS,TBAR
   30 CONTINUE
      CALL TICKER(TSTOP)
      TIME=(TSTOP-TSTART)/2160.
      TBAR13=(W1*T1+W3*TBAR)/W13
      DBWINT=GC(1)*AM/W3
      SBAR=0.
   80 IF(JS5.EQ.0) GO TO 95
      DO 90 I=1,JS5
   90 SBAR=SBAR+Q5(I)*X5(I)/(2.*TANH(X5(I)/(2.*T5)))
   95 TBTOT=W1*T1+W3*TBAR+W5*SBAR
      WRITE(I06,100)DBWINT,TBAR,TIME,TBTOT
  100 FORMAT(//10X22HDEBYE-WALLER INTEGRAL=1PE15.6,10X14HTBAR (MODE 3)=
     1E15.6,10X6HT(CH)=E15.6/10X11HTOTAL TBAR=E15.6//)
      IF(NGPRT.NE.0)WRITE(I06,110)GC(1),    (I,T(I),GC(I),GS(I),I=1,NT)
  110 FORMAT(//10X6HG3(0)=1PE15.6/
     110X23HI, T(I), G3C(I), G3S(I)/ 2(I5,1P3E15.6))
C
C     MAIN LOOP OVER ALPHAS
C
      IF(NP.EQ.0)GO TO 10
      DO 1000 IP=NREST,NP
```

```
      PS=PSQ(IP)
      DBW=1.0
      DO 300 I=1,NE
      SC(I)=SCT(ALPHA(IP),BETA(I),TEMP,TBAR13,W13)
      S1(I)=SC(I)
      S2(I)=0.
  300 S (I)=SC(I)
      IF(ALPHA(IP).GE.ALPSW) GO TO 520
C
C     CHI, MODES 1-4
      CALL TICKER(TSTART)
      DBW=1.0
      IF(W3.EQ.0.) GO TO 410
      DBW=EXP(-PS*GC(1))
      APS=PS*W1/AM
      BPS=PS
      DO 400 I=1,NT
      EX1=EXP(BPS*GC(I))
      EX2=EXP(-APS*T1*T(I)**2)
      Q(I)=(COS(BPS*GS(I))*EX1-1.)*EX2
      R(I)=SIN(BPS*GS(I))*EX1*EX2
  400 CONTINUE
      DBWP=DBW/3.1415927
      GO TO 430
  410 DO 420 I=1,NE
  420 S1(I)=0.
      GO TO 470
  430 CONTINUE
      CALL TICKER(TSTOP)
      TCHI=TCHI+TSTOP-TSTART
C
C     S, MODES 1-4
      CALL TICKER(TSTART)
      IF(NCP.NE.0)WRITE(I06,440)IP,ALPHA(IP),PS,(T(I),Q(I),R(I),I=1,NT)
  440 FORMAT(1H1//20X6HALPHA I2,2H =1PE15.6,8H P**2/2=E15.6/
     110X13HT, Q(T), R(T)/4(1XE9.2,2E11.3))
      CALL ENDPT(NT,NT1R,R,Q(1),CRIT3)
      CALL ENDPT(NT,NT1Q,Q,Q(1),CRIT3)
      NT1=MAX0(NT1R,NT1Q)
      CALL SCINT(T,Q,R,EPSM,S1,APS,DBWP,NT1,NEX)
      DO 450 I=1,NEX
      S1(I)=S1(I)/EB2(I)
  450 IF(S1(I).LT.0.)S1(I)=0.
      IF(NEX1.EQ.0)GO TO 470
      DO 460 I=NEX1,NE
  460 S1(I)=SC(I)
  470 IF(W1.EQ.0.0 .AND. NDAM.NE.0) GO TO 485
  475 CONTINUE
      SZCON=DBW*SQRT(AM/(12.566371*PS*W1*T1))
      DO 480 I=1,NE
  480 S2(I)=SZ2(EPS(I))
  485 CONTINUE
      CALL TICKER(TSTOP)
      TSX=TSX+TSTOP-TSTART
  490 DO 500 I=1,NE
```

```
      S(I)=S1(I)
      IF(NDAM.EQ.0) S(I)=S(I)+S2(I)
      S1EB(I)=S1(I)*EB2(I)
      S2EB(I)=S2(I)*EB2(I)
      SCEB(I)=SC(I)*EB2(I)
  500 SEB(I) = S(I)*EB2(I)
      IF(W3.NE.0.0)WRITE(I06,510)ALPHA(IP),NT1R,NT1Q,DBW,
     1(I,BETA(I),S1(I),S1EB(I),S2(I),S2EB(I),S(I),SEB(I),SCEB(I),I=1,NE)
  510 FORMAT(1H1//10X6HALPHA=1PE15.6,10X2I7,10X20HDEBYE-WALLER FACTOR=
     XE15.6//
     X         5H    I,11X4HBETA,11X4HS1   ,15H S1*EXP(BETA/2),
     111X4HS2   ,15H S2*EXP(BETA/2),12X3HS   ,14H S*EXP(BETA/2),11X3HSCT
     2/(I5,1P8E15.6))
  520 IF(JS5.EQ.0)GO TO 620
      DO 525 K=1,JS5
      CALL BESSL(ARG1(K)*PS     ,BF,20)
      EX=EXP(-PS    *ARG2(K))
      DO 525 I=1,20
  525 ANK(K,I)=BF(I)*EX
C
C     RECURSIVE CONVOLUTION OF S(PART 1) WITH DISCRETE OSCILLATORS
      IF(W3.EQ.0.)GO TO 530
      CALL TICKER(TSTART)
      CALL RCONV
      CALL TICKER(TSTOP)
      TCONV1=TCONV1+TSTOP-TSTART
C
C     CONVOLUTION OF S(PART 2) WITH 2 DISCRETE OSCILLATORS
  530 IF(W1.EQ.0.0.OR.NDAM.NE.0.OR.JS5.NE.2)GO TO 540
      IF(ALPHA(IP).GE.ALPSW) GO TO 540
      CALL TICKER(TSTART)
      CALL ACON2
      CALL TICKER(TSTOP)
      TCONV2=TCONV2+TSTOP-TSTART
  540 CONTINUE
C
C     CONVOLUTION OF S (PART 2) WITH 1 DISCRETE OSCILLATOR
      IF(JS5.NE.1.OR.NDAM.NE.0.OR.W1.EQ.0.0) GO TO 550
      IF(ALPHA(IP).GE.ALPSW) GO TO 550
      CALL ACON1
  550 CONTINUE
C
C
      DO 600 I=1,NE
      S(I)=S1(I)+S2(I)
      S1EB(I)=S1(I)*EB2(I)
      S2EB(I)=S2(I)*EB2(I)
      SCEB(I)=SC(I)*EB2(I)
  600 SEB (I)= S(I)*EB2(I)
      WRITE(I06,610)IP,ALPHA(IP),(I,BETA(I),S1(I),S1EB(I),S2(I),S2EB(I),
     1S(I),SEB(I),SCEB(I),I=1,NE)
  610 FORMAT(1H1//10X6HALPHA I2,3H = ,1PE15.6,15X9HCONVOLVED//
     1         5H    I,11X4HBETA,11X4HS1   ,15H S1*EXP(BETA/2),
     211X4HS2   ,15H S2*EXP(BETA/2),12X3HS   ,14H S*EXP(BETA/2),11X3HSCT
     3/(I5,1P8E15.6))
```

```
C
  620 CONTINUE
      WRITE(I07)(S(I),I=1,NE)
      IF(NSEP.NE.0)WRITE(I07)(S1(I),I=1,NE)
      IF(NSEP.NE.0)WRITE(I07)(S2(I),I=1,NE)
      IF(WARN (XX))1000,630,630
  630 WRITE(6,640)IP
  640 FORMAT(///5X,20(1H*),19HRESTART AFTER ALPHA I3,20(1H*))
      REWIND I07
      CALL EXIT
 1000 CONTINUE
C
      TTOT=TSX+TCONV1+TCONV2+TCHI
      TCHI=TCHI/TTOT
      TSX=TSX/TTOT
      TCONV1=TCONV1/TTOT
      TCONV2=TCONV2/TTOT
      WRITE(I06,1010)TCHI,TSX,TCONV1,TCONV2
 1010 FORMAT(///10X7HT(CHI)=1PE13.5,3X5HT(S)=E13.5,3X9HT(CONV1)=E13.5,3X
     19HT(CONV2)=E13.5)
C
      CALLERRMAP(NE,NP,ALPHA,BETA,EB2,HOL,TEMP,AM,NSEP,EMAX,DBWINT,IRST)
C
      GO TO 10
      END
```

```
@I     FOR PREP/S1,PREP/S1,PREP/R1
       SUBROUTINE PREP(IRST)
       COMMON HOL(20),NT,NP,NE,NDAM,NGPRT,NCP,NMESH,NREST,NCVP,NSEP,
      1NSUMCV,JS3,JS4,JS5,W1,W2,W3,W4,W5,T1,T2,T3,T4,T5,TEMP,AM,DC,
      2BETSW,ALPSW,CRIT1,CRIT2,CRIT3,X3(100),Q3(100),X4(100),Q4(100),
      3X5(20),Q5(20),NPHON(20),ALPHA(100),BETA(150),EB2(150),PSQ(100),
      4EPS(150),T(1000),H(1000),R5(20),ANK(20,21),ARG1(20),ARG2(20),
      5BF(21),SK(150),S1(150),S2(150),S1EB(150),S2EB(150),SEB(150),S(150)
      6,SC(150),W12,R(1000),Q(1000),GS(1000),GC(1000),ZPHON(100),
      7EPSM(150),SCEB(150),IP,W13,TBAR13,NEX,NEX1,TSX,TCONV1,TCONV2,
      8TCHI,SZCON,PS,IPG,TBAR
       COMMON /STERPC/SLOG(150)
       COMMON /IOCOM/I05,I06,I07,IOPCH
       REWIND I07
       READ(I05,10)
      1HOL,NT,NP,NE,NDAM,NGPRT,NCP,NMESH,NREST,NCVP,NSEP,IPG,JS3,JS4,JS5,
      2W1,W2,W3,W4,W5,T1,T2,T3,T4,T5,TEMP,     AM,DC,BETSW,ALPSW,CRIT1,
      3CRIT2,CRIT3
    10 FORMAT(20A4    /11I5/3I5/5E10.4/6E10.4/7E10.4)
       IF(BETSW.EQ.0. )BETSW=100.
       IF(ALPSW.EQ.0. )ALPSW=100.
       IF(CRIT1.EQ.0.)CRIT1=.001
       IF(CRIT2.EQ.0.)CRIT2=.001
       IF(CRIT3.EQ.0.)CRIT3=.00001
       WRITE(I06,20)HOL,NT,NP,NE,NDAM,NGPRT,NCP,NMESH,NREST,NCVP,NSEP,IPG
      1,JS3,JS4,JS5,W1,W2,W3,W4,W5,T1,T2,T3,T4,T5,AM,DC,BETSW,ALPSW,CRIT1
      2,CRIT2,CRIT3
    20 FORMAT(1H1///10X20A4   //5X3HNT=I5,5H  NP=I3,4H NE=I3,6H NDAM=I2,
      17H NGPRT=I2,5H NCP=I2,7H NMESH=I2,7H NREST=I3,6H NCVP=I2,6H NSEP=I
      22,5H IPG=I2//5X4HJS3=I5,6H  JS4=I5,6H  JS5=I3//5X6HW1-W5=
      31P5E15.6//5X6HT1-T5=5E15.6                //5X2HM=E15.6,10X2HD=E15.
      46//5X26HSCT FOR S.LT.0 OR BETA.GT.E15.6,2X12HOR ALPHA.GT.E15.6//
      5 5X36HCRITERION FOR CONVOLUTION OF PART 1=E15.6,
      65X 36HCRITERION FOR CONVOLUTION OF PART 2=E15.6/
      75X 43HCRITERION FOR TRUNCATION OF TIME INTEGRALS= E15.6)
       W12=W1+W2
C      CONVERT MASS IN UNIFIED AMU TO NEUTRON MASS UNITS
       AM=AM/1.0086654
C
     4 FORMAT(7E10.4)
       IF(IPG.NE.0)GO TO 80
       IF(JS3.EQ.0) GO TO 80
       IF(JS3.GT.0)READ(I05,4)(X3(I),I=1,JS3)
       IF(JS3.GT.0)GO TO 50
       READ(I05,4)X3MAX
       JS3=-JS3
       IDEB=0
       IF(X3MAX.LT.0.0) IDEB=1
       IF(X3MAX.LT.0.0) X3MAX=-X3MAX
       DX3=X3MAX/FLOAT(JS3)
       X3(1)=DX3
       DO  40 I=2,JS3
    40 X3(I)=X3(I-1)+DX3
    50 CONTINUE
       IF(IDEB.EQ.0) GO TO 55
```

```
      DO 51 I=1,JS3
   51 Q3(I)=X3(I)**2
      GO TO 56
   55 READ(IO5,4)(Q3(I),I=1,JS3)
   56 DO   60 I=1,JS3
      EX=EXP(X3(I)/(2.*T3))
      SINHEX=0.5*(EX-1./EX)
   60 ZPHON(I)=Q3(I)*EX/(2.*X3(I)*SINHEX)
      WRITE(IO6,5)(I,X3(I),Q3(I),ZPHON(I),I=1,JS3)
    5 FORMAT(//10X6HMODE 3/15X5HOMEGA,5X10HRHO(OMEGA),3X12HOPHON(OMEGA)/
     1(I5,1P3E15.6))
   80 CONTINUE
      IF(JS4.EQ.0) GO TO 120
      IF(JS4.GT.0)READ(IO5,4)(X4(I),I=1,JS4)
      IF(JS4.GT.0) GO TO 100
      READ(IO5,4)X4MAX
      JS4=-JS4
      DX4=X4MAX/FLOAT(JS4)
      X4(1)=DX4
      DO  90 I=2,JS4
   90 X4(I)=X4(I-1)+DX4
  100 CONTINUE
      READ(IO5,4)(Q4(I),I=1,JS4)
      WRITE(IO6,7)(I,X4(I),Q4(I),I=1,JS4)
    7 FORMAT(//10X24HOMEGA, RHO(OMEGA),MODE 4/3(I5,1P2E15.6))
  120 CONTINUE
      IF(JS5.EQ.0) GO TO 150
      READ(IO5,4)(X5(I),I=1,JS5)
      READ(IO5,4)(Q5(I),I=1,JS5)
      READ(IO5,140)(NPHON(I),I=1,JS5)
  140 FORMAT(7I10)
      WRITE(IO6,9)(I,X5(I),Q5(I),NPHON(I),I=1,JS5)
    9 FORMAT(//5X10HOSCILLATOR,7X6HENERGY,7X8HWEIGHT   ,4X8H PHONONS/
     1(I11,4X1P2E15.6,I10))
  150 CONTINUE
      IF(TEMP .EQ.0.)TEMP=AMAX1(T1,T2,T3,T4,T5)
      IF(NMESH.EQ.0) GO TO 160
      CALL MESH(NP,NE,ALPHA,BETA,TEMP,AM)
      IF(NMESH.LT.0)READ(IO5,4)(ALPHA(I),I=1,NP)
      GO TO 170
  160 READ(IO5,4)(ALPHA(I),I=1,NP)
      READ(IO5,4)(BETA(I),I=1,NE)
  170 CONTINUE
      DO 180I=1,NP
  180 PSQ(I)=ALPHA(I)*AM*TEMP
      WRITE(IO6,12)(I,ALPHA(I),PSQ(I),I=1,NP)
   12 FORMAT(//10X13HALPHA, P**2/2/3(I5,1P2E15.6))
      DO 200I=1,NE
  200 EPS(I)=BETA(I)*TEMP
      WRITE(IO6,14)(I,BETA(I),EPS(I),I=1,NE)
   14 FORMAT(//10X9HBETA, EPS/3(I5,1P2E15.6))
      IF(IPG.EQ.0)GO TO 245
      READ(IO5,244)TBAR
      READ(IO5,244)(T(I),I=1,NT)
      READ(IO5,244)(GS(I),GC(I),I=1,NT)
```

```
      RR=W3/AM
      DO 246 I=1,NT
      GS(I)=GS(I)*RR
      GC(I)=GC(I)*RR
  246 T(I)=T(I)/0.65817E-15
  244 FORMAT(8E10.3)
      GO TO 240
  245 CONTINUE
      IF(NT.GT.0)READ(I05,4)(T(I),I=1,NT)
      IF(NT.GT.0) GO TO 240
      NTR=-NT
      T(1)=0.
      NT=1
      WRITE(I06,15)
   15 FORMAT(//10X,10X2HDT,11X4HTMAX/)
      DO 230 I=1,NTR
      READ(I05,4)DT,TMAX
      TMAXP=TMAX-DT/2.
      WRITE(I06,16)I,DT,TMAX
   16 FORMAT(I10,1P2E15.6)
  220 T(NT+1)=T(NT)+DT
      NT=NT+1
      IF(T(NT).LT.TMAXP)GO TO 220
  230 CONTINUE
  240 CONTINUE
C
      SW=W1+W2+W3+W4+W5
      W1=W1/SW
      W2=W2/SW
      W3=W3/SW
      W4=W4/SW
      W5=W5/SW
      IF(JS5.EQ.0) GO TO 270
      SW=0.
      DO 250I=1,JS5
  250 SW=SW+Q5(I)
      DO 260I=1,JS5
  260 Q5(I)=Q5(I)/SW
  270 CONTINUE
C
C     EXP(BETA/2)
      DO 300 I=1,NE
      EPSM(I)=-EPS(I)
  300 EB2(I)=EXP(BETA(I)/2.)
C
C     MODE 5 PRELIMS
      IF(W5.EQ.0.0)GO TO 320
      DO 310 I=1,JS5
      RR=0.5*X5(I)/T5
      U=EXP(RR)
      U=0.5*(U-1./U)
      ARG1(I)=W5*Q5(I)/(AM*X5(I)*U)
  310 ARG2(I)=W5*Q5(I)/(AM*X5(I)*TANH(RR))
  320 CONTINUE
C
```

```
      W13=W1+W3
      TBAR13=(W1*T1+W3*T3)/W13
  330 IF(NREST.EQ.0)NREST=1
      IRST=0
      IF(NREST.EQ.1)GO TO 350
      IF(NREST.LT.0)IRST=-NREST
      IF(NREST.LT.0)NREST=-NREST
      IF(IRST.NE.0)GO TO 350
      NRESTM=NREST-1
      READ(I07)GC,GS,TBAR
      DO 340 I=1,NRESTM
      READ(I07)PS
      IF(NSEP.NE.0)READ(I07)PS
  340 IF(NSEP.NE.0)READ(I07)PS
  350 CONTINUE
      TSX=0.
      TCONV1=0.
      TCONV2=0.
      TCHI=0.
      DO 360 I=1,NE
      NEX=I
      IF(BETA(I).GT.BETSW) GO TO 370
  360 CONTINUE
  370 IF(NEX.EQ.NE)GO TO 380
      NEX1=NEX
      NEX=NEX-1
      GO TO 390
  380 NEX1=0
  390 RETURN
      END
```

```
@I     FOR ERRMAP/S1,ERRMAP/S1,ERRMAP/R1
       SUBROUTINE ERRMAP(JX,IX,ALPHA,BETA,EXBH,HOLL,T,A,NSEP,EMAX,ALAM,
      1IRST)
       DIMENSION ALPHA(1),BETA(1),EXBH(1),HOLL(1),HOL(18),S(80,150),
      1ILT(150),IHT(150),W(150)
       COMMON DUM(1000),S
       COMMON /IOCOM/I05,I06,I07,IOPCH
       EMAX=BETA(JX)*T
       READ(I05,20)ID,NPT,SIGF,EPS
    20 FORMAT(2I10,3E10.4)
       IF(FLOAT(ID+NPT)+SIGF+EPS.EQ.0.) GO TO 930
       IF(IRST.NE.0)CALL RDS(-1,S,HOL,IX,ALPHA,JX,BETA,IDP,ILT,IHT,
      1SIGFP,EPSP,ALAMP,EMAXP,TP,AP)
       IF(IRST.EQ.0)IRST=1
       DO 5 I=1,18
     5 HOL(I)=HOLL(I)
       ISEP=1
     1 REWIND I07
       READ(I07)(DDUM,I=1,2001)
       DO 10 I=IRST,IX
       IF(NSEP.EQ.0)READ(I07)(S(I,J),J=1,JX)
       IF(NSEP.EQ.0)GO TO 10
       GO TO (11,12,13),ISEP
    11 READ(I07)(S(I,J),J=1,JX)
       READ(I07)C
       READ(I07)C
       GO TO 10
    12 READ(I07)C
       READ(I07)(S(I,J),J=1,JX)
       READ(I07)C
       GO TO 10
    13 READ(I07)C
       READ(I07)C
       READ(I07)(S(I,J),J=1,JX)
    10 CONTINUE
       C=0.0
       DO 430 J=1,JX
       DO 430 I=1,IX
       S(I,J)=S(I,J)*T
       IF(S(I,J)*EXBH(J)-C)430,430,420
   420 C=S(I,J)*EXBH(J)
   430 CONTINUE
       C=C*EPS
       DO 480 J=1,JX
       DO 440 I=1,IX
       IL=I
       IF(S(I,J)*EXBH(J)-C)440,440,450
   440 CONTINUE
       ILT(J)=0
       IHT(J)=0
       GO TO 480
   450 ILT(J)=IL
       DO 470 I=IL,IX
       IF(S(I,J)*EXBH(J)-C)470,470,460
   460 IHT(J)=I
```

```
  470 CONTINUE
  480 CONTINUE
C=====PRINT AND PUNCH S==============================================
  500 GO TO (501,502,503),ISEP
  501 WRITE(IO6,505)
      GO TO 508
  502 WRITE(IO6,506)
      GO TO 508
  503 WRITE(IO6,507)
  505 FORMAT(1H1//20X5HS1+S2)
  506 FORMAT(1H1//20X2HS1)
  507 FORMAT(1H1//20X2HS2)
  508 CONTINUE
      WRITE(IO6,509)ID,SIGF,EPS
  509 FORMAT(4H0ID=I5,5X5HSIGF=1PE13.6,5X4HEPS=E13.6)
      DO 530 J=1,JX
      IL=ILT(J)
      IF(IL)530,530,510
  510 IH=IHT(J)
      WRITE(IO6,520)J,BETA(J),(I,S(I,J),I=IL,IH)
  520 FORMAT(25H0SP(ALPHA,BETA) FOR BETA I4,2H= F10.5/(6(I6,1PE12.5)))
  530 CONTINUE
      IF(NPT-1)540,620,540
  540 GO TO (541,542,543),ISEP
  541 IF(IOPCH)2541,3541,2541
 3541 PUNCH 551,HOL,ID
      GO TO 4541
 2541 WRITE(IOPCH,551)HOL,ID
 4541 CONTINUE
      GO TO 544
  542 IF(IOPCH)2542,3542,2542
 3542 PUNCH 552,HOL,ID
      GO TO 4542
 2542 WRITE(IOPCH,552)HOL,ID
 4542 CONTINUE
      GO TO 544
  543 IF(IOPCH)2543,3543,2543
 3543 PUNCH 553,HOL,ID
      GO TO 4543
 2543 WRITE(IOPCH,553)HOL,ID
 4543 CONTINUE
  544 CONTINUE
  551 FORMAT(17A4,A2,5HS1+S2,I5)
  552 FORMAT(17A4,A2,5HS1   ,I5)
  553 FORMAT(17A4,A2,5HS2   ,I5)
 1040 IF(IOPCH)2040,3040,2040
 3040 PUNCH 1050,JX
      GO TO 4040
 2040 WRITE(IOPCH,1050)JX
 4040 CONTINUE
 1050 FORMAT(11HDCC2    402,11X1H4,5X1H5,1XI5)
      EPS=EMAX/T
      IF(IOPCH)2001,3001,2001
 3001 PUNCH 560,SIGF,EPS,A,EMAX,ALAM
      GO TO 4001
```

```
 2001 WRITE(IOPCH,560)SIGF,EPS,A,EMAX,ALAM
 4001 CONTINUE
  560 FORMAT(6(1PE11.4,1X))
      IF(IOPCH)2002,3002,2002
 3002 PUNCH 1060,IX,BETA(1)
      GO TO 4002
 2002 WRITE(IOPCH,1060)IX,BETA(1)
 4002 CONTINUE
 1060 FORMAT(29HDCC1     401      3      4      0I6,13X1PE11.4)
      IF(IOPCH)2003,3003,2003
 3003 PUNCH 560,(ALPHA(I),I=1,IX)
      GO TO 4003
 2003 WRITE(IOPCH,560)(ALPHA(I),I=1,IX)
 4003 CONTINUE
      CALL SPCH(S(1,1),1,IX,1)
      DO 1110 J=2,JX
      IL=ILT(J)
      IF(IL)1090,1090,1070
 1070 IH=IHT(J)
      LDB=IH-IL+1
      IF(IOPCH)2004,3004,2004
 3004 PUNCH 1080,LDB,IL,BETA(J)
      GO TO 4004
 2004 WRITE(IOPCH,1080)LDB,IL,BETA(J)
 4004 CONTINUE
 1080 FORMAT(29HDCC1     401      4      4      0I6,I6,7X1PE11.4)
      CALL SPCH(S(1,J),IL,IH,J)
      GO TO 1110
 1090 IF(IOPCH)2005,3005,2005
 3005 PUNCH 1100,BETA(J)
      GO TO 4005
 2005 WRITE(IOPCH,1100)BETA(J)
 4005 CONTINUE
 1100 FORMAT(29HDCC1     401      4      4      0,6H      2,6H      1,7X1PE11.
     14)
      DAM=C/EXBH(J)
      IF(IOPCH)2006,3006,2006
 3006 PUNCH 1105,DAM,DAM,J
      GO TO 4006
 2006 WRITE(IOPCH,1105)DAM,DAM,J
 4006 CONTINUE
 1105 FORMAT(2(1PE11.4,1X),48XI4,3X1H1)
 1110 CONTINUE
      IF(IOPCH)2007,3007,2007
 3007 PUNCH 1120
      GO TO 4007
 2007 WRITE(IOPCH,1120)
 4007 CONTINUE
 1120 FORMAT(11HEND      500)
      IF(NPT-1)630,620,620
  620 REWIND I07
      WRITE(I07)HOL,ID,T,A,SIGF,ALAM,IX,JX,ALPHA,BETA,ILT,IHT,S
      NTFLAG=1
  630 CONTINUE
C=====ERROR MAP=================================================
```

```
  700 WRITE(I06,710)
  710 FORMAT(24H1INTERPOLATION ERROR MAP)
      DO 760 J=1,JX
      IL=ILT(J)
      IF(IL)760,760,720
  720 IH=IHT(J)
      ILP=IL+2
      IF(ILP-IH)730,730,760
  730 DO 740 I=ILP,IH
      CALL ERROR(ALPHA(I-2),S(I-2,J),ALPHA(I-1),S(I-1,J),
     1ALPHA(I),S(I,J),ER)
  740 W(I)=100.*ER
      WRITE(I06,750)J,BETA(J),(W(I),S(I,J),I,I=ILP,IH)
  750 FORMAT(3H0J=I3,7H  BETA=F10.5/(5(F8.2,E9.2,I5)))
  760 CONTINUE
      DO 840 I=1,IX
      DO 770 J=1,JX
      JL=J
      IF(S(I,J)-C)770,770,780
  770 CONTINUE
      GO TO 840
  780 DO 800 J=JL,JX
      IF(S(I,J)-C)800,800,790
  790 JH=J
  800 CONTINUE
      JLP=JL+2
      IF(JLP-JH)810,810,840
  810 DO 820 J=JLP,JH
      CALL ERROR(BETA(J-2),S(I,J-2),BETA(J-1),S(I,J-1),
     1BETA(J),S(I,J),ER)
  820 W(J)=100.*ER
      WRITE(I06,830)I,ALPHA(I),(W(J),S(I,J),J,J=JLP,JH)
  830 FORMAT(3H0I=I3,8H  ALPHA=F10.5/(5(F8.2,E9.2,I5)))
  840 CONTINUE
C=====TERMINATE=========================================================
  900 IF(NTFLAG)920,920,910
  910 END FILE I07
      REWIND I07
  920 IF(NSEP.EQ.0) GO TO 930
      ISEP=ISEP+1
      IF(ISEP.LE.3) GO TO 1
  930 RETURN
      END
```

```
@I     FOR ERROR/S1,ERROR/S1,ERROR/R1
       SUBROUTINE ERROR(X1,Y1,X2,Y2,X3,Y3,E)
C=====COMPUTES ERROR IN LINEAR INTERPOLATION===========================
       IF(Y1.EQ.0.0.OR.Y2.EQ.0.0.OR.Y3.EQ.0.0) GO TO 20
   10 H1=X3-X2
       H2=X3-X1
       H3=X2-X1
       A2=ABS((H3*ALOG(Y3)-H2*ALOG(Y2)+H1*ALOG(Y1))/(H3*H2*H1))
       E=A2*(H1/2.)**2
   30 RETURN
   20 E=0.
       GO TO 30
       END
```

```
@I    FOR RDS/S1,RDS/S1,RDS/R1
      SUBROUTINE RDS(N,S,HOL,IX,ALPHA,JX,BETA,ID,ILT,IHT,SIGF,EPS,
     1ALAM,EMAX,T,A)
C=====READ S(ALPHA,BETA)===============================================
C     N=-1 READ FROM CARDS IN BNL FORMAT
      COMMON /IOCOM/ I05,I06
      DIMENSION S(80,150),ILT(1),IHT(1),HOL(1),ALPHA(1),BETA(1)
  120 READ(I05,30)HOL,ID
   30 FORMAT(18A4,3X,I5)
      READ(I05,125)JX
  125 FORMAT(30XI5)
      READ(I05,40)SIGF,EPS,A,EMAX,ALAM
   40 FORMAT(6(E11.4,1X))
      T=EMAX/EPS
      READ(I05,130)IX,BETA(1)
  130 FORMAT(30XI5,13XE11.4)
      DO 131 J=1,JX
      DO 131 I=1,IX
  131 S(I,J)=0.
      READ(I05,40)(ALPHA(I),I=1,IX)
      READ(I05,40)(S(I,1),I=1,IX)
      ILT(1)=1
      IHT(1)=IX
      DO 150 J=2,JX
      READ(I05,135)LDB,IL,BETA(J)
  135 FORMAT(29X2I6,7XE11.4)
      IF(IL.LE.0) GO TO 140
      IH=LDB+IL-1
      READ(I05,40)(S(I,J),I=IL,IH)
      ILT(J)=IL
      IHT(J)=IH
      GO TO 150
  140 READ(I05,145)BETA(J)
  145 FORMAT(48XE11.4)
      READ(I05,40)DUM,DUM
  150 CONTINUE
      READ(I05,155)ICHK
  155 FORMAT(8XI3)
      IF(ICHK.NE.500)WRITE(I06,160)ICHK
      IF(ICHK.NE.500)CALL EXIT
  160 FORMAT(////1H0,20(1H*),59HERROR- BNL OUTPUT PUNCHING DOESNT END WI
     1TH 8X 500, BUT WITH    I4//)
      DO 170 J=1,JX
      DO 170 I=1,IX
  170 S(I,J)=S(I,J)/T
  110 CONTINUE
      RETURN
      END
```

```
@I     FOR ENDPT/S1,ENDPT/S1,ENDPT/R1
       SUBROUTINE ENDPT(NT,NTN,X,SCALE,CRIT3)
       DIMENSION X(1)
       NTN=NT
       DO 20 I=1,NT,20
       SUM=0.
       JP=I+19
       DO 10 J=I,JP
    10 SUM=SUM+ABS(X(J))
       IF(SUM/SCALE.LE.CRIT3)GO TO 40
    20 CONTINUE
    30 RETURN
    40 NTN=I
       GO TO 30
       END
```

```
@I     FOR SPCH/S1,SPCH/S1,SPCH/R1
       SUBROUTINE SPCH(S,IL,IH,LAB)
       DIMENSION S(80),P(6)
       COMMON /IOCOM/I05,I06,I07,IOPCH
       NC=1
       DO 10 I=IL,IH,6
       IU=I+5
       L=I
       DO 5 J=1,6
       P(J)=S(L)
       IF(L.GT.IH)P(J)=0.
     5 L=L+1
       IF(IOPCH)1000,2000,1000
  2000 PUNCH 20,P,LAB,NC
       GO TO 3000
  1000 WRITE(IOPCH,20)P,LAB,NC
  3000 CONTINUE
    10 NC=NC+1
    20 FORMAT(6(1PE11.4,1X),2I4)
       RETURN
       END
```

```
@I     FOR MESH/S1,MESH/S1,MESH/R1
       SUBROUTINE MESH(IMAX,JMAX,ALPHA,BETA,T,A)
       DIMENSION ALPHA(1),BETA(1)
       COMMON /IOCOM/IO5,IO6,IO7,IOPCH
       READ(IO5,10)EMAX,DALPHA,ALPHAC,DBETA,BETAC
   10  FORMAT(7E10.4)
       BMAX=EMAX/T
       AMAX=4.*BMAX/A
C=====COMPUTE ALPHA MESH==================================================
  100  ALPHA(1)=DALPHA
       DO 110 I=2,IMAX
       I1=I
       ALPHA(I)=ALPHA(I-1)+DALPHA
       IF(ALPHA(I)-ALPHAC)110,120,120
  110  CONTINUE
  120  I2=IMAX-I1
       FI2=I2
       IF(I2)170,170,130
  130  RHO=(AMAX-ALPHAC)/DALPHA
       RA=1.000
  140  RA=RA+0.0001
       RP=RA*(RA**FI2-1.)/(RA-1.)
       IF(RP-RHO)140,150,150
  150  IA=I1+1
       DO 160 I=IA,IMAX
  160  ALPHA(I)=ALPHA(I-1)+RA*(ALPHA(I-1)-ALPHA(I-2))
  170  IX=IMAX
       IXP=IX+1
C=====COMPUTE BETA MESH===================================================
  200  BETA(1)=0.0
       DO 210 J=2,JMAX
       J1=J
       BETA(J)=BETA(J-1)+DBETA
       IF(BETA(J)-BETAC)210,220,220
  210  CONTINUE
  220  J2=JMAX-J1
       FJ2=J2
       IF(J2)270,270,230
  230  RHO=(BMAX-BETAC)/DBETA
       RB=1.000
  240  RB=RB+0.0001
       RP=RB*(RB**FJ2-1.)/(RB-1.)
       IF(RP-RHO)240,250,250
  250  JA=J1+1
       DO 260 J=JA,JMAX
  260  BETA(J)=BETA(J-1)+RB*(BETA(J-1)-BETA(J-2))
  270  JX=JMAX
C=====PRINT MESHES========================================================
       WRITE(IO6,320)EMAX,IMAX,DALPHA,ALPHAC,RA,(I,ALPHA(I),I=1,IX)
  320  FORMAT(6H0EMAX=E13.6/12H0ALPHA MESH,I5,18H POINTS, INTERVAL=F10.5/
     112X13HTRANSITION ATF10.5,15H   EXPANSION BYF10.5/
     2(7(I5,F10.5)))
       WRITE(IO6,330)JMAX,DBETA,BETAC,RB,(J,BETA(J),J=1,JX)
  330  FORMAT(11H0BETA MESH,I5,18H POINTS, INTERVAL=F10.5/
     112X13HTRANSITION ATF10.5,15H   EXPANSION BYF10.5/
     2(7(I5,F10.5)))
       RETURN
       END
```

```
@I     FOR GTG/S1,GTG/S1,GTG/R1
       SUBROUTINE GTG(RWT,TMP,AM,X,Q,Y,PC,PS,NS,NR,TBAR)
       DIMENSION  X(1),Q(1),Y(1),PC(1),PS(1)
C      COMPUTE NORMALIZER R
       T=Q(1)*X(1)/3.
       CALL INTG(X,Q,A,NS)
       R = RWT / AM /(T+A)
C      CALC FOR Y.GE.Y(2) AND X.GE.X(1)
       CALL FTRANS(TMP,X,Q,Y(2),PC(2),PS(2),NS,NR-1)
C      CALC FOR Y.GE.Y(2) AND 0.LE.X.LT.X(1)
       F=X(1)*0.5/TMP
       T=EXP(F)
       H=(T+1./T)/(T-1./T)
       DO 30 I=2,NR
       T=X(1)*Y(I)
       IF (T.GT.0.005) GO TO 10
       C=0.5*T - T**3/24.
       S=T-T**3/6.
       CS=T/3.-T**3/30.
       GO TO 20
    10 C = COS(T)
       S = SIN(T)
       CS = S/T**2 - C/T
       C=(1.-C)/T
    20 PC(I)=PC(I)+Q(1)/T * (H*(S-C)+C/F)
    30 PS(I)=PS(I) + Q(1) * CS
C      CALC FOR Y(1)=0. AND 0.LE.X.LT.X(1)
       PC(1)=0.5*Q(1)* (1./F + H)
       PS(1)=0.
       TBAR=Q(1)*TMP*X(1)/3.
C      CALC FOR Y(1)=0. AND X.GE.X(1)
       DO 40 I=1,NS
       F=X(I)*0.5/TMP
       T=EXP(F)
       H=(T+1./T)/(T-1./T)
    40 Q(I)=Q(I)*H/X(I)
       CALL INTG (X,Q,A,NS)
       PC(1)=PC(1)+A
       DO 45 I=1,NS
    45 Q(I)=Q(I)*X(I)**2*0.5
       CALL INTG(X,Q,A,NS)
       TBAR=TBAR+A
C      NORMALIZE RESULTS
       DO 50 I=1,NR
       PC(I)=PC(I)*R
    50 PS(I)=PS(I)*R
       TBAR=TBAR*R*AM/RWT
       RETURN
       END
@I     FOR INTG/S1,INTG/S1,INTG/R1
       SUBROUTINE INTG(X,Q,A,N)
       DIMENSION X(1),Q(1)
       A=0.
       DO 10 I=2,N
    10 A=A+(Q(I)+Q(I-1))*(X(I)-X(I-1))
       A=0.5*A
       RETURN
       END
```

```
@I      FOR FTRANS/S1,FTRANS/S1,FTRANS/R1
        SUBROUTINE FTRANS(TMP,X,Q,Y,PC,PS,NS,NR)
        DIMENSION  X(1),Q(1),Y(1),PC(1),PS(1)
        DO 20 I=1,NR
        PC(I)=0.
        PS(I)=0.
        SM=X(1)*Y(I)
        SINSM = SIN(SM)
        COSSM = COS(SM)
        ZM=EXP(X(1)*0.5/TMP)
        DO 10 J=2,NS
        IF (X(J).EQ. X(J-1)) GO TO 10
        S = X(J)*Y(I)
        SINS = SIN(S)
        COSS = COS(S)
        Z = EXP (X(J)*0.5/TMP)
        IF(ABS(S/SM-1.0).LE.5.E-7)GO TO 40
        T = S-SM
        IF (T.GT.0.005) GO TO 30
        ST = T**2/6. - T**4/120.
        CT = 0.5*T - T**3/24.
        GO TO 40
   30   SINT = SINS * COSSM - COSS * SINSM
        COST = COSS * COSSM + SINS * SINSM
        ST = 1. - SINT/T
        CT = (1.-COST)/T
   40   PC(I)=PC(I)+Q(J)/X(J)*(Z+1./Z)/(Z-1./Z)*(ST*SINS+CT*COSS)
      1 -Q(J-1)/X(J-1)*(ZM+1./ZM)/(ZM-1./ZM)*(ST*SINSM - CT*COSSM)
        PS(I)=PS(I)+Q(J)/X(J)*(CT*SINS-ST*COSS)+Q(J-1)/X(J-1)
      1 *(CT*SINSM+ST*COSSM)
        SM=S
        SINSM=SINS
        COSSM=COSS
        ZM=Z
   10   CONTINUE
        PC(I)=PC(I)/Y(I)
   20   PS(I)=PS(I)/Y(I)
        RETURN
        END
```

```
@I    FOR SCINT/S1,SCINT/S1,SCINT/R1
      SUBROUTINE SCINT(T,Q,R,EPS,S,A,F,NT,NE)
      DIMENSION T(1),Q(1),R(1),EPS(1),S(1)
      DO 20 I=1,NE
      AL=EPS(I)+A
      IF(AL.NE.0.0) GO TO 5
      CALL INTG(T,Q,S(I),NT)
      S(I)=S(I)*F
      GO TO 20
    5 S(I)=0.
      SM=T(1)*AL
      SINSM=SIN(SM)
      COSSM=COS(SM)
      VO=0.
      DO 10 J=2,NT
      IF(T(J).EQ.T(J-1)) GO TO 10
      U=T(J)*AL
      SINS=SIN(U)
      COSS=COS(U)
      V=U-SM
      IF(ABS(V/VO-1.0).LE.5.E-7) GO TO 40
      IF(ABS(V).GT.0.005)GO TO 30
      ST=(V**2)/6.-(V**2)**2/120.
      CT=V*0.5-V**3/24.
      GO TO 40
   30 CONTINUE
      SINT=SINS*COSSM-COSS*SINSM
      COST=COSS*COSSM+SINS*SINSM
      ST=1.-SINT/V
      CT=(1.-COST)/V
   40 S(I)=S(I)+(Q(J)*(ST*SINS+CT*COSS)-Q(J-1)*(ST*SINSM-CT*COSSM))
      S(I)=S(I)-(R(J)*(-ST*COSS+CT*SINS)-R(J-1)*(-ST*COSSM-CT*SINSM))
      SM=U
      SINSM=SINS
      COSSM=COSS
      VO=V
   10 CONTINUE
      S(I)=S(I)*F/AL
   20 CONTINUE
      RETURN
      END
```

> NOTE: This alternate version of SCINT with subsidiary program SNCS can be used for machines which require more than about 10 multiplications to generate a sine or cosine. This routine generates sine and cosine recursively when the integration step is constant, recalculating the functions exactly every n^{th} (10 here) time to keep numerical errors generated by the recursion relation from building up.

```
@IL   FOR SCINT/S1,SCINT/S1,SCINT/R1
      SUBROUTINE SCINT(T,Q,R,EPS,S,A,F,NT,NE)
      DIMENSION T(1),Q(1),R(1),EPS(1),S(1)
      DO 20 I=1,NE
      AL=EPS(I)+A
      IF(AL.NE.0.0) GO TO 5
      CALL INTG(T,Q,S(I),NT)
      S(I)=S(I)*F
      GO TO 20
    5 S(I)=0.
      SM=T(1)*AL
      SINSM=SIN(SM)
      COSSM=COS(SM)
      VO=0.
      DO 10 J=2,NT
      IF(T(J).EQ.T(J-1)) GO TO 10
      U=T(J)*AL
      V=U-SM
      CALL       SNCS(SINS,COSS,SINSM,COSSM,U,SM,V,VO)
      IF(V.EQ.VO) GO TO 40
      IF(ABS(V).GT.0.005)GO TO 30
      ST=(V**2)/6.-(V**2)**2/120.
      CT=V*0.5-V**3/24.
      GO TO 40
   30 CONTINUE
      SINT=SINS*COSSM-COSS*SINSM
      COST=COSS*COSSM+SINS*SINSM
      ST=1.-SINT/V
      CT=(1.-COST)/V
   40 S(I)=S(I)+(Q(J)*(ST*SINS+CT*COSS)-Q(J-1)*(ST*SINSM-CT*COSSM))
      S(I)=S(I)-(R(J)*(-ST*COSS+CT*SINS)-R(J-1)*(-ST*COSSM-CT*SINSM))
      SM=U
      SINSM=SINS
      COSSM=COSS
      VO=V
   10 CONTINUE
      S(I)=S(I)*F/AL
   20 CONTINUE
      RETURN
      END
@IL   FOR SNCS
      SUBROUTINE SNCS(SINS,COSS,SINSM,COSSM,U,SM,V,VO)
      DATA K/0/
C     CHECK THAT LAMBDA*DELTA T IS UNCHANGED TO WITHIN 5.E-8
      IF(ABS(V/VO-1.).LT.5.E-8)GO TO 20
C     CALCULATE EXPLICITLY
      SINS=SIN(U)
      COSS=COS(U)
C     SIN AND COS OF NEW LAMBDA*DELTA T
      SINDTL=SIN(V)
      COSDTL=COS(V)
      K=0
   10 RETURN
C     CALCULATE BY RECURSION
   20 K=K+1
      IF(K.GE.10)GO TO 30
      SINS=SINSM*COSDTL+SINDTL*COSSM
      COSS=COSSM*COSDTL-SINSM*SINDTL
      GO TO 10
   30 SINS=SIN(U)
      COSS=COS(U)
      K=0
      GO TO 10
      END
```

```
@I     FOR STERP/S1,STERP/S1,STERP/R1
       SUBROUTINE STERP(B,BETA,NB,SINT)
C      INTERPOLATES LINEARLY IN TABLE OF LOG(S1) TO GIVE S1(B)
       COMMON/STERPC/SLOG(150),IC
       DIMENSION BETA(1)
       IF(B.GT.BETA(1)) GO TO 1
       SINT=EXP(SLOG(1))
       GO TO 40
     1 IF(B.LT.BETA(NB)) GO TO 2
       SINT=0.
       GO TO 40
     2 IF(IC.LE.0.OR.IC.GT.NB)IC=1
    10 IF(B.GE.BETA(IC)) GO TO 20
       IC=IC-1
       GO TO 10
    20 IF(B.LT.BETA(IC+1)) GO TO 30
       IC=IC+1
       GO TO 10
    30 SL=    SLOG(IC)+((B-BETA(IC))/(BETA(IC+1)-BETA(IC)))*(SLOG(IC+1)-
      1SLOG(IC))
       SINT=EXP(SL)
    40 RETURN
       END
```

```
@I     FOR SNEAR/S1,SNEAR/S1,SNEAR/R1
       FUNCTION SNEAR(B,S,BETA,NB)
C      FINDS APPROXIMATE S OVER INTERVAL INCLUDING B
       COMMON/STERPC/SLOG(150),IC
       DIMENSION S(1),BETA(1)
       IF(B.GE.BETA(1))GO TO 1
       SNEAR=S(1)
       GO TO 40
     1 IF(B.LE.BETA(NB))GO TO 2
       SNEAR=S(NB)
       GO TO 40
     2 IF(IC.LE.0.OR.IC.GT.NB)IC=1
    10 IF(B.GE.BETA(IC))GO TO 20
       IC=IC-1
       GO TO 10
    20 IF(B.LT.BETA(IC+1))GO TO 30
       IC=IC+1
       GO TO 10
    30 SNEAR=(S(IC)+S(IC+1))/2.
    40 RETURN
       END
```

```
@I     FOR RCONV/S1,RCONV/S1,RCONV/R1
       SUBROUTINE RCONV
       COMMON HOL(20),NT,NP,NE,NDAM,NGPRT,NCP,NMESH,NREST,NCVP,NSEP,
      1NSUMCV,JS3,JS4,JS5,W1,W2,W3,W4,W5,T1,T2,T3,T4,T5,TEMP,AM,DC,
      2BETSW,ALPSW,CRIT1,CRIT2,CRIT3,X3(100),Q3(100),X4(100),Q4(100),
      3X5(20),Q5(20),NPHON(20),ALPHA(100),BETA(150),EB2(150),PSQ(100),
      4EPS(150),T(1000),H(1000),R5(20),ANK(20,21),ARG1(20),ARG2(20),
      5BF(21),SK(150),S1(150),S2(150),S1EB(150),S2EB(150),SEB(150),S(150)
      6,SC(150),W12,R(1000),Q(1000),GS(1000),GC(1000),ZPHON(100),
      7EPSM(150),SCEB(150),IP,W13,TBAR13,NEX,NEX1,TSX,TCONV1,TCONV2,
      8TCHI,SZCON,PS
       COMMON /STERPC/SLOG(150)
       COMMON /IOCOM/IO5,IO6,IO7,IOPCH
       DO  20 I=1,NE
       SK(I)=0.
       IF(S1(I).LE.0.0)GO TO 10
       SLOG(I)=ALOG(S1(I))
       GO TO 20
    10 SLOG(I)=-100.
    20 CONTINUE
       DO 120 K=1,JS5
       IF(ALPHA(IP).LT.ALPSW)
      1WRITE(IO6,40) (ANK(K,I),I=1,20)
    40 FORMAT(//5X9HANK(K,I)=1P7E15.6/(14X7E15.6))
       NPHO=NPHON(K)
       DO  80 I=1,NE
       N=IFIX(EPS(I)/X5(K))+1
       IN=0
    50 CALL STERP(ABS(BETA(I)-FLOAT(IN)*X5(K)/T5),BETA,NE,SINT)
       INP=IABS(IN)+1
       SK(I)=SK(I)+ANK(K,INP)*SINT
       IN=IN+1
       IF(IN.LE.N) GO TO 50
       IN=-NPHO
    60 IF(IN.GE.0.AND.IN.LE.N) GO TO 70
       ARG=ABS(BETA(I)-FLOAT(IN)*X5(K)/T5)
       INP=IABS(IN)+1
       IF(SNEAR(ARG,S1,BETA,NE).LT.CRIT1*SK(I).OR.ANK(K,INP).EQ.0.) GO
      1 TO 70
       CALL STERP(ARG,BETA,NE,SINT)
       SK(I)=SINT*ANK(K,INP)+SK(I)
    70 IN=IN+1
       IF(IN.LE.NPHO) GO TO 60
    80 CONTINUE
       IF(ALPHA(IP).LT.ALPSW.AND.NCVP.GT.0)
      1WRITE(IO6, 90)K,(I,BETA(I),SK(I),I=1,NE)
    90 FORMAT(//5X21HS1 AFTER CONVOLUTION I2//16X4HBETA,12X3HS1K,
      1/(I5,1P2E15.6))
       DO 110 I=1,NE
       S1(I)=SK(I)
       SK(I)=0.
       IF(JS5.EQ.K) GO TO 110
       IF(S1(I).LE.0.) GO TO 100
       SLOG(I)=ALOG(S1(I))
       GO TO 110
   100 SLOG(I)=-100.
   110 CONTINUE
   120 CONTINUE
       RETURN
       END
```

```
@I      FOR ACON2/S1,ACON2/S1,ACON2/R1
        SUBROUTINE ACON2
        COMMON HOL(20),NT,NP,NE,NDAM,NGPRT,NCP,NMESH,NREST,NCVP,NSEP,
       1NSUMCV,JS3,JS4,JS5,W1,W2,W3,W4,W5,T1,T2,T3,T4,T5,TEMP,AM,DC,
       2BETSW,ALPSW,CRIT1,CRIT2,CRIT3,X3(100),Q3(100),X4(100),Q4(100),
       3X5(20),Q5(20),NPHON(20),ALPHA(100),BETA(150),EB2(150),PSQ(100),
       4EPS(150),T(1000),H(1000),R5(20),ANK(20,21),ARG1(20),ARG2(20),
       5BF(21),SK(150),S1(150),S2(150),S1EB(150),S2EB(150),SEB(150),S(150)
       6,SC(150),W12,R(1000),Q(1000),GS(1000),GC(1000),ZPHON(100),
       7EPSM(150),SCEB(150),IP,W13,TBAR13,NEX,NEX1,TSX,TCONV1,TCONV2,
       8TCHI,SZCON,PS
        COMMON /STERPC/SLOG(150)
        COMMON /IOCOM/I05,I06,I07,IOPCH
C       ANALYTIC FREE GAS S(ALPHA,BETA) FOR MODE 5
        SZ2(E)=SZCON*EXP(-AM*(E**2+(PS*W1/AM)**2)/(4.*PS*T1*W1))
        CONT=AM/(4.*PS*T1*W1)
        CRIT2L=-ALOG(CRIT2)
        DO  60 I=1,NE
        S2(I)=0.
        N2=-NPHON(2)
   10   IN2P=IABS(N2)+1
        IF(ANK(2,IN2P).EQ.0.) GO TO 50
        FN20=FLOAT(N2)*X5(2)
        N1=IFIX((EPS(I)-FN20)/X5(1))+1
        IF(N1.LT.-NPHON(1).OR.N1.GT.NPHON(1)) GO TO 50
        EXMAX= ABS(EPS(I)-FN20-FLOAT(N1)*X5(1))
        EXMAX2=EXMAX**2
        S20=0.
        IN1=-NPHON(1)
   20   EXTST=ABS(EPS(I)-FN20-FLOAT(IN1)*X5(1))
        IN1P=IABS(IN1)+1
        IF(EXTST/T1.GT.BETSW) GO TO 30
        IF(CONT*(EXTST**2-EXMAX2).GT.CRIT2L.OR.ANK(1,IN1P).EQ.0.)GO TO 30
        S20=S20+ANK(1,IN1P)*SZ2(EXTST)
   30   IN1=IN1+1
        IF(IN1.LE.NPHON(1)) GO TO 20
   40   CONTINUE
        S2(I)=S2(I)+ANK(2,IN2P)*S20
   50   N2=N2+1
        IF(N2.LE.NPHON(2)) GO TO 10
        SEB(I)=SZ2(EPS(I))
   60   CONTINUE
        IF(ALPHA(IP).LT.ALPSW.AND.NCVP.GT.0)
       1WRITE(I06, 70)(I,BETA(I),SEB(I),S2(I),I=1,NE)
   70   FORMAT(//5X,11X4HBETA,12X3HS2Z,12X3HS2K /(I5,1P3E15.6))
        RETURN
        END
```

```
@I     FOR ACON1/S1,ACON1/S1,ACON1/R1
       SUBROUTINE ACON1
       COMMON HOL(20),NT,NP,NE,NDAM,NGPRT,NCP,NMESH,NREST,NCVP,NSEP,
      1NSUMCV,JS3,JS4,JS5,W1,W2,W3,W4,W5,T1,T2,T3,T4,T5,TEMP,AM,DC,
      2BETSW,ALPSW,CRIT1,CRIT2,CRIT3,X3(100),Q3(100),X4(100),Q4(100),
      3X5(20),Q5(20),NPHON(20),ALPHA(100),BETA(150),EB2(150),PSQ(100),
      4EPS(150),T(1000),H(1000),R5(20),ANK(20,21),ARG1(20),ARG2(20),
      5BF(21),SK(150),S1(150),S2(150),S1EB(150),S2EB(150),SEB(150),S(150)
      6,SC(150),W12,R(1000),Q(1000),GS(1000),GC(1000),ZPHON(100),
      7EPSM(150),SCEB(150),IP,W13,TBAR13,NEX,NEX1,TSX,TCONV1,TCONV2,
      8TCHI,SZCON,PS
       COMMON /STERPC/SLOG(150)
C      ANALYTIC FREE GAS S(ALPHA,BETA) FOR MODE 5
       SZ2(E)=SZCON*EXP(-AM*(E**2+(PS*W1/AM)**2)/(4.*PS*T1*W1))
       CONT=AM/(4.*PS*T1*W1)
       CRIT2L=-ALOG(CRIT2)
       DO  40 I=1,NE
       S20=0.
       IN1=-NPHON(1)
    20 EXTST=ABS(EPS(I)-FLOAT(IN1)*X5(1))
       IN1P=IABS(IN1)+1
       IF(EXTST/T1.GT.BETSW.OR.CONT*EXTST**2.GT.CRIT2L.OR.ANK(1,IN1P).EQ.
      10.0) GO TO 30
       S20=S20+ANK(1,IN1P)*SZ2(EXTST)
    30 IN1=IN1+1
       IF(IN1.LE.NPHON(1)) GO TO 20
       S2(I)=S20
    40 CONTINUE
       RETURN
       END
```

```
@I      FOR BESSL/S1,BESSL/S1,BESSL/R1
        SUBROUTINE BESSL(X,B,NX)
        DIMENSION B(21),BF(60)
        IF(X.GT.0.05) GO TO 19
        FNFACT=1.0
        X2N=1.0
        X2=X*0.5
        DO 18 I=1,NX
        B(I)=X2N/FNFACT
        X2N=X2N*X2
     18 FNFACT=FNFACT*FLOAT(I)
        GO TO 90
     19 CONTINUE
        DO20L=1,NX
  20    B(L)=0.0
        IF(X-1.0)50,55,55
  50    IORD=-37.0/(.43429*ALOG(.1*X))
        IF(IORD-5)51,51,60
  51    B(1)=1.0
        GOTO80
  55    IORD=30
  60    BF(IORD-1)=1.E-37
        BF(IORD)=0.0
        TA=1.E-37
        IOTA=IORD-1
        DO65L=2,IOTA
        IND=IORD-L
        BF(IND)=FLOAT(IND)*2.0*BF(IND+1)/X+BF(IND+2)
  65    TA=TA+BF(IND)
        TA=2.0*TA-BF(1)
        FACT=EXP(X)/TA
        DO70L=1,NX
        B(L)=FACT*BF(L)
        IF(B(L)-1.E-20)67,67,70
  67    B(L)=0.0
  70    CONTINUE
  80    NERR=1
     90 RETURN
        END
```