LA-3823

LOS ALAMOS SCIENTIFIC LABORATORY
of the
University of California
LOS ALAMOS • NEW MEXICO

Calculation of

Thermal Neutron Scattering Cross Sections

for Crystalline Materials: The TOR Program

This report expresses the opinions of the author or authors and does not necessarily reflect the opinions or views of the Los Alamos Scientific Laboratory.

LOS ALAMOS SCIENTIFIC LABORATORY
of the
University of California
LOS ALAMOS • NEW MEXICO

Calculation of

Thermal Neutron Scattering Cross Sections

for Crystalline Materials: The TOR Program

by

W. W. Clendenin
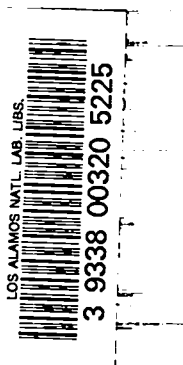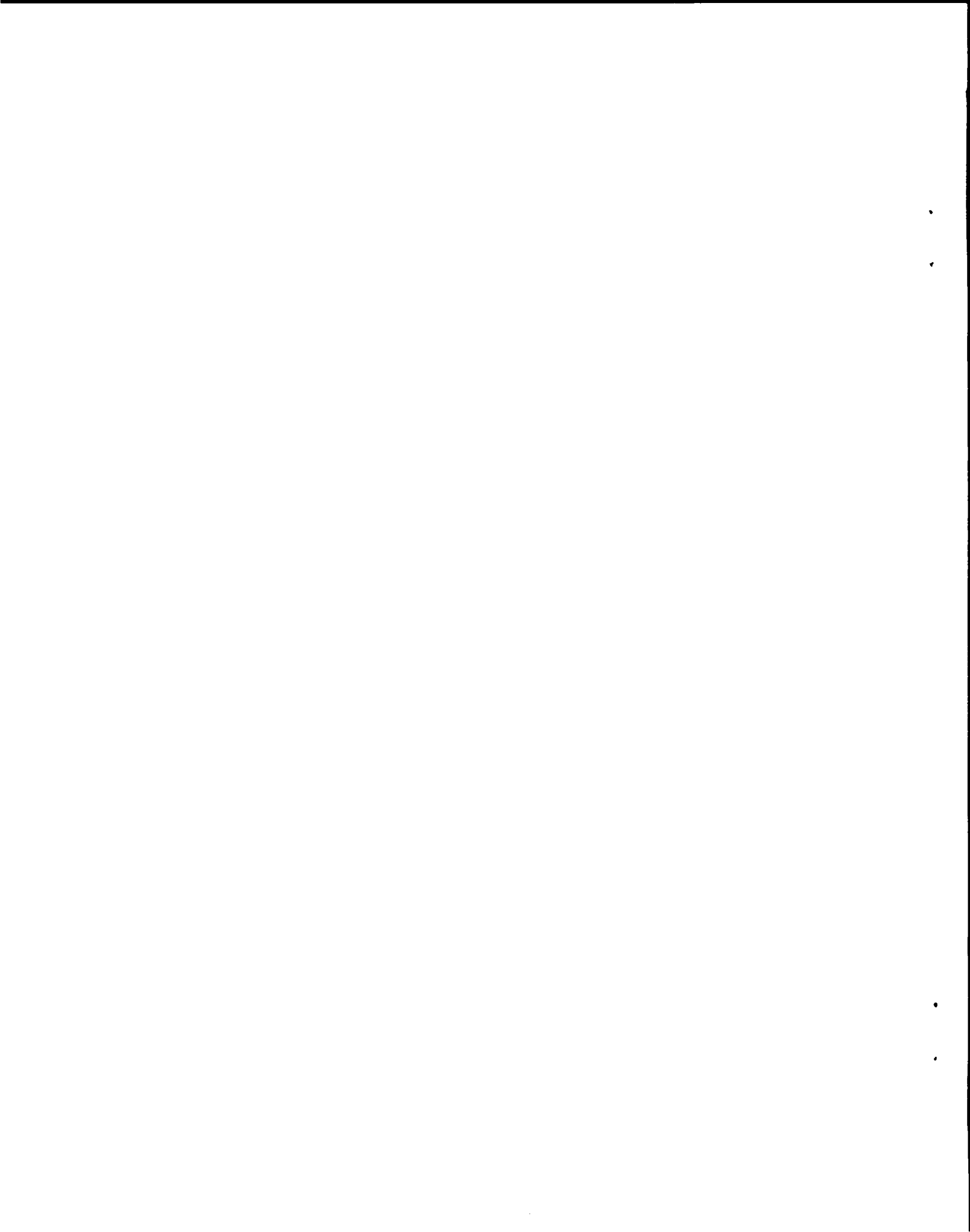
CALCUIATION OF THERMAL NEUTRON SCATTERING CROSS SECTIONS

FOR CRYSTALLINE MATERIALS: THE TOR PROGRAM

W. W. Clendenin

ABSTRACT

The FORTRAN-IV program TOR has been developed for the calculation of
thermal neutron differential scattering cross sections of crystalline ma-
terials. The scattering law is calculated in the incoherent approximation
by direct evaluation of the Fourier integrals. A new numerical integration
technique of improved accuracy is used. This includes a verification based
on the detailed balance condition for each value of the scattering law. A
two parameter function, derived from the scattering law but having more ac-
curate interpolation properties, is provided as card output. The latter
has the form of input for the FORTRAN-IV program GLEN which obtains the to-
tal scattering cross section, thermal neutron diffusion length, and flux-
weighted group cross sections.

I. <u>Introduction</u>. The scattering cross section of
the moderating material, e.g., graphite, beryllium,
H_2O, and D_2O, plays a basic role in determining
the characteristics of a thermal neutron reactor.
For neutrons with energies in the range .0 to about
3 eV the energy change cross section is strongly
dependent both on the nature of the particular ma-
terial and on its temperature. The materials with
simplest cross sections are monatomic gases such
as ^{4}He, the theory of which has been developed with
varying degrees of elaboration[1-5] over a number of
years. Because of its comparative simplicity a
monatomic gas model has sometimes been used as an
approximation for substances in the crystal or liq-
uid form.

One of the most successful of these applications
has been a modification[6] of the monatomic gas model
to fit the room temperature diffusion length of H_2O.
Even in this case there are substantial differences[7]
between the diffusion lengths at higher temperatures
implied by this model and those implied by a model[8]
taking into account in more detail the properties
of the moderator.

For a crystalline material the use of a monatomic
gas model is doubtful because of the special char-
acteristics of the crystal cross section. For ener-
gies near the lower end of the thermal neutron range,
but above the Bragg limit (.00175 eV for graphite
and .0062 eV for beryllium) it is typical of the
crystal cross section that it is primarily an elas-
tic scattering cross section. In contrast to the
monatomic gas case, the energy change cross section
may be an order of magnitude less than the total
scattering cross section, depending on the tempera-
ture of the material.

In attempting to use a monatomic gas as a model for
the crystal cross section, the usual practice has
been to duplicate the high energy total cross sec-
tion. The energy change cross section then differs

so widely from that of the crystal that the neutron spectrum for absorption typical of a reactor is substantially in error.[9]

The diffusion properties of the crystalline moderator depend qualitatively as well as quantitatively on the nature of the cross section. The existence of a diffusion length for the material depends[10] on the smallest value of the total cross section, which occurs at an energy just below the Bragg limit. The diffusion coefficient for neutrons below the Bragg limit differs, by an order of magnitude at some temperatures, from that for neutrons above the Bragg limit. Consequently, it is important, for an accurate treatment of neutron diffusion, to use cross sections which represent correctly the characteristics of the crystalline material.

The TOR and GLEN codes have been programmed to obtain cross sections for crystalline materials in the incoherent approximation, and to carry out group averages for use in transport theory codes[11] using the S_n method. The program TOR calculates the scattering law $G(\alpha,\beta)$ and punches for use in GLEN the related quantity $s(R,\epsilon)$. A fundamental aspect of the computational technique is to make use of the dependence of $s(R,\epsilon)$ on only two parameters. Cross sections corresponding to initial energy E_o, final energy E and angle of deflection θ are obtained by interpolation from a table of values of $s(R,\epsilon)$. The function $s(R,\epsilon)$ is used because of its suitability, examined in Section II, for interpolation.

A significant innovation in TOR is the use of an improved numerical evaluation. The cross sections are obtained by direct computation of the Fourier integrals involved without recourse to a phonon expansion or similar approximation. A new method[12] of numerical calculation of Fourier integrals makes possible rapid and accurate evaluation even for large values of the frequency parameter. Previous methods of the type introduced by Filon[13] were either forced to use a mesh interval which became smaller in proportion to the reciprocal of the frequency implying a lengthening calculation, or were subject to large errors for particular frequencies. The integration formula used in the earlier program GASKET[14] is of this type, but uses a cruder interpolation between mesh points than that in Filon's

method. Comparisons of differential cross section values obtained from TOR with those obtained from GASKET indicate close agreement for some values but differences as large as 10% in other cases.

The accuracy of the TOR values is verified by a check based on the detailed balance condition, described in Sections II and III. This check confirms an accuracy of 1%, within the incoherent approximation, for the differential cross sections computed by TOR.

II. Scattering Cross Section. The incoherent approximation[15-21] to the scattering cross section of a Bravais lattice is obtained by the TOR-GLEN program system. The form[21,22] of the double differential cross section for scattering from initial laboratory system energy E_o to final energy E with deflection through an angle θ is

$$d^2\sigma/d\Omega dE \approx \sigma(E_o \to E,\theta,T) = \sigma_0(E_o \to E,\theta,T) + \sigma_1(E_o \to E,\theta,T).$$
(1)

Here $\sigma_0(E_o \to E,\theta,T)$ is the elastic scattering term[*]

$$\sigma_0(E_o \to E,\theta,T) = (\sigma_b/4\pi)\exp\{-R\gamma(0)\}\delta(\epsilon).$$
(2)

The cross section $\sigma_1(E_o \to E,\theta,T)$, which includes inelastic scattering, is given by

$$\sigma_1(E_o \to E,\theta,T) = (\sigma_b/4\pi)(E/E_o)^{\frac{1}{2}}\exp\{-R\gamma(0)\}$$

$$\cdot (2\pi)^{-1}\int_{-\infty}^{\infty}\exp(i\epsilon t)[\exp\{R\gamma(t)\} - 1]dt.$$
(3)

The basic parameters R and ϵ of the cross section are

$$R = (m/M)(E_o + E - 2E_o^{\frac{1}{2}}E^{\frac{1}{2}}\cos\theta),$$
(4)

$$\epsilon = E - E_o.$$
(5)

The function $\gamma(t)$ is

$$\gamma(t) = \int_{-\infty}^{\infty}\{f(\zeta)/2\zeta\ \sinh(\zeta/2T)\}\exp\{(\zeta/2T)+i\zeta t\}d\zeta.$$
(6)

Here T is the absolute temperature and ζ the phonon frequency, both in energy units. In Eq. (6), $f(\zeta)$ is the phonon frequency distribution of the crystal.

_____

[*]The elastic cross section $\sigma_0(E_o \to E,\theta,T)$ is corrected for the Bragg limit in GLEN; values of Eq. (2) are presented in TOR only as indications of magnitude.

This distribution obeys the normalization and symmetry conditions,

$$\int_{-\infty}^{\infty} f(\zeta)d\zeta = 2,$$ (7)

and

$$f(\zeta) \geq 0, \quad f(-\zeta) = f(\zeta).$$ (8)

On the basis of the second condition of Eq. (8), $\gamma(t)$ may be expressed as

$$\gamma(t) = \gamma_{even}(t) + i\gamma_{odd}(t),$$ (9)

where

$$\gamma_{even}(t) = \int_{0}^{\infty} \zeta^{-1} f(\zeta) \coth(\zeta/2T) \cos(\zeta t)d\zeta,$$ (10)

$$\gamma_{odd}(t) = \int_{0}^{\infty} \zeta^{-1} f(\zeta) \sin(\zeta t)d\zeta.$$ (11)

The cross section $\sigma_1(E_o \to E, \theta, T)$ is

$$\sigma_1(E_o \to E, \theta, T) = (\sigma_b/4\pi)(E/E_o)^{\frac{1}{2}} s(R, \epsilon).$$ (12)

Here the factor $s(R, \epsilon)$ is made up of the two Fourier integrals,

$$s(R, \epsilon) = u(R, \epsilon) + v(R, \epsilon)$$ (13)

where

$$u(R, \epsilon) = \pi^{-1} \int_{0}^{\infty} [\exp\{R\gamma_{even}(t) - R\gamma_{even}(0)\} \cos\{R\gamma_{odd}(t)\}$$

$$- \exp\{-R\gamma_{even}(0)\}] \cos(\epsilon t)dt,$$ (14)

$$v(R, \epsilon) = -\pi^{-1} \int_{0}^{\infty} \exp\{R\gamma_{even}(t)$$

$$- R\gamma_{even}(0)\} \sin\{R\gamma_{odd}(t)\} \sin(\epsilon t)dt.$$ (15)

The integrals of Eqs. (10),(11),(14),(15) are in the forms to which the numerical method used[12] applies directly.

It may be shown[22] that the cross section $\sigma_1(E_o \to E, \theta, T)$ obeys the detailed balance condition, i.e., that

$$\exp(\epsilon/2T)s(R, \epsilon) = \exp(-\epsilon/2T)s(R, -\epsilon).$$ (16)

The scattering law[23], for $\epsilon \neq 0$, is the dimensionless quantity

$$G(\alpha, \beta) = T \exp(\epsilon/2T)s(R, \epsilon),$$ (17)

where

$$\alpha = R/T,$$ (18)

$$\beta = \epsilon/T.$$ (19)

The detailed balance condition of (16), together with the form of Eqs. (13),(14), and (15) may be used to provide a check on $u(R, \epsilon)$ and $v(R, \epsilon)$. These integrals obey the condition

$$u(R, \epsilon)\{\exp(-\epsilon/T)-1\} = v(R, \epsilon)\{\exp(-\epsilon/T)+1\}.$$ (20)

Verification of Eq. (20) for each pair of values R, ϵ provides a check on $s(R, \epsilon)$ with no additional numerical computation.

The dependence of $s(R, \epsilon)$ on only the two parameters R, ϵ suggests a computational scheme based on a table of values either of $s(R, \epsilon)$ or of $G(\alpha, \beta)$. Since values for $-\epsilon$ can be obtained by means of Eq. (16) from those for ϵ, it is only necessary to compute values for one sign of ϵ. It is clear from Eq. (16) that $s(R, \epsilon)$ for $\epsilon > 0$ decreases more rapidly with increasing $|\epsilon|$ than does $s(R, \epsilon)$ for $\epsilon < 0$. It is clear from Eq. (17) that $G(\alpha, \beta)$ also decreases more rapidly with increasing $|\epsilon|$ than does $s(R, \epsilon)$ for $\epsilon < 0$. Consequently, the most favorable choice for a table to be used for interpolation is to compute $s(R, \epsilon)$ for $\epsilon < 0$.

In outline, the program TOR computes such a table of $s(R_n, \epsilon_m)$ for a specified mesh of values R_n, ϵ_m. The calculation is made by first computing a set of values $\gamma_{even}(t_j)$ and $\gamma_{odd}(t_j)$ for a set of mesh values t_j. Needed values of $\gamma_{even}(t)$ and $\gamma_{odd}(t)$ are obtained by quadratic interpolation from this set. The functions $u(R_n, \epsilon_m)$ and $v(R_n, \epsilon_m)$ are calculated by the method[12] for evaluating Fourier integrals. The ratio of the two sides of Eq. (20) is obtained as a check, and $s(R_n, \epsilon_m)$ is obtained from Eq. (13).

III. FORTRAN-IV Program TOR. The primary purpose of the TOR program is to compute values $s(R_n, \epsilon_m)$ over a mesh R_n, ϵ_m suitable for interpolation. For each variable, the mesh uses a succession of systematically increasing intervals in which the ratio of each interval to the preceding one is a fixed multiplier specified as input.

Since R, Eq. (4), is inherently nonnegative, the first interval h_R (HREC) > 0 extends from $R_1 = 0$ to

$R_2 = h_R$. The second interval, of length $A_R h_R$ where A_R(AFAREC) is the multiplying factor, extends from $R_2 = h_R$ to $R_3 = h_R(1+A_R)$. Similarly, the nth interval, of length $A_R^{n-1} h_R$ extends from R_n(REC(N)) to R_{n+1}(REC(N+1)). The mesh limit is specified by the input parameter R_{max}(RECMAX), the upper limit of the mesh being REC(NLIM) where, for $A_R > 1$, NLIM is the positive integer given by

$$\text{NLIM-2} \leq [\log\{1+h_R^{-1}(A_R-1)R_{max}\}]/[\log A_R] < \text{NLIM-1}. \quad (21)$$

For $A_R = 1$, Eq. (21) is replaced by

$$\text{NLIM} - 1 \leq h_R^{-1} R_{max} < \text{NLIM}. \quad (22)$$

The mesh for the variable ϵ is similar, except that an independent set of parameters designated by h_ϵ(HEPS), A_ϵ(AFAEPS), ϵ_{max}(EPSMAX), and ϵ_m(EPS(M) for M = 1, ... MLIM) is used. With these replacements, Eqs. (21) and (22) apply also to the mesh of values ϵ_m. Since ϵ may be negative, the parameters h_ϵ and ϵ_{max} which must have the same sign may be negative--from the accuracy considerations of Section II this is the usual case. Typical values of the input parameters for the mesh R_n, ϵ_m are given in Section IV which describes the input for TOR.

For the case of a crystal cross section, designated by setting the control parameter IDEN > 0, the program TOR calculates $s(R_n,\epsilon_m)$ as given by Eq. (13). A necessary first step is to calculate $\gamma_{even}(t_j)$, Eq. (10), and $\gamma_{odd}(t_j)$, Eq. (11), for a suitable mesh of values t_j. The basis for the form of this mesh is the method[12] for calculating Fourier integrals. Here, a succession of intervals is defined by pairs, the length of each interval in each pair being three times as long as the length of each of the preceding pair of intervals. For the present application it is suitable from the point of view of interpolation to carry out this expansion of the interval through six pairs of intervals. For values of t larger than those in the twelfth interval, the interval size is the same as that of the twelfth interval.

The length of the first interval is given by $\Delta t_1 = 1/(9\,\zeta_{max})$ where ζ_{max} is the largest value of $|\zeta|$ for which $f(\zeta)$ differs from zero. The second

interval $\Delta t_2 = \Delta t_1$, $\Delta t_3 = \Delta t_4 = 3\Delta t_1$, $\Delta t_5 = \Delta t_6 = 9\Delta t_1$, ... $\Delta t_{11} = \Delta t_{12} = 243\,\Delta t_1$, and all intervals with higher indices are equal to Δt_{12}. In each interval values of $\gamma_{even}(t_j)$ and $\gamma_{odd}(t_j)$ are obtained at 28 equally spaced points, including the initial and final points of the interval. The total number of intervals required depends on the particular phonon frequency distribution $f(\zeta)$ considered. For the Egelstaff[23,9] and Young-Koppel[24] phonon distributions for graphite, 36 intervals have been found to give good accuracy based on comparison of values computed with this number with values obtained using a larger number of intervals. For the Debye and Young-Koppel[25] phonon distributions for beryllium, 24 intervals have been found to give good accuracy. The number of intervals is specified as the input parameter INMXO in TOR.

For the crystal cross section, IDEN > 0, the phonon frequency distribution $f(\zeta_k)$, PHOFRE(NZETA), is specified as input at a set of values ζ_k, ZETA(NZETA). The total number, NZEMAX, of such values must lie in the range $4 \leq$ NZEMAX ≤ 201. Quadratic interpolation is used to determine $f(\zeta)$ between these net points, and as a consequence four points are sufficient for a Debye spectrum. The minimum number of four points is set by the subroutine which normalizes the distribution $f(\zeta)$ according to Eq. (7). It is not necessary for the input spectrum to be normalized, or for the values ζ_k to be at equal intervals.

The method[12] for the calculation of Fourier integrals using a double convergence criterion of .001 is used to obtain $\gamma_{even}(t_j)$ and $\gamma_{odd}(t_j)$ from $f(\zeta)$. Quadratic interpolation between mesh points t_j is used to obtain values needed in the calculation of $u(R_n,\epsilon_m)$, Eq. (14), and $v(R_n,\epsilon_m)$, Eq. (15). For this calculation a double convergence criterion of .003 is used. The factor $s(R_n,\epsilon_m)$ designated in TOR as SKE(N,M) is obtained according to Eq. (13) at each mesh point. The check based on detailed balance consists of obtaining the ratio of the right side of Eq. (20) to the left side. This ratio, which thus should approximate unity, is designated as DEBARA(N,M).

The magnitude factor $\exp\{-R_n\gamma_{even}(0)\}$ of Eq. (2) is computed for each value R_n and designated SEID(N). The parameter α_n, ALPHEG(N), determined from R_n according to Eq. (18), is obtained for each R_n. Similarly, the parameter β_m, BETEG(M), given in terms of ϵ_m by Eq. (19), is obtained for each ϵ_m. The scattering law component $G(\alpha_n, \beta_m)$ obtained from $s(R_n, \epsilon_m)$ through Eq. (17) is calculated for each mesh point and designated as SIGEF(N,M). The corresponding quantity derived from the elastic scattering cross section of Eq. (2) is $T\exp\{-R_n\gamma_{even}(0)\}$ which is calculated for each R_n and designated as SIGEID(N).

The output of TOR is described in detail in Section V. All quantities calculated are printed out, and in addition those needed for interpolation to obtain the cross sections for GLEN are punched.

An option in TOR, specified by setting IDEN = 0 substitutes a monatomic gas model for the crystal model of Eqs. (1) - (11). The monatomic gas cross section can be expressed[26] in the form of Eq. (12) provided $s(R,\epsilon)$ is replaced by

$$s'(R,\epsilon) = (4\pi RT)^{-\frac{1}{2}}\exp\{-(\epsilon+R)^2/4RT\}. \qquad (23)$$

For IDEN = 0, SKE(N,M) is computed according to Eq. (23), and DEBARA(N,M) is set to 1. There is no analogue of the elastic cross section of Eq. (2) in the monatomic gas case and the quantities SEID(N) and SIGEID(N) are set to 0.

IV. Input for TOR.

1. Title card   12 A 6
2. IDEN, INMXO   2 I 10
    a. For IDEN = 0, monatomic gas.
    b. For IDEN > 0, crystal specified by phonon spectrum.
    c. INMXO specifies upper limit on integration over t. Typical values are INMXO = 24 for beryllium phonon spectra and INMXO = 36 for graphite spectra. For monatomic gas, calculation is analytic and INMXO should be set to 1. Upper limit on INMXO is 72.
3. a. For IDEN = 0, program goes directly to 4, below.
    b. For IDEN > 0:
        1) NZEMAX (4 ≤ NZEMAX ≤ 201)   I 10

2) ZETA (NZETA), NZETA = 1, NZEMAX

                             4 E 20.8

Energies at which values of phonon frequency distribution are specified. ZETA (1) must be .0 and ZETA (NZETA+1) > ZETA (NZETA).

3) PHOFRE (NZETA), NZETA = 1, NZEMAX

                             4 E 20.8

Values of phonon frequency distribution corresponding to energies in 2) above. PHOFRE (1) must be .0, and PHOFRE (NZETA) ≥ 0.

4. TEMPEN (temperature T in energy units > .0)

                             E 20.8

5. RECMAX, HREC, AFAREC   3 E 20.8
RECMAX > .0 is maximum value of R and HREC (.0 < HREC ≤ RECMAX) is smallest interval of R, both in energy units. AFAREC ≥ 1. is numerical factor which is ratio of successive intervals in R. Typical values are RECMAX = 3.1 eV., HREC = .005 eV., AFAREC = 1.1.

6. EPSMAX, HEPS, AFAEPS   3 E 20.8
EPSMAX is the largest magnitude of ϵ, and HEPS is the interval of ϵ smallest in magnitude, both in energy units. They must have the same sign and EPSMAX/HEPS ≥ 1. Code will accept either sign but for accuracy in computing crystal cross section, negative values are preferable. AFAEPS ≥ 1. is numerical factor which is ratio of successive intervals in ϵ. Typical values are EPSMAX = -3.1 eV., HEPS = -.005 eV., AFAREC = 1.1.

Points to be noted about the input:

1) An energy unit, e.g., electron volts, must be used consistently for all quantities having the dimensions of energy. These include ZETA, TEMPEN, RECMAX, HREC, EPSMAX, HEPS.

2) The program includes a subroutine for normalizing the phonon frequency distribution so that it is not necessary for the input phonon spectrum to be normalized. At least 4 values of ZETA and PHOFRE must be included to specify the input spectrum. Since quadratic interpolation between mesh points is used, 4 points are sufficient for a Debye spectrum. The values of ZETA do not need to be at equal intervals.

3) For the case of a crystal, IDEN > 0, the calcula-

tion of the function $\gamma(t)$ represents a significant investment of machine time, and a provision for data retrieval and use is included in the code. For IDEN $\geq$ 128, the values of $\gamma(t)$ are read in from cards instead of being computed. These cards are placed at the end of the input following EPSMAX, HEPS, AFAEPS. They must be obtained as part of the output of a previous problem. For $16 \leq$ IDEN < 128, a card output specifying $\gamma(t)$ is provided by the code as the first cards printed. The cards to be used as input for $\gamma(t)$ are immediately preceded and followed by the title card. The regular output follows the second title card.

4) In addition to the input checks indicated above, an input check to limit the amount of machine time is included in TOR. The maximum size of the matrix of values SKE(N,M) is given by $N \leq 50$, $M \leq 50$. If the input is such as to imply NLIM > 50, the problem is stopped and either the ratio RECMAX/HREC must be reduced or the parameter AFAREC increased. Similarly, if it is implied that MLIM > 50, the problem is stopped and the ratio EPSMAX/HEPS must be reduced or AFAEPS must be increased.

V. TOR Output.

1. Title card

Following the title card, various check quantities are printed out by the calculating subroutines PHFRNO, TORIN, FIGAFC, and TORCO.

The main output of the code is edited by the subroutine TOSCRI. It consists of printed output and card output. The card deck is to be used intact as part of the input for GLEN. The remainder of the printed output is:

- -

Reprint of input:

2. IDEN, INMXO

3. a. If IDEN = 0 code goes directly to 4. below.
    b. If IDEN > 0 code prints:
       1) NZEMAX
       2) NZETA, ZETA (NZETA), PHOFRE (NZETA), for NZETA = 1, NZEMAX. Note that these are normalized values of PHOFRE differing from the input values by the normalization constant.

4. TEMPEN

5. RECMAX, HREC, AFAREC

6. EPSMAX, HEPS, AFAEPS

- -

7. NLIM. The number of values of R_n, designated REC(N) in the code, in the mesh of values of $s(R_n, \epsilon_m)$, designated SKE(N,M) in the code. $1 \leq N \leq$ NLIM.

8. MLIM. The number of values of ϵ_m, designated EPS(M) in the code, in the mesh of values of $s(R_n, \epsilon_m)$. $1 \leq M \leq$ MLIM.

9. N, REC(N), SEID(N), SIGEID(N) for $1 \leq N \leq$ NLIM. SEID(N) is the coefficient exp $\{-R \gamma(0)\}$ in the elastic scattering term exp $\{-R \gamma(0)\}$ $\delta(\epsilon)$ of Eq. (2), and SIGEID(N) is the coefficient T exp $\{-R \gamma(0)\}$ of the corresponding term T exp $\{-R \gamma(0)\}$ $\delta(\epsilon)$ in the scattering law.

10. For $1 \leq N \leq$ NLIM and $1 \leq M \leq$ MLIM, REC(N), EPS(M), SKE(N,M), ALPHEG(N), BETEG(M), SIGEF(N,M), DEBARA(N,M). The parameter ALPHEG(N) is R_n/T and the parameter BETEG(M) is ϵ_m/T. The quantity SIGEF(N,M) is the scattering law term T exp $(\epsilon_m 2T)$ $s(R_n, \epsilon_m)$. The parameter DEBARA(N,M) is a check quantity based on the detailed balance condition and computed for each value of $s(R_n, \epsilon_m)$. For perfect accuracy DEBARA(N,M) would be exactly 1., and its nearness to 1. indicates the accuracy of $s(R_n, \epsilon_m)$. For the case of a crystal, IDEN > 0, this provides a useful check on the numerical integrations. For a monatomic gas, $s(R_n, \epsilon_m)$ is computed analytically and DEBARA(N,M) is identically 1.

11. The function $\gamma(t)$ is a complex function given in terms of the real functions $\gamma_{even}(t)$ and $\gamma_{odd}(t)$ by $\gamma_{even}(t) + i\gamma_{odd}(t)$. The functions $\gamma_{even}(t)$ and $\gamma_{odd}(t)$ are printed out as functions of t, designated in the printout as TIME. The function $\gamma_{even}(t)$ is designated as GAMEVE, and the function $\gamma_{odd}(t)$ as GAMODD. Note that the running variables N, $1 \leq N \leq$ INMXO, and M, $1 \leq M \leq 28$, used in this printout are not the same as the running variables N, M of 9. and 10. above.

The card output of TOR is:

1. Title card   12 A 6

2. IDEN, TEMPEN, GAMO   I 10, 2 E 20.8

    GAMO is $\gamma(0)$.

3. AFAREC, HREC, AFAEPS, HEPS   4 E 20.8

4. NLIM   I 10

5. REC(N) for N = 1, NLIM   4 E 19.8

6. MLIM   I 9

7. EPS(M) for M = 1, MLIM   4 E 18.8

8. NPROD   I 8

    NPROD is the product NLIM* MLIM

9. SKE(N,M) for N = 1, NLIM and

    M = 1, MLIM   5 E 15.8

It will be noted that a different printing format is used for each type of quantity so that the quantity can be identified by the format.

If $16 \leq$ IDEN < 128 a card output specifying $\gamma(t)$ is provided by the code. This deck, which is to be used as part of the input for TOR when IDEN $\geq$ 128, is punched out before the regular card output above and is preceded by the title card. Only the deck between the two title cards is to be used as input for TOR, and only if IDEN $\geq$ 128.

The regular card output from TOR, outlined above, is to be used intact as part of the input for GLEN.

APPENDIX

The program has been compiled and run on the CDC 6600. The core storage requirement is approximately 26,000.

REFERENCES

1. E. P. Wigner and J. E. Wilkins, Jr., AECD-2275, Div. of Tech. Info. Exten., USAEC (1944).

2. H. D. Brown and D. S. St. John, DP-33, du Pont de Nemours and Co., Savannah River Laboratory (1954).

3. G. J. Marchuk, Soviet J. At. Energy Suppl. 3, 19 (1958).

4. W. W. Clendenin, J. Nucl. Energy A13, 25 (1960).

5. G. L. Blackshaw and R. L. Murray, Nucl. Sci. Eng. 27, 520 (1967).

6. A. Radkowsky, ANL 4476, p. 89, Argonne Laboratory Quarterly Report (1950).

7. W. W. Clendenin, Nucl. Sci. Eng. 18, 351 (1964).

8. M. S. Nelkin, Phys. Rev. 119, 741 (1960).

9. D. E. Parks, J. R. Beyster, and N. F. Wikner, Nucl. Sci. Eng. 13, 306 (1962).

    N. F. Wikner, G. D. Joanou and D. E. Parks, Nucl. Sci. Eng. 19, 108 (1964).

10. N. Corngold, Nucl. Sci. Eng. 19, 80 (1964).

    N. Corngold and P. Michael, Nucl. Sci. Eng. 19, 91 (1964).

11. K. D. Lathrop, IA-3373, Los Alamos Laboratory Report "DTF-IV, a FORTRAN-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering" (1965).

12. W. W. Clendenin, Numerische Mathematik 8, 422 (1966).

13. L. N. G. Filon, Proc. Roy. Soc. Edinburgh 49, 38 (1928).

14. J. U. Koppel, J. R. Triplett and Y. D. Naliboff, GA-7417, General Atomic Report, "GASKET, A Unified Code for Thermal Neutron Scattering" (1966).

15. P. O. Fröman, Ark. Fys. 4, 191 (1951).

16. G. Placzek, Phys. Rev. 86, 377 (1952).

17. G. Placzek and L. Van Hove, Phys. Rev. 93, 1207 (1954).

18. G. C. Wick, Phys. Rev. 94, 1228 (1954).

19. L. van Hove, Phys. Rev. 95, 249 (1954).

20. R. J. Glauber, Phys. Rev. 98, 1692 (1955).

21. A. Sjölander, Ark. Fys. 14, 315 (1958).

22. W. W. Clendenin, IA-DC-9060 (1967).

23. P. A. Egelstaff, Nucl. Sci. Eng. 12, 250 (1962); P. A. Egelstaff and P. Schofield, Nucl. Sci. Eng. 12, 260 (1962).

24. J. A. Young and J. U. Koppel, J. Chem. Phys. 42, 357 (1965).

25. J. A. Young and J. U. Koppel, Phys. Rev. 134, A 1476 (1964).

26. A. C. Zemach and R. J. Glauber, Phys. Rev. 101, 118 (1956).

```
                  PROGRAM TOR(INPUT,TAPE10=INPUT,
                 1OUTPUT,TAPE9=OUTPUT,
                 2PUNCH,TAPE11=PUNCH)
          $IBFIC IOR       DECK
000003            COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
                 1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
                 2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                 3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
                 4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
                 5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000003            COMMON T2(73,5),S(74,6)
000003            COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000003            COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
                 1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
                 2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODU,
                 3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
                 4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
                 5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
                 6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
                 7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
                 8FIALPH,FIBET,FIGAM
000003            COMMON AFACTO,TE2
000003            COMMON FACSIG,SIGMA,SIGMAC,ETINO,
                 1RECMAX,HREC,AFAREC,EPSMAX,HEPS,AFAEPS,
                 2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
                 3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
                 4ALPHEG(50),BETEG(50),AFIELD(12),
                 5INMXO,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000003            READ(10,1)(AFIELD(J),J=1,12)
000015          1 FORMAT(12A6)
000015            WRITE(9,2)
000021          2 FORMAT(55H1                                                              I)
000021            WRITE(9,1)(AFIELD(J),J=1,12)
000033          3 ININCK=0
000034          4 FORMAT(8I10)
000034          5 FORMAT(4E20.8)
000034            READ(10,4)IDEN,INMXO
000044            IF(IDEN)951,8,951
000045        951 IF(INMXO-8)6,8,8
000050          6 WRITE(9,7)
000054          7 FORMAT(18H0INMXO LESS THAN 8)
000054            ININCK=1
000055          8 IF(INMXO-72)11,11,9
000060          9 WRITE(9,10)
000064         10 FORMAT(22H0INMXO GREATER THAN 72)
000064            ININCK=1+ININCK
000066         11 IF(IDEN)12,33,15
000070         12 NZEMAX=2
000071            READ(10,5)ZETA(NZEMAX)
000077            ABC=ZETA(NZEMAX)
000101            IF(ABC)13,13,33
000102         13 WRITE(9,14)
000106         14 FORMAT(30H0ZETA(NZEMAX) NEGATIVE OR ZERO)
000106            ININCK=1+ININCK
000110            GO TO 33
000110         15 READ(10,4)NZEMAX
000116            IF(NZEMAX-4)16,18,18
000121         16 WRITE(9,17)
000125         17 FORMAT(19H0NZEMAX LESS THAN 4)
000125            ININCK=1+ININCK
000127         18 IF(NZEMAX-201)21,21,19
000132         19 WRITE(9,20)
000136         20 FORMAT(24H0NZEMAX GREATER THAN 201)
000136            ININCK=1+ININCK
000140         21 READ(10,5)(ZETA(NZETA),NZETA=1,NZEMAX)
000153            READ(10,5)(PHOFRE(NZETA),NZETA=1,NZEMAX)
000166            ABC=ZETA(1)
000170            IF(ABC)22,24,22
000171         22 WRITE(9,23)
000175         23 FORMAT(17H0ZETA(1) NOT ZERO)
000175            ININCK=1+ININCK
```

```
000177      24 ABC=PHOFRE(1)
000201         IF(ABC)25,261,25
000202      25 WRITE(9,26)
000206      26 FORMAT(19HOPHOFRE(1) NOT ZERO)
000206         ININCK=1+ININCK
000210     261 DO 29 NZETA=2,NZEMAX
000212         ABC=ZETA(NZETA)-ZETA(NZETA-1)
000214         IF(ABC)27,27,29
000216      27 NZELS1=NZETA-1
000220         WRITE(9,28)NZETA,NZELS1
000230      28 FORMAT(6HOZETA(,I4,19H ) LESS/EQUAL ZETA(,I4,2H ))
000230         ININCK=1+ININCK
000232      29 CONTINUE
000235         DO 32 NZETA=2,NZEMAX
000236         ABC=PHOFRE(NZETA)
000240         IF(ABC)30,32,32
000241      30 WRITE(9,31)NZETA
000247      31 FORMAT(8HOPHOFRE(,I4,11H ) NEGATIVE)
000247         ININCK=1+ININCK
000251      32 CONTINUE
000254         ALPHA=.1*ZETA(NZEMAX)
000256      33 READ(10,5)TEMPEN
000264         IF(TEMPEN)34,34,36
000266      34 WRITE(9,35)
000272      35 FORMAT(23HOTEMPEN LESS/EQUAL ZERO)
000272         ININCK=1+ININCK
000274      36 READ(10,5)RECMAX,HREC,AFAREC
000306         IF(RECMAX)37,37,39
000310      37 WRITE(9,38)
000314      38 FORMAT(23HORECMAX LESS/EQUAL ZERO)
000314         ININCK=1+ININCK
000316      39 ABC=RECMAX/HREC
000320         IF(ABC-1.)40,42,42
000322      40 WRITE(9,41)
000326      41 FORMAT(25HORECMAX/HREC LESS THAN 1.)
000326         ININCK=1+ININCK
000330      42 IF(AFAREC-1.)43,45,45
000333      43 WRITE(9,44)
000337      44 FORMAT(20HOAFAREC LESS THAN 1.)
000337         ININCK=1+ININCK
000341      45 READ(10,5)EPSMAX,HEPS,AFAEPS
000353         ABC=EPSMAX/HEPS
000355         IF(ABC-1.)46,48,48
000357      46 WRITE(9,47)
000363      47 FORMAT(25HOEPSMAX/HEPS LESS THAN 1.)
000363         ININCK=1+ININCK
000365      48 IF(AFAEPS-1.)49,51,51
000370      49 WRITE(9,50)
000374      50 FORMAT(20HOAFAEPS LESS THAN 1.)
000374         ININCK=1+ININCK
000376      51 IF(AFAREC-1.)52,52,53
000401      52 NLIM=INT(RECMAX/HREC)+1
000405         GO TO 54
000405      53 NLIM=INT((ALOG(1.+(AFAREC-1.)*RECMAX/HREC))
              1/(ALOG(AFAREC)))+2
000421      54 IF(NLIM-50)57,57,55
000424      55 WRITE(9,56)
000430      56 FORMAT(16HONLIM EXCEEDS 50)
000430         ININCK=1+ININCK
000432      57 IF(AFAEPS-1.)58,58,59
000435      58 MLIM=INT(EPSMAX/HEPS)+1
000441         GO TO 60
000441      59 MLIM=INT((ALOG(1.+(AFAEPS-1.)*EPSMAX/HEPS))
              1/(ALOG(AFAEPS)))+2
000455      60 IF(MLIM-50)63,63,61
000460      61 WRITE(9,62)
000464      62 FORMAT(16HOMLIM EXCEEDS 50)
000464         ININCK=1+ININCK
000466      63 IF(ININCK)64,66,64
000467      64 WRITE(9,65)ININCK
000475      65 FORMAT(22HOINPUT CHECKED, ABOVE ,I3,31H ERRORS FOUND, PROBLEM STOP
              1PED.)
```

```
000475          STOP
000477      66 IF(IDEN)67,67,661
000501     661 CALL PHFRNO
000502      67 FITINT=.001
000504         ETININ=.003
000505         FITNO=.11111111
000507         NINIT=11
000510         CALL TORIN
000511         TNMPL4=INMX0
000513         INMPL5=INMX0+1
000515         IF(IDEN-128)68,72,72
000517      68 CALL CLOCK(ABCDEF)
000521         WRITE(9,681)ABCDEF
000527     681 FORMAT(22HOCLOCK BEFORE FIGAFC =,E15.8)
000527         CALL FIGAFC
000530         CALL CLOCK(ABCDEG)
000532         WRITE(9,682)ABCDFG
000540     682 FORMAT(21HOCLOCK AFTER FIGAFC =,F15.9)
000540         IF(IDEN-16)74,69,69
000543      69 WRITE(11,1)(AFIELD(J),J=1,12)
000555         WRITE(11,4)INMPL4
000563         DO 70 N=1,INMPL4
000565      70 WRITE(11,71)(TIMVAR(N,M),GAEVFC(N,M),GAODFC(N,M),
                1M=1,28)
000613      71 FORMAT(3E17.8)
000613         GO TO 74
000613      72 READ(10,4)INMPL4
000621         INMX0=INMPL4
000623         INMPL5=INMPL4+1
000625         DO 73 N=1,INMPL4
000626      73 READ(10,71)(TIMVAR(N,M),GAEVFC(N,M),GAODFC(N,M),M=1,28)
000654         TIMVAR(INMPL5,1)=TIMVAR(INMPL4,28)
000656         GAMO=GAEVFC(1,1)
000657      74 REC(1)=.0
000660         HRFCNU=HREC
000662         REC(2)=HRECNU
000663         DO 75 N=3,NLIM
000664         HRFCNU=HRECNU*AFAREC
000666      75 REC(N)=REC(N-1)+HRECNU
000672         EPS(1)=.0
000673         HEPSNU=HEPS
000674         EPS(2)=HEPSNU
000675         DO 76 M=3,MLIM
000677         HEPSNU=HEPSNU*AFAEPS
000701      76 EPS(M)=EPS(M-1)+HEPSNU
000705         DO 79 N=1,NLIM
000705         IF(IDEN)78,77,78
000707      77 SEDD(N)=.0
000711         SIGLLD(N)=,0
000712         GO TO 79
000712      78 RECOIL=REC(N)
000714         SEDD(N)=EXP(-RECOIL*GAMO)
000721         SIGELD(N)=TEMPEN*SEDD(N)
000723      79 CONTINUE
000726      80 DO 82 N=1,NLIM
000730         DO 81 M=1,MLIM
000731         SNF(N,M)=.0
000734         DEHARA(N,M)=1.
000736      81 SIGEF(N,M)=.0
000742      82 CONTINUE
000744      83 DO 99 N=1,NLIM
000746         RECOIL=REC(N)
000750         M=1
000751      84 OMEGA=EPS(M)
000753         FACTOR=TEMPEN*EXP(OMEGA/(2.*TEMPFN))
000761         IF(RECOIL)85,85,86
000762      85 SKF(N,M)=.0
000766         DEHARA(N,M)=1.
000770         SIGEF(N,M)=.0
000772         GO TO 89
000772      86 IF(IDEN)88,87,88
000773      87 AMT1=1./((12.566371*RECOIL*TEMPEN)**.5)
```

```
001001          AMT2=(OMEGA+RECOIL)**2
001003          AMT3=4.*RECOIL*TEMPEN
001006          SKE(N,M)=AMT1*EXP(-AMT2/AMT3)
001016          DEBARA(N,M)=1.
001020          SIGEF(N,M)=FACTOR*SKE(N,M)
001023          SKEMAX=.0
001024          GO TO 94
001025      88 CALL TORCO
001026          SKE(N,M)=SIGMA
001033          DEBARA(N,M)=SIGMAC
001034          SIGEF(N,M)=FACTOR*SKE(N,M)
001040      89 IF(M-1)90,90,91
001043      90 SKEMAX=SKE(N,M)
001047          GO TO 93
001050      91 GLNCMP=SKE(N,M)-SKEMAX
001055          IF(GLNCMP)93,93,92
001056      92 SKEMAX=SKE(N,M)
001062      93 GLNCMP=SKE(N,M)-1.E-03*SKEMAX
001070          IF(GLNCMP)931,94,94
001072     931 GLNCMP=ABS(EPS(M))-REC(N)
001076          IF(GLNCMP)94,94,96
001100      94 IF(M-MLIM)95,96,96
001103      95 M=M+1
001105          GO TO 84
001105      96 DO 98 M=1,MLIM
001107          GLNCMP=SKE(N,M)-1.E-03*SKEMAX
001114          IF(GLNCMP)97,98,98
001116      97 SKE(N,M)=.0
001122          DEBARA(N,M)=1.
001124          SIGEF(N,M)=.0
001126      98 CONTINUE
001131      99 CONTINUE
001133          DO 100 N=1,NLIM
001135     100 ALPHEG(N)=REC(N)/TEMPEN
001142          DO 101 M=1,MLIM
001143     101 BETEG(M)=EPS(M)/TEMPEN
001150          CALL TOSCRI
001151          STOP
001153          END
```

```
            $*  ****COMMENT CARD TO BREAK UP BATCH COMPILE
            $IBFTC TOR2    OECK
                    SUBROUTINE TORIN
000002          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
                1SFINAL,ERR,TIMF,FIRST,FINAL,FCN,FSFCN,
                2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
                4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
                5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
                1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
                2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
                3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
                4NFI,NSOF,FISOIF,FISOER,FIALMU,FIBEMU,
                5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
                6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
                7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
                8FIALPH,FIBET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
                1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
                2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
                3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
                4ALPHEG(50),BETEG(50),AFIELD(12),
                5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
```

```
000002            NTYPE=1
000003            INMPL4=INMX0+4
000005            INMPL5=INMX0+5
000007            FACSIG=.31830989
000010            IF(ETININ-3.E-9)1,3,3
000013          1 WRITE(9,2)
000017          2 FORMAT(28H0ETININ NOT IN CORRECT RANGE)
000017            STOP
000021          3 IF(ETININ-1.)4,4,1
000024          4 ETINT=ETININ
000026            IF(IDEN)5,6,5
000027          5 TINTV=ETINO/(ZETA(NZEMAX))
000033            GO TO 7
000033          6 TINTV=(1./(80.*TEMPEN))
                 1*((-ALOG(ETININ/3000.))**.5)
000047          7 WRITE(9,8)NTYPE,FACSIG,ETINT,TINTV
000063          8 FORMAT(7H0NTYPE=,I4,8H FACSIG=,E15.8,
                 17H ETINT=,E15.8,7H TINTV=,E15.8)
000063            RETURN
000064            END
```

```
$*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
*IBFTC TOR3    DECK
                SUBROUTINE TORCO
000002          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
                1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
                2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
                4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
                5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),RHOFRE(201),
                1NTYPE,TEMPEN,ENDIFF,RECOIL,RFSGAM,REGA12,
                2INDFT,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
                3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
                4NFT,NSOF,FISOIF,FISOER,F1ALMU,FIREMU,
                5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
                6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
                7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
                8FIALPH,FIBET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
                1RECMAX,HRFC,AFARFC,EPSMAX,HEPS,AFAEPS,
                2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
                3SKF(50,50),SIGFF(50,50),DEBARA(50,50),
                4ALPHEG(50),BETEG(50),AFIELD(12),
                5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002          IND=0
000003          CALL FORIN
000004          SIGMA=SFINAL
000006          ACSCMP=SFINAL*(EXP(-OMEGA/TEMPEN)-1.)
                1/(EXP(-OMEGA/TEMPEN)+1.)
000015          IF(ERR-.02)3,3,1
000020        1 WRITE(9,2)RECOIL,OMEGA,IND,SFINAL,ERR,J1,J2,ARGPAC
000044        2 FORMAT(5H0REC=,E12.5,5H EPS=,E12.5,
                15H IND=,I3,8H SFINAL=,E14.7,5H ERR=,F14.7,
                24H J1=,I3,4H J2=,I3,8H ARGPAC=,F14.7)
000044        3 IND=1
000045          CALL FORIN
000046          SIGMA=SIGMA+SFINAL
000050          BSICMP=SFINAL
000051          IF(ERR-.02)5,5,4
000053        4 WRITE(9,2)RECOIL,OMEGA,IND,SFINAL,ERR,J1,J2,ARGPAC
000077        5 SIGMA=FACSIG*SIGMA
000101          SIGMAC=BSICMP/ACSCMP
000103          RETURN.
000103          END
```

```
$*    ****COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC PRO    . DECK
             SUBROUTINE PHFRNO
000002       COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
             1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
             2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
             3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
             4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
             5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002       COMMON T2(73,5),S(74,6)
000002       COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002       COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
             1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
             2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODD,
             3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
             4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
             5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
             6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
             7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
             8FIALPH,FIBET,FIGAM
000002       COMMON AFACTO,TE2
000002       COMMON FACSIG,SIGMA,SIGMAC,ETINO,
             1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
             2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
             3SKF(50,50),SIGEF(50,50),DEBARA(50,50),
             4ALPHEG(50),BETEG(50),AFIELD(12),
             5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002       IF(ZETA(1))1,3,1
000003     1 WRITE(9,2)
000007     2 FORMAT(39H0 PHONON SPECTRUM INCORRECTLY SPECIFIED)
000007       STOP
000011     3 IF(PHOFRE(1))1,4,1
000012     4 DO 6 N=2,NZEMAX
000014       ZETDIF=ZETA(N)-ZETA(N-1)
000017       IF(ZETDIF)1,1,5
000021     5 IF(PHOFRE(N))1,6,6
000024     6 NABC=1
000030     7 PHNOIN=ZETA(2)*PHOFRE(2)/3.
000033       ZEDF1=ZETA(2)-ZETA(1)
000035       ZEDF2=ZETA(3)-ZETA(2)
000037       ZEDF3=ZETA(3)-ZETA(1)
000040       ZEDF4=2.*ZETA(3)+ZETA(2)-3.*ZETA(1)
000045       PHDF1=PHOFRE(2)-PHOFRE(1)
000047       PHDF2=PHOFRE(3)-PHOFRE(2)
000051       PHNOIN=PHNOIN+ZEDF2*(PHOFRE(2)
             1+(ZEDF4*PHDF2)/(6.*ZEDF3)
             2+((ZEDF2**2)*PHDF1)/(6.*ZEDF1*ZEDF3))
000067       NZMLS1=NZEMAX-1
000071       DO 8 N=3,NZMLS1
000072       ZEDF1=ZEDF2
000074       ZEDF2=ZETA(N+1)-ZETA(N)
000076       ZEDF3=ZETA(N+1)-ZETA(N-1)
000101       ZEDF4=2.*ZETA(N+1)+ZETA(N)-3.*ZETA(N-1)
000107       PHDF1=PHDF2
000110       PHDF2=PHOFRE(N+1)-PHOFRE(N)
000113     8 PHNOIN=PHNOIN+ZEDF2*(PHOFRE(N)
             1+(ZEDF4*PHDF2)/(6.*ZEDF3)
             2+((ZEDF2**2)*PHDF1)/(6.*ZEDF1*ZEDF3))
000135       DO 9 N=1,NZEMAX
000137     9 PHOFRE(N)=PHOFRE(N)/PHNOIN
000144       WRITE(9,501)PHNOIN                                              OMIT
000151       WRITE(9,502)(PHOFRE(N),N=1,NZEMAX)                              OMIT
000164   501 FORMAT(8H0PHNOIN=,E15,8)                                        OMIT
000164   502 FORMAT(4E20,8)                                                  OMIT
000164       RETURN
000165       END
```

```
$*    ****COMMENT CARD TO BREAK UP BATCH COMPILE
      $IBFTC TOSC    DECK
                SUBROUTINE TOSCRI
000002          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
               1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
               2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
               3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
               4COFC5,COFC6,COFC7,COFC8,CDFCN8,COFCN7,COFCN6,
               5COFCN5,COFCN4,COFCN3,CDFCN2,COFCN1,COFCN0
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
               1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
               2INDF1,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
               3F1STAR,FIFIN,FISOFM,FIINTF,FIERR,
               4NFT,NSOF,FISOIF,FISOER,F1ALMU,FIREMD,
               5NCOUNT,FIHT,FIINTE(9),F1COMP,FICOLD,
               6NSOCNT,FISOIT(9),FSOCOM,FSOCLU,
               7FEVSO,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
               8FIALPH,FIHET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
               1RECMAX,HREC,AFAREC,EPSMAX,HEPS,AFAEPS,
               2NLIM,MLIM,REC(50),FPS(50),SELD(50),SIGELD(50),
               3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
               4ALPHFG(50),BETEG(50),AFIELD(12),
               5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002          WRITE(11,1)(AFIELD(J),J=1,12)
000014        1 FORMAT(12A6)
000014          WRITE(11,901)IDEN,TEMPEN,GAM0
000026      901 FORMAT(I10,2E20.8)
000026          WRITE(11,2)AFAREC,HREC,AFAEPS,HEPS
000042        2 FORMAT(4E20.8)
000042          WRITE(11,3)NLIM
000050        3 FORMAT(I10)
000050          WRITE(11,4)(REC(N),N=1,NLIM)
000063        4 FORMAT(4E19.8)
000063          WRITE(11,5)MLIM
000071        5 FORMAT(I9)
000071          WRITE(11,6)(EPS(M),M=1,MLIM)
000104        6 FORMAT(4F18.8)
000104          NPROD=NLIM*MLIM
000107          WRITE(11,7)NPROD
000114        7 FORMAT(I8)
000114          DO 8 N=1,NLIM
000116        8 WRITE(11,9)(SKE(N,M),M=1,MLIM)
000135        9 FORMAT(5E15.8)
000135       10 WRITE(9,110)
000141      110 FORMAT(55H1                                                    1)
000141          WRITE(9,1)(AFIELD(J),J=1,12)
000153          WRITE(9,11)IDEN,INMX0
000163       11 FORMAT(6HOIDEN=,I4,7H INMX0=,I4)
000163          IF(IDEN)12,18,14
000165       12 WRITE(9,13)ZETA(NZEMAX)
000174       13 FORMAT(14HOZETA(NZEMAX)=,E15.8)
000174          GO TO 18
000175       14 WRITE(9,15)NZEMAX
000203       15 FORMAT(8HONZEMAX=,I4)
000203          WRITE(9,16)
000207       16 FORMAT(35HONZETA          ZETA              PHOFRE)
000207          WRITE(9,17)(NZETA,ZETA(NZETA),PHOFRE(NZETA),
               1NZETA=1,NZEMAX)
000227       17 FORMAT(I5,E17.8,E17.8)
000227       18 WRITE(9,19)TEMPEN
000235       19 FORMAT(8HOTEMPEN=,E15.8)
000235          WRITE(9,20)RECMAX,HREC,AFAREC
000247       20 FORMAT(8HORECMAX=,E15.8,6H HREC=,E15.8,8H AFAREC=,
               1E15.8)
```

```
000247          WRITE(9,21)EPSMAX,HEPS,AFAEPS
000261       21 FORMAT(8HOEPSMAX=,E15,8,6H HEPS=,E15,8,8H AFAEPS=,
                1E15,8)
000261          WRITE(9,22)NLIM
000267       22 FORMAT(6HONLIM=,I4)
000267          WRITE(9,23)MLIM
000275       23 FORMAT(6HOMLIM=,I4)
000275          WRITE(9,24)
000301       24 FORMAT(50H0    N          REC           SELD            SIGELD)
000301          WRITE(9,25)(N,REC(N),SELD(N),SIGELD(N),N=1,NLIM)
000324       25 FORMAT(I4,3E17,8)
000324          WRITE(9,26)
000330       26 FORMAT(115H0    N    M       REC           EPS            SKE
                1       ALPHEG         BETEG          SIGEF          DEBARA)
000330          DO 27 N=1,NLIM
000332       27 WRITE(9,28)(N,M,REC(N),EPS(M),SKF(N,M),
                1ALPHEG(N),BETEG(M),SIGEF(N,M),DEBARA(N,M),
                2M=1,MLIM)
000402       28 FORMAT(2I4,7E16.8)
000402          WRITE(9,29)
000405       29 FORMAT(54H1 N    M         TIME          GAMEVE          GAMODD)
000405          DO 30 N=1,INMPL4
000407       30 WRITE(9,31)(N,M,TIMVAR(N,M),GAEVFC(N,M),
                1GAODFC(N,M),M=1,28)
000443       31 FORMAT(2I4,3E17,8)
000443          RETURN
000443          END


$*    ****COMMENT CARD TO BREAK UP BATCH COMPILE
     $IBFTC FORA    DECK
              SUBROUTINE FORIN
000002        COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
              1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
              2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
              3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
              4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
              5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002        COMMON T2(73,51),S(74,6)
000002        COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002        COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
              1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
              2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODD,
              3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
              4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
              5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
              6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
              7FEVSO,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
              8FIALPH,FIBET,FIGAM
000002        COMMON AFACTO,TE2
000002        COMMON FACSIG,SIGMA,SIGMAC,ETINO,
              1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
              2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
              3SKF(50,50),SIGEF(50,50),DEBARA(50,50),
              4ALPHEG(50),BETEG(50),AFIELU(12),
              5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
            C NUMERICAL CALCULATION OF FOURIER INTEGRAL,
            C INPUT VARIABLES IND, ETINT, TINTV, OMEGA,
            C FUNCTIONAL VALUE FCN SPECIFIED BY SUBROUTINE FCNCAL,
            C CALCULATED INTEGRAL SFINAL, ESTIMATED UNCERTAINTY ERR,
000002        CALL PAR
000003        CALL CONTRO
000004        RETURN
000005        END
```

```
$*     ****COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC FORM      DECK
            SUBROUTINE PAR
000002      COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
           1SFINAL,EPR,TIME,FIRST,FINAL,FCN,FSFCN,
           2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
           3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
           4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
           5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002      COMMON T2(73,5),S(74,6)
000002      COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002      COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PROFRE(201),
           1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
           2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
           3FISTAR,FIFIN,FISOFN,FIINIF,FIEHR,
           4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
           5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
           6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
           7FEVSO,FODSO,FSOEV,FSOOD,FIARG,FIFCN,
           8FIALPH,FIBET,FIGAM
000002      COMMON AFACTO,TE2
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
           1RECMAX,RREC,AFARFC,EPSMAX,REPS,AFAEPS,
           2NLIM,MLIM,REC(50),EPS(50),SELO(50),SIGELO(50),
           3SKF(50,50),SIGEF(50,50),OEBARA(50,50),
           4ALPHEG(50),BETFG(50),AFIELD(12),
           5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002      OMEGAA=ABS(OMEGA)
000004      HT0=TINTV/3,
000006      ARG=.5*HT0*OMEGAA
000011      IF(ARG-.44335956E-05)101,101,102
000013  101 GO TO 30
000014  102 IF(ARG-.13300787E-04)103,103,104
000017  103 HT0=.17734382E-04/OMEGAA
000021      GO TO 30
000022  104 IF(ARG-.39902361E-04)105,105,106
000025  105 HT0=.53203147E-04/OMEGAA
000027      GO TO 30
000030  106 IF(ARG-.11970708E-03)107,107,108
000033  107 HT0=.15960944E-03/OMEGAA
000035      GO TO 30
000036  108 IF(ARG-.35912124E-03)109,109,110
000041  109 HT0=.47882833E-03/OMEGAA
000043      GO TO 30
000044  110 IF(ARG-.10773637E-02)1,1,2
000047    1 HT0=.14364850E-02/OMEGAA
000051      GO TO 30
000052    2 IF(ARG-.32320912E-02)3,3,4
000055    3 HT0=.430945493E-02/OMEGAA
000057      GO TO 30
000060    4 IF(ARG-.96962736E-02)5,5,6
000063    5 HT0=.129283648E-01/OMEGAA
000065      GO TO 30
000066    6 IF(ARG-.29088821E-01)7,7,8
000071    7 HT0=.387850945E-01/OMEGAA
000073      GO TO 30
000074    8 IF(ARG-.87266463E-01)9,9,10
000077    9 HT0=.116355283/OMEGAA
000101      GO TO 30
000102   10 IF(ARG-.26179939)11,11,12
000105   11 HT0=.349065850/OMEGAA
000107      GO TO 30
000110   12 IF(ARG-.78539816)13,13,14
000113   13 HT0=1.04719755/OMEGAA
000115      GO TO 30
000116   14 IF(ARG-2.3561945)15,15,16
000121   15 HT0=3.14159265/OMEGAA
000123      GO TO 30
000124   16 IF(ARG-7.0685835)17,17,18
000127   17 HT0=9.42477796/OMEGAA
000131      GO TO 30
```

18

```
000132      18 IF(ARG-21.205751)19,19,20
000135      19 HT0=28.2743339/OMEGAA
000137         GO TO 30
000140      20 IF(ARG-63.617252)21,21,22
000143      21 HT0=84.8230016/OMEGAA
000145         GO TO 30
000146      22 IF(ARG-190.85175)23,23,24
000151      23 HT0=254.469005/OMEGAA
000153         GO TO 30
000154      24 ARG1=ARG/381.703507
000156         ARG2=AINT(ARG1)
000160         ARG3=.5*ARG2
000161         ARG4=ARG3+.51
000163         ARG5=AINT(ARG3)
000165         ARG6=AINT(ARG4)
000167         IF(ARG6-ARG5)25,25,26
000171      25 ODINT=ARG2+1.
000173         GO TO 27
000174      26 ODINT=ARG2
000176      27 HT0=ODINT*763.407015/OMEGAA
000201      30 TINT0=3.*HT0
000203         RETURN
000204         END


           $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
           $IBFTC FORC     DECK
               SUBROUTINE CONTRO
000002         COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
              1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
              2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
              3COP1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
              4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
              5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002         COMMON T2(73,5),S(74,6)
000002         COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002         COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
              1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
              2INDF1,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
              3FISTAR,FIFIN,FISOFN,FIINIF,FIERR,
              4NFI,NSOF,FISOIF,FISOER,F1ALMU,FIREMU,
              5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
              6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
              7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
              8FIALPH,FIBET,FIGAM
000002         COMMON AFACTO,TE2
000002         COMMON FACSIG,SIGMA,SIGMAC,ETINO,
              1RECMAX,HREC,AFAREC,EPSMAX,HEPS,AFAEPS,
              2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
              3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
              4ALPHEG(50),BETEG(50),AFIELD(12),
              5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002         ARGP=.0
000003         IF(IND)1,37,1
000004       1 IF(OMEGA)3,2,3
000005       2 SFINAL=.0
000006         ERR=.0
000007         RETURN
000007       3 FIPST=.0
000010         TIME=FIRST
000011         CALL FCNCAL
000012         FSFCN=FCN
000014         ARGPAC=.0
000015         J1=0
000016         FINLIM=1.57079633/OMEGAA
000020         IF(FINLIM-TINTV)4,4,5
000022       4 FINAL=FINLIM
000024         TIME=FINAL
```

```
000025          CALL FCNCAL
000026          FNFCN=FCN
000030          IPREIN=0
000031          GO TO 6
000031        5 FINAL=TINTV
000033          TIME=FINAL
000034          CALL FCNCAL
000035          FNFCN=FCN
000037          IPREIN=1
000040        6 J2=1
000041          DO 7 K2=1,5
000043        7 T2(J2,K2)=.0
000051        8 HT=FINAL-FIRST
000053        9 TEMP3=.0
000054          ARGCOR=3.*OMEGAA*HT
000057          CALL FACFIN
000060          T2(J2+1,1)=T2(J2,1)+TFIN
000064          HT=HT/3.
000065          ARGCOR=3.*OMEGAA*HT
000067          CALL FACFIN
000070          CALL ENDSUM(1,2)
000072          CALL CORR1
000073          T2(J2+1,2)=T2(J2,2)+TFIN+TFAC*TEMP3+CORR1
000101       11 HT=HT/3.
000103          ARGCOR=3.*OMEGAA*HT
000105          CALL FACFIN
000106          CALL ENDSUM(1,8)
000110          CALL NEXSUM(2,4,5,7)
000113          CALL CORR1
000114          CALL CORR2
000115          T2(J2+1,3)=T2(J2,3)+TFIN+TFAC*TEMP3+CORR1+COR2
000124          AMAG=ABS(T2(J2+1,1))+ABS(T2(J2+1,2))+ABS(T2(J2+1,3))
000132          IF(AMAG)19,19,10
000134       10 IF(J2-3)310,318,318
000137      318 IF(J2-4)319,319,310
000142      319 IF(ARGP-26.)311,13,13
000145      310 IF(ARGP-80.)311,13,13
000150      311 COMP=ABS(1.-T2(J2+1,3)/T2(J2+1,2))
000155          IF(COMP-ETINT)12,12,13
000157       12 COMP=ABS(1.-T2(J2+1,3)/T2(J2+1,1))
000164          IF(COMP-ETINT)19,19,13
000166       13 HT=HT/3.
000170          ARGCOR=3.*OMEGAA*HT
000172          CALL FACFIN
000173          CALL ENDSUM(1,26)
000175          CALL NEXSUM(2,4,23,25)
000200          CALL FOLSUM(5,7,8,19,20,22)
000204          CALL SMSUM(10,16,3)
000207          CALL SMSUM(11,17,3)
000212          CALL CORR1
000213          CALL CORR2
000214          T2(J2+1,4)=T2(J2,4)+TFIN+TFAC*TEMP3+CORR1+COR2
000223          IF(ARGP-242.)313,15,15
000225      313 COMP=ABS(1.-T2(J2+1,4)/T2(J2+1,3))
000232          IF(COMP-ETINT)14,14,15
000234       14 COMP=ABS(1.-T2(J2+1,4)/T2(J2+1,2))
000241          IF(COMP-ETINT)21,21,15
000243       15 HT=HT/3.
000245          ARGCOR=3.*OMEGAA*HT
000247          CALL FACFIN
000250          CALL ENDSUM(1,80)
000252          CALL NEXSUM(2,4,77,79)
000255          CALL FOLSUM(5,7,8,73,74,76)
000261          CALL SMSUM(10,70,3)
000264          CALL SMSUM(11,71,3)
000267          CALL CORR1
000270          CALL CORR2
000271          T2(J2+1,5)=T2(J2,5)+TFIN+TFAC*TEMP3+CORR1+COR2
000300          DO 16 K2=1,5
000301       16 T2(J2+1,K2)=T2(J2+1,5)
000310          GO TO 23
```

```
000311      19 ABC=1,
000313         DO 20 K2=1,5
000314      20 T2(J2+1,K2)=T2(J2+1,3)
000323         GO TO 23
000324      21 ABC=1,
000326         DO 22 K2=1,5
000327      22 T2(J2+1,K2)=T2(J2+1,4)
000336      23 COMP=ABS(1,-T2(J2,5)/T2(J2+1,5))
000343         ARGP=(FINAL-FIRST)/HT

000346         ARGPAC=ARGPAC+ARGP                            OMIT
000347      24 IF(IPREIN)25,25,27
000351      25 FIRST=FINLIM
000353         FINAL=FINLIM+TINTO
000355         FSFCN=FNFCN
000356         TIME=FINAL
000360         CALL FCNCAL
000361         FNFCN=FCN
000363         J1=1
000364         DO 26 K1=1,6
000365      26 S(J1,K1)=T2(J2+1,5)
000374         GO TO 39
000375      27 IF(COMP-ETINT)271,271,28
000400     271 IF(J2-2)30,272,272
000403     272 COMP=ABS(1,-T2(J2-1,5)/T2(J2+1,5))
000410         IF(COMP-FTINT)29,29,28
000412      28 IF(J2-INMX0)30,29,29
000415      29 SFINAL=T2(J2+1,5)
000417         ERR=COMP
000421         RETURN
000421      30 EINTJ2=FLOAT(J2)
000423         ARGP1=,5*EINTJ2
000424         ARGP2=ARGP1+,51
000426         ARGP3=AINT(ARGP1)
000430         ARGP4=AINT(ARGP2)
000432         IF(ARGP4-ARGP3)301,301,31
000434     301 IF(J2-NINIT)32,32,31
000437      31 ADDEND=FINAL-FIRST
000441         GO TO 33
000442      32 ADDEND=3,*(FINAL-FIRST)
000445      33 GFINAL=FINAL+ADDEND
000447         IF(FINLIM-GFINAL)34,34,35
000452      34 FIRST=FINAL
000454         FSFCN=FNFCN
000455         FINAL=FINLIM
000456         TIME=FINAL
000457         CALL FCNCAL
000460         FNFCN=FCN
000462         IPREIN=0
000463         GO TO 36
000463      35 FIRST=FINAL
000465         FSFCN=FNFCN
000466         FINAL=GFINAL
000467         TIME=FINAL
000470         CALL FCNCAL
000471         FNFCN=FCN
000473         IPREIN=1
000474      36 J2=J2+1
000476         GO TO 8
000476      37 FIRST=,0
000477         TIME=FIRST
000500         CALL FCNCAL
000501         FSFCN=FCN
000503         ARGPAC=,0
000504         J2=0
000505         FINAL=TINTO
000506         TIME=FINAL
000507         CALL FCNCAL
000510         FNFCN=FCN
000512         J1=1
000513         DO 38 K1=1,6
000514      38 S(J1,K1)=,0
```

```
000522      39  INDJ1=0
000523          INDJ1P=0
000524      40  HT=TINTO
000526      41  ARGCOR=OMEGAA*HT
000530      42  IF(INDJ1)43,43,54
000532      43  IF(ARGCOR-3.14159)54,44,44
000535      44  IF(IND)47,45,47
000536      45  ARG1=OMEGAA*FIRST/3.14159265
000541          OMINT1=AINT(ARG1)
000543          IF(ABS(ARG1-OMINT1)-1.E-6)53,53,145
000547     145  IF(ABS(ARG1-OMINT1-1.)-1.E-6)53,53,46
000555      46  FINAL=3.14159265*(OMINT1+1.)/OMEGAA
000561          TIME=FINAL
000562          CALL FCNCAL
000563          FNFCN=FCN
000565          HT=FINAL-FIRST
000567          ARGCOR=OMEGAA*HT
000570          GO TO 52
000571      47  ARG1=OMEGAA*FIRST/1.57079633
000574          OMINT1=AINT(ARG1)
000576          ARG2=.5*OMINT1
000577          ARG3=ARG2+.51
000601          ARG4=AINT(ARG2)
000603          ARG5=AINT(ARG3)
000605          IF(ARG5-ARG4)50,50,48
000607      48  IF(ABS(ARG1-OMINT1)-1.E-6)53,53,49
000614      49  FINAL=1.57079633*(OMINT1+2.)/OMEGAA
000620          TIME=FINAL
000621          CALL FCNCAL
000622          FNFCN=FCN
000624          HT=FINAL-FIRST
000626          ARGCOR=OMEGAA*HT
000627          GO TO 52
000630      50  IF(ABS(ARG1-OMINT1-1.)-1.E-6)53,53,51
000636      51  FINAL=1.57079633*(OMINT1+1.)/OMEGAA
000642          TIME=FINAL
000643          CALL FCNCAL
000644          FNFCN=FCN
000646          HT=FINAL-FIRST
000650          ARGCOR=OMEGAA*HT
000651      52  INDJ1P=1
000652      53  INDJ1=1
000653      54  TEMP3=.0
000654          CALL FACFIN
000655          S(J1+1,1)=S(J1,1)+TFIN
000661          HT=HT/3.
000662          ARGCOR=OMEGAA*HT
000664          CALL FACFIN
000665          CALL ENDSUM(1,2)
000667          CALL CORR1
000670          S(J1+1,2)=S(J1,2)+TFIN+TFAC*TEMP3+COR1
000676      56  HT=HT/3.
000700          ARGCOR=OMEGAA*HT
000701          CALL FACFIN
000702          CALL ENDSUM(1,8)
000704          CALL NEXSUM(2,4,5,7)
000707          CALL CORR1
000710          CALL CORR2
000711          S(J1+1,3)=S(J1,3)+TFIN+TFAC*TEMP3+COR1+COR2
000720          AMAG=ABS(S(J1+1,1))+ABS(S(J1+1,2))+ABS(S(J1+1,3))
000726          IF(AMAG)67,67,55
000730      55  IF(J1-3)155,163,163
000733     163  IF(J1-4)164,164,155
000736     164  IF(ARGP-26.)156,58,58
000741     155  IF(ARGP-80.)156,58,58
000744     156  COMP=ABS(1.-S(J1+1,3)/S(J1+1,2))
000751          IF(COMP-ETINT)57,57,58
000753      57  COMP=ABS(1.-S(J1+1,3)/S(J1+1,1))
000760          IF(COMP-ETINT)67,67,58
000762      58  HT=HT/3.
000764          ARGCOR=OMEGAA*HT
```

```
000765          CALL FACFIN
000766          CALL ENDSUM(1,26)
000770          CALL NEXSUM(2,4,23,25)
000773          CALL FOLSUM(5,7,8,19,20,22)
000777          CALL SMSUM(10,16,3)
001002          CALL SMSUM(11,17,3)
001005          CALL CORR1
001006          CALL CORR2
001007          S(J1+1,4)=S(J1,4)+TFIN+TFAC*TEMP3+COR1+COR2
001016          IF(ARGP-242,)158,60,60
001020      158 COMP=ABS(1.-S(J1+1,4)/S(J1+1,3))
001025          IF(COMP-ETINT)59,59,60
001027       59 COMP=ABS(1.-S(J1+1,4)/S(J1+1,2))
001034          IF(COMP-ETINT)69,69,60
001036       60 HT=HT/3.
001040          ARGCOR=OMEGAA*HT
001041          CALL FACFIN
001042          CALL ENDSUM(1,80)
001044          CALL NEXSUM(2,4,77,79)
001047          CALL FOLSUM(5,7,8,73,74,76)
001053          CALL SMSUM(10,70,3)
001056          CALL SMSUM(11,71,3)
001061          CALL CORR1
001062          CALL CORR2
001063          S(J1+1,5)=S(J1,5)+TFIN+TFAC*TEMP3+COR1+COR2
001072          COMP=ABS(1.-S(J1+1,5)/S(J1+1,4))
001076          IF(COMP-ETINT)61,61,62
001100       61 COMP=ABS(1.-S(J1+1,5)/S(J1+1,3))
001105          IF(COMP-ETINT)71,71,62
001107       62 IF(ABS(ARGCOR-1.04719755)-1.E-6)63,63,71
001114       63 HT=HT/3.
001116          ARGCOR=OMEGAA*HT
001117          CALL FACFIN
001120          CALL ENDSUM(1,242)
001122          CALL NEXSUM(2,4,239,241)
001125          CALL FOLSUM(5,7,8,235,236,238)
001131          CALL SMSUM(10,232,3)
001134          CALL SMSUM(11,233,3)
001137          CALL CORR1
001140          CALL CORR2
001141          S(J1+1,6)=S(J1,6)+TFIN+TFAC*TEMP3+COR1+COR2
001150          DO 64 K1=1,6
001151       64 S(J1+1,K1)=S(J1+1,6)
001160          GO TO 73
001161       67 ABC=1.
001163          DO 68 K1=1,6
001164       68 S(J1+1,K1)=S(J1+1,3)
001173          GO TO 73
001174       69 ABC=1.
001176          DO 70 K1=1,6
001177       70 S(J1+1,K1)=S(J1+1,4)
001206          GO TO 73
001207       71 ABC=1.
001211          DO 72 K1=1,6
001212       72 S(J1+1,K1)=S(J1+1,5)
001221       73 COMP=ABS(1.-S(J1,5)/S(J1+1,5))
001226          ARGP=(FINAL-FIRST)/HT
001231          ARGPAC=ARGPAC+ARGP                              UMIT
001232       76 J1POLD=J1P
001234          J1P=J1-INDJ1P
001235          IF(J1P-J1POLD)180,180,176
001237      176 IF(J1P-4)78,77,77
001242       77 IF(COMP-ETINT)185,185,180
001245      185 COMP=ABS(1.-S(J1-1,5)/S(J1+1,5))
001252          IF(COMP-ETINT)85,85,180
001255       78 IF(IND)178,180,178
001256      178 IF(J1P-3)180,179,179
001261      179 IF(COMP-ETINT)185,185,180
001264      180 EINJ1P=FLOAT(J1P)
001266          ARGP1=.5*EINJ1P
001267          ARGP2=ARGP1+.51
```

```
001271          ARGP3=AINT(ARGP1)
001273          ARGP4=AINT(ARGP2)
001275          IF(ARGP4-ARGP3)79,79,86
001277       79 IF(J1P-NINIT)80,80,86
001302       80 IF(J1P-INMX0)81,84,84
001305       81 FIRST=FINAL
001307          FSFCN=FNFCN
001310          IF(J1P-J1POLD)182,182,181
001313      181 TINTO=3.*TINTO
001315      182 FINAL=FINAL+TINTO
001317          TIME=FINAL
001320          CALL FCNCAL
001321          FNFCN=FCN
001323          IF(OMEGAA*FINAL-5.E+07)82,85,85
001326       82 J1=J1+1
001330          GO TO 40
001330       84 COMP=ABS(1.-S(J1-1,5)/S(J1+1,5))
001335       85 SFINAL=S(J1+1,5)
001337          ERR=COMP
001341          RETURN
001341       86 IF(J1P-INMX0)87,84,84
001344       87 FIRST=FINAL
001346          FSFCN=FNFCN
001347          FINAL=FINAL+TINTO
001351          TIME=FINAL
001352          CALL FCNCAL
001353          FNFCN=FCN
001355          IF(OMEGAA*FINAL-5.E+07)82,85,85
001361          END



        $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
        $IBFTC FORD    DECK
               SUBROUTINE ENDSUM(K1,KN1)
000004         COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
              1SFTNAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
              2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
              3CUR1,COP2,CUFC0,COFC1,COFC2,CUFC3,COFC4,
              4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
              5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000004         COMMON T2(73,5),S(74,6)
000004         COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000004         COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
              1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
              2INDFI,ETININ,FITINT,GAMO,GAMFVE,GAMODU,
              3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
              4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
              5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
              6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
              7FEVSU,FOOSU,FSOEV,FSOOD,FIARG,FIFCN,
              8FIALPH,FIBET,FIGAM
000004         COMMON AFACTO,TE2
000004         COMMON FACSIG,SIGMA,SIGMAC,ETIMO,
              1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
              2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
              3SKF(50,50),SIGEF(50,50),UEBARA(50,50),
              4ALPHEG(50),BETEG(50),AFIELD(12),
              5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000004         CUFC3=COFC1
000005         COFC6=COFC2
000007         COFCN3=COFCN1
000010         COFCN6=COFCN2
000012         IF(IND)2,1,2
000013       1 FN=FLOAT(K1)
000015         TIME=FIRST+EN*HT
000020         CALL FCNCAL
000024         COFC1=FCN*COS(OMEGA*TIME)
```

24

```
000032          COFCN2=COFC1
000033          TEMP3=TEMP3+COFC1
000035          EN=FLOAT(KN1)
000036          TIME=FIRST+EN*HT
000041          CALL FCNCAL
000045          COFCN1=FCN*COS(OMEGA*TIME)
000053          COFC2=COFCN1
000054          TEMP3=TEMP3+COFCN1
000056          RETURN
000056        2 EN=FLOAT(K1)
000060          TIME=FIRST+EN*HT
000063          CALL FCNCAL
000067          COFC1=FCN*SIN(OMEGA*TIME)
000075          COFCN2=COFC1
000076          TEMP3=TEMP3+COFC1
000100          EN=FLOAT(KN1)
000101          TIME=FIRST+EN*HT
000104          CALL FCNCAL
000110          COFCN1=FCN*SIN(OMEGA*TIME)
000116          COFC2=COFCN1
000117          TEMP3=TEMP3+COFCN1
000121          RETURN
000121          END


          $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
          $IBFTC FORE     DECK
                SUBROUTINE NEXSUM(K2,K4,KN4,KN2)
000006          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
               1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
               2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
               3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
               4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
               5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000006          COMMON T2(73,5),S(74,6)
000006          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000006          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
               1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
               2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
               3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
               4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
               5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
               6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
               7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
               8FIALPH,FIBET,FIGAM
000006          COMMON AFACTO,TE2
000006          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
               1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
               2NLIM,MLIM,REC(50),EPS(50),SELO(50),SIGELO(50),
               3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
               4ALPHEG(50),BETEG(50),AFIELD(12),
               5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
000006          IF(IND)2,1,2
000007        1 EN=FLOAT(K2)
000011          TIME=FIRST+EN*HT
000014          CALL FCNCAL
000022          COFC2=FCN*COS(OMEGA*TIME)
000033          COFCN7=COFC2
000034          TEMP3=TEMP3+COFC2
000035          EN=FLOAT(K4)
000036          TIME=FIRST+EN*HT
000041          CALL FCNCAL
000047          COFC4=FCN*COS(OMEGA*TIME)
000060          COFCN5=COFC4
000061          TEMP3=TEMP3+COFC4
000062          EN=FLOAT(KN4)
000063          TIME=FIRST+EN*HT
000066          CALL FCNCAL
```

```
000074          COFCN4=FCN*COS(OMEGA*TIME)
000105          COFC5=COFCN4
000106          TEMP3=TEMP3+COFCN4
000107          EN=FLOAT(KN2)
000110          TIME=FIRST+EN*HT
000113          CALL FCNCAL
000121          COFCN2=FCN*COS(OMEGA*TIME)
000132          COFC7=COFCN2
000133          TEMP3=TEMP3+COFCN2
000134          GO TO 3
000135        2 EN=FLOAT(K2)
000137          TIME=FIRST+EN*HT
000142          CALL FCNCAL
000150          COFC2=FCN*SIN(OMEGA*TIME)
000161          COFCN7=COFC2
000162          TEMP3=TEMP3+COFC2
000163          EN=FLOAT(K4)
000164          TIME=FIRST+EN*HT

000167          CALL FCNCAL
000175          COFC4=FCN*SIN(OMEGA*TIME)
000206          COFCN5=COFC4
000207          TEMP3=TEMP3+COFC4
000210          EN=FLOAT(KN4)
000211          TIME=FIRST+EN*HT
000214          CALL FCNCAL
000222          COFCN4=FCN*SIN(OMEGA*TIME)
000233          COFC5=COFCN4
000234          TEMP3=TEMP3+COFCN4
000235          EN=FLOAT(KN2)
000236          TIME=FIRST+EN*HT
000241          CALL FCNCAL
000247          COFCN2=FCN*SIN(OMEGA*TIME)
000260          COFC7=COFCN2
000261          TEMP3=TEMP3+COFCN2
000262        3 COFC8=COFCN1
000264          COFCN8=COFC1
000265          RETURN
000266          END
```

```
$*    ****COMMENT CARD TO BREAK UP BATCH COMPILE
      $IBFTC FORF    DECK
               SUBROUTINE FOLSUM(K5,K7,K8,KN8,KN7,KN5)
000007         COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
              1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
              2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
              3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
              4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
              5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000007         COMMON T2(73,5),S(74,6)
000007         COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000007         COMMON NIDEN,NINIT,NZFMAX,ZETA(201),PHOFRE(201),
              1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
              2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
              3FISTAR,FIFIN,FISOFN,FIINIF,FIERR,
              4NFI,NSOF,FISOIF,FISOER,F1ALMU,FIREMU,
              5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
              6NSOCNT,FISOIT(9),FSOCOM,FSOCLU,
              7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
              8F1ALPH,FIBET,FIGAM
000007         COMMON AFACTO,TE2
000007         COMMON FACSIG,SIGMA,SIGMAC,ETINO,
              1RECMAX,HREC,AFAREC,EPSMAX,HEPS,AFAEPS,
              2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
```

```
              3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
              4ALPHEG(50),BETEG(50),AFIELD(12),
              5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
000007        IF(IND)2,1,2
000010      1 EN=FLOAT(K5)
000012        TIME=FIRST+EN*HT
000015        CALL FCNCAL
000025        COFC5=FCN*COS(OMEGA*TIME)
000037        TEMP3=TEMP3+COFC5
000040        EN=FLOAT(K7)
000042        TIME=FIRST+EN*HT
000045        CALL FCNCAL
000055        COFC7=FCN*COS(OMEGA*TIME)
000067        TEMP3=TEMP3+COFC7
000070        EN=FLOAT(K8)
000072        TIME=FIRST+EN*HT
000075        CALL FCNCAL
000105        COFC8=FCN*COS(OMEGA*TIME)
000117        TEMP3=TEMP3+COFC8
000120        EN=FLOAT(KN8)
000122        TIME=FIRST+EN*HT
000125        CALL FCNCAL
000135        COFCN8=FCN*COS(OMEGA*TIME)
000147        TEMP3=TEMP3+COFCN8
000150        EN=FLOAT(KN7)
000152        TIME=FIRST+EN*HT
000155        CALL FCNCAL
000165        COFCN7=FCN*COS(OMEGA*TIME)
000177        TEMP3=TEMP3+COFCN7
000200        EN=FLOAT(KN5)
000202        TIME=FIRST+EN*HT
000205        CALL FCNCAL
000215        COFCN5=FCN*COS(OMEGA*TIME)
000227        TEMP3=TEMP3+COFCN5
000230        RETURN
000231      2 EN=FLOAT(K5)
000233        TIME=FIRST+EN*HT
000236        CALL FCNCAL
000246        COFC5=FCN*SIN(OMEGA*TIME)
000260        TEMP3=TEMP3+COFC5
000261        EN=FLOAT(K7)
000263        TIME=FIRST+EN*HT
000266        CALL FCNCAL
000276        COFC7=FCN*SIN(OMEGA*TIME)
000310        TEMP3=TEMP3+COFC7
000311        EN=FLOAT(K8)
000313        TIME=FIRST+EN*HT
000316        CALL FCNCAL
000326        COFC8=FCN*SIN(OMEGA*TIME)
000340        TEMP3=TEMP3+COFC8
000341        EN=FLOAT(KN8)
000343        TIME=FIRST+EN*HT
000346        CALL FCNCAL
000356        COFCN8=FCN*SIN(OMEGA*TIME)
000370        TEMP3=TEMP3+COFCN8
000371        EN=FLOAT(KN7)
000373        TIME=FIRST+EN*HT
000376        CALL FCNCAL
000406        COFCN7=FCN*SIN(OMEGA*TIME)
000420        TEMP3=TEMP3+COFCN7
000421        EN=FLOAT(KN5)
000423        TIME=FIRST+EN*HT
000426        CALL FCNCAL
000436        COFCN5=FCN*SIN(OMEGA*TIME)
000450        TEMP3=TEMP3+COFCN5
000451        RETURN
000452        END
```

```
$*    ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC FORG     DECK
          SUBROUTINE SMSUM(K1,K2,K3)
000005    COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
         1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
         2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
         3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
         4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
         5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000005    COMMON T2(73,5),S(74,6)
000005    COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000005    COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
         1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
         2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
         3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
         4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
         5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
         6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
         7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
         8FIALPH,FIBET,FIGAM
000005    COMMON AFACTO,TE2
000005    COMMON FACSIG,SIGMA,SIGMAC,ETINO,
         1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
         2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
         3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
         4ALPHEG(50),BETEG(50),AFIELD(12),
         5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
000005    TF(INT)3,1,3
000006  1 DO 2 N=K1,K2,K3
000010    FN=FLOAT(N)
000011    TIME=FIRST+EN*HT
000014    CALL FCNCAL
000021  2 TEMP3=TEMP3+FCN*COS(OMEGA*TIME)
000034    RETURN
000034  3 DO 4 N=K1,K2,K3
000036    FN=FLOAT(N)
000037    TIME=FIRST+EN*HT
000042    CALL FCNCAL
000047  4 TEMP3=TEMP3+FCN*SIN(OMEGA*TIME)
000062    RETURN
000062    END
```

```
$*    ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC FORH     DECK
          SUBROUTINE FACFIN
000002    COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
         1SFINAL,FRR,TIME,FIRST,FINAL,FCN,FSFCN,
         2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
         3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
         4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
         5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002    COMMON T2(73,5),S(74,6)
000002    COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002    COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
         1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
         2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
         3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
         4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
         5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
         6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
         7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
         8FIALPH,FIBET,FIGAM
000002    COMMON AFACTO,TE2
000002    COMMON FACSIG,SIGMA,SIGMAC,ETINO,
         1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
         2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
```

```
                3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
                4ALPHEG(50),BETEG(50),AFIELD(12),
                5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
000002          IF(ARGCOR-1.05)4,1,1
000005        1 SIND1=SIN(.5*OMEGA*HT)
000012          TF1=(2.*SIND1)/(HT*(OMEGA**2))
000015          TFAC=2.*SIND1*TF1
000017          IF(IND)3,2,3
000020        2 TIME=FIRST
000022          TFIN=FSFCN*(-SIN(OMEGA*TIME)/OMEGA
               1+TF1*SIN(OMEGA*(TIME+.5*HT)))
000040          TIME=FINAL
000042          TFIN=TFIN+FNFCN*(SIN(OMEGA*TIME)/OMEGA
               1-TF1*SIN(OMEGA*(TIME-.5*HT)))
000061          RETURN
000062        3 TIME=FIRST
000064          TFIN=FSFCN*(COS(OMEGA*TIME)/OMEGA
               1-TF1*COS(OMEGA*(TIME+.5*HT)))
000102          TIME=FINAL
000103          TFIN=TFIN+FNFCN*(-COS(OMEGA*TIME)/OMEGA
               1+TF1*COS(OMEGA*(TIME-.5*HT)))
000122          RETURN
000123        4 TFAC=HT
000125          IF(IND)6,5,6
000126        5 TIME=FIRST
000130          COFCO=FSFCN*COS(OMEGA*TIME)
000135          TFIN=.5*HT*COFCO
000137          TIME=FINAL
000141          COFCNO=FNFCN*COS(OMEGA*TIME)
000146          TFIN=TFIN+.5*HT*COFCNO
000151          RETURN
000152        6 TIME=FIRST
000154          COFCO=FSFCN*SIN(OMEGA*TIME)
000161          TFIN=.5*HT*COFCO
000163          TIME=FINAL
000165          COFCNO=FNFCN*SIN(OMEGA*TIME)
000172          TFIN=TFIN+.5*HT*COFCNO
000175          RETURN
000176          END



        $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
        $IBFTC FORI     DECK
                SUBROUTINE CORR1
000002          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
               1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
               2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
               3COR1,COR2,COFCO,COFC1,COFC2,COFC3,COFC4,
               4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
               5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCNO
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
               1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
               2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODU,
               3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
               4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
               5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
               6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
               7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
               8FIALPH,FIBET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
               1RECMAX,HREC,AFAREC,EPSMAX,HEPS,AFAEPS,
               2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
               3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
               4ALPHEG(50),BETEG(50),AFIELD(12),
               5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
```

```
000002          IF (ARGCOR-1.05)2,1,1
000005        1 COR1=.0
000006          RETURN
000007        2 COR1=-.125*(COFC0+COFCN0)
               1+.166666667*(COFC1+COFCN1)
               2-.416666667E-01*(COFC2+COFCN2)
000022          COR1=HT*COR1
000023          RETURN
000024          END




       $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
       $IBFTC FORJ     DECK
                 SUBROUTINE CORR2
000002           COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
                1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
                2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
                4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
                5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002           COMMON T2(73,5),S(74,6)
000002           COMMON IDEN,ALPHA,BFIA,J1,J2,ARGPAC
000002           COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
                1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
                2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
                3F1STAR,FIFIN,FISOFN,FIINTF,FIERR,
                4NFI,NSOF,FISOIF,FISOER,F1ALMU,FIREMU,
                5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
                6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
                7FEVSU,FODSO,FSOEV,FSOOD,FIARG,FIFCN,
                8FIALPH,FIBET,FIGAM
000002           COMMON AFACTO,TE2
000002           COMMON FACSIG,SIGMA,SIGMAC,ETINO,
                1RECMAX,HREC,AFAREC,EPSMAX,HEPS,AFAEPS,
                2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
                3SKF(50,50),SIGFF(50,50),DEBARA(50,50),
                4ALPHEG(50),BETEG(50),AFIELD(12),
                5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GADDFC(72,28)
000002           IF (ARGCOR-1.05)2,1,1
000005        1  COR2=.0
000006           RETURN
000007        2  COR2=-.919932941E-01*(COFC0+COFCN0)
                1+.448476872*(COFC1+COFCN1)
                2-1.01071006*(COFC2+COFCN2)
                3+1.44171242*(COFC3+COFCN3)
                4-1.46326563*(COFC4+COFCN4)
                5+1.06868454*(COFC5+COFCN5)
                6-.532635224*(COFC6+COFCN6)
                7+.161585864*(COFC7+COFCN7)
                8-.22355485E-01*(COFC8+COFCN8)
000052           COR2=HT*COR2
000053           RETURN
000054           END




       $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
       $IBFTC FORW     DECK
                 SUBROUTINE FIGAFC
000002           COMMON IND,ETINT,TTNTV,OMEGA,OMEGAA,TINTO,
                1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
                2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
                4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
                5COFCN5,COFCN4,COFCN3,CDFCN2,COFCN1,COFCN0
```

```
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BFTA,J1,J2,ARGPAC
000002          COMMON NIDFN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
               1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
               2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODD,
               3FISTAP,FIFIN,FISOFN,FIINTF,FIERR,
               4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
               5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
               6NSOCNT,FISOIT(9),FSOCOM,FSOCLU,
               7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
               8FIALPH,FIBET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
               1RECMAX,HPEC,AFAREC,FPSMAX,HEPS,AFAEPS,
               2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
               3SKE(50,50),SIGEF(50,50),UEBARA(50,50),
               4ALPHEG(50),BETEG(50),AFIELD(12),
               5INMXO,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
000002          TIMVAR(1,1)=.0
000003          TIMVAR(2,1)=TINTV
000005          TIMVAR(3,1)=TIMVAR(2,1)+TINTV
000006          TIMVAR(4,1)=TIMVAR(3,1)+3.*TINTV
000010          TIMVAR(5,1)=TIMVAR(4,1)+3.*TINTV
000013          TIMVAR(6,1)=TIMVAR(5,1)+9.*TINTV
000015          TIMVAR(7,1)=TIMVAR(6,1)+9.*TINTV
000017          TIMVAR(8,1)=TIMVAR(7,1)+27.*TINTV
000022          TIMVAR(9,1)=TIMVAR(8,1)+27.*TINTV
000024          TIMVAR(10,1)=TIMVAR(9,1)+81.*TINTV
000026          TIMVAR(11,1)=TIMVAR(10,1)+81.*TINTV
000031          TIMVAR(12,1)=TIMVAR(11,1)+243.*TINTV
000033          TIMVAR(13,1)=TIMVAR(12,1)+243.*TINTV
000035          DO 110 N=14,INMPL5
000037      110 TIMVAR(N,1)=TIMVAR(N-1,1)+243.*TINTV
000047          DO 1 N=1,INMPL4
000051          TIMINT=(TIMVAR(N+1,1)-TIMVAR(N,1))/27.
000055          DO 111 M=2,27
000056      111 TIMVAR(N,M)=TIMVAR(N,1)+(FLOAT(M)-1.)*TIMINT
000072        1 TIMVAR(N,28)=TIMVAR(N+1,1)
000077          IF(IDFN)2,7,9
000100        2 AMT=ZETA(NZEMAX)/(2.*TEMPEN)
000104          COSHZT=.5*(EXP(AMT)+EXP(-AMT))
000114          IF(AMT-5.E-02)3,3,4
000116        3 SINHZT=AMT+(AMT**3)/6.
000122          GO TO 5
000122        4 SINHZT=.5*(EXP(AMT)-EXP(-AMT))
000132        5 TE2=2.*TEMPEN
000134          TE2IN=1./TE2
000136          TE24=(TE2)**2
000137          TE24IN=1./TE24
000140          IF(AMT-5.E-02)51,51,52
000143       51 AFACTO=1./((TE24)*((AMT**3)/3.)*(1.+.1*(AMT**2)))
000153          GO TO 53
000154       52 AFACTO=1./((TE24)*(AMT*COSHZT-SINHZT))
000161       53 GAMO=AFACTO*TE2*SINHZT
000164          DO 6 N=1,INMPL4
000165          DO 6 M=1,28
000166          TIME=TIMVAR(N,M)
000172          BFACTO=AFACTO/(TIME**2+TE24IN)
000175          CFACTO=COSHZT*SIN(ZETA(NZEMAX)*TIME)
000203          DFACTO=SINHZT*COS(ZETA(NZEMAX)*TIME)
000211          GAEVFC(N,M)=BFACTO*(TE2IN*DFACTO+TIME*CFACTO)
000220        6 GAODFC(N,M)=BFACTO*(TE2IN*CFACTO-TIME*DFACTO)
000234          GO TO 17
000234        7 GAMO=.0
000235          DO 8 N=1,INMPL4
000237          DO 8 M=1,28
000240          TIME=TIMVAR(N,M)
000244          GAEVFC(N,M)=-TEMPEN*(TIME**2)
000251        8 GAODFC(N,M)=TIME
000257          GO TO 17
000260        9 WRITE(9,501)FITINT
```

```
000266      501 FORMAT(8H0FITINT=,E15,8)
000266          INDFI=0
000267          TIME=,0
000270          CALL FILINT
000271          IF (FIERR-,02)12,12,10
000274       10 WRITE(9,11)N,M,INDFI,TIME,FIINTF,FIERR,FISOIF,FISOER
000326       11 FORMAT(3H0N=,I2,3H M=,I2,5H NFI=,I2,
                16H TIME=,E13,6,8H FIINTF=,E13,6,7H FIERR=,E13,6,
                28H FISOIF=,E13,6,8H FISOER=,E13,6)
000320       12 GAMO=FIINTF
000322          DO 16 N=1,INMPL4
000323          DO 16 M=1,28
000324          TIME=TIMVAR(N,M)
000330          INDFI=0
000331          CALL FTLINT
000332          IF (FIERR-,02)14,14,13
000335       13 WRITE(9,11)N,M,INDFI,TIME,FIINTF,FIERR,FISOIF,FISOER
000361       14 GAFVFC(N,M)=FIINTF
000366          INDFI=1
000367          CALL FILINT
000370          IF (FIERR-,02)16,16,15
000373       15 WRITE(9,11)N,M,INDFI,TIME,FIINTF,FIERR,FISOIF,FISOER
000417       16 GAODFC(N,M)=FIINTF
000431       17 RETURN
000432          END




        3*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
        $IBFTC TORX    DECK
                SUBROUTINE FCNCAL
000002          COMMON IND,EIINT,TINTV,OMEGA,OMEGAA,TINTO,
                1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
                2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
                4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
                5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
                1NTYPF,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
                2INDF1,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
                3FISTAR,FIFIN,FISOFN,FIINIF,FIERR,
                4NFI,NSOF,FISOIF,FISOER,FIALMO,FIREMU,
                5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
                6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
                7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
                8FIALPH,FIBET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
                1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
                2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
                3SKF(50,50),SIGEF(50,50),DEBARA(50,50),
                4ALPHEG(50),BETEG(50),AFIELD(12),
                5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002          NTVAR=2
000003        1 TIMARG=TIMVAR(NTVAR,1)
000006          IF (TIME-TIMARG)5,5,2
000010        2 IF (NTVAR-INMPL5)3,4,4
000013        3 NTVAR=NTVAR+1
000015          GO TO 1
000015        4 FCN=.0
000016          RETURN
000017        5 NTVAR=NTVAR-1
000021          TIMINT=TIMVAR(NTVAR,2)-TIMVAR(NTVAR,1)
000024          TIMARG=TIMVAR(NTVAR,2)
000025          IF (TIME-TIMARG)6,6,7
000030        6 ARGOIF=TIME-TIMVAR(NTVAR,I)
```

```
000033          GAMEVE=GAEVFC(NTVAR,1)
                1+(-1.5*GAEVFC(NTVAR,1)+2.*GAEVFC(NTVAR,2)-.5*GAEVFC(NTVAR,3))
                2*(ARGDIF/TIMINT)
                3+(.5*GAEVFC(NTVAR,1)-GAEVFC(NTVAR,2)+.5*GAEVFC(NTVAR,3))
                4*((ARGDIF/TIMINT)**2)
000054          GAMODD=GAODFC(NTVAR,1)
                1+(-1.5*GAODFC(NTVAR,1)+2.*GAODFC(NTVAR,2)-.5*GAODFC(NTVAR,3))
                2*(ARGDIF/TIMINT)
                3+(.5*GAODFC(NTVAR,1)-GAODFC(NTVAR,2)+.5*GAODFC(NTVAR,3))
                4*((ARGDIF/TIMINT)**2)
000075          GO TO 10
000075        7 MTVAR=3
000076        8 TIMARG=TIMVAR(NTVAR,MTVAR)
000103          IF(TIME-TIMARG)9,9,17
000105        9 ARGDIF=TIME-TIMVAR(NTVAR,MTVAR-1)
000113          GAMEVE=GAEVFC(NTVAR,MTVAR-1)
                1+(.5*GAEVFC(NTVAR,MTVAR)-.5*GAEVFC(NTVAR,MTVAR-2))
                2*(ARGDIF/TIMINT)+(.5*GAEVFC(NTVAR,MTVAR)
                3-GAEVFC(NTVAR,MTVAR-1)+.5*GAEVFC(NTVAR,MTVAR-2))
                4*((ARGDIF/TIMINT)**2)
000137          GAMODD=GAODFC(NTVAR,MTVAR-1)

                1+(.5*GAODFC(NTVAR,MTVAR)-.5*GAODFC(NTVAR,MTVAR-2))
                2*(ARGDIF/TIMINT)+(.5*GAODFC(NTVAR,MTVAR)
                3-GAODFC(NTVAR,MTVAR-1)+.5*GAODFC(NTVAR,MTVAR-2))
                4*((ARGDIF/TIMINT)**2)
000161       10 IF(NTYPE)11,14,11
000162       11 IF(IND)13,12,13
000163       12 FCN=EXP(RECOIL*(GAMEVE-GAM0))*COS(RECOIL*GAMODD)
000176          IF(IDEN)21,22,21
000177       21 FCN=FCN-EXP(-RECOIL*GAM0)
000205       22 ABC=1.
000207          RETURN
000207       13 FCN=-EXP(RECOIL*(GAMEVE-GAM0))*SIN(RECOIL*GAMODD)
000222          RETURN
000223       14 IF(IND)16,15,16
000224       15 FCN=EXP(RECOIL*(GAMEVE-GAM0)-REGA12*TIME)
                1*COS(RECOIL*GAMODD)
000241          RETURN
000241       16 FCN=-EXP(RECOIL*(GAMEVE-GAM0)-REGA12*TIME)
                1*SIN(RECOIL*GAMODD)
000256          RETURN
000257       17 IF(MTVAR-28)18,9,9
000262       18 MTVAR=MTVAR+1
000264          GO TO 8
000264          END




         $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
         $IBFTC TRL2    DECK
                SUBROUTINE FILINT
000002          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
                1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
                2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
                4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
                5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
                1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
                2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
                3FISTAP,FIFIN,FISOFN,FIINTF,FIERR,
                4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
                5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
                6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
                7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
                8FIALPH,FIBET,FIGAM
```

33

```
000002              COMMON AFACTO,TE?
000002              COMMON FACSIG,SIGMA,SIGMAC,ETINO,
             1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
             2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
             3SKF(50,50),SIGEF(50,50),DEBARA(50,50),
             4ALPHEG(50),BETEG(50),AFIELD(12),
             5INMXO,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002              IF(INDFI)1,3,1
000003           1 IF(TIME)3,2,3
000004           2 FIINTF=.0
000005             FIERR=.0
000006             RETURN
000006           3 FIFIN=ZETA(NZEMAX)
000011             CALL FIINIT
000012             CALL FICONT
000013             IF(FISTAR)4,4,5
000015           4 FISOIF=.0
000016             FISOER=.0
000017             RETURN
000017           5 IF(FISTAR-ZETA(NZEMAX))13,14,14
000023          13 FISOFN=FISTAR
000025             GO TO 15
000025          14 FISOFN=ZETA(NZEMAX)
000030          15 CALL FISOIN
000031             CALL FISOCO
000032             FIINTF=FIINTF+FISOIF
000034             FIERR=FIERR*ABS((FIINTF-FISOIF)/FIINTF)
             1+FISOER*ABS(FISOIF/FIINTF)
000043             RETURN
000044             END)
```

```
$*    ****COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC IRM2      DECK
                  SUBROUTINE FIINIT
000002            COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
             1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
             2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
             3COR1,COR2,COFCO,COFC1,COFC2,COFC3,COFC4,
             4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
             5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002            COMMON T2(73,5),S(74,6)
000002            COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002            COMMON NIDFN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
             1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
             2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
             3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
             4NFI,NSOF,FISOIF,FISOER,FIALMU,FIBEMU,
             5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
             6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
             7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
             8FIALPH,FIBET,FIGAM
000002            COMMON AFACTO,TE?
000002            COMMON FACSIG,SIGMA,SIGMAC,ETINO,
             1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
             2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
             3SKF(50,50),SIGEF(50,50),DEBARA(50,50),
             4ALPHEG(50),BETEG(50),AFIELD(12),
             5INMXO,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002            IF(INDFI)2,1,2
000003          1 FISTAR=ALPHA
000005         14 FIARG=FIFIN
000007            CALL FIFNCA
000010            FIALMU=FIFCN*SIN(FIFIN*TIME)
000016            FIBEMU=FIFCN*COS(FIFIN*TIME)
000023            FIARG=FISTAR
000024            CALL FIFNCA
000025            FIALMU=FIALMU-FIFCN*SIN(FISTAR*TIME)
```

```
000034          FIBEMU=.5*(FIBEMU+FIFCN*COS(FISTAR*TIME))
000044          GO TO 3
000044        2 ARG1=6.2831853/ABS(TIME)
000047          ARG2=ALPHA/ARG1
000050          ARG3=AINT(ARG2)
000052          FISTAR=(1.57079633/ABS(TIME))+ARG1*ARG3
000057          FIARG=FIFIN
000060          CALL FIFNCA
000061          FIALMU=-FIFCN*COS(FIFIN*TIME)
000067          FIBEMU=FIFCN*SIN(FIFIN*TIME)
000075          FIARG=FISTAR
000076          CALL FIFNCA
000077          FIBEMU=.5*(FIFCN*SIN(FISTAR*TIME)+FIBEMU)
000107        3 RETURN
000110          END




         $*   ***COMMENT CARD TO BREAK UP BATCH COMPILE
         $IBFTC TORN     DECK
                SUBROUTINE FICONT
000002          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
               1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
               2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
               3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
               4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
               5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
               1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
               2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
               3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
               4NFI,NSOF,FISOIF,FISOER,FIALMU,FIBEMU,
               5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
               6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
               7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
               8FIALPH,FIBET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
               1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
               2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
               3SKF(50,50),SIGEF(50,50),DEBARA(50,50),
               4ALPHEG(50),BETEG(50),AFIELD(12),
               5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002          IF(FISTAR-ZETA(NZEMAX))101,100,100
000006      100 FIINTF=.0
000007          FIERR=.0
000010          RETURN
000010      101 NFI=5
000011          FIHT=(FIFIN-FISTAR)/10.
000014          CALL FIEVSU
000015          CALL FIODSU
000016          CALL FIABGA
000017          FIINTE(1)=FIHT*(FIALPH*FIALMU+FIBET*(FIBEMU
               1+FEVSU)+FIGAM*FODSU)
000027          NCOUNT=2
000030          FICOMP=1.
000031        1 NFI=NFI+NFI
000032          FIHT=FIHT/2.
000034          FEVSU=FEVSU+FODSU
000036          CALL FIODSU
000037          CALL FIABGA
000040          FIINTE(NCOUNT)=FIHT*(FIALPH*FIALMU+FIBET*(FIBEMU
               1+FEVSU)+FIGAM*FODSU)
000051          FICOLD=FICOMP
000052          NCOLS1=NCOUNT-1
000054          FICOMP=ABS(1.-FIINTE(NCOUNT)/FIINTE(NCOLS1))
000061          IF(FICOMP-FITINT)2,2,3
```

```
000063      2 IF(FICOLD-FITINT)21,21,3
000066     21 FIINTF=FIINTE(NCOUNT)
000071        FIERR=FICOMP
000072        RETURN
000073      3 IF(NCOUNT-8)4,21,21
000076      4 NCOUNT=NCOUNT+1
000100        GO TO 1
000100        END
```

```
       $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
       $IBFTC TR02    DECK
               SUBROUTINE FIEVSU
000002         COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
              1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
              2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
              3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
              4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
              5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002         COMMON T2(73,5),S(74,6)
000002         COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002         COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
              1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
              2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
              3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
              4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
              5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
              6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
              7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
              8FIALPH,FIBET,FIGAM
000002         COMMON AFACTO,TE2
000002         COMMON FACSIG,SIGMA,SIGMAC,ETINO,
              1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
              2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
              3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
              4ALPHEG(50),BETEG(50),AFIELD(12),
              5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002         FEVSU=.0
000003         NTERM=NFI-1
000005         DO 5 J=1,NTERM
000007         FITRIG=2.*FIHT*FLOAT(J)
000012         FIARG=FISTAR+FITRIG
000014         CALL FIFNCA
000015         IF(INDFI)2,1,2
000016      1 FEVSU=FEVSU+FIFCN*COS(FIARG*TIME)
000025        GO TO 5
000026      2 IF(TIME)3,4,4
000030      3 FEVSU=FEVSU-FIFCN*COS(FITRIG*TIME)
000037        GO TO 5
000040      4 FEVSU=FEVSU+FIFCN*COS(FITRIG*TIME)
000047      5 CONTINUE
000052        RETURN
000052        END
```

```
       $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
       $IBFTC TRP2    DECK
               SUBROUTINE FIODSU
000002         COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
              1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
              2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
              3COR1,COR2,COFC0,CDFC1,COFC2,CUFC3,COFC4,
              4CUFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
              5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
```

```
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
               1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
               2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODD,
               3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
               4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
               5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
               6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
               7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
               8FIALPH,FIBET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
               1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
               2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
               3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
               4ALPHEG(50),BETEG(50),AFIELD(12),
               5INMXD,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
000002          FODSU=.0
000003          DO 5 J=1,NFI
000005          FITRIG=2.*FIHT*FLOAT(J)-FIHT
000010          FIARG=FISTAR+FITRIG
000012          CALL FIFNCA
000013          IF(INDFI)2,1,2
000014        1 FODSU=FODSU+FIFCN*COS(FIARG*TIME)
000023          GO TO 5
000024        2 IF(TIME)3,4,4
000026        3 FODSU=FODSU-FIFCN*COS(FITRIG*TIME)
000035          GO TO 5
000036        4 FODSU=FODSU+FIFCN*COS(FITRIG*TIME)
000045        5 CONTINUE
000050          RETURN
000050          END



          $*    ****COMMENT CARD TO BREAK UP BATCH COMPILE
          $IBFTC TORN     DECK
                SUBROUTINE FIARGA
000002          COMMON IND,ETINT,TINIV,DMEGA,OMEGAA,TINTO,
               1SFTNAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
               2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
               3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
               4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
               5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BFTA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
               1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
               2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODD,
               3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
               4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
               5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
               6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
               7FEVSO,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
               8FIALPH,FIBET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
               1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
               2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
               3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
               4ALPHEG(50),BETEG(50),AFIELD(12),
               5INMXD,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002          IF(TIME)1,2,1
000003        1 THETA=FIHT*TIME
000005          IF(ABS(THETA)-2.E-01)11,11,13
000010       11 IF(ABS(THETA)-1.E-5)2,2,12
000014       12 THETA2=THETA**2
000016          THETA3=THETA**3
```

```
000017          FIALPH=.44444444E-1*THETA3*(1.
              1-.14285714*THETA2*(1.
              2-.66666667E-1*THETA2))
000026          FIHET=.66666667*(1.+.2*THETA2*(1.
              1-.28571429*THETA2))
000035          FIGAM=1.33333333*(1.-.1*THETA2*(1.
              1-.35714286E-1*THETA2))
000043          RETURN
000043       13 THETA2=THETA**2
000045          THETA3=THETA**3
000046          SINTHE=SIN(THETA)
000051          COSTHE=COS(THETA)
000053          SITHE3=SINTHE/THETA3
000055          COTHE2=COSTHE/THETA2
000057          SICOTH=COSTHE*SITHE3
000061          SI2TH3=2.*SINTHE*SITHE3
000063          FIALPH=1./THETA+THETA*SICOTH-SI2TH3
000067          FIHET=4./THETA2-SI2TH3*THETA-4.*SICOTH
000074          FIGAM=4.*(SITHE3-COTHE2)
000076          RETURN
000077        2 FIALPH=.0
000100          FIHET=.666666667
000102          FIGAM=1.33333333
000103          RETURN
000104          END
```

```
                SUBROUTINE FISOIN
000002          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
              1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
              2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
              3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
              4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
              5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002          COMMON T2(73,5),S(74,6)
000002          COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002          COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
              1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
              2IUDFI,ETTNIN,FITINT,GAMO,GAMEVE,GAMODU,
              3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
              4NFI,NSOF,F1SOIF,FISOER,FIALMU,FIREMU,
              5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLU,
              6NSOCNT,FISOIT(9),FSOCOM,FSOCLU,
              7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
              8FIALPH,FIHET,FIGAM
000002          COMMON AFACTO,TE2
000002          COMMON FACSIG,SIGMA,SIGMAC,ETINO,
              1RECMAX,HREC,AFARFC,FPSMAX,HEPS,AFAEPS,
              2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
              3SKE(50,50),SIGFF(50,50),UEBARA(50,50),
              4ALPHEG(50),BETEG(50),AFIELD(12),
              5INMXD,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
000002          FIARG=.0
000003          CALL FIFNCA
000004          IF(IUDFI)2,1,2
000005        1 FIREMU=FIFCN
000007          GO TO 3
000007        2 FIALMU=FIFCN
000011        3 FIARG=FISOFN
000013          CALL FIFNCA
000014          IF(INDFI)5,4,5
```

```
000015      4 FIALMU=FIFCN*SIN(FISOFN*TIME)
000023        FIBEMU=.5*(FIFCN*COS(FISOFN*TIME)+FIBEMU)
000032        GO TO 6
000032      5 FIALMU=FIALMU-FIFCN*COS(FISOFN*TIME)
000041        FIBEMU=.5*FIFCN*SIN(FISOFN*TIME)
000050      6 RETURN
000051        END
```

```
           $*    ****COMMENT CARD TO BREAK UP BATCH COMPILE
           $IBFTC TORS     DECK
                  SUBROUTINE FISOCO
000002            COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
                 1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
                 2FINFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                 3COR1,COR2,COFCO,COFCI,COFC2,COFC3,COFC4,
                 4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
                 5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002            COMMON T2(73,5),S(74,6)
000002            COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002            COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
                 1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
                 2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
                 3FISTAR,FIFIN,FISOFN,FIINIF,FIERR,
                 4NFI,NSOF,FISOIF,FISOER,FIALMU,FIBEMU,
                 5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
                 6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
                 7FEVSU,FODSU,FSOEV,FSOOO,FIARG,FIFCN,
                 8FIALPH,FIBET,FIGAM
000002            COMMON AFACTO,TE2
000002            COMMON FACSIG,SIGMA,SIGMAC,ETINO,
                 1RECMAX,HREC,AFARFC,FPSMAX,HEPS,AFAEPS,
                 2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
                 3SKE(50,50),SIGEF(50,50),UEBARA(50,50),
                 4ALPHEG(50),BETEG(50),AFIELU(121,
                 5INMXO,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002            NSOF=2
000003            FIHT=FISOFN/4.
000005            CALL FISOEV
000006            CALL FISOOD
000007            CALL FIARGA
000010            FISOIT(1)=FIHT*(FIALPH*FIALMU+FIBET
                 1*(FIBEMU+FSOEV)+FIGAM*FSOOO)
000020            NSOCNT=2
000021            FSOCOM=1.
000022          1 NSOF=NSOF+NSOF
000023            FIHT=FIHT/2.
000025            FSOEV=FSOEV+FSODD
000027            CALL FISOOD
000030            CALL FIABGA
000031            FISOIT(NSOCNT)=FIHT*(FIALPH*FIALMU+FIBET
                 1*(FIBEMU+FSOEV)+FIGAM*FSOOO)
000042            FSOCLD=FSOCOM
000043            NSOLS1=NSOCNT-1
000045            FSOCOM=ABS(1.-FISOIT(NSOCNT)/FISOIT(NSOLS1))
000052            IF(FSOCOM-FITINT)2,2,3
000054          2 IF(FSOCLD-FITINT)21,21,3
000057         21 FISOIF=FISOIT(NSOCNT)
000062            FISOER=FSOCOM
000063            RETURN
000064          3 IF(NSOCNT-8)4,21,21
000067          4 NSOCNT=NSOCNT+1
000071            GO TO 1
000071            END
```

```
      $*    ****CUMMENT CARD TO BREAK UP BATCH COMPILE
         $IBFTC TRT2    DECK
               SUBROUTINE FISOEV
000002         COMMON IND,ETINT,TINIV,OMEGA,OMEGAA,TINTO,
              1STINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
              2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
              3COR1,COR2,COFCO,COFC1,COFC2,COFC3,COFC4,
              4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
              5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCNU
000002         COMMON T2(73,5),S(74,6)
000002         COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002         COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
              1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
              2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
              3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
              4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
              5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
              6NSOCNT,FISOIT(9),FSOCOM,FSOCLU,
              7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
              8FIALPH,FIHET,FIGAM
000002         COMMON AFACTU,TE2
000002         COMMON FACSIG,SIGMA,SIGMAC,ETINO,
              1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
              2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
              3SKF(50,50),SIGEF(50,50),DEBARA(50,50),
              4ALPHEG(50),BETEG(50),AFIELD(12),
              5INMXD,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002         FSOEV=.0
000003         NTERM=NSOF-1
000005         DO 3 J=1,NTERM
000007         FITRIG=2.*FIHT*FLOAT(J)
000012         FIARG=FITRIG
000013         CALL FIFNCA
000014         IF(INDFI)2,1,2
000015       1 FSOEV=FSOEV+FIFCN*COS(FITRIG*TIMF)
000024         GO TO 3
000025       2 FSOEV=FSOEV+FIFCN*SIN(FITRIG*TIMF)
000034       3 CONTINUE
000037         RETURN
000037         END
```

```
      $*    ****COMMENT CARD TO BREAK UP BATCH COMPILE
         $IBFTC TRU2    DECK
               SUBROUTINE FISOOD
000002         COMMON IND,ETINT,TINIV,OMEGA,OMEGAA,TINTO,
              1STINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
              2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
              3COR1,COR2,COFCO,COFC1,COFC2,COFC3,COFC4,
              4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
              5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCNU
000002         COMMON T2(73,5),S(74,6)
000002         COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002         COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
              1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
              2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
              3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
              4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
              5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
              6NSOCNT,FISOIT(9),FSOCOM,FSOCLU,
              7FEVSU,FODSU,FSOEV,FSOOO,FIARG,FIFCN,
              8FIALPH,FIHET,FIGAM
000002         COMMON AFACTU,TE2
000002         COMMON FACSIG,SIGMA,SIGMAC,ETINO,
              1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
              2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
              3SKF(50,50),SIGEF(50,50),DEBARA(50,50),
```

```
                          4ALPHEG(50),BETEG(50),AFIELD(12),
                          5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002                     FSOOD=.0
000003                     DO 3 J=1,NSOF
000005                     FITRIG=2.*FIHT*FLOAT(J)-FIHT
000010                     FIARG=FITRIG
000011                     CALL FIFNCA
000012                     IF(INDFI)2,1,2
000013                   1 FSOOD=FSOOD+FIFCN*COS(FITRIG*TIME)
000022                     GO TO 3
000023                   2 FSOOD=FSOOD+FIFCN*SIN(FITRIG*TIME)
000032                   3 CONTINUE
000035                     RETURN
000035                     END


              $*   ****COMMENT CARD TO BREAK UP BATCH COMPILE
              $IBFTC TORV    DECK
                     SUBROUTINE FIFNCA
000002               COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTO,
                    1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
                    2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                    3COR1,COR2,COFC0,COFC1,COFC2,COFC3,CDFC4,
                    4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
                    5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
000002               COMMON T2(73,5),S(74,6)
000002               COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002               COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
                    1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
                    2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODU,
                    3FISTAR,FIFIN,FISOFN,FIINIF,FIERR,
                    4NF1,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
                    5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLU,
                    6NSOCNT,FISOIT(9),FSOCOM,FSOCLD,
                    7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
                    8FIALPH,FIBET,FIGAM
000002               COMMON AFACTO,TE2
000002               COMMON FACSIG,SIGMA,SIGMAC,ETINO,
                    1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
                    2NLIM,MLIM,REC(50),EPS(50),SELU(50),STGELD(50),
                    3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
                    4ALPHEG(50),BETEG(50),AFIELD(12),
                    5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002               1 TEMP=ZETA(NZEMAX)
000005                 IF(FIARG-TEMP)3,3,2
000007               2 FIFCN=.0
000010                 RETURN
000011               3 TEMP=FIARG-ZETA(2)
000013                 IF(TEMP)4,4,13
000015               4 IF(FIARG)5,5,6
000017               5 PARAM=1.E-10*ZETA(2)
000021                 GO TO 7
000022               6 PARAM=FIARG
000024               7 PHFRCU=((PARAM/ZETA(2))**2)
                    1*PHOFRE(2)
000030               8 IF(INDFI)9,12,9
000031               9 IF(FIARG)10,10,11
000033              10 FIFCN=.0
000034                 RETURN
000035              11 FIFCN=PHFRCU/PARAM
000037                 RETURN
000040              12 SIARG=PARAM/(2.*TEMPEN)
000043                 IF(SIARG-10,1111,111,110
000045             110 FIFCN=PHFRCU/PARAM
000047                 RETURN
000050             111 EXPFC2=EXP(-SIARG)
000054                 IF(SIARG-1.E-02)113,113,112
```

```
000056      112 SIHFC=EXP(SIARG)-EXPFC2
000062          GO TO 114
000063      113 IF(SIARG-1.E-05)1113,1113,1114
000066     1113 SIAR26=.0
000067          GO TO 1115
000070     1114 SIAR26=(SIARG**2)/6.
000073     1115 SIHFC=2.*(SIARG*(1.+SIAR26))
000077      114 FIFCN=(SIHFC+2.*EXPFC2)*PHFRCU/(PARAM*SIHFC)
000105          RETURN
000106       13 NZETA=3
000107       14 TEMP=FIARG-ZETA(NZETA)
000112          IF(TEMP)15,16,17
000114       15 DIFF12=ZETA(NZETA-1)-ZETA(NZETA-2)
000120          DIFF01=ZETA(NZETA)-ZETA(NZETA-1)
000123          DIFF02=ZETA(NZETA)-ZETA(NZETA-2)
000126          DEN=DIFF12*DIFF01*DIFF02
000130          AMT1=DIFF12*(PHOFRE(NZETA)-PHOFRF(NZETA-1))
000134          AMT2=DIFF01*(PHOFRE(NZETA-2)-PHOFRE(NZETA-1))
000140          COEF1=PHOFRE(NZETA-1)
000142          COEF2=(DIFF12*AMT1-DIFF01*AMT2)/DEN
000147          COEF3=(AMT1+AMT2)/DEN
000150          ARGINT=FIARG-ZETA(NZETA-1)
000153          PHFRCU=COEF1+COEF2*ARGINT+COEF3*(ARGTNT**2)
000161          IF(PHFRCU)115,116,116
000162      115 PHFRCU=.0
000163      116 PARAM=FIARG
000165          GO TO 8
000165       16 PHFRCU=PHOFRE(NZFTA)
000170          PARAM=FIARG
000171          GO TO 8
000172       17 NZETA=NZETA+1
000174          GO TO 14
000174          END
```