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Calculation of
Thermal Neutron Scattering Cross Sections
for Crystalline Materials: The TOR Program



UNITED STATES
ATOMIC ENERGY COMMISSION
CONTRACT W-7405-ENG. 36

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Printed in the United States of America. Available from
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151

Price: Printed Copy \$3.00; Microfiche \$0.65

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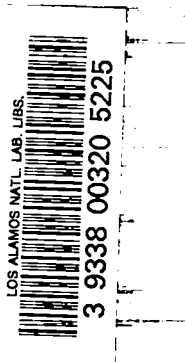
Report written: October 20, 1967

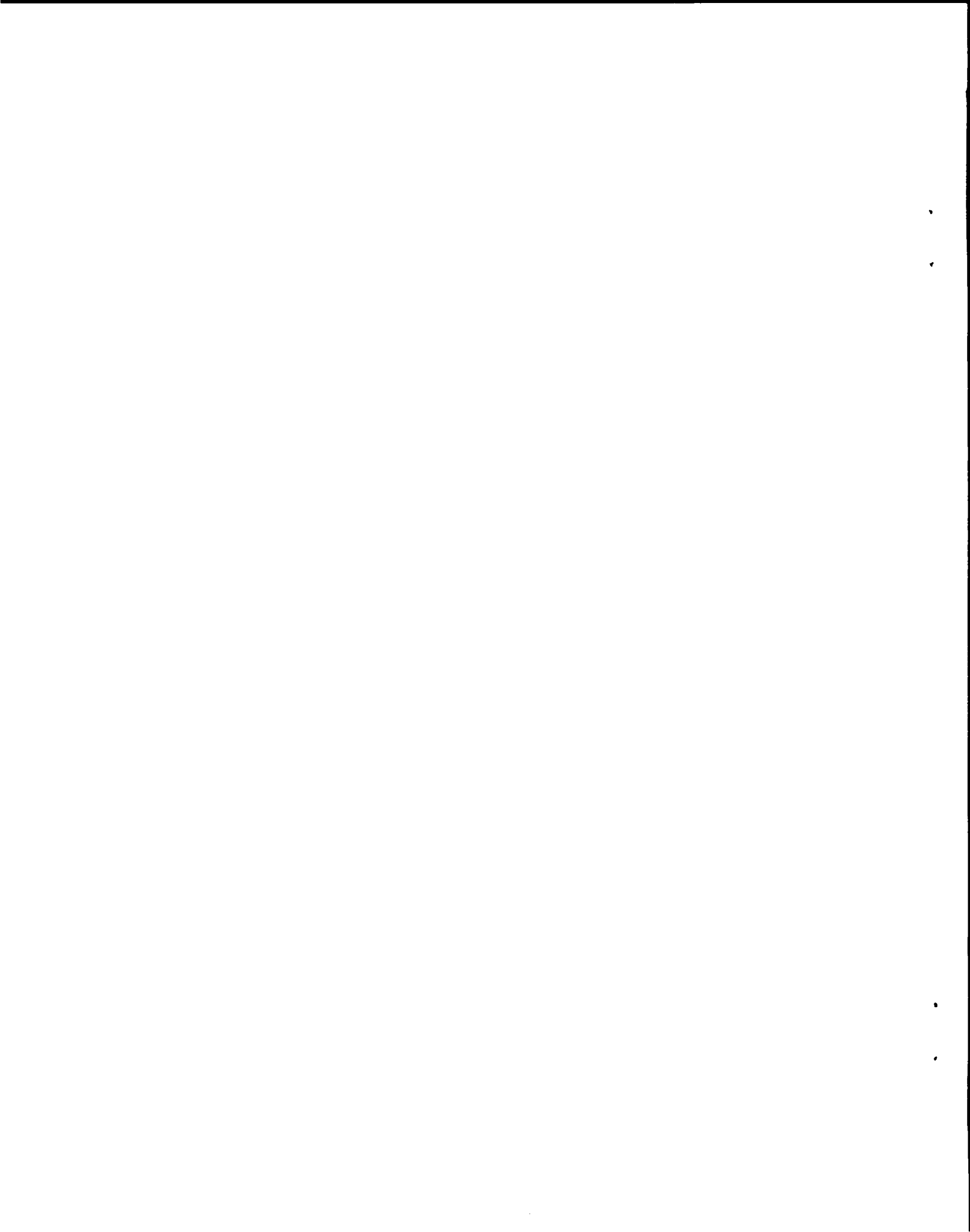
Report distributed: December 18, 1967

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by

W. W. Clendenin





CALCULATION 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 materials. 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 accurate interpolation properties, is provided as card output. The latter has the form of input for the FORTRAN-IV program GLEN which obtains the total scattering cross section, thermal neutron diffusion length, and flux-weighted group cross sections.

I. Introduction. 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 material and on its temperature. The materials with simplest cross sections are monatomic gases such as 4He , the theory of which has been developed with varying degrees of elaboration¹⁻⁵ 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 liquid form.

One of the most successful of these applications has been a modification⁶ of the monatomic gas model to fit the room temperature diffusion length of H_2O . Even in this case there are substantial differences⁷ between the diffusion lengths at higher temperatures

implied by this model and those implied by a model⁸ 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 characteristics of the crystal cross section. For energies 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 elastic 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 temperature 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 section. 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 depends¹⁰ 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 codes¹¹ 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_0 , 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 method¹² 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 Filon¹³ 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 GASKET¹⁴ 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 approximation¹⁵⁻²¹ 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_0 to final energy E with deflection through an angle θ is

$$d^2\sigma/d\Omega dE = \sigma(E_0 \rightarrow E, \theta, T) = \sigma_0(E_0 \rightarrow E, \theta, T) + \sigma_1(E_0 \rightarrow E, \theta, T). \quad (1)$$

Here $\sigma_0(E_0 \rightarrow E, \theta, T)$ is the elastic scattering term*

$$\sigma_0(E_0 \rightarrow E, \theta, T) = (\sigma_b/4\pi) \exp\{-R\gamma(0)\} \delta(\epsilon). \quad (2)$$

The cross section $\sigma_1(E_0 \rightarrow E, \theta, T)$, which includes inelastic scattering, is given by

$$\sigma_1(E_0 \rightarrow E, \theta, T) = (\sigma_b/4\pi) (E/E_0)^{\frac{1}{2}} \exp\{-R\gamma(0)\} \cdot (2\pi)^{-1} \int_{-\infty}^{\infty} \exp(1\epsilon t) [\exp\{R\gamma(t)\} - 1] dt. \quad (3)$$

The basic parameters R and ϵ of the cross section are

$$R = (m/M) (E_0 + E - 2E_0^{\frac{1}{2}} E^{\frac{1}{2}} \cos \theta), \quad (4)$$

$$\epsilon = E - E_0. \quad (5)$$

The function $\gamma(t)$ is

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

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 $\sigma_0(E_0 \rightarrow E, \theta, T)$ 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,

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

and

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

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

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

where

$$\gamma_{\text{even}}(t) = \int_0^{\infty} \zeta^{-1} f(\zeta) \coth(\zeta/2T) \cos(\zeta t) d\zeta, \quad (10)$$

$$\gamma_{\text{odd}}(t) = \int_0^{\infty} \zeta^{-1} f(\zeta) \sin(\zeta t) d\zeta. \quad (11)$$

The cross section $\sigma_1(E_0 \rightarrow E, \theta, T)$ is

$$\sigma_1(E_0 \rightarrow E, \theta, T) = (\sigma_b/4\pi)(E/E_0)^{\frac{1}{2}} s(R, \epsilon). \quad (12)$$

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

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

where

$$u(R, \epsilon) = \pi^{-1} \int_0^{\infty} [\exp\{R\gamma_{\text{even}}(t) - R\gamma_{\text{even}}(0)\} \cos\{R\gamma_{\text{odd}}(t)\} - \exp\{-R\gamma_{\text{even}}(0)\}] \cos(\epsilon t) dt, \quad (14)$$

$$v(R, \epsilon) = -\pi^{-1} \int_0^{\infty} \exp\{R\gamma_{\text{even}}(t) - R\gamma_{\text{even}}(0)\} \sin\{R\gamma_{\text{odd}}(t)\} \sin(\epsilon t) dt. \quad (15)$$

The integrals of Eqs. (10), (11), (14), (15) are in the forms to which the numerical method used¹² applies directly.

It may be shown²² that the cross section $\sigma_1(E_0 \rightarrow E, \theta, T)$ obeys the detailed balance condition, i.e., that

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

The scattering law²³, for $\epsilon \neq 0$, is the dimensionless quantity

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

where

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

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

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

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

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 $\gamma_{\text{even}}(t_j)$ and $\gamma_{\text{odd}}(t_j)$ for a set of mesh values t_j . Needed values of $\gamma_{\text{even}}(t)$ and $\gamma_{\text{odd}}(t)$ 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 method¹² 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 $h_R(\text{HREC}) > 0$ 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 n^{th} 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

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

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

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

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 $M = 1, \dots, \text{MLIM}$) 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 $\gamma_{\text{even}}(t_j)$, Eq. (10), and $\gamma_{\text{odd}}(t_j)$, Eq. (11), for a suitable mesh of values t_j . The basis for the form of this mesh is the method¹² 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 $\Delta t_1 = 1/(9 \zeta_{\text{max}})$ where ζ_{max} is the largest value of $|\zeta|$ for which $f(\zeta)$ differs from zero. The second

interval $\Delta t_2 = \Delta t_1$, $\Delta t_3 = \Delta t_4 = 3\Delta t_1$, $\Delta t_5 = \Delta t_6 = 9\Delta t_1$, \dots , $\Delta t_{11} = \Delta t_{12} = 243 \Delta t_1$, and all intervals with higher indices are equal to Δt_{12} . In each interval values of $\gamma_{\text{even}}(t_j)$ and $\gamma_{\text{odd}}(t_j)$ 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-Koppel²⁴ 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-Koppel²⁵ 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 $4 \leq \text{NZEMAX} \leq 201$. 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 method¹² for the calculation of Fourier integrals using a double convergence criterion of .001 is used to obtain $\gamma_{\text{even}}(t_j)$ and $\gamma_{\text{odd}}(t_j)$ 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 $\exp\{-R_n \gamma_{\text{even}}(0)\}$ of Eq. (2) is computed for each value R_n and designated $\text{SELD}(N)$. The parameter α_n , $\text{ALPHEG}(N)$, determined from R_n according to Eq. (18), is obtained for each R_n . Similarly, the parameter β_m , $\text{BETEG}(M)$, 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 $\text{SIGEF}(N, M)$. The corresponding quantity derived from the elastic scattering cross section of Eq. (2) is $T \exp\{-R_n \gamma_{\text{even}}(0)\}$ which is calculated for each R_n and designated as $\text{SIGELD}(N)$.

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 $\text{IDEN} = 0$ substitutes a monatomic gas model for the crystal model of Eqs. (1) - (11). The monatomic gas cross section can be expressed²⁶ in the form of Eq. (12) provided $s(R, \epsilon)$ is replaced by

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

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

IV. Input for TOR.

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

- 2) ZETA (NZETA), $\text{NZETA} = 1$, NZEMAX 4 E 20.8
Energies at which values of phonon frequency distribution are specified. ZETA (1) must be .0 and $\text{ZETA} (\text{NZETA}+1) > \text{ZETA} (\text{NZETA})$.
- 3) PHOFRE (NZETA), $\text{NZETA} = 1$, NZEMAX 4 E 20.8
Values of phonon frequency distribution corresponding to energies in 2) above. PHOFRE (1) must be .0, and $\text{PHOFRE} (\text{NZETA}) \geq 0$.
4. TEMPEN (temperature T in energy units $> .0$) E 20.8
5. RECMAX , HREC , AFAREC 3 E 20.8
 $\text{RECMAX} > .0$ is maximum value of R and HREC ($.0 < \text{HREC} \leq \text{RECMAX}$) is smallest interval of R , both in energy units. $\text{AFAREC} \geq 1$. is numerical factor which is ratio of successive intervals in R . Typical values are $\text{RECMAX} = 3.1$ eV., $\text{HREC} = .005$ eV., $\text{AFAREC} = 1.1$.
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 $\text{EPSMAX}/\text{HEPS} \geq 1$. Code will accept either sign but for accuracy in computing crystal cross section, negative values are preferable. $\text{AFAEPS} \geq 1$. is numerical factor which is ratio of successive intervals in ϵ . Typical values are $\text{EPSMAX} = -3.1$ eV., $\text{HEPS} = -.005$ eV., $\text{AFAREC} = 1.1$.

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, $\text{IDEN} > 0$, 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, HEFS, 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/HEFS 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, HEFS, 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), SELD(N), SIGELD(N) for $1 \leq N \leq NLIM$. SELD(N) is the coefficient $\exp\{-R \gamma(0)\}$ in the elastic scattering term $\exp\{-R \gamma(0)\} \delta(\epsilon)$ of Eq. (2), and SIGELD(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 $\gamma_{\text{even}}(t)$ and $\gamma_{\text{odd}}(t)$ by $\gamma_{\text{even}}(t) + i\gamma_{\text{odd}}(t)$. The functions $\gamma_{\text{even}}(t)$ and $\gamma_{\text{odd}}(t)$ are printed out as functions of t, designated in the printout as TIME. The function $\gamma_{\text{even}}(t)$ is designated as GAMEVE, and the function $\gamma_{\text{odd}}(t)$ 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 GAMO is $\gamma(0)$.	I 10, 2 E 20.8
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 NPROD is the product NLIM* MLIM	I 8
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 $16 \leq \text{IDEN} < 128$ 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 $\text{IDEN} \geq 128$, 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 $\text{IDEN} \geq 128$.

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

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PROGRAM TOR(INPUT,TAPE10=INPUT,
1OUTPUT,TAPE9=OUTPUT,
2PUNCH,TAPE11=PUNCH)
*IBFIC TOR DECK
000003 COMMON IND,ETINT,TINTV,OMEGA,OMEGA,TINTO,
15FINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
3COP1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFCN8,CNFCN7,COFCN6,
5COFC15,COFCN4,COFCN3,COFCN2,COFCN1,CNFCN0
000003 COMMON TD(73,5),S(74,6)
000003 COMMON IDEN,ALPHA,RETA,J1,J2,ARGPAC
000003 COMMON NIDEN,NINIT,NZFMAX,ZETA(201),PHOFRE(201),
INTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
3FISTAR,FIFIN,FISOFN,FIINF,FIERR,
4NFI,NSOF,FISUIF,FISDER,FIALMU,FIEMU,
5NCOUNT,FIHT,FIINT(9),FICOMP,FICOLD,
6NSCNT,FISOIT(9),FSOCOM,FSOCLD,
7FEVSU,FOSU,FSOEV,FSOOD,FIARG,FIFCN,
8FIALPH,FIHEI,FIGAM
000003 COMMON AFACTO,TFP
000003 COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAH,HREC,AFAREC,FMSMAX,HEPS,AFAPPS,
2NLM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
3SKE(50,50),SIGEF(50,50),UEBARA(50,50),
4ALPHEG(50),HETEG(50),AFIELD(12),
5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,2H),GAODFC(72,2H)
000003 READ(10,1)(AFIELD(J),J=1,12)
000015 1 FORMAT(12A6)
000015 WRITE(9,2)
000021 2 FORMAT(55H1)
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,INMX0
000044 IF(IDEN)951,8,951
000045 951 IF(INMX0-8)6,8,8
000050 6 WRITE(9,7)
000054 7 FORMAT(18H0INMX0 LFSS THAN 8)
000054 ININCK=1
000055 8 IF(INMX0-72)11,11,9
000060 9 WRITE(9,10)
000064 10 FORMAT(22H0INMX0 GRFATER THAN 72)
000064 ININCK=1+ININCK
000066 11 IF(IDEN)12,33,15
000070 12 NZFMAX=2
000071 READ(10,5)ZETA(NZFMAX)
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)16,1R,1R
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 ZERU)
000175 ININCK=1+ININCK

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000177      24 ABC=PHOFRE(1)
000201      IF (ABC)25,261,25
000202      25 WRITE(9,26)
000206      26 FORMAT(19H0PHOFRE(1) NOT ZERO)
000206      ININCK=1+ININCK
000210      261 DO 29 NZETA=2,NZEMAX
000212      ABC=ZETA(NZETA)-7ETA(NZETA=1)
000214      IF (ABC)27,27,29
000216      27 NZELSI=NZETA-1
000220      WRITE(9,28)NZETA,NZELSI
000230      28 FORMAT(6H0ZETA(,I4,19H ) LESS/EQUAL 7ETA(,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(8H0PHOFRE(,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(23H0TEMPEN 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(23H0RECMAX 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(25H0RECMAX/HREC LESS THAN 1.)
000326      ININCK=1+ININCK
000330      42 IF (AFAREC-1.)43,45,45
000333      43 WRITE(9,44)
000337      44 FORMAT(20H0AFAREC 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(25H0EPSMAX/HEPS LESS THAN 1.)
000363      ININCK=1+ININCK
000365      48 IF (AFAEPS-1.)49,51,51
000370      49 WRITE(9,50)
000374      50 FORMAT(20H0AFAEPS 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(16H0NLIM 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(16H0MLIM EXCEEDS 50)
000464      ININCK=1+ININCK
000466      63 IF (ININCK)64,66,64
000467      64 WRITE(9,65)ININCK
000475      65 FORMAT(22H0INPUT CHECKED. ABOVE ,I3,31H ERRORS FOUND. PROBLEM STOP
1PED.)

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000475      STOP
000477      66 IF (IDEN) 67,67,661
000501      661 CALL PHFRNO
000502      67 FITINT=.001
000504      EITIN=.003
000505      EITNO=.11111111
000507      NINIF=11
000510      CALL TORIN
000511      INMPL4=INMX0
000513      INMPL5=INMX0+1
000515      IF (IDEN=128) 68,72,72
000517      68 CALL CLOCK(AHCDEF)
000521      WRITE(9,681) ABCDEF
000527      681 FORMAT(22HOCLOCK BEFORE FIGAFC =,E15.8)
000527      CALL FIGAFC
000530      CALL CLOCK(AHCDEF)
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),
      M=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      GAM0=GAEVFC(1,1)
000657      74 REC(1)=.0
000660      HRECNU=HREC
000662      REC(2)=HRECNU
000663      DO 75 N=3,NLIM
000664      HRECNU=HRECNU*AFAREC
000666      75 REC(N)=REC(N-1)+HRECNU
000672      EPS(1)=.0
000673      HEPSNU=HEPS
000674      EPS(2)=HEPSMU
000675      DO 76 M=3,MLIM
000677      HEPSNU=HEPSNU*AFAEPS
000701      76 EPS(M)=EPS(M-1)+HEPSMU
000705      DO 79 N=1,NLIM
000706      IF (IDEN) 78,77,78
000707      77 SELD(N)=.0
000711      SIGLD(N)=.0
000712      GO TO 79
000712      78 RECOIL=REC(N)
000714      SELD(N)=EXP(-RECOIL*GAM0)
000721      SIGLD(N)=TEMPFN*SELD(N)
000723      79 CONTINUE
000726      80 DO 82 N=1,NLIM
000730      DO 81 M=1,MLIM
000731      SIF(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=TEMPFN*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*TEMPFN)**.5)

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```

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 RETEG(M)=EPS(M)/TEMPEN
001150      CALL TOSCRI
001151      STOP
001153      END

```

\$* ***COMMENT CARD TO BREAK UP BATCH COMPILE

\$IBFTC TOR2 DECK

```

SUBROUTINE TORIN
COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
1SFINAL,ERR,TIMF,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
3CURL,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFC9,COFCN6,
5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
COMMON T2(73,5),S(74,6)
COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHUFRE(201),
1INTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMOND,
3FISTAR,FIFIN,FIS0FN,FIINTF,FIERR,
4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIBEMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NS0CNT,FIS0IT(9),FS0COM,FS0CLU,
7FEVSU,F0DSU,FS0EV,FS0OD,FIARG,FI0CN,
8FIALPH,FIBET,FIGAM
COMMON AFACTO,TE2
COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,FP5MAX,HEPS,AFAP5,
2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
4ALPHEG(50),RETEG(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(2#H0ETININ 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.*TEMPFN))
000047      1*((-ALOG(ETININ/3000.))**.5)
000063      7 WRITE(9,8) NTYPE,FACSIG,ETINT,TINTV
000064      8 FORMAT(7#H0NTYPE=,I4,8# FACSIG=,E15.8,
17# ETINT=,E15.8,7# TINTV=,E15.8)
000063      RETURN
000064      END)

```

***COMMENT CARD TO BREAK UP BATCH COMPILE

```

*IHFTC TOR3 DECK
SUBROUTINE TORCO
000002      COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCON,TFAC,TFIN,
3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFC9,COFCN0,COFCN1,COFCN2,
5COFCN3,COFCN4,COFCN5,COFCN6,COFCN7,COFCN8,COFCN9
000002      COMMON T2(73,5),S(74,6)
000002      COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002      COMMON NIDEN,NINIT,NZEMAX,ZETA(20),PHOFRE(20),
1NTYPE,TEMPEN,ENDIFF,RECOIL,RFSGAM,HEGAL2,
2INDFT,ETININ,FITINT,GAM0,GAMEVE,GAMOND,
3FISTAR,FIFIN,FISOFN,FIINIF,FIHR,
4NFJ,NSOF,FISUIF,FISOER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSCNT,FISUIT(9),FSOCOM,FSOCLD,
7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
8FIALPH,FIHET,FIGAM
000002      COMMON AFACTO,TEP
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HRFC,AFARFC,EPSSMAX,HEPS,AFHEPS,
2NLTM,MLTM,REC(50),EPS(50),SELD(50),STGELD(50),
3SKF(50,50),SIGFF(50,50),UEBARA(50,50),
4ALPHEG(50),HETEG(50),AFIELD(12),
5INMX0,INMPL4,INMPL5,IMVAR(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(5#H0REC=,E12.5,5# EPS=,E12.5,
15# IND=,I3,8# SFINAL=,E14.7,5# ERR=,F14.7,
24# J1=,I3,4# J2=,I3,8# ARGPAC=,F14.7)
000044      3 IND=1
000045      CALL FORIN
000046      SIGMA=SIGMA+SFINAL
000050      RSICMP=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=RSICMP/ACSCMP
000103      RETURN
000103      END)

```



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S* ***COMMENT CARD TO BREAK UP BATCH COMPILE
SIBFTC PRO DECK
SUBROUTINE PHFRNO
000002 COMMON IND,ETINT,TINTV,OMEGA,OMEGA,TINT0,
1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCON,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,GAMOND,
3FISTAR,FIFIN,FIS0FN,FIINTF,FIERR,
4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NS0CNT,FIS0IT(9),FS0COM,FSUCLD,
7FEVSU,FODSU,FS0EV,FS0OD,FIARG,FIFCN,
8FIALPH,FIHET,FIGAM
000002 COMMON AFACT0,TE2
000002 COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,EPSSMAX,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),GAVFC(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 ZEDIF=ZETA(N)-ZETA(N-1)
000017 IF(ZEDIF)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

```

```

5* ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IRFTC TOSC DECK
SURROUTINE TOSCR1
000002 COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
3CUR1,CUR2,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,RETA,J1,J2,ARGPAC
000002 COMMON NIDEN,NINIT,NZEMAX,ZETA(20),PHOFRE(20),
1NTYPE,TEMPEN,ENDJFF,HECUIL,RESGAM,REGAL2,
2INDF1,ETININ,FITINT,GAM0,GAMEVE,GAMOD0,
3FLSTAR,FIFIN,FISOFN,FINTIF,FEHR,
4NFT,NSOF,FISUIF,FIS0ER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSCNT,FIS0II(9),FSOCOM,FSUCLD,
7FEVSU,FONSU,FS0EV,FSOOD,FIARG,FIFCN,
8FIALPH,FIHET,FIGAM
000002 COMMON AFACTO,TE2
000002 COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
2NLIM,MLIM,REC(50),FPS(50),SELU(50),SIGELD(50),
3SKE(50,50),SIGEF(50,50),DEBARA(50,50),
4ALPHFG(50),BETEG(50),AFIELD(12),
5INMXU,INMPL4,INMPL5,IMVAR(73,28),GAVFC(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(110,2E20.8)
000026 WRITE(11,2)AFAREC,HREC,AFAEPS,HEPS
000042 2 FORMAT(4E20.8)
000042 WRITE(11,3)NLIM
000050 3 FORMAT(110)
000050 WRITE(11,4)(HEC(N),N=1,NLIM)
000063 4 FORMAT(4F19.8)
000063 WRITE(11,5)MLIM
000071 5 FORMAT(19)
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(1H)
000114 DO 8 N=1,NLIM
000116 8 WRITE(11,9)(SKF(N,M),M=1,MLIM)
000135 9 FORMAT(5E15.8)
000135 10 WRITE(9,110)
000141 110 FORMAT(55H1
000141 WRITE(9,1)(AFIELD(J),J=1,12)
000153 WRITE(9,11)IDEN,INMXU
000163 11 FORMAT(6H0IDEN=,I4,7H INMXU=,I4)
000163 IF(IDEN)12,1H,14
000165 12 WRITE(9,13)ZETA(NZEMAX)
000174 13 FORMAT(14H0ZETA(NZEMAX)=,E15.8)
000174 GO TO 18
000175 14 WRITE(9,15)NZEMAX
000203 15 FORMAT(8H0NZEMAX=,I4)
000203 WRITE(9,16)
000207 16 FORMAT(35H0ZETA ZETA PHOFRE)
000207 WRITE(9,17)(NZETA,ZETA(NZETA),PHOFRE(NZETA),
1NZETA=1,NZEMAX)
000227 17 FORMAT(15,E17.8,F17.8)
000227 18 WRITE(9,19)TEMPEN
000235 19 FORMAT(8H0TEMPEN=,E15.8)
000235 WRITE(9,20)RECMAX,HREC,AFAREC
000247 20 FORMAT(8H0RECMAX=,E15.8,6H HREC=,E15.8,8H AFAREC=,
1E15.8)

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1)

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000247      WRITE(9,21)EPSMAX,HEPS,AFAEPS
000261      21 FORMAT(8H0EPSMAX=,E15.8,6H HEPS=,E15.8,8H AFAEPS=,
      1E15.8)
000261      WRITE(9,22)NLIM
000267      22 FORMAT(6H0NLIM=,I4)
000267      WRITE(9,23)MLIM
000275      23 FORMAT(6H0MLIM=,I4)
000275      WRITE(9,24)
000301      24 FORMAT(50H0 N          REC          SELD          SIGELD)
000301      WRITE(9,25)(N,REC(N),SELD(N),SIGFLD(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          HETEG          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,OMEGA,TTINTO,
      1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
      2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
      3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
      4COFC5,COFC6,COFC7,COFC8,COFC9,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),
      1INTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGAL2,
      2INDFI,ETININ,FIINT, GAMO,GAMEVE,GAMODD,
      3FISTAR,FIFIN,FIS0FN,FIINTF,FIERR,
      4NFI,NSOF,FISUIF,FIS0ER,FIALMU,FIREFU,
      5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
      6NS0CNT,FIS0IT(9),FS0COM,FSUCLU,
      7FEVSU,F0DSU,FS0EV,FS0OD,FIARG,FIFCN,
      8FIALPH,FIBET,FIGAM
000002      COMMON AFACTO,TEP
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
      1RECMAX,HREC,AFARFC,EPSSMAX,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)
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 CONTR0
000004      RETURN
000005      END

```

\$* **COMMENT CARD TO BREAK UP BATCH COMPILE

\$IBFTC FORM DECK

```
000002      SUBROUTINE PAR
             COMMON INI,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
             1SFINAL,EPR,TIME,FIRST,FINAL,FCN,FSFCN,
             2FNFCN,HT,TEMP3,ARGCON,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,HECOIL,RESGAM,REGA12,
             2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
             3FISTAR,FIFIN,FISOFN,FIINIF,FIENR,
             4NFI,NSOF,FISUIF,FISNER,FIALMU,FIEMU,
             5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
             6NSCNT,FISOIT(9),FSOCOM,FSOCLD,
             7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
             8FIALPH,FIBET,FIGAM
000002      COMMON AFACTO,TEP
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
             1HRCMAX,HREC,AFARFC,EPSMAX,HEPS,AFΔEPS,
             2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
             3SMF(50,50),SIGFF(50,50),VEHARA(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-.44335956F-05)101,101,102
000013      101 GO TO 30
000014      102 IF (ARG-.13300787E-04)103,103,104
000017      103 HT0=.17734382E-04/OMEGAA
             GO TO 30
000021      104 IF (ARG-.39902361F-04)105,105,106
000022      105 HT0=.53203147E-04/OMEGAA
             GO TO 30
000027      106 IF (ARG-.11970708E-03)107,107,108
000030      107 HT0=.15960944E-03/OMEGAA
             GO TO 30
000033      108 IF (ARG-.35912124F-03)109,109,110
000035      109 HT0=.47882833E-03/OMEGAA
             GO TO 30
000036      110 IF (ARG-.10773637E-02)1,1,2
000041      1 HT0=.14364850E-02/OMEGAA
             GO TO 30
000044      2 IF (ARG-.32320912E-02)3,3,4
000047      3 HT0=.430945493E-02/OMEGAA
             GO TO 30
000051      4 IF (ARG-.96962736F-02)5,5,6
000052      5 HT0=.129283648E-01/OMEGAA
             GO TO 30
000055      6 IF (ARG-.29088821F-01)7,7,8
000057      7 HT0=.387850945E-01/OMEGAA
             GO TO 30
000060      8 IF (ARG-.87266463F-01)9,9,10
000063      9 HT0=.116355283/OMEGAA
             GO TO 30
000065      10 IF (ARG-.26179939)11,11,12
000066      11 HT0=.349065850/OMEGAA
             GO TO 30
000071      12 IF (ARG-.78539816)13,13,14
000073      13 HT0=1.04719755/OMEGAA
             GO TO 30
000074      14 IF (ARG-2.3561945)15,15,16
000077      15 HT0=3.14159265/OMEGAA
             GO TO 30
000101      16 IF (ARG-7.0685835)17,17,18
000102      17 HT0=9.42477796/OMEGAA
000105      GO TO 30
000107
000110
000113
000115
000116
000121
000123
000124
000127
000131
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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
000175      27 HT0=ODINT*763.407015/OMEGAA
000201      30 TINT0=3.*HT0
000203      RETURN
000204      END

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$* ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC FORC DECK

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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,CnFCN7,COFCN6,
5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,CnFLN0
000002      COMMON T2(73,5),S(74,6)
000002      COMMON IDEN,ALPHA,RETA,J1,J2,ARGPAC
000002      COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
1NTYPE,TEMPEN,ENDIFF,HECUIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAMU,GAMEVE,GAMODU,
3FIPSTAR,FIFIN,FIS0FN,FIINIF,FIERR,
4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NS0CNT,FIS0IT(9),FS0COM,FS0CLD,
7FEVSU,FO0SU,FS0EV,FS0OD,FIARG,FIFCN,
8FIALPH,FIHET,FIGAM
000002      COMMON AFACTU,TE2
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAH,HREC,AFAREC,EPSMAX,HEPS,AFAEPS,
2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),
3SKE(50,50),SIGEF(50,50),DEHARA(50,50),
4ALPHEG(50),BETEG(50),AFIELU(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

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000025      CALL FCNCAL
000026      FNFCN=FCN
000030      IPRF.IN=0
000031      GO TO 6
000031      5 FINAL=TINTV
000033      TIME=FINAL
000034      CALL FCNCAL
000035      FNFCN=FCN
000037      IPRF.IN=1
000040      6 J2=1
000041      DU 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)=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+CUR1
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+CUR1+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+CUR1+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+CUR1+COR2
000300      DU 16 K2=1,5
000301      16 T2(J2+1,K2)=T2(J2+1,5)
000310      GO TO 23

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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
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-FINT)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

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OMIT

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000522      39 INDJ1=0
000523      INDJ1P=0
000524      40 HT=IINT0
000526      41 ARGCOR=OMEGAA*HT
000530      42 IF (INDJ1)43,43,54
000532      43 TF (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      TF (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/J.
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

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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
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 E1NJ1P=FLOAT(J1P)
001266      ARGP1=.5*E1NJ1P
001267      ARGP2=ARGP1+.51

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001271      ARGP3=AIN(T(ARGP1)
001273      ARGP4=AIN(T(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 TINT0=3.*TINT0
001315      182 FINAL=FINAL+TINT0
001317      TIME=FINAL
001320      CALL FCNCAL
001321      FNFCN=FCN
001323      IF (OMEGA*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+TINT0
001351      TIME=FINAL
001352      CALL FCNCAL
001353      FNFCN=FCN
001355      IF (OMEGA*FINAL-5.E+07) 82,85,85
001361      END

```

\$* ***COMMENT CARD TO BREAK UP BATCH COMPILE

```

$IHFTC FOR( DECK
SUBROUTINE ENDSUM(K1,KN1)
000004      COMMON IND,ETINT,TINTV,OMEGA,OMEGA*,TINT0,
1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCON,TFAC,TFIN,
3CUR1,COF2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFCN8,CNFCN7,COFCN6,
5COFC15,COFCN4,COFCN3,COFCN2,COFCN1,CNFCN0
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),
1INTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGAL2,
2INDP1,ETININ,FITINT,GAM0,GAMVF,GAMODU,
3FISTAR,FIFIN,FIS0FN,FIINTF,FIERR,
4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINT(9),FICOMP,FICOLD,
6NS0CNT,FIS0IT(9),FS0COM,FSOCLU,
7FEVSU,F0DSU,FS0EV,FS0OD,FIARG,FIFCN,
8FIALPH,FIBET,FIGAM
000004      COMMON AFACT0,TEP
000004      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
2NLJM,MLIM,REC(50),EPS(50),SELU(50),STGLD(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      COFC3=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)

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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

```

S* ***COMMENT CARD TO BREAK UP BATCH COMPILE

```

$IBFTC FORE DECK
000006      SUBROUTINE NEXSUM(K2,K4,KN4,KN2)
COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
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),
INTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
2INFI,ETININ,FITINT,GAM0,GAMEVE,GAMOD,
3FISTAR,FIFIN,FIS0FN,FIINTF,FIERR,
4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIEMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NS0CNT,FIS0IT(9),FS0COM,FS0CLD,
7FEVSU,F0DSU,FS0EV,FS0OD,FIARG,FIFCN,
8FIALPH,FIBET,FIGAM
000006      COMMON AFACT0,TE2
000006      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),GA0DFC(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

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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 FN=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

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\$* ***COMMENT CARD TO BREAK UP BATCH COMPILE

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$IBFTC FORH DECK
SUBROUTINE FULSUM(K5,K7,K8,KN8,KN7,KN5)
COMMON IND,ETINT,TINTV,OMEGA,OMEGA,TIME0,
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
COMMON T2(73,5),S(74,6)
COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
INTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGAL2,
2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMOND,
3FISTAR,FIFIN,FIS0FN,FIINTF,FIERR,
4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIEMU,
5NCOUNT,FIHT,FIINT(9),FICOMP,FICOLD,
6NS0CNT,FIS0IT(9),FS0COM,FS0CLU,
7FEVSU,FODSU,FS0EV,FS0OD,FIARG,FIFCN,
BF1ALPH,FIBET,FIGAM
COMMON AFACTO,TEP
COMMON FACSIG,SIGMA,SIGMAC,ETINO,
IRECMAX,HREC,AFAREC,EP5MAX,HEPS,AFAEPS,
2NLIM,MLIM,REC(50),EPS(50),SELD(50),SIGELD(50),

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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

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$* ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC FORH DECK
SUBROUTINE SMSUM(K1,K2,K3)
000005 COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCON,TFAC,TFIN,
3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFCN8,CNFCN7,COFCN6,
5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,CNFCN0
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,HFCOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
3F1STAR,FIFIN,FIS0FN,FIINTF,FIERR,
4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIHEMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSOCNT,FIS0IT(9),FSOCOM,FSOCLD,
7FEVSU,FODSU,FS0EV,FS0OD,FIARG,FIFCN,
8FIALPH,FIBET,FIGAM
000005 COMMON AFACT0,TE2
000005 COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
2NLIM,MLIM,REC(50),EPS(50),SELU(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 IF(INN)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 ENI

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$* ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IHFTC FORH DECK
SUBROUTINE FACFIN
000002 COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
1SFINAL,FRR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCON,TFAC,TFIN,
3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFCN8,CNFCN7,COFCN6,
5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,CNFCN0
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,HFCOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
3F1STAR,FIFIN,FIS0FN,FIINTF,FIERR,
4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIHEMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSOCNT,FIS0IT(9),FSOCOM,FSOCLD,
7FEVSU,FODSU,FS0EV,FS0OD,FIARG,FIFCN,
8FIALPH,FIBET,FIGAM
000002 COMMON AFACT0,TE2
000002 COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,EPSMAX,HEPS,AFAEPS,
2NLIM,MLIM,REC(50),EPS(50),SELU(50),SIGELD(50),

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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     COFC0=FSFCN*COS(OMEGA*TIME)
000135     TFIN=.5*HT*COFC0
000137     TIME=FINAL
000141     COFC0=FNFCN*COS(OMEGA*TIME)
000146     TFIN=TFIN+.5*HT*COFC0
000151     RETURN
000152   6 TIME=FIRST
000154     COFC0=FSFCN*SIN(OMEGA*TIME)
000161     TFIN=.5*HT*COFC0
000163     TIME=FINAL
000165     COFC0=FNFCN*SIN(OMEGA*TIME)
000172     TFIN=TFIN+.5*HT*COFC0
000175     RETURN
000176     END

```

```

S* ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC FORI   DECK
SUBROUTINE CORR1
000002   COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
3CURL,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFC9,COFCN0,COFCN1,COFCN2,
5COFCN3,COFCN4,COFCN5,COFCN6,COFCN7,COFCN8,COFCN9
000002   COMMON T2(73,5),S(74,6)
000002   COMMON IDEN,ALPHA,RETA,J1,J2,ARGPAC
000002   COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
INTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODU,
3FISTAR,FIIFIN,FIS0FN,FIINTF,FIERR,
4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NS0CNT,FIS0IT(9),FS0COM,FS0CLD,
7FEVSU,FODSU,FS0EV,FS0OD,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 CUR1=.0
000006      RETURN
000007      2 CUR1=-.125*(COFC0+COFCN0)
          1+.106666667*(COFC1+COFCN1)
          2=-.416666667E-01*(COFC2+COFCN2)

000022      CUR1=HT*COR1
000023      RETURN
000024      END

```

```

S* ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC FORJ DECK

```

```

SUBROUTINE CORR2
000002      COMMON IND,ETINT,TINTV,OMEGA,OMEGA,OMEGA,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,NINT,NZEMAX,ZETA(201),PHOFRE(201),
          1NTYPE,TEMPEN,ENDIFF,RECUIL,RESGAM,REGAL2,
          2JNDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODD,
          3F1STAR,FIFIN,FISOFN,FIINTF,FIERR,
          4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIREMU,
          5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
          6NS0CNT,FIS0IT(9),FS0COM,FS0CLD,
          7FEVSU,F0DSU,FS0EV,FS0OD,FIARG,FIFCN,
          8FIALPH,FIRET,FIGAM
000002      COMMON AFACTO,TEP
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
          1RECMAX,HREC,AFARFC,EP5MAX,HEPS,AFAPES,
          2NLM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
          3SKF(50,50),SIGFF(50,50),DEBARA(50,50),
          4ALPEG(50),BETEG(50),AFIELD(12),
          5INMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
000002      IF (ARGCOR=1.05)2,1,1
000005      1 CUR2=.0
000006      RETURN
000007      2 CUR2=-.419432941E-01*(COFC0+COFCN0)
          1+.444476872*(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-.72355485E-01*(COFC8+COFCN8)
000052      CUR2=HT*COR2
000053      RETURN
000054      END

```

```

S* ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC FORW DECK

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```

SUBROUTINE FIGAFC
000002      COMMON IND,ETINT,TINTV,OMEGA,OMEGA,OMEGA,TINTO,
          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,BFTA,J1,J2,ARGPAC
000002      COMMON NIDFN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
INTYPE,TEMPEN,ENDIFF,WFCOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODD,
3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
4NFI,INSOF,FISOIF,FISOER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSOCNT,FISOIT(9),FSOCOM,FSUCLD,
7FEVSU,FODSU,FSDEV,FSOOD,FIARG,FIICN,
8FIALPH,FIHET,FIGAM
000002      COMMON AFACTO,TE2
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMA,HPREC,AFAREC,FPSMAX,HEPS,AFAPES,
2NLIM,MLIM,REC(50),EPS(50),SELU(50),SIGELD(50),
3SKE(50,50),SIGEF(50,50),UEBARA(50,50),
4ALPHEG(50),BETEG(50),AFIELD(12),
5INMX0,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)
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

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000266 501 FORMAT(8HOFITINT=,E15.8)
000266 INDFI=0
000267 TIME=.0
000270 CALL FTLINT
000271 IF (FIERR=.02)12,12,10
000274 10 WRITE(9,11)N,M,INDFI,TIME,FIINTF,FIERR,FISOIF,FISDER
000320 11 FORMAT(3HON=,I2,3H M=,I2,5H NFI=,I2,
16H TIME=,E13.6,8H FIINTF=,E13.6,7H FIERR=,E13.6,
28H FISOIF=,E13.6,8H FISDER=,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,FISDER
000361 14 GAUVFC(N,M)=FIINTF
000366 INDFI=1
000367 CALL FTLINT
000370 IF (FIERR=.02)16,16,15
000373 15 WRITE(9,11)N,M,INDFI,TIME,FIINTF,FIERR,FISOIF,FISDER
000417 16 GAUVFC(N,M)=FIINTF
000431 17 RETURN
000432 END

```

3* ***COMMENT CARD TO BREAK UP BATCH COMPILE

```

$IBFTC TORX DECK
SUBROUTINE FCNCL
000002 COMMON IND,EIINT,TINTV,OMEGA,UMEGAA,TINTO,
1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2NF1,HT,TEMP3,ARGCON,TFAC,TFIN,
3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFC9,CNFCN7,COFCN6,
5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,CNFCN0
000002 COMMON T2(73,5),S(74,6)
000002 COMMON IDEN,ALPHA,RETA,J1,J2,ARGPAC
000002 COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
1NTYFF,TEMPEN,ENDIFF,RECOIL,RESGAM,REGAL2,
2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
3FISTAR,FIFIN,FISDFN,FIINTF,FIERR,
4NF1,NSOF,FISOIF,FISDER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSCNT,FISOIT(9),FSOCOM,FSUCLU,
7FEVSU,FODSU,FSOEV,FSOOD,FIARG,FIFCN,
8FIALPH,FIHET,FIGAM
000002 COMMON AFACTO,TE2
000002 COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,EPSSMAX,HEPS,AFALPS,
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),
5INMXU,INMPL4,INMPL5,TIMVAR(73,28),GAUVFC(72,28),GAUVFC(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 ARGUIF=TIME-TIMVAR(NTVAR,1)

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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 AHC=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)
            RETURN
000241      16 FCN=-EXP(RECOIL*(GAMEVE-GAM0)-REGA12*TIME)
            1*SIN(RECOIL*GAMODD)
            RETURN
000256      17 IF (MTVAR-28) 18,9,9
000257      18 MTVAR=MTVAR+1
000262      GO TO 8
000264      ENN
000264

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$* ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IBFTC IRL2 DECK

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```

SUBROUTINE FILINT
000002      COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
            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,TEMPE,ENDIFF,RECOIL,RESGAM,REGA12,
            2INOFI,ETININ,FITINT,GAM0,GAMEVE,GAMODD,
            3FISTAP,FIFIN,FIS0FN,FIINTF,FIERR,
            4NFI,NSOF,FISOIF,FISOER,FIALMU,FIEMU,
            5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
            6NSNCNT,FISOIT(9),FSOCOM,FSOCLD,
            7FEVSU,FODSU,FS0EV,FSOOD,FIARG,FIFCN,
            8FIALPH,FIBET,FIGAM

```

```

000002      COMMON AFACTO,TEP
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO.
                1HRCMAX,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),RETEG(50),AFIELD(12),
                5INMXU,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      FIEKR=.0
000006      RETURN
000006      3 FIFIN=ZETA(NZEMAX)
000011      CALL FIINIT
000012      CALL FICONT
000013      IF (FISTAR) 4,4,5
000015      4 FIS0IF=.0
000016      FIS0ER=.0
000017      RETURN
000017      5 IF (FISTAR=ZETA(NZEMAX)) 13,14,14
000023      13 FIS0FN=FISTAR
000025      GO TO 15
000025      14 FIS0FN=ZETA(NZEMAX)
000030      15 CALL FIS0IN
000031      CALL FIS0CO
000032      FIINTF=FIINTF+FI0IF
000034      FIFRR=FIFRR+ABS((FIINTF-FIS0IF)/FIINTF)
                1+FIS0ER*ABS(FIS0IF/FIINTF)
000043      RETURN
000044      END

```

```

$* ***COMMENT CARD TO BREAK UP HATCH COMPILE
$IRBTC IRM2 DECK

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```

000002      SUBROUTINE FIINIT
                COMMON IND,ETINT,TINTV,OMEGA,UMEGAA,TINT0,
                1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
                2FINFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
                3CURL,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
                4COFC5,COFC6,COFC7,COFC8,COFC9,COFC10,COFC11,COFC12,
                5COFC13,COFC14,COFC15,COFC16,COFC17,COFC18,COFC19,COFC20
                COMMON T2(73,5),S(74,6)
000002      COMMON IDEN,ALPHA,RETA,J1,J2,ARGPAC
000002      COMMON NIDFN,NINIT,NZEMAX,ZETA(201),PHUFRE(201),
                1NTYPE,TEMPEN,ENDIFF,HECOIL,RESGAM,REGAL2,
                2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMOND,
                3FISTAR,FIFIN,FIS0FN,FIINTF,FIERR,
                4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIHEMU,
                5NCOUNT,FINT,FIINTE(9),FICOMP,FICOLD,
                6NSCNT,FIS0IT(9),FS0COM,FSUCLD,
                7FEVSU,FODSU,FS0EV,FS0OD,fIARG,FIFCN,
                8FIALPH,FIHET,FIGAM
000002      COMMON AFACTO,TEP
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO.
                1HRCMAX,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),RETEG(50),AFIELD(12),
                5INMXU,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      FIHEMU=FIFCN*COS(FIFIN*TIME)
000023      FIARG=FISTAR
000024      CALL FIFNCA
000025      FIALMU=FIALMU-FIFCN*SIN(FISTAR*TIME)

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```

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=ATN(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

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```

000002      SUBROUTINE FICONT
COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINTD,
1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
3COR1,COR2,COFCN,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFCN8,CNFCN7,COFCN6,
5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,CNFCN0
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),
INTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMOND,
3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
4NFI,NSOF,FISUIF,FISOER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSNCNT,FISOIT(9),FSNCOM,FSOCLD,
7FEVSU,FODSU,FSOEV,FSUOD,FIARG,FIFCN,
8FIALPH,FIRET,FIGAM
000002      COMMON AFACTO,TEP
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,EPSSMAX,HEPS,AFAEPS,
2NLM,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      IF(FISTAR-ZETA(NZEMAX))101,100,100
000006      100 FIINTF=.0
000007      FIEKR=.0
000010      RETURN
000010      101 NFI=5
000011      FIHT=(FIFIN-FISTAR)/10.
000014      CALL FIEVSU
000015      CALL FIODSU
000016      CALL FIARGA
000017      FIINTE(1)=FIHT*(FIALPH*FIALMU+FIRET*(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 FIARGA
000040      FIINTE(NCOUNT)=FIHT*(FIALPH*FIALMU+FIRET*(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 IR02 DECK

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```

000002      SUBROUTINE FIEVSU
          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
          1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
          2FNFCN,HT,TEMP3,ARGCON,TFAC,TFIN,
          3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
          4COFC5,COFC6,COFC7,COFC8,COFCN8,C0FCN7,COFCN6,
          5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,C0FCN0
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),
          INTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
          2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMOD,
          3FISTAR,FIFIN,FIS0FN,FIINTF,FIERR,
          4NFI,NS0F,FIS0IF,FIS0ER,FIALMU,FIREMU,
          5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
          6NS0CNT,FIS0IT(9),FS0COM,FS0CLD,
          7FEVSU,F0DSU,FS0EV,FS0OD,FIARG,FIFCN,
          8FIALPH,FIHET,FIGAM
000002      COMMON AFACT0,TE2
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
          1RECMA, HREC,AFARFC,EPSSMAX,MEPS,AFAPES,
          2NLIM,MLIM,REC(50),EPS(50),SEL(50),SIGELD(50),
          3SKE(50,50),SIGEF(50,50),UEBARA(50,50),
          4ALPHEG(50),BETEG(50),AFIELD(12),
          5JNMX0,INMPL4,INMPL5,TIMVAR(73,28),GAFVFC(72,28),GAODFC(72,28)
          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 IRP2 DECK

```

```

000002      SUBROUTINE FIODSI
          COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
          1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
          2FNFCN,HT,TEMP3,ARGCON,TFAC,TFIN,
          3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
          4COFC5,COFC6,COFC7,COFC8,COFCN8,C0FCN7,COFCN6,
          5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,C0FCN0

```

```

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),
INIYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODD,
3FISTAR,FIFIN,FISQFN,FIINTF,FIERR,
4NFI,NSOF,FISQIF,FISQER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSQNT,FISQIT(9),FSQCOM,FSQCLD,
7FEVSU,FODSU,FSQEV,FSQOD,FIARG,FIFCN,
8FIALPH,FIBET,FIGAM
000002      COMMON AFACTO,TE2
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,EPSSMAX,HEPS,AFAPES,
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),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 TORQ DECK

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```

000002      SUBROUTINE FIARGA
COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
1SFINAL,ERR,TIME,FIIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCOM,TFAC,TFIN,
3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFC9,COFCN0,COFCN1,COFCN2,
5COFCN3,COFCN4,COFCN5,COFCN6,COFCN7,COFCN8,COFCN9
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),
INIYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODD,
3FISTAR,FIFIN,FISQFN,FIINTF,FIERR,
4NFI,NSOF,FISQIF,FISQER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSQNT,FISQIT(9),FSQCOM,FSQCLD,
7FEVSU,FODSU,FSQEV,FSQOD,FIARG,FIFCN,
8FIALPH,FIBET,FIGAM
000002      COMMON AFACTO,TE2
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,EPSSMAX,HEPS,AFAPES,
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),GAEVFC(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.)F-5)2,2,12
000014      12 THETA2=THETA**2
000016      THETA3=THETA**3

```

```

000017      FIALPH=.44444444F-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      SINTE=SIN(THETA)
000051      COSTHE=COS(THETA)
000053      SITHE3=SINTE/THETA3
000055      COTHE2=COSTHE/THETA2
000057      SICOTH=COSTHE*SITHE3
000061      SI2TH3=2.*SINTE*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=.66666667
000102      FIGAM=1.33333333
000103      RETURN
000104      END

```

** ***COMMENT CARD TO BREAK UP BATCH COMPILE
\$IBFTC IRR2 DECK

```

000002      SUBROUTINE FISOIN
            COMMON IND,ETINT,TINIV,OMEGA,OMEGAA,TINT0,
            1SFINAL,FRR,TIME,FIRST,FINAL,FCN,FSFCN,
            2FNFCN,HT,TEMP3,ARGCON,TFAC,TFIN,
            3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
            4COFC5,COFC6,COFC7,COFC8,COFCN8,CNFCN7,COFCN6,
            5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,CNFCN0
            COMMON T2(73,5),S(74,6)
000002      COMMON IDEN,ALPHA,REFIA,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,FISUIF,FISLER,FIALMU,FIEMU,
            5NCOUNT,FIHT,FIINTE(9),FICOMP,FIOLU,
            6NSCNT,FISOIT(9),FSOCOM,FSOCLU,
            7FEVSU,FONSU,FSOEV,FSOOD,FIARG,FIFCN,
            8FIALPH,FIHET,FIGAM
000002      COMMON AFACTO,TE2
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
            1RECMAX,HREC,AFARFC,FPSMAX,HEPS,AFAPES,
            2NLM,MLIM,REC(50),EPS(50),SELU(50),STWELD(50),
            3SKE(50,50),SIGFF(50,50),UEBARA(50,50),
            4ALPHEG(50),BETEG(50),AFIELU(12),
            5INMX0,INMPL4,INMPL5,IMVAR(73,28),GAEVFC(72,28)
000002      FIARG=.0
000003      CALL FIFNCA
000004      IF(INDFI)2,1,2
000005      1 FIHEMU=FIFCN
000007      GO TO 3
000007      2 FIALMU=FIFCN
000011      3 FIARG=FISOFN
000013      CALL FIFNCA
000014      IF(INDFI)5,4,5

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```

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

```

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$* ***COMMENT CARD TO BREAK UP BATCH COMPILE
$IRFTC TORR   DECK

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```

000002      SUPROUTINE FISOCN
COMMON IND,ETINT,TINTV,OMEGA,UMEGA,TINTO,
1SFINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCON,TFAC,TFIN,
3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFCN8,COFCN7,COFCN6,
5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,COFCN0
COMMON T2(73,5),S(74,6)
000002      COMMON IDEN,ALPHA,BETA,J1,J2,ARGPAC
000002      COMMON NIDEN,NINIT,NZEMAX,ZETA(201),PHOFRE(201),
000002      INTYPE,TEMPEN,ENDIFF,RECOIL,REGAM,REGA12,
2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMODU,
3FISTAR,FIFIN,FISOFN,FIINTF,FIERR,
4NFI,NSOF,FISOF,FISOFER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
6NSOCNT,FISOIT(9),FSOCOM,FSOCLU,
7FEVSU,FOISU,FSOEV,FSOOD,FIARG,FIFCN,
8FIALPH,FIBET,FIGAM
000002      COMMON AFACTO,TE2
000002      COMMON FACSIG,SIGMA,SIGMAC,ETINO,
1RECMAX,HREC,AFARFC,FPSMAX,HEPS,FAEPS,
2NLM,MLM,REC(50),EPS(50),SEL(50),SIGELD(50),
3SKF(50,50),SIGFF(50,50),UEBARA(50,50),
4ALPHFG(50),BETFG(50),AFILLU(12),
5INMXU,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+FIRET
1*(FIBEMU+FSOEV)+FIGAM*FSOOD)
000020      NSOCNT=2
000021      FSOCOM=1.
000022      1 NSOF=NSOF+NSOF
000023      FIHT=FIHT/2.
000025      FSOEV=FSOEV+FSOOD
000027      CALL FISOOD
000030      CALL FIABGA
000031      FISOIT(NSOCNT)=FIHT*(FIALPH*FIALMU+FIBET
1*(FIBEMU+FSOEV)+FIGAM*FSOOD)
000042      FSOCLU=FSOCOM
000043      NSOLS1=NSOCNT-1
000045      FSOCOM=ABS(1.-FISOIT(NSOCNT)/FISOIT(NSOLS1))
000052      IF (FSOCOM-FITINT) 2,2,3
000054      2 IF (FSOCLU-FITINT) 21,21,3
000057      21 FISOIF=FISOIT(NSOCNT)
000062      FISUER=FSOCOM
000063      RETURN
000064      3 IF (NSOCNT-8) 4,21,21
000067      4 NSOCNT=NSOCNT+1
000071      GO TO 1
000071      END

```

** ***COMMENT CARD TO BREAK UP BATCH COMPILE
 \$IBFTC TRT2 DECK

```

000002  SURROUTINE FIS0EV
        COMMON IN0,ETINT,TINTV,OMEGA,OMEGA,TINT0,
        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,NINJT,NZEMAX,ZETA(201),PHOFRE(201),
        1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
        2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMOND,
        3F1STAR,FIFIN,FIS0FN,FIINTF,FIERR,
        4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIEMU,
        5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
        6NS0CNT,FIS0IT(9),FS0COM,FS0CLU,
        7FEVSU,F0DSU,FS0EV,FS0OD,FIARG,FIFCN,
        8FIALPH,FIHET,FIGAM
000002  COMMON AFACT0,TEP
000002  COMMON FACSIG,SIGMA,SIGMAC,ETINO,
        1RECMAX,HREC,AFARFC,EP5MAX,HEPS,AFAPES,
        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),
        5TIMX0,INMPL4,INMPL5,IMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
000002  FS0EV=.0
000003  NITERM=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 FS0EV=FS0EV+FIFCN*COS(FITRIG*TIME)
000024  GO TO 3
000025  2 FS0EV=FS0EV+FIFCN*SIN(FITRIG*TIME)
000034  3 CONTINUE
000037  RETURN
000037  END
  
```

** ***COMMENT CARD TO BREAK UP BATCH COMPILE
 \$IBFTC TRU2 DECK

```

000002  SURROUTINE FIS00F
        COMMON IN0,ETINT,TINTV,OMEGA,OMEGA,TINT0,
        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,NINJT,NZEMAX,ZETA(201),PHOFRE(201),
        1NTYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
        2INDFI,ETININ,FITINT,GAM0,GAMEVE,GAMOND,
        3F1STAR,FIFIN,FIS0FN,FIINTF,FIERR,
        4NFI,NSOF,FIS0IF,FIS0ER,FIALMU,FIEMU,
        5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLD,
        6NS0CNT,FIS0IT(9),FS0COM,FS0CLU,
        7FEVSU,F0DSU,FS0EV,FS0OD,FIARG,FIFCN,
        8FIALPH,FIHET,FIGAM
000002  COMMON AFACT0,TEP
000002  COMMON FACSIG,SIGMA,SIGMAC,ETINO,
        1RECMAX,HREC,AFARFC,EP5MAX,HEPS,AFAPES,
        2NLIM,MLIM,REC(50),EPS(50),SELD(50),STGELD(50),
        3SKF(50,50),SIGEF(50,50),UEBARA(50,50),
  
```

```

4ALPHEG(50),BETEG(50),AFIELU(12),
SINMX0,INMPL4,INMPL5,TIMVAR(73,28),GAEVFC(72,28),GAODFC(72,28)
000002   FS00)=.0
000003   DO 3 J=1,NSOF
000005   FITRIG=2,*FIHT*FLUAT(J)=FIHT
000010   FIARG=FITRIG
000011   CALL FIFNCA
000012   IF(INDFI)2,1,2
000013   1 FS00D=FS00D+FIFCN*COS(FITRIG*TIME)
000022   GO TO 3
000023   2 FS00D=FS00D+FIFCN*SIN(FITRIG*TIME)
000032   3 CONTINUE
000035   RETURN
000035   END

```

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$* ****COMMENT CARD TO BREAK UP BATCH COMPILE
$IRFTC TORV DECK

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```

SURROUTINE FIFNCA
000002   COMMON IND,ETINT,TINTV,OMEGA,OMEGAA,TINT0,
1STINAL,ERR,TIME,FIRST,FINAL,FCN,FSFCN,
2FNFCN,HT,TEMP3,ARGCOR,TFAC,TFIN,
3COR1,COR2,COFC0,COFC1,COFC2,COFC3,COFC4,
4COFC5,COFC6,COFC7,COFC8,COFCN8,CNFCN7,COFCN6,
5COFCN5,COFCN4,COFCN3,COFCN2,COFCN1,CNFCN0
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),
INIYPE,TEMPEN,ENDIFF,RECOIL,RESGAM,REGA12,
2INDFI,ETININ,FITINT,GAMO,GAMEVE,GAMODU,
3FISTAR,FIFIN,FISOFN,FIINIF,FIERR,
4NFI,NSOF,FISOIF,FISOER,FIALMU,FIREMU,
5NCOUNT,FIHT,FIINTE(9),FICOMP,FICOLU,
6NSCNT,FISOI(9),FS0COM,FSOCLD,
7FEVSU,FONSU,FS0EV,FS00D,FIARG,FIFCN,
8FIALPH,FIBET,FIGAM
000002   COMMON AFACTO,TE2
000002   COMMON FACSIG,SIGMA,SIGMAC,ETINO,
IRECMAX,HREC,AFARFC,EPSSMAX,HEPS,AFAEPS,
2NLM,MLIM,REC(50),EPS(50),SELU(50),STGELD(50),
3SKE(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)
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-10.111,111,110)
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 SIAK26=.0
000067      GO TO 1115
000070      1114 SIAK26=(SIARG**2)/6.
000073      1115 SIHFC=2.*(SIARG*(1.+SIAK26))
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)-PHOFRE(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*(ARGINT**2)
000161      IF(PHFRCU)115,116,116
000162      115 PHFRCU=.0
000163      116 PARAM=FIARG
000165      GO TO 8
000165      16 PHFRCU=PHOFRE(NZETA)
000170      PARAM=FIARG
000171      GO TO 8
000172      17 NZETA=NZETA+1
000174      GO TO 14
000174      END

```