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CODAC

A FORTRAN IV Programme to Process a TIMOC Library from the ENDF/B File

by

H. KRAINER

1970

Joint Nuclear Research Center
Ispra Establishment - Italy
Reactor Theory and Calculation

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CODAC generates the group averaged values of σ_c, σ_{el}, σ_{in}, σ_f and ν, the angular distribution function for elastic scattering and different inelastic scattering models. With this code one has the possibility to obtain group averaged data for special, problem orientated group limits.

CODAC is written in FORTRAN IV for an IBM 360/65 using no programming tricks and nearly no machine features, so that it will run, except for minor modifications, on any other machine which is large enough. For the sake of saving computer space, it is built up in an overlay structure.

CODAC uses the retrieval subroutines developed by H.C. Honeck and parts of the ETOM-ETOG code of Westinghouse which produces inputs for MUFT and GAM.

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ABSTRACT

The processing of nuclear data from standard cross section libraries is of particular importance for Monte Carlo programmes which can handle a large number of nuclear input parameters. The CODAC code is designed to produce these parameters from the ENDF/B data file in the form of group averaged cross sections and scattering models. The output formats of CODAC agree with the input specifications of the Monte Carlo code TIMOC.

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KEYWORDS

MONTE CARLO METHOD
FORTRAN
MATHEMATICS
INELASTIC SCATTERING
ANGULAR DISTRIBUTION
DOCUMENTATION
CROSS SECTIONS

C O D A C

A FORTRAN IV PROGRAMME TO PROCESS A TIMOC LIBRARY FROM THE ENDF/B FILE *)

1. INTRODUCTION

The processing of nuclear data from standard cross section libraries is of particular importance for Monte Carlo programmes which can handle a large number of nuclear input parameters. The CODAC code is designed to produce these parameters from the ENDF/B data file[2,3] in the form of group averaged cross sections and scattering models. The output formats of CODAC agree with the input specifications of the Monte Carlo code TIMOC.[1]

CODAC generates the group averaged values of σ_c, σ_{el}, σ_{in}, σ_f and ν, the angular distribution function for elastic scattering and different inelastic scattering models. With this code one has the possibility to obtain group averaged data for special, problem orientated group limits.

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CODAC uses the retrieval subroutines developed by H.C. Honeck[4] and parts of the ETOM-ETOG code of Westinghouse[5,6] which produces inputs for MUFT and GAM.

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*) Manuscript received on 15 June 1970

2. PROGRAMME DESCRIPTION

2.1 General Informations

In this report reference is made to TIMOC input formats and to the ENDF/B structure and notation; however, the ENDF/B notation and TIMOC input parameters will not be explained in detail here.

In the following a quantity without an argument (e.g. σ_{el}) will denote a group averaged value, while a quantity with an argument (e.g. $\sigma_{el}(E)$) will represent an energy dependent description.

Group averaged values are usually calculated as

$$\sigma^i = \frac{\int_i \sigma(E)\, W(E)\, dE}{\int_i W(E)\, dE}$$

In this expression the integral is taken over the energy range of group i ($E_i - E_{i+1}$). W(E) is the weighting function and may be given in four different ways:

a) Constant weighting with W = 1.0

b) Weighting function W = 1/E

c) Weighting spectrum given point by point together with the interpolation codes and ranges (ENDF/B standard)

d) Weighting spectrum given as a polynomial in E. Input: the coefficients of the polynomial.

2.2 Smooth Cross Sections

Input block II of the TIMOC code (all microscopic group averaged cross sections) requires the group mean values of the cross sections for capture, elastic scattering, inelastic scattering, fission, and of the particle multiplication factor for fission. The last value is obtained from ENDF/B file 1, while most of the other required data are contained in ENDF/B file 3. If the resonance representation

contributes to the smooth cross sections, the results obtained from ENDF/B file 2 are added to the smooth part.

Cross sections less than 10^{-4} are set equal to zero in the output.

2.2.1 Smooth Capture

The basic part of the smooth capture cross section is calculated as

$$\sigma_c^i = \sigma_{n\gamma}^i + \sigma_{np}^i + \sigma_{nd}^i + \sigma_{nt}^i + \sigma_{n\,He^3}^i + \sigma_{n\alpha}^i + \sigma_{n2\alpha}^i ,$$

where the averaged quantities, σ_{nx}^i , are calculated as

$$\sigma_{nx}^i = \frac{\int_i \sigma_{nx}(E)\, W(E)\, dE}{\int_i W(E)\, dE} .$$

The $\sigma_{nx}(E)$ tabulations are obtained from ENDF/B file 3.
In the tabulations, the reaction type number has the following meaning:

x = γ	MT = 102
x = p,	MT = 103
x = d,	MT = 104
x = t,	MT = 105
x = He^3,	MT = 106
x = α ,	MT = 107
x = 2α ,	MT = 108

If there exists a resonance contribution, this will be added to the smooth capture cross section (sections 2.3 and 2.4).

2.2.2 Elastic Scattering

The elastic scattering cross section for group i is defined by

$$\sigma_{el}^{i} = \frac{\int_{i} \sigma_{el}(E)\, W(E)\, dE}{\int_{i} W(E)\, dE}$$

where $\sigma_{el}(E)$ is given in ENDF/B file 3, MT = 2.

If the resonance options require, the resonance contributions are added to the smooth cross section (see sections 2.3 and 2.4). The energy dependent smooth part (TAB1 for $\sigma(E)$ or $\sigma(E)\cdot W(E)$, respectively) above the resonance region is temporarily stored in COMMON/DENS/ since it is necessary for the computation of μ_l^i (averaged cosine of the elastic scattering in the Lab. system) and of the secondary angular distribution (TIMOC block III).

2.2.3 Inelastic Scattering

The inelastic scattering cross section is calculated as

$$\sigma_{in}^{i} = \frac{\int_{i} \sigma_{in}(E)\, W(E)\, dE}{\int_{i} W(E)\, dE}$$

where $\sigma_{in}(E)$ is given in ENDF/B file 3, MT = 4.

According to a special input option, n-2n scattering is partly or fully added to σ_{in}^{i} under certain conditions (see sections 2.2.7 and 4.2.10). In addition $\sigma_{in}(E)$ is stored in /DENS/ for later use in the construction of the inelastic scattering matrix.

2.2.4 Fission Cross Section

The basic smooth fission cross section for group i is calculated as

$$\sigma_f^i = \frac{\int_i \sigma_f(E)\, W(E)\, dE}{\int_i W(E)\, dE} .$$

$\sigma_f(E)$ is obtained from ENDF/B file 3, MT = 18.

Again, certain resonance conditions may exist such that a resonance contribution must be added to the smooth fission cross section (see sections 2.3 and 2.4). Under certain circumstances the n, 2n scattering cross section will, according to the corresponding input option, be added half or fully to the smooth fission cross section (see sec. 2.2.7 and 4.2.10). Therefore a non fissionable isotope may show a σ_f.

2.2.5 Neutrons Per Fission

The average number of neutrons per fission is obtained from

$$\nu^i = \frac{(\nu \sigma_f)^i}{\sigma_f{}^i}$$

where

$$(\nu \sigma_f)^i = \frac{\int_i (\nu(E)\, \sigma_f(E))\, W(E)\, dE}{\int_i W(E)\, dE} .$$

$\nu(E)$ is contained in ENDF/B file 1, MT = 452. If $\nu(E)$ is given as a polynomial in E, it is converted into a tabulated (TAB1-) function. $\nu(E)$ is multiplied times the smooth and resonance part of $\sigma_f(E)$ (and possibly with $\sigma_{n,2n}(E)$ or $\frac{1}{2}\sigma_{n,2n}(E)$) and then the above integral is calculated. Thus, a non fissionable isotope can, according to the n-2n treatment (input option), have a factor $\nu = 1$ or $\nu = 2$ (cf. Section 4.2.10).

2.2.6 Averaged Cosine For Anisotropic Scattering

The averaged cosine of the elastic scattering in the Lab. system is calculated for energies above the resonance region as

$$\mu_L^i = \frac{(\mu_L \sigma_{el})^i}{\sigma_{el}^i}$$

where

$$(\mu_L \sigma_{el})^i = \frac{\int_i \mu_L(E)\, \sigma_{el}(E)\, W(E)\, dE}{\int_i W(E)\, dE}$$

and $\mu_L(E)$ is obtained from ENDF/B file 3, MT = 251.

If μ_L is not given for the whole energy range, it is assumed to be $\mu_L = \frac{2}{3A}$ outside the range. The atomic mass ratio A = AWR is given in ENDF/B file 1. $\sigma_{el}(E)$ is the smooth part of file 3.

In and below the resonance region μ_L^i is calculated as

$$\mu_L^i = \frac{\int_i \mu_L(E)\, W(E)\, dE}{\int_i W(E)\, dE} ,$$

Thus in this region the assumption has been made that the elastic scattering is nearly isotropic (or μ_L^i is very small). In the group which covers both ranges, the computational techniques are combined. In practice this is done by assuming the $\sigma_{el}(E)$-curve to be constant in and below the resonance region with the value of the first $\sigma_{el}(E)$-point above the resonance region.

If no $\mu_L(E)$ data are given in file 3, but μ_L^i is desired according to input option N3, it is calculated from ENDF/B file 4, MT = 2 (see section 4.2.5).

2.2.7 n-2n Scattering

TIMOC has no means to explicitly treat the n-2n scattering. Therefore an input option is provided which allows one to treat the n-2n reaction in three different ways:

a) n-2n is added to inelastic scattering
b) n-2n is added half to inelastic, scattering, half to fission
c) n-2n is added to fission

If the isotope is fissile only option a) can be used.

For further details see section 4.2.10.

2.3 Resolved Resonance Treatment

TIMOC contains no specific treatment of the resonances. Therefore the resonance contributions for σ_{el}, σ_c (σ_γ) and σ_f are calculated at a point mesh for each group; these values are then averaged for each group and simply added to the corresponding smooth cross section. For the calculations the single level Breit-Wigner formulation is used:

$$\sigma_{el} = \frac{\sigma_0 \Gamma_n}{\Gamma} \cdot \frac{1}{1+x^2} + 4\pi R^2 + \frac{2x}{1+x^2}\sqrt{\sigma_0 4\pi R^2 \varrho \frac{\Gamma_n}{\Gamma}}$$

$$\sigma_\gamma = \frac{\sigma_0 \Gamma_\gamma}{\Gamma} \cdot \frac{1}{1+x^2}\sqrt{\frac{E_0}{E}}$$

$$\sigma_f = \frac{\sigma_0 \Gamma_f}{\Gamma} \quad \frac{1}{1+x^2}\sqrt{\frac{E_0}{E}} \;,$$

where R is designated as AP in ENDF/B and

$$\sigma_o = \frac{2.6037 \cdot 10^6 \, \Gamma_n \, g}{|E_o| \, \Gamma} \left(\frac{Z + 1.008665}{Z} \right)^2$$

$$\chi = \frac{(E - E_o)}{\Gamma/2}$$

$$g = \frac{2J+1}{2(2I+1)}$$

The accuracy of the calculation of the resonance contribution depends on the choice of the point mesh at which the cross sections are computed. For instance it would be possible to take a mesh of equal lethargy or energy spacing, but, in this case, one is forced to use a large number of points to insure that no resonance or its principal contribution is missed. Therefore it is better to use a variable spacing of the mesh which depends on the number and position of the resonances in the group.

Consequently, the fine mesh is constructed by taking into account the N resonances within the group and the nearest one on each side of the group. Each of the interior resonances are then calculated at 400/(N+1) points. Half of the allotted points go from $(E_o - \frac{\Gamma}{2})$ to $(E_o + \frac{\Gamma}{2})$, the other half from $E_o \pm \frac{\Gamma}{2}$ to the midpoint between two resonances, all with an equal energy spacing. The two resonances on each side of the group are ach covered with 200/(N+1) points, one half going from E_o to $E_o \pm \frac{\Gamma}{2}$ and the other half going from $E_o \pm \frac{\Gamma}{2}$ to the midpoint. Thus the complete fine mesh is taken from the peak of the first resonance below to that of the first resonance above the group. Then the resonance contribution at each point is calculated by summing up the contributions of all the resonances (also that one outside the group) at this point. The resulting tabulation is then averaged with the weighting function and added to the smooth cross section.

2.4 Unresolved Resonance Treatment

As in the case of the resolved resonances the resonance contributions are calculated at a point mesh for each group. These values are then averaged and simply added to the corresponding smooth cross sections.

The technique used here is the same as that used by the Argonne code MC^2 [7] and ETOM [5], which evaluate the resonance part of the cross section at an energy mesh in the unresolved region.

In MC^2, the effective unresolved resonance capture cross section at an energy point is calculated as

$$\sigma_c(E) = \sum \frac{\frac{\sigma_p \Gamma_\gamma}{\langle D \rangle} \int_0^\infty P_n(r) \int_0^\infty P_k(s) \int_0^\infty \frac{\psi}{\psi+\beta} \, dx \, dr \, ds}{1 - \frac{1}{\langle D \rangle} \int_0^\infty P_n(r) \int_0^\infty P_k(s) \, \Gamma \int_0^\infty \frac{\psi}{\psi+\beta} \, dx \, dr \, ds},$$

where the sum is taken over all J states for all ℓ states and

$$P_n(r)\,dr = \frac{n}{2} \frac{1}{\Gamma(\frac{n}{2})} \left(\frac{nr}{2}\right)^{\frac{n}{2}-1} \exp\left(-\frac{nr}{2}\right) dr.$$

This equation is for fissile isotopes while for fertile isotopes the $P_k(s)$ integral must be omitted. A similar equation [7] is used for the calculation of the fission cross section.

CODAC does not include temperature dependence, therefore, a zero temperature is assumed. In this case

$$\int_0^\infty \frac{\psi}{\psi+\beta} \, dx = \frac{\sqrt{\pi}/2}{\sqrt{\beta(1+\beta)}}$$

holds, where β is defined as $\frac{\Sigma_p}{N\sigma_o}$, $\frac{\Sigma_p}{N}$ is the macroscopic potential scattering cross section for the mixture per absorber atom and σ_o is the cross section at the resonance peak.

Since CODAC does not permit mixture dependence, it cannot calculate $\frac{\Sigma_p}{N}$. Hence, the quantity $(\Sigma_p/N - 4\pi R^2)$ must be provided as an input item. Thus, it is possible for the user to select the best $\frac{\Sigma_p}{N}$ -value vor his applications, taking into account the resonance self shielding. Σ_p/N only effects the unresolved resonance treatment.

CODAC calculates the capture, fission and elastic scattering cross section for each group at 100 points, equally spaced in lethargy. These values are then averaged within each group using the input weight and then added to the smooth cross sections.

2.5 Elastic Scattering Secondary Angular Distribution

Block III of the TIMOC input needs all the information on elastic isotropic or anisotropic scattering for each group with $\sigma_{el} \neq 0$. There are four different possibilities (c.f. also section 4.2.5 and 5.4) to represent the angular distribution by:

1) isotropic scattering in the c.m. system
2) a Legendre polynomial expansion in the c.m. system
3) a polygon along the μ-axis in the $\frac{d\sigma}{d\mu}$ -table in the c.m. system
4) the averaged cosine in the Lab. system.

2.5.1 Isotropic Scattering in the c.m. system

For this case no calculation is necessary.

2.5.2 Legendre Polynomial

In this case the coefficients of the Legendre polynomial expansion $\sigma_{el}^{i}(\mu) = \sum_{\ell=0}^{\infty} \alpha_\ell^i P_\ell(\mu)$ are needed. These are calculated as

$$\alpha_\ell^i = \frac{\frac{2\ell+1}{2} \int_i \sigma_{el}(E)\, W(E)\, f_\ell^{c.m.}(E)\, dE}{\int_i \sigma_{el}(E)\, W(E)\, dE},$$

where $f_\ell^{c.m.}(E)$ is given on ENDF/B file 4, MT = 2 and $\sigma_{el}(E)*W(E)$ is already stored in /DENS/ (c.f. sections 2.2.2 and 2.2.6).

2.5.3 Polygon Along the μ-axis

If the elastic secondary angular distribution is calculated as a table in μ in the c.m. system, this is done according to

$$\sigma_{el}^i(\mu_n) = \frac{\int_i \sigma_{el}(E)\, W(E)\, p^{c.m.}(\mu_n, E)\, dE}{\int_i \sigma_{el}(E)\, W(E)\, dE},$$

where $p^{c.m.}(\mu, E)$ is again tabulated on ENDF/B file 4, MT = 2 and $\sigma_{el}(E)*W(E)$ is already stored in /DENS/.

Values less than 10^{-10} are set equal to zero in the output.

2.5.4 Averaged Cosine in the Lab. System

If the $\mu_L(E)$ data are given on ENDF/B file 3, MT = 251, μ_L^i is simply calculated as

$$\mu_L^i = \frac{\int_i \sigma_{el}(E)\, W(E)\, \mu_L(E)\, dE}{\int_i \sigma_{el}(E)\, W(E)\, dE}.$$

$\mu_L(E)$ possibly may not be found on file 3. In this case it is calculated from file 4, MT = 2. If the data given there are in terms of a polygon in the Lab. system, this calculation is done as

$$\mu_L^i = \frac{\int_i dE\, \sigma_{el}(E) W(E) \int_{-1}^{1} p^L(\mu,E)\, \mu\, d\mu}{\int_i dE\, \sigma_{el}(E) W(E) \int_{-1}^{1} p^L(\mu,E)\, d\mu}$$

with $p^L(\mu,E)$ given on ENDF/B file 4, MT = 2. However, data may also be given in the Legendre polynomial version. In this case the averaged cosine results from

$$\mu_L^i = \frac{\int_i \sigma_{el}(E) W(E) f_1^L(E) dE}{\int_i \sigma_{el}(E) W(E) dE}$$

Again $f_\ell(E)$ is given on file 4, MT = 2, but possibly in the c.m. system. In this case $f_\ell^{c.m.}$ is transformed to f_ℓ^L by use of the transfer matrix.

$\sigma_{el}(E) \cdot W(E)$ is already stored in COMMON/DENS/. (c.f. sections 2.2.2 and 2.2.6).

If μ_L^i differs from $\frac{2}{3A}$ by less than 5%, scattering in this group is assumed to be isotropic in the c.m. system.

2.6 Inelastic Matrix Treatment

The TIMOC library requires one of three representations of the inelastic scattering secondary energy distribution. The first two representations (statistical model and excited level description) are not treated by CODAC. So CODAC produces an inelastic scattering matrix as output and input for TIMOC block IV. All necessary information for the calculation of the matrix is found on ENDF/B file 5, MT = 4. There are ten different possible representations on ENDF/B. The present version of CODAC will

handle LF = 2 through 10, although inelastic data usually will be given only as discrete levels (LF = 3) plus a Maxwellian distribution (LF = 8 or 9). The other distribution representation (LF = 1) is not treated by the programme and is ignored by simply returning from the corresponding subroutine.

The transfer matrix is calculated as

$$\sigma_{in}^{i\to j} = \sum_{m} \sigma_{in,m}^{i\to j}$$

where the sum is taken over all different representations LF and, therefore, also over all discrete levels.

For LF = 6, 8 or 10, an E' mesh is constructed which covers the entire energy range and the corresponding LF-function, $f_{LF}(E)$, is calculated at this mesh. Next, the fractional amount in each sink group is computed. The contribution of this LF-function to the probability matrix element is then calculated by multiplying by the average probability for the special LF-function:

$$\sigma_{in,LF}^{i\to j} = \int_i P_{LF}(E)\,\sigma_{in}(E)\,W(E)\,dE \cdot \frac{\int_j f_{LF}(E')\,dE'}{\int_{\substack{\text{all groups}\\ \text{and below}}} f_{LF}(E')\,dE'}$$

The same formula is also used for LF = 4. For LF = 5, 7 or 9 the programme first averages the value Θ,

$$\Theta_{LF}^{i} = \frac{\int_i \Theta_{LF}(E)\,dE}{\int_i dE}$$

The rest of the calculation is now the same as before with $f_{LF}(E)$ replaced by $f_{LF}(E,\Theta_{LF}^{i})$.

For LF = 2, $\sigma_{in}^{i\to j}$ is calculated as

$$\sigma_{in,2}^{i\to j} = \begin{cases} \int_i P_{LF}(\theta)\,\sigma_{in}(E)\,W(E)\,dE & \text{if } \Theta \text{ is in the group} \\ \tfrac{1}{2}\int_i P_{LF}(\theta)\,\sigma_{in}(E)\,W(E)\,dE & \text{if } \Theta = \text{group limit} \\ 0 & \text{all else} \end{cases}$$

The contribution to the matrix elements from LF = 3 is calculated as

$$\sigma_{in_{|LF}}^{i\to j} = \int_i P_{LF}(E)\,\sigma_{in}(E)\,W(E)\,dE \cdot \frac{\int_j P_{LF}(E'-\Theta_{LF})\,dE'}{\int_{\substack{\text{all groups}\\ \text{and below}}} P_{LF}(E'-\Theta_{LF})\,dE'}.$$

This is only valid if $E_{i+1} > \Theta_{LF}$, otherwise the result is zero.

Thus, each element of the matrix is the sum of contributions from one or more LF subsections. Since TIMOC does not need a normalized matrix, this is not done, and, therefore, the output is unnormalized due to integration and other calculational round-off errors (elements less than $10^{-4} \cdot \sigma_{in}^{i}$ are set equal to zero in the output).

TIMOC also needs $\mu_{in,L}^{i\to j}$. The present version of CODAC, however, ignores this feature and puts all $\mu_{in,L}^{i\to j}$ equal to zero.

If n-2n scattering is added to σ_{in} (c.f. section 2.2.7) the n-2n scattering matrix is built in the same way and added to the inelastic matrix.

2.7 Fission Spectrum

Block I of the TIMOC input requires the coefficients of the source spectrum. If the isotope is fissile, the source is given by the secondary energy distribution of fission neutrons while, for fertile isotopes, it may be given by the secondary energy distribution of the n-2n reaction (see sections 2.2.7 and 4.2.10).

CODAC will only treat a source spectrum represented by or as a combination of a simple fission spectrum (LF = 6, 7), a Maxwellian distribution (LF = 8, 9), or a Watt spectrum (LF = 10). Up to 3 spectra, different in their representation and in the values of their parameters, may be combined. All needed data are given on ENDF/B file 5, MT = 18 or 16, respectively.

Simple fission spectrum LF = 6:

$$\chi(E') = b\sqrt{E'}\, e^{-E'/a}$$

where a is designated as Θ in ENDF/B and b is calculated as

$$b = \sqrt{\frac{4}{\pi \Theta^3}} \int_{\text{range}} p(E)\, dE \Big/ \int_{\text{range}} dE, \qquad \text{and}$$

where the integration runs over the entire energy range.

Maxwell spectrum LF = 8:

$$\chi(E') = b\, E'\, e^{-E'/a}$$

where again a is designated as Θ and

$$b = \frac{\langle p(E) \rangle}{\Theta^2}.$$

For the simple fission spectrum LF = 7 and the Maxwellian distribution LF = 9 we have the same representation as before but with

$$a = \Theta = \langle \Theta(E) \rangle.$$

Watt spectrum LF = 10:

$$\chi(E') = c \cdot e^{-E'/a} \cdot \sinh\sqrt{bE'}$$

where a and b are given in ENDF/B and c is calculated as

$$c = \sqrt{\frac{4}{\pi a^3 b}}\, e^{-ab/4} \langle p(E) \rangle.$$

CODAC only calculates the coefficients a, b and c as output items.

3. EXECUTION INFORMATION

3.1 Summary Description

CODAC is a programme to process data from the ENDF/B tapes with MODE = 1 or 3 and produces a library deck for TIMOC. The CODAC output consists of printed information and tabulations of the data and optionally a punched card deck or library tape in the proper format.

3.2 Limitations

3.2.1 Restrictions of Input Items

1) IM: Number of multigroups: $3 \leq IM \leq 50$. The lower limit is a TIMOC limitation and also is checked by the input part of CODAC.

2) ENE(I): Group limits: $ENE(1) \geq 0.021$ eV
$ENE(IM+1) \leq 20$ MeV

3) EPS: Error criterion: $0.0 < EPS < 0.1$
If EPS = 0,0 it is set equal 10^{-3}.

4) MODE: Mode of the ENDF/B tape: MODE = 1 or 3.

5) N1: Number of interpolation ranges for the weight:
$N1 \leq 100$, but keep it as small as possible.

6) N2: Number of weighting function points:
$N2 \leq 4000$, but keep it as small as possible.

7) X(1): First energy point of the weight $\leq ENE(1)$

8) X(N2): Last energy point of the weight $\geq ENE(IM+1)$

9) Y(I): Weight at point X(I) : $Y(I) > 0.0$

10) N1: Number of coefficients of the weighting polynomial:
$1 \leq N1 \leq 24$

11) CONST(I): Coefficients of the weighting polynimial:
Must be chosen in such a way that the resulting weight is greater or equal zero throughout the range ENE(1) - ENE(IM+1).

3.2.2 ENDF/B Data Restrictions

3.2.2.1 File 1 - General Information

1) ν is represented as a polynomial with the maximum number of coefficients: NC = 10.

3.2.2.2 File 2 - Resonance Parameters

1) Number of isotopes: ≤ 6

2) Number of ℓ-states: ≤ 2

3) Number of J-states per ℓ-state ≤ 3

4) Maximum number of points in the fission width tabulation: 1000/(total number of states)

5) Only one resolved and one unresolved region are allowed

6) Only data for the single level Breit-Wigner formulation are accepted.

3.2.2.3 File 3 - Smooth Cross Sections

1) Number of points in all file 3 tables: up to 4000

2) Number of interpolation ranges ≤ 50

3.2.2.4 File 4 - Secondary Angular Distributions

1) Energy interpolation table ≤ 50

2) Number of transformation matrix elements ≤ 2000

3) Number of energy points where data are given ≤ 996

3.2.2.5 File 5 - Secondary Energy Distributions

1) Maximum number of points in the P(E) tabulation: 1000

2) Maximum number of interpolation ranges for P(E): 10

3) Number of incident energies for LF = 1: $\leq$ 20

4) Maximum number of interpol.ranges between incident energies for LF = 1: 10

5) Maximum number of g(E - E') - matrix points: 2000

6) Maximum number of g(E - E') total interpolation ranges: 70

7) Maximum number of points in the g(x) tabulation per subsection: 1000 for LF = 4,5

8) Maximum number of interpolation ranges for g(x) per subsection: 10 for LF = 4,5

9) Maximum number of points in the Θ(E) tabulation per subsection: 1000

10) Maximum number of interpolation ranges for Θ(E) per subsection: 10

3.2.2.6 Data On Several Files

If inelastic (MT = 4), n-2n (MT = 16), and/or fission data (MT = 18) are given on file 3, the corresponding secondary energy distribution must be given on file 5.

If elastic data (MT = 2) are given on file 3, the corresponding secondary angular distribution must be given on file 4.

4. INPUT DESCRIPTION

In the following input list, the various items are listed and described and the corresponding columns for each item designated. All formats are standard FORTRAN formats. A more detailed description of the input options and data is given in the next section.

4.1 Input Card Deck

4.1.1 Units

Card 1) (I5)

Cols.	Name	Description
1 - 5	IPUNCH	Logical unit of the output tape or the card puncher. If = 0, IPUNCH is set = 7.

4.1.2 Energy group structure

Card 2) (I5)

Cols.	Name	Description
1 - 5	IM	Number of multigroups

Card 3) (6(E11.4,1X))

1 - 11	ENE(1)	Group breakpoint 1 (lowest energy in eV)
13 - 23	ENE(2)	Group breakpoint 2
.	.	.
.	.	.
.	.	.
67 - 71	ENE(6)	Group breakpoint 6
.	.	.
.	.	.
.	.	.
etc. using (IM+1)/6 cards		.
.	.	.

ENE(IM)	Group breakpoint IM
ENE(IM+1)	Group breakpoint IM+1 (highest energy)

Cards 2) and 3) must only be given once for one run. Therefore the group sturcture is the same for all the following isotopes.

4.1.3 Isotope Identification and Data

Card 4) (A6, 1X, I5, 1X, 2(E11.4), 3(I5, 1X))

Cols.	Name	Description
1 - 6	ISOT	TIMOC identification name for the material (Hollerith)
8 - 12	MATNO	ENDF/B tape material number MAT
14 - 24	SIGP	Non-resonance isotope potential scattering cross section per absorber atom, i.e., $\left(\frac{\Sigma_p}{N} - 4\pi R^2\right)$ where Σ_p is the mixture macroscopic potential cross section, N is the resonance isotope number density and $4\pi R^2$ is the resonance isotope potential scattering.
26 - 36	EPS	Error criterion for combining two TAB1 functions.
38 - 42	N3	Option for the treatment of TIMOC block III, elastic scattering data.
44 - 48	INALL	0 = only card 4) is read for this isotope 1 = all isotope input cards are read
50 - 54	IREW	0 = ENDF/B tape is not rewound by CODAC 1 = ENDF/B tape is rewound by CODAC

4.1.4 Weighting Spectrum and Other General Data

This card and the following ones are read only if INALL = 1 on card 4).

Card 5) (A4, 3X, 5 (I5, 1X))

Cols.	Name	Description
1 - 4	SPEC	Weighting function to be used
8 - 12	NDFB	Logical unit on which the ENDF/B library tape is mounted
14 - 18	IN2N	Option for the treatment of the n-2n reaction
20 - 24	MODE	Mode of the ENDF/B tape
26 - 30	IDTAP	ENDF/B tape identification number
32 - 36	IPUN	Option for punched output

4.1.5 Weighting Spectrum Data

These cards are only necessary if the weighting function SPEC needs further data, i.e. if SPEC = POIN or POLY.

a) SPEC = POIN:

The set consists of the desired weighting function in the form of tabulated points plus the interpolation tables defining the interpolation schemes to be used between the tabulated points. The weighting function must be given from low to high energy (c.f. TAB1 functions on ENDF/B).

Card 6a) (2(I11,1X))

Cols.	Name	Description
1 - 11	N1	Number of interpolation ranges
13 - 23	N2	Number of weighting function points

Card(s) 7a) (6(I11,1X))

Cols.	Name	Description
1 - 11	NBT(1)	Last point number in 1st interpolation region
13 - 23	JNT(1)	Interpolation scheme for 1st region
.	.	.
.	.	.
.	.	.
49 - 59	NBT(3)	Last point number of 3rd interpolation region
61 - 71	JNT(3)	Interpolation scheme for 3rd region
.	.	.
.	.	.
.	.	.
etc. using N1/3 cards		.
		.
	.	.
	.	.
	.	.
	NBT(N1)	Last point number in N1 interpolation region
	JNT(N1)	Interpolation scheme for N1 region

Card(s) 8a) (6(E11.4,1X))

Cols.	Name	Description
1 - 11	X(1)	1st energy point ($\lesssim$ ENE(1)) in eV
13 - 23	Y(1)	Weight at this energy
.	.	.
.	.	.
.	.	.
49 - 59	X(3)	3rd energy point
61 - 71	Y(3)	Weight at this energy
.	.	.
.	.	.
.	.	.
etc. using N2/3 cards		.
		.
	.	.
	.	.
	.	.
	X(N2)	Last energy point ($\gtrsim$ ENE(IM+1))
	Y(N2)	Weight at this energy

b) SPEC = POLY:

The weighting spectrum is input as a polynimial in E(eV): $W(E) = a_o + a_1 \cdot E + a_2 E^2 + ... + a_{N1-1} E^{N1-1}$. The set consists of the desired coefficients, a_i, starting with i = 0 in increasing order of i.

Card 6b) (I11)

Cols.	Name	Description
1 - 11	N1	Number of coefficients, a_i = highest power of E plus 1.

Card(s) 7b) (6(E11.4, 1X))

1 - 11	CONST(2)	Coefficient a_o
.	.	.
.	.	.
.	.	.
61 - 71	CONST(7)	Coefficient a_5
.	.	.
.	.	.
.	.	.
		.
etc. using N1/6 cards		,
	.	.
	.	.
	.	.
	CONST(N1+1)	Coefficient a_{N1-1}

4.2 Input Items

4.2.1 IM: Number of multigroups, must be limited to $3 \leq IM \leq 50$. This is a TIMOC restriction. The upper limit is also a CODAC limitation.

4.2.2 ENE(I): Group break points in eV. There must be IM+1 break points in increasing order, limited to the range (0.021 eV - 20.0 MeV).

4.2.3 SIGP: Non-resonance isotope potential scattering cross section per absorber atom. See unresolved resonance treatment, section 2.4.

4.2.4 EPS: Combining two TAB1 functions to give a third one (for instance combining a cross section with the weight to give $\sigma \cdot W$) is done to an accuracy of EPS (0.0 EPS 0.1). If EPS is left blank, a value 10^{-3} is assumed.

4.2.5 N3: Option for the treatment of data for TIMOC block III. If N3

= 0: the programme tries to compute the secondary angular distribution $\sigma_{el}(\mu)$ as a Legendre series or as a $\frac{d\sigma}{d\mu}$ -table in μ for 33 μ-points ($+1 \geq \mu \geq -1$) in the c.m. system.

If the ENDF/B data in file 4 have one of the foregoing representations in the c.m. system, the Legendre coefficients or $\frac{d\sigma}{d\mu}$ -values at the 33 μ-points, respectively, are computed for each group with $\sigma_{el} \neq 0$. Ohterwise μ_L^i is determined from file 3, or if not given there, from file 4 data.

= 1: CODAC tries to compute μ_L^i. This is done from file 3 or, if there are no data, from file 4. If file 4 contains a Legendre representation in the c.m. system (and no transformation matrix) or a point by point representation in the c.m. system, the computation runs as for N3 = 0 (if no μ_L-data in file 3), this means that instead of μ_L^i , the corresponding representation is calculated. See also section 2.5.

4.2.6 INALL: 0 = only card 4) is read for this isotope.

1 = card 4) is read, together with card 5), and, if necessary, cards 6)-8).

For the first isotope in the data deck INALL must be 1, since the items on card 5) (weighting function, logical ENDF/B unit etc.) must first be defined. If one wants to change one of the card 5) - parameters for some isotopes, card 4) of the first of these isotope must contain the value INALL = 1 and then be followed by the changed card 5).

4.2.7 IREW: 0 = ENDF/B tape is not rewound by CODAC

1 = ENDF/B tape is rewound by CODAC

IREW = 1 would, for instance, be necessary if one needs data from one isotope twice with different data on cards 4) or 5) during one run.

4.2.8 SPEC: The weighting function to be used.

SPEC = ␣␣␣␣, 1.0␣, or ␣1.0: no weighting is used.

SPEC = 1/E␣ or ␣1/E: a 1/E weighting is used.

SPEC = POIN: Weighting function is input as a TAB1 function. The energy range must span the multigroup structure, the weight always being positive. Cards 6a)-8a) must follow.

SPEC = POLY: Weighting function is input as the coefficients of a polynomial in E. From this polynomial CODAC generates a TAB1 function which must be positive in the multigroup range. Cards 6b) and 7b) must follow.

SPEC = SAME: The same weighting function as for the previous isotope is used.

If one only wants to change an option on card 5), SPEC = SAME avoids cards 6)-8) if SPEC = POIN or POLY for the previous isotope.

4.2.9 NDFB: Logical unit on which the ENDF/B library is mounted.

ENDF/B data are usually written on more than one tape or physical file. If the corresponding isotope is on a different file (or tape) then the previous isotope, its data can be read during the same run by changing the logical unit NDFB, for example. In this case the correspondence between each file (or tape) and its logical unit must be fixed on control cards.

Another method to read data from more than one ENDF/B file is to read beyond the file ends, always closing the proceeding file and opening the next one. This is possible, for instance, on the IBM 360 (see section 6.2.1).

4.2.10 IN2N: Option for the treatment of the n-2n reaction. Three possibilities are provided for.

IN2N = 1: n-2n is added to smooth fission. Therefore one has

$$\sigma_f' = \sigma_f + \sigma_{n,2n}$$

$$\nu = \frac{\nu \cdot \sigma_f + 2.0 \cdot \sigma_{n,2n}}{\sigma_f + \sigma_{n,2n}}$$

IN2N = 2: n-2n is treated half as fission (with a ν -value of 1) and half as inelastic scattering:

$$\sigma_f = \sigma_f + 0.5 \cdot \sigma_{n,2n}$$

$$\sigma_{in} = \sigma_{in} + 0.5 \cdot \sigma_{n,2n}$$

$$\nu = \frac{\nu \cdot \sigma_f + 1.0 \cdot 0.5 \cdot \sigma_{n,2n}}{\sigma_f + 0.5 \cdot \sigma_{n,2n}}$$

IN2N = 3: The n-2n reaction is added to the inelastic scattering

$$\sigma_{in} = \sigma_{in} + \sigma_{n,2n} .$$

If the isotope is fissionable, this option is overridden and all n-2n is added to σ_{in}. If n-2n is added to fission, this fact is also taken into account in computing the fission spectrum parameters for TIMOC block II, while addition to σ_{in} also affects an n-2n matrix, which is added to the inelastic one.

4.2.11 MODE: Mode of the ENDF/B tape

MODE = 1: ENDF/B tape is binary mode (standard arrangement)
MODE = 3: ENDF/B tape is BCD mode (standard arrangement)

If MODE = 3, CODAC internally changes it to MODE = 2.

4.2.12 IDTAP: ENDF/B tape identification number. Each ENDF/B tape (or physical file) contains a tape identification number at the beginning (first record) which is tested by the programme.

IDTAP must only be given in the data card 5) for the first material treated in a file (or tape) or if IREW = 1 (since after the ENDF/B tape is rewound, reading starts again at the very beginning).

The present ENDF/B version contains five files with the following labels IDTAP:

1. File : 114
2. File : 115
3. File : 116
4. File : 5003
5. File : 117

4.2.13 IPUN: Option for the output.

IPUN = 1: no punched output (only a printed one).
IPUN = 0: CODAC produces a punched output or an output on a tape, mounted at the logical unit IPUNCH, defined on card 1).
IPUN = -1: If the first isotope in the data deck contains IPUN = -1, first the energy structure is punched; then continued as for IPUN = 0.

4.3 Programme Lapse and Input Preparation

CODAC will process any number of materials during one run. The first material request (via card 4)) must be accompanied by all input data (INALL = 1) and the ENDF/B tape should be rewound by the programme (IREW = 1). Simultaneously, the tape identification number of the file containing this isotope must be given (IDTAP).

Subsequent material requests will, in general, only require card 4) (INALL = 0) unless one wants to change parameters on cards 5)-8). Usually it is not necessary to rewind the ENDF/B tape (IREW = 0). If the ENDF/B tape is not rewound, the material requests should be in ascending order according to ENDF/B material number (MATNO on card 4)). This means that materials should be requested in increasing order of MATNO within each file, and so on, file by file, starting with the first file. For the first requested material in each file define the proper label IDTAP on card 5). Therefore, the first material in each file must also contain INALL = 1 (IREW = 0) and all input data. The weighting spectrum can be refered to by SPEC = SAME.

For maximum efficiency, rewind the ENDF/B tape only if the same material is requested twice (for instance with a different weighting).

5. OUTPUT

The printed output is easy to read and needs no explanation. Therefore in the following only the punched output is described.

5.1 Energy-Group Structure

5.1.1

Card 1) (I6) = IM: Number of energy groups

5.1.2

Cards 2) (E11.4) =(ENE(I), I = 1, IM + 1)

ENE(I) : The lower energy limits (in eV) of the IM energy groups in increasing order, ENE(IM+1) = upper limit of the top group.
The above set of cards is produced once during one run (and only if the first material contains IPUN = -1) and thus the boundaries are the same for all isotopes.
The following cards 3) to 11) are produced for each isotope.

5.2 Block I: Parameters which are Independent of the Energy-Group Structure

5.2.1

Card 3) (A6) = ISOT: Isotope identification

5.2.2

Cards 4) 3(12A6) = TEXT: Three cards, which contain a description of this isotope (origin of the cross sections, etc.)

5.2.3

Cards 5) (A6, E11.4, I6) = ISOT, ATW, IMF

ISOT: Isotope identification

ATW: Atomic weight of the isotope (measured in neutron masses)

IMF: Number of different fission spectrum representations to be used (always ≤ 3)

5.2.4

Card 6) (I6, 5E11.4) = LTT, EMIN, EMAX, (ELCO(I), I = 1,3)

LTT: Symbol defining fission spectrum description

LTT = 6 or 7: Simple fission spectrum

$$\chi(E') = b\sqrt{E'}\, e^{-E'/a}$$

LTT = 8 or 9: Maxwellian distribution

$$\chi(E') = b\, E'\, e^{-E'/a}$$

LTT = 10: Watt spectrum

$$\chi(E') = c \cdot e^{-E'/a} \sinh\sqrt{b\,E'}$$

EMIN, EMAX: Lower and upper limit (in eV) for the corresponding fission spectrum

ELCO(1): Coefficient a

ELCO(2): Coefficient b

ELCO(3): Coefficient c (non zero only for LTT = 10)

5.3 Block II: All Microscopic Group Averaged Cross Sections

These are split into the capture, elastic scattering, inelastic scattering and fission parts and the particle multiplication factor for fission.

5.3.1

Card 7) (A6, 6E11.4) = ISOT, ENCH, (CROM(I), I = 1,5)

ISOT: Isotope identification

ENCH: Lower boundary of the energy group (eV)

CROM(1): Is σ_c, the microscopic capture cross section. Unit: barns.

CROM(2): Is σ_{el}, the microscopic elastic scattering cross section. Unit: barns

CROM(3): Is σ_{in}, the microscopic inelastic scattering cross section. Unit: barns

CROM(4): Is σ_f, the microscopic fission cross section. Unit: barns

CROM(5): Is ν, the particle multiplication factor to be used for the product $\nu \sigma_f$.

5.4 Block III: All Information On Elastic Isotropic Or Anisotropic Scattering

A card 8) must be present for each energy group (in increasing order) in which $\sigma_{el} \neq 0$. If required, card 8) must be followed by the corresponding card 9). The(se) card(s) describe(s) the differential cross section for the elastic anisotropic scattering.

5.4.1

Card 8) (A6, E11.4, 2I6) = ISOT, ENCH, LTT, NE

ISOT: Isotope identification

ENCH: Lower boundary of the energy group (eV)

NE: Number of points or coefficients given

LTT: Symbol defining angular distribution description

LTT = 0: Isotropic scattering distribution in the c.m. system. Card 9) is omitted. NE = 0 in this case.

LTT = 1: The distribution is described by a Legendre polynomial in the c.m. system. Card 9) contains the first NE Legendre coefficients for the anisotropic scattering distribution:

$$\frac{d\sigma}{d\cos\vartheta} = \sum_{n=0}^{NE-1} ELCO(n+1) \cdot P_n(\cos\vartheta)$$

LTT = 2: NE is the number of equidistant points (= 33) along the μ-axis in the $\frac{d\sigma}{d\cos\vartheta}$-table, describing anisotropic scattering in the c.m. system by a polygon. Card 9) contains the values of $\frac{d\sigma}{d\mu}$ for the 33 points.

LTT = 3: The averaged value of cos Θ of the angular distribution in the Lab. system is used. μ_L^i is placed as ELCO(1) on card 9). NE = 1.

5.4.2 Card(s) 9) (6E11.4) = (ELCO(I), I = 1, NE)

If LTT = 0: This card is omitted

If LTT = 1: The ELCO(I) are the first NE coefficients of the Legendre polynomial expansion.

If LTT = 2: The ELCO(I) are the NE(=33) values of the angular distribution $\frac{d\sigma}{d\mu}$ at NE equidistant points between $[+1,-1]$, including the boundary . The number of intervals is therefore NE -1. The ELCO(I) are given for the distribution in the c.m. system and in decreasing order of cos ϑ $[+1 \rightarrow -1]$.

If LTT = 3: ELCO(1) is the averaged value μ_L^i of cos Θ in the Lab. system.

Note that in different energy groups different types of representations may be produced.

5.5 Block IV: All Information On Inelastic Scattering and Transfer Matrices

Only energy groups which contain a $\sigma_{in} \neq 0$ on card 7) require a corresponding card 10) and eventually card 11) in this block.

5.5.1

Card 10) (A6, E11.4, 2I6) = ISOT, ENCH, LTT, NU

ISOT: Isotope identification

ENCH: Lower energy boundary (eV)

NU: Number of data given

LTT: Symbol defining inelastic scattering description

LTT = 1: NU is twice the number of excited levels. Card(s) 11) follow(s).

LTT = 2: The statistical model is used. The corresponding parameter (nuclear temperature) for the group is on card 11).

LTT = 3: NU is the number of transfer matrix elements. It is always three times the number of energy groups into which scattering occurs. Card(s) 11) follow(s).

The present version of CODAC produces only LTT = 3 data with $\overline{\cos \Theta} = 0$ (see below).

5.5.2

Card(s) 11) 2(I6, 2E11.4) = ELCO(1), ELCO(2), ELCO(3), ... for LTT = 3.

ELCO(1): Is the number of energy groups which the neutron skips after the collision

ELCO(1) = -0: Only down scattering in the same group

ELCO(1) = -m: Down scattering into a group defined by substracting m from the actual energy group index.

ELCO(2): Relative probability for the particle to jump into the energy group specified by ELCO(1).

ELCO(3): Averaged value of the angular distribution ($\overline{\cos \Theta}$) in the Lab. system for the corresponding scattering process.

The present version of CODAC assumes $\overline{\cos \Theta} = 0.0$.

ELCO(4): Like ELCO(1) and so on.

Cards 3) to 11) are repeated for the next isotope, etc. Each card gets a label. The card containing the number of groups gets the label "NRGROUPS" while the group limits are labeled with "ENERGY + number of the limit". For instance the 3rd limit has the label "ENERGY 3". The deck for an isotope is labeled in the following way: the first 4 columns contain the ENDF/B-MAT-number, while the other 4 columns contain the card number, starting with 0001.

6. PROGRAMMER'S INFORMATION

This section contains some internal details of CODAC. It should be helpful to the programmer in adding, altering, or modifying parts of the programme and in understanding the meaning of programme messages and also should prove to be helpful in making the programme operational at another installation.

6.1 General Features

CODAC is written in FORTRAN IV for an IBM 360/65 but uses no machine features or nearly so (see section 6.2). Most of the subroutines and steps within are headed by comments, so that the different working steps can easily be understood.

The programme is written in an OVERLAY structure, although the main storage of the 360/65 is sufficient for a run without OVERLAY. The main programme is simply a series of calls for the different OVERLAY segments (CODAC1 , CODAC2 , etc.).

Most of the data handling is done with large common storage blocks. ENDF/B data are first read into these blocks before processing. Many data manipulations are done in the blocks. The blocks also serve as temporary storage for some processed or read data.

For each material, data are processed in the order they appear on ENDF/B with the results being stored and output accomplished in the last OVERLAY. The output consists of printed tabulations and a punched one (or a tape) in the proper TIMOC library formats.

6.2 Special Features

6.2.1 Reading Several ENDF/B-Files

Since the FORTRAN IV version of the IBM 360 has the ability to read beyond file ends, a special part is inserted into subroutine TRID, allowing for this feature. If the different physical ENDF/B files are posi-

tioned successively on one tape, this allows one to read all these files during one run, therefore only the right file identification number IDTAP must be defined for the first processed material in each file. The logical unit NDFB can be the same for all files and only the control cards must contain the definition of all files used.

If one only wants to work with one file or with several files by assigning to each another logical unit, one must omit the corresponding part of subroutine TRID (which is explicitly marked).

6.2.2 End of the Input Card Deck

The input card deck must be closed by an end-of-file card. Subroutine ISOTO contains a special READ-statement which tests for this card.

6.2.3 Hollerith Description

The Hollerith data needed by the printed output are prepared by using an EQUIVALENCE statement, since storing with a DO-loop did not work on the compiler which has been used.

It is possible to change these parts. In doing so , some care must be taken, since the IBM 360 stores only 4 characters per word.

6.3 Labeled COMMON

In the following, the most important COMMON blocks are listed in alphabetical order. The labeled COMMON block name is given first and its general category described. The variables in the block are then described in the same order as they appear in the block.

Many common blocks are part of the package of Retrieval Subroutines for the ENDF/B System written by H.C. Honeck[4] and of the ETOG-ETOM Code[5,6]. In CODAC, many of the dimensions and items have been changed.

/BLOCK/	floating point storage
B	general floating point storage space
/BLOKS/	counters for BLOK1-BLOK4 and IBLK1-IBLK4, which are connected with /RECS/ arrays via EQUIVALENCE
LBK12	usually the number of data pairs in BLOK1 and BLOK2
LBK34	same as LBK12 but usually for BLOK3 and BLOK4
LIBK12,	
LIBK34	same as above but associated with IBLK1-IBLK4.
/CONS/	storage of the weighting polynomial input
CONST(1)	number of coefficients of the polynomial
CONST(I≠1)	coefficients of the polynomial
/CONSTS/	data constants
PI	π
HAFPI	$\pi/2$
EZERO	$1.0 \cdot 10^7$
UZERO	$\ln(10^7)$
/CONTF1/	control information file 1
ZA	material (Z,A) designation
AWR	atomic weight ratio
LRP	resonance indicator
LFI	fissile indicator
LDD	radioactive decay indicator
LFP	fission product indicator
NWD	number of (computer) words in material description
LNU	ν representation indicator
NC	number of ν polynomial terms
C	ν polynomial coefficients
NR1	interpolation table length for ν
NP1	data list length for ν
/CONTF2/	control information - file 2
NIS	number of isotopes
ZAI	isotope (Z,A) designation

ABN	abundance
LFW	fission width indicator
NER	number of energy ranges
LISR,LISRX	resolved scattering calculation indicator
EL	range lower energy limit
EH	range higher energy limit
LRU	data type indicator
LRF	resonance formula indicator
LISU,LISUX	unresolved scattering calculation indicator
SPIR	nuclear spin-resolved
AP,AM,AA	scattering length
NLSR	number of ℓ states - resolved
CR	penetration factor constant - resolved
LR	ℓ value - resolved
SPIU	nuclear spin - unresolved
NLSU	number of ℓ states - unresolved
CU	penetration factor constant - unresolved
NEX	number of points in fission width tabulation
LU	ℓ - unresolved
NRS	number of resonances
NJS	number of J states
MUF	number of degrees of freedom in fission width tabulation
ELOR	lowest energy - resolved region
EHIR	highest energy - resolved region
ELOU	lowest energy - unresolved region
EHIU	highest energy - unresolved region
XPOTR, XPOTU	not used
LLRR	resolved data indicator
LLRU	unresolved data indicator
LFWX	fission width data indicator
/CONTF3/	control information - file 3
LFS	final state number
NR3	interpolation table length
NP3	data list length

/CONTF4/	control information - file 4
LVT	transformation matrix indicator
LTT	data representation indicator
LCT	system indicator
NK4	number of matrix elements
NM4	number of rows minus one in the transform. matrix
NRE4	number of codes to interpolate between tabulated energy values
NE4	number of energies given
NL4	number of Legendre coefficients
NR4	number of interpolation codes between tabulated μ-values
NP4	number of μ-values given
E4	special energy value of the NE different values
/CONTF5/	control information - file 5
NK	number of representations (subsections)
THETA	θ
LF	function representation indicator
NE	number of E-values in g-tabulation
NR5	interpolation table length
NP5	data list length
EINIT	E values in g-tabulation
AWATT	constant "a" in Watt spectrum
BWATT	constant "b" in Watt spectrum
LTHET	length of theta array
LITHET	length of theta interpolation table
LPP	length of P-list
LIPP	length of P interpolation tables
LGG	length of g-list
LIGG	length of g-interpolation tables
/COUNT/	counter to assure a correct initial P (E)-value for LF = 3
NKK	counter for NK representations of /CONTF5/
/DENS/	dense (multi-record) storage
JMT	record indentifier
JAT	record starting location
JTT	record type

JLT	record length
A	record bulk storage array
JNS,MNS	pointers for next record
JX	maximum length of the A array
MX	maximum length of the JMT,JAT,JTT and JLT arrays
/ELMU/	programme control indicator
NOMU	μ_L^i indicator
/ENERG/	energy group structure
IM	number of energy groups
IM1	IM+1
ENE	group limits
/EPSIL/	error criterion for combining 2 TAB1 functions
EPSMIN	input criterion EPS
EPSMAX	10 times input criterion EPS
FACEPS	increase factor of EPSMIN ($\approx \sqrt{10}$)
/FILE3/	storage for group averaged results
XS	elastic scattering and temporary storage
XIN	inelastic scattering
XF	fission
XC	capture
GNU	ν
XSMU	μ_L and temporary storage
XNF	$\nu \cdot \sigma_f$ and temporary storage
ZETA	group integral of the weight
/FILE4/	elastic data
LAST	indicator for form of elastic data (c.f. input option N3)
/FILE5/	inelastic matrix
PMX	inelastic matrix
/FILE6/	storage for group averaged results
TRUM	temporary storage

/FIPAR/	source spectrum
PARA(I,1)	fission spectrum indicator
PARA(I,2)	lower limit for the corresponding spectrum
PARA(I,3)	upper limit
PARA(I,3-6)	the corresponding coefficients "a", "b", and "c"
NLF	counter for the number of different fission spectra
/FLAGS/	programme control indicators
KEY	data presence indicator
NOXS	elastic scattering cross section indicator
NOXIN	σ_{in} indicator
NON2N	$\sigma_{n,2n}$ indicator
NOXF	σ_{f} indicator
NONG	σ_{γ} indicator
NONP	$\sigma_{n,p}$ indicator
NOND	$\sigma_{n,d}$ indicator
NONT	$\sigma_{n,t}$ indicator
NOHE	σ_{n,He^3} indicator
NONA	$\sigma_{n,\alpha}$ indicator
NON2A	$\sigma_{n,2\alpha}$ indicator
NOCAP	unused
/HOLLTH/	hollerith storage
TEXT	storage for a part of the material heading description
/IMODE/	ENDF/B mode
MO	mode of the ENDF/B tape
/INDEX/	control check
IND	indicator, if group structure is already read in

/ISOTOP/ + DOUBLE PRECISION ISOT: input items

	see input description
ISOT	used as double precision, since the IBM 360 stores only 4 characters/word
N4	is not used

/LETHAR/	lethargy group structure
UGRP	lethargy group limits
/OPT5/	n-2n treatment
INEL	indicator, if n-2n is present and if it is added to σ_f or σ_{in} (c.f. input option IN2N)
/OPTION/	input items (see input description)
FISP,EMIN,EMAX	not used
/PUNCH/	punched output label
NCARD	counter for the label of the punched output
/RECS/	single record storage
MAT	material number
MF	file number
MT	reaction type number
C1,C2	floating point constants
L1,L2	integer constants (usually test numbers)
N1	count of items in a list to follow
N2	count of items in a second list to follow
NBT,JNT	general integer storage space
X,Y	general floating point storage space
N1X	maximum length of the NBT and JNT arrays
N2X	maximum length of the X and Y arrays
NS	card sequence number
/SPE/	spectrum indicator
ISPC	indicator for type of weighting function SPEC
IFIS	unused
/TAPES/	tape and unit names and data mode
MODE	mode of the ENDF/B library tape (is set = 2 if MODE = 3)
NDFB	ENDF/B library tape
IPUNCH	output punch tape
IPRINT	output print tape
ISCTP1	prepared for a scratch tape, but used to count the files in the special IBM-360 version (c.f. section 6.2.1)
ICR	cardreader or input tape

6.4 Overlay Structure and Subroutines

In the following, the programmes, subroutines, functions and commons used by CODAC are listed. Each control flow programme name is followed first by a table of all labelled common blocks (in brackets) which appear in the subroutines inserted into the corresponding overlay. Next comes the list of names of the subroutines used and labelled common blocks to be inserted into the corresponding overlay. This means, for instance, that if a common block appears in the list of the overlay root segment, its data are needed in different overlays, while a common block which only appears in the list of a certain overlay segment is only used to transfer data within this overlay.

A brief summary of the purpose of each subroutine is included. The table and list are arranged in alphabetical order within each overlay, Since the list is ordered segment by segment, it serves as an overlay structure description.

6.4.1 Root Segment

MAIN	controls flow of main programme (COMMONS: BLOCK, BLOKS, CONSTS, CONTF1, CONTF2, DENS, ELMU, ENERG, EPSIL, FILE3, FILE4, FILE5, FILE6, FIPAR, FLAGS, HOLLTH, INDEX, ISOTOP+D.PREC.ISOT, LETHAR, NUMEN, OPT5, OPTION, RECS, SPE, TAPES)
COMB	combines two TAB1 functions
COMBP	combines one panel of two TAB1 functions
CONT	reads control (CONT) record
DELETE	deletes record from dense storage
ECSI	computes integral of y(x)
ERROR	prints error message
FETCH	fetches record from dense storage
FPDS	fetches point from dense storage
GPAV	averages over selected groups
GRATE	integrates TAB1 function
INTGRT	integrates a TAB1 function
IPDS	interpolates point in dense storage

LIST	reads LIST record
LRIDS	locates record in dense storage
MULT	combining function for multiplication
STORE	stores record in dense storage
TAB1	reads TAB1 record
TAB2	reads TAB2 record
TERP1	interpolates one point
TERPO	interpolates a data array
TPOS	positions ENDF/B tape to file MF and reaction MT
XTND	extends data array

ADD,DIV,SUB,TERP combining functions for addition, division, substraction, and interpolation between two points.

The COMMON blocks to be inserted are the same as in the above table.

6.4.2 1. Overlay A

CODAC1	controls flow of programme in the 1st overlay (COMMONS: BLOKS, CONS, CONSTS, CONTF1, CONTF2, DENS, ENERG, EPSIL, FILE3, HOLLTH, IMODE, INDEX, ISOTOP+D.PREC.ISOT, LETHAR, NUMEN, OPTION, RECS, SPE, TAPES)
ENERGY	reads and tests group structure
ERR	prints error message
GENT1	generates TAB1 function
HOLL	reads hollerith material description
INDENS	initializes dense storage
ISOTO	reads all input cards for one material
OUTEN	writes group structure
OUTSIO	prints input description for one material
OUTSPE	prints spectrum and common input data
POLY	functions to evaluate a polynomial
STORNU	converts ν -polynomial to TAB1 function and store
TITLE	prints titles of the output

TMAT	positions ENDF/B tape to material MAT
TMF1	reads ENDF/B file 1
TRID	reads ENDF/B tape identification (see also section 6.2.1)
UNITS	reads and define units
WEAV	calculates group integral values of the weight
ZERO	initializes named common
/CONS/	
/IMODE/	

6.4.3 2. Overlay A

CODAC2	controls flow of programme in the 2nd overlay (COMMONS: BLOCK, CONSTS, CONTF2, ENERG, EPSIL, FILE3, ISOTOP+D.PREC.ISOT, LETHAR, RECS, TAPES)
RESR	calculates averaged cross sections from resolved resonances
RESU	calculates averaged cross sections from unresolved resonances
TMF2	reads ENDF/B file 2

No labelled COMMON is inserted.

6.4.4 3. Overlay A

CODAC3	controls flow in the 3rd overlay (COMMONS: CONTF1, CONTF2, CONTF3, ELMU, ENERG, EPSIL, FILE3, FLAGS, OPTION, RECS, SPE, TAPES)
CROS	calculates smooth cross sections
RESTOR	restores σ_{el} and σ_{in} in dense storage
TMF3	reads ENDF/B file 3
/CONTF3/	

6.4.5 4. Overlay A

CODAC4	controls flow in the 4th overlay (COMMONS: BLOCK, BLOKS, CONTF1, CONTF4, ELMU, ENERG, EPSIL, FILE3, FILE4, FLAGS, ISOTOP+D.PREC.ISOT, RECS, TAPES)

ELSCAT	computes elastic scattering angular distribution
LEGCO	computes Legendre coefficients for $\sigma_{el}(\mu)$
MUB1	computes μ_L from Legendre data, file 4
MUB2	computes μ_L from file 4, tabulated form in the Lab. system
SIPOIN	computes 33-point table in μ for $\sigma_{el}(\mu)$
TERP2	forms new table by interpolation
TMF4	reads ENDF/B file 4

6.4.6 5. Overlay A

CODAC5	controls flow in the 5th overlay (COMMONS: BLOKS, CONSTS, CONTF1, CONTF5, COUNT, ENERG, EPSIL, FILE3, FILE5, FILE6, FIPAR, FLAGS, LETHAR, OPT5, OPTION, RECS, SPE, TAPES)
AVRG	averages over a selected range
CWAX	combines weight and a cross section
FISSPC	computes parameters of the fission spectrum
FSSPAR	determines fission spectrum parameters
IMAT	calculates constribution to inelastic matrix
INF5	initializes file 5 parameters in common blocks named
INSCAT	computes inelastic and n-2n matrix
RSTR	restores weighting
TMF5	reads ENDF/B file 5
/CONTF5/	
/COUNT/	

6.4.7 6. Overlay A

CODAC6	controls flow in the 6th overlay (COMMONS: BLOCK, CONTF1, ELMU, ENERG, FILE3, FILE4, FILE5, FIPAR, FLAGS, HOLLTH, ISOTOP+D.PREC.ISOT, OPT5, OPTION, PUNCH, SPE, TAPES)
OUT1	prints and punch output for TIMOC block I
OUT2	prints and punch output for TIMOC block II
OUT3	prints and punch output for TIMOC block III
OUT4	prints and punch output for TIMOC block IV
/PUNCH/	

6.5 Messages and Error Stops

Many of the subroutines contain write statements which directly print out error and other messages. Other error messages are printed by the error printing subroutines ERR and ERROR.

Most of the errors detected in the input cards are printed by subroutine ERR in an interpreted form.

All other errors run via subroutine ERROR, which only prints out an error number and the control words, MAT, MF, and MT. A list of the error numbers, the subroutines which detect the error (although it may occur in another subroutine) and a short explanation of the errors follow .

Error No.	Sub-routine	Explanation
110	ECSI	Interpolation code out of range
130	TERP2	X(N) not in increasing order
131	"	XP(N) "
132	"	Interpolation table incorrect
133	TERP1	Interpolation code out of range
134	"	Zero or negative value cannot be interpolated by logs
135	"	X1 = X2, discontinuity
300	STORE	JT not in range 1-6
301	"	MA = 0 not allowed
310	COMB	XL $\geqslant$ XH
311	"	MA or MB is zero
314	IPDS	Improper interpolation table
315	GRATE	Interpolation table incorrect
1000	OUTEN	Input option IPUN $\neq$ 0 or 1 or -1
1004	OUTSPE	Weighting spectrum W (MA = 1) not in /DENS/
1005	"	"
1010	GPAV	Data to be averaged will not fit in /DENS/, MA = 2
1011	"	JLO or JHI not in range 1-IM
1012	"	MA =1 (W) or MB =2 (data to be averaged) not in /DENS/

Error No.	Sub-routine	Explanation
1013	GPAV	Result of combining MA = 1 with MB = 2 will not fit in /RECS/
1210	AVRG	Data to be averaged will not fit in /DENS/, MA = 2
1211	"	MA = 1 (W) or MB = 2 (data to be averaged) not in /DENS/
1212	"	Result of comb. MA = 1 and MB = 2 will not fit in /RECS/
1213	"	MA = 1 (W) not in /DENS/
1300	RESR	$\sigma_{f,res}$ for one group will not fit in /DENS/, MA = 2
1301	"	MA = 2 ($\sigma_{f,res}$) or MB = 3 (ν) not in /DENS/
1302	"	Result of comb. MA = 2 and MB = 3 will not fit in /RECS/
1310	STORNU	TAB1 for ν will not fit in /RECS/
1311	"	" /DENS/
1312	"	NC > 10 on ENDF/B file 1, second section
1500	TMF5	More than 10 interpolation regions for TAB2, ENDF/B file 5, LF = 1
1501	"	More than 20 incident energies, " LF = 1
1502	"	More than 2000 points in the g(E'-E) matrix, " LF = 1
1503	"	More than 70 interpol. regions for g(E'-E) matrix, " LF = 1
1504	"	More than 10 interpol. regions in TAB 1, ENDF/B file 5
1505	"	More than 1000 energy points in TAB 1, ENDF/B file 5
1510	RESU	$\sigma_{f,unres}$ for 1 group will not fit in /DENS/, MA = 2
1511	"	MA = 2 ($\sigma_{f,unres}$) or MB = 3 (ν) not in /DENS/
1512	"	Result of comb. MA = 2 and MB = 3 will not fit in /RECS/
1520	CROS	$\sigma_{f,smooth}$ will not fit in /DENS/, MA = 2
1521	"	LNU ≠ 1 or 2 on ENDF/B file 1, second section
1522	"	MA = 2 ($\sigma_{f,smooth}$) or MB = 3 (ν) not in /DENS/
1523	"	Result of comb. MA = 2 and MB = 3 will not fit in /RECS/
1524	"	$\sigma_{n,2n}$ will not fit in /DENS/, MA = 6
1525	"	$\sigma_{el,smooth}$ " , MA = 4
1526	"	σ_{in} " , MA = 5
1527	"	μ_L " , MA = 4
1528	"	MA = 3 (σ_{el} • W) or MB = 4 (μ_L) not in /DENS/
1529	"	Result of comb. MA = 3 and MB = 4 will not fit in /RECS/

Error No.	Sub-routine	Explanation
1701	ELSCAT	LTT ≠ 1 or 2 on ENDF/B file 4, MT = 2
1702	"	LCT ≠ 1 or 2 "
1703	"	LVT ≠ 0 or 1 "
1704	"	Key for presence of μ_L-data, NOMU ≠ 1 or 2
1710	LEGCO	Energy interpolation table for LTT = 1 or value NE incorrect on ENDF/B file 4, MT = 2
1711	"	Legendre polynomial expansion at an energy point contains less than 1 coefficient, ENDF/B file 4, MT = 2
1712	"	TAB1 for a Legendre coefficient at 2 energy points will not fit in /DENS/, MA = 4
1713	"	MA = 3 (σ_{el} * W) or MB = 4 (TAB1 above) not in /DENS/
1714	"	Result of comb. MA = 3 and MB = 4 will not fit in /RECS/
1720	MUB1	Legendre coefficients given for more than 996 energy points, ENDF/B file 4, MT = 2
1721	"	Interpol. table between energies for LTT = 1 is greater than 50, ENDF/B file 4, MT = 2
1722	"	TAB1 for a Leg. coefficient at all energy points will not fit in /DENS/, MA = 4
1723	"	MA = 3 (σ_{el} * W) or MB = 4 (TAB1 above) not in /DENS/
1724	"	Result of comb. MA=3 and MB=4 will not fit in /RECS/
1730	SIPO	NE or energy interpolation table for LTT = 2 is incorrect, ENDF/B file 4, MT = 2
1731	"	TAB1 for a μ-point at 2 energies will not fit in /DENS/, MA = 4
1732	"	MA = 4 (see above) or MB = 3 (σ_{el} * W) not in /DENS/
1733	"	Result of comb. MB = 3 and MA = 4 will not fit in /RECS/
1735	"	MA = 3 (σ_{el} * W) not in /DENS/
1740	MUB2	Data for LTT = 2 given for more than 996 energy points, ENDF/B file 4, MT = 2
1741	"	TAB1 at one energy for all μ-points will not fit in /DENS/, MA = 4
1742	"	TAB1 for Y = μ ($-1 \leq \mu \leq +1$) will not fit in /DENS/, MB = 5
1743	"	MA = 4 ($\sigma_{el}(\mu)$) or MB = 5 (μ) not in /DENS/
1744	"	Result of comb. MA = 4 and MB = 5 will not fit in /RECS/
1745	"	Energy interpolation table > 50, ENDF/B file 4, MT = 2
1746	"	TAB1 for $Y(E) = \int_{-1}^{+1} P_{Lab}(\mu, E)\, \mu\, d\mu$ will not fit in /DENS/, MA = 4

Error No.	Sub-routine	Explanation
1747	MUB2	MB = 3 (σ_{el} * W) or MA = 4 (see above) not in /DENS/
1748	"	Result of comb. MB = 3 and MA = 4 will not fit in /RECS/
1760	RESTOR	MA = 1 (W) or MB = 4 (σ_{el}) not in /DENS/
1761	"	Result of comb. MA = 1 and MB = 4 will not fit in /RECS/
1762	"	MB = 4 (σ_{el}) not in /DENS/
1763	"	Interpolation table for $\sigma_{el}(E)$ incorrect
1764	"	Expanded σ_{el} * W-table exceeds size of /RECS/
1765	"	No σ_{el}-data given for energies below the resonance region, ENDF/B file 3, MT = 2
1766	"	σ_{el} * W will not fit in /DENS/, MA = 3
1767	"	MA = 5 (σ_{in}) not in /DENS/
1768	"	σ_{in} will not fit in /DENS/, MA=2
1850	CWAX	MA = 1 (W) not in /DENS/
1851	"	MB = 7 (W) will not fit in /DENS/
1852	"	MB = 7 or MA = MA not in /DENS/
1853	"	Result of comb. MA = MA and MB = 7 will not fit in /RECS/
1854	"	MA = MA not in /DENS/
1855	"	MA * Weight will not fit in /DENS/, MA = 1
1860	RSTR	MA = 7 (W) not in /DENS/
1861	"	Weight will not fit in /DENS/, MA = 1
1870	INSCAT	σ_{in} given on ENDF/B file 3 but no data in file 5
1871	"	MA = 6 ($\sigma_{n,2n}$) not in /DENS/
1872	"	MA = 6 ($\frac{1}{2}\sigma_{n,2n}$) will not fit in /DENS/
1873	"	$\sigma_{n,2n}$ given on ENDF/B file 3 but no data in file 5
1880	FISSPC	σ_{f} "
1881	"	More than 3 different representations for the fission (or n-2n)-spectrum on ENDF/B file 5
1891	FSSPAR	More than 3 different representations for the fission (or n-2n)-spectrum on ENDF/B file 5
1892	"	At least two equal representations for the fission (or n-2n)-spectrum on ENDF/B file 5
1897	OUT1	Wrong fission (or n-2n)-spectrum on ENDF/B file 5
1898	OUT4	Number of sink groups for an exit group (σ_{in} $(E_k \rightarrow E_i)$) is $\leq$ 0.

Overflows can usually be avoided by decreasing EPS or using smaller energy groups (c.f.:"data will not fit in /DENS/" or "RECS").

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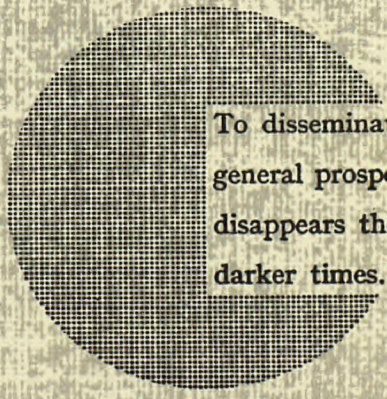

To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

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