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Manual

The NJOY Nuclear Data Processing System, Volume III: The GROUPR, GAMINR, and MODER Modules

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by

R. E. MacFarlane and D. W. Muir

ABSTRACT

The NJOY Nuclear Data Processing System is a comprehensive computer code package for producing pointwise and multigroup cross sections and related quantities from ENDF/B-IV, V, or VI evaluated nuclear data. A concise description of the code system and references to the ancestors of NJOY are given in Vol. I of this report. This volume describes the GROUPR module, which produces multigroup neutron interaction cross sections and group-to-group production cross sections for neutrons and photons; the GAMINR module, which produces multigroup photon-interaction cross sections and group-to-group matrices; and the MODER module, which converts ENDF/B and NJOY interface files back and forth between formatted (i.e., BCD, ASCII) and binary modes and performs several associated editing functions.

XIV. INTRODUCTION TO VOLUME III

The NJOY nuclear data processing system is a comprehensive computer code package for producing pointwise and multigroup cross sections from evaluated nuclear data in ENDF/B format. Volume I[1] of this report gives a concise description of the code system and functions as a User's Manual. Volume II[2] describes the main modules for producing detailed pointwise (that is, energy dependent) cross sections, including heating, radiation-damage, and thermal-scattering parameters. This volume provides detailed descriptions of the GROUPR and GAMINR modules, which are used to generate multigroup neutron and photon cross sections. It also describes the MODER program, which is used to convert files back and forth between coded (for example BCD or ASCII) and binary modes. MODER also has

some useful editing functions such as selecting one material out of an ENDF/B tape and combining several ENDF, PENDF, or GENDF materials together onto one tape. Volume IV[3] describes the ERROR and COVR modules, which are used to generate, plot, and reformat cross-section covariances.

XV. GROUPR

GROUPR produces selfshielded multigroup cross sections, anisotropic group-to-group scattering matrices, and anisotropic photon production matrices from ENDF/B-IV or V evaluated nuclear data. Special features are provided for ratio quantities (for example, $\bar{\mu}$, $\bar{\nu}$, or photon yield), inverse velocity, delayed neutron spectra by time group, and anisotropic thermal neutron scattering. Fission is represented as a group-to-group matrix for full generality. Scattering matrices and photon production matrices may be selfshielded if desired.

The Bondarenko narrow-resonance weighting scheme[4] is usually used. Optionally, a weighting flux can be computed for various mixtures of heavy absorbers with light moderators. An accurate pointwise solution of the integral slowing down equation is used. This option is normally called on to account for intermediate resonance effects in the epithermal range.

Neutron data and photon-production data are processed in a parallel manner using the same weight function and quadrature scheme. This helps to assure consistent cross sections for coupled neutron-photon problems. Two-body scattering is computed with a center-of-mass (CM) Gaussian quadrature, which gives accurate results even for small Legendre components of the group-to-group matrix. A special projection interpolation scheme is used to multigroup the coupled angle-energy thermal scattering distributions. The method helps to give smooth results even for rather coarse incident energy grids.

User conveniences include free-form input and complete control over which reactions are processed. The neutron group structure, photon group structure, and weight function can each be read in or set to one of the internal options. Output can be printed and/or written to an output "groupwise-ENDF" (GENDF) file for further processing by a formatting module (DTFR, CCCCR, MATXSR), by the covariance module (ERRORR), or by the MCNP continuous-energy Monte-Carlo module (ACER).

A. Multigroup Constants

Multigroup constants are normally used by computer codes that calculate the distributions of neutrons and/or photons in space and energy, and that compute various responses to these distributions, such as criticality, dose to personnel, or activation of materials. These distributions are solutions of the neutral particle

transport equation:*

$$\mu\frac{\partial}{\partial x}\phi(x,\mu,E) + \sigma_t(x,E)\phi(x,\mu,E)$$

$$= \int d\Omega' \int dE' \sigma_X(x,E'{\to}E,\Omega'{\to}\Omega)\phi(x,\mu',E')$$

$$+ Q(x,\mu,E), \qquad (1)$$

where the flux ϕ is allowed to vary with position x, direction Ω with polar cosine μ, and energy E. Similarly, the macroscopic total cross section σ_t varies with position and energy. The right-hand side of the equation contains the source due to transfers from other directions Ω' and energies E' (as described by the macroscopic transfer cross section σ_X), and a fixed or external source Q.

The macroscopic cross sections (in units of cm^{-1}) in Eq.(1) can be calculated from microscopic cross sections for the component isotopes or elements (in barns) using

$$\sigma_t(x,E) = \sum_i \rho_i(x)\,\sigma_t^i(T[x],E), \qquad (2)$$

where ρ_i is the number density for a constituent (in barns^{-1}cm^{-1}), which may vary with position, and T is the temperature, which may also vary with position. A similar formula holds for σ_X.

The transfer cross section σ_X (which includes both scattering and fission processes) is normally assumed to depend only on the cosine of the scattering angle, $\mu_0 = \Omega \cdot \Omega'$. This allows σ_X to be expanded using Legendre polynomials:

$$\sigma_X(x,E'{\to}E,\Omega'{\to}\Omega) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}\,\sigma_{X\ell}(x,E'{\to}E)\,P_\ell(\mu_0). \qquad (3)$$

Application of the addition theorem and integration over azimuthal angle then gives

$$\mu\frac{\partial}{\partial x}\phi(x,\mu,E) + \sigma_t(x,E)\phi(x,\mu,E)$$

$$= \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(\mu)\int \sigma_{X\ell}(x,E'{\to}E)\,\phi_\ell(x,E')\,dE'$$

$$+ Q(x,\mu,E), \qquad (4)$$

where

$$\phi_\ell(x,E) = \int P_\ell(\mu)\,\phi(x,\mu,E)\,d\mu. \qquad (5)$$

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*The following development uses a notation based on Bell and Glasstone[5], where the lower-case sigma is used for both macroscopic and microscopic cross sections, depending on the context. One-dimensional slab geometry is used throughout for simplicity.

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The desired responses are then given by

$$R(x) = \int \sigma_r(x,E)\,\phi_0(x,E)\,dE, \tag{6}$$

where σ_r is the reaction cross section for the response. The next step is to integrate Eqs.(4) and (6) over a ranges of energies chosen to lie in group g. The results are

$$\mu\frac{\partial}{\partial x}\phi_g(x,\mu) \;+\; \sum_{\ell=0}^{\infty} P_\ell(\mu)\,\sigma_{t\ell g}(x)\,\phi_{\ell g}(x)$$

$$= \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(\mu)\sum_{g'}\sigma_{X\ell g'\to g}(x)\,\phi_{\ell g'}(x) + Q_g(x,\mu), \tag{7}$$

and

$$R(x) = \sum_{g}\sigma_{rg}(x)\,\phi_{0g}(x), \tag{8}$$

where

$$\phi_{\ell g}(x) = \int_g \phi_\ell(x,E)\,dE, \tag{9}$$

$$\sigma_{t\ell g}(x) = \frac{\displaystyle\int_g \sigma_t(x,E)\,\phi_\ell(x,E)\,dE}{\displaystyle\int_g \phi_\ell(x,E)\,dE}, \tag{10}$$

$$\sigma_r(x) = \frac{\displaystyle\int_g \sigma_r(x,E)\,\phi_0(x,E)\,dE}{\displaystyle\int_g \phi_0(x,E)\,dE}, \tag{11}$$

and

$$\sigma_{X\ell g'\to g} = \frac{\displaystyle\int_g dE \int_{g'} dE'\, \sigma_{X\ell}(x,E'\to E)\,\phi_\ell(x,E)}{\displaystyle\int_g \phi_\ell(x,E)\,dE}. \tag{12}$$

The last three equations provide the fundamental definitions for the multigroup cross sections and the group-to-group matrix. Note that the values of the group constants depend upon the basic energy-dependent cross sections obtained from ENDF/B by way of the RECONR, BROADR, UNRESR, HEATR, and THERMR modules of NJOY, and the shape of ϕ within the group.

B. Group Ordering

Since neutrons normally lose energy in scattering, the scattering source into group g depends on the flux at higher-energy groups g' and the cross section for transferring neutrons from g' to g. For this reason, Eq.(7) is usually solved by

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sweeping from high energies to low energies. (Any thermal upscatter or fission is handled by iteration.) Data libraries for use with transport codes normally number the groups such that group 1 is the highest-energy group, and all the scattering matrix elements that transfer neutrons into group 1 are given first, followed by those for scattering into group 2, and so on.

However, in ENDF/B the evaluated nuclear data are always given in order of increasing incident energy, and secondary neutron distributions are described by giving emission spectra for given incident energies. Therefore, GROUPR numbers its groups such that group 1 is the lowest-energy group, and it calculates that scattering out of group 1, followed by the scattering out of group 2, and so on.

The "backward" energy-group numbering convention used by GROUPR is a possible source of confusion in interpreting output produced by the various modules of NJOY. All group indices printed by GROUPR or written to the GROUPR output file use the increasing-energy order. The covariance modules and photon interaction module follow the GROUPR ordering convention. Output modules such as DTFR, CCCCR, and MATXSR invert the group order and rearrange the scattering matrices from the GROUPR outscatter organization to the "transport" inscatter form. Any group indices printed by these three output modules will be in the conventional "transport" decreasing-energy order.

C.   Basic ENDF/B Cross Sections

The basic energy-dependent cross sections and angle-energy distributions needed for Eqs.(10), (11), and (12) are obtained from evaluated nuclear data in ENDF/B format[6]. These data are indexed by material (MAT), type of information (MF), and reaction (MT). Materials can be single isotopes, elements, or compounds. Type of information includes energy-dependent cross section (MF=3), angular distributions (MF=4), and secondary energy distributions (MF=5). Reactions include the total (MT=1) required for Eq.(10), the partial scattering reactions that must be summed for Eq.(12) [that is, elastic (MT=2), discrete-level inelastic, (n,2n), etc.], and the many partial reactions that can be used to calculate responses [for example, (n,2n) or (n,α) for activation, gas production, heat production (KERMA), radiation damage (DPA), etc.]. A list of the MT numbers for partial reactions is included in Vol. I of this report[1].

Before using GROUPR, the basic ENDF/B cross sections should have been converted into energy and temperature dependent pointwise cross sections in PENDF (pointwise ENDF) format using RECONR and BROADR. For heavy isotopes,

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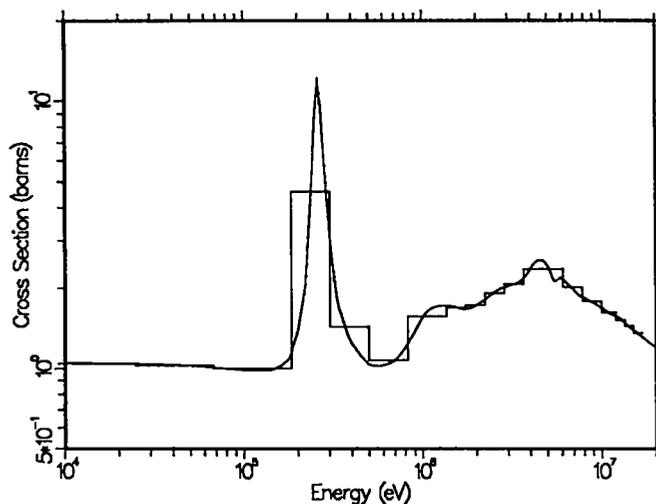
Figure 1: A comparison of the pointwise and multigroup representations for the total cross section of Li-7. The Los Alamos 30-group structure is shown.

unresolved selfshielding data should have been added to the PENDF tape* using UNRESR. If needed, heat production cross sections (KERMA), radiation damage production (or DPA), and thermal upscatter data could have also been added to the PENDF tape using HEATR and THERMR. See Vol. II of this report[2] for the details of preparing a PENDF tape.

The detailed methods used for evaluating Eqs.(10), (11), and (12) from ENDF and PENDF tapes are given below (see Sections K, L, and M). An example of an ENDF/B pointwise cross section compared with group-averaged cross sections from GROUPR is given in Fig.1.

D. Weighting Flux

In general, the weighting flux ϕ is not known; it is, after all, the particle distribution being sought in the transport calculation. However, it is often possible to obtain fairly accurate group constants for a particular application if the shape of the flux is reasonably well known over the broad energy ranges of a few-group structure (for example, a fission spectrum, thermal Maxwellian, or $1/E$ slowing-down spectrum). Alternatively, one can use many small groups so that mistakes in guessing the shape inside the group are not very important. The key to using the multigroup method effectively is balancing the tradeoffs between the choice of

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*The term "tape" is used loosely in this report to refer to any input or output file. Of course, such files would usually be on disk storage in a modern system.

weight function and the number of groups used for each different class of problem being solved.

In many cases of practical interest, the flux ϕ will contain dips corresponding to the absorption resonances of the various materials. In the reaction rate $\sigma(E)*\phi(E)$, these dips clearly reduce (selfshield) the effect of the corresponding resonance. GROUPR provides two methods to estimate the effect of this selfshielding: the Bondarenko model and the flux calculator.

In the Bondarenko model[4], the narrow resonance (NR) approximation, and the B_N approximation for large systems[5] are invoked to obtain

$$\phi_\ell(E) = \frac{W_\ell(E)}{[\sigma_t(E)]^{\ell+1}}, \tag{13}$$

where ϕ_ℓ is the ℓ-th Legendre component of the angular flux, the $W_\ell(E)$ are smooth functions of energy (such as $1/E$+fission), and $\sigma_t(E)$ is the total macroscopic cross section for the material. GROUPR takes all of the W_ℓ to be equal to the single function $C(E)$, where $C(E)$ can be read in or set to one of several internally-defined functions. It is further assumed that the important self-shielding effect of the flux can be obtained for isotope i by representing all the other isotopes with a constant "background cross section", σ_0. Therefore,

$$\phi_\ell^i(E) = \frac{C(E)}{[\sigma_t^i(E) + \sigma_0^i]^{\ell+1}}, \tag{14}$$

where σ_t^i is the microscopic total cross section for isotope i. The qualitative behavior of Eq.(14) is easy to understand. If σ_0 is larger than the tallest peaks in σ_t, the weighting flux ϕ is approximately proportional to the smooth weighting function $C(E)$. This is called "infinite dilution"; the cross section in the material of interest has little or no effect on the flux. On the other hand, if σ_0 is small with respect to σ_t, the weighting flux will have large dips at the locations of the peaks in σ_t, and a large selfshielding effect will be expected.

Each component material of a mixture now has a different weight function. The macroscopic total cross sections are given by

$$\sigma_{t\ell g} = \sum_i \rho_i\, \sigma_{t\ell g}^i(\sigma_0^i, T), \tag{15}$$

where

$$\sigma_{t\ell g}^i(\sigma_0, T) = \frac{\displaystyle\int_g \frac{\sigma_t^i(E,T)}{[\sigma_0 + \sigma_t^i]^{\ell+1}} C(E)\, dE}{\displaystyle\int_g \frac{1}{[\sigma_0 + \sigma_t^i]^{\ell+1}} C(E)\, dE}. \tag{16}$$

Similar equations are used for σ_R and $\sigma_{X\ell g\to g'}$. On the GROUPR level, σ_0 and T are simply parameters. Subsequent codes, such as 1DX[7] or TRANSX[8], can compute an appropriate value for σ_0, and then interpolate in tables of cross section versus σ_0 and T to get the desired selfshielded group constants.

The appropriate value for σ_0^i is obvious when a single resonance material is mixed with a moderator material (for example, $^{238}UO_2$), because the admixed materials typically have a constant cross section in the energy range where the heavy isotopes have resonances. For a mixture of resonance materials, the normal procedure is to preserve the average of Eq.(14) in each group by using

$$\sigma_{0g}^i = \frac{1}{\rho_i} \sum_{j\neq i} \rho_j\, \sigma_{t0g}^j(\sigma_{0g}^j, T), \tag{17}$$

where the ρ_i are atomic densities or atomic fractions. Eq.(17) is solved by iteration. Interference between resonances in different materials is handled in an average sense only.

In the unresolved energy range (see UNRESR), the explicit dependence of cross section on energy is not known. The integrands are replaced by their expected values:

$$\sigma_{x\ell g}(\sigma_0) = \frac{\displaystyle\int_g \left\langle \frac{\sigma_x}{[\sigma_0 + \sigma_t]^{\ell+1}} \right\rangle W_\ell\, dE}{\displaystyle\int_g \left\langle \frac{1}{[\sigma_0 + \sigma_t]^{\ell+1}} \right\rangle W_\ell\, dE}, \tag{18}$$

where the expected values are averages over the distributions of resonance position and width expected in the vicinity of energy E. The UNRESR module produces effective selfshielded point cross sections defined by

$$\langle \sigma_x \rangle_\ell = \frac{\left\langle \dfrac{\sigma_x}{[\sigma_0 + \sigma_t]^{\ell+1}} \right\rangle}{\left\langle \dfrac{1}{[\sigma_0 + \sigma_t]^{\ell+1}} \right\rangle}. \tag{19}$$

Substituting Eq.(19) into Eq.(18) gives an equation with the form of Eqs.(10) and (11), except that σ is replaced by $\langle \sigma \rangle$, and the flux is replaced by an average effective flux. This effective flux can be obtained by manipulating the effective

total cross section as follows:

$$\langle \sigma_t \rangle_\ell = \frac{\left\langle \dfrac{\sigma_0 + \sigma_t - \sigma_0}{[\sigma_0 + \sigma_t]^{\ell+1}} \right\rangle}{\left\langle \dfrac{1}{[\sigma_0 + \sigma_t]^{\ell+1}} \right\rangle} = \frac{\left\langle \dfrac{1}{[\sigma_0 + \sigma_t]^\ell} \right\rangle}{\left\langle \dfrac{1}{[\sigma_0 + \sigma_t]^{\ell+1}} \right\rangle} - \sigma_0, \tag{20}$$

from which

$$\left\langle \frac{1}{[\sigma_0 + \sigma_t]^{\ell+1}} \right\rangle = \frac{\left\langle \dfrac{1}{[\sigma_0 + \sigma_t]^\ell} \right\rangle}{\sigma_0 + \langle \sigma_t \rangle_k}. \tag{21}$$

Eq.(21) defines a recursion relation which can be used to compute the effective flux to any order:

$$\left\langle \frac{1}{[\sigma_0 + \sigma_t]^{\ell+1}} \right\rangle = \prod_{k=0}^{\ell} \frac{1}{\sigma_0 + \langle \sigma_t \rangle_k}. \tag{22}$$

This equation reduces to Eq.(14) in the resolved range. It is the formula used in GENFLX to compute $\phi_\ell(E)$ for the Bondarenko option.

When heterogeneity effects are important, the background cross section method can be extended as follows. In an infinite system of two regions (fuel and moderator), the neutron balance equations are

$$V_f \sigma_f \phi_f = (1 - P_f) V_f S_f + P_m V_m S_m, \tag{23}$$

and

$$V_m \sigma_m \phi_m = P_f V_f S_f + (1 - P_m) V_m S_m, \tag{24}$$

where V_f and V_m are the region volumes, σ_f and σ_m are the corresponding total macroscopic cross sections, S_f and S_m are the sources per unit volume in each region, P_f is the probability that a neutron born in the fuel will suffer its next collision in the moderator, and P_m is the probability that a neutron born in the moderator will suffer its next collision in the fuel. As usual, use is made of the reciprocity theorem,

$$V_f \sigma_f P_f = V_m \sigma_m P_m, \tag{25}$$

and the Wigner rational approximation to the fuel escape probability,

$$P_f = \frac{\sigma_e}{\sigma_e + \sigma_f}, \tag{26}$$

where σ_e is a slowly-varying function of energy called the escape cross section, to obtain an equation for the fuel flux in the form

$$(\sigma_f + \sigma_e)\phi_f = \frac{\sigma_e S_m}{\sigma_m} + S_f. \tag{27}$$

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In the limit where the resonances are narrow with respect to both fuel and moderator scattering, the source terms S_f and S_m take on their asymptotic forms of σ_p/E and σ_m/E respectively, and this equation becomes equivalent to the Bondarenko model quoted above with

$$\sigma_0^f = \frac{\sigma_e}{\rho_f}, \tag{28}$$

and

$$C(E) = \frac{\sigma_e + \sigma_p}{\rho_f E}. \tag{29}$$

Note that a large escape cross section (that is, a sample small relative to the average distance to collision) corresponds to infinite dilution as discussed above. To illustrate the general case, consider a neutron traveling through a lump of uranium oxide with an energy close to a resonance energy. If the neutron scatters from an oxygen nucleus, it will lose enough energy so that it can no longer react with the uranium resonance. Similarly, if the neutron escapes from the lump it can no longer react with the uranium resonance. The processes of moderator scattering and escape are equivalent in some way. Comparing Eq.(28) with Eq.(17) gives an "equivalence principle" that says that a lump of particular dimensions and a mixture of particular composition will have the same selfshielded cross sections when the narrow resonance approximation is valid. The effects of material mixing and escape can simply be added to obtain the effective σ_0 for a lump containing admixed moderator material. Therefore, Eq.(17) is extended to read

$$\sigma_{0g}^i = \frac{1}{\rho_i}\left\{\sigma_e + \sum_{j \neq i} \rho_j \, \sigma_{i0g}^j(\sigma_{0g}^j, T)\right\}, \tag{30}$$

where the escape cross section for simple convex objects (such as plates, spheres, or cylinders) is given by $(4V/S)^{-1}$, where V and S are the volume and surface area of the object, respectively. Many codes that use the background cross section method modify the escape cross section as defined above to correct for errors in the Wigner rational approximation ("Bell factor", "Levine factor"), or to correct for the interaction between different lumps in the moderating region ("Dancoff corrections"). These enhancements will not be discussed here.

E.   Flux Calculator

This narrow-resonance approach is quite useful for practical fast reactor problems. However, for nuclear systems sensitive to energies from 1 to 500 eV, there are many broad and intermediate-width resonances which cannot be selfshielded with sufficient accuracy using the Bondarenko approach. The GROUPR flux calculator is designed for just such problems.

Consider an infinite homogeneous mixture of two materials and assume isotropic scattering in the center-of-mass system. The integral slowing down equation becomes

$$\sigma(E)\phi(E) = \int_E^{E/\alpha_1} \frac{\sigma_{s1}(E')}{(1-\alpha_1)E'} \phi(E')\, dE'$$
$$+ \int_E^{E/\alpha_2} \frac{\sigma_{s2}(E')}{(1-\alpha_2)E'} \phi(E')\, dE'. \tag{31}$$

Furthermore, assume that material 1 is a pure scatterer with constant cross section and transform to the σ_0 representation. The integral equation becomes

$$[\sigma_0 + \sigma_{t2}(E)]\,\phi(E) = \int_E^{E/\alpha_1} \frac{\sigma_0}{(1-\alpha_1)E'} \phi(E')\, dE'$$
$$+ \int_E^{E/\alpha_2} \frac{\sigma_{s2}(E')}{(1-\alpha_2)E'} \phi(E')\, dE'. \tag{32}$$

Finally, assume that the moderator (material 1) is light enough so that all the resonances of material 2 are narrow with respect to scattering from material 1. This allows the first integral to be approximated by its asymptotic form $1/E$. More generally, the integral is assumed to be a smooth function of E given by $C(E)$. In this way, material 1 can represent a mixture of other materials just as in the Bondarenko method. Fission source and thermal upscatter effects can also be lumped in $C(E)$. The integral equation has now been reduced to

$$[\sigma_0 + \sigma_t(E)]\,\phi(E) = C(E)\,\sigma_0 + \int_E^{E/\alpha} \frac{\sigma_s(E')}{(1-\alpha)E'} \phi(E')\, dE'. \tag{33}$$

This is the simplest problem that can be solved using the flux calculator. The results still depend on the single parameter σ_0, and they can be used easily by codes that accept Bondarenko cross sections.

For heterogeneous problems when the narrow-resonance approximation fails, both S_f and S_m in Eq.(27) will show resonance features. To proceed further with the solution of this equation, it is necessary to eliminate the moderator flux that is implicit in S_m. As a sample case, consider a fuel pin immersed in a large region of water. The fission neutrons appear at high energies, escape from the pin, slow down in the moderator (giving a $1/E$ flux), and are absorbed by the resonances in the pin. In this limit, any dips in the moderator flux caused by resonances in the fuel are small. On the other hand, in a closely-packed lattice, the flux in the moderator is very similar to the flux in the fuel, and resonance dips in the moderator flux become very evident. Intermediate cases can be approximated[9] by

assuming

$$\phi_m = (1 - \beta) C(E) + \beta \phi_f, \tag{34}$$

where β is a heterogeneity parameter given by

$$\beta = \frac{V_f \sigma_e}{V_m \sigma_m}. \tag{35}$$

Note that $\beta \to 0$ gives the isolated rod limit and $\beta \to 1$ gives the close-packed lattice limit. This substitution reduces the calculation of the fuel flux to

$$(\sigma_f + \sigma_e) \phi_f = (1 - \beta) C(E) \sigma_e + S_\beta, \tag{36}$$

where S_β is the source term corresponding to a homogeneous mixture of the fuel isotopes with the isotopes from the moderator region changed by the factor $\beta \sigma_e / \sigma_m$. If the fuel and moderator each consisted of a single isotope and for isotropic scattering in the center-of-mass system, the integral equation would become

$$
\begin{aligned}
[\sigma_0 + \sigma_t(E)] \phi_f(E) &= (1 - \beta) C(E) \sigma_0 \\
&+ \int_E^{E/\alpha_m} \frac{\beta \sigma_0}{(1 - \alpha_m) E'} \phi_f(E') \, dE' \\
&+ \int_E^{E/\alpha_f} \frac{\sigma_{sf}(E')}{(1 - \alpha_f) E'} \phi_f(E') \, dE',
\end{aligned} \tag{37}
$$

where σ_0 is σ_e divided by the fuel density (units are barns/atom), α_m and α_f are the maximum fractional energy change in scattering for the two isotopes, and $\sigma_{sf}(E')$ is the fuel scattering cross section.

This result has a form parallel to that of Eq.(33), but the solution depends on the two parameters β and σ_0. For any given data set, β must be chosen in advance. This might not be difficult if the data are to be used for one particular system, such as pressurized water reactors. The routine also has the capability to include one more moderator integral with a different α value and a constant cross section. This allows calculations with H_2O as the moderator and an oxide as the fuel. The flux calculator can thus obtain quite realistic flux shapes for a variety of fuel, admixed moderator, and external moderator combinations. An example comparing the Bondarenko flux to a more realistic computed flux is given in Fig.2.

In practice, a fuel rod rarely contains only one resonance isotope. As an example, consider a mixture of a few percent of ^{239}Pu with ^{238}U as the major component. There will be a strong dip in the flux associated with the 6.7 eV ^{238}U resonance
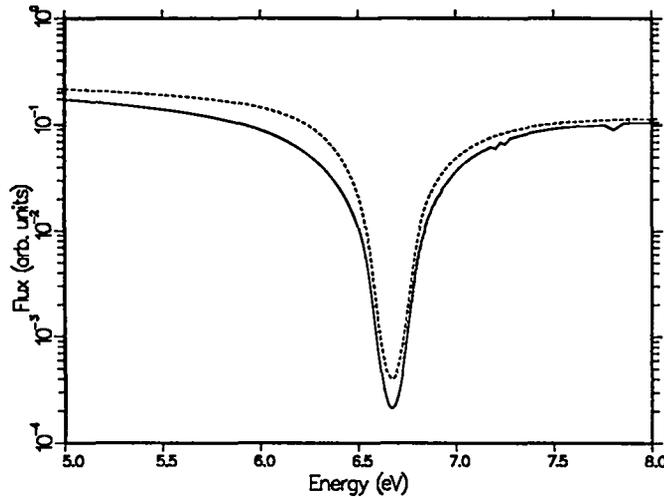
Figure 2: A comparison of the Bondarenko flux model (dashed) with a realistic computed flux (solid) for a ^{238}U oxide pin in water in the region of the 6.7 eV resonance.

that will affect the flux in the region of the 7.8 eV ^{239}Pu resonance (the interference effect), and there will also be a dip in the flux corresponding to the 7.8 eV resonance (the selfshielding effect). This additional complication in the flux shape would be expected to change the group constants for ^{239}Pu since both features lie in the same group for typical group structures. However, the effect of the ^{239}Pu on the ^{238}U group constants should be minimal. This argument suggests that the full flux calculation be used for ^{238}U as a single resonance material. The resulting flux would then be used to estimate the flux to be used in averaging the ^{239}Pu cross sections as follows:

$$\phi_{239}(E, \sigma_0) = \frac{\phi_{238}(E, 50)}{\sigma_0 + \dfrac{\sigma_{239}(E)}{1 + \dfrac{\sigma_{238}(E)}{50}}}, \tag{38}$$

where the ^{238}U flux is characteristic of a background of 50 barns/atom, which is representative of many thermal reactor systems. This formula assumes that the effect of ^{239}Pu on the scattering source for the mixture is small, but it retains the absorption effects. The selfshielding of ^{239}Pu is treated in the narrow resonance approximation only. The GROUPR flux calculator includes an option to write out a file containing the calculated flux and cross section needed for this formula (e.g., for ^{238}U) and another option to skip the flux calculation and use the formula above to obtain the weighting flux (e.g., for ^{239}Pu).

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The slowing down integral equation of Eq.(33) or (37) is solved point-by-point (see subroutine GENFLX) using the total and elastic cross sections on the PENDF tape produced by RECONR. In order to keep this task within bounds, the flux is computed from the lower limit of the first group to a specified energy EHI or until NFMAX values have been computed. The flux at higher energies is continued using the Bondarenko model described above.

F. Fission Source

The fission source was included in the transfer cross section σ_X in the development above. It is usually convenient to separate fission from scattering. Assuming isotropy, the source of fission neutrons into group g is given by

$$S_g = \sum_{g'} \sigma_{fg' \to g}\, \phi_{0g'},\tag{39}$$

where the group-to-group matrix for fission is defined as in Eq.(12), but with ℓ equal to zero. Most existing transport codes do not use this matrix form directly because the upscatter is expensive to handle and a reasonably accurate alternative exists. Except for relatively high neutron energies, the spectrum of fission neutrons is only weakly dependent on initial energy. Therefore, the fission source can be written

$$S_g = \chi_g \sum_{g'} \overline{\nu}_{g'}\, \sigma_{fg'}\, \phi_{0g'},\tag{40}$$

where $\overline{\nu}_g$ is the fission neutron yield, σ_{fg} is the fission cross section, and χ_g is the average fission spectrum (the familiar "chi" vector), which can be defined by

$$\chi_g \doteq \frac{\displaystyle\sum_{g'} \sigma_{fg' \to g}\, \phi_{0g'}}{\displaystyle\sum_g \sum_{g'} \sigma_{fg' \to g}\, \phi_{0g'}}.\tag{41}$$

The fission neutron yield is given by

$$\overline{\nu}_g = \sum_{g'} \sigma_{fg \to g'} \,/\, \sigma_{fg}.\tag{42}$$

Clearly, χ_g as given by Eq.(41) depends on the flux in the system of interest. The dependence is weak except for high incident energies, and a rough guess for ϕ_{0g} usually gives an accurate spectrum. When this is not the case, the problem can be iterated, or the full matrix representation can be used.

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The fission matrix computed by GROUPR represents the prompt part of fission only. The delayed component of fission is represented by a delayed-neutron yield $\overline{\nu}_g^D$, decay constants for six time groups, λ_i^D, and emission probability spectra for six time groups, χ_{ig}^D. Steady-state fission can be obtained using

$$\overline{\nu}_g^{SS} = \overline{\nu}_g + \overline{\nu}_g^D \tag{43}$$

and

$$\chi_g^{SS} = \frac{\sum_{g'} \sigma_{fg' \to g} \, \phi_{0g'} + \chi_g^D \sum_{g'} \overline{\nu}_{g'}^D \, \sigma_{fg'} \, \phi_{0g'}}{\sum_{g} \sum_{g'} \sigma_{fg' \to g} \, \phi_{0g'} + \sum_{g'} \overline{\nu}_{g'}^D \, \sigma_{fg'} \, \phi_{0g'}}, \tag{44}$$

where

$$\chi_g^D = \sum_i \chi_{ig}^D. \tag{45}$$

Note that χ_g^D sums to unity, but the χ for each time group sums to the fraction of the delayed neutron yield that appears in that time group.

In the ENDF/B files, the total fission reaction is represented by MT=18. Important isotopes also give the partial fission reactions (n,f), (n,n'f), (n,2nf), and sometimes (n,3nf) using MT=19, 20, 21, and 38 respectively. The MT=18 representation is adequate for most fission reactor applications, but the partial reactions should be processed for applications with significant flux above 6 MeV. Caution: although the cross section for MT=18 equals the sum of its parts, the group-to-group fission matrix $\sigma_{fg \to g'}$ computed from MT=18 will not, in general, equal the sum of the partial matrices for MT=19, 20, 21, and 38 above the 6-MeV threshold for second-chance fission. The delayed neutron data are given in MT=455. Sample input instructions for processing the various combinations of fission reactions used in ENDF/B will be found in Section M below. GROUPR outputs all the components of fission separately in order to give succeeding modules or codes complete flexibility.

G. Diffusion Cross Sections

The diffusion equation is very commonly used in reactor physics calculations. Starting with Eq.(7), use the Legendre expansion for ϕ_g in the derivative term, and make use of the recursion relation for $\mu P_\ell(\mu)$ and the orthogonality relation for the Legendre polynomials to obtain the transport equation in spherical harmonic form

$$\frac{n+1}{2n+1} \frac{\partial \phi_{n+1,g}}{\partial x} + \frac{n}{2n+1} \frac{\partial \phi_{n-1,g}}{\partial x} \, \sigma_{tng} \, \phi_{ng}$$

$$= \sum_{g'} \sigma_{sng' \to g} \, \phi_{ng'} + S_{fg} + Q_{ng}, \tag{46}$$

where the transfer term has been separated into a scattering term with cross section σ_s, and a fission source term S_f. When this set of equations is truncated at $n = N$, the result is usually called the "P_N equations". Now, all terms with $n > 1$ are dropped, and Q is assumed to be isotropic. Thus,

$$\frac{\partial \phi_{1g}}{\partial x} + \sigma_{t0g} \, \phi_{0g} = \sum_{g'} \sigma_{s0g' \to g} \, \phi_{0g'} + S_f + Q_{0g}, \tag{47}$$

and

$$\frac{1}{3} \frac{\partial \phi_{0g}}{\partial x} + \sigma_{t1g} \, \phi_{1g} = \sum_{g'} \sigma_{s1g' \to g} \, \phi_{1g'}. \tag{48}$$

The second equation can be written in the form of Fick's Law as follows:

$$\phi_{1g} = -D_g \frac{\partial \phi_{0g}}{\partial x}, \tag{49}$$

and

$$D_g = \frac{1}{3} \frac{1}{\sigma_{t1g} - \sum_{g'} \sigma_{s1g' \to g} \, \phi_{1g'} \, / \, \phi_{1g}}, \tag{50}$$

where D_g is the diffusion constant. The term in the denominator of the second factor is the transport cross section for diffusion, σ_{trD}. Unfortunately, it depends on a fairly complete knowledge of the neutron current in the system, perhaps from a previous calculation. However, for many problems, σ_{trD} can be simplified by assuming that

$$\sum_{g'} \sigma_{s1g' \to g} \, \phi_{1g'} \approx \sum_{g'} \sigma_{s1g \to g'} \, \phi_{1g}, \tag{51}$$

with the result that

$$\sigma_{trD,g} = \sigma_{t1g} - \sum_{g'} \sigma_{s1g \to g'}, \tag{52}$$

or

$$\sigma_{trD,g} = \sigma_{t1g} - \overline{\mu}_g \, \sigma_{s0g}, \tag{53}$$

where $\overline{\mu}_g$ is the average scattering cosine for neutrons in group g. These forms depend only on the shape of the weighting flux within the group, as usual. Substituting for ϕ_{1g} in Eq.(47) gives

$$\frac{\partial}{\partial x} \left(-D_g \frac{\partial \phi_{0g}}{\partial x} \right) + \sigma_{0tg} \, \phi_{0g} = \sum_{g'} \sigma_{s0g' \to g} \, \phi_{0g'} + S_{fg} + Q_{0g}, \tag{54}$$

which is the standard diffusion equation in slab geometry. Neither the diffusion coefficient nor the transport cross section for diffusion are produced directly by GROUPR. However, the components such a $\sigma_{t\ell}$ and $\sigma_{s0g'\to g}$ are made available to subsequent modules.

H. Cross Sections for Transport Theory.

The S_N (discrete ordinates) transport codes solve the equation

$$
\begin{aligned}
\mu\frac{\partial}{\partial x}\phi_g(\mu,x) \quad &+ \quad \sigma_g^{SN}\phi_g(\mu,x) \\
&= \quad \sum_{\ell=0}^{N}\frac{2\ell+1}{2}P_\ell(\mu)\sum_{g'}\sigma_{s\ell g'\to g}^{SN}(x)\,\phi_{\ell g'} \\
&+ \quad S_{fg}+Q_g(\mu,x),
\end{aligned}
\tag{55}
$$

where once again one-dimensional slab geometry has been used for simplicity.* By comparing Eq.(55) with Eq.(7), it is seen that the S_N equations require the following cross sections:

$$
\sigma_{s\ell g'\to g}^{SN} = \sigma_{s\ell g'\to g}, \qquad g' \neq g,
\tag{56}
$$

and

$$
\sigma_{s\ell g\to g}^{SN} = \sigma_{s\ell g\to g} - \sigma_{t\ell g} + \sigma_g^{SN},
\tag{57}
$$

where σ_g^{SN} is not determined, and can be chosen to improve the convergence of the S_N calculation. A particular choice of σ_g^{SN} gives rise to a "transport approximation", and various recipes are in use.

Consistent-P approximation:

$$
\sigma_g^{SN} = \sigma_{t0g},
\tag{58}
$$

Inconsistent-P approximation:

$$
\sigma_g^{SN} = \sigma_{t,N+1,g},
\tag{59}
$$

Diagonal transport approximation:

$$
\sigma_g^{SN} = \sigma_{t,N+1,g} - \sigma_{s,N+1,g\to g},
\tag{60}
$$

---

*The following development is based on the work of Bell, Hansen, and Sandmeier[10].

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Bell-Hansen-Sandmeier or extended transport approximation:

$$\sigma_g^{SN} = \sigma_{t,N+1,g} - \sum_{g'} \sigma_{s,N+1,g \to g'},$$ (61)

Inflow transport approximation:

$$\sigma_g^{SN} = \sigma_{t,N+1,g} - \frac{\sum_{g'} \sigma_{s,N+1,g' \to g}\, \phi_{N+1,g'}}{\phi_{N+1,g}}.$$ (62)

The first two approximations are most appropriate when the scattering orders above N are small. The inconsistent option removes most of the delta function of forward scattering introduced by the correction for the anisotropy of the total scattering rate, and should normally be more convergent than the consistent option. The diagonal and Bell-Hansen-Sandmeier (BHS) recipes make an attempt to correct for anisotropy in the scattering matrix and are especially effective for forward-peaked scattering. The BHS form is more often used, but the diagonal option can be substituted when BHS produces negative values. The inflow recipe makes the $N+1$ term of the P_N expansion vanish, but it requires a good knowledge of the $N+1$ flux moment from some previous calculation. Inflow reduces to BHS for systems in equilibrium by detail balance (i.e., the thermal region). In the absence of selfshielding (that is, $\sigma_0 \to \infty$), the distinction between σ_{t1} and σ_{t0} disappears, and so does the distinction between the inconsistent-P and consistent-P options. Also note that the inflow and BHS versions of σ_g are equivalent to the definitions of $\sigma_{trD,g}$ given in Eqs.(50) and (52), respectively, when $N = 0$.

These transport-corrected cross sections are not computed directly by GROUPR, but the components needed are written to the GROUPR output file for use by subsequent modules.

I. Photon Production and Coupled Sets

Photon transport is treated with an equation similar to Eq.(7), except that the flux, cross sections, and groups are all referred to photon interactions and photon energies instead of to the corresponding neutron quantities. Methods of producing the photon interaction cross sections are described in the GAMINR chapter of this volume. The external photon source Q_g depends on the neutron flux and the photon production cross sections through

$$Q_g(x,\mu) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{2} P_\ell(\mu) \sum_{g'} \sigma_{\gamma \ell g' \to g}(x)\, \phi_{\ell g'}(x),$$ (63)

group

1		N		N+G
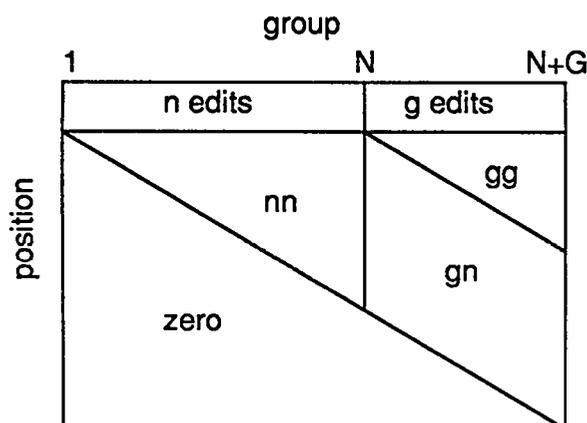
Figure 3: Arrangement of neutron (n) and photon (g) cross sections in a coupled transport table.

where $\sigma_{\gamma \ell g' \to g}$ is defined by Eq.(12) with X replaced by γ. The ENDF/B files define σ_γ using a combination of photon production cross sections (MF=13), photon yields (MF=12) with respect to neutron cross sections (MF=3), discrete lines (MF=12 and 13), and continuous γ distributions (MF=15). Methods for working with these representations will be discussed in more detail below.

For many practical problems, it is convenient to combine the neutron and photon transport calculations into a single application of Eq.(7) where the photons are treated as additional groups of low-energy neutrons. Since (γ,n) events are not usually very important, the down-scattering structure (see Section B) of the transport calculation is preserved for both n→γ and n→n events. Cross sections for this application are called "coupled sets". Coupled sets are not produced directly by GROUPR, but the n→n and n→γ components are made available to the other modules where they can be combined with γ→γ cross sections from GAMINR. As an example, the MATXSR module can format data for the TRANSX code[8], which can, in turn, prepare coupled sets for use by standard transport codes such as ONEDANT[11]. The normal arrangement of data in a coupled set is shown schematically in Fig.3.

J.   Thermal Data

GROUPR uses thermal data written onto the PENDF tape by the THERMR module. It does not process ENDF File-7 data directly. Three different represen-

tations of thermal scattering are used in ENDF.

For crystalline materials like graphite, coherent elastic (with zero energy change) scattering can take place. The cross section for this process shows well-defined "Bragg edges" at energies that correspond to the various lattice-plane spacings in the crystalline powder. As shown in the THERMR chapter of Vol.II of this report[2], the angular dependence of the coherent elastic cross section can be written as

$$\sigma^{coh}(E,\mu) = \sum_i \frac{b_i}{E} \delta(\mu - \mu_i), \tag{64}$$

where

$$\mu_i = 1 - 2\frac{E_i}{E}, \tag{65}$$

and where the E_i are the energies of the Bragg edges. THERMR integrates Eq.(64) over all angles, and writes the result to the PENDF tape. Clearly, the b_i can be recovered from

$$E\,\sigma^{coh}(E) = \sum_i{}' b_i, \tag{66}$$

where the primed sum is over all i such that $E_i < E$. It is only necessary to locate the steps in $E\,\sigma^{coh}(E)$. The size of the step gives b_i and the E for the step gives E_i. The Legendre cross sections become

$$\sigma_\ell^{coh}(E) = \sum_i{}' \frac{b_i}{E} P_\ell(\mu_i), \tag{67}$$

where any terms with $\mu_i < -1$ are omitted from the primed sum. An example of a pointwise cross section for coherent elastic scattering is given in Fig.4.

For materials with partial order, such as polyethylene and zirconium hydride, the process of incoherent elastic scattering is important. Here the angular cross section is given by

$$\sigma^{iel}(E,\mu) = \frac{\sigma_b}{2} \exp\left[-\frac{2EW}{A}(1-\mu)\right] \tag{68}$$

(see the THERMR chapter of Vol.II of this report). THERMR converts this into an integrated cross section, $\sigma^{iel}(E)$, and a set of N equally probable emission cosines, $\overline{\mu}_i$. These angles are present in File 6 on the PENDF tape. GROUPR can easily determine the Legendre components of the scattering cross section using

$$\sigma_\ell^{iel}(E) = \sigma^{iel}(E)\frac{1}{N} \sum_{i=1}^{N} P_\ell(\mu_i). \tag{69}$$

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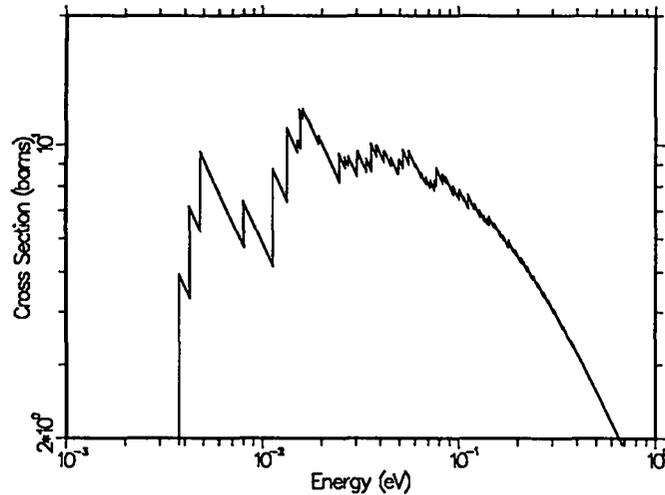
Figure 4: The coherent elastic scattering cross section for BeO showing the Bragg edges. The shape of $\sigma(E)$ between edges is $1/E$. Therefore, the function $E\sigma(E)$ is a stairstep function, where the height of each step depends on the structure factor for scattering from that set of lattice planes [see Eq.(66)].

The third thermal process is incoherent inelastic scattering. Here the neutron energy can either increase or decrease. The data from THERMR are given as a cross section in File 3 and an energy-angle distribution using a special form of File 6. The distribution is represented by sets of secondary-energy values E' for particular incident energies E. For each $E \rightarrow E'$, a scattering probability $f^{inc}(E \rightarrow E')$ and a set of equally probable cosines $\mu_i(E \rightarrow E')$ are given. The scattering probabilities for each value of E integrate to unity. Although the thermal scattering cross section is a smooth function of incident neutron energy, this is not true for the scattering from E to one particular final energy group g', since the differential cross section tends to peak along the line $E' = E$ and at E' values corresponding to well-defined excitations in the molecule or lattice. If interpolation between adjacent values of E were to be performed along lines of constant E', the excitation peaks would be well represented, but the $E = E'$ feature would produce two peaks in the intermediate spectrum, as shown in Figure 5. To avoid this problem, while still using a relatively sparse incident energy grid, GROUPR uses a new method called "projection interpolation". First, the spectrum at E_{lo} is divided into NBIN regions of equal area (probability). Then the spectrum at E_{hi} is divided similarly. Imaginary lines are drawn between the corresponding bin edges at E_{lo} and E_{hi}. The shape of the spectrum inside each bin at E_{lo} is projected up along these lines, and the shape in each bin at E_{hi} is projected down. The bin
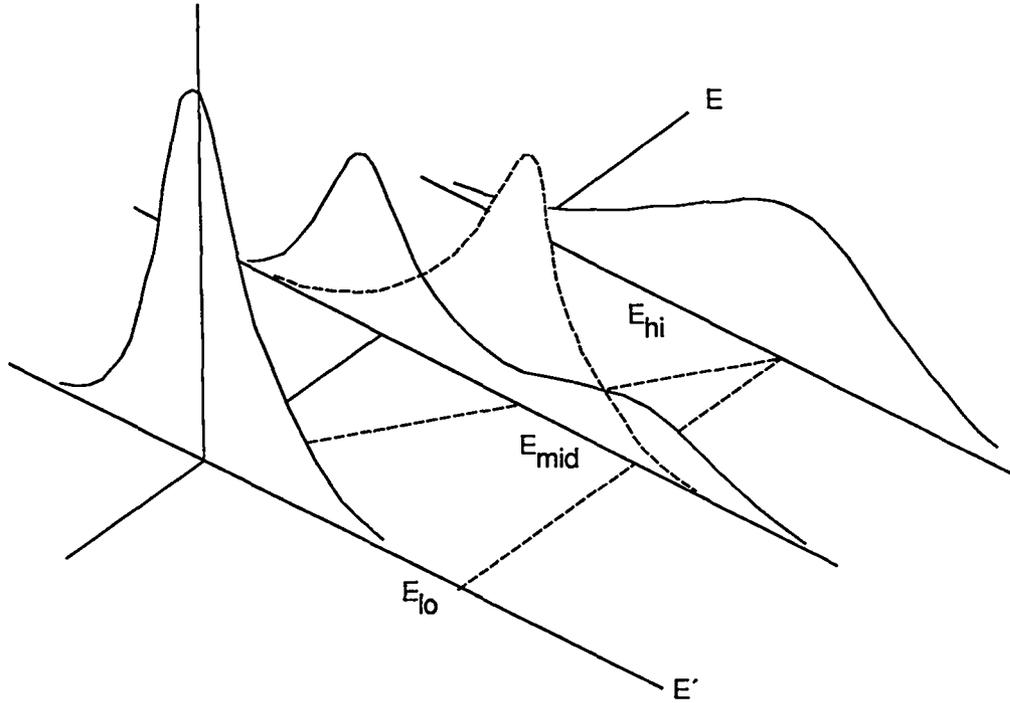
Figure 5: Illustration of projection interpolation showing the double-humped curve resulting from simple Cartestian interpolation (solid) and the more realistic curve obtained by projection (dashed).

lines thus provide both vertical and horizontal scaling of the spectrum shapes at E_{lo} and E_{hi}. The average of these two rescaled shapes at $E = E_{mid}$ normally is a relatively smooth spectrum at all intermediate energies (see the dashed line in Fig.5).

K. Generalized Group Integrals

In order to unify many formerly different processing tasks, GROUPR uses the concept of a generalized group integral

$$\sigma_g = \frac{\displaystyle\int_g \mathcal{F}(E)\,\sigma(E)\,\phi(E)\,dE}{\displaystyle\int_g \phi(E)\,dE}, \tag{70}$$

where the integrals are over all initial neutron energies in group g, $\sigma(E)$ is a cross section at E, and $\phi(E)$ is an estimate of the flux at E. The function $\mathcal{F}(E)$ is called the "feed function". It alone changes for different data types. To average a neutron cross section, $\mathcal{F}$ is set to 1. To average a ratio quantity like $\bar{\mu}$ with respect

to elastic scattering, $\mathcal{F}$ is set to $\bar{\mu}$. For photon production, $\mathcal{F}$ is the photon yield. For matrices, $\mathcal{F}$ is the ℓ-th Legendre component of the normalized probability of scattering into secondary-energy group g' from initial energy E. This definition is clearly independent of whether the secondary particle is a neutron or a photon.

The question of integration grid or quadrature scheme is important for the evaluation of Eq.(70). Each factor in the integrands has its own characteristic features, and it is important to account for them all. First, a grid must be established for each factor. As an example, the grid of $\sigma(E)$ is generated in RECONR such that sigma can be obtained to within a given tolerance by linear interpolation. GROUPR contains a subroutine GETSIG which carries out this interpolation at E and also returns the next grid energy in ENEXT. Subroutines GETFLX and GETFF perform similar functions for the flux and feed function. It is now easy to generate a union grid for the three-factor integrand using the following FORTRAN:

```
      ...
      CALL GETSIG(E,ENEXT,...)
      CALL GETFLX(E,EN,...)
      IF (EN.LT.ENEXT) ENEXT=EN
      CALL GETFF(E,EN,...)
      IF (EN.LT.ENEXT) ENEXT=EN
      ...
```

On occasion, there will be a discontinuity at ENEXT for one of the factors. In order to flag such a case, each "GET" routine also sets a discontinuity flag IDISC. The grid logic actually used throughout NJOY is as follows:

```
      ...
      CALL GETSIG(E,ENEXT,IDISC,...)
      CALL GETFLX(E,EN,IDIS,...)
      IF (EN.EQ.ENEXT.AND.IDIS.GT.IDISC) IDISC=IDIS
      IF (EN.LT.ENEXT) IDISC=IDIS
      IF (EN.LT.ENEXT) ENEXT=EN
      CALL GETFF(E,EN,IDIS,...)
      IF (EN.EQ.ENEXT.AND.IDIS.GT.IDISC) IDISC=IDIS
      IF (EN.LT.ENEXT) IDISC=IDIS
      IF (EN.LT.ENEXT) ENEXT=EN
      ...
```

This union grid for the integrand in the numerator is used to subdivide the generalized group integral of Eq.(70) into "panels". The main program of GROUPR carries out the integrals with the following logic:

```
      ...
      ELO=EGN(IG)
      EHI=EGN(IG+1)
      ENEXT=EHI
  230 CALL PANEL(ELO,ENEXT,...)
```

```
         IF (ENEXT.EQ.EHI) GO TO 240
         ELO=ENEXT
         ENEXT=EHI
         GO TO 230
     240 CONTINUE
         . . .
```

A panel is first defined by the energy bounds of group g. Subroutine PANEL is called to sum in the contributions from this panel. However, PANEL discovers that the integrand has a grid point at ENEXT less than EHI. It adds in the contributions for the smaller panel ELO to ENEXT and returns. GROUPR now sees that ENEXT is less than EHI, so it tries a new panel from the top of the last panel (ELO=ENEXT) to EHI. This loop continues until a panel with EHI as its upper bound is summed in. The integral for this group is then complete.

In this simple way, the algorithm accounts for the user's group structure and for all structure in the integrand. The method used for establishing the RECONR grid makes this integration algorithm equivalent to adaptive integration as used in MINX[12]. It has the great advantage that no "stack" of intermediate results is carried along. This single-pass feature of the quadrature scheme allows many different integrals to be accumulated simultaneously within reasonable storage limits. In this way, GROUPR accumulates cross sections for all values of σ_0 simultaneously. Similarly, group-to-group cross sections are computed for all secondary energy groups and all Legendre orders simultaneously.

Any degree of complexity can be used for the integral over each subpanel. Because $\sigma(E)$ has been linearized, PANEL is based on trapezoidal integration. Both $\phi(E)$ and $R(E) = \sigma(E)*\phi(E)$ are assumed to vary linearly across each panel. In some cases, the feed function is oscillatory over a certain energy range (see Two-Body Scattering). It is then convenient to integrate inside the panel using Lobatto quadrature[13] (note the variable NQ in PANEL). As discussed in more detail later, this method can obtain accurate results for an oscillatory function whose integral is small with respect to its magnitude. This behavior is characteristic of the higher Legendre components of two-body scattering cross sections.

The generalized integration scheme discussed here is also used by the GAMINR and ERRORR modules.

L.   Two-Body Scattering

Elastic scattering (ENDF/B MT=2) and discrete inelastic scattering (with MT=51–90) are both examples of two-body kinematics and are treated together by GROUPR. The feed function required for the group-to-group matrix calculation

may be written

$$\mathcal{F}_{\ell g'}(E) = \int_{g'} dE' \int_{-1}^{+1} d\omega \, f(E \rightarrow E', \omega) \, P_\ell(\mu[\omega]), \tag{71}$$

where $f(E \rightarrow E', \omega)$ is the probability of scattering from E to E' through a center-of-mass cosine ω and P_ℓ is a Legendre polynomial for laboratory cosine μ. The laboratory cosine corresponding to ω is given by

$$\mu = \frac{1 + R\omega}{\sqrt{1 + R^2 + 2R\omega}}, \tag{72}$$

and the cosine ω is related to secondary energy E' by

$$\omega = \frac{E'(1 + A)^2 - E(1 + R^2)}{2RE}. \tag{73}$$

In Eqs.(72) and (73), R is the effective mass ratio

$$R = A\sqrt{1 - \frac{(A + 1)(-Q)}{AE}}, \tag{74}$$

A is the ratio of target mass to neutron mass, and $-Q$ is the energy level of the excited nucleus ($Q = 0$ for elastic scattering). Integrating Eq.(71) over secondary energy gives

$$\mathcal{F}_{\ell g'}(E) = \int_{\omega_1}^{\omega_2} f(E, \omega) \, P_\ell(\mu[\omega]) \, d\omega, \tag{75}$$

where ω_1 and ω_2 are evaluated using Eq.(73) for E' equal to the upper and lower bounds of g' respectively.

The scattering probability is given by

$$f(E, \omega) = \sum_{\ell=0}^{L} f_\ell(E) \, P_\ell(\omega), \tag{76}$$

where the Legendre coefficients are either retrieved directly from the ENDF/B File 4 or computed from File 4 tabulated angular distributions (see subroutines GETFLE and GETCO).

The integration in Eq.(75) is performed (see subroutine GETFF) simultaneously for all Legendre components using Gaussian quadrature[13]. The quadrature order is selected based on the estimated polynomial order of the integrand. A reasonable estimate is given by

$$ND + NL + \log(300/A), \tag{77}$$

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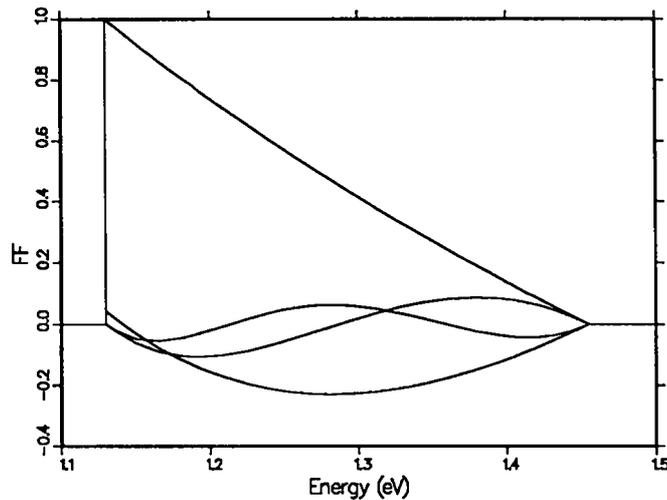
Figure 6: A typical feed function for two-body scattering showing the oscillations that must be treated correctly by the integration over incident energy.

where ND is the number of Legendre components desired for the feed function and NL is the number of components required to represent $f(E,\omega)$. The log term approximates the number of additional components required to represent the center-of-mass to lab transformation.

The two-body feed function for higher Legendre orders is a strongly oscillatory function in some energy ranges. An example is shown in Figure 6. Furthermore, the integral of the oscillatory part is often small with respect to the magnitude of the function. Such functions are very difficult to integrate with adaptive techniques, which converge to some fraction of the integral of the absolute value. This is the reason that MINX[12] gives poor answers for small Legendre components of the scattering matrix. Gaussian methods, on the other hand, are capable of integrating such oscillatory functions exactly if they are polynomials. Since a polynomial representation of the feed function is fairly accurate, a Gaussian quadrature scheme was chosen. The scheme used is also well-adapted to performing many integrals in parallel. In GROUPR, all Legendre components and all final groups are accumulated simultaneously (see PANEL).

The boundaries of the various regions of the feed function are called "critical points." Between critical points, the feed function is a smooth analytic function of approximately known polynomial order. It is only necessary to add these critical points to the incident energy grid of the feed function (the ENEXT variable) and to tell PANEL what quadrature order (NQ) to use. The critical points are determined

in GETFF by solving Eq.(73) for the values of E for which $\omega = +1$ and $\omega = -1$ when E' is equal to the various group boundaries. This can be done by writing

$$\frac{E_g}{E} = \frac{1}{(1+A)^2}[R^2 \pm 2R + 1], \tag{78}$$

substituting for E using Eq.(74), and then solving for R. The result is

$$E_{crit} = \frac{\dfrac{(A+1)(-Q)}{A}}{1 - \dfrac{F^2}{A^2}}, \tag{79}$$

where

$$F = \frac{1 \pm \sqrt{D}}{1 + \dfrac{E_F}{(-Q)}}, \tag{80}$$

$$D = \left[A^2\left(1 + \frac{E_F}{(-Q)}\right) - 1\right]\frac{E_F}{(-Q)}, \tag{81}$$

and

$$E_F = \frac{1+A}{A}E_g. \tag{82}$$

M.   Continuum Scattering and Fission

In ENDF/B, scattering from many closely-spaced levels or multi-body scattering such as (n,2n), (n,n'α), and fission is often represented using a separable function of scattering cosine and secondary neutron energy:

$$f(E \rightarrow E', \mu) = F(E, \mu)\, g(E \rightarrow E'), \tag{83}$$

where F is the probability that a neutron will scatter through a laboratory angle with cosine μ irrespective of final energy E'. It is obtained from MF=4. Similarly, g is the probability that a neutron's energy will change from E to E' irrespective of the scattering angle, and it is given in MF=5. Continuum reactions are easily identified by MT numbers of 6 through 49 and 91. The secondary-energy distributions can be represented in the ways listed below.

Law	Description
1	Arbitrary tabulated function
5	General evaporation spectrum (Used for delayed neutrons only)
7	Simple Maxwellian fission spectrum
9	Evaporation spectrum
11	Energy-dependent Watt fission spectrum
12	Energy-dependent spectrum of Madland and Nix

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The feed functions for continuum scattering are simply

$$\mathcal{F}_{\ell g'}(E') = \int_{-1}^{+1} P_\ell(\mu) \, f(E, \mu) \, d\mu \int_{g'} g(E, E') \, dE'. \tag{84}$$

The first integral is returned by GETFLE ["FLE" for $f_\ell(E)$] as described above, and the second integral is returned by GETSED ("SED" for secondary energy distribution).

For law 1, g is given as a tabulated function of E' for various values of E. When $E_1 \leq E < E_2$, the term $\int_{g'} g(E, E') \, dE'$ is obtained by interpolating between pre-computed values of $\int_{g'} g(E_1, E') \, dE'$ and $\int_{g'} g(E_2, E') \, dE'$ in subroutine GETSED. Since E always increases in successive calls to GETSED, it is only necessary to store two sets of the precomputed values at any time. Whenever E increases to or past E_2, the E_2 data are moved down to the E_1 positions, and new values are generated for the next higher energy in File 5. Except in the case of fission, any apparant upscatter produced by the "stair step" treatment near $E = E'$ is added to the in-group scattering term ($g' = g$).

For law 5, $g(x)$ is given versus $x = E'/\theta(E)$ and $\theta(E)$ is given vs E in File 5. This secondary neutron distribution leads to the following group integral:

$$\int_{g'} g(E, E') \, dE' = \theta(E) \int_{E_1/\theta}^{E_2/\theta} g(x) \, dx, \tag{85}$$

with E_1 and E_2 being the lower and upper boundary energies for group g'.

For law 7, the secondary-energy distribution is given by

$$g(E, E') = \frac{\sqrt{E'}}{I} \exp\left(-\frac{E'}{\theta(E)}\right), \tag{86}$$

where the effective temperature $\theta(E)$ is tabulated in File 5 and the normalization factor is given by

$$I = \theta^{3/2} [\sqrt{\frac{\pi}{4}} \operatorname{erf}(x) - x e^{-x}], \tag{87}$$

where

$$x = \frac{E - U}{\theta}. \tag{88}$$

Here U is a constant used to define the upper limit of secondary neutron energy $\theta \leq E' \leq E - U$. The desired group integral is given by

$$\begin{aligned}
\int_{g'} g(E, E') \, dE' &= \int_{E_1}^{E_2} g(E, E') \, dE' \\
&= \frac{X_1 - X_2 - Y_1 + Y_2}{\sqrt{\pi/4} - Y - X},
\end{aligned} \tag{89}$$

where

$$X = \sqrt{x}\, e^{-x}, \tag{90}$$

$$Y = \sqrt{\frac{\pi}{4}}\, \mathrm{rerfc}(\sqrt{x}), \tag{91}$$

and where X_1, Y_1, X_2, and Y_2 refer to X and Y evaluated at E_1/θ and E_2/θ. The integral of Eq.(89) is computed in ANASED ("ANA" for analytic). The function "rerfc" is the reduced complementary error function[13].

For law 9, the secondary energy distribution is given by

$$g(E, E') = \frac{E'}{I} \exp\left(-\frac{E'}{\theta(E)}\right), \tag{92}$$

where

$$I = \theta^2[1 - e^{-x}(1 + x)]. \tag{93}$$

Here x has the same meaning as above—see Eq.(88). The group integral is

$$\int_{g'} g(E, E')\, dE' = \frac{(1 + x_1)e^{-x_1} - (1 + x_2)e^{-x_2}}{1 - (1 + x)e^{-x}}, \tag{94}$$

where x_1 and x_2 refer to E_1/θ and E_2/θ, respectively. This result is also computed in ANASED.

For law 11, the secondary energy distribution is given by

$$g(E, E') = \frac{e^{-E'/a}}{I} \sinh(\sqrt{bE'}), \tag{95}$$

where

$$I = \frac{1}{2}\sqrt{\frac{\pi a^3 b}{4}}\, e^{x_0}[\mathrm{erf}(\sqrt{x} - \sqrt{x_0}) + \mathrm{erf}(\sqrt{x} + \sqrt{x_0})] - ae^{-x}\sinh(abx). \tag{96}$$

In this case, $a(E)$ and $b(E)$ are given in File 5,

$$x = \frac{E - U}{a}, \tag{97}$$

and

$$x_0 = \frac{ab}{4}. \tag{98}$$

The group integrals are given by

$$\int_{g'} g(E, E') = \frac{H(x_1, x_2, x_0)}{H(0, x, x_0)}, \tag{99}$$

30

where

$$
\begin{aligned}
H(x_1, x_2, x_0) &= H_2(\sqrt{x_1} - \sqrt{x_0}, \sqrt{x_2} - \sqrt{x_0}) \\
&+ \sqrt{x_0} H_1(\sqrt{x_1} - \sqrt{x_0}, \sqrt{x_2} - \sqrt{x_0}) \\
&- H_2(\sqrt{x_1} + \sqrt{x_0}, \sqrt{x_2} + \sqrt{x_0}) \\
&+ \sqrt{x_0} H_1(\sqrt{x_1} + \sqrt{x_0}, \sqrt{x_2} + \sqrt{x_0}),
\end{aligned}
\tag{100}
$$

and where

$$
H_n(a, b) = \frac{1}{\pi} \int_a^b z^n e^{-z^2} \, dz.
\tag{101}
$$

The methods for computing H_n are described in the BROADR chapter of Vol.II of this report[2]. When $\sqrt{x_2} < .01$, a short-cut calculation can be used for the numerator of Eq.(99):

$$
\frac{4\sqrt{x_0} e^{-x_0}}{3\sqrt{\pi/4}} [x_2^{3/2} - x_1^{3/2}].
\tag{102}
$$

For law 12, the Madland-Nix option, the secondary-energy distribution is given by

$$
g(E, E') = \frac{1}{2}[G(E', E_{fl}) + G(E', E_{fh})],
\tag{103}
$$

where

$$
\begin{aligned}
G(E', &E_f) \\
&= \frac{1}{3\sqrt{E_f T_m}} \left[u_2^{3/2} E_1(u_2) - u_1^{3/2} E_1(u_1) + \gamma(3/2, u_2) - \gamma(3/2, u_1) \right],
\end{aligned}
\tag{104}
$$

$$
u_1 = (\sqrt{E'} - \sqrt{E_f})^2 / T_m,
\tag{105}
$$

$$
u_2 = (\sqrt{E'} + \sqrt{E_f})^2 / T_m,
\tag{106}
$$

and where E_{fl}, E_{fh}, and $T_m(E)$ are given in File 5. The special functions used are the first-order exponential integral, $E_1(x)$, and the incomplete gamma function, $\gamma(n, x)$. The group integrals of this function are very complex[14]. Let

$$
\alpha = \sqrt{T_m},
\tag{107}
$$

$$
\beta = \sqrt{E_f},
\tag{108}
$$

$$
A = \frac{(\sqrt{E_1} + \beta)^2}{\alpha^2},
\tag{109}
$$

$$
B = \frac{(\sqrt{E_2} + \beta)^2}{\alpha^2},
\tag{110}
$$

$$A' = \frac{(\sqrt{E_1} - \beta)^2}{\alpha^2}, \tag{111}$$

$$B' = \frac{(\sqrt{E_2} - \beta)^2}{\alpha^2}. \tag{112}$$

Then the integral over the range (E_1, E_2) of G is given by one of the following three expression, depending on the region of integration in which E_1 and E_2 lie:

Region I $(E_1 \geq E_f, E_2 > E_f)$

$$3\sqrt{E_f T_m} \int_{E_1}^{E_2} G(E', E_f) dE'$$

$$= [(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2) E_1(B) - (\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2) E_1(A)]$$

$$-[(\frac{2}{5}\alpha^2 B'^{5/2} + \frac{1}{2}\alpha\beta B'^2) E_1(B') - (\frac{2}{5}\alpha^2 A'^{5/2} + \frac{1}{2}\alpha\beta A'^2) E_1(A')]$$

$$+[(\alpha^2 B - 2\alpha\beta B^{1/2})\gamma(3/2, B) - (\alpha^2 A - 2\alpha\beta A^{1/2})\gamma(3/2, A)]$$

$$-[(\alpha^2 B' + 2\alpha\beta B'^{1/2})\gamma(3/2, B') - (\alpha^2 A' + 2\alpha\beta A'^{1/2})\gamma(3/2, A')]$$

$$-\frac{3}{5}\alpha^2 [\gamma(5/2, B) - \gamma(5/2, A) - \gamma(5/2, B') + \gamma(5/2, A')]$$

$$-\frac{3}{2}\alpha\beta [e^{-B}(1 + B) - e^{-A}(1 + A) + e^{-B'}(1 + B') - e^{-A'}(1 + A')]. \tag{113}$$

Region II $(E_1 < E_f, E_2 \leq E_f)$

$$3\sqrt{(E_f T_m)} \int_{E_1}^{E_2} G(E', E_f) dE'$$

$$= [(\frac{2}{5}\alpha^2 B^{5/2} - \frac{1}{2}\alpha\beta B^2) E_1(B) - (\frac{2}{5}\alpha^2 A^{5/2} - \frac{1}{2}\alpha\beta A^2) E_1(A)]$$

$$-[(\frac{2}{5}\alpha^2 B'^2) E_1(B') - (\frac{2}{5}\alpha^2 A'^{5/2} - \frac{1}{2}\alpha\beta A'^2) E_1(A')]$$

$$+[(\alpha^2 B - 2\alpha\beta B^{1/2})\gamma(3/2, B) - (\alpha^2 A - 2\alpha\beta A^{1/2})\gamma(3/2, A)]$$

$$-[(\alpha^2 B' - 2\alpha\beta B'^{1/2})\gamma(3, 2, B') - (\alpha^2 A' - 2\alpha\beta A'^{1/2})\gamma(3/2, A')]$$

$$-\frac{3}{5}\alpha\beta [\gamma(5/2, B) - \gamma(5/2, A) - \gamma(5/2, B') + \gamma(5/2, A')]$$

$$-\frac{3}{2}\alpha\beta [e^{-B}(1 + B) - e^{-A}(1 + A) - e^{-B'}(1 + B') + e^{-A'}(1 + A')]. \tag{114}$$

Region III $(E_1 < E_f, E_2 > E_f)$

$$3\sqrt{E_f T_m} \int_{E_1}^{E_2} G(E', E_f) dE'$$

$$
\begin{aligned}
&= [(\tfrac{2}{5}\alpha^2 B^{5/2} - \tfrac{1}{2}\alpha\beta B^2)E_1(B) - (\tfrac{2}{5}\alpha^2 A^{5/2} - \tfrac{1}{2}\alpha\beta A^2)E_1(A)] \\
&\quad -[(\tfrac{2}{5}\alpha^2 B'^{5/2} + \tfrac{1}{2}\alpha\beta B'^2)E_1(B') - (\tfrac{2}{5}\alpha^2 A'^{5/2} - \tfrac{1}{2}\alpha\beta A'^2)E_1(A')] \\
&\quad +[(\alpha^2 B - 2\alpha\beta B^{1/2})\gamma(3/2,B) - (\alpha^2 A - 2\alpha\beta A^{1/2})\gamma(3/2,A)] \\
&\quad -[(\alpha^2 B' + 2\alpha\beta B'^{1/2})\gamma(3/2,B') - (\alpha^2 A' - 2\alpha\beta A'^{1/2})\gamma(3/2,A')] \\
&\quad -\tfrac{3}{5}\alpha^2[\gamma(5/2,B) - \gamma(5/2,A) - \gamma(5/2,B') + \gamma(5/2,A')] \\
&\quad -\tfrac{3}{2}\alpha\beta[e^{-B}(1+B) - e^{-A}(1+A) + e^{-B'}(1+B') + e^{-A'}(1+A') - 2].
\end{aligned}
\tag{115}
$$

N. GENDF Output

The group constants produced by GROUPR are normally written to an output file in GENDF (groupwise ENDF) format for use by other modules of NJOY. For example, DTFR can be used to convert a GENDF material to DTF (or "transport") format; CCCCR produces the standard interface files[15] ISOTXS, BRKOXS, and DLAYXS; MATXSR produces a file in MATXS format[8]; and POWR produces libraries of the Electric Power Research Institute (EPRI) codes EPRI-CELL and EPRI-CPM. Other formats can easily be produced by new modules, and some functions, such as group collapse, are conveniently performed directly in GENDF format. The GENDF format is also used for GAMINR output, and ACER and ERRORR both use GENDF input for some purposes.

Depending on the sign of NGOUT2 (see below), the GENDF file will be written in either formatted mode (i.e., BCD, ASCII, EBCDIC, etc.) or in the special NJOY blocked-binary mode. Conversion between these modes can be performed subsequently by the MODER module, as described in Chapter XVII of this report.

The GENDF material begins with a header record (MF=1, MT=451), but the format of this first section is different from MT=451 on an ENDF or PENDF tape. The section consists of a "CONT" record containing

ZA	Standard 1000*Z+A value
AWR	Atomic weight ratio to neutron
0	Zero
NZ	Number of σ_0 values
-1	Identifies a GENDF-type data file
NTW	Number of words in title

and a single "LIST" record containing

TEMPIN	Material temperature (Kelvin)
0.	Zero
NGN	Number of neutron groups
NGG	Number of photon groups
NW	Number of words in LIST
0	Zero
TITLE	Title from GROUPR input (NTW words)
SIGZ	Sigma-zero values (NZ words)
EGN	Neutron group boundaries, high to low (NGN+1 words)
EGG	Photon group boundaries, high to low (NGG+1 words).

The word count is seen to be NW=NTW+NZ+NGN+1+NGG+1. The LIST record is followed by a standard ENDF file-end record (FEND). The normal ENDF section-end (SEND) is omitted.

This header is followed by a series of records for reactions. The ENDF ordering requirements are relaxed, and MF and MT values can occur in any order. Each section starts with a "CONT" record:

ZA	Standard 1000*Z+A value
AWR	Standard atomic weight ratio
NL	Number of Legendre components
NZ	Number of sigma-zero values
LRFLAG	Break-up identifier flag
NGN	Number of groups.

It is followed by a series of LIST records, one for every incident-energy group with nonzero result:

TEMP	Material temperature (Kelvin)
0.	Zero
NG2	Number of secondary positions
IG2LO	Index to lowest nonzero group
NW	Number of words in LIST
IG	Group index for this record
A(NW)	Data for LIST (NW words)

where NW=NL*NZ*NG2LO. The last LIST record in the sequence is the one with IG=NGN. It must be given even if its contents are zero. The last LIST record is followed by a SEND record.

The contents of A(NW) change for various types of data. For simple cross section "vectors" (MF=3), NG2 is 2, and A contains the two FORTRAN arrays

FLUX(NL,NZ), SIGMA(NL,NZ)

in that order. For ratio quantities like fission $\bar{\nu}$, NG2 is three, and A contains

FLUX(NL,NZ), RATIO(NL,NZ), SIGMA(NL,NZ).

For transfer matrices (MF=6 or 16), A contains

FLUX(NL,NZ), MATRIX(NL,NZ,NG2-1).

The actual secondary group indices for the last index of MATRIX are IG2LO, IG2LO+1, etc., using the GROUPR convention of labeling groups in order of increasing energy. Finally, for delayed neutron spectra (MF=5), NL is used to index the 6 time groups, NZ is one, and there is only one incident energy record (IG=IGN). The array A contains

LAMDA(NL), CHID(NL,NG2-1),

where LAMDA contains the six delayed-neutron time constants and CHID contains the six spectra.

The GENDF material ends with a material-end (MEND) record, and the GENDF tape ends with a tape-end (TEND) record.

O. Running GROUPR

The input instructions as reproduced from the comment cards at the beginning of the 6/83-3 version of the GROUPR module follow. Since the code changes from time to time, it is a good idea to check these comment cards in the current version to obtain up-to-date input instructions.

```
*---INPUT SPECIFICATIONS (FREE FORMAT)-------------------------------*
*                                                                    *
* CARD1                                                              *
*    NENDF    UNIT FOR ENDF/B TAPE                                   *
*    NPEND    UNIT FOR PENDF TAPE                                    *
*    NGOUT1   UNIT FOR INPUT GOUT TAPE (DEFAULT=0)                   *
*    NGOUT2   UNIT FOR OUTPUT GOUT TAPE (DEFAULT=0)                  *
* CARD2                                                              *
*    MATB     MATERIAL TO BE PROCESSED                               *
*             MATB LT 0 IS A FLAG TO ADD MTS TO AND/OR REPLACE       *
*             INDIVIDUAL MTS ON NGOUT1.                              *
*    IGN      NEUTRON GROUP STRUCTURE OPTION                         *
*    IGG      GAMMA GROUP STRUCTURE OPTION                           *
*    IWT      WEIGHT FUNCTION OPTION                                 *
*    LORD     LEGENDRE ORDER                                         *
*    NTEMP    NUMBER OF TEMPERATURES                                 *
*    NSIGZ    NUMBER OF SIGMA ZEROES                                 *
```

```
*     IPRINT  LONG PRINT OPTION (0/1=MINIMUM/MAXIMUM)              *
*             (DEFAULT=1)                                         *
* CARD3                                                           *
*     TITLE   RUN LABEL (UP TO 80 CHARACTERS DELIMITED BY *,      *
*             ENDED WITH /)  (DEFAULT=BLANK)                      *
* CARD4                                                           *
*     TEMP    TEMPERATURES IN KELVIN                              *
* CARD5                                                           *
*     SIGZ    SIGMA ZERO VALUES (INCLUDING INFINITY)              *
*                                                                 *
*             IF IGN=1, READ NEUTRON GROUP STRUCTURE (6A AND 6B)  *
* CARD6A                                                          *
*     NGN     NUMBER OF GROUPS                                    *
* CARD6B                                                          *
*     EGN     NGN+1 GROUP BREAKS (EV)                             *
*                                                                 *
*             IF IGG=1, READ GAMMA GROUP STRUCTURE (7A AND 7B)    *
* CARD7A                                                          *
*     NGG     NUMBER OF GROUPS                                    *
* CARD7B                                                          *
*     EGG     NGG+1 GROUP BREAKS (EV)                             *
*                                                                 *
*             WEIGHT FUNCTION OPTIONS (8A,8B,8C,8D)               *
* CARD8A      FLUX CALCULATOR PARAMETERS (IWT.LT.0 ONLY)          *
*     EHI     BREAK BETWEEN COMPUTED FLUX AND BONDARENKO FLUX     *
*                 (MUST BE IN RESOLVED RANGE)                     *
*     SIGPOT  ESTIMATE OF POTENTIAL SCATTERING CROSS SECTION      *
*     NFLMAX  MAXIMUM NUMBER OF COMPUTED FLUX POINTS              *
*     NINWT   TAPE UNIT FOR NEW FLUX PARAMETERS (DEFAULT=0)       *
*     JSIGZ   INDEX OF REFERENCE SIGMA ZERO IN SIGZ ARRAY         *
*             (DEFAULT=0)                                         *
*     ALPHA2  ALPHA FOR ADMIXED MODERATOR (DEF=0=NONE)            *
*     SAM     ADMIXED MODERATOR XSEC IN BARNS PER ABSORBER        *
*             ATOM (DEF=0=NONE)                                   *
*     BETA    HETEROGENEITY PARAMETER (DEF=0=NONE)                *
*     ALPHA3  ALPHA FOR EXTERNAL MODERATOR (DEF=0=NONE)           *
*     GAMMA   FRACTION OF ADMIXED MODERATOR CROSS SECTION IN      *
*             EXTERNAL MODERATOR CROSS SECTION (DEF=0)            *
* CARD8B      TABULATED (IWT=1 OR -1 ONLY)                        *
*     WGHT    READ WEIGHT FUNCTION AS TAB1 RECORD.                *
*             END WITH A /.                                       *
* CARD8C      ANALYTIC FLUX PARAMETERS (IWT=4 OR -4 ONLY)         *
*     EB      THERMAL BREAK (EV)                                  *
*     TB      THERMAL TEMPERATURE (EV)                            *
*     EC      FISSION BREAK (EV)                                  *
*     TC      FISSION TEMPERATURE (EV)                            *
* CARD8D      INPUT RESONANCE FLUX (IWT=0 ONLY)                   *
*     NINWT   TAPE UNIT FOR FLUX PARAMETERS                       *
*                                                                 *
* CARD9                                                           *
*     MFD     FILE TO BE PROCESSED                                *
*     MTD     SECTION TO BE PROCESSED                             *
*     MTNAME  DESCRIPTION OF SECTION TO BE PROCESSED              *
*             REPEAT FOR ALL REACTIONS DESIRED                    *
*             MFD=0/ TERMINATES THIS TEMPERATURE/MATERIAL.        *
* CARD10                                                          *
*     MATD    NEXT MAT NUMBER TO BE PROCESSED                     *
*             MATD=0/ TERMINATES GROUPR RUN.                      *
```

```
*                                                                    *
*---OPTIONS FOR INPUT VARIABLES----------------------------------------*
*                                                                    *
*     IGN              MEANING                                       *
*     ---              -------                                       *
*      1               ARBITRARY STRUCTURE (READ IN)                *
*      2               CSEWG 239 GROUP STRUCTURE                     *
*      3               LANL 30 GROUP STRUCTURE                       *
*      4               ANL 27 GROUP STRUCTURE                        *
*      5               RRD 50 GROUP STRUCTURE                        *
*      6               GAM-I 68 GROUP STRUCTURE                      *
*      7               GAM-II 100 GROUP STRUCTURE                    *
*      8               LASER-THERMOS 35 GROUP STRUCTURE              *
*      9               EPRI-CPM 69 GROUP STRUCTURE                   *
*     10               LANL 187-GROUP STRUCTURE                      *
*     11               LANL 70-GROUP STRUCTURE                       *
*     12               SAND-II 620-GROUP STRUCTURE                   *
*     13               LANL 80-GROUP STRUCTURE                       *
*     14               EURLIB 100-GROUP STRUCTURE                    *
*     15               SAND-IIA 640-GROUP STRUCTURE                  *
*                                                                    *
*     IGG              MEANING                                       *
*     ---              -------                                       *
*      0               NONE                                         *
*      1               ARBITRARY STRUCTURE (LIST RECORD)            *
*      2               CSEWG 94 GROUP STRUCTURE                     *
*      3               LANL 12 GROUP STRUCTURE                      *
*      4               STEINER 21 GROUP GAMMA-RAY STRUCTURE         *
*                            (ORNL-TM-2564)                         *
*      5               STRAKER 22 GROUP STRUCTURE                   *
*      6               LANL 48-GROUP STRUCTURE                      *
*      7               LANL 24-GROUP STRUCTURE                      *
*                                                                    *
*     IWT              MEANING                                       *
*     ---              -------                                       *
*      1               READ IN SMOOTH WEIGHT FUNCTION               *
*      2               CONSTANT                                     *
*      3               1/E                                          *
*      4               1/E + FISSION SPECTRUM + THERMAL MAXWELLIAN  *
*      5               EPRI-CELL LWR                                *
*      6               (THERMAL) -- (1/E) -- (FISSION + FUSION)     *
*      7               FAST REACTOR                                 *
*      8               THERMAL--1/E--FAST REACTOR--FISSION + FUSION *
*      9               CLAW WEIGHT FUNCTION                         *
*     -N               COMPUTE FLUX WITH WEIGHT N                   *
*      0               READ IN RESONANCE FLUX FROM NINWT            *
*                                                                    *
*     MFD              MEANING                                       *
*     ---              -------                                       *
*      3               CROSS SECTION OR YIELD VECTOR                *
*      5               FISSION CHI BY SHORT-CUT METHOD              *
*      6               NEUTRON-NEUTRON MATRIX                       *
*     12               PHOTON PROD. XSEC (PHOTON YIELDS GIVEN, MF12) *
*     13               PHOTON PROD. XSEC (PHOTON XSECS GIVEN, MF13)  *
*     16               NEUTRON-GAMMA MATRIX (PHOTON YIELDS GIVEN)   *
*     17               NEUTRON-GAMMA MATRIX (PHOTON XSECS GIVEN)    *
*     90+N             RADIOACTIVE NUCLIDE PRODUCTION FROM NTH      *
*                        SUBSECTION FOR MTD IN FILE 9.             *
```

```
*    100+N          RADIOACTIVE NUCLIDE PRODUCTION FROM NTH      *
*                   SUBSECTION FOR MTD IN FILE 10.               *
*            NOTE: MFD=13 WILL AUTOMATICALLY CHANGE TO 12        *
*                   IF NECESSARY, AND MFD=16 WILL AUTOMATICALLY  *
*                   CHANGE TO 17 IF NECESSARY.                   *
*                                                               *
*    MTD            MEANING                                      *
*    ---            -------                                      *
*    -N             PROCESS ALL MT NUMBERS FROM THE PREVIOUS     *
*                   ENTRY TO N INCLUSIVE                         *
*    221-250        RESERVED FOR THERMAL SCATTERING             *
*    258            AVERAGE LETHARGY                             *
*    259            AVERAGE INVERSE VELOCITY (M/SEC)            *
*                                                               *
****************************************************************
```

In the instructions, CARD1 defines the input and output units for GROUPR. The module requires both ENDF and PENDF input tapes, because the PENDF tapes produced by RECONR, BROADR, etc., do not contain angle (MF=4), energy (MF=5), or photon (MF=12,15) distributions. For materials that do not use resonance parameters to represent part of the cross section, it is possible to use a copy of the ENDF tape in place of the PENDF tape. The normal mode for GROUPR is to use NGOUT1=0; however, sometimes it is convenient to add a new material or reaction to an existing GENDF tape. The old GENDF tape is then mounted on unit NGOUT1, and the revised GENDF tape will be written to NGOUT2.

CARD2 selects the first material to be processed (MATB) and sets up the group structures, weighting option, Legendre order, and selfshielding parameters for all the materials to be processed in this run.

The names of the available group structures are given in the input instructions, and the energy bounds are tabulated in Appendix A of this report. Of course, it is always possible to read in an arbitrary group structure (see CARD6A through CARD7B). The energies must be given in <u>increasing</u> order (note that this is opposite from the usual convention). Here is an example of the input cards for the conventional 4 group structure used in many thermal reactor codes:

```
4/ CARD6A
1E-5 .625 5530 .821E6 10E6 / CARD6B.
```

These cards are read by the standard NJOY free-format input routine (FREE). Fields are delimited by space, and "/" terminates the processing of input on a card. Anything after the slash is a comment.

The available weight function options are listed in the input instructions under IWT, and they are plotted in Appendix B of this report. Just as in the case of

group structures, an arbitrary weight function can be read in (see CARD8B). This function is presented to GROUPR as an ENDF/B "TAB1" record. This means that a count of $E, C(E)$ pairs and one or more interpolation schemes are given. For the case of a single interpolation scheme, the input cards would be

```
0. 0. 0 0 1 N N INT
E1 C(E1) E2 C(E2) ... / CARD8B,
```

where N is the count of E,C pairs, and INT specifies the interpolation law to be used for values of E between the grid values E_1, E_2,... according to the "graph paper" schemes below.

INT	Meaning
1	histogram
2	linear-linear
3	linear-log
4	log-linear
5	log-log

For example, I=5 specifies that $\ln C$ is a linear function of $\ln E$ in each panel $E_i \leq E < E_j$. Similarly, I=4 specifies that $\ln C$ is a linear function of E in each panel. As many physical lines as are needed can be used for "CARD8B", as long as the terminating slash is included.

One of the weighting options is a generalized "$1/E$+fission+thermal" function where the thermal temperature, fission temperature, and breakpoint energies (all in eV) are given on CARD8C. The weight function used for the Los Alamos LIB-IV cross section library[16] used

```
.10 .025 820.3E3 1.4E6 / CARD8C.
```

A plot of this function will be found in Appendix B.

The GROUPR flux calculator is selected by a negative sign on IWT. The additional CARD8A is then read. The calculator option used is determined by the number of parameters given and their values. EHI and NFLMAX are used to select the energy range for the flux calculation, and they also determine the cost in time and storage. The actual value for SIGPOT is not very critical—a number near 10 barns is typical for fissionable materials.

Nonzero values for NINWT and JSIGZ will cause the computed flux for a given fissionable isotope (such as ^{238}U) to be written out onto a file. This saved flux can be used as input for a subsequent run for a fissile material (such as ^{239}Pu) with IWT=0 to get an approximate correction for resonance-resonance interference. See Eq.(38).

Nonzero values for some of the last five parameters on CARD8A select the extended flux calculation of Eq.(37). The simplest such calculation is for an isolated pin containing a heavy absorber with an admixed moderator. For $^{238}UO_2$, the card might be

        400 10.6 5000 0 0 .7768 7.5 / CARD8A,

where 7.5 barns is twice the oxygen cross section and α is computed from $[(A-1)/(A+1)]^2$ with $A \doteq 15.858$. A more general case would be a PWR-like lattice of $^{238}UO_2$ fuel rods in water:

        400 10.6 5000 0 0 .7768 7.5 .40 1.7E-7 .086 / CARD8A,

where .086 is computed using 3.75 barns for O and 40 barns for for the two H atoms bound in water. A third example would compute the flux for a homogeneous mixture of ^{238}U and hydrogen:

        400 10.6 5000 0 0 0 0 1. 1.7E-7 / CARD8A.

The maximum Legendre expansion order used for scattering matrices is set by LORD. The number of tables produced is LORD+1; that is, $\ell = 0, 1, ...$ LORD. When more than 1 value of σ_0 is requested, both the $\ell = 0$ and $\ell = 1$ components of the total cross section are produced.

CARD3 contains a short descriptive title that is printed on the listing and added to the output GENDF tape. CARD4 gives the NTEMP values of temperature for the run. They must be in <u>ascending</u> order, and if unresolved data are included on the PENDF tape, the temperatures in this list must match the first NTEMP values in MF=2, MT=153 from UNRESR (see STOUNR and GETUNR). CARD5 gives the σ_0 values for the run in <u>descending</u> order, starting with infinity (represented by 10^{10} barns).

The above completes the description of the global input parameters for GROUPR. The rest of the input cards request reactions to be processed for the various temperatures and materials desired. Because of the many types of data that it can process, GROUPR does not have a completely automatic mode for choosing reactions to be processed. On the basic level, it asks the user to request each separate cross section or group-to-group matrix using the parameters MFD, MTD, and MTNAME. However, simplified input modes are also available. For example, the one "CARD9" containing

        3/

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will process the cross section "vectors" for all of the reaction MT numbers found on the PENDF tape.

For completeness, the full input for MATD, MFD, and MTNAME will be described first. The value of MFD depends on the output desired (vector, matrix) and the form of the data on the ENDF evaluation. Simple cross section "vectors" σ_{xg} are requested using MFD=3 and the MTD numbers desired from the list of reactions available in the evaluation (check the "dictionary" in MF=1, MT=451 of the ENDF and PENDF tapes for the reactions available). A typical example would be

```
3    1 *TOTAL*/
3    2 *ELASTIC*/
3   16 *(N,2N)*/
3   51 *(N,NPRIME)FIRST*/
3  -66 *(N,NPRIME)NEXT*/
3   91 *(N,NPRIME)CONTINUUM*/
3  102 *RADIATIVE CAPTURE*/.
```

The combination of "3 51" followed by "3 16" means process all the reactions from 51 through 66; that is, (n,n_1'), (n,n_2'), etc. If selfshielding is requested, the following reactions will be processed using NSIGZ values of background cross section: total (MT=1), elastic (MT=2), fission (MT=18 and 19), radiative capture (MT=102), heat production (MT=301), kinematic KERMA (MT=443), and damage energy production (MT=444). The other File 3 reactions will be computed at $\sigma_0 = \infty$ only. This list of reactions can be altered by small changes in INIT if desired.

There are several special options for MTD available when processing cross section vectors:

MTD	Option
259	Average inverse neutron velocity for group in sec/meter.
258	Average lethargy for group.
251	Average elastic scattering cosine $\bar{\mu}$ computed from File 4.
252	Continuous-slowing-down parameter $\bar{\xi}$: the average logarithmic energy decrement for elastic scattering, computed from File 4.
253	Continuous-slowing-down parameter $\bar{\gamma}$: the average of the square of the logarithmic energy decrement for elastic scattering, divided by twice the average logarithmic energy decrement for elastic scattering, all computed from File 4.
452	$\bar{\nu}$: the average total fission yield, computed from MF=1 and MF=3.
455	$\bar{\nu}^D$: the average delayed neutron yield, computed from MF=1 and MF=3.

456 $\overline{\nu}^P$: the average prompt fission neutron yield, computed from MF=1 and MF=3.

There are also some special options for MFD as follows:

MFD	Option
12	Photon production cross section computed from File 12 and File 3.
13	Photon production cross section computed from File 13. Recent versions of GROUPR will automatically shift between 12 and 13, if necessary.
91–99	Isomer production cross sections computed from yields in File 9. MFD=91 is for the first state given in the file (usually the ground state), MFD=92 is for the second state given (usually the first isomeric state), etc.
101–109	Isomer production cross sections as above, except for data given as isomer production cross sections in File 10.

An example of the isomer production capability would be the radiative capture reaction of ENDF/B-V ^{109}Ag(n,γ) from Tape 532:

```
91 102 *(N,G) TO G.S.*/
92 102 *(N,G) TO ISOMER*/.
```

The next class of reactions usually processed is the group-to-group neutron scattering matrices. The complete list of MTD values is most easily found under File 4 in the MF=1, MT=451 "dictionary" section of the evaluation. An example follows:

```
6    2 *ELASTIC MATRIX*/
6   16 *(N,2N) MATRIX*/
6   51 *(N,NPRIME)FIRST MATRIX*/
6  -66 *(N,NPRIME)NEXT MATRIX*/
6   91 *(N,NPRIME)CONTINUUM MATRIX*/.
```

The elastic matrix will be computed for NSIGZ values of background cross section, but the other reactions will be computed for $\sigma_0 = \infty$ only. The list of matrices to be selfshielded can be changed by making small changes to INIT if desired. There are a few cases in ENDF/B-V where File 4 will be found for reactions with MT in the range 103–107. These are angular distributions for charged particles and should not be processed in GROUPR.

The case of fission is more complex. For the minor isotopes, only the total fission reaction is used, and the following input is appropriate for the prompt component:

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```
3 18 *FISSION XSEC*/
6 18 *PROMPT FISSION MATRIX*/.
```

For the important isotopes, partial fission reactions are given. They are really not needed for most fission reactor problems, and the input above is adequate. However, for problems where high-energy neutrons are important, the following input should be used:

```
3 18 *TOTAL FISSION*/
3 19 *(N,F)*/
3 20 *(N,NF)*/
3 21 *(N,2NF)*/
3 38 *(N,3NF)*/
6 19 *(N,F)*/
6 20 *(N,NF)*/
6 21 *(N,2NF)*/
6 38 *(N,3NF)*/.
```

Note that "6 18" is omitted because it will, in general, be different than the sum of the partial matrices (see Section F). Some materials don't have data for (n,3nf); in these cases, omit the two lines with MTD=38 from the input. The fission matrix is not selfshielded. Since resonance-to-resonance fission-spectrum variations are not described in ENDF/B, it is sufficient to selfshield the cross section and then to use the selfshielding factor for the cross section to selfshield the fission neutron production.

Delayed fission data are available for the important actinide isotopes, and the following input to GROUPR is used to process them:

```
3 455 *DELAYED NUBAR*/
5 455 *DELAYED SPECTRA*/.
```

The line for MFD=5 automatically requests spectra for all six time groups of delayed neutrons. The six time constants are also extracted from the evaluation. As discussed in Section F, formatting modules such as DTFR and CCCCR must combine the prompt and delayed fission data written onto the GENDF tape in order to obtain steady-state fission parameters for use in transport codes.

Photon production reactions can be found in the ENDF "dictionary" under MF=12 and 13. To request a neutron-to-photon matrix, add 4 to this number *. For example,

---

*Beginning with version 6/83-3, GROUPR will automatically shift between 16 and 17 using data read from the ENDF dictionary by the CONVER subroutine. Thus, use of MFD=17 is no longer recommended.

```
17    3 *NONELASTIC PHOTONS*/
16    4 *INELASTIC PHOTONS*/
16   18 *FISSION PHOTONS*/
16  102 *CAPTURE PHOTONS*/.
```

Yields (MF=12) are normally used with resonance reactions like MT=18 or
MT=102, or for low-lying inelastic levels (MT=51, 52, ...). MT=3 is often used
by evaluators as a catch-all reaction at high energies where it is difficult to sepa-
rate the source reactions in total photon emission measurements. In these cases,
photon production cross sections from other reactions like MT=102 are normally
set equal to zero at high energies. The general rule for photon emission is that
the total production is equal to the sum of all the partial production reactions
given in the evaluation. Since resonance-to-resonance variations in photon spectra
are not given in ENDF/B, GROUPR does not normally selfshield the photon pro-
duction matrices (although this can be done if desired by making a small change
in INIT); instead, it is assumed that only the corresponding cross section needs
to be shielded. Subsequent codes can use the cross section selfshielding factor
with the infinite-dilution photon production matrix to obtain selfshielded photon
production numbers.

The user will normally process all reactions of interest at the first tempera-
ture (for example, 300 K). At higher temperatures, the threshold reactions should
be omitted, because their cross sections do not change significantly with tem-
perature except at the most extreme conditions. This means that only the fol-
lowing reactions should be included for the higher temperatures (if present): total
(MT = 1), elastic (MT = 2), fission (MT = 18), radiative capture (MT = 102), heat-
ing (MT = 301), kinematic KERMA (MT = 443), damage (MT = 444), and any
thermal cross sections (MT = 221-250). Only the elastic and thermal matrices
should be included at the higher temperatures.

Warning: when using the explicit-input option, it is a fatal error to request
a reaction that does not appear in the evaluation, cannot be computed from the
evaluation, or was not added to the PENDF tape by a previous module. Reactions
with thresholds above the upper boundary of the highest energy group will be
skipped after printing a message on the output file.

Beginning with the 6/83-3 version, automated processing of essentially all re-
actions.included in an ENDF/B evaluation is also available. As mentioned above,
the single card

3/

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will process all the reactions found in File 3 of the input PENDF tape. However, this list <u>excludes</u> thermal data (MT = 221–250) and special options such as MTD = 251–253, 258–259, and 452–456. If any of these reactions are needed, they should be given explicitly (see example below). Similarly, the single card

      6/

will process the group-to-group matrices for all reactions appearing in File 4 of the ENDF/B tape, except for MT = 103–107 and thermal scattering matrices (MT = 221–250). If MT = 18 and 19 are both present, only MT = 19 will be processed into a fission matrix. Photon production cross sections are requested using

      13/

and photon-production matrices are requested with the single card

      16/

In both cases, all reactions in both File 12 and File 13 will be processed without the need for using MFD = 12 or MFD = 17. There is no automatic option for delayed neutron data. An example of a rather complete processing run for a fissionable isotope with thermal cross sections follows:

```
3/
3 221/ THERMAL XSEC
3 229/ AV.INVERSE VELOCITY
3 455/ DELAYED NUBAR
5 455/ DELAYED SPECTRA
6/
6 221/ THERMAL MATRIX
16/ PHOTON PRODUCTION MATRIX.
```

P.   Coding Details

GROUPR begins by reading most of the user's input (see RUINB). It then locates the desired material and temperature on the input ENDF, PENDF, and GENDF tapes, and reads in the selfshielded unresolved cross sections (if any) from the PENDF tape using STOUNR. If selfshielding was requested, GENFLX is used to compute the weighting flux as described in Section D. The next step is to write the header record for this material on the output GENDF tape.

The code is now ready to begin the loop over reactions for this material and temperature. Either an input card is read to get MFD, MTD, and reaction name, or the next reaction in an automatic sequence is selected. First, the default Legendre order, secondary group count, and σ_0 count are selected for the reaction

in INIT, and the retrieval routines are initialized. GROUPR then processes the reaction using the PANEL logic described in Section J, or for energy-independent data like delayed neutron spectra, using the short-cut method of FSPECT. As the cross sections for each group are obtained, they are printed out (see DISPLA) and written to the GENDF tape. When the last group has been processed, GROUPR loops back to read a new input card for a new reaction.

This loop over reaction continues until a terminating "0/" card is read. GROUPR then proceeds to the next temperature, if any, and repeats the loop over reactions. After the last temperature has been processed for the first material, an opportunity is provided to change to a new material, keeping all the other input parameters unchanged. A "0/" card at this point terminates the GROUPR run and closes out all the files.

Automatic choice of the next reaction to be processed is done in one of two ways. For a simple range of MT numbers, such as the example 51–66 used above, the negative value is stored in the variable MTDP in the GROUPR subroutine. When MTDP is negative, MTD is incremented after each reaction until it is greater than the absolute value of MTDP. MTDP is then reset to one, and the code proceeds to the next input card. A more automatic method is triggered by MTD=0. In this case, a subroutine called NEXTR is called to return the next value of MTD to be used, and a subroutine called NÁMER is called to generate the reaction name (in the 6/83-3 version, NAMER returns only blanks). For MFD = 3, NEXTR finds the next reaction in File 3 on the input PENDF tape. MT = 251–253 and thermal data (MT = 221–250) are excluded. The MT values for the special option (258, 259, etc.) do not appear on the PENDF tape, and they must be requested explicitly if needed. When MFD = 6 or 16 on entry, NEXTR uses lists of reactions found in the File 4, File 12, and File 13 sections of the MF = 1, MT = 451 dictionary of the ENDF tape by the CONVER routine. Each subsequent call returns the next element of one of these lists until it is exhausted. The subroutine then resets the AUTO flag to force the reading of a new card from the input stream. The MF = 12 and MF = 13 lists are linked, so that a single card with "16/" will process all the photon production matrices automatically.

Subroutine GENGPN generates the group bounds in /GROUPN/ for the neutron group structure from input cards, from DATA statements, or by calculation. Some of the DATA statements use energies in eV and some use lethargy. GENGPG generates the photon group structure in /GROUPG/ from input cards or DATA statements; in this case, all bounds are in eV.

Subroutine GENWTF sets up the weight function option requested with IWT

by reading the input cards into /WEIGHTS/, transferring numbers from DATA statements to /WEIGHTS/, or simply reporting the analytic weight option requested. GETWTF returns the values of the weight function at energy E by calculation or by interpolating in the table established by GENWTF. The current version returns the same value for all Legendre orders. Choosing ENEXT is difficult for GETWTF because the functions have not been explicitly linearized. It is important to generate extra grid points in energy regions where the weight function may vary faster than the cross section (for example, in the fusion peak).

Subroutine GENFLX computes the selfshielded weighting flux using either the Bondarenko model or the flux calculator, and it writes the result on a scratch tape using the LOADA routine from the NJOY level. When fluxes are needed for the generalized group integrals, they are read from this scratch file using FINDA (see GETFLX). GENFLX starts by checking for the weighting option. If the Bondarenko model was selected, it initializes GETY1 and GETWTF to read the total cross section from the PENDF tape and the smooth weighting function $C(E)$ set up by GENWTF. It then steps through the union grid of $\sigma_t(E)$ and $C(E)$ computing the flux vs σ_0 and Legendre order by means of Eq.(14). In the unresolved energy range, GETUNR is used to retrieve the unresolved cross sections as a function of σ_0, and Eq.(22) is used to compute the weighting flux. In both cases, the data at each energy are stored as the 1+(LORD+1)*NSIGZ components

E, PHI(IL,IZ),

where IL runs from 1 to LORD+1 and IZ runs from 1 to NSIGZ.

If the flux calculator option was requested, GENFLX sets up the parameters for the calculation and requests needed storage space. Next, the cross section retrieval routines GETY1 and GETY2 are set up to return total and elastic cross sections from the PENDF tape. A lower energy limit (ELO) is chosen, and the cross sections are read into storage in /ECS/ until a maximum energy EHI or a maximum number of points NEMAX is reached.

The slowing-down equation, either Eq.(33) or Eq.(37), is then solved from the break energy down to ELO. The scattering source from energies above the break is based on the NR approximation. When the calculation is finished, fluxes from 10^{-5} eV to ELO are written to the scratch file using LOADA in the same format used for the Bondarenko option. From ELO to the energy break point, fluxes are transferred from /ECS/ to the LOADA file. Finally, above the break point, fluxes are computed and saved using the Bondarenko model.

Subroutine INIT is used to set up the number of σ_0 values, secondary energy

groups, and Legendre components for each combination of MFD and MTD, and to initialize the retrieval routines for cross section (GETSIG), flux (GETFLX), and feed function (GETFF). If MFD = 5, FSPECT is initialized instead. If MFD = 6, a special copy of File 6 is made for use in GETAED. The list of reactions to be selfshielded can be changed if desired. The number of secondary groups NG helps determine the storage required for the accumulating group integrals (see dynamic storage array ANS with pointer IANS in GROUPR). For simple cross section vectors, NG = 2. The NZ*NL flux components are stored first, followed by the NZ*NL cross section components. When all the panels for one group have been processed, dividing position 2 by position 1 gives the group-averaged cross section. For ratio quantities like $\overline{\nu}$ and $\overline{\mu}$ (MTD = 251–253, 452, 455, 456), NG is 3. Once again, the flux components are stored first, followed by the NL*NZ components of RATIO*SIGMA, followed by the components of the cross section. This arrangement allows for the calculation of group-averaged values of RATIO*SIGMA, RATIO, or cross section by dividing position 2 by 1, position 2 by 3, or position 3 by 1, respectively. For matrices, NG is set to one more than the number of secondary groups (NGN or NGG). The NL*NZ flux components are stored first, followed by the NL*NZ integrals for each secondary energy group in turn.

Subroutine PANEL performs the generalized group integrals using the logic described in Section J. For most calls to PANEL, the lower point of each "panel" was computed as the upper point of the previous panel. Therefore, PANEL is careful to save these previous values. However, if the bottom of the panel is just above a discontinuity, new values of cross section and flux are retrieved. Once the values at the lower boundary of the panel are in place, new values for the top of the panel are retrieved (see FLUX, SIG). If the top of the panel is at a discontinuity in σ or at a group boundary, the energy used is just below the nominal top of the panel. "Just below" and "just above" are determined by RNDOFF and DELTA. For maximum accuracy, these numbers should be chosen such that RNDOFF>1, DELTA<1, and RNDOFF*DELTA<1 for the precision of the machine being used.

For simple average cross sections, the integrals of $\sigma*\phi$ and ϕ are computed for the panel using trapezoids. This is justified by the linearization of σ; the value of $\sigma*\phi$ at the midpoint is too uncertain to justify a fancier treatment. For two-body scattering, the feed function is far from linear over the panel. In fact, it can show oscillations as described in Section L. The integral of the triple product $\mathcal{F}*\sigma*\phi$ is obtained by Lobatto quadrature of order 6 or 10 using the quadrature points and weights given in the DATA statements (see QP6, QW6, QP10, and QW10). The cross section and reaction rate are determined at each quadrature point by interpolation, and the feed function is obtained by GETFF. For many reactions,

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FF will be nonzero for only a certain range of secondary groups. IG1 is the index to the first nonzero result, and NG1 is the number of nonzero values of FF in the range. PANEL maintains the two corresponding values IGLO and NG to specify the nonzero range of values in array ANS. Finally, the flux and cross section at the top of the panel are transferred to FLST and SLST, and control is returned to the panel loop in GROUPR.

Subroutine DISPLA is used to print cross sections and group-to-group matrices on the output listing (NSYSO). Small values are removed for efficiency. Note that different formats are used in different circumstances. Infinitely-dilute data are printed without σ_0 labels. Isotropic matrices are printed with several final groups on each line. Delayed neutron spectra are printed using the Legendre order variable for time groups and with the time constants given on a heading line.

Subroutine GETFLX returns NL by NZ components of the weighting flux. If NSIGZ is 1, the flux is computed using GETWTF, and all Legendre orders are taken to be equal. When selfshielding has been requested, the flux components are obtained by interpolating between adjacent values retrieved with FINDA from the scratch tape written by GENFLX. The grid energies found on the scratch tape are used to get ENEXT. The flux is taken to be continuous, so IDIS is always set to zero.

Subroutine GETYLD returns the yield needed by GETFF for fission (MT = 452, 455, or 456 from File 1) or radionuclide production yields from File 9 (MFD = 91–99). This routine also retrieves the delayed neutron time constants when MTD = 455. Tabulated yields are obtained by interpolation using the utility routine TERPA. Polynomial data are expanded by direct computation in this subroutine.

Subroutine GETSIG returns NL*NZ components of the cross section using point data from the PENDF tape and selfshielded unresolved data, if present, from GETUNR. The routine starts by adjusting MF and MT for the special options (MTD = 258–259, MFD = 91–99, etc.) and locating the desired section on the PENDF tape. GETSIG is then called for each desired energy value E in increasing order. For MTD = 258 or 259, the appropriate velocity or lethargy is computed from E and returned. In the more general cases, GETY1 is used to retrieve the pointwise cross section from the PENDF tape, and GETUNR is called to replace this value with selfshielded unresolved cross sections if necessary.

The unresolved cross sections are handled using STOUNR and GETUNR. STOUNR locates the desired material and temperature in MF = 2, MT = 152 of the PENDF tape, and then it copies the data into the dynamic storage array with

pointer IUNR. The σ_0 grid on the PENDF tape does not have to agree with the list requested for GROUPR, but a diagnostic message will be printed if they are different. However, the NTEMP values of temperature requested by GROUPR must agree with the first NTEMP temperatures on the PENDF tape, or a fatal error will result. GETUNR checks whether E is in the unresolved energy range and whether MT is one of the resonance reactions. If so, it locates the desired interpolation range in the UNR array in dynamic storage, and interpolates for the selfshielded cross sections. If this is an energy range where resolved and unresolved ranges overlap, the resolved part is added to the backgroud σ_0 before interpolation. The subroutine TERPU is used for interpolating in the unresolved cross section tables. MT = 261 is used to select the $\ell = 1$ component of the total cross section. Note that GETSIG uses this $\ell = 1$ value for $\ell = 2, 3, ...$ also.

Subroutine GETFF returns the feed function FF using different portions of the coding for different options. First is the section used for cross sections and ratio quantities. The same yield YLD is returned for every ℓ-component in FF.

The second section of GETFF is for neutron continuum transfer matrices. The yield is either determined from MT [for example, YLD = 2 for MT = 16, the (n,2n) reaction], or it is obtained using GETYLD for fission. Next, the angular distribution is obtained using GETFLE [see F in Eq.(83)], and the secondary energy distribution is obtained using GETSED [see g in Eq.(83)]. Finally, the product of the three factors is loaded in FF. Note that the range of groups returned extends from IGLO = 1 to the highest nonzero result, for a total of NG groups. Since FF for these reactions is a smooth function of incident energy, NQ is set to zero, and no additional quadrature points will be used in PANEL.

The third section of GETFF is for gamma production matrices. The photon yields are obtained using GETGYL. In general, there are NYL different yields, each one corresponding to a different discrete gamma ray, or to the continuum. The angular distributions for these gamma rays are obtained using GETGFL (most ENDF/B photons are given as isotropic). The energy distribution for the continuum (if any) is obtained by GETSED. Now, the code loops through the photon group structure placing each discrete photon in the appropriate group and adding in the continuum part. During this loop, the range of nonzero values (IGLO,IGHI) is determined. Finally, the nonzero values are packed into FF, and IGLO and NG are returned to describe the distribution. Once again, NQ = 0 is used.

The fourth section of GETFF handles two-body scattering, either elastic or discrete-level inelastic. First, the angular distribution is retrieved with GETFLE, and an appropriate quadrature order is selected using Eq.(77). Then, a group

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loop from low energy to high energy is used to compute the ω_1 and ω_2 limits of Eq.(75), and the range (ω_1, ω_2) is subdivided using the appropriate Gauss-Legendre quadrature points (see QP4, QP8, QP12, and QP20). The function $f(E, \omega)$ is computed at each of these quadrature points using Eq.(76) and the angular distribution previously returned by GETFLE. The laboratory cosine at the quadrature point, $\mu[\omega]$, is computed using Eq.(72). Finally, the integrand of Eq.(75) is multiplied by the appropriate quadrature weight (QW4, QW8, QW12, or QW20) and added into the accumulating integral. This process is continued until $\omega_2 = 1$. The nonzero values of FF and the parameters IGLO and NG are then complete for this value of E.

The next step is to determine ENEXT based on the next critical point as given by Eqs.(79)–(82). Special cases are used for elastic scattering to avoid numerical problems. Note that the discontinuity flag IDISC is set for critical points. The NQ variable is also set to force PANEL to subdivide the initial-energy integration.

The last section of GETFF is used for thermal scattering matrices. These matrices have both upscatter and energy-angle correlation. The bulk of the work is done by GETAED, which is discussed below. GETFF takes the output of GETAED, finds the range of nonzero elements (IGLO, NG), and packs them into the final result, FF.

Subroutine GETFLE retrieves or computes the Legendre coefficients for the angular distribution of a reaction at incident energy E. When called with $E = 0$, GETFLE requests storage for the raw data, reads in the File 4 information for the first two incident energies on the file, and then uses GETCO to retrieve the corresponding coefficients. On subsequent entries with $E > 0$, GETFLE simply interpolates for the desired coefficients. When E exceeds the upper energy in storage, the values for the upper energy are moved to the lower positions, and new upper values are read and converted to coefficients. An isotropic distribution is returned if E is outside the range of the angular data from File 4.

Subroutine GETAED retrieves angle-energy data for thermal scattering reactions. For coherent elastic scattering, the routine reads through the cross section on the PENDF tape using GETY1 and locates the Bragg edges. On each subsequent call to GETAED, the Legendre components of the cross section are computed using Eq.(67). For incoherent elastic scattering, the routine is first initialized by reading in the raw data for the first energy. On subsequent entries, a test is made to see whether E is in the range ELO to EHI. If not, the high data are moved to the low positions, and new high data are read. The Legendre components are then computed using Eq.(69). For incoherent inelastic scattering, GETAED is

initialized by reading in the raw data for the first incident energy and dividing the energy distribution into NBIN = 30 equally-probable bins using BINA. On subsequent entries, the subroutine checks to see whether E is between ELO and EHI. If not, the binned data for EHI are moved to the low positions, and new raw data are read from File 6 and binned. Once the correct data are in place, the desired energy-angle distribution is computed by using projection interpolation for each secondary group.

Subroutine GETGFL returns the Legendre coefficients for the angular distributions for all discrete and continuum photons for a reaction simultaneously. When called with ED = 0, the routine reads File 14 into scratch storage and finds the starting location for the subsection describing each photon. On subsequent entries with ED>0, GETGFL sets up a loop over the NG photons on this section of File 14. For each photon, it searches for the energy panel that contains ED, uses GETCO to retrieve or compute the Legendre coefficients at the upper and lower File 14 energies, and interpolates for the desired coefficients at ED using TERP1. Since most ENDF/B photons are represented as isotropic, a special short-cut calculation is provided for that case. Isotropic results are also returned if ED is outside the range of the data in File 14.

Subroutine GETCO is used by both GETFLE and GETGFL to retrieve or compute Legendre coefficients from data in File 4 or File 14 format. The user can request output in either the the LAB or CM system, and the raw data can be either Legendre coefficients or tabulated probability versus emission cosine. However, if the raw data are in the laboratory system, CM coefficients cannot be produced. If the raw data are already in the form of coefficients in the desired sytem, GETCO simply checks for the maximum Legendre order needed using a tolerance of TOLER = 1E-6 and returns the coefficients in FL and the order in NL. If coordinate conversion is required, or if the raw data are tabulated, GETCO sets up the integral over cosine using Gauss-Legendre quadrature of order 20 (see QP and QW). The scattering probability for the quadrature point is computed from the coefficients or obtained by interpolating in the tabulation. The Legendre polynomials in the desired reference system are then computed. If the raw data are in the CM system (ω) and the result is to be in the lab system (μ), the desired polynomials are $P_\ell(\mu[\omega])$; otherwise, the quadrature angle is used directly to compute the polynomials. Once the coefficients have been computed, they are checked using TOLER to determine the maximum order required, NL, and the final results are returned in FL.

Subroutine GETGYL is used to retrieve the yields for all photons emitted in a

specified reaction simultaneously. The raw data are obtained from the ENDF/B tape as either yields (MF = 12) or production cross sections (MF = 13). In the latter case, GETGYL actually returns the fraction of the total yield assigned to each photon. The cross section returned by GETSIG is the total photon production cross section from MF = 13 on the PENDF tape, which makes the resulting integral correct. Using the normal GROUPR procedure, GETGYL is initialized by calling it with ED = 0. The entire File 12 or File 13 is read into scratch storage, and the starting location for each subsection is determined. On subsequent entries (ED>0), the routine loops over the NYL photons found, and uses TERPA to compute the yield at ED. If this is a primary photon, a discontinuity is set up at the energy where the photon will change groups. For MF = 12, the calculation is finished. For MF = 13, the numbers calculated above are converted to fractions of the total yield by dividing by the total production subsection from File 13. This routine does not handle ENDF/B transition probability arrays directly, because they will have been converted to File 12 yields by CONVER.

Subroutine CONVER converts ENDF/B evaluations to a standard form for GROUPR. If transition probability arrays were used in File 12, they are converted to yields and written back into File 12. If MF = 1, MT = 456 is missing from the evaluation, and a copy of MT = 452 is added to the tape as MT = 456. In addition, a second copy of the modified tape is made on .unit NSCR. While CONVER is reading through the tape, lists of the reactions in File 4, File 12, and File 13 are written to /RLIST/ for use by the automatic reaction selection logic in NEXTR.

Subroutine GETSED returns the secondary energy distribution for neutrons or continuum photons for all groups simultaneously. Both tabulated and analytic functions are handled. GETSED is initialized for a particular reaction by calling it with ED = 0. First, scratch storage is allocated, and all the analytic subsections (if any) are read in. The array LOC contains pointers for each subsection. If tabulated data are present, the raw data for the first energy are read in. On subsequent entries (ED>0), GETSED loops over the the subsections for this reaction. It first retrieves the fractional probability for the subsection using TERPA. If an analytic law is specified, ANASED is used to compute the group integral for each secondary energy group. Each integral is multiplied by the fractional probability for the law and accumulated into SED. For tabulated data, the routine checks whether ED is between the current values of ELO and EHI. If not, the high data are moved to the low positions, and new high data are read from File 5 or File 15. The raw data are then integrated over the secondary energy groups using INTEGA. Once ED is in the correct energy range, GETSED simply interpolates for the group integrals using TERP1, and accumulates them into SED. Note that this

storage procedure requires that all analytic subsections occur before the tabulated subsection, and that there be only one tabulated subsection. All current ENDF/B evaluations obey these restrictions. "Upscatter" is not allowed in secondary-energy distributions except for fission or photon production. If found, it is put into the "in-group" $(g' = g)$.

Secondary-energy distributions for fission and photon production typically vary slowly with energy, and are constant at low energies. GETSED takes advantage of this to speed up its calculation. After computing SED at E, it calculates a value for ECON. On the next entry, if ED<ECON, the previously computed SED is used. For ED<10 keV, ECON is set to 10 keV. This means that one array SED is used over the entire resonance range where energy values are closely spaced. Above 10 keV, ECON increases in 10% steps.

Subroutine ANASED is used to calculate the integral from E1 to E2 for one of the analytic laws [see Eqs.(86)–(115)]. The routine starts with statement functions for the reduced complementary error function, rerfc. The parameters are then retrieved from the raw data, and the code branches to the appropriate block of coding. The resulting integral is returned in G.

Subroutine HNAB is used to compute the special functions required for analytic law 11, the energy-dependent Watt spectrum. The method used is described in the BROADR chapter of Vol.II of this report.

Subroutine FSPECT is used to compute a secondary energy spectrum at incident energy E by means of a single call to GETSED. It is normally used for delayed-neutron spectra, which are independent of incident energy. However, it can also be used as a short-cut method for prompt or total fission induced by relatively low-energy neutrons because the energy dependence is weak. Note that FSPECT also recovers the delayed neutron time constants from /DELAYN/ and loads them into FS.

Q. Error Messages

GROUPR***UNABLE TO FIND MAT,T.

Check for input error or wrong PENDF tape mounted.

GROUPR***STORAGE EXCEEDED.

Main container array is not big enough. See the variables IA-MAX = 14500 in GROUPR and A(14500) in /GSTORE/.

GROUPR***ILLEGAL MFD.

Check input MFD, legal values are 3, 5, 6, 16, 17, 91–99, 101–109.

RUINB***NTEMP=0 NOT ALLOWED.

There must be at least one temperature requested.

RUINB***TOO MANY TEMPERATURES.

The maximum number of temperatures is 10. See the variables NT-MAX and TEMP(10) in /TEMPR/.

RUINB***NSIGZ=0 NOT ALLOWED.

There must be at least one background cross section. The first input value is automatically changed to 1E10.

RUINB***TOO MANY SIGMA ZEROES.

The maximum number of sigma-zero values is 10. See NZMAX and SIGZ(10) in /SIGZER/.

GENGPN***TOO MANY GROUPS.

The maximum number of neutron group boundaries is 641. See NG-MAX and EG(641) in /GROUPN/.

GENGPN***READ-IN GROUP STRUCTURE IS OUT OF ORDER.

Group structures must be given in ascending energy order.

GENGPN***ILLEGAL GROUP STRUCTURE REQUESTED.

Check input, current legal values are 1 through 15.

GENGPG***TOO MANY GROUPS.

The maximum number of photon group boundaries is 150. See the variables NGMAX and EGG(150) in /GROUPG/.

GENGPG***ILLEGAL GROUP STRUCTURE REQUESTED.

Check input, current legal values are 1 through 7.

GENWTF***ILLEGAL WEIGHT FUNCTION REQUESTED.

Check input, current legal values are -9 through +9.

GENFLX***TOTAL NOT DEFINED OVER ENERGY RANGE.

A complete total cross section is needed for selfshielding. This means that "dosimetry" and "activation" tapes, which normally give only a few key reactions, must be processed using NSIGZ = 1 (infinite dilution).

GETFWT***E OUTSIDE RANGE OF DATA IN NINWT.

A premature end-of-file was found on the input flux tape when using the IWT = 0 option. Check to be sure the tape was the output from a legal flux calculator run.

GETFWT*REQUESTED E IS OUT OF ORDER.**

Could be an improper input tape. Check as above.

GETFWT*TEMPERATURE NOT ON NINWT.**

The IWT = 0 calculation must be consistent with the previous flux calculator run. Check to see if the correct tape was mounted.

PANEL*ELO.GT.EHI.**

This indicates some error in the energy grid for PANEL. It usually occurs if RNDOFF and DELTA are incorrect for your machine. Make sure that RNDOFF>1, that DELTA<1, and that the product RNDOFF*DELTA< 1 when evaluated on your machine (for example, 1.00000001 is not greater than unity on a 32-bit machine).

GETYLD*ILLEGAL LND.**

The maximum number of time groups is 6. See NDN and DNTC(6) in /DELAYN/.

GETSIG*ILLEGAL MT.**

Check input for MTD. Legal values are 1–150, 201–250, 251–253, 258–259, 300–450, 452, 455, and 456.

STOUNR*STORAGE EXCEEDED.**

Not enough storage for unresolved cross section data on PENDF tape. This means that there is no more room in the main container array. See IAMAX = 14500 and A(14500) in /GSTORE/.

STOUNR*CANT FIND TEMP.**

The list of temperatures requested for the GROUPR run must agree with the first NTEMP temperatures on the PENDF tape. Check your BROADR and UNRESR runs.

GETFF*OPTION NOT AVAILABLE FOR MF.**

The legal values for MFD are 3, 5, 6, 12, 13, 16, 17, 91–99, 101–109.

GETFF*ILLEGAL NQP GT 20.**

The highest quadrature order available is currently 20. See DATA statements for QP and QW.

GETFF*DISC LT 0.**

Error in solving quadratic equation for next critical point.

GETFLE*DESIRED ENERGY ABOVE HIGHEST ENERGY GIVEN.**

Should not occur for well-constructed ENDF files. Check the evaluation to be sure File 3 and File 4 are consistent.

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GETFLE*NOT ENOUGH STORAGE FOR RAW DISTRIBUTIONS.

There are 350 words allocated for raw distribution data. See NC-MAX = 350. This can be changed at will.

GETAED*NOT CODED FOR ENDF-FORMATTED FILE 6.

This subroutine uses a special form of File 6 that is not consistent with the one described in ENDF-102[6].

GETAED*STORAGE EXCEEDED.

This message also indicates that the main container array is too small. See IAMAX = 14500 in GROUPR and A(14500) in /GSTORE/.

GETGFL*DESIRED ENERGY AT HIGHEST GIVEN ENERGY.

Should not occur in a well-constructed ENDF file. Check Files 3, 12, 13, and 14 for consistency.

GETCO*LIMITED TO 21 LEGENDRE COEFFICIENTS.

This limit is consistent with ENDF/B procedures. See NLMAX/21/ and P(21). If NLMAX is increased, it might also be advisable to increase the quadrature order (currently 20).

GETCO*LAB TO CM CONVERSION NOT CODED.

The need for this type of conversion rarely occurs on the current ENDF evaluations, because CM is consistently used for two-body reactions, and the laboratory frame is consistently used for continuum reactions. There are a few exceptions for the heavy isotopes where CM and lab are essentially equivalent, but they were errors when the files were generated.

GETGYL*LO=2 NOT CODED.

This message should not occur, because any transition probability arrays on the ENDF tape should have been converted to yields by CONVER.

GETGYL*TOO MANY GAMMAS.

The current limit is 100 photons. See NYLMAX/100/ and LOCA(100).

GETGYL*STORAGE EXCEEDED.

Main container array is too small. See the variables IAMAX in GROUPR and A(14500) in /GSTORE/.

GETSED*TABULATED SUBSECTION MUST BE LAST.

If an evaluation contains a combination of analytic and tabulated subsections for a reaction, the tabulated subsection must be last. This is not an ENDF requirement, but it is satisfied by all current ENDF evaluations. Also, there must be only one tabulated subsection. This is a reasonable limit, since a single tabulated subsection can represent any function.

GETSED***TOO MANY SUBSECTIONS.

The current limit is 20. See NKMAX/20/ and LOC(20).

GETSED***INSUFFICIENT STORAGE FOR RAW ENDF DATA.

The space allocated for raw File 5 or File 15 data is determined by MAXRAW/1200/. It can be increased at will, if there is enough room in the main container array.

ANASED***ILLEGAL LF.

Legal values are 5, 7, 9, 11, and 12.

R. **References**

1. R. E. MacFarlane, D. W. Muir, and R. M. Boicourt, "The NJOY Nuclear Data Processing System, Volume I: User's Manual," Los Alamos National Laboratory report LA-9303-M, Vol.I (ENDF-324) (May 1982).

2. R. E. MacFarlane, D. W. Muir, and R. M. Boicourt, "The NJOY Nuclear Data Processing System, Volume II: The NJOY, RECONR, BROADR, HEATR, and THERMR Modules," Los Alamos National Laboratory report LA-9303-M, Vol.II (ENDF-324) (May 1982).

3. D. W. Muir and R. E. MacFarlane, "The NJOY Nuclear Data Processing System, Volume IV: The ERRORR and COVR Modules," Los Alamos National Laboratory report LA-9303-M, Vol.IV (ENDF-324) (December 1985).

4. I. I. Bondarenko, Ed., *Group Constants for Nuclear Reactor Calculations* (Consultants Bureau, New York, 1964).

5. G. I. Bell and S. Glasstone, *Nuclear Reactor Theory* (Van Nostrand Reinhold, New York, 1970).

6. R. Kinsey, Ed., "ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF," Brookhaven National Laboratory report BNL-NCS-50496 (ENDF-102) 2nd Edition (ENDF/B-V) (October 1979).

7. R. W. Hardie and W. W. Little, Jr., "1DX, A One-Dimensional Diffusion Code for Generating Effective Nuclear Cross Sections," Battelle Northwest Laboratory report BNWL-954 (1969).

8. R. E. MacFarlane, "TRANSX-CTR: A Code for Interfacing MATXS Cross-Section Libraries to Nuclear Transport Codes for Fusion Systems Analysis," Los Alamos National Laboratory report LA-9863-MS (February 1984).

9. R. E. MacFarlane, "ENDF/B-IV and -V Cross Sections for Thermal Power Reactor Analysis," in Proc. Intl. Conf. of Nuclear Cross Sections for Technology, Knoxville, TN (October 22-26, 1979), National Bureau of Standards Publication 594 (September 1980).

10. G. I. Bell, G. E. Hansen, and H. A. Sandmeier, "Multitable Treatments of Anisotropic Scattering in S_N Multigroup Transport Calculations," Nucl. Sci. Eng. 28, 376 (1967).

11. R. D. O'Dell, F. W. Brinkley, Jr., and D. R. Marr, "User's Manual for ONEDANT: A Code Package for One-Dimensional Diffusion-Accelerated, Neutral-Particle Transport," Los Alamos National Laboratory report LA-9184-M (February 1982).

12. C. R. Weisbin, P. D. Soran, R. E. MacFarlane, D. R. Harris, R. J. LaBauve, J. S. Hendricks, J. E. White, and R. B. Kidman, "MINX, A Multigroup Interpretation of Nuclear X-Sections from ENDF/B," Los Alamos Scientific Laboratory report LA-4750-MS (ENDF-237) (September 1976).

13. M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions* (Dover Publications, New York, 1965).

14. D. G. Madland, "New Fission Neutron Spectrum Representation for ENDF," Los Alamos National Laboratory report LA-9285-MS (ENDF-321) (April 1982).

15. R. D. O'Dell, "Standard Interface Files and Procedures for Reactor Physics Codes, Version IV," Los Alamos Scientific Laboratory report LA-6941-MS (September 1977).

16. R. B. Kidman and R. E. MacFarlane, "LIB-IV, A Library of Group Constants for Nuclear Reactor Calculations," Los Alamos Scientific Laboratory report LA-6260-MS (March 1976).

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XVI. GAMINR

The GAMINR module of NJOY is designed to produce complete and accurate multigroup photo-atomic interaction cross sections from ENDF/B-IV, -V, or -VI data[1,2]. Total, coherent, incoherent, pair production, and photoelectric cross sections can be averaged using a variety of group structures and weighting functions. The Legendre components of the group-to-group coherent and incoherent scattering cross sections are calculated using the form factors[3] now available in ENDF/B. These form factors account for the binding of the electron in its atom. Consequently, the cross sections are accurate for energies as low as 1 keV. GAMINR also computes partial heating cross sections or KERMA factors (Kinetic Energy Release in MAterials) for each reaction and sums them to obtain the total heating factor. The resulting multigroup constants are written on an intermediate interface file for later conversion to any desired format. Photonuclear reactions such as (γ,n) are not computed by this module.

GAMINR differs from the previously used GAMLEG code[4] in the following ways:

- Coherent form factors are processed thereby allowing higher Legendre components of the coherent scattering cross section to be produced. GAMLEG processed the P_0 cross section only.

- Incoherent structure factors are processed giving accurate results at low energies where the Klein-Nishina formula fails.

- Heat-production cross sections (KERMA factors) are generated.

- Variable dimensioning and dynamic storage allocation allow arbitrarily complex problems to be run.

- GAMINR is much slower than GAMLEG since charge scaling of the incoherent matrix can no longer be used at all energies.

A. Description of ENDF/B Photon Interaction Files

In the ENDF/B-IV, -V, or -VI photon interaction files, the coherent scattering of photons by electrons is represented by

$$\sigma_C(E, E', \mu)\, dE' d\mu = \frac{3\sigma_T}{8}(1 + \mu^2)\,|F(q, Z)|^2 \delta(E - E')\, dE' d\mu, \qquad (1)$$

where E is the energy of the incident photon, E' is the energy of the scattered photon, μ is the scattering cosine, σ_T is the classical Thomson cross section (0.66524486 b), Z is the atomic number of the scattering atom, and F is the atomic form factor. The coherent form factor is a function of momentum transfer q given by

$$q = 2k\sqrt{\frac{1 - \mu}{2}}, \qquad (2)$$

where k is the energy in free-electron units ($k = E/511003.4$ eV), but F is actually tabulated versus the quantity $x = 20.60744q$. The coherent form factor is given as MT=502 in File 27.

Incoherent scattering is represented by the expression

$$\sigma_I(E, E', \mu)\, dE' d\mu = S(q, Z)\, \sigma_{KN}(E, E', \mu)\, dE' d\mu, \qquad (3)$$

where S is the incoherent scattering function and σ_{KN} is the free-electron Klein-Nishina cross section

$$\sigma_{KN}(E, E', \mu) = \frac{3\sigma_T}{8k^2}\left[\frac{k}{k'} + \frac{k'}{k} + 2\left(\frac{1}{k} - \frac{1}{k'}\right) + \left(\frac{1}{k} - \frac{1}{k'}\right)^2\right]. \qquad (4)$$

The scattering angle and momentum transfer for incoherent scattering are given by

$$\mu = 1 + \frac{1}{k} - \frac{1}{k'}, \qquad (5)$$

and

$$q = 2k\sqrt{\frac{1 - \mu}{2}}\,\frac{\sqrt{1 + (k^2 + 2k)(1 - \mu)/2}}{1 + k(1 - \mu)}. \qquad (6)$$

As was the case for coherent scattering, $S(q, Z)$ is actually tabulated vs $x = 20.60744q$. It is important to note that S is essentially equal to Z for x greater than Z. The incoherent scattering function is given as MT=504 in File 27.

The ENDF/B-IV, -V, and -VI photon interaction files also contain tabulated cross sections for total, coherent, incoherent, pair production, and photoelectric reactions. They are given in File 23 as MT=501, 502, 504, 516, and 602 respectively

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(in ENDF/B-VI files, 602 is changed to 522). The coherent and incoherent cross sections were obtained by the evaluator by integrating Eqs.(1) and (3) and are therefore redundant. Due care must be taken to avoid introducing inconsistencies.

The existing photon interaction data libraries contain no photonuclear data.

B. Calculational Method

The multigroup cross sections produced by GAMINR are defined as follows:

$$\sigma_{xg} = \frac{\int_g \sigma_x \, \phi_0(E) \, dE}{\int_g \phi_0(E) \, dE}, \tag{7}$$

$$\sigma_{T\ell g} = \frac{\int_g \sigma_T(E) \, \phi_\ell(E) \, dE}{\int_g \phi_\ell(E) \, dE}, \tag{8}$$

$$\sigma_{x\ell g \to g'} = \frac{\int_g \mathcal{F}_{x\ell g'}(E) \, \sigma_x(E) \, \phi_\ell(E) \, dE}{\int_g \phi_\ell(E) \, dE}. \tag{9}$$

In these expressions, g represents an energy group for the initial energy E, g' is a group of final energies E', x stands for one of the reaction types, T denotes the total, and ϕ_ℓ is a Legendre component of a guess for the photon flux. In the last equation, $\mathcal{F}$ is the "feed function"; that is, the total normalized probability of scattering from E into group g'. The feed function for coherent scattering is

$$\begin{aligned}
\mathcal{F}_{C\ell g'}(E) &= \frac{\int_{-1}^{+1} \sigma_C(E, E', \mu) \, P_\ell(\mu) \, d\mu}{\sigma_C(E)} \\
&= \frac{\int_{-1}^{+1} (1 - \mu^2) \, |F(x)|^2 P_\ell(\mu) \, d\mu}{\int_{-1}^{+1} (1 - \mu^2) \, |F(x)|^2 d\mu},
\end{aligned} \tag{10}$$

for E in g' and zero elsewhere.

Here $P_\ell(\mu)$ is a Legendre polynomial. Note that $\mathcal{F}_{C0g'} = 1$; this form assures that the coherent scattering cross sections are consistent with the values tabulated in File 23.

For incoherent scattering,

$$\mathcal{F}_{I\ell g'} = \frac{\int_{g'} S(q, Z) \, \sigma_{KN}(E, E', \mu) \, P_\ell(\mu) \, dE'}{\int_{g'} S(q, Z) \, \sigma_{KN}(E, E', \mu) \, dE'}, \tag{11}$$

Because S is simply equal to Z for high values of q, it is not necessary to completely recompute the incoherent matrix when processing a series of elements in the order

of increasing Z. GAMINR automatically determines that some groups for element Z_{now} can be obtained from element Z_{last} by scaling by the factor Z_{now}/Z_{last}.

Finally, pair production is represented as a $(\gamma, 2\gamma)$ scattering event where

$$\mathcal{F}_{PP\ell g'}(E) = \begin{cases} 2, & \text{if } g' \text{ includes } 511003.4 \text{ eV}; \\ 0, & \text{otherwise.} \end{cases} \tag{12}$$

In addition, GAMINR computes multigroup heating cross sections or KERMA factors (Kinetic Energy Release in MAterials) as follows:

$$\sigma_{Hxg} = \frac{\int_g [E - \overline{E}_x(E)] \, \sigma_x(E) \, \phi_0(E) \, dE}{\int_g \phi_0(E) \, dE}, \tag{13}$$

where $\overline{E}_x(E)$ is the average energy of photons scattered from E by reaction type x. The average energies are computed using

$$\overline{E}_C = E, \tag{14}$$

$$\overline{E}_{PP} = 1.022007 \, \text{MeV}, \tag{15}$$

$$\overline{E}_{PE} = 0, \tag{16}$$

$$\overline{E}_I(E) = \int_0^\infty E' \, \sigma_I(E, E', \mu) \, dE' / \sigma_I(E). \tag{17}$$

These separate contributions to the heating cross section are summed to get a quantity that can be combined with a calculated flux to obtain the total heating rate.

C. Integrals Involving Form Factors

The integrals of Eqs.(10) and (11) that involve the form factors are very difficult to perform because of the extreme forward peaking of the scattering at high energies. Figure 1 illustrates the problem for coherent scattering.

For coherent scattering, the integral of Eq.(10) is broken up into panels naturally by the tabulation values of x. Each panel is integrated in the x domain using Lobatto quadrature of order 6 for $\ell = 3$ or less and order 10 for larger Legendre orders. Eq.(2) is used to compute the μ value for each x and to obtain the Jacobian required.

Since μ is quadratic in x, the polynomial order of the integrand in the numerator of Eq.(10) is $2\ell + 2$ plus twice the polynomial order of F in the panel. For $\ell = 3$,

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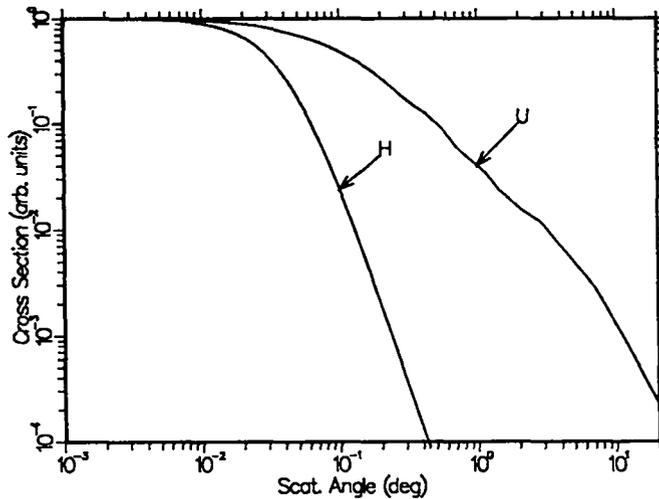
Figure 1: Angular distribution for coherent scattering from uranium at high photon energy.

the theory of Gaussian quadrature implies that the integral will be exact if F can be represented as a quadratic function over the panel.

The incoherent integral of Eq.(11) is also broken up into panels, but here the panels are defined by the union of the tabulation values of x and the momenta corresponding to the secondary energy group bounds. The relationship between x, μ, and secondary energy is given in Eqs.(5) and (6). This time the integral is performed vs E' using Lobatto quadrature of order 6 for ℓ less than or equal to 5 and order 10 for larger ℓ values.

All form factors and structure factors are interpolated using ENDF/B log-log interpolation as specified by the format. However, the cross sections in the file were evaluated using a special log-log-quadratic scheme. Ignoring this complication may lead to a 5% error in the incoherent cross section at 0.1 keV with a negligible error at the higher energies that are of most practical concern[3].

D. Coding Details

The code begins by reading the user's input. It then locates the position for the new material on the old GENDF tape (if any) and copies the earlier results to the new output tape. The desired material is also located on the input PENDF tape prepared previously using RECONR. A new material header is then written onto the output tape leaving the code ready to begin the loop over reaction types.

For each of the preset reaction types, GAMINR uses the panel logic of GROUPR to average the cross sections (see subroutine GPANEL and the GROUPR writeup). If this is the first material in a series of elements, the incoherent matrix is saved to a scratch area. For subsequent materials, the higher energy matrix elements are obtained by scaling these saved values by the appropriate Z ratio. The resulting cross sections and group-to-group matrix elements are then printed out and written to the output tape. The heat production contribution from each reaction is summed into a storage area. After all reactions have been processed for this material, a special pass through the output logic is used to create a heating section using MT=621 (or MT=525 for ENDF/B-VI). Finally, the rest of the old output tape is copied to the new output tape. A description of the format of the multigroup output tape will be found in the GROUPR writeup.

As with PANEL in GROUPR, GPANEL integrates the triple product $\mathcal{F}*\sigma*\phi$. The feed into secondary group g' for Legendre order ℓ from initial energy E is computed in GTFF as described in Section C above. Cross sections are read from the PENDF tape (see GTSIG). Flux can be read in, constant, or $1/E$ with high and low energy rolloffs (see GNWTF and GTFLX).

E. User Input

The following description of the user input is reproduced from the comment cards at the beginning of the GAMINR module.

```
*---INPUT SPECIFICATIONS (FREE FORMAT)----------------------------*
*                                                                 *
* CARD1                                                           *
*    NENDF   UNIT FOR ENDF/B TAPE                                 *
*    NPEND   UNIT FOR PENDF TAPE                                  *
*    NGAM1   UNIT FOR INPUT NGAM TAPE (DEFAULT=0)                 *
*    NGAM2   UNIT FOR OUTPUT NGAM TAPE (DEFAULT=0)                *
* CARD2                                                           *
*    MATB    MATERIAL TO BE PROCESSED                             *
*            INPUT MATERIALS IN ASCENDING ORDER                   *
*    IGG     GAMMA GROUP STRUCTURE OPTION                         *
*    IWT     WEIGHT FUNCTION OPTION                               *
*    LORD    LEGENDRE ORDER                                       *
*    IPRINT  PRINT OPTION (0/1=MINIMUM/MAXIMUM) (DEFAULT=1)       *
* CARD3                                                           *
*    TITLE   RUN LABEL UP TO 80 CHARACTERS (DELIMITED BY *,       *
*            ENDED WITH /)                                        *
* CARD4      (IGG=1 ONLY)                                         *
*    NGG     NUMBER OF GROUPS                                     *
*    EGG     NGG+1 GROUP BOUNDS (EV)                              *
* CARD5      (IWT=1 ONLY)                                         *
*    WGHT    WEIGHT FUNCTION AS TAB1 RECORD                       *
* CARD6                                                           *
*    MFD     FILE TO BE PROCESSED                                 *
```

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```
*    MTD      SECTION TO BE PROCESSED                              *
*    MTNAME   DESCRIPTION OF SECTION TO BE PROCESSED               *
*             REPEAT FOR ALL REACTIONS DESIRED                     *
*             MFD=0/ TERMINATES THIS MATERIAL                      *
*             MFD=-1/ IS A FLAG TO PROCESS ALL SECTIONS PRESENT    *
*             FOR THIS MATERIAL  (TERMINATION IS AUTOMATIC)        *
* CARD7                                                            *
*    MATD     NEXT MAT NUMBER TO BE PROCESSED                      *
*             TERMINATE GAMINR RUN WITH MATD=0.                    *
*                                                                  *
*---OPTIONS FOR INPUT VARIABLES----------------------------------*
*                                                                  *
*         IGG      MEANING                                         *
*         ---      -------                                         *
*         0        NONE                                            *
*         1        ARBITRARY STRUCTURE (READ IN)                   *
*         2        CSEWG 94 GROUP STRUCTURE                        *
*         3        LANL 12 GROUP STRUCTURE                         *
*         4        STEINER 21-GROUP GAMMA-RAY STRUCTURE            *
*         5        STRAKER 22 GROUP STRUCTURE                      *
*         6        LANL 48-GROUP STRUCTURE                         *
*         7        LANL 24-GROUP STRUCTURE                         *
*         8        VITAMIN-C 36-GROUP STRUCTURE                    *
*         9        VITAMIN-E 37-GROUP STRUCTURE                    *
*                                                                  *
*         IWT      MEANING                                         *
*         ---      -------                                         *
*         1        READ IN                                         *
*         2        CONSTANT                                        *
*         3        1/E + ROLLOFFS                                  *
*                                                                  *
********************************************************************
```

Note that both an ENDF/B tape and a PENDF tape from RECONR are required. [The photon interaction tapes are available from the Radiation Shielding Information Center (RSIC) at the Oak Ridge National Laboratory as DLC7E (for ENDF/B-IV) or DLC-99/HUGO (for ENDF/B-V). A photoatomic library in ENDF-VI format based on DLC-99 is available from the National Nuclear Data Center (NNDC) at the Brookhaven National Laboratory.] Material numbers (MATB) are simply the element Z number for versions IV and V; they are equal to 100*Z for ENDF/B-VI. The values of MATD on card 7 should be given in increasing order for maximum economy. The normal mode of operation uses MFD= -1. This automatically processes MT=501, 502, 504, 516, 602, and 621. For ENDF/B-VI, the photoelectric cross section is changed from 602 to 522 and the heating cross section is changed from 621 to 525.

The following sample run prepares a GENDF tape for two elements. The numbers on the left are for reference; they are not part of the input.

```
1.    0
2.    4
```

```
 3.    *RECONR*
 4.    20 21
 5.    *PENDF TAPE FOR 2 ELEMENTS FROM DLC7E*/
 6.    1 1 0
 7.    .001 0./
 8.    *1-HYDROGEN*/
 9.    92 1 0
10.    .001 0./
11.    *92-URANIUM*/
12.    0/
13.    *GAMINR*
14.    20 21 0 22
15.    1 3 3 4 0
16.    *12-GROUP PHOTON INTERACTION LIBRARY*/
17.    -1/
18.    92
19.    -1/
20.    0/
21.    *STOP*
```

The input for RECONR is described more completely in the RECONR chapter in Vol.II of this series. On card 4, an ENDF/B tape containing File 23 has been mounted on logical unit 20. The title on line 5 will appear on the PENDF tape. Material 1 is hydrogen (cards 6-8) and material 92 is uranium (cards 9-11). The element names on cards 8 and 11 will appear on the PENDF tape in MF1, MT451. Linearization is accurate to better than 0.1%.

GAMINR uses the same ENDF tape as RECONR (actually only MF=27 is read by GAMINR), but GAMINR also reads the RECONR output tape on unit 21. The GAMINR GENDF tape will be on unit 22. Card 15 specifies hydrogen as the first material, 12 groups, $1/E$ weight with rolloffs, Legendre components through P_3, and the full printed output. Cards 17 and 19 select the default list of reaction types. Card 18 specifies uranium as the second material to be processed, and card 20 terminates the element loop and the GAMINR run.

Figures 2 through 4 give plots of the results of this sample run. These graphs were made using the DTFR module.

The plots of photon transport matrices require some explanation. These curves are given for the "positions" of the transport table; that is, the back curve is for ingroup scattering, the next one is the scattering into a group from the next higher-energy group, and so on. The horizontal axes are determined by group index, irrespective of the actual energy width of the group. The vertical scale is logarithmic, and the "max" and "min" values are also logarithms.
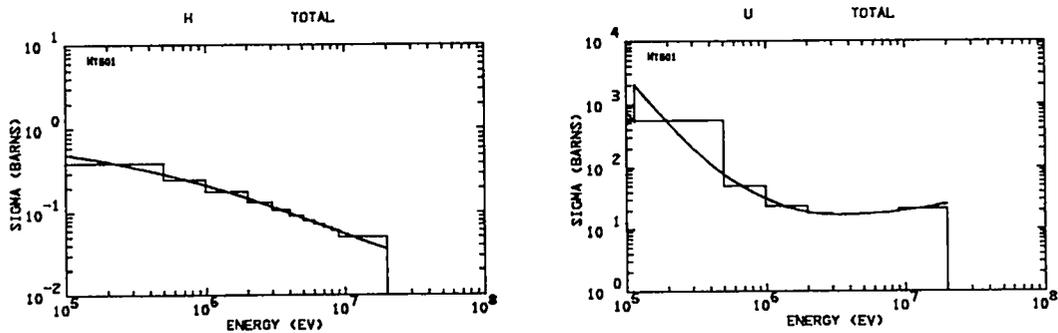
Figure 2: Comparison of pointwise and 12-group total photon interaction cross sections for hydrogen and uranium. Note the photoelectric absorption edge near 100 keV in uranium.
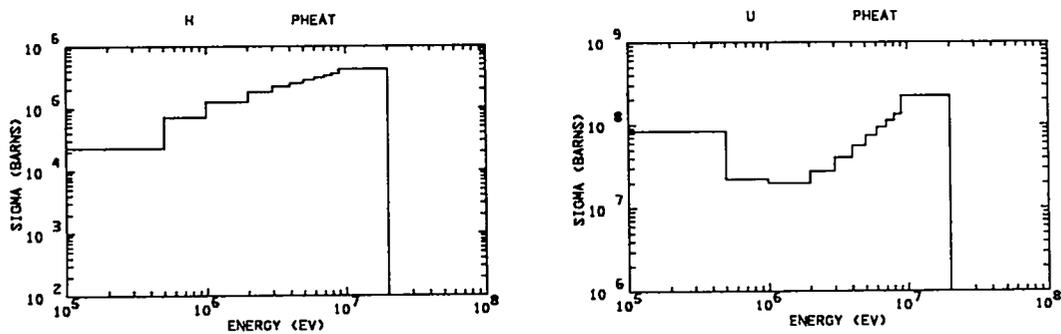
Figure 3: Comparison of 12-group photon heat production cross sections for hydrogen and uranium. The ordinate should actually read "eV-barns".
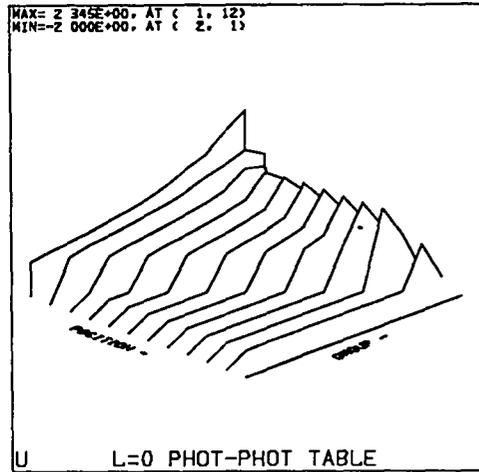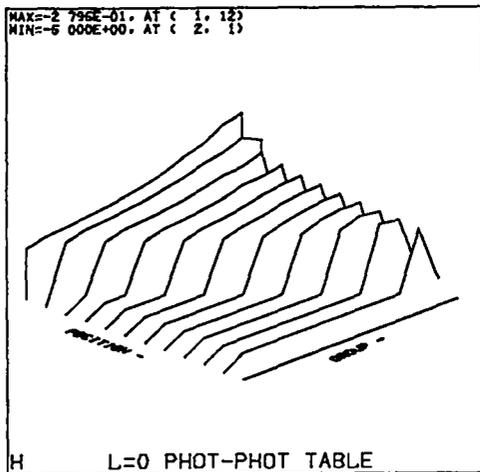
Figure 4: Comparison of photon transport matrices for hydrogen and uranium. These curves are given for the "positions" in the transport table (see text).

F. Error Messages

RESERV***STORAGE EXCEEDED.

Increase the size of the STORAG container array /STORE/A(28000) and increase IAMAX to match. Both of these variables will be found in the main routine of GAMINR.

GENGPG***TOO MANY GROUPS.

Increase /GROUPG/ in GAMINR and NGMAX=150 in subroutine GENGPG.

GTFF***INSUFFICIENT STORAGE FOR FORM FACTOR.

Increase size of container array as above.

GTFF***ILLEGAL FILE TYPE.

Only files 23 and 26 can be requested.

GTFF***ILLEGAL REACTION FOR CROSS SECTION=---.

Only reactions 501, 502, 504, 516, 602, and 621 (heat) can be requested for ENDF/B-IV or -V, or only 501, 502, 504, 516, 522, and 525 for ENDF/B-VI.

GPANEL***ELO GT EHI.

Something wrong with the energy grids during integration over incident energy. Usually means there is a problem with the choice of RNDOFF and/or DELTA. Be sure that RNDOFF<1, DELTA>1, and RNDOFF*DELTA<1 as represented on your machine.

GENGPG***ILLEGAL GROUP STRUCTURE REQUESTED.

Values of IGG must lie between 1 and 9.

70

G. I/O Units

There are no scratch files used in GAMINR. The only restriction on the files assigned on CARD1 of the user input is that NGAM1 and NGAM2 must be in the same mode (that is, both binary or both formatted).

H. References

1. R. Kinsey, "ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF," Brookhaven National Laboratory report BNL-NCS-50496 (ENDF-102) (October 1979).

2. R. W. Roussin, J. R. Knight, J. H. Hubbell, and R. J. Howerton, "Description of the DLC-99/HUGO Package of Photon Interaction Data in ENDF/B-V Format," Oak Ridge National Laboratory report ORNL/RSIC-46 (ENDF-335) (December 1983).

3. J. H. Hubbell, Wm. J. Viegle, E. A. Briggs, R. T. Brown, D. T. Cromer, and R. J. Howerton, "Atomic Form Factors, Incoherent Scattering Functions, and Photon Scattering Cross Sections," J. Phys. Chem. Ref. Data 4, 471 (1975).

4. K. D. Lathrop, "GAMLEG–A FORTRAN Code to Produce Multigroup Cross Sections for Photon Transport Calculations," Los Alamos Scientific Laboratory report LA-3267 (March 1965).

XVII. MODER

The MODER module is used to convert ENDF and PENDF tapes from the NJOY blocked-binary mode to formatted mode (BCD, EBCDIC, ASCII, etc.) and vice versa. It can also be used to copy data from one logical unit to another without change of mode and to perform several other file-management tasks. MODER handles all ENDF/B-IV, ENDF/B-V and ENDF/B-VI formats, plus special-purpose formats developed for NJOY, such as the GROUPR and ERRORR output formats.

A. Code Description

At the beginning of execution, MODER rewinds the output tape NOUT. Additionally, each time a new input tape NIN is specified, that unit is rewound. MODER then processes NIN one file at a time, either for all materials on NIN, or optionally (see following section) for a single specified material. As each file is identified, the main program calls a subroutine dedicated to that file. Each subroutine makes the series of calls to CONTIO, LISTIO, etc., that is appropriate to that file.

If NIN and NOUT are of opposite sign, then mode conversion is performed automatically by the utility I/O subroutines. If NIN and NOUT have the same sign, then no mode conversion is performed; runs of this type can be used simply to make an extra copy of the input tape or to retrieve selected materials without mode change. Only a little more than one page of scratch storage is needed, so there are no limitations on which tapes can be processed.

B. Input Instructions for MODER

As an aid to discussions of the user input to MODER, we list below the input instructions that appear as comment cards at the beginning of the current (6/83-3) version of this module. Since code changes are possible, it is always advisable to consult the comment-card instructions contained in the version of the code actually being used before proceeding with an actual calculation.

```
*---INPUT SPECIFICATIONS (FREE FORMAT)-------------------------*
*                                                              *
* CARD 1       UNIT NUMBERS                                    *
*      NIN     INPUT UNIT                                      *
*      NOUT    OUTPUT UNIT                                     *
*                                                              *
* A POSITIVE UNIT IS CODED (MODE 3).                           *
* A NEGATIVE UNIT IS BLOCKED BINARY (NJOY MODE).               *
*                                                              *
* NOTE: ABS(NIN) GE 1 AND LE 19 IS A FLAG TO SELECT VARIOUS    *
```

```
    *       MATERIALS FROM ONE OR MORE INPUT TAPES, WITH OR         *
    *       WITHOUT MODE CONVERSION.  THE KIND OF DATA TO BE        *
    *       PROCESSED IS KEYED TO NIN AS FOLLOWS:                   *
    *            NIN=1, FOR ENDF OR PENDF INPUT AND OUTPUT,         *
    *               2, FOR GENDF INPUT AND OUTPUT,                  *
    *               3, FOR ERRORR-FORMAT INPUT AND OUTPUT.          *
    *                                                               *
    *     CARDS 2 AND 3 FOR ABS (NIN) GE 1 AND LE 19 ONLY.         *
    *                                                               *
    * CARD 2                                                        *
    *     TPID    TAPEID FOR NOUT.  66 CHARACTERS ALLOWED           *
    *             (DELIMITED WITH *, ENDED WITH /)                  *
    * CARD 3                                                        *
    *     NIN     INPUT UNIT                                        *
    *             TERMINATE MODER BY SETTING NIN=0                  *
    *     MATD    MATERIAL ON THIS TAPE TO ADD TO NOUT              *
    *****************************************************************
```

NIN and NOUT are positive or negative logical unit numbers, with absolute magnitudes normally in the range 20–99, inclusive. Positive unit numbers refer to formatted tapes, and negative unit numbers refer to blocked-binary tapes. No other input is required to copy or convert the entire contents of the data file on unit NIN, writing the results to unit NOUT.

A positive value of NIN in the range 1–3 is used as a "trigger" to specify that the data to be copied or converted is not the entire contents of a single tape, but, instead, selected materials from one or more input tapes. The type of data to be processed (ENDF/PENDF vs. GENDF vs. ERRORR-format) is keyed to the value of NIN, as detailed in the instructions above. If NIN is in the range 1-3, and in this case only, additional input is supplied to specify (on card 2) the tape-identification information to be written on the first record of the output tape and to specify (on card 3) both the MAT-numbers of the materials to be included and the logical units where each of the desired materials is to be found. Note that the slash terminating the Hollerith information on card 2 is required. In the case of GENDF processing of a material MATD which is present on the specified input tape at a series of temperatures, a single card 3 causes the retrieval of all temperatures. Card 3 is repeated as many times as needed, and input is terminated with a card containing 0/.

C. Sample Input

It is good practice to convert the mode of the ENDF/B tape before proceeding with any NJOY run. The time spent in MODER is normally much less than the time saved in the subsequent modules. The required input for this is extremely simple.

```
0
5
*MODER* / MOUNT FORMATTED ENDF TAPE ON UNIT 20
20 -21
*RECONR*
-21 -22
...
```

Although it requires 3 additional input cards, the following will result in even greater efficiency, since in this case unit 21 will contain only the single needed material.

```
0
5
*MODER* / MOUNT FORMATTED ENDF TAPE ON UNIT 20
1 -21
*B-10*/
20 1305
0/
*RECONR*
-21 -22
...
```

The final example (taken from an example problem discussed in Vol. I) shows the use of MODER to prepare a special multi-material ENDF tape for a covariance calculation involving the 5 primary fissionable isotopes. Since, in this particular example problem, the resonance region is of no interest, a copy of the ENDF serves as the PENDF for later modules.

```
0
5
*MODER* / MOUNT ENDF TAPE 515, 516, 555 ON UNITS 20, 21, 22
1 -23
*ENDF/B-V NUBAR COVARIANCE MATERIALS*/
20 1380
20 1381
21 1390
22 1395
22 1398
20 1399
0/
*MODER* / COPY ENDF FOR USE AS A PENDF
-23 -24
*GROUPR* / PREPARE GENDF WITH MULTIGROUPED NUBARS
-23 -24 0 25
...
```

D. Error Messages in MODER

MODER***CONVERSION ASKED FOR A FILE NOT YET CODED.

Illegal or unrecognizable MF-value on NIN.

MODER***SHOULD HAVE FOUND SEND CARD.

MODER is lost. The listed data display the contents of the last card read. Input data file may be bad.

MODER***ILLEGAL COVARIANCE FILE= ---.

ERRORR-format file is missing the required MF=3.

MODER***ENDF MATERIALS MUST BE IN ASCENDING ORDER.

ENDF and PENDF tapes must be MAT ordered.

MODER***UNIT NIN = --- IS NOT AN ENDF OR PENDF TAPE.

User has specified NIN=1 on card 1, thereby requesting selective multi-tape ENDF or PENDF processing, but input data file on the unit NIN specified on card 3 is not an ENDF/PENDF.

MODER***UNIT NIN = --- IS NOT A GENDF TAPE.

User has requested GENDF processing, but input data file is not a GENDF tape.

MODER***UNIT NIN = --- IS NOT AN ERRORR OUTPUT TAPE.

User has requested ERRORR-format processing, but input data file is not an ERRORR-format tape.

MODER***MAT = --- IS NOT A GENDF MATERIAL.

Input file contains an illegal mixture of data, namely, an initial GENDF material, followed by the indicated non-GENDF MAT.

Appendix A. GROUP STRUCTURES

1. IGN=2...CSEWG 240 Group

This set of group bounds was proposed[1] as a "super-group" structure to be used for fine-group libraries that could be collapsed to several other group structures in general use at the time. It was felt that such a collapse would be more economical than producing a set of group constants directly in the target group structure. A large 171-group subset of these group bounds was used for the VITAMIN-C library[2] generated at the Oak Ridge National Laboratory for shielding and fusion applications.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e-05	4.1399e-01	5.3158e-01	6.2506e-01	6.8256e-01
6	8.3368e-01	8.7642e-01	1.1254e+00	1.4450e+00	1.8554e+00
11	2.3824e+00	3.0590e+00	3.9279e+00	5.0435e+00	6.4760e+00
16	8.3153e+00	1.0677e+01	1.3710e+01	1.7603e+01	2.2603e+01
21	2.9023e+01	3.7267e+01	4.7851e+01	6.1442e+01	7.8893e+01
26	1.0130e+02	1.3007e+02	1.6702e+02	2.1445e+02	2.7536e+02
31	3.5358e+02	4.5400e+02	5.8295e+02	7.4852e+02	9.6112e+02
36	1.2341e+03	1.3639e+03	1.5073e+03	1.5846e+03	1.6659e+03
41	1.8411e+03	2.0347e+03	2.2487e+03	2.4852e+03	2.6126e+03
46	2.7465e+03	2.8635e+03	3.0354e+03	3.3546e+03	3.7074e+03
51	4.0973e+03	4.3074e+03	4.5283e+03	5.0045e+03	5.5308e+03
56	6.2673e+03	7.1017e+03	8.0473e+03	9.1188e+03	1.0333e+04
61	1.1709e+04	1.3268e+04	1.5034e+04	1.7036e+04	1.9305e+04
66	2.1335e+04	2.1875e+04	2.3579e+04	2.4176e+04	2.4788e+04
71	2.6058e+04	2.8088e+04	3.1828e+04	3.4307e+04	3.5175e+04
76	3.6066e+04	4.0868e+04	4.6309e+04	5.2475e+04	5.6562e+04
81	5.9462e+04	6.2511e+04	6.7379e+04	7.6351e+04	8.6517e+04
86	9.8037e+04	1.1109e+05	1.1679e+05	1.2277e+05	1.2907e+05
91	1.3569e+05	1.4264e+05	1.4996e+05	1.5764e+05	1.6163e+05
96	1.6573e+05	1.6992e+05	1.7422e+05	1.8316e+05	1.9255e+05
101	2.0242e+05	2.1280e+05	2.2371e+05	2.3518e+05	2.4724e+05
106	2.5991e+05	2.7324e+05	2.8015e+05	2.8725e+05	2.9452e+05
111	3.0197e+05	3.0962e+05	3.1746e+05	3.3373e+05	3.5084e+05
116	3.6883e+05	3.8774e+05	4.0762e+05	4.2852e+05	4.5049e+05
121	4.7359e+05	4.9787e+05	5.1047e+05	5.2340e+05	5.3665e+05
126	5.5023e+05	5.7844e+05	6.0810e+05	6.3928e+05	6.7206e+05
131	7.0651e+05	7.4274e+05	7.8082e+05	8.2085e+05	8.6294e+05
136	9.0718e+05	9.5369e+05	9.6164e+05	9.7783e+05	1.0026e+06
141	1.0540e+06	1.1080e+06	1.1648e+06	1.1943e+06	1.2246e+06
146	1.2873e+06	1.3534e+06	1.4227e+06	1.4957e+06	1.5335e+06
151	1.5724e+06	1.6122e+06	1.6530e+06	1.7377e+06	1.8268e+06
156	1.8731e+06	1.9205e+06	1.9691e+06	2.0190e+06	2.1225e+06
161	2.2313e+06	2.2689e+06	2.3069e+06	2.3457e+06	2.3653e+06
166	2.3852e+06	2.4251e+06	2.4660e+06	2.5924e+06	2.7253e+06
171	2.8650e+06	3.0119e+06	3.0882e+06	3.1664e+06	3.2465e+06
176	3.3287e+06	3.4994e+06	3.6788e+06	3.8674e+06	4.0657e+06
181	4.2741e+06	4.4933e+06	4.6070e+06	4.7237e+06	4.8432e+06

186	4.9659e+06	5.2205e+06	5.4881e+06	5.7695e+06	5.9156e+06
191	6.0653e+06	6.2189e+06	6.3763e+06	6.5377e+06	6.5924e+06
196	6.6476e+06	6.7032e+06	6.8729e+06	7.0469e+06	7.2253e+06
201	7.4082e+06	7.5957e+06	7.7880e+06	7.9852e+06	8.1873e+06
206	8.3946e+06	8.6071e+06	8.8250e+06	9.0484e+06	9.2774e+06
211	9.5123e+06	9.7531e+06	1.0000e+07	1.0253e+07	1.0513e+07
216	1.0779e+07	1.1052e+07	1.1331e+07	1.1618e+07	1.1912e+07
221	1.2214e+07	1.2523e+07	1.2840e+07	1.3165e+07	1.3499e+07
226	1.3840e+07	1.4191e+07	1.4550e+07	1.4918e+07	1.5296e+07
231	1.5683e+07	1.6080e+07	1.6487e+07	1.6905e+07	1.7333e+07
236	1.7771e+07	1.8221e+07	1.8682e+07	1.9155e+07	1.9640e+07
241	1.9970e+07				

2. IGN=3...LANL 30 Group

This is a small structure with complete energy coverage, and it is very economical to use. This makes it useful for survey calculations for fusion systems, fast fission systems, and radiation shields. The group size at low energies is "one lethargy". At higher energies, some one-half and one-quarter lethargy groups are used. Finally, the fusion energy range is represented by bounds close to even energy values. This structure was used in the CLAW-3 and CLAW-4 libraries[3] that are available from the Radiation Shielding Information Center at the Oak Ridge National Laboratory, and in the MATXS1 and MATXS5 libraries used with the TRANSX code[4].

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.3900e-04	1.5200e-01	4.1400e-01	1.1300e+00	3.0600e+00
6	8.3200e+00	2.2600e+01	6.1400e+01	1.6700e+02	4.5400e+02
11	1.2350e+03	3.3500e+03	9.1200e+03	2.4800e+04	6.7600e+04
16	1.8400e+05	3.0300e+05	5.0000e+05	8.2300e+05	1.3530e+06
21	1.7380e+06	2.2320e+06	2.8650e+06	3.6800e+06	6.0700e+06
26	7.7900e+06	1.0000e+07	1.2000e+07	1.3500e+07	1.5000e+07
31	1.7000e+07				

3. IGN=4...ANL 27 Group

This small group structure with even one-half lethargy spacings has been used for fast breeder reactor studies. It is most appropriate for data that have been collapsed from a finer structure for use in two- or three-dimensional calculations; however, it has also been used for processing code comparison studies.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)

1	5.0435e+00	2.2603e+01	3.7267e+01	6.1442e+01	1.0130e+02
6	1.6702e+02	2.7536e+02	4.5400e+02	7.4852e+02	1.2341e+03
11	2.0347e+03	3.3546e+03	5.5308e+03	9.1188e+03	1.5034e+04
16	2.4788e+04	4.0868e+04	6.7379e+04	1.1109e+05	1.8316e+05
21	3.0197e+05	4.9787e+05	8.2085e+05	1.3534e+06	2.2313e+06
26	3.6788e+06	6.0653e+06	1.0000e+07		

4. IGN=5...RRD 50 Group

This structure was specified for a standardized library[5] of group constants based on ENDF/B-IV to be used in the U.S. fast breeder reactor program (base techology was then under the Office of Reactor Research and Development [RRD]). It is still useful for this application, but comparisons with more detailed structures suggested that more groups were needed in the region where U-238 epithermal capture is important and in the region of the 27 keV iron resonance (see the 70 and 80 group structures below). The RRD structure uses quarter lethargy spacing in the middle energy range, with one-half lethargy groups above 500 keV and below 275 eV.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e-05	6.8256e-01	1.1254e+00	1.8554e+00	3.0590e+00
6	5.0435e+00	8.3153e+00	1.3710e+01	2.2603e+01	3.7267e+01
11	6.1442e+01	1.0130e+02	1.6702e+02	2.7536e+02	3.5358e+02
16	4.5400e+02	5.8295e+02	7.4852e+02	9.6112e+02	1.2341e+03
21	1.5846e+03	2.0347e+03	2.6126e+03	3.3546e+03	4.3074e+03
26	5.5308e+03	7.1017e+03	9.1188e+03	1.1709e+04	1.5034e+04
31	1.9305e+04	2.4788e+04	3.1828e+04	4.0868e+04	5.2475e+04
36	6.7379e+04	8.6517e+04	1.1109e+05	1.4264e+05	1.8316e+05
41	2.3518e+05	3.0197e+05	3.8774e+05	4.9787e+05	8.2085e+05
46	1.3534e+06	2.2313e+06	3.6788e+06	6.0653e+06	1.0000e+07
51	1.9971e+07				

5. IGN=6...GAM-I 68 Group

This group structure uses a simple uniform quarter-lethargy spacing. It is accurate for the epithermal portion of thermal reactor calculations, and has been used extensively for both water-moderated and graphite-moderated designs. In addition to its use in the GAM-I code at General Atomic, this structure is used in libraries[6] produced for the state-of-the-art EPRI-CELL code developed by the Electric Power Research Institute for the U.S. electric utilities.

GROUP	GROUP LOWER BOUNDARIES (EV)

INDEX N	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	4.1399e-01	5.3158e-01	6.8256e-01	8.7642e-01	1.1254e+00
6	1.4450e+00	1.8554e+00	2.3824e+00	3.0590e+00	3.9279e+00
11	5.0435e+00	6.4760e+00	8.3153e+00	1.0677e+01	1.3710e+01
16	1.7603e+01	2.2603e+01	2.9023e+01	3.7267e+01	4.7851e+01
21	6.1442e+01	7.8893e+01	1.0130e+02	1.3007e+02	1.6702e+02
26	2.1445e+02	2.7536e+02	3.5358e+02	4.5400e+02	5.8295e+02
31	7.4852e+02	9.6112e+02	1.2341e+03	1.5846e+03	2.0347e+03
36	2.6126e+03	3.3546e+03	4.3074e+03	5.5308e+03	7.1017e+03
41	9.1188e+03	1.1709e+04	1.5034e+04	1.9305e+04	2.4788e+04
46	3.1828e+04	4.0868e+04	5.2475e+04	6.7379e+04	8.6517e+04
51	1.1109e+05	1.4264e+05	1.8316e+05	2.3518e+05	3.0197e+05
56	3.8774e+05	4.9787e+05	6.3928e+05	8.2085e+05	1.0540e+06
61	1.3534e+06	1.7377e+06	2.2313e+06	2.8650e+06	3.6788e+06
66	4.7237e+06	6.0653e+06	7.7880e+06	1.0000e+07	

6. IGN=7...GAM-II 100 Group

This structure was a successor to the GAM-I set described above. It is the same as GAM-I below 100 keV, but for groups above that point it shifts to one-tenth lethargy. It also includes several groups above 10 MeV to represent the D-T fusion source and the high-energy tail of the fission spectrum. The upper limit of the highest group was changed at Los Alamos (from 14.918 to 17.0 MeV) to permit more accurate averaging over the fusion peak.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e-05	4.1399e-01	5.3158e-01	6.8256e-01	8.7642e-01
6	1.1254e+00	1.4450e+00	1.8554e+00	2.3824e+00	3.0590e+00
11	3.9279e+00	5.0435e+00	6.4760e+00	8.3153e+00	1.0677e+01
16	1.3710e+01	1.7603e+01	2.2603e+01	2.9023e+01	3.7267e+01
21	4.7851e+01	6.1442e+01	7.8893e+01	1.0130e+02	1.3007e+02
26	1.6702e+02	2.1445e+02	2.7536e+02	3.5358e+02	4.5400e+02
31	5.8295e+02	7.4852e+02	9.6112e+02	1.2341e+03	1.5846e+03
36	2.0347e+03	2.6126e+03	3.3546e+03	4.3074e+03	5.5308e+03
41	7.1017e+03	9.1188e+03	1.1709e+04	1.5034e+04	1.9305e+04
46	2.4788e+04	3.1828e+04	4.0868e+04	5.2475e+04	6.7379e+04
51	8.6517e+04	1.1109e+05	1.2277e+05	1.3569e+05	1.4996e+05
56	1.6573e+05	1.8316e+05	2.0242e+05	2.2371e+05	2.4724e+05
61	2.7324e+05	3.0197e+05	3.3373e+05	3.6883e+05	4.0762e+05
66	4.5049e+05	4.9787e+05	5.5023e+05	6.0810e+05	6.7206e+05
71	7.4274e+05	8.2085e+05	9.0718e+05	1.0026e+06	1.1080e+06
76	1.2246e+06	1.3534e+06	1.4957e+06	1.6530e+06	1.8268e+06
81	2.0190e+06	2.2313e+06	2.4660e+06	2.7253e+06	3.0119e+06
86	3.3287e+06	3.6788e+06	4.0657e+06	4.4933e+06	4.9659e+06
91	5.4881e+06	6.0653e+06	6.7032e+06	7.4082e+06	8.1873e+06
96	9.0484e+06	1.0000e+07	1.1052e+07	1.2214e+07	1.3499e+07
101	1.7000e+07				

7. IGN=8...LASER-THERMOS 35 Group

This is a thermal group structure. It is based on the THERMOS equal-velocity structure with additional groups added in the vicinity of the Pu-240 resonance. It is used for the thermal calculation in EPRI-CELL.

GROUP INDEX N	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
		GROUP LOWER BOUNDARIES (EV)			
1	2.5300e-04	2.2770e-03	6.3250e-03	1.2397e-02	2.0493e-02
6	3.0613e-02	4.2757e-02	5.6925e-02	8.1972e-02	1.1159e-01
11	1.4573e-01	1.8444e-01	2.2770e-01	2.5104e-01	2.7053e-01
16	2.9075e-01	3.0113e-01	3.2064e-01	3.5768e-01	4.1704e-01
21	5.0326e-01	6.2493e-01	7.8211e-01	9.5070e-01	1.0137e+00
26	1.0428e+00	1.0525e+00	1.0624e+00	1.0722e+00	1.0987e+00
31	1.1664e+00	1.3079e+00	1.4575e+00	1.5950e+00	1.7262e+00
36	1.8550e+00				

8. IGN=9...EPRI-CPM 69 Group

This group structure is designed for water-moderated thermal reactor data sets. It is the same as the WIMS structure, and it was used at Los Alamos to prepare libraries[6] for the EPRI-CPM code. The portion above 4 eV is basically one-half lethargy, except that the boundaries of several groups have been shifted to approximately center important resonances within their groups. The portion below 4 eV is a detailed thermal structure including extra detail for the Pu-240 resonance.

GROUP INDEX N	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
		GROUP LOWER BOUNDARIES (EV)			
1	1.0000e-05	5.0000e-03	1.0000e-02	1.5000e-02	2.0000e-02
6	2.5000e-02	3.0000e-02	3.5000e-02	4.2000e-02	5.0000e-02
11	5.8000e-02	6.7000e-02	8.0000e-02	1.0000e-01	1.4000e-01
16	1.8000e-01	2.2000e-01	2.5000e-01	2.8000e-01	3.0000e-01
21	3.2000e-01	3.5000e-01	4.0000e-01	5.0000e-01	6.2500e-01
26	7.8000e-01	8.5000e-01	9.1000e-01	9.5000e-01	9.7200e-01
31	9.9600e-01	1.0200e+00	1.0450e+00	1.0710e+00	1.0970e+00
36	1.1230e+00	1.1500e+00	1.3000e+00	1.5000e+00	2.1000e+00
41	2.6000e+00	3.3000e+00	4.0000e+00	9.8770e+00	1.5968e+01
46	2.7700e+01	4.8052e+01	7.5501e+01	1.4873e+02	3.6726e+02
51	9.0690e+02	1.4251e+03	2.2395e+03	3.5191e+03	5.5300e+03
56	9.1180e+03	1.5030e+04	2.4780e+04	4.0850e+04	6.7340e+04
61	1.1100e+05	1.8300e+05	3.0250e+05	5.0000e+05	8.2100e+05
66	1.3530e+06	2.2310e+06	3.6790e+06	6.0655e+06	1.0000e+07

9. IGN=10...LANL 187 Group

This structure is intended to be a single set of fine-lethargy bounds that can be used for thermal reactors, fast breeder reactors, fusion systems, and shielding calculations. As such, it has a thermal structure below 4 eV that is somewhat finer than either the 69-group or the 35-group structures. It is superior to all the other structures in the epithermal range (say, 4 eV to 100 keV). Finally, it has a high-energy structure that is finer that the 80-group set, but not as detailed as the 100- or 240-group structures.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e-05	2.5399e-04	7.6022e-04	2.2769e-03	6.3247e-03
6	1.2396e-02	2.0492e-02	2.5500e-02	3.0612e-02	3.5500e-02
11	4.2755e-02	5.0000e-02	5.6922e-02	6.7000e-02	8.1968e-02
16	1.1157e-01	1.4572e-01	1.5230e-01	1.8443e-01	2.2769e-01
21	2.5103e-01	2.7052e-01	2.9074e-01	3.0112e-01	3.2063e-01
26	3.5767e-01	4.1499e-01	5.0323e-01	6.2506e-01	7.8208e-01
31	8.3368e-01	8.7642e-01	9.1000e-01	9.5065e-01	9.7100e-01
36	9.9200e-01	1.0137e+00	1.0427e+00	1.0525e+00	1.0623e+00
41	1.0722e+00	1.0987e+00	1.1254e+00	1.1664e+00	1.3079e+00
46	1.4574e+00	1.5949e+00	1.7261e+00	1.8554e+00	2.1024e+00
51	2.3824e+00	2.6996e+00	3.0590e+00	3.4663e+00	3.9279e+00
56	4.4509e+00	5.0435e+00	5.7150e+00	6.4760e+00	6.8680e+00
61	7.3382e+00	8.3153e+00	9.4225e+00	1.0677e+01	1.2099e+01
66	1.3710e+01	1.5535e+01	1.7603e+01	1.9947e+01	2.2603e+01
71	2.5613e+01	2.9023e+01	3.2888e+01	3.7267e+01	4.2229e+01
76	4.7851e+01	5.4222e+01	6.1442e+01	6.9623e+01	7.8893e+01
81	8.9398e+01	1.0130e+02	1.1479e+02	1.3007e+02	1.4739e+02
86	1.6702e+02	1.8926e+02	2.1445e+02	2.4301e+02	2.7536e+02
91	3.1203e+02	3.5358e+02	4.0065e+02	4.5400e+02	5.1445e+02
96	5.8295e+02	6.6057e+02	7.4852e+02	8.4818e+02	9.6112e+02
101	1.0891e+03	1.2341e+03	1.3984e+03	1.5846e+03	1.7956e+03
106	2.0347e+03	2.3056e+03	2.6126e+03	2.9604e+03	3.3546e+03
111	3.8013e+03	4.3074e+03	4.8810e+03	5.5308e+03	6.2673e+03
116	7.1017e+03	8.0473e+03	9.1188e+03	1.0333e+04	1.1709e+04
121	1.3268e+04	1.5034e+04	1.7036e+04	1.9305e+04	2.1875e+04
126	2.4788e+04	2.6058e+04	2.8088e+04	3.1828e+04	3.6066e+04
131	4.0868e+04	4.6309e+04	5.2475e+04	5.9462e+04	6.7379e+04
136	7.6351e+04	8.6517e+04	9.8037e+04	1.1109e+05	1.2588e+05
141	1.4264e+05	1.6163e+05	1.8316e+05	2.0754e+05	2.3518e+05
146	2.6649e+05	3.0197e+05	3.4218e+05	3.8774e+05	4.3937e+05
151	4.9787e+05	5.6416e+05	6.3928e+05	7.2440e+05	8.2085e+05
156	9.3014e+05	1.0540e+06	1.1943e+06	1.3534e+06	1.5335e+06
161	1.7377e+06	1.9691e+06	2.2313e+06	2.5284e+06	2.8650e+06
166	3.2465e+06	3.6788e+06	4.1686e+06	4.7237e+06	5.3526e+06
171	6.0653e+06	6.8729e+06	7.7880e+06	8.8250e+06	1.0000e+07
176	1.1000e+07	1.2000e+07	1.3000e+07	1.3500e+07	1.3750e+07
181	1.3940e+07	1.4200e+07	1.4420e+07	1.4640e+07	1.5000e+07
186	1.6000e+07	1.7000e+07	2.0000e+07		

10. IGN=11...LANL 70 Group

This structure was designed for the ENDF/B-V follow-on to the 50-group library. More groups were added in the region between 450 eV and 3 keV where U-238 capture is important in fast breeder reactors, and a few more groups were added for important resonances in iron and oxygen. The low limit was left at a relatively high 10 eV to discourage the use of the corresponding library (which was produced with a specific fast-reactor weight function) at inappropriate energies. Later consideration showed this to be a mistake, because the library doesn't work well in the outlying blanket and shield regions of some benchmark assemblies and reactor systems. The 80-group structure is preferred.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0677e+01	6.1442e+01	1.0130e+02	1.3007e+02	1.6702e+02
6	2.1445e+02	2.7537e+02	3.5358e+02	4.5400e+02	5.8295e+02
11	7.4852e+02	9.6112e+02	1.0891e+03	1.2341e+03	1.3984e+03
16	1.5846e+03	1.7956e+03	2.0347e+03	2.3056e+03	2.6126e+03
21	2.9605e+03	3.3546e+03	3.8013e+03	4.3074e+03	4.8810e+03
26	5.5308e+03	6.2673e+03	7.1017e+03	8.0473e+03	9.1188e+03
31	1.0333e+04	1.1709e+04	1.3268e+04	1.5034e+04	1.7036e+04
36	1.9305e+04	2.1875e+04	2.4788e+04	2.8088e+04	3.1828e+04
41	4.0868e+04	5.2475e+04	6.7380e+04	8.6517e+04	1.1109e+05
46	1.4264e+05	1.8316e+05	2.3518e+05	3.0197e+05	3.8774e+05
51	4.3937e+05	4.9787e+05	5.6416e+05	6.3928e+05	7.2440e+05
56	8.2085e+05	9.3015e+05	1.0540e+06	1.1943e+06	1.3534e+06
61	1.7377e+06	2.2313e+06	2.8651e+06	3.6788e+06	4.7237e+06
66	6.0653e+06	7.7880e+06	1.0000e+07	1.2840e+07	1.6487e+07
71	2.0000e+07				

11. IGN=12...SAND-II 620 Group

This very fine group structure is used in dosimetry applications for flux unfolding. It has also been used for processing code comparisons[7], where it is almost as accurate as pointwise cross sections without the complication of different grid structures for different codes. Many users now use the 640-group version of this structure (see IGN=15 below) that has 20 additional groups above 18 MeV for high-energy dosimetry.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e-04	1.0500e-04	1.1000e-04	1.1500e-04	1.2000e-04
6	1.2750e-04	1.3500e-04	1.4250e-04	1.5000e-04	1.6000e-04

11	1.7000e-04	1.8000e-04	1.9000e-04	2.0000e-04	2.1000e-04
16	2.2000e-04	2.3000e-04	2.4000e-04	2.5500e-04	2.7000e-04
21	2.8000e-04	3.0000e-04	3.2000e-04	3.4000e-04	3.6000e-04
26	3.8000e-04	4.0000e-04	4.2500e-04	4.5000e-04	4.7500e-04
31	5.0000e-04	5.2500e-04	5.5000e-04	5.7500e-04	6.0000e-04
36	6.3000e-04	6.6000e-04	6.9000e-04	7.2000e-04	7.6000e-04
41	8.0000e-04	8.4000e-04	8.8000e-04	9.2000e-04	9.6000e-04
46	1.0000e-03	1.0500e-03	1.1000e-03	1.1500e-03	1.2000e-03
51	1.2750e-03	1.3500e-03	1.4250e-03	1.5000e-03	1.6000e-03
56	1.7000e-03	1.8000e-03	1.9000e-03	2.0000e-03	2.1000e-03
61	2.2000e-03	2.3000e-03	2.4000e-03	2.5500e-03	2.7000e-03
66	2.8000e-03	3.0000e-03	3.2000e-03	3.4000e-03	3.6000e-03
71	3.8000e-03	4.0000e-03	4.2500e-03	4.5000e-03	4.7500e-03
76	5.0000e-03	5.2500e-03	5.5000e-03	5.7500e-03	6.0000e-03
81	6.3000e-03	6.6000e-03	6.9000e-03	7.2000e-03	7.6000e-03
86	8.0000e-03	8.4000e-03	8.8000e-03	9.2000e-03	9.6000e-03
91	1.0000e-02	1.0500e-02	1.1000e-02	1.1500e-02	1.2000e-02
96	1.2750e-02	1.3500e-02	1.4250e-02	1.5000e-02	1.6000e-02
101	1.7000e-02	1.8000e-02	1.9000e-02	2.0000e-02	2.1000e-02
106	2.2000e-02	2.3000e-02	2.4000e-02	2.5500e-02	2.7000e-02
111	2.8000e-02	3.0000e-02	3.2000e-02	3.4000e-02	3.6000e-02
116	3.8000e-02	4.0000e-02	4.2500e-02	4.5000e-02	4.7500e-02
121	5.0000e-02	5.2500e-02	5.5000e-02	5.7500e-02	6.0000e-02
126	6.3000e-02	6.6000e-02	6.9000e-02	7.2000e-02	7.6000e-02
131	8.0000e-02	8.4000e-02	8.8000e-02	9.2000e-02	9.6000e-02
136	1.0000e-01	1.0500e-01	1.1000e-01	1.1500e-01	1.2000e-01
141	1.2750e-01	1.3500e-01	1.4250e-01	1.5000e-01	1.6000e-01
146	1.7000e-01	1.8000e-01	1.9000e-01	2.0000e-01	2.1000e-01
151	2.2000e-01	2.3000e-01	2.4000e-01	2.5500e-01	2.7000e-01
156	2.8000e-01	3.0000e-01	3.2000e-01	3.4000e-01	3.6000e-01
161	3.8000e-01	4.0000e-01	4.2500e-01	4.5000e-01	4.7500e-01
166	5.0000e-01	5.2500e-01	5.5000e-01	5.7500e-01	6.0000e-01
171	6.3000e-01	6.6000e-01	6.9000e-01	7.2000e-01	7.6000e-01
176	8.0000e-01	8.4000e-01	8.8000e-01	9.2000e-01	9.6000e-01
181	1.0000e+00	1.0500e+00	1.1000e+00	1.1500e+00	1.2000e+00
186	1.2750e+00	1.3500e+00	1.4250e+00	1.5000e+00	1.6000e+00
191	1.7000e+00	1.8000e+00	1.9000e+00	2.0000e+00	2.1000e+00
196	2.2000e+00	2.3000e+00	2.4000e+00	2.5500e+00	2.7000e+00
201	2.8000e+00	3.0000e+00	3.2000e+00	3.4000e+00	3.6000e+00
206	3.8000e+00	4.0000e+00	4.2500e+00	4.5000e+00	4.7500e+00
211	5.0000e+00	5.2500e+00	5.5000e+00	5.7500e+00	6.0000e+00
216	6.3000e+00	6.6000e+00	6.9000e+00	7.2000e+00	7.6000e+00
221	8.0000e+00	8.4000e+00	8.8000e+00	9.2000e+00	9.6000e+00
226	1.0000e+01	1.0500e+01	1.1000e+01	1.1500e+01	1.2000e+01
231	1.2750e+01	1.3500e+01	1.4250e+01	1.5000e+01	1.6000e+01
236	1.7000e+01	1.8000e+01	1.9000e+01	2.0000e+01	2.1000e+01
241	2.2000e+01	2.3000e+01	2.4000e+01	2.5500e+01	2.7000e+01
246	2.8000e+01	3.0000e+01	3.2000e+01	3.4000e+01	3.6000e+01
251	3.8000e+01	4.0000e+01	4.2500e+01	4.5000e+01	4.7500e+01
256	5.0000e+01	5.2500e+01	5.5000e+01	5.7500e+01	6.0000e+01
261	6.3000e+01	6.6000e+01	6.9000e+01	7.2000e+01	7.6000e+01
266	8.0000e+01	8.4000e+01	8.8000e+01	9.2000e+01	9.6000e+01
271	1.0000e+02	1.0500e+02	1.1000e+02	1.1500e+02	1.2000e+02
276	1.2750e+02	1.3500e+02	1.4250e+02	1.5000e+02	1.6000e+02
281	1.7000e+02	1.8000e+02	1.9000e+02	2.0000e+02	2.1000e+02
286	2.2000e+02	2.3000e+02	2.4000e+02	2.5500e+02	2.7000e+02
291	2.8000e+02	3.0000e+02	3.2000e+02	3.4000e+02	3.6000e+02
296	3.8000e+02	4.0000e+02	4.2500e+02	4.5000e+02	4.7500e+02

301	5.0000e+02	5.2500e+02	5.5000e+02	5.7500e+02	6.0000e+02
306	6.3000e+02	6.6000e+02	6.9000e+02	7.2000e+02	7.6000e+02
311	8.0000e+02	8.4000e+02	8.8000e+02	9.2000e+02	9.6000e+02
316	1.0000e+03	1.0500e+03	1.1000e+03	1.1500e+03	1.2000e+03
321	1.2750e+03	1.3500e+03	1.4250e+03	1.5000e+03	1.6000e+03
326	1.7000e+03	1.8000e+03	1.9000e+03	2.0000e+03	2.1000e+03
331	2.2000e+03	2.3000e+03	2.4000e+03	2.5500e+03	2.7000e+03
336	2.8000e+03	3.0000e+03	3.2000e+03	3.4000e+03	3.6000e+03
341	3.8000e+03	4.0000e+03	4.2500e+03	4.5000e+03	4.7500e+03
346	5.0000e+03	5.2500e+03	5.5000e+03	5.7500e+03	6.0000e+03
351	6.3000e+03	6.6000e+03	6.9000e+03	7.2000e+03	7.6000e+03
356	8.0000e+03	8.4000e+03	8.8000e+03	9.2000e+03	9.6000e+03
361	1.0000e+04	1.0500e+04	1.1000e+04	1.1500e+04	1.2000e+04
366	1.2750e+04	1.3500e+04	1.4250e+04	1.5000e+04	1.6000e+04
371	1.7000e+04	1.8000e+04	1.9000e+04	2.0000e+04	2.1000e+04
376	2.2000e+04	2.3000e+04	2.4000e+04	2.5500e+04	2.7000e+04
381	2.8000e+04	3.0000e+04	3.2000e+04	3.4000e+04	3.6000e+04
386	3.8000e+04	4.0000e+04	4.2500e+04	4.5000e+04	4.7500e+04
391	5.0000e+04	5.2500e+04	5.5000e+04	5.7500e+04	6.0000e+04
396	6.3000e+04	6.6000e+04	6.9000e+04	7.2000e+04	7.6000e+04
401	8.0000e+04	8.4000e+04	8.8000e+04	9.2000e+04	9.6000e+04
406	1.0000e+05	1.0500e+05	1.1000e+05	1.1500e+05	1.2000e+05
411	1.2750e+05	1.3500e+05	1.4250e+05	1.5000e+05	1.6000e+05
416	1.7000e+05	1.8000e+05	1.9000e+05	2.0000e+05	2.1000e+05
421	2.2000e+05	2.3000e+05	2.4000e+05	2.5500e+05	2.7000e+05
426	2.8000e+05	3.0000e+05	3.2000e+05	3.4000e+05	3.6000e+05
431	3.8000e+05	4.0000e+05	4.2500e+05	4.5000e+05	4.7500e+05
436	5.0000e+05	5.2500e+05	5.5000e+05	5.7500e+05	6.0000e+05
441	6.3000e+05	6.6000e+05	6.9000e+05	7.2000e+05	7.6000e+05
446	8.0000e+05	8.4000e+05	8.8000e+05	9.2000e+05	9.6000e+05
451	1.0000e+06	1.1000e+06	1.2000e+06	1.3000e+06	1.4000e+06
456	1.5000e+06	1.6000e+06	1.7000e+06	1.8000e+06	1.9000e+06
461	2.0000e+06	2.1000e+06	2.2000e+06	2.3000e+06	2.4000e+06
466	2.5000e+06	2.6000e+06	2.7000e+06	2.8000e+06	2.9000e+06
471	3.0000e+06	3.1000e+06	3.2000e+06	3.3000e+06	3.4000e+06
476	3.5000e+06	3.6000e+06	3.7000e+06	3.8000e+06	3.9000e+06
481	4.0000e+06	4.1000e+06	4.2000e+06	4.3000e+06	4.4000e+06
486	4.5000e+06	4.6000e+06	4.7000e+06	4.8000e+06	4.9000e+06
491	5.0000e+06	5.1000e+06	5.2000e+06	5.3000e+06	5.4000e+06
496	5.5000e+06	5.6000e+06	5.7000e+06	5.8000e+06	5.9000e+06
501	6.0000e+06	6.1000e+06	6.2000e+06	6.3000e+06	6.4000e+06
506	6.5000e+06	6.6000e+06	6.7000e+06	6.8000e+06	6.9000e+06
511	7.0000e+06	7.1000e+06	7.2000e+06	7.3000e+06	7.4000e+06
516	7.5000e+06	7.6000e+06	7.7000e+06	7.8000e+06	7.9000e+06
521	8.0000e+06	8.1000e+06	8.2000e+06	8.3000e+06	8.4000e+06
526	8.5000e+06	8.6000e+06	8.7000e+06	8.8000e+06	8.9000e+06
531	9.0000e+06	9.1000e+06	9.2000e+06	9.3000e+06	9.4000e+06
536	9.5000e+06	9.6000e+06	9.7000e+06	9.8000e+06	9.9000e+06
541	1.0000e+07	1.0100e+07	1.0200e+07	1.0300e+07	1.0400e+07
546	1.0500e+07	1.0600e+07	1.0700e+07	1.0800e+07	1.0900e+07
551	1.1000e+07	1.1100e+07	1.1200e+07	1.1300e+07	1.1400e+07
556	1.1500e+07	1.1600e+07	1.1700e+07	1.1800e+07	1.1900e+07
561	1.2000e+07	1.2100e+07	1.2200e+07	1.2300e+07	1.2400e+07
566	1.2500e+07	1.2600e+07	1.2700e+07	1.2800e+07	1.2900e+07
571	1.3000e+07	1.3100e+07	1.3200e+07	1.3300e+07	1.3400e+07
576	1.3500e+07	1.3600e+07	1.3700e+07	1.3800e+07	1.3900e+07
581	1.4000e+07	1.4100e+07	1.4200e+07	1.4300e+07	1.4400e+07
586	1.4500e+07	1.4600e+07	1.4700e+07	1.4800e+07	1.4900e+07

591	1.5000e+07	1.5100e+07	1.5200e+07	1.5300e+07	1.5400e+07
596	1.5500e+07	1.5600e+07	1.5700e+07	1.5800e+07	1.5900e+07
601	1.6000e+07	1.6100e+07	1.6200e+07	1.6300e+07	1.6400e+07
606	1.6500e+07	1.6600e+07	1.6700e+07	1.6800e+07	1.6900e+07
611	1.7000e+07	1.7100e+07	1.7200e+07	1.7300e+07	1.7400e+07
616	1.7500e+07	1.7600e+07	1.7700e+07	1.7800e+07	1.7900e+07
621	1.8000e+07				

12.   IGN=13...LANL 80 Group

This structure has been optimized for fast breeder reactors and fusion systems. The resonance-region treatment uses numerous one-eighth lethargy groups to give an accurate treatment of U-238 capture, and extra group bounds are provided around the important sodium resonance near 3 keV and the iron resonance near 27 keV. A fairly high level of resolution is used in the fission spectrum range to accommodate the differences between different reactor designs and fast critical assemblies such as GODIVA and JEZEBEL, and to represent the resonances and "window" in oxygen. The structure above 10 MeV is similar to that of the 30-group set, which is adequate for practical fusion blanket calculations of quantities like tritium production and radiation damage. A finer structure should only be needed for careful high-threshold dosimetry work. Finally, a few low-energy groups were provided to represent the soft flux in outlying blanket and shield regions of reactor systems. The 80-group structure is recommended over the 50- or 70-group structures for these kinds of problems.

| GROUP INDEX N | GROUP LOWER BOUNDARIES (EV) |
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.3888e-04	1.5230e-01	4.1399e-01	1.1254e+00	3.0590e+00
6	5.0435e+00	8.3153e+00	1.3710e+01	2.2603e+01	3.7267e+01
11	6.1442e+01	1.0130e+02	1.6702e+02	2.7536e+02	3.5358e+02
16	4.5400e+02	5.8295e+02	7.4852e+02	9.6112e+02	1.0891e+03
21	1.2341e+03	1.3984e+03	1.5846e+03	1.7956e+03	2.0347e+03
26	2.3056e+03	2.6126e+03	2.9604e+03	3.3546e+03	3.8013e+03
31	4.3074e+03	4.8810e+03	5.5308e+03	6.2673e+03	7.1017e+03
36	8.0473e+03	9.1188e+03	1.0333e+04	1.1709e+04	1.3268e+04
41	1.5034e+04	1.7036e+04	1.9305e+04	2.1875e+04	2.4788e+04
46	2.6058e+04	2.8088e+04	3.1828e+04	4.0868e+04	5.2475e+04
51	6.7379e+04	8.6517e+04	1.1109e+05	1.4264e+05	1.8316e+05
56	2.3518e+05	3.0197e+05	3.8774e+05	4.3937e+05	4.9787e+05
61	5.6416e+05	6.3928e+05	7.2440e+05	8.2085e+05	9.3014e+05
66	1.0540e+06	1.1943e+06	1.3534e+06	1.7377e+06	2.2313e+06
71	2.8650e+06	3.6788e+06	4.7237e+06	6.0653e+06	7.7880e+06
76	1.0000e+07	1.1912e+07	1.3499e+07	1.4918e+07	1.6905e+07
81	2.0000e+07				

13. IGN=14...EURLIB 100 Group

This structure has been used extensively in Western Europe in the analysis of integral experiments and in NEA shielding benchmark exercises. It is very similar to the constant-lethargy-step GAM-II structure (see IGN=7 above). The only changes are the removal of 7 of the 16 group boundaries below 17 eV, the insertion of 4 new boundaries at high energy (7.0469, 6.3763, 4.7237, and 2.3457 MeV), and the addition of 3 new boundaries near the iron minimum (26.058, 23.579, and 21.875 keV).

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e-05	4.1399e-01	6.2506e-01	1.1254e+00	1.8554e+00
6	3.0590e+00	5.0435e+00	8.3153e+00	1.0677e+01	1.7603e+01
11	2.2603e+01	2.9023e+01	3.7267e+01	4.7851e+01	6.1442e+01
16	7.8893e+01	1.0130e+02	1.3007e+02	1.6702e+02	2.1445e+02
21	2.7536e+02	3.5358e+02	4.5400e+02	5.8295e+02	7.4852e+02
26	9.6112e+02	1.2341e+03	1.5846e+03	2.0347e+03	2.6126e+03
31	3.3546e+03	4.3074e+03	5.5308e+03	7.1017e+03	9.1188e+03
36	1.1709e+04	1.5034e+04	1.9305e+04	2.1875e+04	2.3579e+04
41	2.4788e+04	2.6058e+04	3.1828e+04	4.0868e+04	5.2475e+04
46	6.7379e+04	8.6517e+04	1.1109e+05	1.2277e+05	1.3569e+05
51	1.4996e+05	1.6573e+05	1.8316e+05	2.0242e+05	2.2371e+05
56	2.4724e+05	2.7324e+05	3.0197e+05	3.3373e+05	3.6883e+05
61	4.0762e+05	4.5049e+05	4.9787e+05	5.5023e+05	6.0810e+05
66	6.7206e+05	7.4274e+05	8.2085e+05	9.0718e+05	1.0026e+06
71	1.1080e+06	1.2246e+06	1.3534e+06	1.4957e+06	1.6530e+06
76	1.8268e+06	2.0190e+06	2.2313e+06	2.3457e+06	2.4660e+06
81	2.7253e+06	3.0119e+06	3.3287e+06	3.6788e+06	4.0657e+06
86	4.4933e+06	4.7237e+06	4.9659e+06	5.4881e+06	6.0653e+06
91	6.3763e+06	6.7032e+06	7.0469e+06	7.4082e+06	8.1873e+06
96	9.0484e+06	1.0000e+07	1.1052e+07	1.2214e+07	1.3499e+07
101	1.4918e+07				

14. IGN=15...SAND-IIA 640 Group

This fine-group structure is used for dosimetry work with flux unfolding codes. It is an extension of the 620-group structure (see above) that includes 20 extra groups above 18 MeV.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e-04	1.0500e-04	1.1000e-04	1.1500e-04	1.2000e-04
6	1.2750e-04	1.3500e-04	1.4250e-04	1.5000e-04	1.6000e-04
11	1.7000e-04	1.8000e-04	1.9000e-04	2.0000e-04	2.1000e-04
16	2.2000e-04	2.3000e-04	2.4000e-04	2.5500e-04	2.7000e-04

21	2.8000e-04	3.0000e-04	3.2000e-04	3.4000e-04	3.6000e-04
26	3.8000e-04	4.0000e-04	4.2500e-04	4.5000e-04	4.7500e-04
31	5.0000e-04	5.2500e-04	5.5000e-04	5.7500e-04	6.0000e-04
36	6.3000e-04	6.6000e-04	6.9000e-04	7.2000e-04	7.6000e-04
41	8.0000e-04	8.4000e-04	8.8000e-04	9.2000e-04	9.6000e-04
46	1.0000e-03	1.0500e-03	1.1000e-03	1.1500e-03	1.2000e-03
51	1.2750e-03	1.3500e-03	1.4250e-03	1.5000e-03	1.6000e-03
56	1.7000e-03	1.8000e-03	1.9000e-03	2.0000e-03	2.1000e-03
61	2.2000e-03	2.3000e-03	2.4000e-03	2.5500e-03	2.7000e-03
66	2.8000e-03	3.0000e-03	3.2000e-03	3.4000e-03	3.6000e-03
71	3.8000e-03	4.0000e-03	4.2500e-03	4.5000e-03	4.7500e-03
76	5.0000e-03	5.2500e-03	5.5000e-03	5.7500e-03	6.0000e-03
81	6.3000e-03	6.6000e-03	6.9000e-03	7.2000e-03	7.6000e-03
86	8.0000e-03	8.4000e-03	8.8000e-03	9.2000e-03	9.6000e-03
91	1.0000e-02	1.0500e-02	1.1000e-02	1.1500e-02	1.2000e-02
96	1.2750e-02	1.3500e-02	1.4250e-02	1.5000e-02	1.6000e-02
101	1.7000e-02	1.8000e-02	1.9000e-02	2.0000e-02	2.1000e-02
106	2.2000e-02	2.3000e-02	2.4000e-02	2.5500e-02	2.7000e-02
111	2.8000e-02	3.0000e-02	3.2000e-02	3.4000e-02	3.6000e-02
116	3.8000e-02	4.0000e-02	4.2500e-02	4.5000e-02	4.7500e-02
121	5.0000e-02	5.2500e-02	5.5000e-02	5.7500e-02	6.0000e-02
126	6.3000e-02	6.6000e-02	6.9000e-02	7.2000e-02	7.6000e-02
131	8.0000e-02	8.4000e-02	8.8000e-02	9.2000e-02	9.6000e-02
136	1.0000e-01	1.0500e-01	1.1000e-01	1.1500e-01	1.2000e-01
141	1.2750e-01	1.3500e-01	1.4250e-01	1.5000e-01	1.6000e-01
146	1.7000e-01	1.8000e-01	1.9000e-01	2.0000e-01	2.1000e-01
151	2.2000e-01	2.3000e-01	2.4000e-01	2.5500e-01	2.7000e-01
156	2.8000e-01	3.0000e-01	3.2000e-01	3.4000e-01	3.6000e-01
161	3.8000e-01	4.0000e-01	4.2500e-01	4.5000e-01	4.7500e-01
166	5.0000e-01	5.2500e-01	5.5000e-01	5.7500e-01	6.0000e-01
171	6.3000e-01	6.6000e-01	6.9000e-01	7.2000e-01	7.6000e-01
176	8.0000e-01	8.4000e-01	8.8000e-01	9.2000e-01	9.6000e-01
181	1.0000e+00	1.0500e+00	1.1000e+00	1.1500e+00	1.2000e+00
186	1.2750e+00	1.3500e+00	1.4250e+00	1.5000e+00	1.6000e+00
191	1.7000e+00	1.8000e+00	1.9000e+00	2.0000e+00	2.1000e+00
196	2.2000e+00	2.3000e+00	2.4000e+00	2.5500e+00	2.7000e+00
201	2.8000e+00	3.0000e+00	3.2000e+00	3.4000e+00	3.6000e+00
206	3.8000e+00	4.0000e+00	4.2500e+00	4.5000e+00	4.7500e+00
211	5.0000e+00	5.2500e+00	5.5000e+00	5.7500e+00	6.0000e+00
216	6.3000e+00	6.6000e+00	6.9000e+00	7.2000e+00	7.6000e+00
221	8.0000e+00	8.4000e+00	8.8000e+00	9.2000e+00	9.6000e+00
226	1.0000e+01	1.0500e+01	1.1000e+01	1.1500e+01	1.2000e+01
231	1.2750e+01	1.3500e+01	1.4250e+01	1.5000e+01	1.6000e+01
236	1.7000e+01	1.8000e+01	1.9000e+01	2.0000e+01	2.1000e+01
241	2.2000e+01	2.3000e+01	2.4000e+01	2.5500e+01	2.7000e+01
246	2.8000e+01	3.0000e+01	3.2000e+01	3.4000e+01	3.6000e+01
251	3.8000e+01	4.0000e+01	4.2500e+01	4.5000e+01	4.7500e+01
256	5.0000e+01	5.2500e+01	5.5000e+01	5.7500e+01	6.0000e+01
261	6.3000e+01	6.6000e+01	6.9000e+01	7.2000e+01	7.6000e+01
266	8.0000e+01	8.4000e+01	8.8000e+01	9.2000e+01	9.6000e+01
271	1.0000e+02	1.0500e+02	1.1000e+02	1.1500e+02	1.2000e+02
276	1.2750e+02	1.3500e+02	1.4250e+02	1.5000e+02	1.6000e+02
281	1.7000e+02	1.8000e+02	1.9000e+02	2.0000e+02	2.1000e+02
286	2.2000e+02	2.3000e+02	2.4000e+02	2.5500e+02	2.7000e+02
291	2.8000e+02	3.0000e+02	3.2000e+02	3.4000e+02	3.6000e+02
296	3.8000e+02	4.0000e+02	4.2500e+02	4.5000e+02	4.7500e+02
301	5.0000e+02	5.2500e+02	5.5000e+02	5.7500e+02	6.0000e+02
306	6.3000e+02	6.6000e+02	6.9000e+02	7.2000e+02	7.6000e+02

311	8.0000e+02	8.4000e+02	8.8000e+02	9.2000e+02	9.6000e+02
316	1.0000e+03	1.0500e+03	1.1000e+03	1.1500e+03	1.2000e+03
321	1.2750e+03	1.3500e+03	1.4250e+03	1.5000e+03	1.6000e+03
326	1.7000e+03	1.8000e+03	1.9000e+03	2.0000e+03	2.1000e+03
331	2.2000e+03	2.3000e+03	2.4000e+03	2.5500e+03	2.7000e+03
336	2.8000e+03	3.0000e+03	3.2000e+03	3.4000e+03	3.6000e+03
341	3.8000e+03	4.0000e+03	4.2500e+03	4.5000e+03	4.7500e+03
346	5.0000e+03	5.2500e+03	5.5000e+03	5.7500e+03	6.0000e+03
351	6.3000e+03	6.6000e+03	6.9000e+03	7.2000e+03	7.6000e+03
356	8.0000e+03	8.4000e+03	8.8000e+03	9.2000e+03	9.6000e+03
361	1.0000e+04	1.0500e+04	1.1000e+04	1.1500e+04	1.2000e+04
366	1.2750e+04	1.3500e+04	1.4250e+04	1.5000e+04	1.6000e+04
371	1.7000e+04	1.8000e+04	1.9000e+04	2.0000e+04	2.1000e+04
376	2.2000e+04	2.3000e+04	2.4000e+04	2.5500e+04	2.7000e+04
381	2.8000e+04	3.0000e+04	3.2000e+04	3.4000e+04	3.6000e+04
386	3.8000e+04	4.0000e+04	4.2500e+04	4.5000e+04	4.7500e+04
391	5.0000e+04	5.2500e+04	5.5000e+04	5.7500e+04	6.0000e+04
396	6.3000e+04	6.6000e+04	6.9000e+04	7.2000e+04	7.6000e+04
401	8.0000e+04	8.4000e+04	8.8000e+04	9.2000e+04	9.6000e+04
406	1.0000e+05	1.0500e+05	1.1000e+05	1.1500e+05	1.2000e+05
411	1.2750e+05	1.3500e+05	1.4250e+05	1.5000e+05	1.6000e+05
416	1.7000e+05	1.8000e+05	1.9000e+05	2.0000e+05	2.1000e+05
421	2.2000e+05	2.3000e+05	2.4000e+05	2.5500e+05	2.7000e+05
426	2.8000e+05	3.0000e+05	3.2000e+05	3.4000e+05	3.6000e+05
431	3.8000e+05	4.0000e+05	4.2500e+05	4.5000e+05	4.7500e+05
436	5.0000e+05	5.2500e+05	5.5000e+05	5.7500e+05	6.0000e+05
441	6.3000e+05	6.6000e+05	6.9000e+05	7.2000e+05	7.6000e+05
446	8.0000e+05	8.4000e+05	8.8000e+05	9.2000e+05	9.6000e+05
451	1.0000e+06	1.1000e+06	1.2000e+06	1.3000e+06	1.4000e+06
456	1.5000e+06	1.6000e+06	1.7000e+06	1.8000e+06	1.9000e+06
461	2.0000e+06	2.1000e+06	2.2000e+06	2.3000e+06	2.4000e+06
466	2.5000e+06	2.6000e+06	2.7000e+06	2.8000e+06	2.9000e+06
471	3.0000e+06	3.1000e+06	3.2000e+06	3.3000e+06	3.4000e+06
476	3.5000e+06	3.6000e+06	3.7000e+06	3.8000e+06	3.9000e+06
481	4.0000e+06	4.1000e+06	4.2000e+06	4.3000e+06	4.4000e+06
486	4.5000e+06	4.6000e+06	4.7000e+06	4.8000e+06	4.9000e+06
491	5.0000e+06	5.1000e+06	5.2000e+06	5.3000e+06	5.4000e+06
496	5.5000e+06	5.6000e+06	5.7000e+06	5.8000e+06	5.9000e+06
501	6.0000e+06	6.1000e+06	6.2000e+06	6.3000e+06	6.4000e+06
506	6.5000e+06	6.6000e+06	6.7000e+06	6.8000e+06	6.9000e+06
511	7.0000e+06	7.1000e+06	7.2000e+06	7.3000e+06	7.4000e+06
516	7.5000e+06	7.6000e+06	7.7000e+06	7.8000e+06	7.9000e+06
521	8.0000e+06	8.1000e+06	8.2000e+06	8.3000e+06	8.4000e+06
526	8.5000e+06	8.6000e+06	8.7000e+06	8.8000e+06	8.9000e+06
531	9.0000e+06	9.1000e+06	9.2000e+06	9.3000e+06	9.4000e+06
536	9.5000e+06	9.6000e+06	9.7000e+06	9.8000e+06	9.9000e+06
541	1.0000e+07	1.0100e+07	1.0200e+07	1.0300e+07	1.0400e+07
546	1.0500e+07	1.0600e+07	1.0700e+07	1.0800e+07	1.0900e+07
551	1.1000e+07	1.1100e+07	1.1200e+07	1.1300e+07	1.1400e+07
556	1.1500e+07	1.1600e+07	1.1700e+07	1.1800e+07	1.1900e+07
561	1.2000e+07	1.2100e+07	1.2200e+07	1.2300e+07	1.2400e+07
566	1.2500e+07	1.2600e+07	1.2700e+07	1.2800e+07	1.2900e+07
571	1.3000e+07	1.3100e+07	1.3200e+07	1.3300e+07	1.3400e+07
576	1.3500e+07	1.3600e+07	1.3700e+07	1.3800e+07	1.3900e+07
581	1.4000e+07	1.4100e+07	1.4200e+07	1.4300e+07	1.4400e+07
586	1.4500e+07	1.4600e+07	1.4700e+07	1.4800e+07	1.4900e+07
591	1.5000e+07	1.5100e+07	1.5200e+07	1.5300e+07	1.5400e+07
596	1.5500e+07	1.5600e+07	1.5700e+07	1.5800e+07	1.5900e+07

601	1.6000e+07	1.6100e+07	1.6200e+07	1.6300e+07	1.6400e+07
606	1.6500e+07	1.6600e+07	1.6700e+07	1.6800e+07	1.6900e+07
611	1.7000e+07	1.7100e+07	1.7200e+07	1.7300e+07	1.7400e+07
616	1.7500e+07	1.7600e+07	1.7700e+07	1.7800e+07	1.7900e+07
621	1.8000e+07	1.8100e+07	1.8200e+07	1.8300e+07	1.8400e+07
626	1.8500e+07	1.8600e+07	1.8700e+07	1.8800e+07	1.8900e+07
631	1.9000e+07	1.9100e+07	1.9200e+07	1.9300e+07	1.9400e+07
636	1.9500e+07	1.9600e+07	1.9700e+07	1.9800e+07	1.9900e+07
641	2.0000e+07				

15. IGG=2...CSEWG 94 Group

This structure is a "super-group" structure for photons that was developed at the same time as the 240-group neutron structure given above. As such, it was designed to contain a number of the photon group structures in use at that time as subsets. This has made it much more detailed than needed for practical calculations of the comparatively smooth photon spectra found in actual systems. It is also lacking in the detail above 10 MeV needed to represent the emission of "primary" photons from capture reactions in systems with a large flux of 14-MeV neutrons.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	5.0000e+03	1.0000e+04	1.5000e+04	2.0000e+04	3.0000e+04
6	3.5000e+04	4.0000e+04	4.5000e+04	5.5000e+04	6.0000e+04
11	6.5000e+04	7.5000e+04	8.0000e+04	9.0000e+04	1.0000e+05
16	1.2000e+05	1.4000e+05	1.5000e+05	1.6000e+05	1.9000e+05
21	2.2000e+05	2.6000e+05	3.0000e+05	3.2500e+05	3.5000e+05
26	3.7500e+05	4.0000e+05	4.2500e+05	4.5000e+05	5.0000e+05
31	5.2500e+05	5.5000e+05	5.7500e+05	6.0000e+05	6.2500e+05
36	6.5000e+05	6.7500e+05	7.0000e+05	7.5000e+05	8.0000e+05
41	8.2500e+05	8.6500e+05	9.0000e+05	1.0000e+06	1.1250e+06
46	1.2000e+06	1.2500e+06	1.3300e+06	1.4200e+06	1.5000e+06
51	1.6000e+06	1.6600e+06	1.7500e+06	1.8750e+06	2.0000e+06
56	2.1660e+06	2.3330e+06	2.5000e+06	2.6660e+06	2.8330e+06
61	3.0000e+06	3.1660e+06	3.3330e+06	3.5000e+06	3.6500e+06
66	3.8000e+06	3.9000e+06	4.0000e+06	4.2000e+06	4.4000e+06
71	4.5000e+06	4.7000e+06	5.0000e+06	5.2000e+06	5.4000e+06
76	5.5000e+06	5.7500e+06	6.0000e+06	6.2500e+06	6.5000e+06
81	6.7500e+06	7.0000e+06	7.2500e+06	7.5000e+06	7.7500e+06
86	8.0000e+06	8.5000e+06	9.0000e+06	9.5000e+06	1.0000e+07
91	1.0600e+07	1.1000e+07	1.2000e+07	1.4000e+07	2.0000e+07

16. IGG=3...LANL 12-Group

This is a comparatively coarse photon structure that has been used extensively at Los Alamos. It is part of the 42-group structure used in the CLAW-3 and CLAW-4 coupled libraries[3] available from RSIC, and also in the MATXS1 and

MATXS5 libraries used with TRANSX[4]. It is most suitable for systems containing a reasonable concentration of heavy atoms; strongly hydrogenous systems have a very soft photon flux that is not well represented by the single group below 100 keV. The 24-group option (see below) is better in this low range, and it also does a better job of calculating photon energy deposition because of more detail above 9 MeV.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e+04	1.0000e+05	5.0000e+05	1.0000e+06	2.0000e+06
6	3.0000e+06	4.0000e+06	5.0000e+06	6.0000e+06	7.0000e+06
11	8.0000e+06	9.0000e+06	2.0000e+07		

17. IGG=4...Steiner 21 Group

This structure was used extensively in early fusion-reactor systems studies at the Oak Radge National Laboratory and elsewhere.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e+04	1.0000e+05	2.0000e+05	4.0000e+05	1.0000e+06
6	1.5000e+06	2.0000e+06	2.5000e+06	3.0000e+06	3.5000e+06
11	4.0000e+06	4.5000e+06	5.0000e+06	5.5000e+06	6.0000e+06
16	6.5000e+06	7.0000e+06	7.5000e+06	8.0000e+06	1.0000e+07
21	1.2000e+07	1.4000e+07			

18. IGG=5...Straker 22 Group

This structure has been used in air-transport and weapons effects calculations.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e+04	3.0000e+04	6.0000e+04	1.0000e+05	1.5000e+05
6	3.0000e+05	4.5000e+05	6.0000e+05	8.0000e+05	1.0000e+06
11	1.3300e+06	1.6600e+06	2.0000e+06	2.5000e+06	3.0000e+06
16	3.5000e+06	4.0000e+06	5.0000e+06	6.0000e+06	7.0000e+06
21	8.0000e+06	1.0000e+07	1.4000e+07		

19. IGG=6...LANL 48 Group

This is intended to be a comprehensive photon structure that includes all the detail needed for practical photon transport calculations. It includes enough detail

at low energies to represent systems dominated by light elements, and enough detail at high energies to give accurate energy deposition results, even in systems with many primary photons from 14 MeV capture events. In addition, several groups are provided for "signatures" of fissionable materials needed for nondestructive assays in safeguards work. The only applications that require more groups would be those that depend on the observation of particular discrete gamma rays, such a quantitative analysis. The 12- and 24-group structures are both subsets of this 48-group set.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e+03	1.0000e+04	2.0000e+04	3.0000e+04	4.5000e+04
6	6.0000e+04	8.0000e+04	1.0000e+05	1.5000e+05	2.0000e+05
11	3.0000e+05	4.0000e+05	4.5000e+05	5.0000e+05	5.2500e+05
16	6.0000e+05	7.0000e+05	8.0000e+05	9.0000e+05	1.0000e+06
21	1.1250e+06	1.2000e+06	1.3300e+06	1.5000e+06	1.6600e+06
26	1.8750e+06	2.0000e+06	2.3330e+06	2.5000e+06	2.6660e+06
31	3.0000e+06	3.5000e+06	4.0000e+06	4.5000e+06	5.0000e+06
36	5.5000e+06	6.0000e+06	6.5000e+06	7.0000e+06	7.5000e+06
41	8.0000e+06	9.0000e+06	1.0000e+07	1.2000e+07	1.4000e+07
46	1.7000e+07	2.0000e+07	3.0000e+07	5.0000e+07	

20. IGG=7...LANL 24 Group

This structure is intended for practical calculations of photon transport in fission and fusion systems. It includes enough detail at low energies for normal shield compositions, and it gives reasonably good results for photon energy deposition in fusion blanket calculations. It has been used with the 80-group neutron structure in the MATXS6 library used with the TRANSX[4] code. It should be used in preference to the 12-group structure when practical.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e+04	3.0000e+04	6.0000e+04	1.0000e+05	2.0000e+05
6	3.0000e+05	5.0000e+05	5.2500e+05	7.5000e+05	1.0000e+06
11	1.3300e+06	1.6600e+06	2.0000e+06	2.5000e+06	3.0000e+06
16	4.0000e+06	5.0000e+06	6.0000e+06	7.0000e+06	8.0000e+06
21	9.0000e+06	1.0000e+07	1.2000e+07	1.7000e+07	3.0000e+07

21. IGG=8...VITAMIN-C 36 Group

This structure was designed for use with the VITAMIN-C library[2], which was intended for fusion and fast-reactor shielding applications. It is a combination of

the 21-group and 22-group structures described above, with an extra group added to transport the annihilation radiation at 511 keV, and an extra bound added at 70 keV. The main problem with this structure is the upper limit of 14 MeV (see IGG=9 below).

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e+04	2.0000e+04	3.0000e+04	4.5000e+04	6.0000e+04
6	7.0000e+04	1.0000e+05	1.5000e+05	2.0000e+05	3.0000e+05
11	4.0000e+05	4.5000e+05	5.1000e+05	5.1200e+05	6.0000e+05
16	7.0000e+05	8.0000e+05	1.0000e+06	1.3300e+06	1.5000e+06
21	1.6600e+06	2.0000e+06	2.5000e+06	3.0000e+06	3.5000e+06
26	4.0000e+06	4.5000e+06	5.0000e+06	5.5000e+06	6.0000e+06
31	6.5000e+06	7.0000e+06	7.5000e+06	8.0000e+06	1.0000e+07
36	1.2000e+07	1.4000e+07			

22. IGG=9...VITAMIN-E 38 Group

This is a slightly extended version of the previous group structure that was selected for use with the VITAMIN-E library[8]. There were only two changes made: a new group was added above 14 MeV, and a new bound was inserted at 75 keV. The structure given in the reference is not exactly correct; contact the Radiation Shielding Information Center (RSIC) at Oak Ridge for a full description of the VITAMIN-E library as issued.

GROUP INDEX N	GROUP LOWER BOUNDARIES (EV)				
	EL(N+0)	EL(N+1)	EL(N+2)	EL(N+3)	EL(N+4)
1	1.0000e+04	2.0000e+04	3.0000e+04	4.5000e+04	6.0000e+04
6	7.0000e+04	7.5000e+04	1.0000e+05	1.5000e+05	2.0000e+05
11	3.0000e+05	4.0000e+05	4.5000e+05	5.1000e+05	5.1200e+05
16	6.0000e+05	7.0000e+05	8.0000e+05	1.0000e+06	1.3300e+06
21	1.5000e+06	1.6600e+06	2.0000e+06	2.5000e+06	3.0000e+06
26	3.5000e+06	4.0000e+06	4.5000e+06	5.0000e+06	5.5000e+06
31	6.0000e+06	6.5000e+06	7.0000e+06	7.5000e+06	8.0000e+06
36	1.0000e+07	1.2000e+07	1.4000e+07	2.0000e+07	

23. References

1. C. R. Weisbin and R. J. LaBauve, "Specifications of a Generally Useful Multi-group Structure for Neutron Transport," Los Alamos Scientific Laboratory report LA-5277-MS (May 1973).

2. R. W. Roussin, C. R. Weisbin, J. E. White, N. M. Greene, R. Q. Wright, and J. B. Wright, "The CTR Processed Multigroup Cross Section Library for Neutronics Studies," Oak Ridge National Laboratory report ORNL/RSIC-37 (1978).

3. R. J. Barrett and R. E. MacFarlane, "Coupled Neutron and Photon Cross Sections of Transport Calculations," Los Alamos Scientific Laboratory report LA-7808-MS (April 1979).

4. R. E. MacFarlane, "TRANSX-CTR: A Code for Interfacing MATXS Cross-Section Libraries to Nuclear Transport Codes for Fusion Systems Analysis," Los Alamos National Laboratory report LA-9863-MS (February 1984).

5. R. B. Kidman and R. E. MacFarlane, "LIB-IV, A Library of Group Constants for Nuclear Reactor Calculations," Los Alamos Scientific Laboratory report LA-6260-MS (March 1976).

6. R. E. MacFarlane, "ENDF/B-V Cross-Section Library for Reactor Cell Analysis," Electric Power Research Institute report EPRI NP-3418 (February 1984).

7. D. E. Cullen, "Report on the IAEA Cross Section Processing Code Verification Project," International Atomic Energy Agency Nuclear Data Section report INDC(NDS)-170/NI (May 1985).

8. C. R. Weisbin, R. W. Roussin, J. J. Wagschal, J. E. White, and R. Q. Wright, "VITAMIN-E: An ENDF/B-V Multigroup Cross-Section Library for LMFBR Core and Shield, LWR Shield, Dosimetry, and Fusion Blanket Technology," Oak Ridge National Laboratory report ORNL-5505 (ENDF-274) (February 1979).

Appendix B. WEIGHT FUNCTIONS

1. Neutron Weight Functions in GROUPR

Most of the weight functions available in GROUPR are shown in Figures 1 and 2. As mentioned in the main text of this report, the accuracy of a set of multigroup constants is determined by the group structure and the weight function. If only a few groups are used, it is necessary to have a weight function that is similar to the flux in the kinds of nuclear systems to be calculated with that particular group structure. If the flux is not well enough known, or if it varies strongly between different regions of the device, it is necessary to use more groups. The weight functions provided in the code are representative of a few typical nuclear systems, as described below. For systems with unusual spectra, or for very high accuracy calculations, the user should consider entering custom weight functions.

IWT=2 The weight function is constant (not shown). This option is usually chosen for very fine group structures such as the 620-group or 640-group dosimetry structures.

IWT=3 The weight function is proportional to 1/E (not shown). The slowing-down of neutrons in water gives a 1/E flux from about 1 eV up to 100 keV, or so. This weight function is traditionally used for calculating "resonance integrals", but it is not useful at the lower and higher energies needed for a full set of transport constants. The graph of this function is a flat line on a flux-per-unit-lethargy plot, such as Fig. 1.

IWT=4 This weight function combines a thermal Maxwellian at low energies, a 1/E function at intermediate energies, and a fission spectrum at high energies to obtain a function appropriate for several different applications. The temperatures of the Maxwellian and fission parts and the energies where the components join can be chosen by the user. Therefore, option 4 can be used to produce a typical thermal reactor weight function like that shown in Figs. 1 and 2, a pure fission spectrum for calculating some kinds of dosimetry cross sections, or a pure thermal spectrum for getting effective thermal average cross sections. The function shown in the figures was produced using a thermal temperature of 0.025 eV joined to 1/E at 0.1 eV, and a fission temperature of 1.40 MeV joined to 1/E at 820.3 keV.

IWT=5 This is a mid-life PWR (pressurized water reactor) flux spectrum with a fusion peak added (see below for a discussion of the fusion peak used). Note the peaks and dips resulting from oxygen resonances and windows at high energies, and the hardening apparent in the epithermal region. The thermal part of the function is also hardened with respect to a simple Maxwellian shape. The dips that should show up in the eV range due to resonances and U-238 have been removed to allow the selfshielding method to work without risk of counting the shielding effects twice. This weight function has been used for several libraries[1] prepared for the Electric Power Research Institute (EPRI), and for the MATXS7 library used with the TRANSX code[2].

IWT=6 This function is similar to option 4, but the breakpoints were chosen to keep the curves continuous. The thermal Maxwellian is calculated for 300 K. In this case, the fusion peak (see below) was added to the high-energy tail of the fission spectrum for smoothness.

IWT=7 Reserved for future use.

IWT=8 This function is intended for cross sections libraries to be used for fast reactor analysis (typically, fast breeder designs), but is also useful for fusion-blanket problems. It has a fusion peak at high energies, followed by a fission spectrum, a slowing-down spectrum typical of a fast reactor, and a thermal tail. The tail is provided to help give reasonable results in shields far from the core; its characteristic temperature is 300 K. Note the sharp drop in the flux as energy decreases from 19 keV. This region is important for U-238 absorbtion, and this dropoff helps to give good group constants for fast reactors. Of course, it would be entirely wrong for a thermal reactor.

IWT=9 This is another typical thermal+1/E+fission+fusion function that has been used for many libraries at the Los Alamos National Laboratory in the 30-group structure. The CLAW-3 and CLAW-4 libraries are available from the Radiation Shielding Information Center at the Oak Ridge National Laboratory.

2. Shape of the Fusion Peak

Because of the finite width of the distribution of ion energies in a D-T fusion plasma, the emitted "14-MeV" neutrons clearly will not have a delta-function energy spectrum. In fact, owing to the presence of a cross-product term in the kinematic relations, the typical ion-energy spread of the few tens of kilovolts is magnified into a neutron-energy spread of around 1 MeV.

For an assumed isotropic Maxwellian plasma, the neutron peak shape (for example, see the review article by Lehner[3]) is given by

$$S(E) = C \int_0^\infty \exp\{-b[v^2 + v_0(g)^2] - cg^2\} \sinh(2bvv_0) \frac{g^3\sigma(g)}{v_0(g)} \, dg. \qquad (1)$$

Here $S(E)$ is the number of neutrons emitted with laboratory energy between E and $E+dE$, C is a normalization factor, v is the laboratory velocity corresponding to energy E, and v_0 is the velocity of the neutron in the CM system. Both v_0 and the fusion cross section σ are determined by the relative velocity g of the reacting ions, the integration variable in Eq.(1). The coefficient b is equal to $M/2kT$ where M is the total mass of the reacting ions and kT is the plasma temperature. Similarly, c is $\mu/2kT$, where μ is the reduced mass of the ion system.

The only approximation involved in Lehner's derivation of Eq.(1) is that all particles may be treated non-relativistically. At 14 MeV, the relativistic factor

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}} \qquad (2)$$

is very close to unity (1.015), and it varies negligibly over the range of interest (say, 13 to 17 MeV). It is sufficient then to invoke relativistic mechanics in defining the
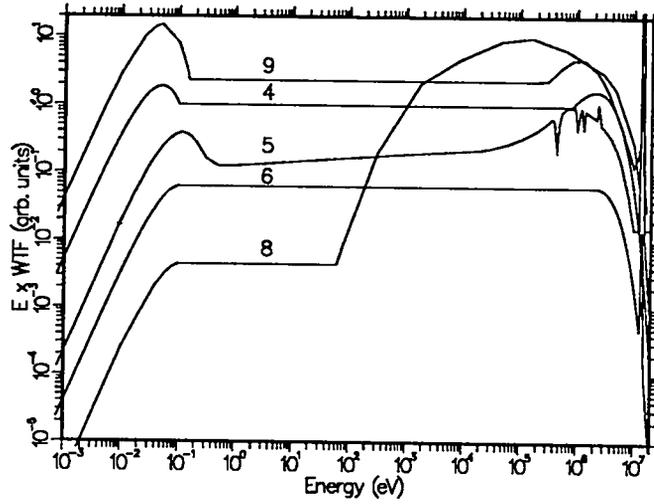
96

Figure 1: Built-in neutron weight functions of GROUPR on a logarithmic flux-per-unit-lethargy plot that emphasizes the low energy range.
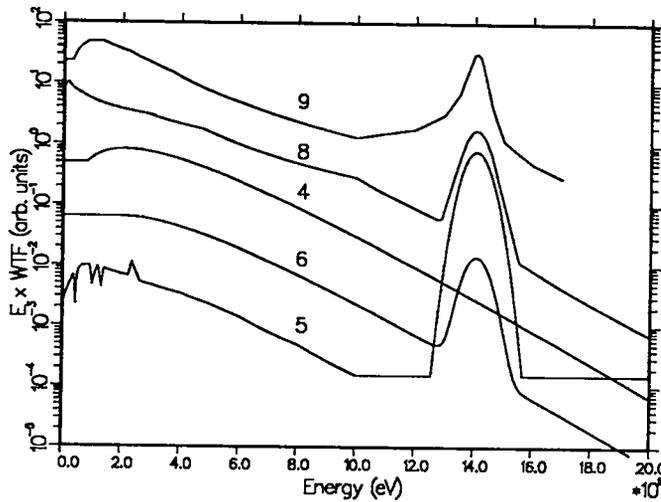

Figure 2: Built-in neutron weight functions on a linear plot that emphasizes the high-energy range.

location of the 14-MeV peak but not in discussing the shape. This effect moves the peak toward lower neutron energies, but only by about 20 keV.

Although the expression for $S(E)$ in Eq.(1) is accurate, it has the disadvantage of requiring a numerical integration at each point E in the energy spectrum. For this reason, we consider what simplifications can be made without serious loss of accuracy. In the energy range around the 14-MeV peak, the product $2bvv_0$ in Eq.(1) has a numerical value of about 6000. Thus the hyperbolic sine can obviously be replaced by just the positive exponential term. If we make this change in Eq.(1), we can write the following, still nearly exact, expression for the neutron spectrum:

$$S_1(E) = C_1 \int_0^\infty \exp[-b(v - v_0)^2]\, P(v_0)\, dv_0. \tag{3}$$

Here we also have inverted the function $v_0(g)$ and changed the integration variable. The spectrum then is a linear superposition of velocity exponentials with slightly different peak locations. For normal plasma temperatures, the velocity distribution $P(v_0)$ is very narrow, since the expression for v_0 is dominated by the nuclear Q-value (17.586 MeV) rather than the contribution from the ion kinetic energy (typically around 50 keV). Thus it seems reasonable to approximate $P(v_0)$ as a delta function:

$$P(v_0) \approx \delta(v_0 - v_p). \tag{4}$$

This gives a second approximate form,

$$S_2(E) = C_2 \exp[-b(v - v_p)^2], \tag{5}$$

where v_p has the obvious meaning of the laboratory neutron velocity at the center of the peak. We shall refer to this as the velocity exponential form of the neutron energy spectrum. An expression essentially identical to Eq.(5) was given in an early paper by Nagle and coworkers[4].

In order to examine the accuracy of the velocity exponential form, we have calculated $S(E)$ from Eq.(1) and $S_2(E)$ from Eq.(5) at 20 keV, a typical plasma temperature in current fusion-reactor concepts. In performing the numerical integration over g in Eq.(1), we used numerical values for the D-T fusion cross section taken from the compilation by Jarmie and Seagrave[5]. In evaluating $S_2(E)$ using Eq.(5), a value of v_p was chosen so as to force agreement between $S_2(E)$ and $S(E)$ at 17 MeV. As discussed by Muir[6], the overall agreement is remarkably good, the maximum error over the range from 13.5 to 17 MeV being about 2%. The value of v_p thus derived corresponds to a peak-center energy E_p of 14.07 MeV. This value includes the small (~ 20 keV) relativistic correction mentioned above.

If we approximate the mass of the D+T system as 5 times the neutron mass, then we obtain the recommended peak shape

$$S_{\text{rec}}(E) = \exp[-\frac{5}{kT}(\sqrt{E} - \sqrt{E_p})^2], \tag{6}$$

where E_p=14.07 MeV. The functional form in Eq.(6) was used to calculate the fusion peak shapes appearing in two of the data statements in GENWTF (namely, those utilized for IWT=5 and 8) and also is used explicitly in GETWTF to calculate analytically the weight function for IWT=6. In all three cases, kT=25 keV is used as an average or typical fusion-reactor plasma temperature. See Fig. 2 for a graphical display of the resulting weight functions in the 14-MeV region.
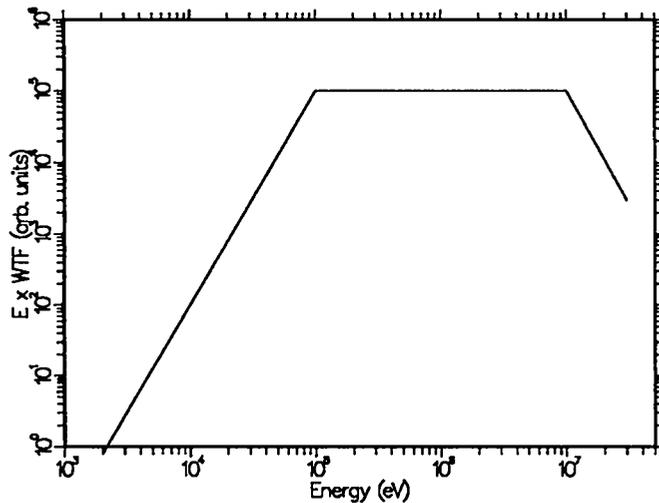
3.   Photon Weight Functions in GAMINR

The main features of a typical photon spectrum are a 1/E region at intermediate energies, a drop-off at low energies caused by photoelectric absorbtion, and a shoulder at high energies corresponding to the maximum Q-value for capture. The relative size and importance of these features depends on the composition of the system. With light materials like water and concrete, the 1/E portion is very obvious and extends to low energies. As heavy materials are added, the low-energy range is supressed. The highest energy photons in a system are normally primary photons from capture, with maximum energies of about $Q + (A/A+1)E$, where E is the neutron energy and A is the atomic weight ratio to the neutron for the absorber. Thus, the shape of the high-energy part of the photon flux may be different for fusion and fission systems, with energies above 10 MeV being important for fusion.

IWT=2   The weight function is constant (not shown). This option is most useful for fine-group libraries, or for benchmark comparisons of different codes where simplicity is useful.

IWT=3   The weight function is basically 1/E; however, low and high-energy "roll offs" are included to keep the first and last group from being unrealistically biased by unimportant regions of the cross-section energy range. See Fig. 3.

4.   References

1. R. E. MacFarlane, "ENDF/B-V Cross-Section Library for Reactor Cell Analysis," Electric Power Research Institute report EPRI NP-3418 (February 1984).

2. R. E. MacFarlane, "TRANSX-CTR: A Code for Interfacing MATXS Cross-Section Libraries to Nuclear Transport Codes for Fusion Systems Analysis," Los Alamos National Laboratory report LA-9863-MS (February 1984).

Figure 3: Built-in photon weight function of GAMINR showing the high- and low-energy rolloffs.

3. G. Lehner, "Reaction Rates and Energy Spectra for Nuclear Reactions in High Energy Plasmas," Z. Physik **232**, 174 (1970).

4. D. E. Nagle, W. E. Quinn, W. B. Riesenfeld, and W. Leland, "Ion Temperature in Scylla, as Determined from the Reaction D(d,p)T," Phys. Rev. Letters **3**, 318 (1959).

5. Nelson Jarmie and John D. Seagrave (editors), "Charged Particle Cross Sections," Los Alamos Scientific Laboratory report LA-2014 (March 1956).

6. D. W. Muir, "Sensitivity of Neutron Multigroup Cross Sections to Thermal Broadening of the Fusion Peak," Proc. 1st Topical Meeting on the Technology of Controlled Nuclear Fusion, San Diego, Calif., April 1974, CONF-740402-P2, p.166 (1975).

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