6. FILE 6. PRODUCT ENERGY-ANGLE DISTRIBUTIONS

6.1. General Description

This file is provided to represent the distribution of reaction products (*i.e.*, neutrons, photons, charged particles, and residual nuclei) in energy and angle. It works together with File 3, which contains the reaction cross sections, and replaces the combination of File 4 and File 5. Radioactive products are identified in File 8. The use of File 6 is recommended when the energy and angular distributions of the emitted particles must be coupled, when it is important to give a concurrent description of neutron scattering and particle emission, when so many reaction channels are open that it is difficult to provide separate reactions, or when accurate charged-particle or residual-nucleus distributions are required for particle transport, heat deposition, or radiation damage calculations.

For the purposes of this file, any reaction is defined by giving the production cross section for each reaction product in barns/steradian assuming azimuthal symmetry:

$$\sigma_i(\mu,E,E') = \sigma(E)\,y_i(E)\,f_i(\mu,E,E')/2\pi \tag{6.1}$$

where i denotes one particular product,
E is the incident energy,
E' is the energy of the product emitted with cosine μ,
$\sigma(E)$ is the interaction cross section (File 3),
y_i is the product yield or multiplicity, and
f_i is the normalized distribution with units (eV-unit cosine)$^{-1}$ where

$$\int dE' \int d\mu \;\; f_i(\mu,E,E') = 1 \tag{6.2}$$

This representation ignores most correlations between products and most sequential reactions; that is, the distributions given here are those which would be seen by an observer outside of a "black box" looking at one particle at a time. The process being described may be a combination of several different reactions, and the product distributions may be described using several different representations.

6.2. Formats

The following quantities are defined for all representations.

ZA,AWR Standard material charge and mass parameters.

LCT Reference system for secondary energy and angle (incident energy is always given in the LAB system).
LCT=1, laboratory (LAB) coordinates used for both;
LCT=2, center-of-mass (CM) system used for angle;
LCT=3, center-of-mass system for both angle and energy of light particles (A≤4), laboratory system for heavy recoils (A>4).

NK Number of subsections in this section (MT). Each subsection describes one reaction product. There can be more than one subsection for a given particle or residual nucleus (see LIP). NK≤1000.

ZAP Product identifier 1000*Z+A with Z=0 for photons and A=0 for electrons and positrons. A section with A=0 can also be used to represent the average recoil energy or spectrum for an elemental target (see text).

AWP Product mass in neutron units.

LIP Product modifier flag. Its main use is to identify the isomeric state of a product nucleus. In this case, LIP=0 for the ground state, LIP=1 for the first isomeric state, *etc.* These values should be consistent with LISO in File 8, MT=457.
In some cases, it may be useful to use LIP to, distinguish between different subsections with the same value of ZAP for light particles. For example, LIP=0 could be the first neutron out for a sequential reaction, LIP=1 could be the second neutron, and so on. Other possible uses might be to indicate which compound system emitted the particles, or to distinguish between the neutron for the (n,np) channel and that from the (n,pn) channel. The exact meaning assigned to LIP should be explained in the File 1, MT=451 comments.

LAW Flag to distinguish between different representations of the distribution function, f_i:
LAW=0, unknown distribution;
LAW=1, continuum energy-angle distribution;
LAW=2, two-body reaction angular distribution;
LAW=3, isotropic two-body distribution;
LAW=4, recoil distribution of a two-body reaction;
LAW=5, charged-particle elastic scattering;
LAW=6, n-body phase-space distribution; and
LAW=7, laboratory angle-energy law.

NR,NP,E_{int} Standard TAB1 parameters.

A section of File 6 has the following form:

```
[MAT, 6, MT/  ZA, AWR,   0, LCT,  NK,   0]HEAD
[MAT, 6, MT/ ZAP, AWP, LIP, LAW,  NR,  NP/Eint/yi(E)]TAB1
```
[LAW-dependent structure for product 1]

<repeat TAB1 and LAW-dependent structures for rest of the NK subsections>

```
[MAT, 6, MT/ 0.0, 0.0,   0,   0,   0,   0]SEND
```

File 6 should have a subsection for every product of the reaction or sum of reactions being described except for MT = 3, 4, 103-107 when they are being used to represent lumped photons. The subsections are arranged in the following order: (1) particles (n, p, d, *etc.*) in order of ZAP and LIP, (2) residual nuclei and isomers in order of ZAP and LIP, (3) photons, and (4) electrons. The contents of the subsection for each LAW are described below.

6.2.1. Unknown Distribution (LAW=0)

This law simply identifies a product without specifying a distribution. It can be used to give production yields for particles, isomers, radioactive nuclei, or other interesting nuclei in materials which are not important for particle transport, heating, or radiation damage calculations. No law-dependent structure is given.

6.2.2. Continuum Energy-Angle Distributions (LAW=1)

This law is used to describe particles emitted in multi-body reactions or combinations of several reactions, such as scattering through a range of levels or reactions at high energies where many channels are normally open. For isotropic reactions, it is very similar to File 5, LF=1 except for a special option to represent sharp peaks as "delta functions" and the use of LIST instead of TAB1.

The following quantities are defined for LAW=1:

LANG Indicator which selects the angular representation to be used; if
LANG=1, Legendre coefficients are used,
LANG=2, Kalbach-Mann systematics are used,
LANG=11-15, a tabulated angular distribution is given using NA/2 cosines and the interpolation scheme specified by LANG–10 (for example, LANG=12 selects linear-linear interpolation).

LEP Interpolation scheme for secondary energy;
LEP=1 for histogram,
LEP=2 for linear-linear, *etc*.

NR,NE,E_{int} Standard TAB2 parameters.
INT=1 is allowed (the upper limit is implied by file 3),
INT=12-15 is allowed for corresponding-point interpolation,
INT=21-25 is allowed for unit base interpolation.

NW Total number of words in the LIST record; NW = NEP (NA+2).

NEP Number of secondary energy points in the distribution.

ND Number of discrete energies given.
The first ND≥0 entries in the list of NEP energies are discrete, and the remaining (NEP-ND)≥0 entries are to be used with LEP to describe a continuous distribution. Discrete primary photons should be flagged with negative energies.

NA Number of angular parameters.
Use NA=0 for isotropic distributions (note that all options are identical if NA=0).
Use NA=1 with LANG=2 (Kalbach-Mann).

The structure of a subsection is

```
[MAT, 6, MT/  0.0,      0.0,    LANG,  LEP,   NR,   NE/Eint]TAB2
[MAT, 6, MT/  0.0,       E1,      ND,   NA,   NW,  NEP/
                E′1, b0(E1,E′1),b1(E1,E′1),------ bNA(E1,E′1),
                E′2, b0(E1,E′2), ---------------------
               E′NEP,b0(E1,E′NEP), ------------  bNA(E1,E′NEP)]LIST
              -------------------------------------
              <continue with LIST structures for the rest of the NE incident energies>
              -------------------------------------
```

where the contents of the b_i depend on LANG.

The angular part of f_i can be represented in several different ways (denoted by LANG).

LANG=1

If LANG=1, Legendre coefficients are used as follows:

$$f_i(\mu, E, E') = \sum_{l=0}^{NA} \frac{2l+1}{2} f_l(E, E') P_l(\mu) \tag{6.3}$$

where NA is the number of angular parameters, and the other parameters have their previous meanings. Note that these coefficients are not normalized like those for discrete two-body scattering (LAW=2); instead, $f_0(E,E')$ gives the total probability of scattering from E to E′ integrated over all angles. This is just the function $g(E,E')$ normally given in File 5. The Legendre coefficients are stored with f_0 in b_0, f_1 in b_1, *etc*.

LANG=2

For LANG=2, the angular distribution is represented by using the Kalbach-Mann systematics [Ref.1] in the extended form developed by Kalbach [Ref.2], hereinafter referred to as KA88. This formulation addresses reactions of the form

$$A + a \rightarrow C \rightarrow B + b,$$

where: A is the target, a is the incident projectile,
C is the compound nucleus,
b is the emitted particle, B is the residual nucleus.

The following quantities are defined:

E_a energy of the incident projectile a in the *laboratory system*

ε_a entrance channel energy, the kinetic energy of the incident projectile a and the target particle A in the *center-of-mass system*

$$\varepsilon_a = E_a \times \frac{AWR_A}{AWR_A + AWR_a}$$

E_b energy of the emitted particle in the *laboratory system*

ε_b emission channel energy, the kinetic energy of the emission particle b and the residual nucleus B in the *center-of-mass system*

$$\varepsilon_b = E_b \times \frac{AWR_B}{AWR_B + AWR_b}$$

μ_b cosine of the scattering angle of the emitted particle b in the *center-of-mass system*

It is ***required*** that LCT=2 with LANG=2.

The KA88 distribution is represented by

$$f(\mu_b, E_a, E_b) = f_0(E_a, E_b)\left[\frac{a(E_a,E_b)}{\sinh\left(a(E_a,E_b)\right)}\left[\begin{array}{l}\cosh\left(a(E_a,E_b)\mu_b\right)\\ +r(E_a,E_b)\sinh\left(a(E_a,E_b)\mu_b\right)\end{array}\right]\right] \quad (6.4)$$

where *r(E* $r(E_a,E_b)$ is the pre-compound fraction as given by the evaluator and $a(E_a,E_b)$ is a simple parameterized function that depends mostly on the center-of-mass emission energy E_b, but also depends slightly on particle type and the incident energy at higher values of E_a.

The center-of-mass energies and angles E_b and μ_b are transformed into the laboratory system using the expressions

$$\begin{aligned} E_{b,lab} &= E_{b,cm} + \frac{AWR_a AWR_b}{(AWR_A + AWR_a)^2} E_{a,lab} + 2\frac{\sqrt{AWR_a}\sqrt{AWR_b}}{AWR_A + AWR_a}\sqrt{E_{a,lab}E_{b,cm}}\,\mu_{b,cm} \\ \mu_{b,lab} &= \sqrt{\frac{E_{b,cm}}{E_{b,lab}}}\mu_{b,cm} + \frac{\sqrt{AWR_a}\sqrt{AWR_b}}{AWR_A + AWR_a}\sqrt{\frac{E_{a,lab}}{E_{b,lab}}} \end{aligned} \quad (6.5)$$

The pre-compound fraction r, where r goes from 0.0 to 1.0, is usually computed by a model code, although it can be chosen to fit experimental data.

The formula for calculating the slope value $a(E_a,E_b)$[1] is:

$$a(E_a, E_b) = C_1 X_1 + C_2 X_1^3 + C_3 M_a m_b X_3^4$$

where

$e_a = \varepsilon_a + S_a$	$e_b = \varepsilon_b + S_b$
R_1 = minimum(e_a,E_{t1})	R_3 = minimum(e_a,E_{t3})
$X_1 = R_1 e_b/e_a$	$X_3 = R_3 e_b/e_a$

The parameter values for light particle induced reactions as given in KA88[2] are:

C_1 = 0.04/MeV	$C_2 = 1.8\times10^{-6}$/MeV^3
$C_3 = 6.7\times10^{-7}$/MeV^4	
E_{t1} = 130 MeV	E_{t3} = 41 MeV
$M_n = 1$	$M_p = 1$
$M_d = 1$	$M_\alpha = 0$
$m_n = 1/2$	$m_p = 1$
$m_d = 1$	$m_t = 1$
$m_{3He} = 1$	$m_\alpha = 2$

S_a and S_b are the separation energies for the incident and emitted particles, respectively, neglecting pairing and other effects for the reaction A + a → C → B + b. The formulae for the separation energies in MeV[3] are:

[1] Equation 10 of Ref. 2.

[2] Table V of ref. 2.

[3] Equation 4 of Ref. 2.

$$S_a = 15.68\left[A_C - A\ \right] - 28.06\left[\frac{(N_C - Z_C)^2}{A_A} - \frac{(N_A - Z_A)^2}{A_A}\right]$$
$$-18.56\left[A_C^{2/3} - A_A^{2/3}\right] + 33.22\left[\frac{(N_C - Z_C)^2}{A_C^{2/3}} - \frac{(N_A - Z_A)^2}{A_A^{2/3}}\right]$$
$$-0.717\left[\frac{Z_C^2}{A_C^{1/3}} - \frac{Z_A^2}{A_A^{1/3}}\right] + 1.211\left[\frac{Z_C^2}{A_C} - \frac{Z_A^2}{A_A}\right] - I_a$$

and

$$S_b = 15.68\left[A_C - A_B\right] - 28.07\left[\frac{(N_C - Z_C)^2}{A_A} - \frac{(N_B - Z_B)^2}{A_B}\right]$$
$$-18.56\left[A_C^{2/3} - A_B^{2/3}\right] + 33.22\left[\frac{(N_C - Z_C)^2}{A_C^{2/3}} - \frac{(N_B - Z_B)^2}{A_B^{2/3}}\right]$$
$$-0.717\left[\frac{Z_C^2}{A_C^{1/3}} - \frac{Z_B^2}{A_B^{1/3}}\right] + 1.211\left[\frac{Z_C^2}{A_C} - \frac{Z_B^2}{A_B}\right] - I_b$$

where

subscripts A, B, and C refer to the target nucleus, the residual nucleus, and the compound nucleus, as before,

N, Z, and A are the neutron, proton, and mass numbers of the nuclei,

I_a and I_b are the energies required to separate the incident and emitted particles into their constituent nucleons (see Appendix H for values used for given particles).

The parameter $f_0(E_a,E_b)$ has the same meaning as f_0 in Eq. (6.3); that is, the total emission probability for this E_a and E_b. *The number of angular parameters (NA) is always 1 for LANG=2*, and f_0 and r are stored in the positions of b_0 and b_1, respectively.

This formulation uses a single-particle-emission concept; it is assumed that each and every secondary particle is emitted from the original compound nucleus C. When the incident projectile a and the emitted particle b are the same, $S_a = S_b$, regardless of the reaction. For incident projectile z, if neutrons emitted from the compound nucleus C are detected, there will be one and only one S_b appropriate for all reactions, for example, (z,nα), (z,n3α), (z,2nα), (z,np), (z,2n2α), and (z,nt2α). Furthermore, if the incident projectile is a neutron (z=n in previous examples), then $S_a = S_b$ in all cases; even for neutrons emitted in neutron-induced reactions, S*a* and S_b will be identical.

LANG = 11-15

For LANG=11-15, a tabulated function is given for $f(\mu)$ using the interpolation scheme defined by LANG minus 10. For example, if LANG=12, use linear-linear interpolation (don't use log interpolation with the cosine). The cosine grid of NA/2 values, μ_i, must span the entire angular range open to the particle for E and E′, and the integral of $f(\mu)$ over all angles must give the total emission probability for this E and E′ (that is, it must equal f_0, as defined above). The value of f below $\mu_{NA/1}$ or above $\mu_{NA/2}$ is zero.

The tabulation is stored in the angular parameters as follows:

$b_0 = f_0$,
$b_1 = \mu_1$,
$b_2 = 0.5f_1(\mu_1)/f_0$,
$b_3 = \mu_2$,
...
...
$b_{NA} = 0.5f_{NA/2}(\mu_{NA/2})/f_0$.

The preferred values for NA are 4, 10, 16, 22, *etc*.

In order to provide a good representation of sharp peaks, LAW=1 allows for a superposition of a continuum and a set of delta functions. These discrete lines could be used to represent particle excitations in the CM frame because the method of corresponding points can be used to supply the correct energy dependence. However, the use of LAW=2 together with MT=50-90, 600-650, *etc*., is preferred. This option is also useful when photon production is given in File 6.

6.2.3. Discrete Two-Body Scattering (LAW=2)

This law is used to describe the distribution in energy and angle of particles described by two-body kinematics. It is very similar to File 4, except its use in File 6 allows the concurrent description of the emission of positrons, electrons, photons, neutrons, charged particles, residual nuclei, and isomers. Since the energy of a particle emitted with a particular scattering cosine μ is determined by kinematics, it is only necessary to give

$$\begin{aligned} p_i(\mu,E) &= \int dE' f_i(\mu,E,E') \\ &= 0.5 + \sum_{l+1}^{NL} \frac{2l+1}{2} a_l(E) P_l(\mu) \quad , \end{aligned} \tag{6.6}$$

where the P_l are the Legendre polynomials with the maximum order NL. Note that the angular distribution pi is normalized.

The following quantities are defined for LAW=2:

LANG	flag that indicates the representation: LANG=0, Legendre expansion; LANG=12, tabulation with $p_i(\mu)$ linear in μ; LANG=14, tabulation with *1n* p_i linear in μ.
NR,NE,E_{int}	standard TAB2 parameters.
NL	for LANG=0, NL is the highest Legendre order used; for LANG>0, NL is the number of cosines tabulated.
NW	number of parameters given in the LIST record: for LANG=0, NW=NL; for LANG>0, NW=2*NL.
A_l	for LANG=0, the Legendre coefficients, for LANG>0, the, μ,p_i pairs for the tabulated angular distribution

The format for a subsection with LAW=2 is

```
[MAT, 6, MT/ 0.0, 0.0,    0,  0,  NR,   NE/ Eint ]TAB2
[MAT, 6, MT/ 0.0,  E1 ,LANG,  0,  NW,   NL/A1(E)]LIST
               ---------------------------
               <continue with LIST records for the
                  rest of the incident energies>
               ---------------------------
```

Note that LANG=0 is very similar to File 4, LTT=1, and LVT=0. The tabulated option is similar to File 4, LTT=2, LVT=0, except that a LIST record is used instead of TAB1. The kinematical equations require AWR and AWP from File 6 and QI from File 3.
LAW=2 can be used in sections with MT=50-90, 600-648, 650-698, *etc*., only, and the center-of-mass system must be used (LCT=2).

6.2.4. Isotropic Discrete Emission (LAW=3)

This law serves the same purpose as LAW=2, but the angular distribution is assumed to be isotropic in the CM system for all incident energies. No LAW-dependent structure is given. This option is similar to LI=1 in File 4. The energy of the emitted particle is completely determined by AWR and AWP in this section and QI from File 3.

6.2.5. Discrete Two-Body Recoils (LAW=4)

If the recoil nucleus of a two-body reaction (*e.g.*, nn?, pn) described using LAW=2 or 3 doesn't break up, its energy and angular distribution can be determined by kinematics. No LAW-dependent structure is given. If isomer production is possible, multiple subsections with LAW=4 can be given to define the energy-dependent branching ratio for the production of each excited nucleus. Finally, LAW=4 may be used to describe the recoil nucleus after radiative capture (MT=102), with the understanding that photon momentum at low energies must be treated approximately.

6.2.6. Charged-Particle Elastic Scattering (LAW=5)

Elastic scattering of charged particles includes components from Coulomb scattering, nuclear scattering, and the interference between them. The Coulomb scattering is represented by the Rutherford formula and electronic screening is ignored.

The following parameters are defined.

$\sigma_{cd}(\mu,E)$	differential Coulomb scattering cross section (barns/sr) for distinguishable particles
$\sigma_{ci}(\mu,E)$	cross section for identical particles
E	energy of the incident particle in the *laboratory system* (eV)
μ	cosine of the scattering angle in the *center-of-mass system*
m_1	incident particle mass (AMU)
Z_1 and Z_2	charge numbers of the incident particle and target, respectively
s	spin (identical particles only, s = 0, 1/2, 1, 3/2, *etc*.)
A	target/projectile mass ratio
k	particle wave number (barns-1/2)
η	dimensionless Coulomb parameter

The cross sections can then be written

$$\sigma_{cd}(\mu,E)=\frac{\eta^2}{k^2(1-\mu)^2} \tag{6.7}$$

and

$$\sigma_{ci}(\mu,E)=\frac{2\eta^2}{k^2(1-\mu)^2}\left[\frac{1+\mu^2}{1-\mu^2}+\frac{(-1)^{2s}}{2s+1}\cos\eta\left(\ln\frac{1+\mu}{1-\mu}\right)\right] \tag{6.8}$$

where

$$k=\frac{A}{1+A}\left[\frac{2}{\hbar}m_1 E\right]^{1/2} \tag{6.9}$$

$$\eta=Z_1Z_2\left[\left(\frac{e^4}{2\hbar^2}\right)\frac{m_1}{E}\right]^{1/2} \tag{6.10}$$

Note that A = 1 and $Z_1 = Z_2$ for identical particles.

The net elastic scattering cross section for distinguishable particles may be written as

$$\begin{aligned}\sigma_{ed}(\mu,E)=\sigma_{cd}(\mu,E)-\frac{2\eta}{1-\mu}\mathrm{Re}\left\{\exp\left(i\eta\;\ln\frac{1-\mu}{2}\right)\sum_{l=0}^{NL}\frac{2l+1}{2}a_l(E)P_l(\mu)\right\}\\ +\sum_{l=0}^{NL}\frac{2l+1}{2}b_l(E)P_l(\mu)\end{aligned} \tag{6.11}$$

and the cross section for identical particles is

$$\begin{aligned}\sigma_{ei}(\mu,E)&=\sigma_{ci}(\mu,E)\\ &-\frac{2\eta}{1-\mu^2}\mathrm{Re}\left\{\sum_{l=0}^{NL}\left[\begin{array}{l}(1+\mu)\exp\left(i\eta\;\ln\frac{1-\mu}{2}\right)\\ +(-1)^l(1-\mu)\exp\left(i\eta\;\ln\frac{1+\mu}{2}\right)\end{array}\right]\frac{2l+1}{2}a_l(E)P_l(\mu)\right\}\\ &+\sum_{l=0}^{NL}\frac{4l+1}{2}b_l(E)P_{2l}(\mu)\end{aligned} \tag{6.12}$$

where the a_l are complex coefficients for expanding the trace of the nuclear scattering amplitude matrix and the b_l are real coefficients for expanding the nuclear scattering cross section. The value of NL represents the highest partial wave contributing to nuclear scattering. Note that $\sigma_{ei}(-\mu,E) = \sigma_{ei}(\mu,E)$.

The three terms in Equations (6.11) and (6.12) are Coulomb, interference, and nuclear scattering, respectively. Since an integrated cross section is not defined for this representation, a value of 1.0 is used in File 3.

When only experimental data are available, it is convenient to remove the infinity due to σ_C by subtraction and to remove the remaining infinity in the interference term by multiplication, thereby obtaining the residual cross sections

$$\sigma_{Rd}(\mu,E)=(1-\mu)\left[\sigma_{ed}(\mu,E)-\sigma_{cd}(\mu,E)\right] \tag{6.13}$$

and

$$\sigma_{Ri}(\mu,E) = (1-\mu^2)\left[\sigma_{ei}(\mu,E) - \sigma_{ci}(\mu,E)\right] \tag{6.14}$$

Then σ_R can be given as a Legendre polynomial expansion in the forms

$$\sigma_{Rd}(\mu,E) = \sum_{l=0}^{NL} \frac{2l+1}{2} c_{ld}(E) P_l(\mu) \tag{6.15}$$

and

$$\sigma_{Ri}(\mu,E) = \sum_{l=0}^{NL} \frac{4l+1}{2} c_{li}(E) P_{2l}(\mu) \tag{6.16}$$

A cross section value of 1.0 is used in File 3.

Because the interference term oscillates as μ goes to 1, the limit of the Legendre representation of the residual cross section at small angles may not be well defined. However, if the coefficients are chosen properly, the effect of this region will be small because the Coulomb term is large.

It is also possible to represent experimental data using the "nuclear plus interference" cross section and angular distribution in the CM system defined by

$$\sigma_{NI}(\mu,E) = \int_{\mu_{\min}}^{\mu_{\max}} \left[\sigma_e(\mu,E) - \sigma_c(\mu,E)\right] d\mu \tag{6.17}$$

and

$$\begin{aligned} P_{NI}(\mu,E) &= \frac{\sigma_e(\mu,E) - \sigma_c(\mu,E)}{\sigma_{NI}(E)}, \;\; \mu_{\min} \le \mu \le \mu_{\max} \\ &= 0, \quad \text{otherwise,} \end{aligned} \tag{6.18}$$

where μ_{min} is -1 for different particles and 0 for identical particles. The maximum cosine should be as close to 1.0 as possible, especially at high energies where Coulomb scattering is less important. The Coulomb cross section $\sigma_c(\mu,E)$ is to be computed using Eqs. (6.7) or (6.8) for different or identical particles, respectively. The angular distribution p_{NI} is given in File 6 as a tabulated function of μ, and $\sigma_{NI}(E)$ in barns is given in File 3.

The following quantities are defined for LAW=5:

SPI Spin of the particle. Used for identical particles (SPI=0, 1/2, 1, *etc*.).

LIDP Indicates that the particles are identical when LIDP=1; otherwise, LIDP=0.

LTP Indicates the representation:
- LTP=1, nuclear amplitude expansion (Eq. 6.11, 6.12);
- LTP=2, residual cross section expansion as Legendre coefficients (Eq. 6.13 through 6.16);
- LTP=12, nuclear plus interference distribution with p_{NI} linear in μ (Eq. 6.17 and 6.18);
- LTP=14, tabulation with *ln* P_{NI} linear in μ (Eq. 6.17 and 6.18).

NR,NE,E_{int} Standard TAB2 parameters.

NL For LTP≤2, NL is the highest Legendre order of nuclear partial waves used; For LTP>2, NL is the number of cosines tabulated.

NW Number of parameters given in the LIST record:
for LTP=1 and LIDP=0, NW=4*NL+3;
for LTP=1 and LIDP=1, NW=3*NL+3;
for LTP=2, NW=NL+1; and for LTP>2, NW=2*NL.

A_l(E) Coefficients(a_i, b_i, or c_i as described below) in barns/sr or μ,p pairs with p dimensionless.

A subsection for LAW=5 has the following form:

```
[MAT, 6, MT/ SPI, 0.0, LIDP,  0,  NR,  NE/ Eint ]TAB2
[MAT, 6, MT/ 0.0,  E1,  LTP,  0,  NW,  NL/Al(E1)]LIST
                ------------------------------
```

<continue with LIST records for the rest of the NE incident energies>

```
                ------------------------------
```

The coefficients in the text of the LIST are organized as follows:

LTP=1 and LIDP=0,
b_0, b_1, ...b_{2NL}, Ra_0, Ia_0, Ra_1, Ia_1, ...Ia_{NL};

LTP=1 and LIDP=1,
b_0, b_1, ...b_{2NL}, Ra_0, Ia_0, Ra_1, Ia_1, ...Ia_{NL};

LTP=2,
c_0, c_1, ... c_{NL}; and

LTP>2,
μ_1, $p_{NI}(\mu_1)$, ... μ_{NL}, $p_{NI}(\mu_{NL})$.

6.2.7. N-Body Phase-Space Distributions (LAW=6)

In the absence of detailed information, it is often useful to use n-body phase-space distributions for the particles emitted from neutron and charged- particle reactions. These distributions conserve energy and momentum, and they provide reasonable kinematic limits for secondary energy and angle in the LAB system.

The phase-space distribution for particle i in the CM system is

$$P_i^{cm}(\mu,E,E') = C_n\sqrt{E'}(E_i^{\max} - E')^{(3n/2)-4} \tag{6.19}$$

where E_i^{max} is the maximum possible center-of-mass energy for particle i,
μ and E′ are in the cm system, and
C_n are normalization constants:

$$C_3 = \frac{4}{\pi(E_i^{\max})^2} \tag{6.20}$$

$$C_4 = \frac{105}{32(E_i^{\max})^{7/2}} \tag{6.21}$$

$$C_5 = \frac{256}{14\pi(E_i^{\max})^5} \tag{6.22}$$

In the laboratory system, the distributions become

$$P_i^{lab}(\mu,E,E') = C_n\sqrt{E'}\left[E_i^{\max} - \left(E_{cm} + E' - 2\mu\sqrt{E_{cm}E'}\right)\right]^{(3n/2)-4} \tag{6.23}$$

where E_{cm} is the energy of the center-of-mass motion in the laboratory, and μ and E' are in the laboratory system.

In the general case, the range of both E' and μ is limited by the condition that the quantity in curly brackets remain non-negative.

The value of E_i^{max} is a fraction of the energy available in CM,

$$E_i^{\max} = \frac{M - m_i}{M} E_a \tag{6.24}$$

where M is the total mass of the n particles being treated by this law.

Note that M may be less than the total mass of products for reactions such as

$$\alpha + {}^9\mathrm{Be} \rightarrow \mathrm{n} + 3\alpha$$

where the neutron can be treated as a two-body event and the alphas by a 3-body phase-space law. The parameter APSX is provided so that E_i^{max} can be determined without having to process the other subsections of this section.

The energy available in CM for one-step reactions is

$$E_a = \frac{m_T}{m_p + m_T} E + Q \tag{6.25}$$

where m_T is the target mass,
m_p is the projectile mass,
E is the LAB energy, and
Q is the reaction QI value from File 3.

For two-step reactions such as the one discussed above, E_a is just the recoil energy from the first step.

The following quantities are defined for LAW=6:

APSX total mass in neutron units of the n particles being treated by the law.
NPSX number of particles distributed according to the phase-space law.

Only a CONT record is given

```
[MAT, 6, MT/ APSX, 0.0,  0,  0,  0, NPSX]CONT
```

6.2.8. Laboratory Angle-Energy Law (LAW = 7)

The continuum energy-angle representation (LAW=1) is good for nuclear model code results and for experimental data that have been converted to Legendre coefficients. However, since experiments normally give spectra at various fixed angles, some evaluators may prefer to enter data sorted according to (E,μ,E′), rather than the LAW=1 ordering (E,E′,μ).

The following quantities are defined for LAW=7:

NR,NE,$\mathbf{E_{int}}$ normal TAB2 parameters for incident energy, E.
NRM,NMU,$\boldsymbol{\mu_{int}}$ normal TAB2 parameters for emission cosine, μ.
NRP,NEP,$\mathbf{E'_{int}}$ normal TAB1 parameters for secondary energy, E′.

The structure of a subsection is:

```
[MAT, 6, MT/ 0.0,      0.0,     0,  0,    NR,   NE/Eint ]TAB2
[MAT, 6, MT/ 0.0,       E1 ,     0,  0,   NRM,  NMU/μint ]TAB2
[MAT, 6, MT/ 0.0,       μ1 ,     0,  0,   NRP,  NEP/E′int/
              E′1 ,f(μ1,E1,E′1), E′2,f(μ1,E1,E′2), -----
              ------------------ E′NEP, f(μ1,E1,E′NEP)]TAB1
              --------------------------------------
              <continue with TAB2 structures for the rest of the
                    NMU emission cosines>
              --------------------------------------
              <continue with TAB2/TAB1 structures for the rest
                   of the NE incident energies>
              --------------------------------------
```

where f(μ,E,E′) is defined as in Eq. (6.1).

Emission cosine and secondary energy must be given in the laboratory system for LAW=7. Also, both variables must cover the entire angle-energy range open to the emitted particle.

6.3. Procedures

File 6 and incident charged particles are new for ENDF/B-VI, and it will take time for detailed procedures to evolve. The following comments are in tended to clarify some features of the format.

6.3.1. Elastic Scattering

For ENDF/B-VI, neutron elastic scattering is represented by giving a cross section in File 3, MT=2 (with resonance contributions in File 2) and an angular distribution in File 4, MT=2. This representation is compatible with previous versions of the ENDF format.

Charged-particle elastic scattering uses MF=3, MT=2, and MF=6, MT=2, but the cross section in File 3 is set equal to 1.0 at all energies represented using LTP=1 and LTP=2. For LTP=12 and LTP=14, File 3 must contain $\sigma_{NI}(E)$ in barns. The elastic File 6 uses LAW=5.

Whenever possible, the nuclear amplitude expansion should be used. Note that the a and b coefficients are not independent, being related by their mutual dependence on the nuclear scattering amplitudes, which are themselves constrained by unitarity and various conservation conditions. Thus, any attempt to fit data directly with expressions (6.13) or (6.14) would underdetermine the a's and b's, giving spurious values for them. The only feasible procedure is to fit the experimental data in terms of a direct parametrization of the nuclear scattering amplitudes (phase shifts, *etc.*) and extract the a and b coefficients from them.

The second representation (LTP=2) can be used when an approximate direct fit to the experimental data is desired. The simple pole approximation for the Coulomb amplitude implied by this representation becomes increasingly poor at lower energies and smaller angles. Since the deficiencies of the approximation are masked by the dominance of the Rutherford cross section in the same region, however, one could expect a reasonable representation of the net scattering cross section at all energies and angles, provided that the coefficients C_1 are determined by fitting data *excluding* the angular region where the Rutherford cross section is dominant.

Tabulated distributions (LTP=12 or 14) are also useful for direct fits to experimental data. In this case, the choice of the cutoff cosine is used to indicate the angular region where Rutherford scattering is dominant.

Figures 6.1 and 6.2 illustrate a typical cross section computed with amplitudes and the corresponding residual cross-section representation.

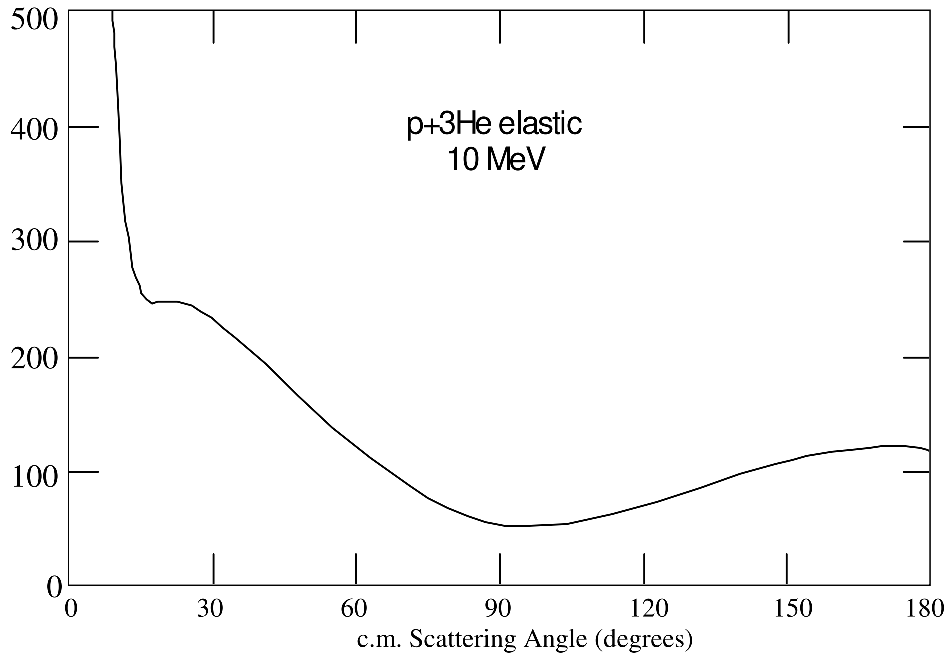

Figure 6.1
Example of Chargewd-Particle Elastic Scattering Cross Section

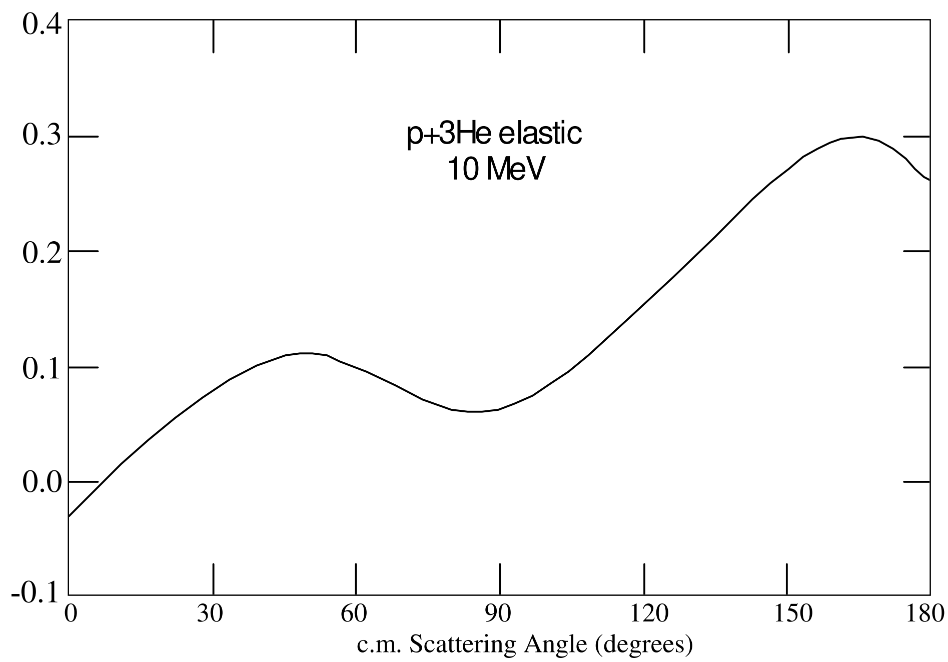

Figure 6.2
Example of Residual Cross Section for Elastic Scattering

6.3.2.Photons

Emitted photons are described using a subsection with ZAP=0. The spectrum is obtained as a sum of discrete photons (delta functions) and a continuum distribution packed into one LIST record. The discrete photons (if any) are given first. They are tabulated in order of decreasing energy, and their energy range may overlap the continuum. The continuum (if any) is given next, and the energies must be in increasing order. Corresponding-point or unit-base interpolation is applied separately to the discrete and continuum segments of the record. A separate angular distribution can be attached to each discrete photon or to each energy of a distribution, but the isotropic form (NA=0) is usually adequate.

For a two-body discrete-level reaction, all the discrete photons produced by cascades from the given level should be included under the same reaction (MT) so that the reaction explicitly conserves energy. This scheme also gives simple energy-independent yields and simple spectra. If the level structure is not known well enough to separate the contributions to the intensity of a particular photon by reaction, the photons can be lumped together in a summation MT with the restriction that energy be conserved for the sum of all reactions.

As an example, consider the typical level structure for the reaction A(i,p)R shown in Figure 6.3. Assume that the secondary protons are described by discrete levels in MT=600-603 and a continuum in MT=649. As many discrete photons as possible should be given with their associated direct level. Thus, the production of arising from direct excitation of the first level should be given in MT=601 (the yield will be 1.0 in the absence of internal conversion).

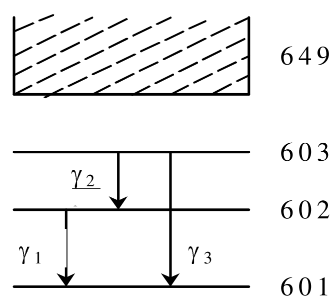

Figure 6.3
Typical Level Structure for Proton-Induced Photon Production

Photons (γ_1, γ_2, and γ_3) should be given in MT=602 using the simple constant yields computed from the branching factors and conversion ratios. This process should be continued until the knowledge of the cascades begins to get fuzzy. All the remaining production of γ_1, γ_2, γ_3, and all photons associated with higher levels (603 and 649 in this case), are then given in the redundant MT=103 using energy-dependent yields and a combination of discrete bins and a continuous distribution.

Photons produced during multi-body reactions should also be tabulated under the reaction MT number so that each reaction independently conserves energy when possible. If necessary, the photons can be lumped together under the redundant MT=3 as long as energy is conserved for the sum of all reactions.

6.3.3.Particles

Isotropic or low-order distributions are often sufficient for the charged particles emitted in continuum reactions because of their short ranges. The angular distributions of emitted neutrons may be needed in more detail because of their importance in shielding calculations.

Note that the angular distributions of identical particles must be symmetric in the CM system; this is true whether the identical particles are in the entrance channel or the exit channel. Symmetry is enforced by setting all odd Legendre components to zero, or by making $p_i(\mu) = p_i(-\mu)$.

6.3.4.Neutron Emission

It is important to represent the spectrum of emitted neutrons as realistically as possible due to their importance for shielding, activation, and fission. Small emission probabilities for low-energy neutrons may acquire increased importance due to the large cross sections at low energies. However, many modern evaluations are done with nuclear model codes that represent emission in energy bins (that is, histograms). Direct use of such calculations would severely distort the effects of emitted neutrons (although the representation would be reasonable for emitted charged particles). In such cases, the evaluator should fit a realistic evaporation shape to his low-energy neutron emission and use this shape to generate additional points for the energy distribution.

6.3.5.Recoil Distributions

The energy distribution of the recoil nucleus is needed to compute radiation damage and should be provided for structural materials whenever possible. Nuclear heating depends on the average recoil energy, and an average or full distribution should be provided for all isotopes that are used in reasonable concentrations in the common applications. All recoil information can be omitted for minor isotopes that only affect activation. Recoil angular distributions are rarely needed. Particle, photon, and recoil distributions taken together should conserve energy.

To enter only recoil average energy, use NEP=1 and ND=1; the recoil spectrum becomes a delta function at the average energy. Average energy must be entered even though it can be computed from the other distributions.

At high energies, it becomes difficult to represent the recoil distribution in the center-of-mass frame, even when that frame remains appropriate for the distribution of light particles ($A \leq 4$). In such cases, use LCT=3,[4] giving the light particles in the CM frame (normally with Kalbach systematics), and the heavy recoil energy spectrum as isotropic in the laboratory frame. Such isotropic distributions are normally adequate for representing energy deposition and damage.

6.3.6.Elements as Targets

Targets which are elements can be represented by using a ZA with A=0 as usual. An attempt should be made to tabulate every product of a reaction with an element.

[4] LCT=3 is only appropriate for LAW=1 and LANG≠2.

As an example, ^{nat}Fe(n,2n) will produce ^{53}Fe and ^{54}Fe in addition to more ^{56}Fe and ^{57}Fe. The product yields in File 6 can be converted to production or activation cross sections for each of these species without having recourse to isotopic evaluations. However, it would be difficult to give a recoil spectrum for each of these nuclei in full detail. Therefore, the evaluator is allowed to give a single total recoil spectrum with ZAP=ZA, where A=0. The yield should be 1.0 and AWP should be an appropriate average recoil mass. This subsection is redundant, and the user should be careful to avoid double counting.

6.3.7. CM versus LAB

Some energy-angle distributions show relatively sharp features (from levels) superimposed on a smoother continuum (see Figure 6.4). If such a distribution is given in the CM system, the position of these peaks in E′ is independent of the scattering angle as shown in Eq. (C.5). This helps assure that the angular distribution given for each E and E′ will be fairly simple. Further more, the E′ for a given sharp peak is a linear function of incident energy E, thus the corresponding-point or unit-base interpolation schemes can be set up to follow the peak exactly. Sharp lines can be represented as delta functions as described for photons, or a more realistic width and shape can be given in tabulated form.

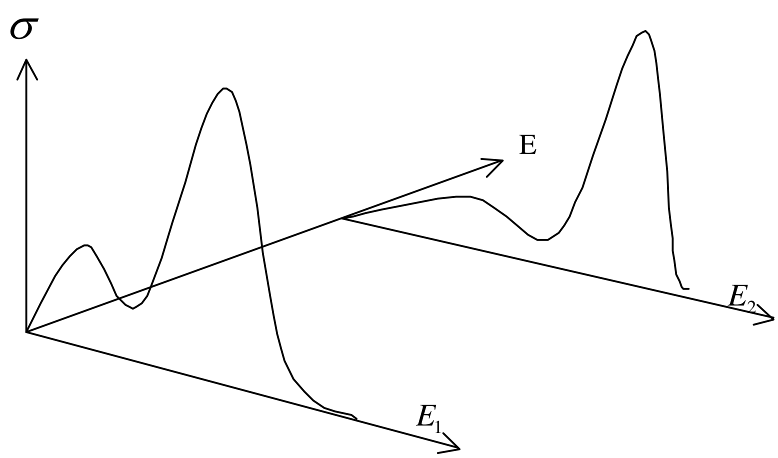

Figure 6.4
Typical Energy Spectrum Showing Levels on a Continuum

Therefore, the CM system should be used for representing secondary energy and scattering angle whenever relatively sharp features are found, even for reactions with three or more particles in the final state. The transformation to LAB coordinates is made by doing vector sums of the emitted particle CM velocities and the LAB velocity of the center of mass of the initial colliding system.

Experimental data are usually provided at fixed angles in the LAB system. It may often be difficult to convert the data to constant energies in the CM system as recommended by this format. However, transport calculations require data for the full range of angle and energy, and full ranges are required to get accurate values of the integrated cross sections from the experimental distributions. The most accurate way to do this process of interpolation and extrapolation is probably to model the distribution in the CM and adjust it to represent the LAB data. The numbers recommended for this format automatically arise from this process.

6.3.8. Phase Space

Comparison of experimental data with a phase-space prediction will often show overall qualitative agreement except for several broad or narrow peaks. It is desirable to represent those peaks using LAW=2 or 3. The remainder may be small enough to represent reasonably well with one of the phase-space laws.

In the absence of complete experimental data, it is recommended that the evaluator supply a phase-space distribution. This assures that energy will be conserved and gives reasonable kinematic limits on energy and angle in the laboratory system. Later comparisons between the evaluation and data may indicate possible improvements in the evaluation.

REFERENCES

1. C. Kalbach and F. M. Mann, *Phenomenology of continuous angular distributions. I. Systematics and parametrization*, ***Phys. Rev. C*** **23** (1981) 112
2. C. Kalbach, *Systematics of Continuum Angular Distributions: Extensions to Higher Energies*, ***Phys. Rev. C*** **37** (1988) 2350