12. FILE 12. PHOTON PRODUCTION MULTIPLICITIES AND TRANSITION PROBABILITY ARRAYS

File 12 can be used to represent the neutron energy dependence of photon production cross sections by means of either multiplicities or transition probability arrays. Both methods rely upon processing codes that use neutron cross sections from File 2 and/or File 3 to generate absolute photon production cross sections.

Multiplicities can be used to represent the cross sections of discrete photons and/or the integrated cross sections of continuous photon spectra. The MT numbers in File 12 designate the particular neutron cross sections (File 2 and/or File 3) to which the multiplicities are referred. The use of multiplicities is the recommended method of presenting (n,γ) capture γ-ray cross sections, provided, of course, that the (n,γ) cross section is adequately represented in File 2 and/or File 3.

For well-established level decay schemes, the use of transition probability arrays offers a concise method for presenting (n,xγ) information. With this method, the actual decay scheme of the residual nucleus for a particular reaction (defined by MT number) is entered in File 12. This information can then be used by a processing code together with discrete level excitation cross sections from File 3 to calculate discrete γ-ray production cross sections. This option cannot be used to represent the integrals of continuous photon spectra.

12.1. Formats

Each section of File 12 gives information for a particular reaction type (MT number), either as multiplicities (LO=1) or as transition probability arrays (LO=2). Each section always starts with a HEAD record and ends with a SEND record.

12.1.1. Option 1 (LO=1): Multiplicities

The neutron energy dependence of photon production cross section is represented by tabulating a set of neutron energy and multiplicity pairs $\{E,y_k(E)\}$ for each discrete photon and for the photon energy continuum[1]. The subscript k designates a particular discrete photon or a photon continuum, and the total number of such sets is represented by NK.

The multiplicity or yield $y_k(E)$ is defined by

$$y_k(E) = \frac{\sigma_k^{\gamma}}{\sigma(E)} \quad \text{(photons)} \tag{12.1}$$

where E designates neutron energy and σ(E) is the neutron cross section in File 2 and/or File 3 to which the multiplicity is referred (by the MT number). For discrete photons, $\sigma_k^{\gamma}(E)$ is the photon production cross section for the discrete photon designated by k. For photon continua, $\sigma_k^{\gamma}(E)$ is the cross section for the photon continuum integrated over photon energy.

In the continuum case,

$$\begin{aligned} y_k(E) &= \frac{\sigma_k^{\gamma}(E)}{\sigma(E)} = \frac{\int \frac{d\sigma_k^{\gamma}}{dE_{\gamma}}\left(E_{\gamma} \leftarrow E\right) dE_{\gamma}}{\sigma(E)} \\ &= \frac{\int \sigma(E)\, y_k\left(E_{\gamma} \leftarrow E\right) dE_{\gamma}}{\sigma(E\ )} = \int_0^{E_{\gamma}^{\max}} y_k\left(E_{\gamma} \leftarrow E\right) dE_{\gamma} \end{aligned} \tag{12.2}$$

[1] There should be no more than one energy continuum for each MT number used. If the decomposition of a continuum into several parts is desired, this can be accomplished in File 15.

where E_γ designates photon energy (eV),

$$\frac{d\sigma_k^\gamma}{E_\gamma}(E_\gamma \leftarrow E)$$

is the absolute photon energy distribution in barns/eV, and $y_k(E_\gamma \leftarrow E)$ is the relative energy distribution in photons/eV. The quantity $y_k(E_\gamma \leftarrow E)$ can be broken down further as

$$y_k(E_\gamma \leftarrow E) = y_k(E) f_k(E_\gamma \leftarrow E) \quad ,$$

which results in the requirements that

$$\int_0^{E_\gamma^{\max}} f_k(E_\gamma \leftarrow E)\, dE_\gamma = 1$$

Any time a continuum representation is used for a given MT number in either File 12 or 13, then the normalized energy distribution $f_k(E_\gamma \leftarrow E)$ must be given in File 15 under the same MT number.

As a check quantity, the total yield NK

$$Y(E) = \sum_{k=1}^{NK} y_k(E) \qquad \text{(photons)}$$

is also tabulated for each MT number if NK>1.

The structure of a section for LO=1 is

```
[MAT, 12, MT/  ZA, AWR, LO,  0, NK,  0] HEAD                    (LO=1)
[MAT, 12, MT/ 0.0, 0.0,  0,  0, NR, NP/ Eint / Y(E)] TAB1 [2]
          <subsection for k =1>
          <subsection for k=2>
                    ......
                    ......
          <subsection for k=NK>
[MAT, 12,  0/ 0.0, 0.0,  0,  0,  0,  0] SEND ,
```

and the structure of each subsection is

```
[MAT, 12, MT/ EGk,  ESk, LP, LF, NR, NP/ Eint / yk(E)] TAB1,
```

where

NK = number of discrete photons including the continuum.

ES_k = energy of the level from which the photon originates. If the level is unknown or if a continuous photon spectrum is produced, then $ES_k \equiv 0.0$ should be used.

EG_k = photon energy for LP=0 or 1 or Binding Energy for LP=2. For a continuous photon energy distribution, $EG_k \equiv 0.0$ should be used.

LP = indicator of whether or not the particular photon is a primary:

LP=0, origin of photons is not designated or not known, and the photon energy is EG_k;

LP=1, for non-primary photons where the photon energy is again simply EG_k;

LP=2, for primary photons where the photon energy EG_k' is given by

$$EG_k' = EG_k + \frac{AWR}{AWR+1} E_n \ .$$

[2] If the total number of discrete photons and photon continua is one (NK=1), this TAB1 record is omitted.

LF = the photon energy distribution law number, which presently has only two values defined:

LF=1, a normalized tabulated function (in File 15), and
LF=2, a discrete photon energy.

12.1.2. Option 2 (LO=2): Transition Probability Arrays

With this option, the only data required are the level energies, de-excitation transition probabilities, and (where necessary) conditional photon emission probabilities. Given this information, the photon energies and their multiplicities can readily be calculated. Photon production cross sections can then be computed for any given level from the excitation cross sections in File 3, along with the transition probability array. Similarly, multiplicities and photon production cross sections can be constructed for the total cascade. For any given level, the transition and photon emission probability data given in the section are for photons originating at that level only; any further cascading is determined from the data for the lower levels.

Now define the following variables.

LG LG=1, simple case (all transitions are γ emission).
LG=2, complex case (internal conversion or other competing processes occur).

NS Number of levels below the present one, including the ground state. (The present level is also uniquely defined by the MT number and by its energy level).

NT Number of transitions for which data are given in a list to follow (*i.e.*, number of nonzero transition probabilities), NT≤NS.

ES_i Energy of the i^{th} level, i=0,1,2... NS.
ES ≡ 0.0, ground state

TP_i $TP_{NS,i}$, probability of a direct transition from level NS to level i, i=0,1,2... (NS-1).

GP_i $GP_{NS,i}$, the probability that, given a transition from level NS to level i, the transition is a photon transition (*i.e.*, the conditional probability of photon emission).

B_i Array of NT doublets or triplets depending on LG value.

Note that each level can be identified by its NS number. Then the energy of a photon from a transition to level i is given by $E_\gamma = ES_{NS} - ES_i$, and its multiplicity is given by $y(E_\gamma \leftarrow E) = (TP_i)(GP_i)$. It is implicitly assumed that the transition probability array is independent of incident neutron energy.

The structure of a section for LO=2 is

```
[MAT, 12, MT/   ZA, AWR,  LO,  LG,        NS,     0] HEAD        (LO=2)
[MAT, 12, MT/ ESNS, 0.0,  LP,   0,(LG+1)*NT, NT/B] LIST
[MAT, 12,  0/ 0.0, 0.0,   0,    0,         0,     0] SEND
```

If LG=1, the array B_i consists of NT doublets $\{ES_i,TP_i\}$; if LG=2, it consists of NT triplets $\{ES_i,TP_i,GP_i\}$. Here the subscript i is a running index over the levels below the level for which the transition probability array is being given (*i.e.*, below level NS). The doublets or triplets are given in decreasing magnitude of energy ES_i.

12.2. Procedures

1. Under Option 1, the subsections are given in decreasing magnitude of EG_k.
2. Under Option 1, the convention is that the subsection for the continuum photons, if present, is last. In this case, the last value of EG_k (EG_{NK}) is set equal to 0.0, and logical consistency with Procedure 1 is maintained.
3. Under Option 1, the values of EG_k should be consistent to within four significant figures with the corresponding EG_k values for the File 14 photon angular distributions. This allows processing and "physics" checking codes to match photon yields with the corresponding angular distributions.
4. Under Option 1, ES_k is the energy of the level from which the photon originates. If ES_k is unknown or not meaningful (as for the continuous photon spectrum), the value 0.0 should be entered.
5. If capture and fission resonance parameters are given in File 2, photon production for these reactions should be given by using Option 1 of File 12, instead of using photon production cross sections in File 13. This is due to the voluminous data required to represent the resonance structure in File 13 and the difficulty of calculating multigroup photon production matrices from such data.
6. Under Option 1, the total yield table, Y(E), should exactly span the same energy range as the combined energy range of all the $y_k(E)$. Within that range,

$$Y(E) = \sum_{k=1}^{NK} y_k(E)$$

   should hold within four significant figures.
7. The excitation cross sections for all the levels appearing in the transition probability arrays must, of course, be given in File 3.
8. The join of all sections, regardless of the option used, should represent the photon production data, with no redundancy. For example, MT=4 cannot include any photons given elsewhere under MT=51 through 91. Likewise, there can be no redundancy between Files 12 and 13.
9. If only one energy distribution is given under Option 1 (NK=1), the TAB1 record for the Y(E) table is deleted to avoid repetitive entries.
10. Data should not be given in File 12 for reaction types that do not appear in Files 2 and/or 3.
11. Under Option 2, the level energies, ES_i, in the transition probability arrays are given in decreasing magnitude.
12. The MT numbers for which transition probability data are given should be for consecutive levels, beginning at the first level, with no embedded levels omitted.
13. The energies of photons arising from level transitions should be consistent within four significant figures with the corresponding EG_k values in File 14. Therefore, care must be taken to specify level energies to the appropriate number of significant figures.

14. Under Option 2, the sum of the transition probabilities (TP_i) over i should equal 1.0000 (that is, should be unity to within five significant figures).

15. The limit on the number of energy points in any tabulations of Y(E) or $y_k(E)$ is 1000. This is an upper limit that will rarely be approached in practice because yields are normally smoothly varying functions of incident neutron energy.

16. The limit on the number of interpolation regions is 10.

17. Tabulations of non-threshold data should normally cover at least the energy range 10^{-5} eV $\leq E \leq 2\times10^7$ eV, where practical. Threshold data should be given from threshold energy up to 2×10^7 eV, where practical.

18. Transition Probability Arrays for (n,n′γ) photons.

    a. The use of transition probability arrays (File 12, LO=2) is a convenient way to represent a portion of the γ-rays produced by de-excitation of discrete levels populated by (n,n′γ) and other reactions.

    b. Several conditions must be met before this representation can be used. Level excitation cross sections (given in File 3 as MT=51,...) must be given from threshold energies up to the same maximum energy (no exceptions). Decay properties of all n levels must be known. The information given in File 12 must be consistent with data given in File 3.

    c. Usually, not all the conditions can be met. Part of the problem is the recommendation that level excitation cross sections for the first few levels be given for neutron energies up to 20 MeV. It is seldom that all level data can be given for neutron energies up to 15 MeV.