Dunn, Michael E.

From: Andrej Trkov [Andrej.Trkov@ijs.si]
Sent: Friday, October 12, 2007 5:01 PM
To: Dunn, Michael E.
Subject: Definition of "stable nuclide" for cumulative yields

Mike,

Another item has been raised at the WPEC meeting related to the definition of "stable nuclides" in constructing the cumulative yields.

Comparing the cumulative yields between JEFF-3.1 and other labraries, very large differences for some nuclides are observed. Such an analysis was done by Liu Tingjin within the scope of the Th-U CRP of the IAEA. It turned out that the reson for the differences is in the definitions. There exist nuclides with extremely long half-lives. If a formalistic approach is adopted, cumulative yields should include all precursors, even if their half-lives are longer that 10**10 years. From a practical point this is nonsense, but the question is, where to draw the line. The JEFF evaluator placed it at some practical limit applicable to waste disposal studies.
Other evaluators assumed a higher limit, and hence the differences.

The ENDF manual should contain a recommendation to the evaluators that would unify the definition of cumulative yields in different libraries.
Please discuss the issue at CSEWG and provide a recommendation to be entered into the ENDF manual.

Best regards, Andrej

--
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Dunn, Michael E.

From: Andrej Trkov [Andrej.Trkov@ijs.si]
Sent: Thursday, October 25, 2007 2:02 PM
To: Dunn, Michael E.
Subject: [Fwd: Re: Definition of "stable nuclides" for cumulative yields]

Mike,

I'm forwarding the e-mail from Robert Mills.

What is required for ENDF-6 is to define the cutoff half-life in the ENDF-6 manual so that all evaluators would use the same value.

An alternative would be to enter the cutoff half-life as a parameter in the dataset for cumulative yields in MF8/MT459.

Best regards, Andrej

---------- Original Message ----------
Subject: Re: Definition of "stable nuclides" for cumulative yields
From: robert.w.mills@nexiasolutions.com
Date: Wed, October 24, 2007 11:22 am
To: Andrej.Trkov@ijs.si
Cc: colin.h.zimmerman@nexiasolutions.com
daniel.p.mathers@nexiasolutions.com

Dear Andrej,

The cutoff half-life I used in the JEF-2.2 and JEFF-3 files was 1E13 seconds (317 thousand years). This was chosen as the lowest power of 10 seconds that removed all long lived alpha decaying fission products. The following is a section of a 1995 report that describes what I did.

> Chain yields can be calculated simply by summing the cumulative yields of all stable nuclides within each mass chain (this allows for cases where there are several stable nuclei in a particular mass chain). It must be noted, however, that several fission products exist that a decay; these have half-lives of greater than one million years. If this type of decay is incorporated into the calculation it will subtract a certain fraction from the chain yield for the parent mass and add to the mass chain four masses below. In practice, however, no yield measurement will observed this transfer of yield due to the human time-scales of the experiment.
>
> The JEF2.2 file contains 36 fission products with half-lives greater than one thousand years and fifteen greater than 1010 years. Of the fission products with half-lives greater than one hour just eight decay to different mass chains, in all cases by a emission. These are listed in table below:
>
> Fission product nuclides with half-lives greater than a one hour which a decay.

Nuclide	Half-life /years
58-Ce-142	4.99658E+16
60-Nd-144	2.09858E+15
62-Sm-146	1.03002E+08

62-Sm-147	1.05927E+11
62-Sm-148	6.97138E+15
62-Sm-149	2.00003E+15
64-Gd-150	1.79003E+06
64-Gd-152	1.07926E+14

Thus the decision was taken in the UKFY evaluations, in view of the very long half-lives that the alpha branches of these nuclides should be ignored in the calculation of cumulative and chain yields. To simpify processing, this was implemented by assuming nuclides with half-lives greater than 1013 seconds were stable. It should be noted that in very long term calculations of these few nuclides and their daughter products cumulative yields cannot be used in simple calculations. For calculation involving these nuclides the independent yields must be used with a full solution of the full radioactive decay equations. These calculations are usually carried out by a computer code such as FISPIN or ORIGEN. This is not regarded as a significant problem given the small number of cases and the extremely long half-lives.

On another issue in the current manual, on page 8.4, there is a reference to interpolation rules being given in appendix E. It appears this should reference section 0.6.2 on page 0.21 to 0.26.

Do you want me be draft a revised section of 8.2?

Best Regards,
Robert

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"Andrej Trkov" <Andrej.Trkov@ijs.si> wrote on 12/10/2007 20:31:42:

> Robert,

> The CSEWG meeting is approaching and this is the right time to come up
> with format proposals for ENDF-6.

> There are differences in cumulative yields in different libraries that
> originate from the definition. What cutoff half-life would you like to
> have in the format specifications to define cumulative yields, in
> order
to
> avoid similar problems in the future.

> Best regards, Andrej
> --
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--
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8. FILE 8, RADIOACTIVE DECAY AND FISSION PRODUCT YIELD DATA

Information concerning the decay of the reaction products (any MT) is given in this file. In addition, fission product yield data (MT=454 and 459) for fissionable materials (see Section 8.2) and spontaneous radioactive decay data (MT=457) for the nucleus (see Section 8.3) are included. See descriptions of File 9 and File 10 for information on isomeric state production from the various reactions. Since a reaction may result in more than one unstable end product, data for the most important product should be entered, while others are allowed.

8.1. Radioactive Nuclide Production

For any isotope, sections may be given which specify that the end product from the interaction of any incident particle or photon is radioactive. Information is given for any MT by identifying the end products in the reaction by their ZAP (ZA for the product), and noting how these end products decay. A section will contain only minimal information about the chain that follows each reaction. One or more isomeric states of the target or the radioactive end product isotope will be described.

The following quantities are defined:

ZA Designation of the original nuclide (ZA = 1000Z + A).

ZAP Designation of the nuclide produced in the reaction (ZAP = 1000Z + A).

MATP Material number for the reaction product (ZAP).

NS Total number of states (LFS) of the radioactive reaction product for which decay data are given.

LMF File number (3, 6, 9, or 10) in which the multiplicity or cross section for this MT number will be found.

LIS State number (including ground and all levels) of the target (ZA).

LISO Isomeric state number of the target.

LFS Level number (including ground and all levels) of the state of ZAP formed by the neutron interaction (to be given in ascending order).

ELFS Excitation energy of the state of ZAP produced in the interaction (in eV above ground state).

NO Flag denoting where the decay information is to be given for an important radioactive end product.
NO = 0, complete decay chain given under this MT.
NO = 1, decay chain given in MT = 457 in MATP.

ND Number of branches into which the nuclide ZAP decays.

HL Half-life of the nuclide ZAP in seconds.

ZAN Z and mass identifier of the next nuclide produced along the chain.

BR Branching ratio for the production of that particular ZAN and level.

END End-point energy of the particle or quantum emitted (this does not include the gamma energy, following beta decay, for example).

CT Chain terminator that gives minimal information about the formation and decay of ZAN. The hundredths digit of CT designates the excited level in which ZAN is formed.
$1.0 \leq CT < 2.0$ indicates that the chain terminates with ZAN, possibly after one or more gamma decays.
$CT \geq 2.0$ indicates that ZAN is unstable and decays further to other nuclides. For example, consider the nuclide (ZAP) formed via a neutron reaction (MT number) in a final state (LFS number); ZAP then decays to a level in ZAN; the

level number is part of the CT indicator and includes non-isomeric states in the count.

The following examples may help explain the use of CT:

CT = 1.00, ZAN was formed in the ground state which is stable.

CT = 1.06, ZAN was formed in the sixth excited state; the sixth state decayed to the ground state which is stable.

CT = 2.00, ZAN was formed in the ground state which is unstable. (No delayed gammas are associated with the formation and decay of this particular ZAN). The next decay in the chain is specified under the RTYP.

CT = 2.11, ZAN was formed in the 11th excited state but the chain does not terminate with that ZAN. The next decay in the chain is specified under the RTYP.

It is readily apparent from the above that CT = "1." indicates that the chain terminates with that particular ZAN and CT = "2." means that one or more decays are involved before stability is reached. Note, however, that stability can be reached ***instantaneously*** upon occasion with the emission of one or more light particles.

RTYP Mode of decay using the same definitions specified in MT=457 (see Section 8.3).

As an example, consider MT=102. Then RTYP = 1.44 would be interpreted as follows:

The first two columns of the RTYP (1.) indicates β^- decay of ZAP; the third and fourth columns (44) indicate that the nucleus ZAN (formed in the β^- decay) then immediately emits two α particles.

This example is represented by the following reaction:

$n + {}^{7}Li \rightarrow \gamma + {}^{8}Li$ (ground state)

β^- (MT=102)

↘

$\underline{2.94\ 2^{+},0}$

^{8}Be

↘

2α

For this example:

$ZA({}^{7}Li) = 3.007E+03$ $LIS({}^{7}Li) = 0$ $LISO({}^{7}Li) = 0$

$ZAP({}^{8}Li) = 3.008E+03$ $LFS({}^{8}Li) = 0$

$ZAN({}^{8}Be) = 4.008E+03$ $CT({}^{8}Be) = 2.01$

Since Be has a half-life of the order of compound-nucleus formation times, decay data for MT = 457 are not required, and the complete chain can easily be represented and read from the information given here.

8.1.1. Formats

The structure of each section always starts with a HEAD record and ends with a SEND record. Subsections contain data for a particular final state of the reaction product (LFS).

The number of subsections NS is given on the HEAD record for the section. The subsections are ordered by increasing value of LFS.

The structure of a section is:

```
[MAT, 8, MT/  ZA,  AWR,  LIS, LISO,   NS,   NO] HEAD
                <subsection for LFS1>
                <subsection for LFS2>
             ---------------------------------
                <subsection for LFSNS>
[MAT, 8,  0/ 0.0,  0.0,    0,    0,    0,    0] SEND
For NO=0 the structure of the subsection is:
[MAT, 8, MT/ ZAP, ELFS,  LMF, LFS,  6*ND, MATP/
           HL1, RTYP1, ZAN1,  BR1,   END1,  CT1,
           HL2, RTYP2, ZAN2,  BR2,   END2,  CT2,
           --------------------------------
           HLND,RTYPND, ZANND, BRND,  ENDND,  CTND] LIST
```

If NO=1, then the reaction gives rise to a significant product which is radioactive, and the evaluator wishes only to identify the radioactive product. The evaluator must supply MF=8, MT=457 data elsewhere to describe the decay of the product. It is understood that the cross section for producing this radioactive product can be determined from the data in File 3, 6, 9, or 10 depending upon the value of LMF.

For NO=1, the structure of the subsection is:

```
[MAT, 8, MT/  ZAP, ELFS,  LMF,  LFS,   0,  MATP] CONT
```

8.1.2. Procedures

1. Data should be given for all ***unstable*** states of the reaction product nucleus for which cross sections are given in File 3 or File 10 or multiplicities in File 6 or File 9. No information of this type is allowed in evaluations for mixtures of elements, molecules, or elements with more than one naturally occurring isotope.
2. In order to provide more general usefulness as these files are being constructed, the following procedures are mandatory. For each reaction type (MT), File 6 yields, File 9 multiplicities, or File 10 cross sections must be provided, except when LMF=3.
3. If the ENDF/B file also contains a complete evaluation of the neutron cross sections for the reaction product nucleus (ZAP, LIS), then the radioactive decay data for the evaluation of (ZAP, LIS) found in MF=8, MT=457 must be consistent with the decay data in this section.
4. The method for calculating the nuclide production cross section is determined by the choice of LMF:
   - LMF = 3 implies that the production cross section is taken directly from the corresponding sections in File 3.
   - LMF = 6 implies that the production cross section is the product of the cross section in File 3 and the yield in File 6.
   - LMF = 9 implies that the production cross section is the product of the cross section in File 3 and the multiplicity in File 9.

   LMF = 10 implies that the production cross section is given explicitly in File 10 (in barns).

8.2. Fission Product Yield Data (MT = 454 and MT = 459)

MT numbers 454 and 459 specify the energy-dependent fission product yield data for each incident particle or photon. These MT numbers can also be used to identify yields for spontaneous fission. A complete set of fission product yield data is given for a particular incident neutron energy. Data sets should be given at sufficient incident energies to completely specify yield data for the energy range given for the fission cross section (as determined from Files 2 or 3). These data are given by specifying fission product identifiers and fission product yields.

MT=454 is used for independent yields (YI), and MT=459 is used for cumulative yields (YC). The formats for MT=454 and MT=459 are identical. Independent yields (YI) are direct yields per fission prior to delayed neutron, beta, *etc.*, decay. The sum of all independent yields is 2.0 for any particular incident neutron energy. Cumulative yields (YC) are specified for the same set of fission products. These account for all decay branches, including delayed neutrons.

The fission products are specified by giving an excited state designation (FPS) and a (charge, mass) identifier (ZAFP). Thus, fission product nuclides are given, not mass chains. More than one (Z,A) may be used to represent the yields for a particular mass chain.

The following quantities are defined

NFP Number of fission product nuclide states to be specified at each incident energy point (this is actually the number of sets of fission product identifiers - fission product yields). (NFP≤2500).

ZAFP (Z,A) identifier for a particular fission product. (ZAFP = (1000Z + A).

FPS State designator (floating-point number) for the fission product nuclide (FPS = 0.0 means the ground state, FPS = 1.0 means the first excited state, *etc.*)

YI (MT=454), independent yield for a particular fission product prior to particle decay.

DYI (MT=454) 1σ uncertainty in YI.

YC (MT=459) cumulative yield.

DYC (MT=459) 1σ uncertainty in YC.

$C_n(E_i)$ Array of yield data for the i^{th} energy point. This array contains NFP sets of four parameters in the order ZAFP, FPS, YI, and DYI in MT=454 and ZAFP, FPS, YC, and DYC in MT=459.

NN Number of items in the $C_n(E_i)$ array, equal to 4*NFP.

E_i Incident neutron energy of the i^{th} point (eV).

LE Test to determine whether energy-dependent fission product yields given:

LE = 0, implies no energy-dependence (only one set of fission product yield data given);

LE > 0, indicates that (LE + 1) sets of fission product yield data are given at (LE + 1) incident neutron energies.

I_i Interpolation scheme (see Appendix E) to be used between the E_{i-1} and E_i energy points.

8.2.1. Formats

The structure of a section always starts with a HEAD record and ends with a SEND record. Sets of fission product yield data are given for one or more incident energies. The sets are ordered by increasing incident energy. For a particular energy the data are presented by giving four parameters (ZAFP, FPS, YI, and DYI in MT=454 and ZAFP, FPS, YC, and DYC in MT 459) for each fission product state. The data are first ordered by increasing values of ZAFP. If more than one yield is given for the same (Z,A) the data are ordered by increasing value of the state designator (FPS).

The structure for a section is

```
[MAT, 8, MT/ ZA,  AWR, LE+1,    0,  0,    0] HEAD
[MAT, 8, MT/  E1, 0.0,   LE,    0, NN, NFP/ Cn(E1) ] LIST
[MAT, 8, MT/  E2, 0.0,    I,    0, NN, NFP/ Cn(E2) ] LIST
[MAT, 8, MT/  E3, 0.0,    I,    0, NN, NFP/ Cn(E3) ] LIST
             ------------------------
[MAT, 8, 0 / 0.0, 0.0,    0,    0,  0,    0] SEND
```

where MT = 454 for independent yield data, and MT = 459 for cumulative yield data. There are (LE + 1) LIST records.

8.2.2. Procedures

The data sets for fission product yields should be given over the same energy range as that used in Files 2 and/or File 3 for the fission cross section. The yields are given as a fractional value at each energy, and normally the independent yields will sum to 2.0.

This format provides for the yields (YI or YC) to each excited state (FPS) of the nuclide designated by ZAFP, and hence accommodates the many metastable fission products having direct fission yields. Data may be given for one or more fission product nuclide states to represent the yield for a particular mass chain. If independent yield data are given for more than one nuclide, the yield for the lowest Z (charge) nuclide state for a particular mass chain should be the same as the cumulative yield in MT=459, and all other independent yields for this same chain should be direct yields.

The direct fission product yields are those prior to delayed neutron emission; for this reason, the summation of independent yields over the nuclides in each mass chain does ***not*** necessarily equal the isobaric chain yield. The cumulative yield for each nuclide (ZAFP, FPS) can be determined by use of the branching fractions in MT=457 or directly from MT=459.

Yields for the same fission product nuclides should be given at each energy point. This will facilitate interpolation of yield data between incident energy points. Also, a linear-linear interpolation scheme should be used.

8.3. Radioactive Decay Data (MT=457)

The spontaneous radioactive decay data are given in Section 457. This section is restricted to single nuclides in their ground state or an isomeric state. (An isomeric state is a "long-lived" excited state of the nucleus.) The main purpose of MT=457 is to describe the energy spectra resulting from radioactive decay and give average parameters useful for applications such as decay heat, waste disposal, depletion and buildup studies, shielding, and fuel integrity. The information in this section can be divided into three parts:

a. General information about the material

ZA	Designation of the original (radioactive) nuclide (=1000Z+A).
AWR	Ratio of the LIS state nuclide mass to that of neutron.
LIS	State of the original nuclide (LIS=0, ground state, LIS=1, first excited state, *etc*.)
LISO	Isomeric state number for the original nuclide (LISO=0, ground state; LISO=1, first isomeric state; *etc*.)
NST	Nucleus stability flag (NST=0, radioactive; NST=1, stable)
$T_{1/2}$	Half-life of the original nuclide (seconds).
NC	Total number of decay energies (eV) given (NC = 3 or 17).
$E_{"x"}$	Average decay energy (eV) of "x" radiation, ***e.g.***, for decay heat applications. The average energies must be given in an order specified in Section 8.3.2. Unknown average radiation energies are indicated by a value of –1.0.
SPI	Spin of the nuclide in its LIS state. (SPI = –77.777 = spin unknown)
PAR	Parity of the nuclide in its LIS state (±1.0).

b. Decay mode information - for each mode of decay

NDK	Total number of decay modes given (cannot be zero).
RTYP	Mode of decay of the nuclide in its LIS state.

Decay modes defined:

RTYP	**Decay Mode**	
0. γ	γ-ray (not used in MT457)	
1.	β^-	Beta decay
2.	e.c., (β^+)	Electron capture and/or positron emission
3.	IT	Isomeric transition (will in general be present only when the state being considered is an isomeric state)
4.	α	Alpha decay
5.	n	Neutron emission (***not*** *delayed neutron decay*, below)
6.	SF	Spontaneous fission
7.	p	Proton emission
10.	-	Unknown origin

Multiple particle decay is also allowed using any combination of the above RTYP variables as illustrated in the following examples:

RTYP	**Decay Mode**	
1.5	β^-,n	Beta decay followed by neutron emission (*delayed neutron decay*)
1.4	β^-,α	Beta decay followed by alpha emission (^{16}N decay)
2.4	β^+,α	Positron decay followed by alpha emission.

RFS Isomeric state flag for daughter nuclide.
RFS=0.0, ground state;
RFS=1.0, first isomeric state, *etc*.

Q Total decay energy (eV) available in the corresponding decay process. This is not necessarily the same as the maximum energy of the emitted radiation. In the case of an isomeric transition Q will be the energy of the isomeric state. For both β^+ and β^-, Q equals the energy corresponding to the mass difference between the initial and final atoms).

BR Fraction of the decay of the nuclide in its LIS state which proceeds by the corresponding decay mode, *e.g.*, if only β^- occurs and no isomeric states in the daughter nucleus are excited then BR = 1.0 for β^- decay.

c. Resulting radiation spectra

NSP Total number of radiation types (STYP) for which spectral information is given (NSP may be zero).

STYP Decay radiation type
Decay radiations defined:

STYP	Radiation type	
0.	γ	Gamma rays
l.	β^-	Beta rays
2.	e.c., (β^+)	Electron capture and/or positron emission
4.	α	Alpha particles
5.	n	Neutrons
6.	SF	Spontaneous fission fragments
7.	p	Protons
8.	e^-	"Discrete electrons"
9.	x	X-rays and annihilation radiation (photons not arising as transitions between nuclear states)

ER discrete energy (eV) of radiation produced(E_γ,$E_{\beta\text{-}}$,$E_{e.c.}$,*etc*.)

RI intensity of discrete radiation produced (relative units).

RP spectrum of the continuum component of the radiation in units of probability/eV such that $\int RP(E)dE = 1$.

TYPE Type of transition for beta and electron capture.
Types Defined:

TYPE	Spectrum Definition
0.0	not required for STYP
1.0	allowed, non-unique
2.0	First-forbidden unique
3.0	Second-forbidden unique

RICC Total internal conversion coefficient (STYP=0.0 only)

RICK K-shell internal conversion coefficient (STYP=0.0 only)

RICL L-shell internal conversion coefficient (STYP=0.0 only)

RIS	Internal pair formation coefficient (STYP=0.0) STYP=2.0, positron intensity, STYP=0.0 otherwise.
LCON	[1]Continuum spectrum flag LCON = 0, no continuous spectrum given LCON = 1, only continuous spectrum given LCON = 2, both discrete and continuum spectra.
NT	Number of entries given for each discrete energy (ER).
FC	[1]Continuum spectrum normalization factor (absolute intensity/relative intensity).
FD	[1]Discrete spectrum normalization factor (absolute intensity/relative intensity).
NER	Total number of tabulated discrete energies for a given spectral type (STYP).
ER_{AV}	[2]Average decay energy of radiation produced.
NR	Number of interpolation ranges for the continuum spectrum.
NP	Number of points at which the distribution will be given.
E_{int}	Interpolation scheme for the continuum spectrum.
NK	Number of partial energy distributions when LCON = 5 is used.
Δ	Uncertainty in any quantity.
LCOV	Flag indicating whether covariance data are given for continuum spectrum data. (LCON = 1 or 2). LCOV=0, no covariance data given LCOV=1, covariance data given
LB	Flag indicating the meaning of the numbers given in the array $\{E_k,F_k\}$. (Only LB=2 presently allowed, See chapter 33).
NPP	Number of pairs of numbers in the $\{E_k,F_k\}$ array.

$\{E_k,F_k\}$ is an array of pairs of numbers, referred to as an E_k table. In each E_k table the first member of a pair is an energy, E_k, the second member of the pair, F_k, is a number associated with the energy interval between the two entries E_k and E_{k+1}.

The E_k table must cover the complete range of secondary particle energies. Some of the F_k's may be zero, as must be the case below threshold for a threshold reaction, and the last value of F in an E table must be zero or blank since it is not defined.

The meaning of the F_k values in the E_k table for the allowed LB=2 is as follows:

LB=2 Fractional components fully correlated over all E_k intervals

$$\mathrm{COV}(X_i, X_j) = \sum_{kk'} S_i^k S_j^{k'} F_k F_{k'} X_i X_j$$

where S_i^k = 1 when the energy E_i is in the interval E_k to E_{k+1} of the E_k table
= 0 otherwise

Here X_i is the normalized spectral intensity at decay particle emitted kinetic energy range E_i obtained from the {E,RP} TAB1 record indicated.

[1] Spontaneous _v for RTYP = 6. and STYP = 5., LCON = 1 and FC = $\_v_p$ and FD = $\_v_d$.

[2] For STYP = 2, this is the average positron energy, for STYP = 4, this includes energy of recoil nucleus.

8.3.1. Formats

The structure of this section always starts with a HEAD record and ends with a SEND record.

For a radioactive nucleus (NST=0), this section is divided into subsections as follows:

```
[MAT, 8,457/    ZA,    AWR, LIS, LISO,    NST,  NSP] HEAD   (NST=0)
[MAT, 8,457/   T1/2,  ΔT1/2,   0,    0,  2*NC,    0/ (E"x",ΔE"x")[3] / LIST
[MAT, 8,457/   SPI,    PAR,   0,    0, 6*NDK,  NDK/
             RTYP1,   RFS1,   Q1,  ΔQ1,    BR1, ΔBR1,
            ---------------------------------
            RTYPNDK, RFSNDK,  QNDK, ΔQNDK, BRNDK,ΔBRNDK] LIST
                <Subsection for Spectrum1>
                <Subsection for Spectrum2>
            ---------------------------------
                <Subsection for SpectrumNSP>
[MAT, 8,  0/   0.0,   0.0,   0,    0,     0,    0] SEND
```

The structure of a subsection is:

```
[MAT, 8,457/   0.0, STYP,   LCON,    0,     6,   NER/
                FD,   ΔFD,   ERAV, ΔERAV,    FC,   ΔFC] LIST
[MAT, 8,457/   ER1,  ΔER1,     0,    0,    NT,     0/
             RTYP1, TYPE1,   RI1,  ΔRI1,  RIS1, ΔRIS1,
             RICC1,ΔRICC1, RICK1,ΔRICK1, RICL1,ΔRICL1] LIST
            ------------------------------------
              ERNER, ΔERNER,    0,    0,    NT,     0/
            RTYPNER,TYPENER, RINER, RINER, ------------] LIST
```

(omit these LIST records if LCON=1)

```
[MAT, 8,457/ RTYP,   0.0,    0, LCOV,    NR,    NP/ Eint / RP(E) ] TAB1
```

(omit if LCON=0)

```
[MAT, 8,457/  0.0,   0.0,    0,   LB, 2*NPP,   NPP/ (Ek,Fk) ] LIST
```

(omit if LCOV=0 or LCON=0)

For a stable nucleus (NST=1), this section is divided into subsections as follows:

```
[MAT, 8,457/    ZA,  AWR,  LIS,  LISO,   NST,    0] HEAD  (NST=1)
[MAT, 8,457/   0.0,  0.0,    0,     0,     6,    0/
               0.0,  0.0,  0.0,   0.0,   0.0,  0.0] LIST
[MAT, 8,457/   SPI,  PAR,    0,     0,     6,    0]
               0.0,  0.0,  0.0,   0.0,   0.0,  0.0] LIST
```

8.3.2. Procedures

1. The initial state of the parent nucleus is designated by LISO, which equals 0 for the ground state and equals n for the n^{th} isomeric state. Only isomeric states are included in the count of LISO. (In other files isomeric and non-isomeric states may be included in the count of levels.)
2. The average decay energy $\underline{E}_{"x"}$ for decay heat application is given for three general radiation types, E_{LP} (for light particles), E_{EM} (for electromagnetic radiation), and E_{HP} (for heavy particles), followed by the individual components. The sum of these three general quantities is the total

[3] Data must be given in order specified in Section 8.3.2.

average (neutrino energies excluded) energy available per decay to the decay heat problem. The three quantities are more precisely defined as

$$\overline{E}_{LP} = \overline{E}_{\beta^-} + \overline{E}_{\beta^+} + \overline{E}_{e^-} + \ldots$$
$$\overline{E}_{EM} = \overline{E}_{\gamma} + \overline{E}_{x-ray} + \overline{E}_{ann.rad.} + \ldots$$
$$\overline{E}_{HP} = \overline{E}_{\alpha} + \overline{E}_{SF} + \overline{E}_{p} + \overline{E}_{n} + \ldots$$

where $\overline{E}_{LP}$ means the average energy of ***all*** "electron-related" radiation such as β^-, β^+ conversion-electrons, Auger, *etc*. The quantity $\overline{E}_{EM}$, means the average energy of all "electromagnetic" radiations such as gamma rays, x-rays, and annihilation radiation. The quantity $\overline{E}_{HP}$ is the average energy of ***all*** heavy charged particles and neutrons, and also includes the recoil energy; but the alpha energy alone can be separated out by the usual $M_R/(M_R+M_\alpha)$ factor, where M_R and M_α are the recoil nucleus and alpha masses, respectively.

The average decay energies $\overline{E}_{"x"}$ must be given in the following order:

$\overline{E}_{LP}$	Average energy of all light particles.
$\overline{E}_{EM}$	Average energy of all electromagnetic radiation.
$\overline{E}_{HP}$	Average energy of all heavy particles.
$\overline{E}_{\beta^-}$	Average β^- energy.
$\overline{E}_{\beta^+}$	Average β^+ energy.
$\overline{E}_{Ae^-}$	Average Auger-electron energy.
$\overline{E}_{ce^-}$	Average conversion-electron energy.
$\overline{E}_{\gamma}$	Average gamma-ray energy.
$\overline{E}_{x-ray}$	Average x-ray energy.
$\overline{E}_{InB}$	Average internal Bremsstrahlung energy.
$\overline{E}_{ann.rad.}$	Average annihilation energy.
$\overline{E}_{\alpha}$	Average α energy.
$\overline{E}_{recoil}$	Average recoil energy.
$\overline{E}_{SF}$	Average SF energy.
$\overline{E}_{n}$	Average prompt and/or delayed neutron energy.
$\overline{E}_{p}$	Average proton energy.
$\overline{E}_{\nu}$	Average neutrino or antineutrino energy.

3. The symbol RTYP indicates the mode of decay as determined by the initial event. A nucleus undergoing beta decay to an excited state of the daughter nucleus, which subsequently decays by gamma emission, is in the beta decay mode. RTYP = 0.0 is not allowed in MT = 457 (although used under 8.l).

   An isomeric state of the daughter nuclide resulting from the decay of parent nuclides is designated by RFS following the procedures used for LISO. Q represents the total energy available in the decay process and is equal to the energy difference available between the initial and final states (both of which may be isomeric). The branching ratio BR for each decay mode

is given as a fraction and the sum over all decay modes must equal unity.

Multiple particle emission is also allowed by using any combination of the RTYP variables. This will account for particle emission from nuclear states excited in the decay of the parent ("delayed-particle" emission) whose half-lives are too short to warrant separate entry in the file. It will also allow users and processing codes to identify the various intermediate states, without having to examine all the spectrum listings to determine radiation types. The multiple-particle RTYP should be constructed in the order in which the particles are emitted. (*e.g.*, RTYP = 1.5 indicates decay followed by neutron emission).

4. The source-of-radiation should be specified for each spectral line or continuous spectra. The source of radiation is a floating-point integer corresponding to the RTYP definitions. If the source-of-radiation is not known RTYP = 10. should be used.
5. The energy spectra should be specified if they are known and identified by STYP. Gamma spectra are described using STYP = 0.0. Relative intensities and errors in the relative intensity should be specified. Absolute normalization is made through multiplication by FC and FD. If absolute discrete spectra are given FD must equal unity. The radiation intensity should total the contributions from all decays leading to radiation within a particular decay type, STYP, having energy $E_r \pm \Delta E_r$.

   a. For gamma ray emission (STYP = 0.0), no other information is required if X-ray, Auger electron, conversion electron, and pair formation intensities have not been calculated for these transitions. In this case NT = 6.

      The amount of additional information depends upon the detail in which quantities were obtained for inclusion in STYP = 8. or 9. spectra, and the number of decay modes. (This detail will also be reflected in the uncertainties assigned in STYP = 8. or 9. spectra.) If only the total conversion electron emission is calculated, RICC and ΔRICC should be included and NT is specified as 8. If contributors from the individual K, L, and M shells are calculated, the K and L shell conversion coefficients should be included and NT = 12. In the rare case (*i.e.*, $^{16}_{7}N$), where internal pair formation is needed, the internal pair formation coefficient should be included as the quantities RIS and ΔRIS.

   b. For electron capture (STYP = 2.), the quantity RIS is 0.0 provided $E_{e.c.} \leq 1.022$ MeV. If positron emission is energetically possible, RIS and ΔRIS must be specified (as $I_{\beta+}$ and $\Delta i_{\beta+}$).

   c. The spectra should be ordered in increasing values of STYP, and discrete spectral data should be specified before continuous spectra.

   d. For STYP = 5. (spontaneous fission neutrons), LCON = 0, NER = 0, and EAV and ΔEAV should be given.

   e. For STYP = 6. (spontaneous fission fragments) LCON = 0, NER = 0, and $\underline{E}_{SF}$ and $\Delta \underline{E}_{SF}$ should be given.

6. The specification of data uncertainties is an important quantity which is difficult to represent in a simple way. Although a one sigma variance is desired, a number should be entered that at least indicates qualitatively how well the parameter is known.

For STYP = 8. and 9., ΔE will reflect the detail in which these values were derived. For example, if only the total conversion electron emission has been calculated, ΔE would be the spread between K-conversion and M-conversion electron energies. If a very detailed calculation has been made, ΔE would reflect the uncertainties in the electron binding energy and the transition energy.

7. The spontaneous fission spectrum is specified using MF = 5 in sub-library 4 (no incoming projectile).

8. Every effort should be made to determine the spin and parity of the original nucleus, either by experimental evidence or by strong theoretical arguments. If the spin cannot be determined, it should be reported as -77.777; if the parity cannot be determined it should be reported as zero.

9. Because the continuum spectrum is normalized, the absolute covariance matrix of a multi-component normalized spectrum processed from this file must have zero for the sum of each row and column. (Processing codes should perform this check).

   Since the covariance form for radioactive product spectra is confined to LB = 2, meeting this test is equivalent to the following condition on the F_k of the E_k covariance table:

$$\sum_k F_k \, y_k = 0,$$

$$\text{where, } y_k = \int_{E_k}^{E_{k+1}} RP(E)\, dE$$

   and y_k is the energy spectrum on the uncertainty evaluation grid. $\Sigma y_k = 1$. If the initial F_k do not meet this condition, the corrected values F'_k are given by:

$$F'_k = F_k - \sum_k F_k \, y_k$$

   Note that unlike the case for File 33, some of the F_k' will be negative. Also, the processed multigroup correlation matrix will show some off-diagonal components that are -1 as well as others that are +1.

   When a processing code constructs the absolute covariance V_{mn} on the user's energy grid E_m, the simplest relations to use are

$$V_{mn} = \sigma_m \sigma_n \, ,$$

$$\text{where, } \sigma_n = \int_{E_n}^{E_{n+1}} F(E)\, RP(E)\, dE$$

   and the integral is easy because F(E) is piece-wise continuous on the E_k grid. By this construction we are assured that the null sum condition will be retained for the covariance matrix of the processed multigroup spectrum.