3. FILE 3, REACTION CROSS SECTIONS

3.1. General Description

Reaction cross sections and auxiliary quantities are given in File 3 as functions of energy E, where E is the incident energy in the laboratory system. They are given as energy-cross section (or auxiliary quantity) pairs. An interpolation scheme is given that specifies the energy variation of the data for incident energies between a given energy point and the next higher point. File 3 is divided into sections, each containing the data for a particular reaction (MT number); see Section 0.5 and Appendix B. The sections are ordered by increasing MT number. As usual, each section starts with a HEAD record and ends with a SEND record. The file ends with a FEND record.

3.2. Formats

The following quantities are defined

ZA,AWR	Standard material charge and mass parameters.
QM	Mass-difference Q value (eV): defined as the mass of the target and projectile minus the mass of the residual nucleus in the ground state and masses of all other reaction products; that is, for $a+A \rightarrow b+c+...+B$, $QM=[(m_a+m_A)-(m_b+m_c+...+m_B)](9.315016 \times 10^8)$ if the masses are in amu. (See paragraph 3.3.2).
QI	Reaction Q value for the (lowest energy) state defined by the given MT value in a simple two-body reaction or a breakup reaction. Defined as QM for the ground state of the residual nucleus (or intermediate system before breakup) minus the energy of the excited level in this system. Use QI=QM for reactions with no intermediate states in the residual nucleus and without complex breakup (LR=0). (See paragraph 3.3.2.)
LR	Complex or "breakup" reaction flag. Indicates that additional particles not specified by the MT number will be emitted. See Sections 0.5.5 and 3.4.4.
NR,NP,E_{int}	Standard TAB1 parameters.
σ(E)	Cross section (barns) for a particular reaction (or the auxiliary quantity) given as a table of NP energy-cross section pairs.

The structure of a section is

```
[MAT, 3, MT/  ZA,  AWR,  0,  0,  0,  0] HEAD
[MAT, 3, MT/  QM,   QI,  0, LR, NR, NP/ Eint / σ(E)] TAB1
[MAT, 3,  0/ 0.0,  0.0,  0,  0,  0,  0] SEND
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3.3. General Procedures

3.3.1. Cross Sections, Energy Ranges, and Thresholds

For incident neutrons, the cross-section data must cover an energy range up to a common upper limit of at least 20 MeV, and the data must extend to a lower limit of the reaction threshold or 10^{-5} eV whichever is higher. For other reactions, the cross section should start at the reaction threshold energy (with a value of 0.0 barns) and should continue up to a **common upper energy limit**.

In the case where there is a change in the representation above a given energy, *e.g.*, a change from separate reactions to MT=5 (sum of reactions not given separately in other sections), the following procedure should be used. For the cross sections in the lower energy region, there should be a duplicate point with a value of zero at the last energy for a which a non-zero cross section is given, and a point with a value of zero at the common upper energy limit. Similarly, for the cross sections in the upper energy region, there should be a duplicate point with a value of zero at the first energy for a which a non-zero cross section is given, and a zero value at the low energy limit. The evaluator should document the change in representation in the File 1 comments.

For charged-particle emission, the cross section is usually very small from the threshold (or lower limit) up to an ***effective threshold*** defined by a noticeable cross section (for example, 10^{-10} barns). The evaluator should tabulate a cross section of 0.0 in such a range in order to avoid interpolation problems.

Sometimes ENDF reactions have an apparent upper limit lower than the upper limit for the material due to changes in representation in different sections. For example, there might be a change from discrete levels to a continuum rule, or from separate reactions to MT=5. Such cross sections must be ***double valued*** at the highest energy for which the cross section is nonzero. The second cross section at the discontinuity must be zero, and it must be followed by another zero value at the upper limit. This will positively show that the cross section has been truncated. For such reactions, there will be another reaction with an artificial threshold at the discontinuity. The cross sections must be chosen in such a way that their sum is continuous.

The limit on the number of energy points (NP) to be used to represent a particular cross section is given in Appendix G. The evaluator should not use more points than are necessary to represent the cross section accurately. When appropriate, resonance parameters can be used to help reduce the number of points needed. The evaluator should avoid sharp features such as triangles or steps (except for the required discontinuities at the limits of the resonance ranges or where reactions change representation), because such features cannot be realistically Doppler broadened.

3.3.2. Q Values

Accurate Q values should be given for all reactions, if possible. If QI is not well defined (as for a range of levels in MT=91, 649, 699, 749, 799, or 849), use the value of QI which corresponds to the threshold of the reaction. Similarly, if the value of QM is not well defined (as in elements or for summation reactions like MT=5), use the value of QM which gives the threshold. If there is no threshold, use the most positive Q value of the component reactions. Note that these ill-defined values of QM cannot be relied on for energy-release calculations.

As an example to clarify the use of QM and QI, consider the reaction $\alpha+{}^{9}\text{Be}\rightarrow\text{n}+\text{X}$. After the neutron has been emitted, the compound system is ^{12}C with QM=5.702 MeV and energy levels (E_x) at 0.0, 4.439, 7.654, and 9.641 MeV. The ground state is stable against particle breakup, the first level decays by photon emission, and the higher levels decay with high probability by breaking up into three alpha particles (7.275 MeV is required). This pattern can be represented as follows.

Reaction	QM	QI	EX	MT
$9Be(a,n_0)12C$	5.702	5.702	0.000	50
$9Be(a,n_1)12C$	5.702	1.263	4.439	51
$9Be(a,n_2)12C(3\alpha)$	-1.573	-1.952	7.654	52
$9Be(a,n_3)12C(3\alpha)$	-1.573	-3.939	9.641	53
$9Be(a,n_C)12C(3\alpha)$	-1.573	-1.573		91

The gamma for the second reaction is not written explicitly in this notation. The last reaction includes the contributions of all the levels above 9.641 MeV, any missed levels, and any direct four-body breakup; therefore, the threshold for MT=91 may be lower than implied by the fourth level of ^{12}C. Note the value used for QI.

3.3.3. Relationship Between File 3 and File 2

If File 2 (Resonance Parameters) contains resolved and/or unresolved parameters (LRP=1), then the cross sections or self-shielding factors computed from these parameters in the resonance energy range for elastic scattering (MT=2), fission (MT=18), and radiative capture (MT=102) must be combined with the cross sections given in File 3. The resonance contributions must also be included in any summation reactions that involve the three resonance reactions (for example, MT=1, 3, or 5). The resonance energy range is defined in File 2. Double-valued energy points will normally be given in File 3 at the upper and lower limits of the unresolved and resolved resonance regions.

Some materials will not have resonance parameters but will have a File 2 (LRP=0) that contains only the effective scattering radius. This quantity is sometimes used to calculate the potential scattering cross section in self-shielding codes. For these materials, the potential scattering cross section computed from File 2 *must not* be added to the cross section given in File 3. The File 3 data for such materials comprise the entire scattering cross section.

In certain derived libraries, the resonance cross sections have been reconstructed and stored in File 3. Such files may have LRP=0 as described in the preceding paragraph. Alternatively, they may have LRP=2 and include a full File 2 with complete resonance parameters. In this case, resonance cross sections or self-shielding factors computed from File 2 *are not* to be combined with the cross sections in File 3.

3.4. Procedures for Incident Neutrons

Cross section data for non-threshold reaction types must cover the energy range from a lower limit of 10^{-5} eV to an upper limit of ***at least*** 20 MeV for all materials. For non-threshold reactions, a cross section value must be given at 0.0253 eV. The limit on the number of energy points (NP) to be used to represent a particular cross section is 50,000. The evaluator should not use more points than are necessary to represent the cross section accurately.

The choice of data to be included in an evaluation depends on the intended application. For neutron sublibraries, it is natural to define "transport" evaluations and "reaction" evaluations. The transport category can be further subdivided into "low-energy transport" and "high-energy transport."

A ***reaction evaluation*** will contain File 1, File 2, File 3, and sometimes File 32 and/or File 33. File 2 can contain resonance parameters. If radioactive products must be described, Files 8, 9, 10, 39, and/or 40 may be present. File 3 may tabulate one or more reaction cross sections. The total cross section is not usually well defined in reaction evaluations since they are incomplete. Examples of this class of evaluations include activation data and dosimetry data.

A ***low-energy transport evaluation*** should be adequate for calculating neutron transport and simple transmutations for energies below about 6-10 MeV. Photon production and covariance data should be included when possible. Typical evaluations will include Files 1, 2, 3, 4, 5, and sometimes Files 8, 9, 10, 12, 13, 14, 15, 31, 32, 33, 34, 35, 39, and/or 40. Resonance parameters will usually be given so that self shielding can be computed. Charged-particle spectra (MT=600-849) and neutron energy-angle correlation (MF=6) will usually not be given. File 3 should include all reactions important in the target energy range, including the total (MT=1) and elastic scattering (MT=2). Other reactions commonly included are inelastic scattering (MT=4,51-91), radiative capture (MT=102), fission (MT=18,19-21,38), absorption (MT=103,104,105,...), and other neutron emitting reactions such as MT=16,17,22,28,.... Specific procedures for each reaction are given below. Examples of this class of evaluations include fission-product data and actinide data.

A ***high-energy transport evaluation*** should be adequate for calculating neutron transport, transmutation, photon production, nuclear heating, radiation damage, gas production, radioactivity, and charged-particle source terms for energies up to at least 20 MeV. In some cases, the energy limit needs to be extended to 40-100 MeV. These evaluations use Files 1, 2, 3, 4, 5, 6, 12, 13, 14, 15, and sometimes 8, 9, 10, 31, 32, 33, 34, 35, 39, and/or 40. Once again, File 3 should give cross sections for all reactions important in the target energy range, including MT=1 and 2. This will normally include many of the reactions mentioned above plus the series MT=600-849. At high energies, some reactions may be combined using the "complex reaction" identifier MT=5. File 6 will normally be needed at high energies to represent energy-angle correlation for scattered neutrons and to give particle and recoil energies for heating and damage calculations. Special attention to energy balance is required. High-energy evaluations are important for materials used in fusion reactor designs, in shielding calculations, and in medical radiation-therapy equipment (including the components of the human body).

3.4.1. Total Cross Section (MT=1)

The total is often the best-known cross section, and it is generally the most important cross section in a shielding material. Considerable care should be exercised in evaluating this cross section and in deciding how to represent it.

Cross section minima (potential windows) and cross section structure should be carefully examined. Sufficient energy points must be used in describing the structure and minima to reproduce the experimental data to the measured degree of accuracy.

The total cross section, as well as any partial cross section, must be represented by 50,000 incident-energy points or fewer. The set of points or energy mesh for the total cross section must be a union of all energy meshes used for the partial cross sections. Within the above constraints, every attempt should be made to minimize the number of points used. The total cross section must be the sum of MT=2 (elastic) and MT=3 (nonelastic). If MT=3 is not given, then the elastic cross section plus all nonelastic components must sum to the total cross section.

The fact that the total cross section is given at every energy point at which at least one partial cross section is given allows the partial cross sections to be added together and checked against the total for any possible errors. In certain cases, more points may be necessary in the total cross section over a given energy range than are required to specify the corresponding partial cross sections. For example, a constant elastic scattering cross section and a 1/v radiative capture cross section could be exactly specified over a given energy range by log-log interpolation (INT=5), but the sum of the two cross sections would not be exactly linear on a log-log scale. If a precise total cross section is required between the energy points provided, it is recommended that the total be calculated from the sum of the partials rather than interpolated directly from MT=1.

3.4.2. Elastic Scattering Cross Section (MT=2)

The elastic scattering cross section is generally not known to the same accuracy as the total cross section. Frequently, the elastic scattering cross section is obtained by subtracting the nonelastic cross section from the total cross section. This procedure can cause problems. The result is an elastic scattering cross section that contains unreal structure. There may be several causes. First, the nonelastic cross section, or any part thereof, is not generally measured with the same energy resolution as the total cross section. When the somewhat poorer resolution nonelastic data are subtracted from the total, the resolution effects appear in the elastic cross section. Second, if the evaluated structure in the nonelastic cross section is incorrect or improperly correlated with the structure in the total cross section (energy-scale errors), an unrealistic structure is generated in the elastic scattering cross section.

The experimental elastic cross section is obtained by integrating measured angular distributions. These data may not cover the entire angular range or may contain contributions from nonelastic neutrons. Such contamination is generally due to contributions from inelastic scattering to low-lying levels that were not resolved in the experiment. Care must be taken in evaluating such results to obtain integrated cross sections. Similarly, experimental angular distribution data can also cause problems when used to prepare File 4.

3.4.3. Nonelastic Cross Section (MT=3)

The nonelastic cross section is not required unless any part of the photon production multiplicities given in File 12 uses MT=3. In this case, MT=3 is required in File 3. If MT=3 is given, then the set of points used to specify this cross section must be a union of the sets used for its partials.

3.4.4. Inelastic Scattering Cross Sections (MT=4,51-91)

A total inelastic scattering cross section (MT=4) must be given if any partials are given; that is, discrete level excitation cross sections (MT=51-90), or continuum inelastic scattering (MT=91). The set of incident energy points used for the total inelastic cross section must be a union of all the sets used for the partials.

Values should be assigned to the level excitation cross sections for as many levels as possible and extended to as high an energy as possible. Any remaining inelastic scattering should be treated as continuum. In particular, low-lying levels with significant direct interaction contributions (such as deformed nuclei with 0^+ ground states) should be extended to the upper limit of the file (at least 20 MeV) in competition with continuum scattering. The secondary energy distribution for such neutrons resembles elastic scattering more than an evaporation spectrum.

Level excitation cross sections must start with zero cross section at the threshold energy. If the cross section for a particular level does not extend to the upper limit for the file (*e.g.*, 20 MeV), it must be ***double-valued*** at the highest energy point for which the cross section is non-zero. The second cross section value at the point must be zero, and it should be followed by another zero value at the upper limit. This will positively show that the cross section has been truncated.

If LR=0, a particular section (MT) represents (n,n'gamma). The angular distribution for the scattered neutron must be given in the corresponding section of File 4 or 6. The associated photons should be given in a corresponding section of File 6 or 12, if possible. If the inelastic photons cannot be assigned to particular levels, they can be represented using MT=4 in File 6, 12 or 13. When inelastic photons cannot be separated from other nonelastic photons, they can be included in MF=13, MT=3.

A LR flag greater than zero indicates inelastic scattering to levels that de-excite by breakup, particle emission, or pair production rather than by photon emission (see Section 0.6)[1] . If LR=1, the identities, yields, and distributions for all particles and photons can be given in File 6. If LR>1, angular distributions for the neutron must be given in File 4, and distributions are not available for the emitted particles. In this case, photon production is handled as described above for LR=0.

If a particular level decays in more than one way, then File 6 can be used or several sections can be given in File 3 for that level. Consider the case in which an excited state sometimes decays by emitting a proton, and sometimes by emitting an alpha particle. That part of the reaction that represents (n,n'α) would use LR=22, and the other part would be given the next higher section number (MT) and would use LR=28 (n,n'p). The angular distribution for the neutron would have to be given in two different MT numbers in File 4, even though they represent the same neutron. The sections must be ordered by decreasing values of QI (increasing excitation energy).

3.4.5. Fission (MT=18,19-21,38)

The total fission cross section is given in MT=18 for fissionable materials. Every attempt should be made to break this cross section up into its various parts:first-chance fission (n,f), MT=19; second-chance fission (n,n'f), MT=20; third-chance fission (n,2nf), MT=21; and fourth-chance fission (n,3nf), MT=38. The data in MT=18 must be the sum of the data in MT=19, 20, 21, and 38. The energy grid for MT=18 must be the union of the grids for all the partials.

[1] LR=31 is still allowed, however, to uniquely define the γ-decay when using MF=3, and MF=12 (or 15) and MF=4.

If resolved or unresolved resonance parameters are given in File 2, the fission cross section computed from the parameters must be included in both MT=18 and MT=19.

The Q value for MT=18, 19, 20, 21, and 38 is the energy released per fission minus the neutrino energy. It should agree with the corresponding value given in MT=458 in File 1.

Secondary neutrons from fission are usually stated to be isotropic in the laboratory system in File 4. Energy distributions are given in File 5. The complex rules associated with the partial fission reactions are described in Section 5.

3.4.6. Charged-Particle Emission to Discrete and Continuum Levels (MT=600-849)

The (n,p) reaction can be represented using a summation cross section, discrete levels, and a continuum (MT=103, 600-648, and 649) in the same way that the (n,n') reaction is represented using MT=4, 51-90, and 91 (see Section 3.4.4). Similarly, (n,d) uses MT=104 and 650-699, and so on for t, ^{3}He, and α. Of course, MT=600, 650, 700, *etc*., represent the ground state and would not have corresponding sections in the photon production files, unless the flag LR>0 (such as in the ^{10}B(n,t)^{8}Be reaction).

3.5. Procedures for Incident Charged Particles and Photons

See Table 0.1 for sublibrary numbers for incident charged particles and photons. Procedures for incident charged particles are generally the same as for neutrons as given in section 3.4. The exceptions are noted below.

3.5.1. Total Cross Sections

The total cross section is undefined for incident charged particles. MT=1 should be used for the photonuclear total cross section, while MT=501 is used for the total atomic photon interaction cross section.

3.5.2. Elastic Scattering Cross Sections

As discussed in detail in Section 6.2.6, it is not possible to construct an integrated cross section for charged-particle elastic scattering because of the Coulomb term. Therefore, σ is either set to 1.0 or to a "nuclear plus interference" value using a cutoff angle. This value may in theory be 0.0, and, in this case, should be set to epsilon, *e.g.*, 10^{-38}. The first and last energy points used for MT=2 in File 3 define the range of applicability of the cross section representation given in File 6. The cross section need not cover the complete range from 10^{-5} eV to 20 MeV. MT=2 is used for the elastic scattering cross section for all incident particles and photons (resonance fluorescence). For photons, MT=502 and 504 are used for coherent and incoherent atomic scattering, respectively.

3.5.3. Inelastic Scattering Cross Sections

The procedure for inelastic cross section for incident charged particles and photons is the same as for neutrons. The following MT combinations should be used.

Incident Particle	MT's for Excited States	MT's for Total Inelastic σ
γ	undefined	102
n	51-91	4
p	601-649	103
d	651-699	104
t	701-749	105
^{3}He	751-799	106
α	801-849	107

3.5.4. Stopping Power

The total charged-particle stopping power in eV×barns is given in MF=3, MT=500. This is basically an atomic property representing the shielding of the nuclear charge by the electrons, but it should be repeated for each isotope of the element. It is a "total" stopping power in that most tabulations implicitly include large-angle coulomb scattering which is also represented here in File 6. In practice, this contribution is probably small enough to keep double counting from being a problem. At low particle energies, mixture effects are sometimes noticeable. They are not accounted for by this representation.