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Title: Lib81 ACE neutron sublibrary erratum for 190-198Pt and 180mTa

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Memorandum
X-Computational Physics (XCP-5)

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Subject: Lib81 ACE neutron sublibrary erratum for $^{190-198}$Pt and ^{180m}Ta

The ACE library based on the neutron-induced ENDF/B-VIII.1 sub-library, Lib81, was released in September 2025. This memorandum documents the release of 80 errata files for the Lib81 library, which fix a problem in the neutron capture γ-ray energy distributions. This Lib81 erratum does not correspond to an ENDF/B library erratum.

1 Discrete Primary γ rays in Incident Neutron Evaluations

Discrete primary γ rays[1] are γ rays that de-excite the compound state immediately to a known discrete excited level in the product nucleus (or the ground state of the product nucleus). The distinction between discrete and continuum primary γ rays is somewhat artificial, based more on experimental capabilities than on physical characteristics, but the discrete primary γ rays typically represent the highest-energy γ rays emitted by low-energy nuclear reactions aside from fission. For this reason, accurate primary γ-ray spectra are important for modeling shielding and energy balance in many applications.

The energy of discrete primary γ rays will increase linearly with the energy of the incident neutron causing the reaction and can be calculated with the following equation (neglecting recoil),

$$E_\gamma = (S_n - E_x) + \frac{M}{M + m_n} E_n, \tag{1}$$

where E_γ is the energy of the emitted primary γ ray, S_n is the neutron separation energy (the binding energy of the least-bound neutron) of the compound nucleus, E_x is the energy of the discrete excited level (or ground state) that this primary leaves the product nucleus in, M is mass of the target, m_n is the mass of the neutron, and E_n is the incident neutron energy. The ACE format has been updated with a new distribution type that holds the quantity $(S_n - E_x)$ for a discrete primary γ ray, allowing MCNP6.3 [1] to calculate the precise energy of the emitted γ ray given the energy of the reaction.

The ENDF-6 format [2] allows two different formats for capture γ-ray data — in File 6, or in Files 12, 14, and 15. In the case of the File 6 format, correlated energy-angle information can be stored. In the case of Files 12, 14, and 15, the discrete energies, angular distribution information, and continuous energy spectra are separated and correlations cannot be recorded. However, correlated energy-angle distributions for capture γ rays are not currently available for incident neutron evaluations above the light elements, and the simpler File 12/14/15 format is more frequently used in the ENDF/B library for $A > 20$ nuclei when discrete primary γ rays are flagged.

[1] Primary capture γ rays are the first to be emitted in a capture cascade. They are emitted directly from the compound state of the reaction, and scale linearly with incident neutron energy if recoil is neglected.

The JENDL library has made much more extensive use of the File 6 format for discrete primary γ rays than the ENDF/B library, with 480 of the 795 evaluations in the incident neutron sublibrary containing flagged discrete primary γ rays in File 6 in the most recent release, JENDL-5.0 [3].

1.1 ENDF/B and JENDL Library Format Divergence

The discrete primary γ rays represent a divergence in the format between the ENDF/B and JENDL libraries. The ENDF-6 format manual [2] Section 6.2.3 states "discrete primary photons should be flagged with negative energies" but does not specify whether in this case the energy in the file should be the neutron-energy-dependent energy of the emitted γ ray, or the neutron-energy-independent quantity $(S_n - E_x)$.

In this format, the energies of the discrete secondary γ rays[2] and the bin edges of the continuous spectra all refer to emitted γ ray[3]. The continuous spectra contain all of the other γ rays in the cascade that are not associated with discrete excited levels in the product nucleus, and as such contain some energy-dependent γ-ray energies and some independent. It is reasonable to assume that the discrete primary γ-ray energies listed in File 6 should also be the emitted γ-ray energy, and this is the choice made by the ENDF/B library.

However, it is also reasonable to assume that the listed energies should be the neutron-energy-independent quantity $(S_n - E_x)$, as this is the clearly-stated rule for formatting discrete primary γ rays in File 12. In Section 12.2.1 of the ENDF-6 manual [2], the listed energy EG_k is defined as the "photon energy for LP=0 or 1 or Binding Energy for LP=2"[4]. Applying this formatting rule to File 6 is the choice made by the JENDL library.

`NJOY2016` [4] was updated in December 2010 to handle the JENDL primary γ-ray format. The change notes are reproduced below:

```
*ident up360
*/ acer -- 09dec2010
*/ - fourth of several updates for acer, recommended by JAEA
*/   colleagues for processing JENDL-4 evaluations.
*/   - modifications to handle a variable number of discrete photons
*/     as a function of incident neutron energy (this is a legal endf
*/     format, but mcnp expects ND to be constant for all incident
*/     energies)
*/     - NOTE:  original JAEA coding modified at LANL (1/21+/2011).
```

The specific part of `NJOY2016` that processes File 6 discrete primary γ rays has not been updated since.

[2]Secondary γ ray is used to refer to all γ rays emitted in the cascade after the primary γ ray.

[3]For the discrete secondary γ rays the emitted energy is not dependent on the incident neutron energy so the distinction is meaningless.

[4]"LP" is a flag indicating whether the listed γ ray is of unknown origin (LP=0), is a secondary γ ray (LP=1), or is a discrete primary (LP=2). The term "Binding Energy" refers to the quantity $(S_n - E_x)$.

1.2 $^{190-198}$Pt and ^{180m}Ta ENDF/B-VIII.1 Evaluations

New incident neutron evaluations were performed for the ENDF/B-VIII.1 library [5] in the fast region by M. Herman and T. Kawano (LANL). The Hauser-Feshbach code EMPIRE [6] was used to both produce the evaluation and format it into the ENDF-6 format [2]. These were the first evaluations in the ENDF/B neutron sublibrary to make use of the discrete primary γ-ray format option in File 6 for capture, and used the ENDF/B format choice to put the emitted γ-ray energy (E_γ) into the file. These ten evaluations were, therefore, the first evaluations in ENDF/B to be impacted by the changes to `NJOY2016` explained above.

2 Processing File 6 Capture γ rays

The `NJOY2016` [4] module `acefm` processes all outgoing γ-ray energy distributions in File 6 into an NJOY-specific section called File 16 (`mfd16`). The data in File 16 is then processed into the ACE distribution type LAW=4. The ENDF-6 format allows the evaluation to contain different discrete (primary and secondary) γ rays in the distributions for different incident neutron energies but ACE format does not, because MCNP expects the same discrete values in each distribution. To handle this, the `acefm` module first loops through each incident energy distribution to collect a full list of all unique discrete γ-ray energies:

```
             !--compare discrete photon list at higher incident
             !--neutron energies with a union list from lower
             !--incident neutron energies.  endf formats allow
             !--these to differ but mcnp doesn't.  let the
             !--dise array accumulate a union list.
             do ki=1,nd
                ep=scr(5+2*ki)
                if (ep.eq.zero) then
                   call mess('acelpp',&
                            '2discrete photon energy must .ne. 0',&
                            'reset to 1.e-5 eV')
                   ep=1.e-5_kr
                endif
                if (law.eq.2) ep=ep-awr*ei/(awr+1)
```

In this part of the code, the (negative) discrete primary γ-ray energy is not converted back to the energy-independent quantity $(S_n - E_x)$, as there is no check for `law` equal to one.

When a discrete primary γ ray is detected (by the negative energy), `NJOY2016` treats it as the negative of the quantity $(S_n + E_x)$, so it negates the value and then adds the second term on the right side of Eqn. 1 to the value. Each unique discrete γ-ray energy is added to each incident distribution, with a probability of zero if it was not originally included. In this way, `NJOY2016` creates outgoing discrete γ-ray distributions that comply with the ACE format. A snippet of `acefm.f90` that performs this calculation is shown here:

```
            !--loop over union list of photons, inserting
            !--missing energies with zero probability.  also
            !--check law and/or sign of photon energy to know
            !--if this is a primary or secondary photon.  if
            !--a primary photon, its energy must be increased
            !--to account for the incident neutron energy.
            do m=nd0,1,-1
               ep=dise(m)
               if (law.eq.1.and.ep.lt.zero)ep=-ep+ei*awr/(awr+1)
```

Under these circumstances, the variable `law` is equal to 1, so the energy will be negated and the recoil-corrected neutron energy will be added to it.

2.1 $^{190-198}$Pt and ^{180m}Ta ENDF/B-VIII.1 Evaluations

When `NJOY2016` was used to process the new ENDF/B-VIII.1 evaluations for $^{190-198}$Pt and ^{180m}Ta, the flagged discrete primary γ rays were processed incorrectly due to the formatting inconsistency. `NJOY2016` expects the flagged primary γ-ray energies to represent the incident-energy-independent quantity $(S_n - E_x)$, which is the same in each distribution. In that case, the first snippet of code above, which collects a union list of all unique discrete γ-ray energies across all distributions, would have added each discrete primary γ-ray energy only once. In these evaluations, the same set of discrete (primary and secondary) γ-ray transitions are listed in all of outgoing distributions, so the length of the union set of γ rays should be the same as the length of the discrete γ rays in any one distribution. However, because the discrete primary γ-ray energies are listed as the neutron-energy-dependent quantity E_γ (emitted γ-ray energy) instead, the union set compiled contained all of the discrete secondary γ rays once, and all of the discrete primary γ rays as many times as there were outgoing distributions. This created a very long list of discrete γ rays for each evaluation - for example, 1592 for ^{190}Pt. The γ-ray energies were incorrect in the set as well, due to the addition of the neutron energy to the emitted energy in the file. The "union grid" that `NJOY2016` created is not actually the same at all incident energies, shown in Fig. 1 — as the incident neutron energy increases, the outgoing energy grid increases as well.

2.2 MCNP

The very large LAW=4 distributions hit a maximum size limit in MCNP6.3, which can only handle distributions with fewer than 1000 energy values. A distribution larger than this leads to an infinite loop in the code, causing the simulation to hang. This effect was discovered in the Lib81 ACE library [7] by a user and diagnosed by the XCP-3 team. The hardcoded size limit may be modified in future versions of MCNP, in case future evaluations do have over 1000 unique discrete γ-ray lines in individual outgoing spectra. However, these Pt and Ta evaluations do not - the large number of discrete γ-ray energies in the ACE files is a product of the File 6 format divergence and the fact that `NJOY2016` was modified to handle the JENDL format choice, and never updated to also handle the ENDF/B format choice.

3 Processing File 12 Capture γ rays

The other option for storing discrete capture γ rays in the ENDF evaluation is to use the combination of Files 12, 14, and 15. In this format, there is a dedicated flag indicating whether a discrete

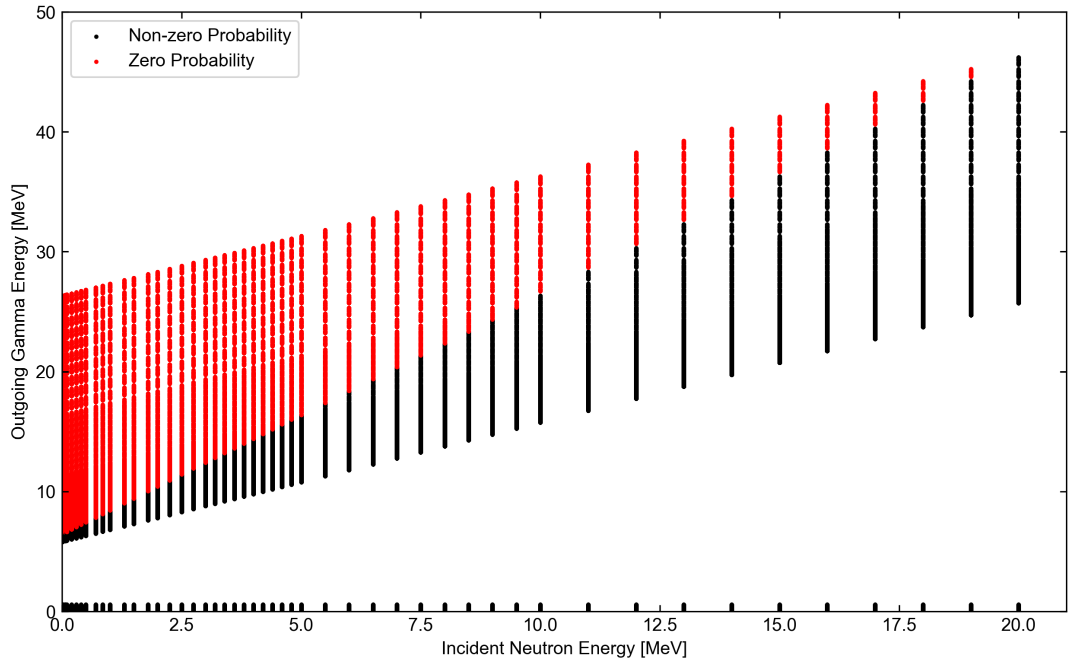

Figure 1: The outgoing discrete γ-ray energies for each incident energy in the ^{190}Pt ACE file in the Lib81 library. In processing, `NJOY2016` attempted to create a union grid at each of the incident energy LAW=4 distributions, but the misinterpretation of the energies in the ENDF-6 file led to different outgoing energies at each incident energy. The multiplicity values are also not correct due to this indexing error. The discrete secondary γ-ray energies, which do not change with incident energy, are seen at the lower energies, consistent across incident energy.

γ ray is a primary or a secondary, so there is no need for negated energies. The ENDF-6 formats manual [2] is much clearer about the format for this file, due to a concerted effort in 2021 to clear up the language. `NJOY2016` processes Files 12/14/15 into a different ACE distribution type, LAW=2, which is specifically for discrete photon energies, and has a flag indicating whether or not the γ ray is a primary or secondary. The `NJOY2016` processing of File 12/14/15 into LAW=2 is done correctly.

3.1 Modified $^{190-198}$Pt and ^{180m}Ta ENDF/B-VIII.1 Evaluations

To create errata files for the Lib81 ACE library, the capture γ-ray information in File 6 of the original ENDF/B-VIII.1 library was converted to File 12/14/15 in new ENDF-6 formatted files using `ENDFtk` [8] for these ten evaluations. Those converted files were then processed with `NJOY2016` using the same processing script (`ndvv`), to produce new ACE files for each isotope at each of the eight temperatures in the Lib81 library. The same processing script was used to ensure that the only changes in the ACE files are the γ-ray spectra changes described here. As a result the erratum files will lead to the same results in any simulations for which the original files worked. The only change will be seen in simulations for which the original files caused MCNP to crash.

3.2 MCNP

The new ACE files (at room temperature) were tested with MCNP6.3 using a simple simulation with photon production and transportation turned on. During these tests, MCNP6.3 did not hang or crash with the new files.

4 Erratum Availability

The erratum files were given the same suffixes as the original files in the Lib81 ACE library in an attempt to ensure that they replace the original files in simulations. Any simulations that ran successfully with the original files will not see any changes in the results. Simulations using photon production and transport will now run without crashing.

The erratum is available on the Lib81 webpage at `https://nucleardata.lanl.gov/ace/lib81` and has the following structure:

```
Pt-Ta-Lib81/
 ├── docs/
 ├── Lib81/
 │   ├── Pt/
 │   └── Ta/
 ├── xsdir
 └── README.md
```

The complete list of files in the erratum are listed in Table 1.

4.1 Availability on LANL Systems

The erratum files will replace the original files on the HPC systems and the ALDX LAN systems on July 1, 2026. Prior to this replacement date, the new files will be available in new `data/nuclear/mc/special/Lib81-erratum/` directories for testing. The original ACE files will be archived on both systems, in new `data/nuclear/mc/archive/` directories.

Table 1: Complete list of files in the erratum.

Temp [K]	^{180m}Ta	^{190}Pt	^{191}Pt	^{192}Pt	^{193}Pt
293.6	1073180.10c	78190.10c	78191.10c	78192.10c	78193.10c
600	1073180.11c	78190.11c	78191.11c	78192.11c	78193.11c
900	1073180.12c	78190.12c	78191.12c	78192.12c	78193.12c
1200	1073180.13c	78190.13c	78191.13c	78192.13c	78193.13c
2500	1073180.14c	78190.14c	78191.14c	78192.14c	78193.14c
0.1	1073180.15c	78190.15c	78191.15c	78192.15c	78193.15c
233.15	1073180.16c	78190.16c	78191.16c	78192.16c	78193.16c
273.15	1073180.17c	78190.17c	78191.17c	78192.17c	78193.17c
Temp [K]	^{194}Pt	^{195}Pt	^{196}Pt	^{197}Pt	^{198}Pt
293.6	78194.10c	78195.10c	78196.10c	78197.10c	78198.10c
600	78194.11c	78195.11c	78196.11c	78197.11c	78198.11c
900	78194.12c	78195.12c	78196.12c	78197.12c	78198.12c
1200	78194.13c	78195.13c	78196.13c	78197.13c	78198.13c
2500	78194.14c	78195.14c	78196.14c	78197.14c	78198.14c
0.1	78194.15c	78195.15c	78196.15c	78197.15c	78198.15c
233.15	78194.16c	78195.16c	78196.16c	78197.16c	78198.16c
273.15	78194.17c	78195.17c	78196.17c	78197.17c	78198.17c

5 Conclusions

New incident-neutron ACE files for $^{190-198}$Pt and ^{180m}Ta were produced as an erratum to the Lib81 ACE library to address the error in processing the discrete γ rays. The new files do not cause MCNP to hang or crash on photon production. The errata files use the same suffixes as the original files and will replace the original files on the LANL systems on July 1, 2026. The full erratum, available at https://nucleardata.lanl.gov/ace/lib81, has the structure laid out in Section 4.

To resolve this issue and prevent similar issues from happening again, the XCP-5 Nuclear Data Team will take the following steps:

1. `NJOY2016` has been updated to correctly handle the ENDF/B-VIII.1 files, based on the library, version, and release numbers in the file. These changes are part of the `NJOY2016.79` release, available at https://github.com/njoy/NJOY2016/releases/tag/2016.79. This version will only correctly process evaluations using this format if the library, version, and release numbers in the descriptive File 1 section indicate the evaluation is part of the ENDF/B-VIII.1 release. It is expected that a resolution to this format discrepancy will be found before the next ENDF/B release, at which point `NJOY2016` will be updated as needed.
2. The format divergence was raised at the 2025 Cross Section Evaluation Working Group meeting (January 2026), but a resolution was not found at the time. It will be raised again at future meetings.
3. The new version of NJOY, `njoy3`, will include the ability to determine the format and process it correctly. Additionally, `njoy3` will always pick one format when multiple are possible. In the case of capture γ rays, it was already decided that the File 12 format would be used instead of the File 6 format in `njoy3`. The File 12 format is clear in this situation, and using `njoy3` to produce evaluations will avoid this particular File 6 format issue.
4. The ACE library validation for Lib81 did not include MCNP simulations with photon production and transport mode. The validation workflow is under active development and will include simulations for all evaluations with all particle modes to catch issues like this in the future.

References

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