ENDF/B-VIII.1: Automated updates to masses, Q-values, thresholds and electrons

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What am I doing?

- I was asked to look into bad mass values in ENDF/B-VIII.1
  - Expanded to Q-values and thresholds (maybe)

- FUDGE also complains about ZAP for photons in the electron sub-library.

- Outline
  - Firstly, the ZAP issue
  - Secondly, bad masses
  - Thirdly, Q-values and thresholds

Electron ZAP for photons

Electron sub-library changes?

- The ENDF-6 manual, section 26.2 states:
  - In particular, the AWI and ZAP will be considered here.
  - For MT=526 (bremsstrahlung), ENDF/B-VIII.0 has ZAP=11 for the photon data instead of ZAP=0 as stated in the documentation.

26.2   Formats

The following quantities are defined:

ZA,AWR Standard material charge and mass parameters

AWI Standard projectile mass parameter

NK Number of subsections in this section (MT). Each subsection describes one reaction product (in this case, photons or electrons), or a subsection can describe the energy transfer associated with excitation or bremsstrahlung.

ZAP Product identifier: zero for photons, and 11 for electrons.

LAW Distinguishes between different representations of the product distributions:

```
1000.00000 .999241400        0        0        2        0 10026527
11.00000005.438673E-4        0        1        1        2 10026527
```

- This is similar to section 6.2:
  - Note: AWP here is AWI above.

Is anyone using the ZAP, AWI data?

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. When ZAP=0, this field can contain the energy of a primary photon. In that case, this section will contain an angular distribution (LAW=2) for the primary photon.

Changes to ENDF/B-VIII.1

- Made a branch in the git repo dubbed "fixElectronZAP11" which changes the photon ZAP=11 to 0 per the ENDF-6 documentation.

> **ZAP** Product identifier: zero for photons, and 11 for electrons.

- The masses are still that of AWI

> **AWI** Standard projectile mass parameter

> The structure of a section is:
>
> ```
> [MAT,26, MT/ ZA, AWR, 0,    0, NK,   0]HEAD
> [MAT,26, MT/ZAP, AWI, 0, LAW, NR, NP/E_int / y(E)] TAB1
> ```

- Does this seem correct?

- Should AWI really be AWP?

Bad, bad mass

There are some bad mass values in ENDF/B-VIII.0 and .1

- I have been asked to fix many of these in ENDF/B-VIII.1.

- I am comparing masses to AME 2020 values.
  - AME = Atomic Mass Evaluation.
  - I turned the AME 2020 database into a GNDS PoPs database.

- There are several types of mass issues.
  - For products with Z <= 2, mass should be nuclear mass and not atomic mass
  - Some masses are way off in an absolute sense

Z <= 2 whose masses include the electron mass

- Example of deuteron mass with electron
  - From "n + O16", MT=28, MF=6, the proton section starts as

```
1.002000+3 1.996800+0                    0          1          1          3 825 6 32
```

  - AWP * neutron_mass = 1.9968 * 1.0086649159 = 2.01410210406912 (~1875.129 MeV)
  - Masses from AME2020
    - d (h2) mass is 2.01355321275 amu (~1874.618 MeV)
      - 1875.129 - 1874.618 = 0.511
    - H2 mass is 2.01410177784 amu (~1875.129 MeV)

- I found ~1279 protares/isotopes with this problem

Some masses are way off

- Example from gammas/g-006_C_012.endf for B10 (MF=6, MT=111)
  - Here is what is in the file

```
4.010000+3 1.004200+1          0          1          1          2 625 6111
```

  - This mass is 107 MeV/c^2 too heavy
  - AME 2020 value is 9.9269209

- There are 79 evaluations/isotopes whose masses are off by at least 4 MeV/c^2
  - Some of the worst are off by (in MeV/c^2): 1018.6 1863.1, 8388.2 and -107.5.
  - This is an absolute test
  - 1661 evaluations/isotopes whose masses are off by at least 0.4 MeV/c^2

- I also did a relative test
  - Current reporting is for 1e-5 relative difference
    - abs(fileMass / PoPsMass – 1) > 1e-5.
  - I found "2460" evaluations/isotopes that failed this test.

What to do?

- If I have a criteria for masses that should be fixed, I can replace just the masses.

- Here is an example of the information I have (from neutrons/n-008_O_016.endf):

```
ZA                      mass ratio    MT     MF        line
-------------------------------------------------------------
1002:

                           1.9968     32      6         186
                           1.99626     5      6        1101
```

- I would only change the masses and leave the rest of the file the same except for a note in the documentation about what was done.
  - If I change a mass for one ZA in a file, do I change all masses for that ZA in that file.
  - I would probably not change the masses in the resonance data (MT=151).

- All changes would go into one git branch.

Q-values and thresholds

Q-values and thresholds

- I have not tested these yet.

- What is needed if anything?

An aside

- The ENDF-6 manual states:

| 151 | (n,RES) | Resonance parameters that can be used to calculate cross sections at different temperatures in the resolved and unresolved en- | Incident neutrons only. |

- What about charged particles?