OAK RIDGE National Laboratory

Format Proposal for Isotopic Distribution in TSL Files for ENDF/B-VIII.1

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Proposed Format: MF7/MT451 File

- A ‘footer’ file for ENDF6-format TSL files
- Would contain several pieces of pertinent information for the scattering atom:
  - Number of scattering atoms in molecule
  - Isotopic distribution within scattering atom
  - Free atom and atomic weight ratios for each isotope
- Will not require significant changes to processing codes or to other sections of the MF7 file

Proposed Format

ZA,AWR Standard charge and mass parameters.

NA Number of unique scattering atoms in the material.

NI Number of unique isotopes in the scattering system.

IZA ZA number corresponding to a specific isotope in the neutron sub-library.

ILIS LIS flag corresponding to a specific isomer of the isotope in the neutron sub-library.

IFR Isotopic fraction of isotope in the scattering system.

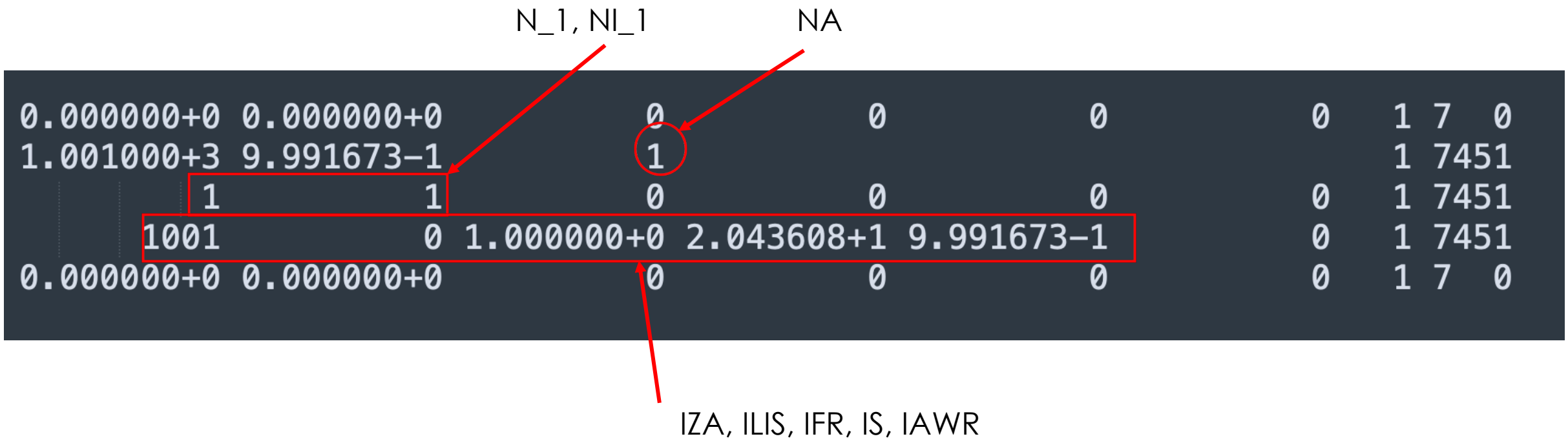
ISF Free atom scattering cross section of this isotope.

IAWR Atomic weight ratio of this isotope.

The structure of the section is

```
[MAT, 7, 451 /   ZA,   AWR,   NA,    0,   0,  0] HEAD
[MAT, 7, 451 /   N1,   NI1,    0,    0,   0,  0] LIST
[MAT, 7, 451 /  IZA,  ILIS,  IFR,  ISF, IAWR,  0] LIST
   ----------------------------
<continue with LIST records for all isotopes NIi >
   ----------------------------
[MAT, 7, 451 / N2, NI2,    0,    0,  0,  0] LIST
   ----------------------------
<continue with LIST records for all remaining NAi >
   ----------------------------
[MAT, 7,   0 /    0,     0,   0,    0,  0,  0] SEND
```

Example 1 – HinH2O



Example 2 – ZrinZrH2

```
 0.000000+0 0.000000+0          0          0          0          0  58 7  0
 1.580000+2 9.043999+1          1          0          0          0  58 7451
          1          5          0          0          0          0  58 7451
      40090          0 5.145000-1 4.987461+0 8.913240+1          0  58 7451
      40091          0 1.132000-1 9.488273+0 9.012470+1          0  58 7451
      40092          0 1.719000-1 6.751001+0 9.111550+1          0  58 7451
      40094          0 1.728000-1 8.222414+0 9.309960+1          0  58 7451
      40096          0 2.760000-2 3.721314+0 9.508440+1          0  58 7451
 0.000000+0 0.000000+0          0          0          0          0  58 7  0
```

Example 3 – SiO2-beta

```
0.000000+0 0.000000+0          0          0          0          0  49 7  0
1.490000+2 2.784423+1          2                                    49 7451
         1          3          0          0          0          0  49 7451
     14028          0 9.223000-1 2.120000+0 2.773700+1          0  49 7451
     14029          0 4.670000-2 2.780000+0 2.872800+1          0  49 7451
     14030          0 3.100000-1 2.640000+0 2.971600+1          0  49 7451
         2          3          0          0          0          0  49 7451
      8016          0 9.976200-1 3.744801+0 1.585751+1          0  49 7451
      8017          0 3.800000-4 3.742671+0 1.685310+1          0  49 7451
      8018          0 2.000000-3 3.846775+0 1.784450+1          0  49 7451
0.000000+0 0.000000+0          0          0          0          0  49 7  0
```

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