

Proposed Generalized Header File for TSLs

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Overview

- Several recent issues have been raised over the past few years regarding:
 1. Inconsistent definitions for number of scattering atoms between incoherent elastic and inelastic (MT2 and MT4 files, respectively) in the same MF7 file
 2. Isotopic distribution of primary scattering atoms
- Processing codes handle these potential issues in different ways
 1. NJOY internally corrects for number of scattering atoms in MT2 by reading in flag from MT4
 2. NJOY and AMPX both manually define isotopes to link TSL files
- Preferred solution would be to automate this to reduce possibility of user error

Proposed Solution – MF7/MT1 file

- A generalized ‘header’ file for ENDF6-format TSL files
- Would contain pertinent information for the scattering atom
 - Number of scattering atoms in molecule (2 for H in polyethylene, 8 for H in Lucite, etc.)
 - Isotopic distribution within scattering atom (100% ^{238}U for U-in- UO_2 , natural Silicon for Si-in-SiC, etc.)
- Should not require significant changes to processing codes or to other sections in MF7 file
 - Some information would be redundant (e.g., scattering atoms in molecule is defined in MT4) and *could* be consolidated into MT1 file

Preliminary Examples – H in CH2

N_atom N_isotopes ZAID, abundance, σ_b

0.000000+0	0.000000+0	0	0	0	0	37	0	0
2	1					37	7	1
1001	1.000000+0	8.202000+1				37	7	1
0.000000+0	0.000000+0	0	0	0	0	37	7	0
1.370000+2	9.991673-1	2	0	0	0	37	7	2
1.640400+2	0.000000+0	0	0	1	11	37	7	2
11	2					37	7	2
2.936000+2	2.734691+1					37	7	2
0.000000+0	0.000000+0	0	0	0	0	37	7	0
1.370000+2	9.991673-1	0	1	0	0	37	7	4
0.000000+0	0.000000+0	0	0	12	1	37	7	4
4.097584+1	1.976285+2	9.991673-1	5.000001+0	0.000000+0	2.000000+0	37	7	4
1.000000+0	4.739180+0	1.189800+1	0.000000+0	0.000000+0	1.000000+0	37	7	4

Self Consistent
N_atom* σ_b

Self Consistent σ_f

Self Consistent N_atom

Preliminary Examples – Si in SiC

N_atom

N_isotopes

ZAID, abundance, σ_b

0.000000+0	0.000000+0	0	0	0	0	43	0	0
1	3					43	7	1
14028	9.223000-1	2.120000+0	14029	4.670000-2	2.780000+0	43	7	1
14030	3.100000-2	2.640000+0				43	7	1
0.000000+0	0.000000+0	0	0	0	0	43	7	0
1.430000+2	2.784400+1	1	0	0	0	43	7	2
3.000000+2	0.000000+0	7	0	1	685	43	7	2
685	1					43	7	2
1.066463-3	3.928144-3	2.132926-3	3.928144-3	3.199390-3	6.916109-3	43	7	2
..								
2.271338-1						43	7	2
						43	7	0
1.430000+2	2.784400+1	0	1	0	0	43	7	4
0.000000+0	0.000000+0	0	0	6	0	43	7	4
2.019294+0	1.976285+2	2.784400+1	5.000001+0	0.000000+0	1.000000+0	43	7	4

Self Consistent σ_f

Self Consistent N_atom

Discussion

- Is this something the community would like?
 - These issues are not present in GNDS
- How should checking codes be changed to account for potential duplicate information?
- What other information should be included?

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