Thermal Data Testing at LLNL

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Thermal Library Study

LLNL-TR-645096, "A Comparative Study of COG Thermal Libraries", available on http://cog.llnl.gov/pdf/LLNL-TR-645096.

What we learned:

- Problems with normalization inconsistencies

- Problems with some BNL ACE files

- Problems with some ENDF/B-VI.0 data

- Problems with some JEFF3.1.1 data

- SABtoCOG and NJOY/SAB.ACEtoCOG produce consistent results

Normalization inconsistencies

- For benzene (C6H6):

    – T.ENDFB7R0 transitions smoothly across the thermal boundary
    – T.ENDFB7R0.LANL is off by a factor of 6
   – T.ENDFB7R1.LANL is off by a factor of 12
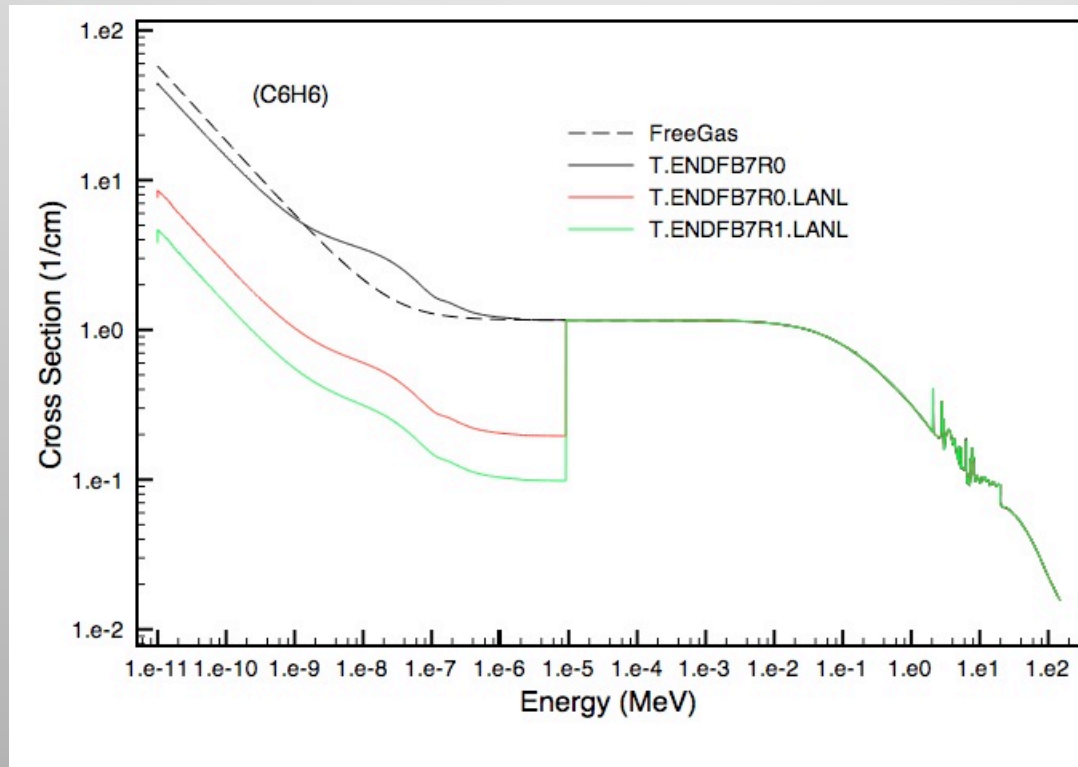
Normalization factors – summary

|	T.ENDFB3R0	T.ENDFB6R0	T.ENDFB6R2	T.ENDFB7R0	T.ENDFB7R0.BNL	T.ENDFB7R0.LANL	T.ENDFB7R1	T.ENDFB7R1.BNL	T.ENDFB7R1.LANL	T.IAEA2007	T.JEF2.2	T.JEFF3.0	T.JEFF3.1	T.JEFF3.1.1	T.JEFF3.1.2
Al				1	1	1	1	1	1						
Be	1	1	1	1	1	1	1	1	1		1	1	1	1	1
Be.BeO				1	2	1	1	2	1						
BeO	1	1	1											6.4	
C	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Ca.CaH2														1	1
C6H6	1			1	12	6	1	12	12						
D.D2O	0.5	0.5		0.5	1	1	0.5	1	1	0.5	0.5	0.5	0.5	1	0.5
Fe56				1	1	1	1	1	1						
H.CH2	0.5	0.5		0.5	1	1	0.5	1	1		0.5	0.5	0.5	1	0.5
H.CaH2														1	1
H.CeH2										0.5					
H.H2O	0.5	0.5	0.5	0.5	1	1	0.5	1	1	0.5	0.5	0.5	0.5	1	0.5
H.TiH2										0.5					
H.YH2										0.5					
H.ZrH	1	1	1	1	1	1	1	1	1	1			1	2	1
Mg													1		1
O.BeO				1	2	1	1	2	1						
O.UO2				1	2	1	1	2	1						
SiO2							1.6		3.3						
U.UO2				1	1	1	1	1	1						
UO2	1														
Zr.ZrH	1	1	1	1	1	1	1	1	1						

Problems with ENDF/B-VI.0 data

- Extra edge structure – non-physical "saw-teeth" – observed for:

    – Be, BeO and C (shown)
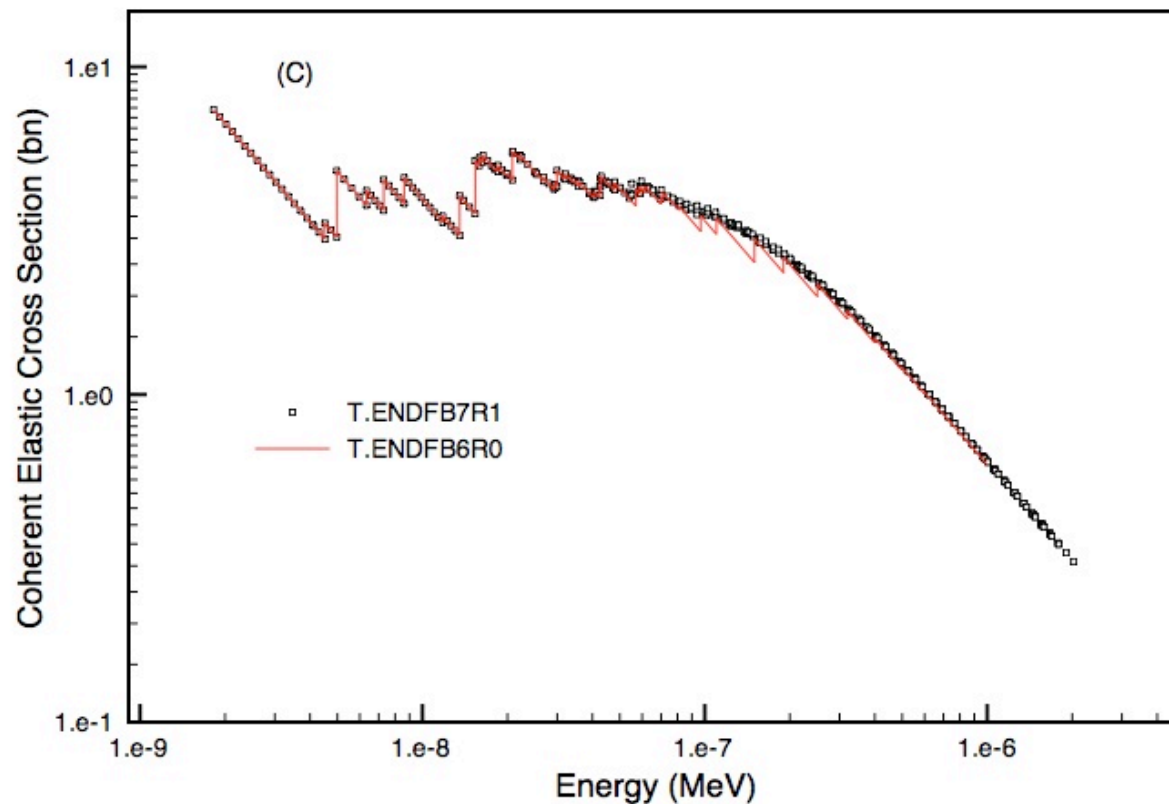
Problems with JEFF3.1.1 data

- There appears to be problems for JEFF3.1.1 data for:

  – BeO (shown) and H.ZrH
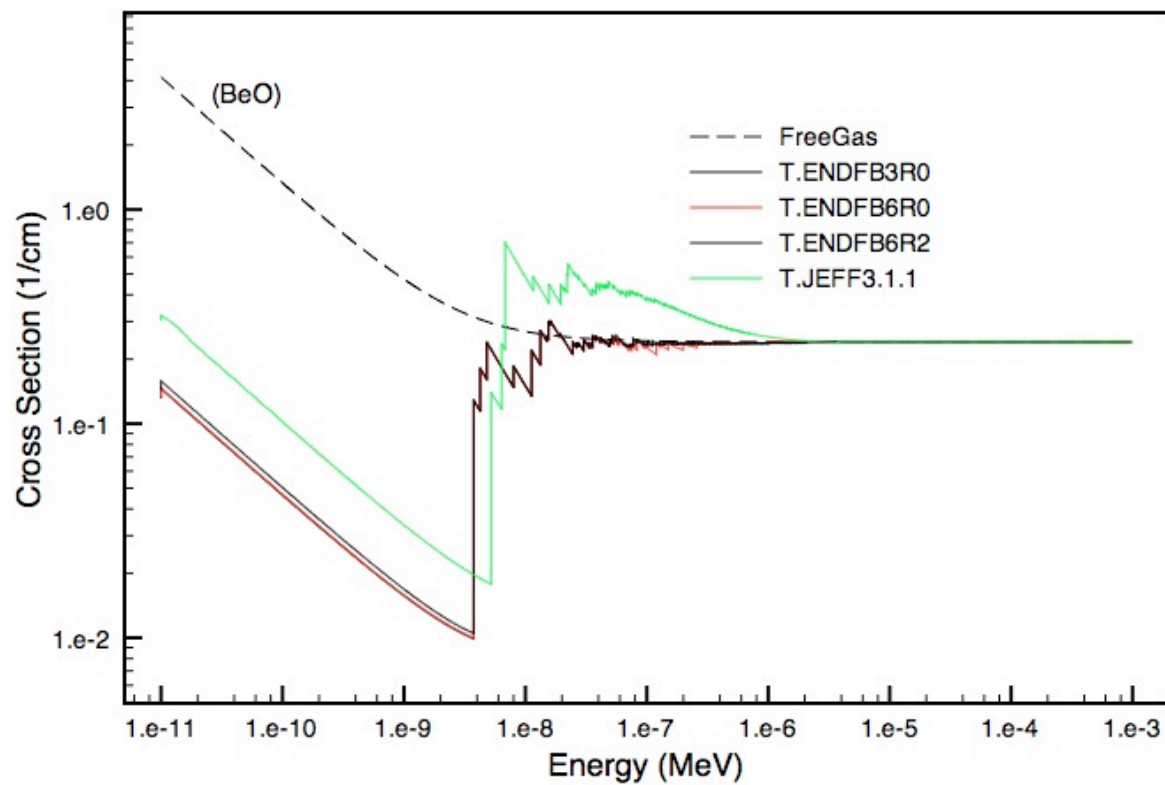
Conclusion

- No problems encountered "processing" File 7 or ACE formats

- SABtoCOG

- NJOY/SAB.ACEtoCOG

Produce consistent results