

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:

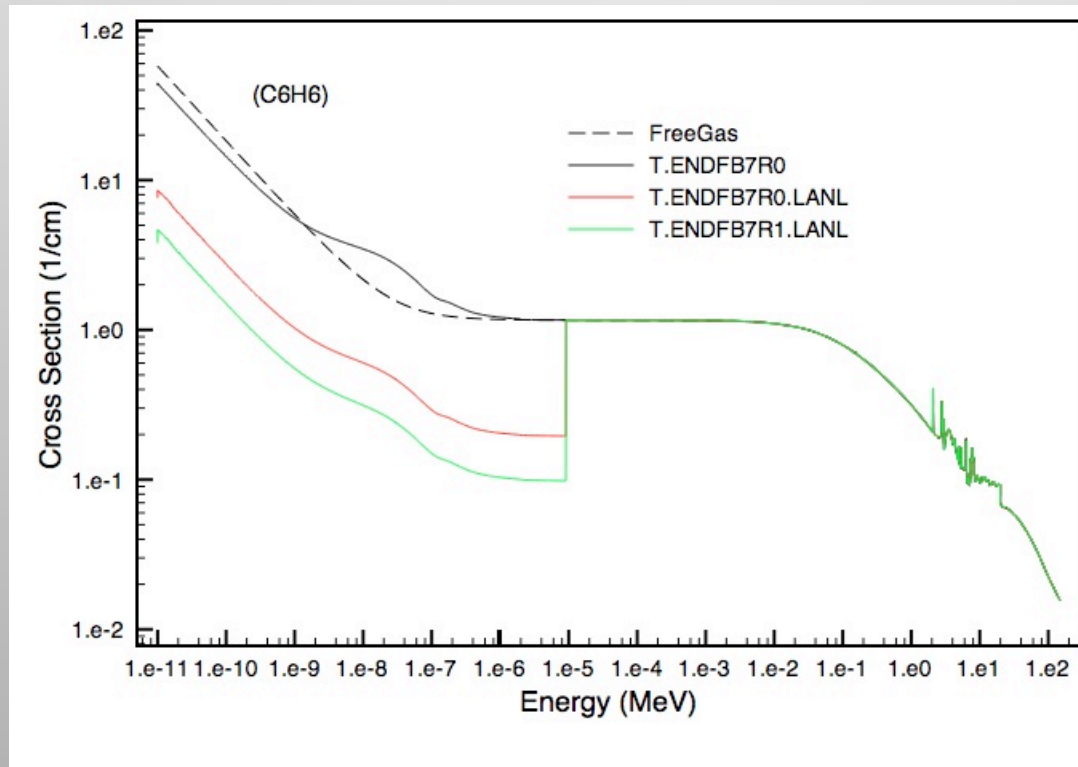
- Problems with normalization inconsistencies
- Problems with some BNL ACE files
- Problems with some ENDF/B-VI.0 data
- Problems with some JEFF3.1.1 data
- SABtoCOG and NJOY/SAB.ACETO COG produce consistent results

Since then we've noticed:

- Hawari and JEFF3.2 corrections for SiO₂, CaH₂ and ZrH
- No BeO in JEFF3.2
- Problems with CAB ENDF (File 7) data near 1 eV

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

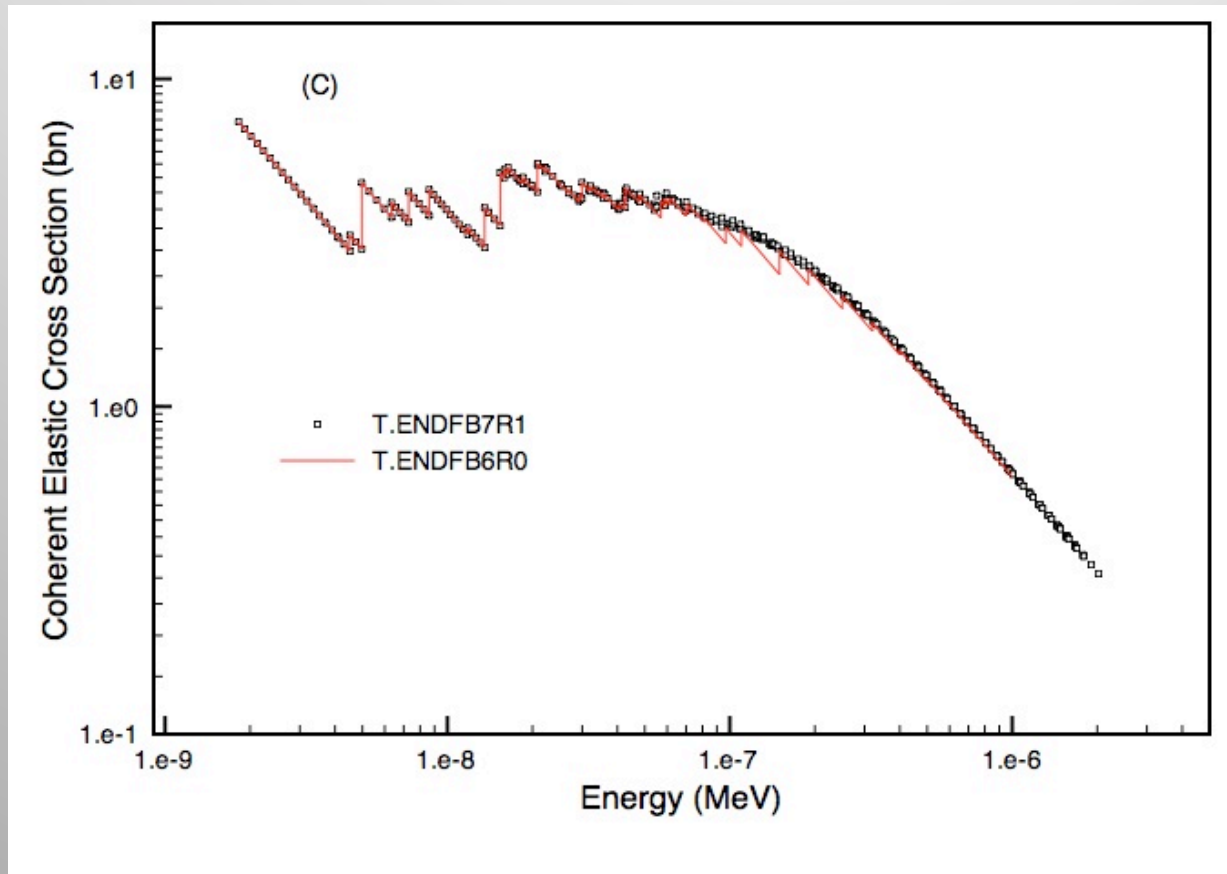


Normalization factors – summary

	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	T.JEFF3.2	T.NCSU (Hawari)	T.CAB2015
Al				1	1	1	1	1	1									
Be	1	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	1		
C.SiC																	1	
Ca.CaH2													1		1	2		
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	1		1
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	1		
H.CaH2													1		1	2		
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	1		1
H.TiH2										0.5								
H.YH2										0.5								
H.ZrH	1	1	1	1	1	1	1	1	1	1			1	2	1	2		
Mg													1		1	1		
O.BeO				1	2	1	1	2	1									
O.D2O																		1
O.UO2				1	2	1	1	2	1									
Si.SiC																	1	
SiO2							1.6		3.3								1	
U.UO2				1	1	1	1	1	1									
UO2	1																	
Zr.ZrH	1	1	1	1	1	1	1	1	1									

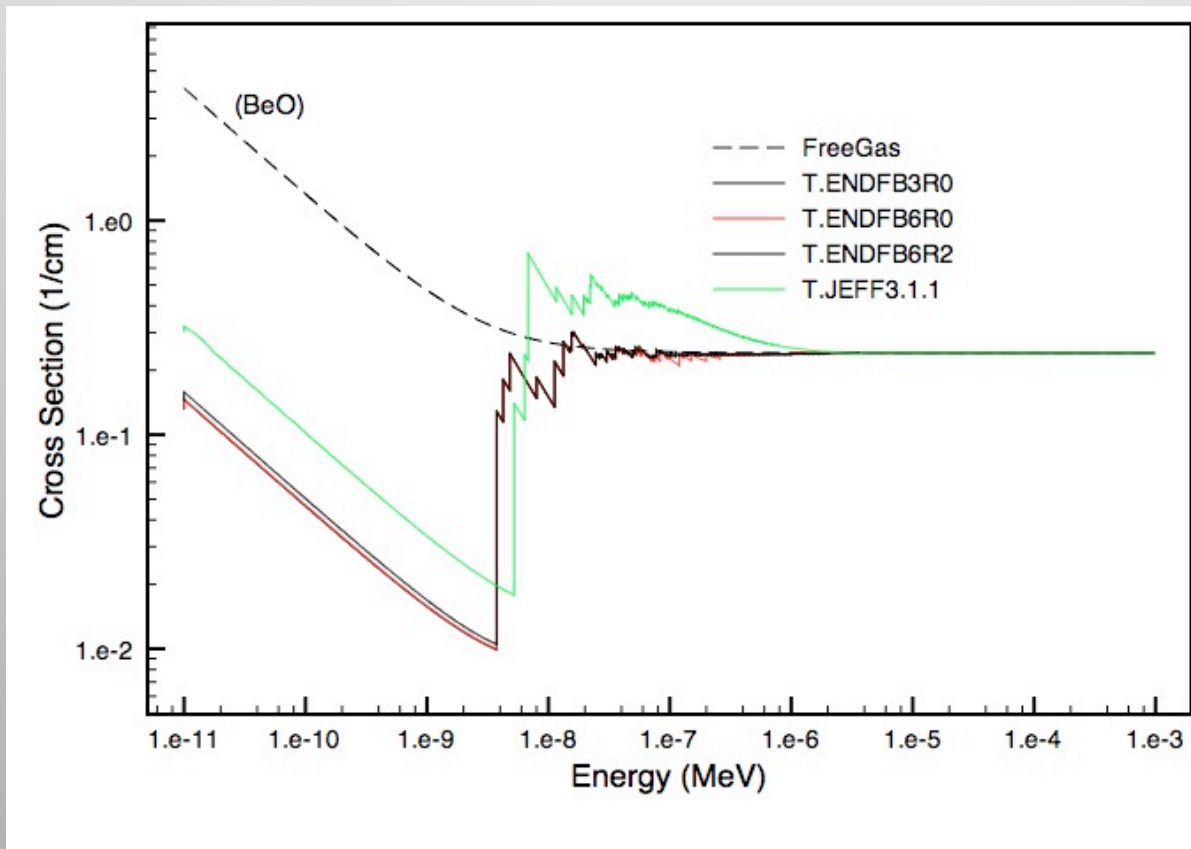
Problems with ENDF/B-VI.0 data

- Extra edge structure – non-physical “saw-teeth” – observed for:
 - Be, BeO and C (shown)



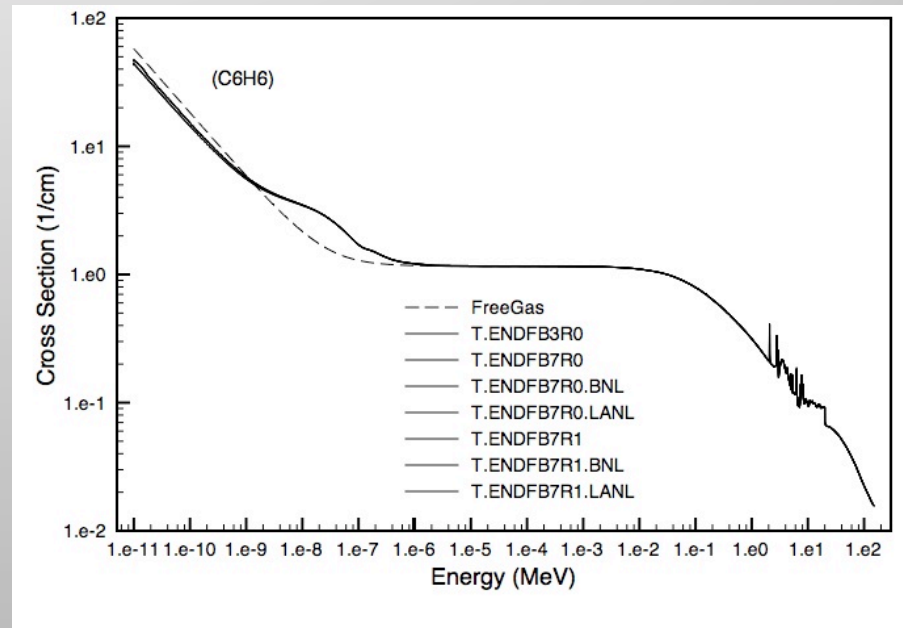
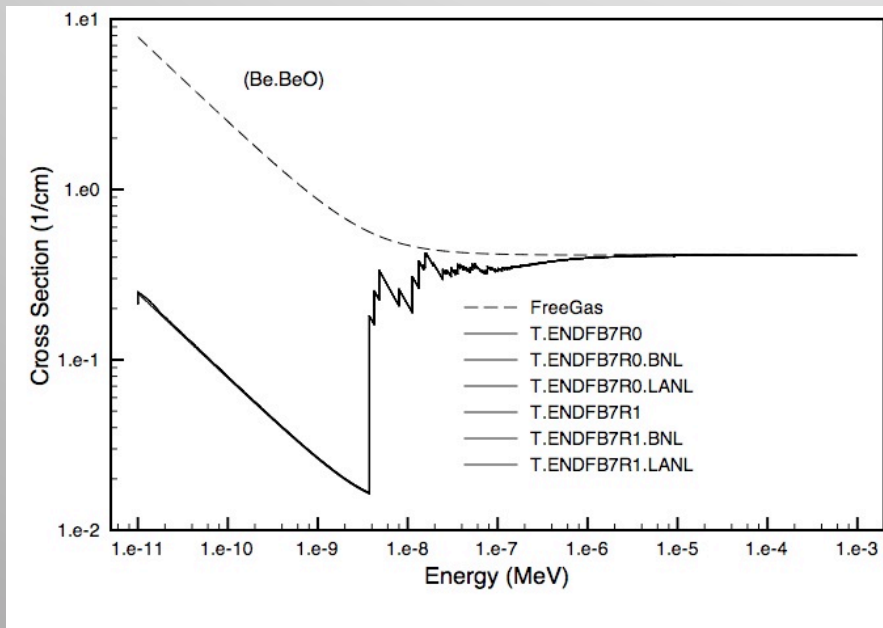
Problems with JEFF3.1.1 data

- There appears to be problems for JEFF3.1.1 data for:
 - BeO (shown) and H.ZrH



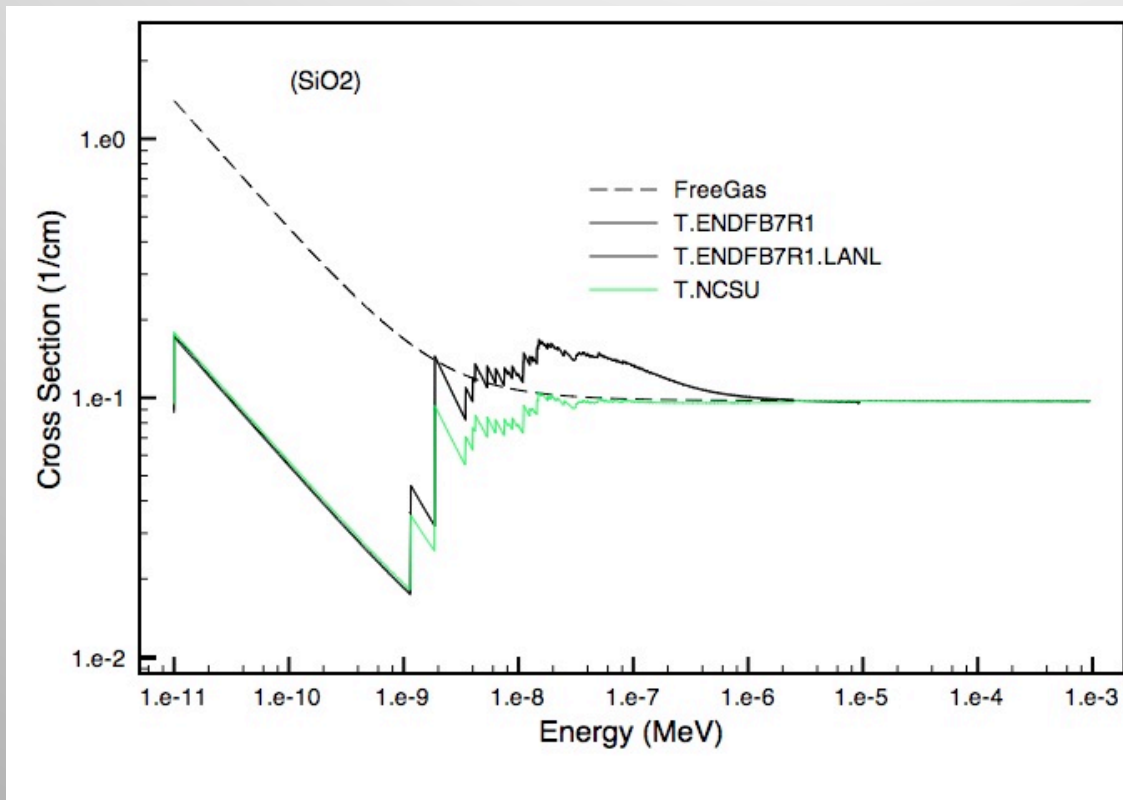
Conclusion

- No problems encountered “processing” File 7 or ACE formats
 - SABtoCOG
 - NJOY/SAB.ACEtoCOG
- } Produce consistent results



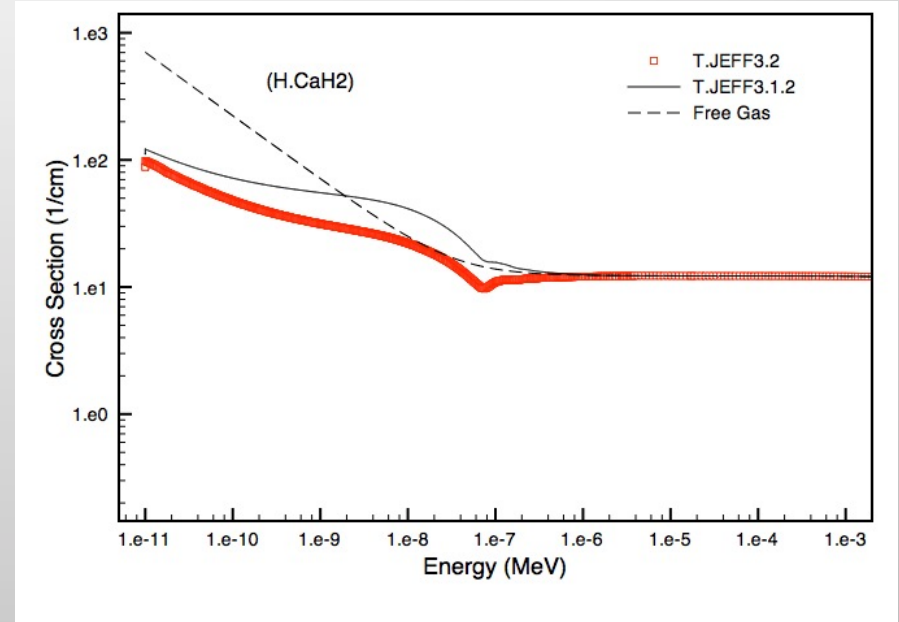
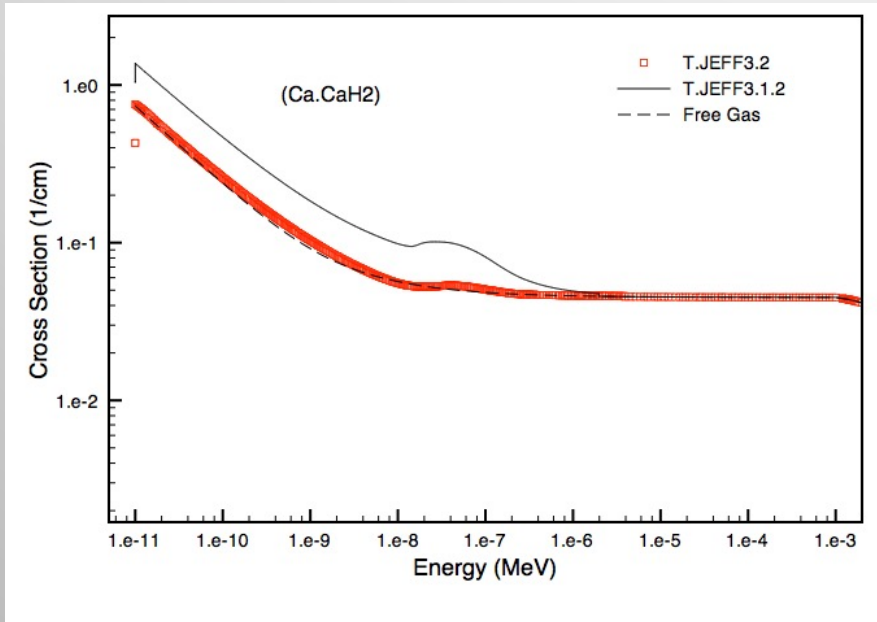
Recent work (1)

- Hawari corrections for SiO₂



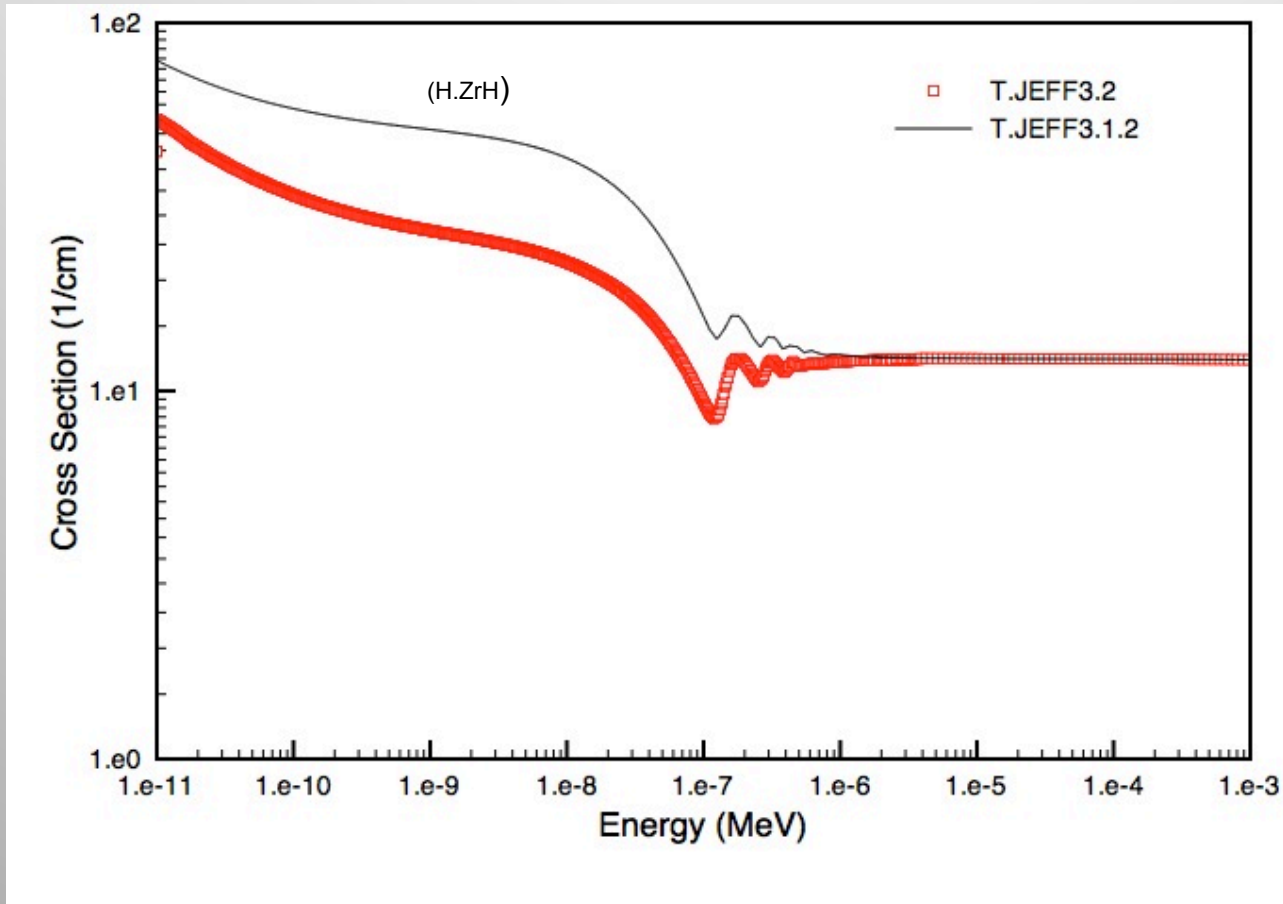
Recent work (2)

- JEFF3.2 corrections for CaH_2



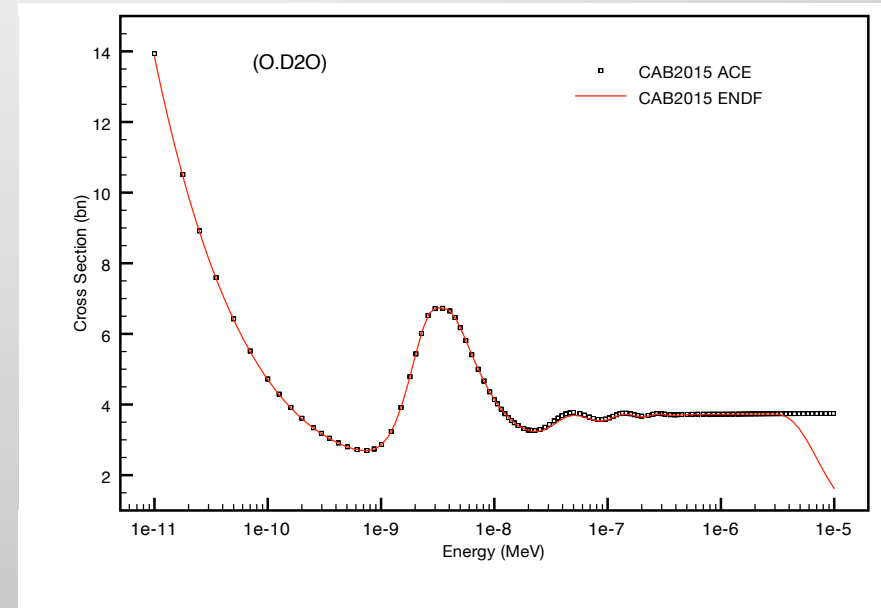
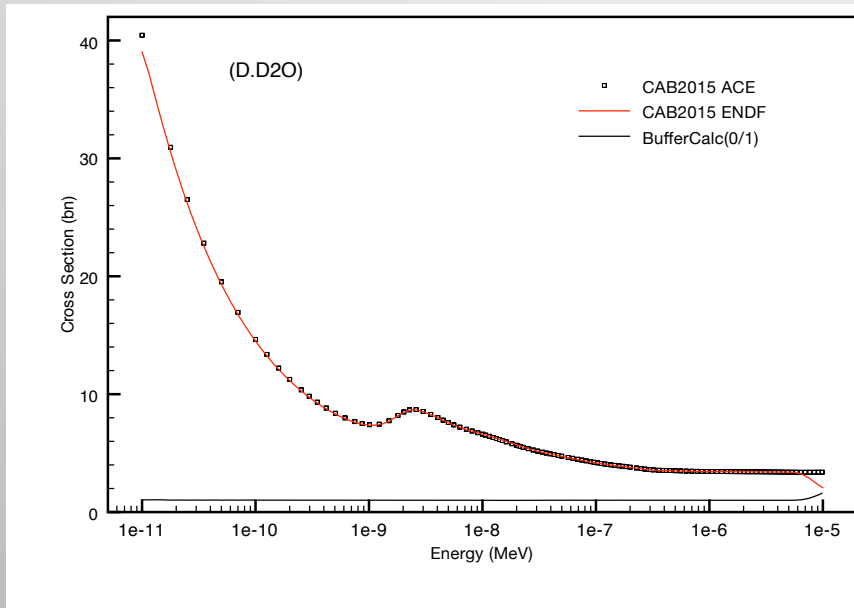
Recent work (3)

- JEFF3.2 corrections for ZrH



Recent work (4)

- Centro Atómico Bariloche (CAB) data for D₂O (and H₂O)



- ACE files look good while ENDF (File 7) trail off above 1 eV

Recommendations

- Evaluators should normalize their data and ensure a smooth transition across the thermal boundary
- This check should be added to ENDF “checker codes”