

Library comparisons of Neutron Capture Rates

Boris Pritychenko
National Nuclear Data Center
November 6, 2007



SIXTY YEARS
OF DISCOVERY
1947-2007

BROOKHAVEN
NATIONAL LABORATORY



Project Motivation

- ❑ ENDF keV region astrophysics applications
- ❑ JENDL-3.3 calculations always agree with ENDF
- ❑ NNDC group project under the same umbrella
- ❑ Complimentary
- ❑ ENDF validation

TABLE I. Maxwellian-averaged (n,γ) cross sections (barns) from the evaluated nuclear reaction libraries, Atlas of Neutron Resonances and Bao *et al.* compilation.

Nucleus	ENDF/B-VII.0	JEFF-3.1	JENDL-3.3	ENDF/B-VI.8	Atlas	Bao <i>et al.</i>	Recommended Library	Recommended Value
1-H-1	1.53E-04	1.53E-04	1.53E-04	1.53E-04		2.54E-04	ENDF/B-VII.0	1.53E-04
1-H-2	2.03E-06	2.03E-06	2.37E-06	2.03E-06			ENDF/B-VII.0	2.03E-06
1-H-3								
2-He-3	2.51E-08	2.51E-08	1.73E-05	2.51E-08	7.70E-06	7.60E-06	JENDL-3.3	1.73E-05
2-He-4								
3-Li-6	3.39E-05	3.39E-05	3.91E-05				ENDF/B-VII.0	3.39E-05
3-Li-7	4.68E-05	4.68E-05	3.96E-05	4.68E-05	3.93E-05	4.20E-05	JENDL-3.3	3.96E-05
4-Be-7								
4-Be-9	1.20E-04	1.47E-05	6.74E-06	1.20E-04			JEFF-3.1	1.47E-05
5-B-10	4.36E-04	4.36E-04	4.45E-04	4.36E-04			ENDF/B-VII.0	4.36E-04
5-B-11	6.59E-05	6.59E-05	5.64E-05	6.59E-05			JENDL-3.3	5.64E-05
16-C-12	1.57E-06	1.57E-06	1.97E-05	1.57E-06	1.54E-05	1.54E-05	Bao	1.54E-05
7-N-14	6.87E-05	6.87E-05	7.29E-05	6.87E-05		4.10E-05	JENDL-3.3	7.29E-05
7-N-15	9.70E-06	9.70E-06	7.49E-06		5.32E-06	5.80E-06	JENDL-3.3	7.49E-06
8-O-16	1.72E-07	1.72E-07	3.51E-05	1.72E-07	3.80E-05	3.80E-05	JENDL-3.3	3.51E-05
8-O-17	4.75E-06	4.75E-06					ENDF/B-VII.0	4.75E-06
9-F-19	4.37E-03	4.37E-03	5.73E-03	6.94E-03	6.20E-03	5.80E-03	JENDL-3.3	5.73E-03
11-Na-22	8.21E-03	8.21E-03					ENDF/B-VII.0	8.21E-03
11-Na-23	1.83E-03	1.83E-03	1.74E-03	1.83E-03		2.10E-03	ENDF/B-VII.0	1.83E-03
12-Mg-24	3.79E-03	3.79E-03	3.79E-03		1.70E-03	3.30E-03	ENDF/B-VII.0	3.79E-03
12-Mg-25	5.29E-03	5.29E-03	5.29E-03		4.40E-03	6.40E-03	ENDF/B-VII.0	5.29E-03
12-Mg-26	8.65E-05	8.65E-05	8.65E-05		1.60E-03	1.26E-04	Bao	1.26E-04
13-Al-27	3.31E-03	3.31E-03	3.35E-03	4.78E-03		3.74E-03	ENDF/B-VII.0	3.31E-03
14-Si-28	3.61E-03	3.61E-03	1.69E-03	3.61E-03	1.19E-03	2.90E-03	ENDF/B-VII.0	3.61E-03
14-Si-29	7.77E-03	5.76E-03	5.76E-03	7.77E-03	6.58E-03	7.90E-03	ENDF/B-VII.0	7.77E-03
14-Si-30	4.43E-03	5.75E-03	5.75E-03	4.43E-03	1.34E-03	6.50E-03	JENDL-3.3	5.75E-03
15-P-31	1.29E-02	1.63E-03	1.63E-03			1.74E-03	JENDL-3.3	1.63E-03
16-S-32	5.66E-03	5.66E-03	5.66E-03	4.23E-03	4.60E-03	4.10E-03	ENDF/B-VI.8	4.23E-03
16-S-33	2.28E-03	2.28E-03	2.28E-03			7.40E-03	ENDF/B-VII.0	2.28E-03
16-S-34	2.33E-04	2.33E-04	2.33E-04			2.26E-04	ENDF/B-VII.0	2.33E-04
16-S-36	6.45E-04	6.45E-04	6.45E-04		1.87E-04	1.71E-04	Bao	1.71E-04
17-Cl-35	7.54E-03	7.54E-03	8.54E-03	8.54E-03		1.00E-02	ENDF/B-VI.8	8.54E-03
17-Cl-37	2.06E-03	2.06E-03	2.47E-03	2.48E-03		2.15E-03	ENDF/B-VII.0	2.06E-03
18-Ar-36	8.84E-03	8.84E-03				9.00E-03	ENDF/B-VII.0	8.84E-03
18-Ar-38	1.60E-04	1.60E-04				3.00E-03	Bao	3.00E-03
18-Ar-40	2.25E-03	2.25E-03	2.25E-03	3.59E-03	5.80E-05	2.60E-03	ENDF/B-VII.0	2.25E-03

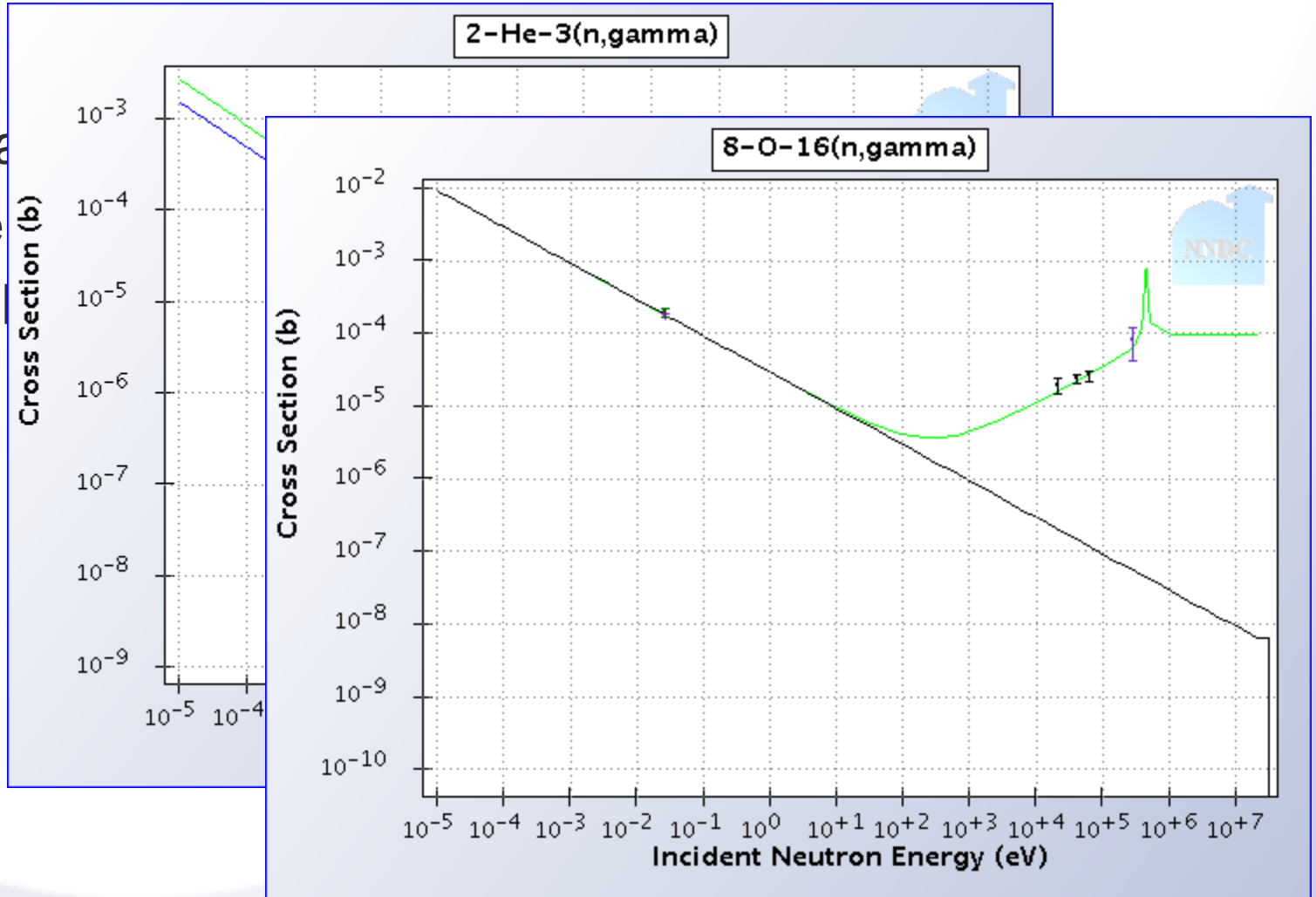


Comparison of Evaluated Libraries

- ❑ 400 different neutron materials in four libraries
- ❑ ^{240}Cm and ^{247}Bk are not in ENDF/B-VII.0
- ❑ Evaluated data for (n,γ) , (n,tot) , (n,el) , (n,inel) , (n,f) , $(n,2n)$, (n,p) , (n,α) reactions was compared with experimental results using Sigma Web interface
- ❑ 3200 spectra were analyzed in total, painstaking but very productive effort
- ❑ Possible problems with data were rated by severity into three categories

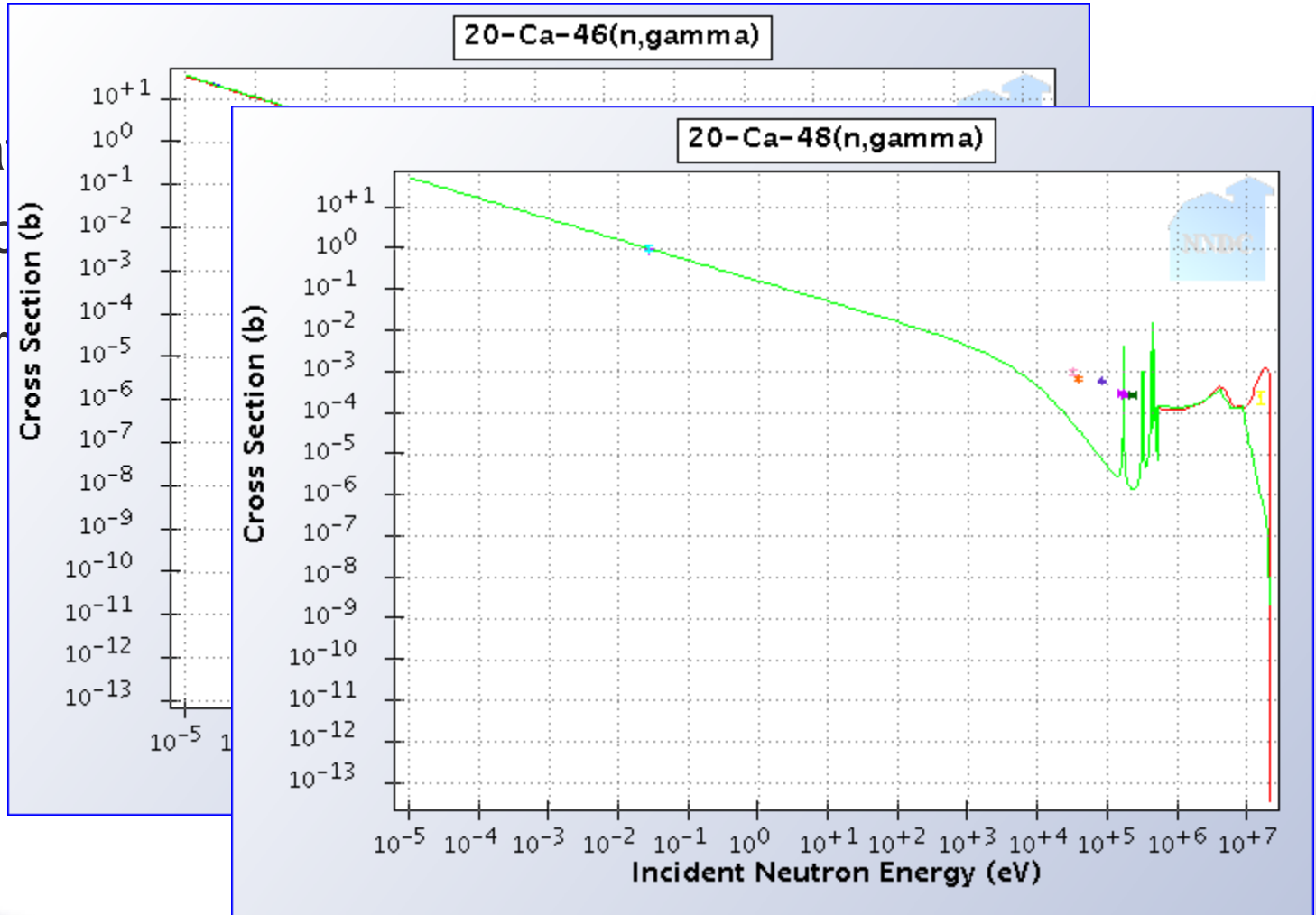
(n,γ) Reactions I

□ Evaluate the high energy



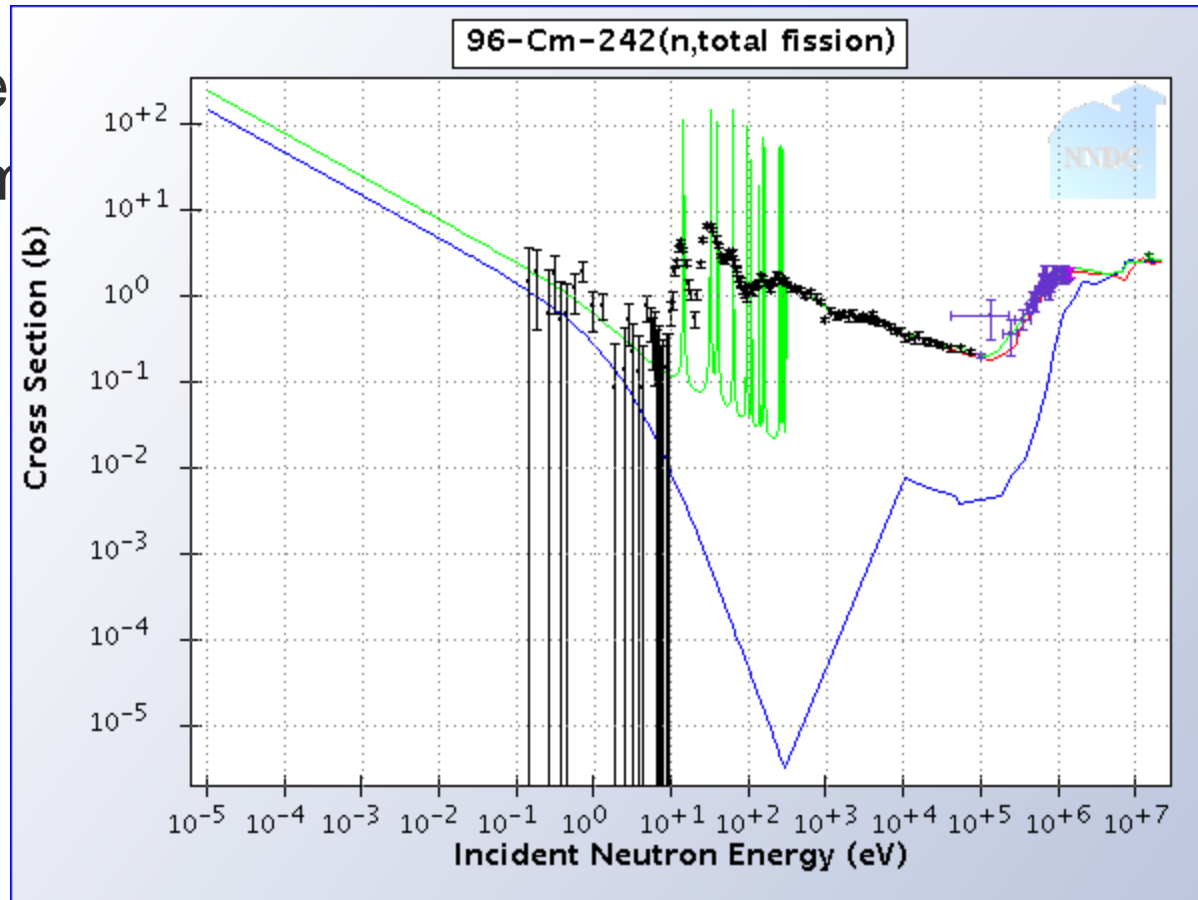
(n,γ) Reactions II

- Macroscopic cross section
- Large cross section



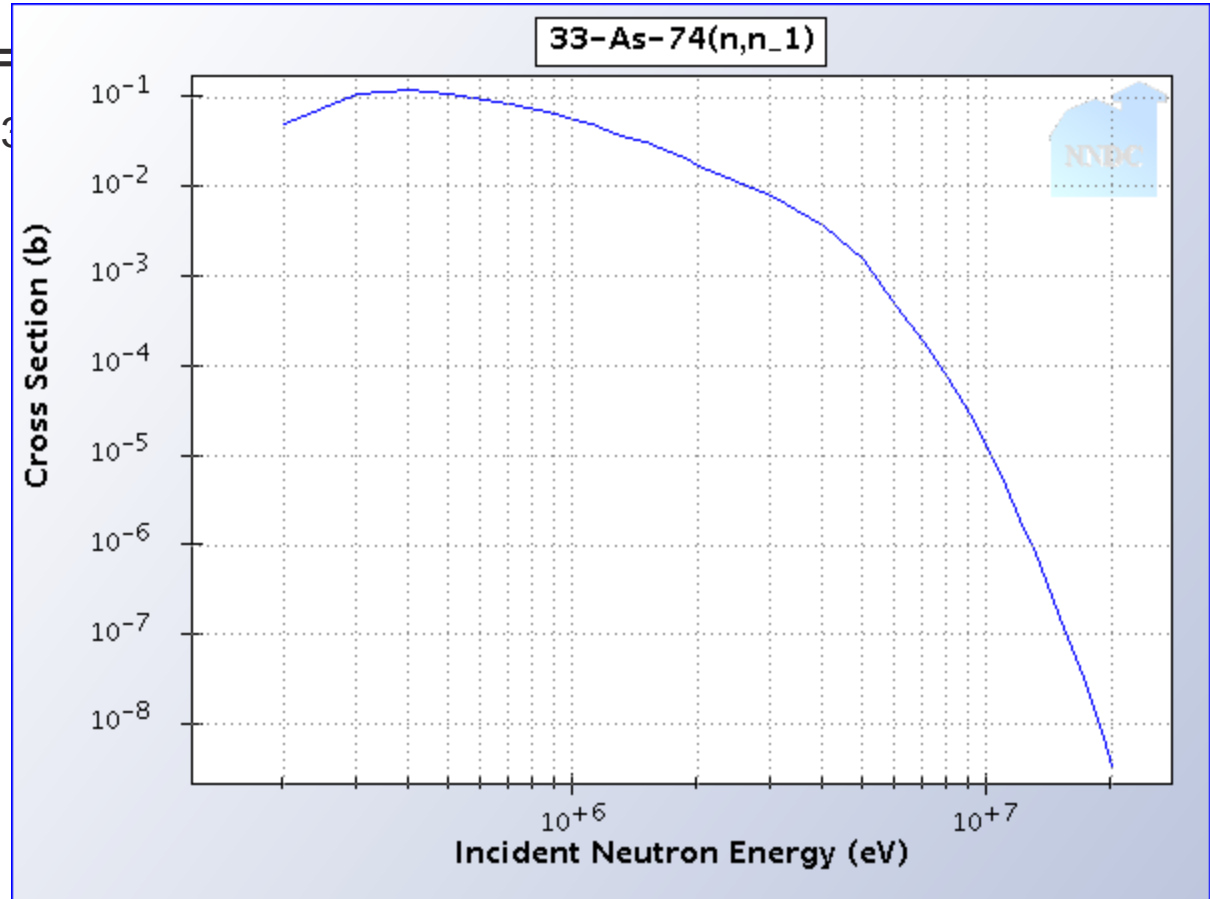
(n,fission) reactions

- Older e problem



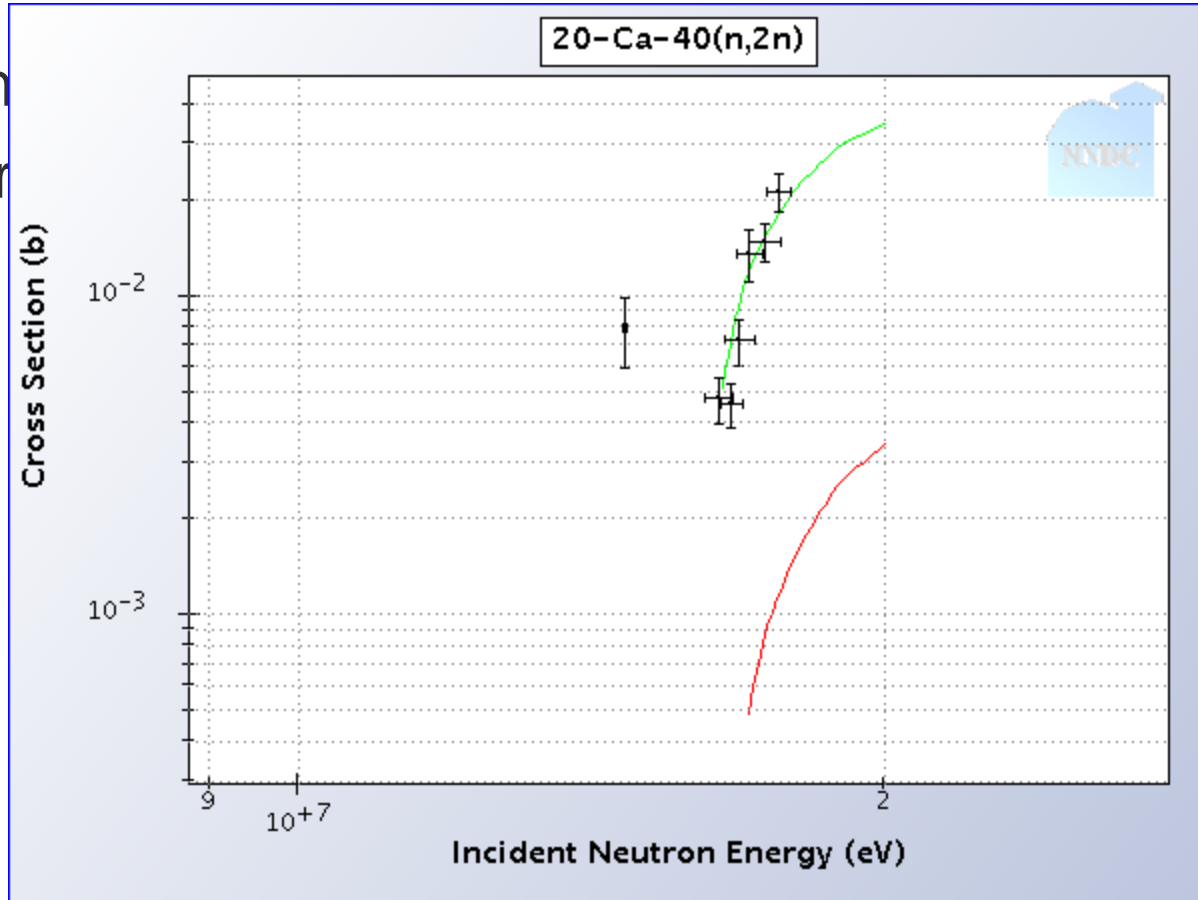
(n,inel) reactions

□ MF=3, MT=
 ^{74}As , ^{90}Y , ^{23}Na



(n,2n) reactions

- Adopting good practice



ENDF/B-VII.0 Validation

- All problems were separated into three categories by severity (1-big, 2-medium, 3-minor)

Severity	1	2	3
(n,tot)	3	12	15
(n,el)	0	6	21
(n,inel)	4	4	13
(n, α)	1	14	25
(n, γ)	5	8	12
(n,f)	3	1	2
(n,p)	0	11	11
(n,2n)	1	8	17
Total	17	64	116

Conclusion & Outlook

- ❑ Severity 1 should be addressed in ENDF/B-VII.1 release
- ❑ Severity 2 should be further investigated and possibly addressed in future releases
- ❑ Preliminary rating of evaluated cross sections: JENDL-3.3, ENDF/B-VII.0, JEFF-3.1, ENDF/B-VI.8
- ❑ ENDF library quality assurance (QA) group has to be established
- ❑ Zip file with 197 potentially problematic spectra is available for CSEWG