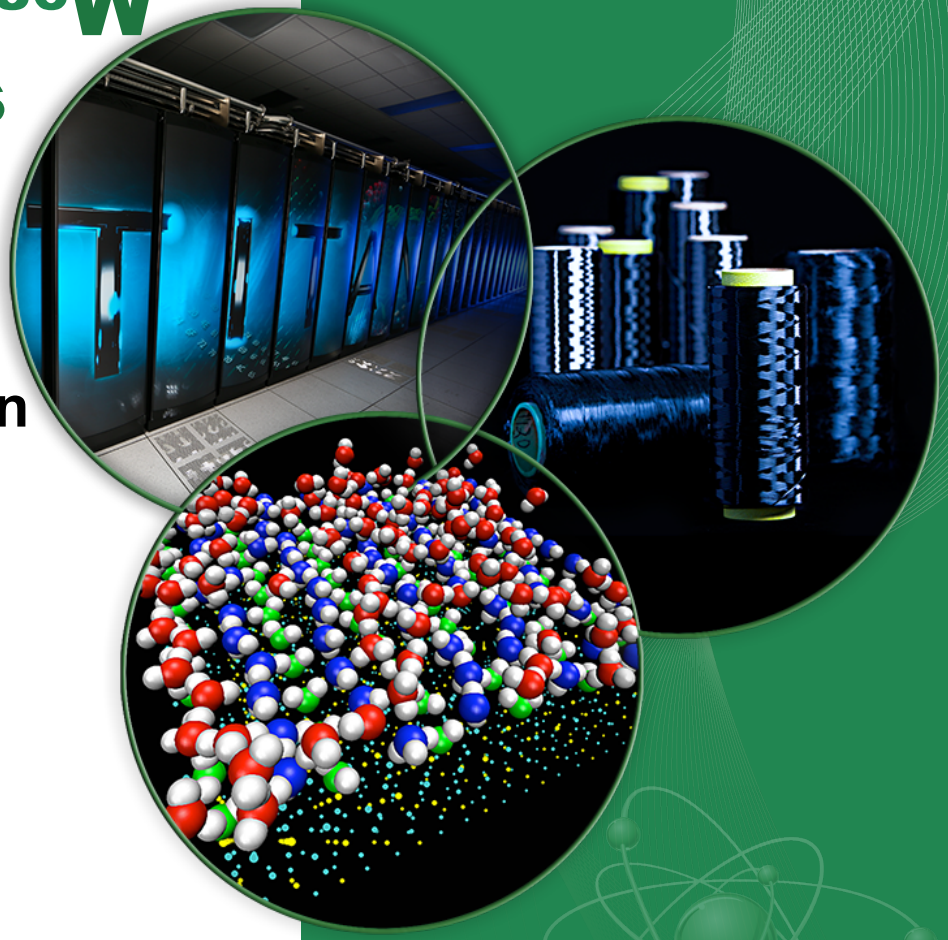
Nuclear Data Evaluations for Tungsten $^{182\text{-}184,186}$W and ^{63,65}Cu isotopes



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NCSP Annual Technical Program
Lawrence Livermore National Laboratory
March 2015

Outline

- Nuclear Data Evaluation Overview
- Evaluation Procedure with SAMMY
  - Details on the differential data evaluation procedure (cross section from resonance parameters)
  - Link to benchmarks (integral data)
- (Completed) Evaluation work on ^{183}W (Pigni)
- (Completed) Evaluation work on ^{182,184,186}Tungsten (Leal)
- (Completed) Evaluation work on ^{63,65}Cu (Sobes)
- (On going) Evaluation work on Ca (Pigni)
- Conclusions

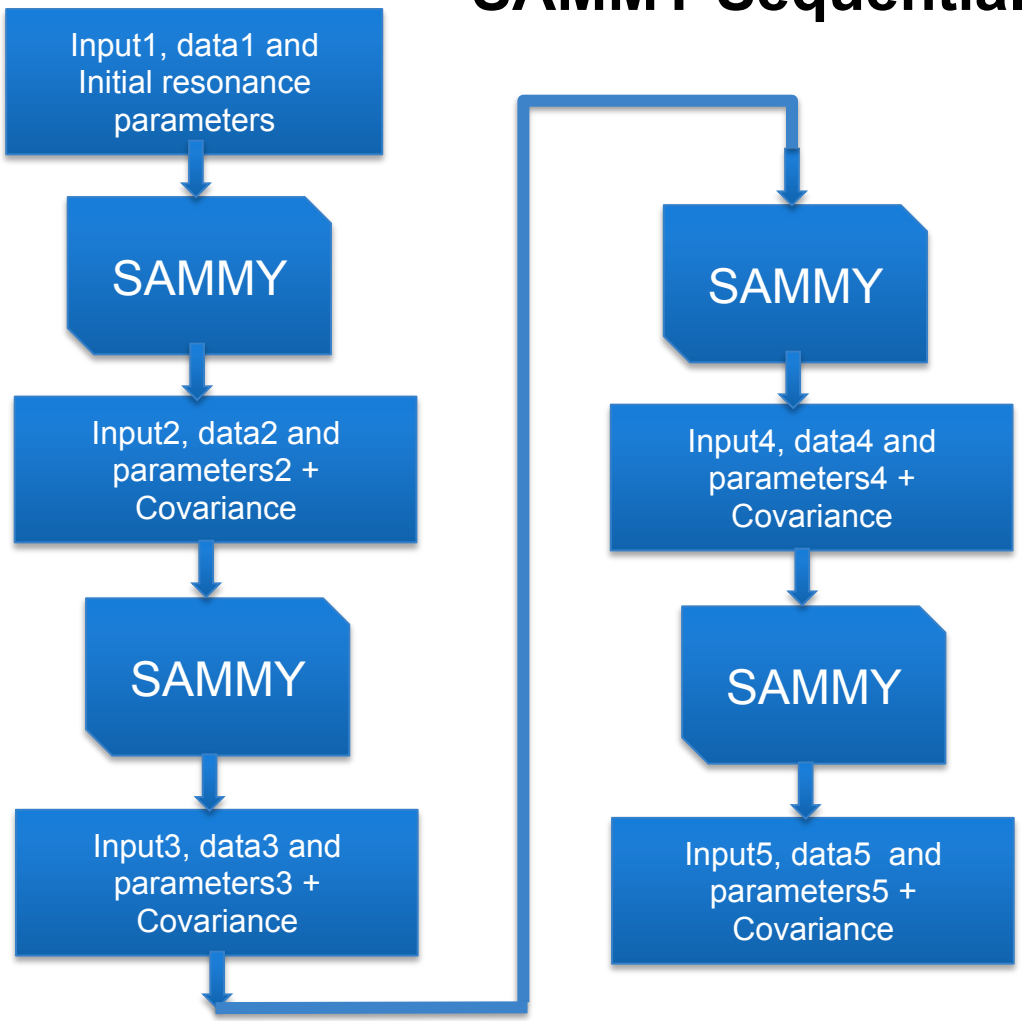
Nuclear Data Evaluation Status Overview

Resolved Resonance Region (RRR) Cross Section Evaluations							
No.	**Nucleus (I^{π})**	$E_{\min} - E_{\max}^{ORNL}(E_{\max}^{existing})$	**Method**	**No. Levels(*)**	**J_0**	**J_1**	**Evaluator**
1 ✓	^{182}W (0^+)	10^{-5} eV–10 (5.0) keV	RM	306	171	135	L. C. Leal
2 ✓	^{183}W ($1/2^-$)	10^{-5} eV–5 (2.2) keV	RM	387	346	21	M. T. Pigni
3 ✓	^{184}W (0^+)	10^{-5} eV–10 (4.0) keV	RM	178	94	84	L. C. Leal
4 ✓	^{186}W (0^+)	10^{-5} eV–10 (8.3) keV	RM	169	95	74	L. C. Leal
5 ✓	^{63}Cu ($3/2^-$)	10^{-5} eV-300 (100) keV	RM	527	323	204	V. Sobes
6 ✓	^{65}Cu ($3/2^-$)	10^{-5} eV-300 (100) keV	RM	762	525	237	V. Sobes
7 ✗	^{40}Ca (0^+)	10^{-5} eV-1.0 (0.5) MeV	RM	On going			M.T. Pigni

RM – Reich-Moore Approximation (*) bound and external levels not included

SAMMY Evaluation Procedure (differential data analysis)

SAMMY Sequential Evaluation



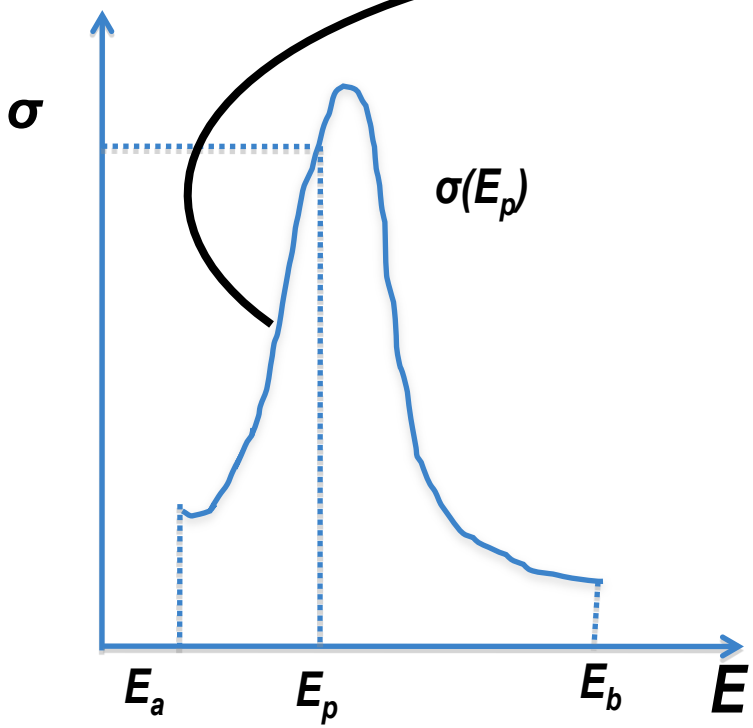
- A final set of parameters should fit reasonably well (small chi-square) the set of experimental data (e.g., data1, data2, data3, data4, data5)
- Generally there are multiple issues to be addressed by the evaluator:
  - Experimental data have different resolution
  - Experimental data have different energy range. Careful analysis of external levels is needed
  - Normalization of experimental data
  - Wrong spin assignment of resonance parameters
  - Missing information in old experiments

SAMMY Evaluation Procedure (link to Integral data)

- All experimental data have been reasonably represented by a set of resonance parameters and covariance (uncertainty) is obtained
  - SAMMY resonance parameter and covariance are converted into the ENDF/B format - file 2 (parameter) and 32 (covariance matrix)
- Process ENDF/B file with NJOY or AMPX in order to generate cross section in pointwise and/or group representation
- Find in the ICSBEP database integral benchmark experiments sensitive to the data of the evaluated isotope(s)
- Run MCNP and/or KENO codes
  - sensitivity analysis using TSUNAMI and TSURFER in order to improve agreement with benchmark experiments
  - Goal: improve results of integral data calculations and, at the same time, have reasonable description of differential data
- SAMMY analysis together with TSUNAMI/TSURFER is the way to go

SAMMY Evaluation Procedure (link to Integral data)

Differential and Integral



σ(E) as a function of energy

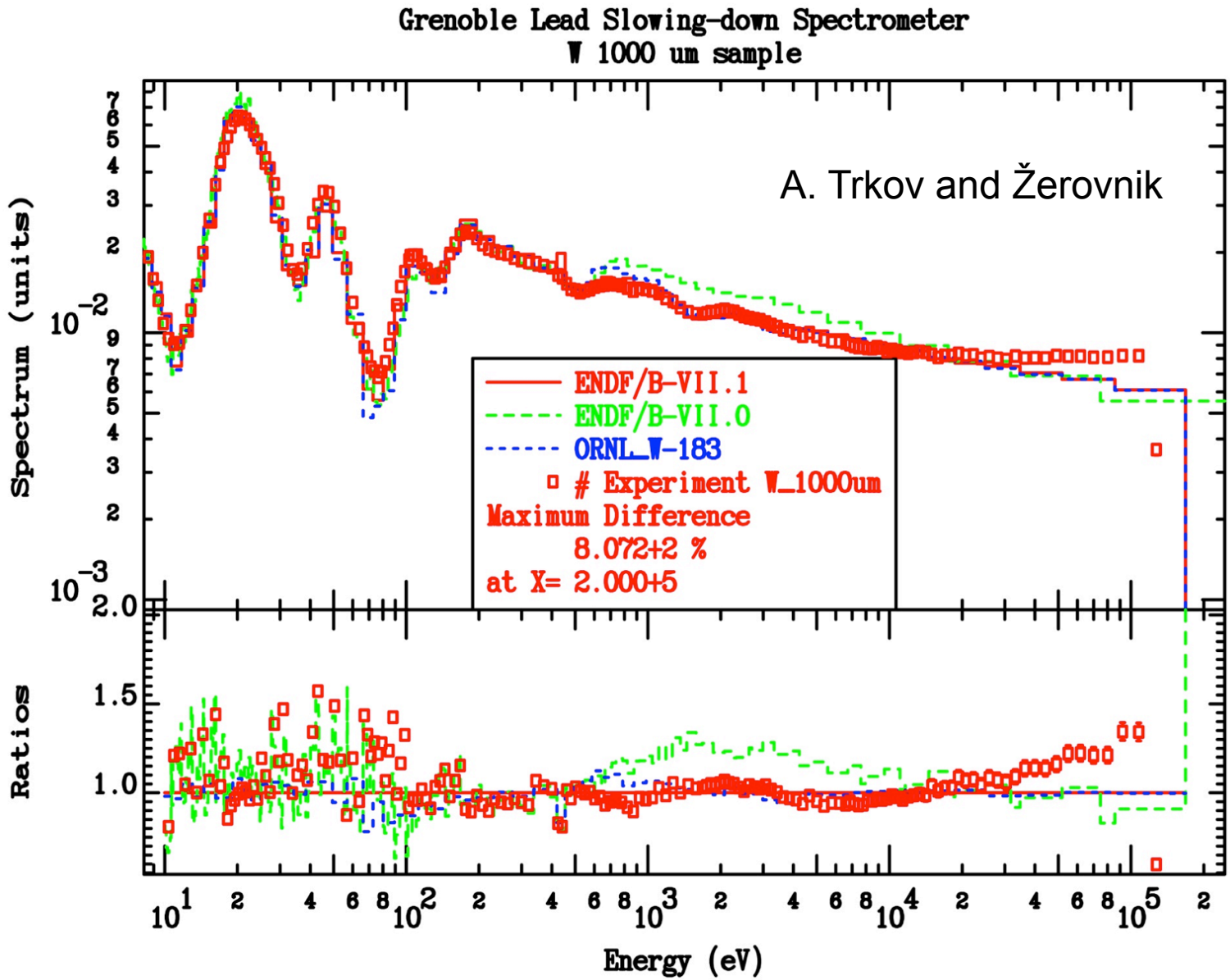
$$R = \int_{E_a}^{E_b} \sigma(E)\varphi(E) \quad dE$$

R **is the reaction rate (measured quantity)**

Differential

Integral

SAMMY Evaluation Procedure (link to Integral data)



M.T. Pigni et al., International Conference on Nuclear Data for Science and Technology (ND2013), New York, NY March 4-8 2013 (published)

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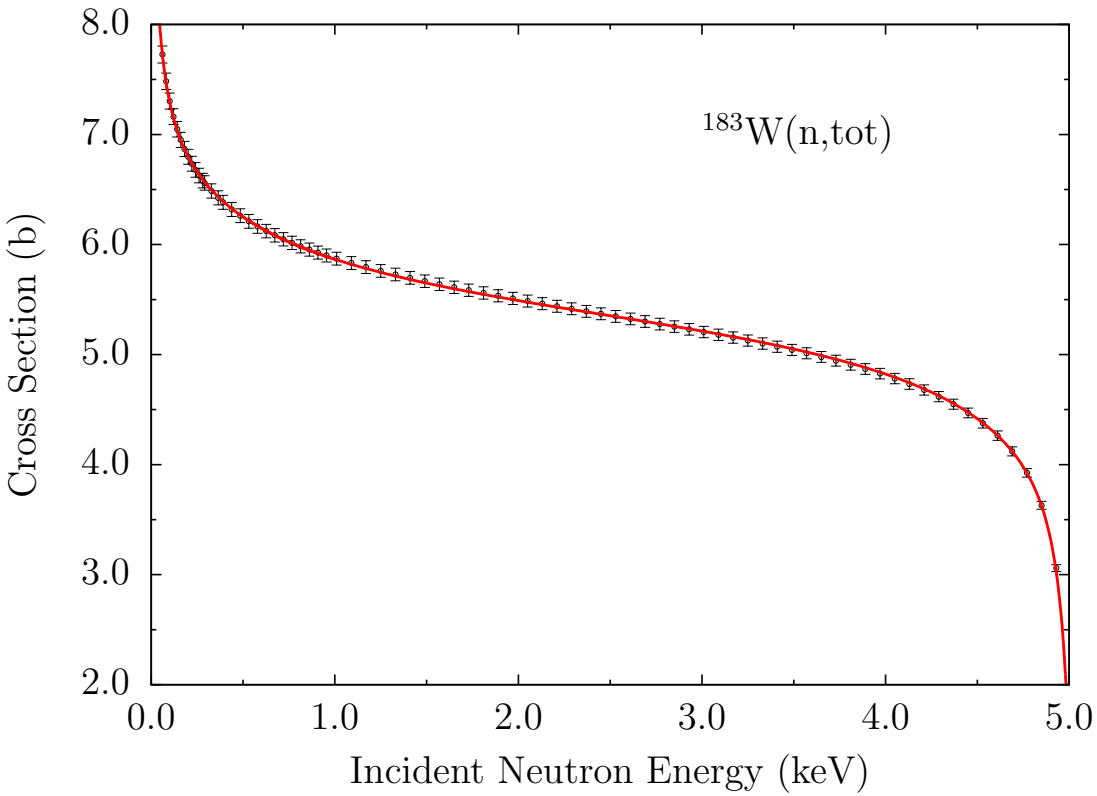
Starting Point: External Levels and Database

- External levels: bound levels (negative resonances) and levels above the resonance region
  - Careful determination of the external levels is needed before starting a SAMMY evaluation
  - It provides a good understanding of the scattering potential cross section
  - Indicates whether background effects a properly calculated
  - (Effective) nuclear scattering radii are well defined once the external levels have been determined
  - Provides an insight whether a direct reaction component is present
- Consistency of the database
  - Resolution function (ORELA, GELINA, …)
  - Data normalization
  - …

External Levels Evaluation

Contribution from the external levels - bound levels (negative resonances) and levels above the resonance region - and potential scattering cross section



- At low energies the effective radius is well defined and the potential scattering cross section is depending by the channel radius, a, and distant-level parameter, R∞, as

$$\sigma^{pot} \xrightarrow{E->0} 4\pi a^2 (1 - R^{\infty})^2 = 4\pi R'^2$$

- R∞(E) is essentially the difference between the contribution to the R-matrix from the resonances below and above E
- External levels important to avoid troublesome edge effects near the boundaries of the internal region

Figure 1. The potential scattering cross section calculated for a channel radius $a_c = 7.3$ fm and a distant-level parameter $\mathcal{R}_c^{J,\infty} = 0$ plus the contribution of 2 bound, i.e., negative levels below and 3 levels above the RRR 5 keV upper limit. The continuous red curve is a fit to the cross sections obtained by extrapolating the known RRR levels below and above the RRR.

^{183}W cross section evaluation (Pigni)

Step 1: Determination of number of partial waves

- The magnitude of the penetrability factors determines the strength of the partial-wave components responsible of the quasi-stationary compound state.

$$\Gamma_{\lambda c} = 2\gamma_{\lambda c}^2 P_\ell$$

	ℓ	s	J^π	g_J	wave
^{183}W $(1/2^-)$	0	0	0^-	1/4	s
		1	1^-	3/4	
	1	0	1^+	3/4	p
		1	0^+ 1^+ 2^+	1/4 3/4 5/4	
	2	0	2^-	5/4	d
		1	1^- 2^- 3^-	3/4 5/4 7/4	

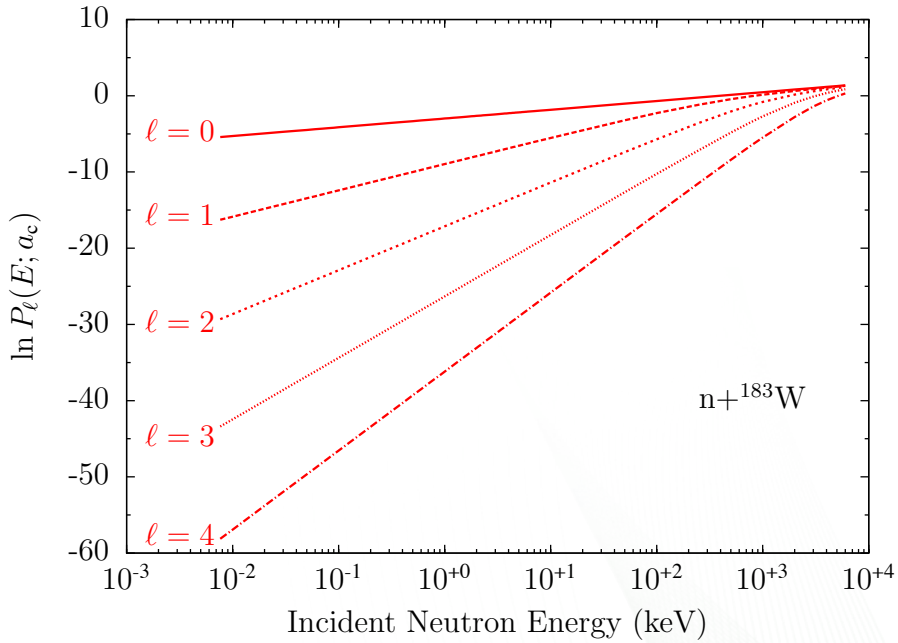
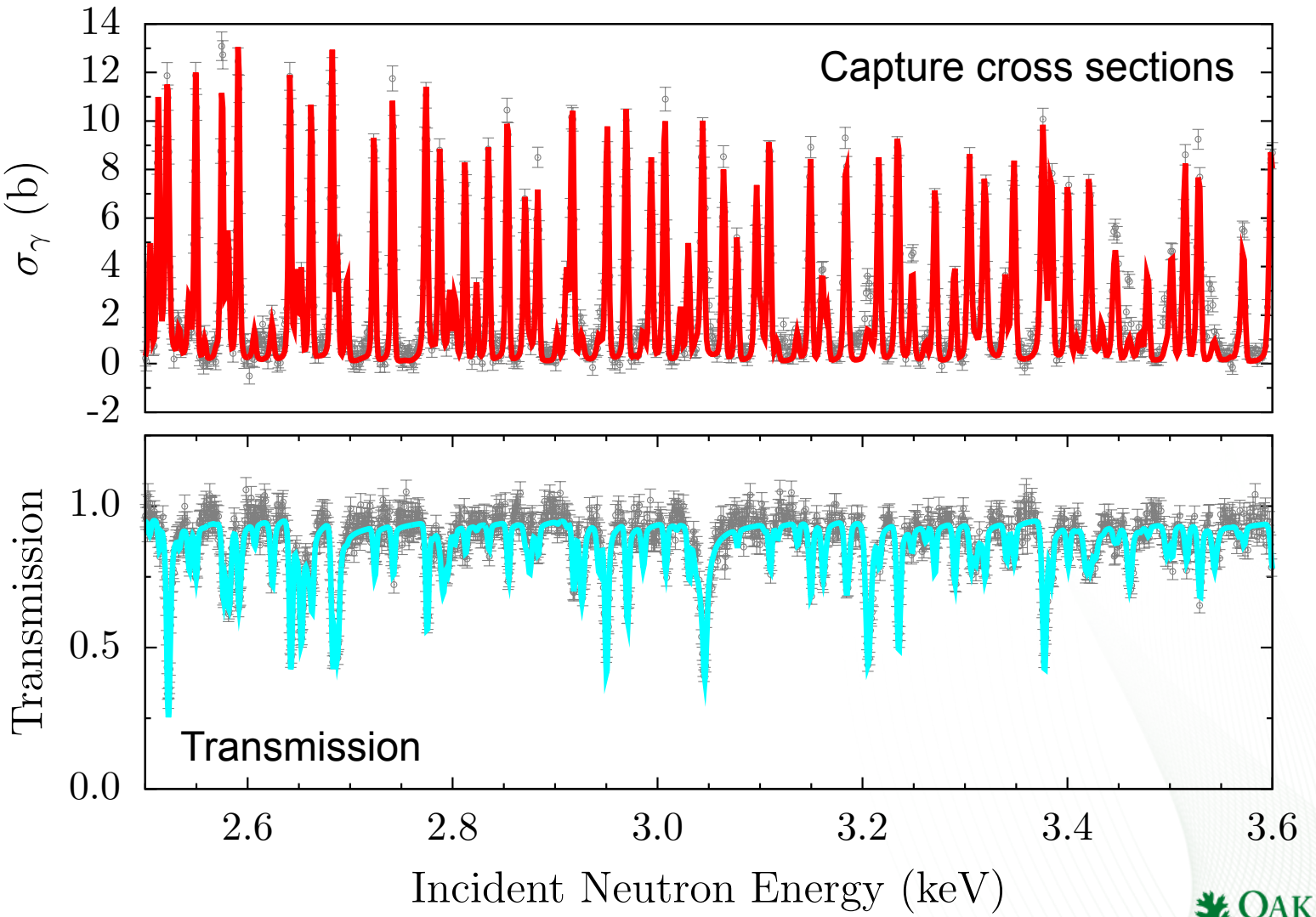


Figure 2. Hard-sphere penetrability factors $P_\ell \equiv P_\ell(E; a_c)$ of n+^{183}W for different angular momentum ℓ calculated at the channel radius $a_c = 7.3$ fm .

Note: for all Tungsten isotopes s- and p-waves were included

^{183}W cross section evaluation (Pigni)

Step 2: Fitting procedure



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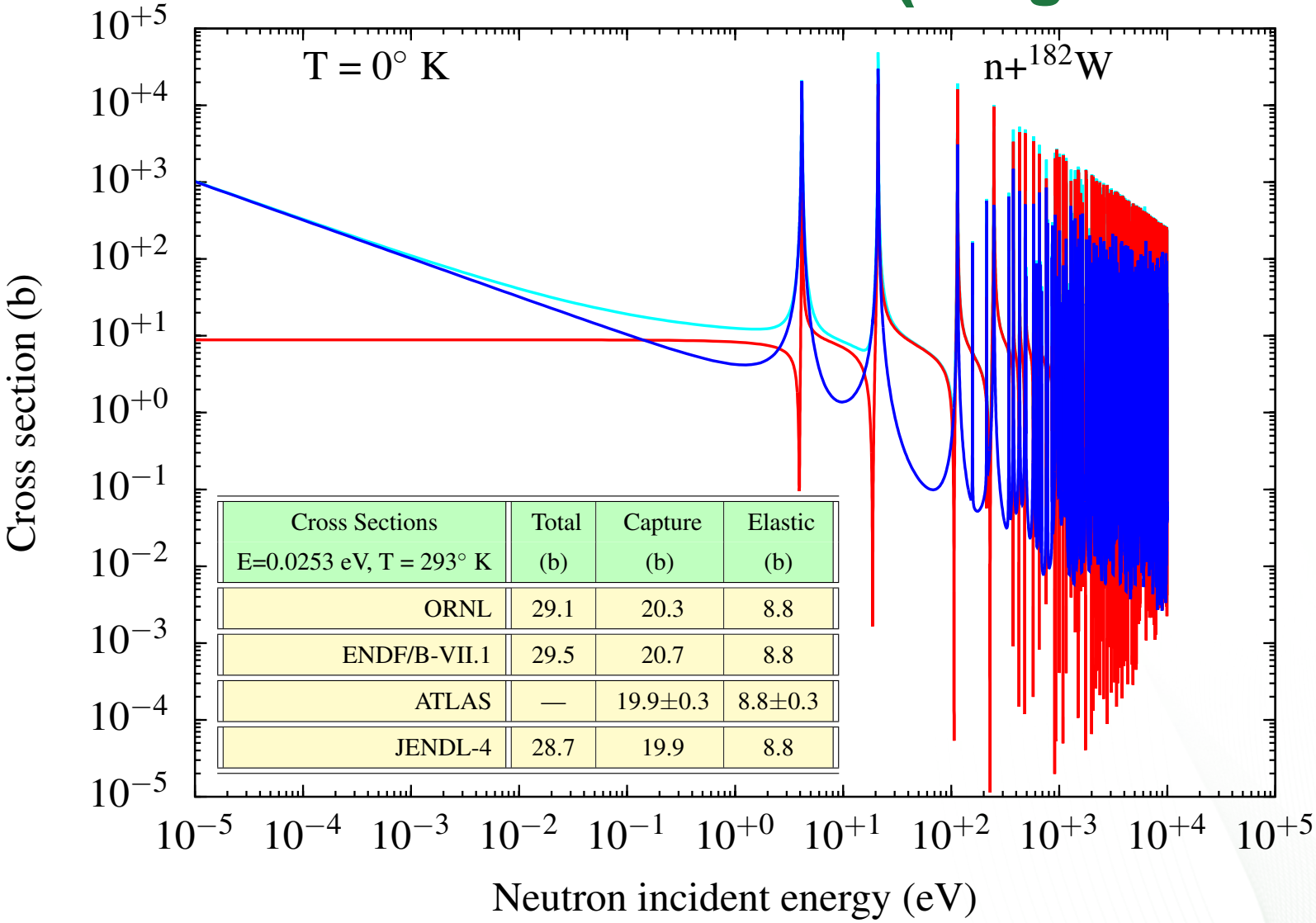
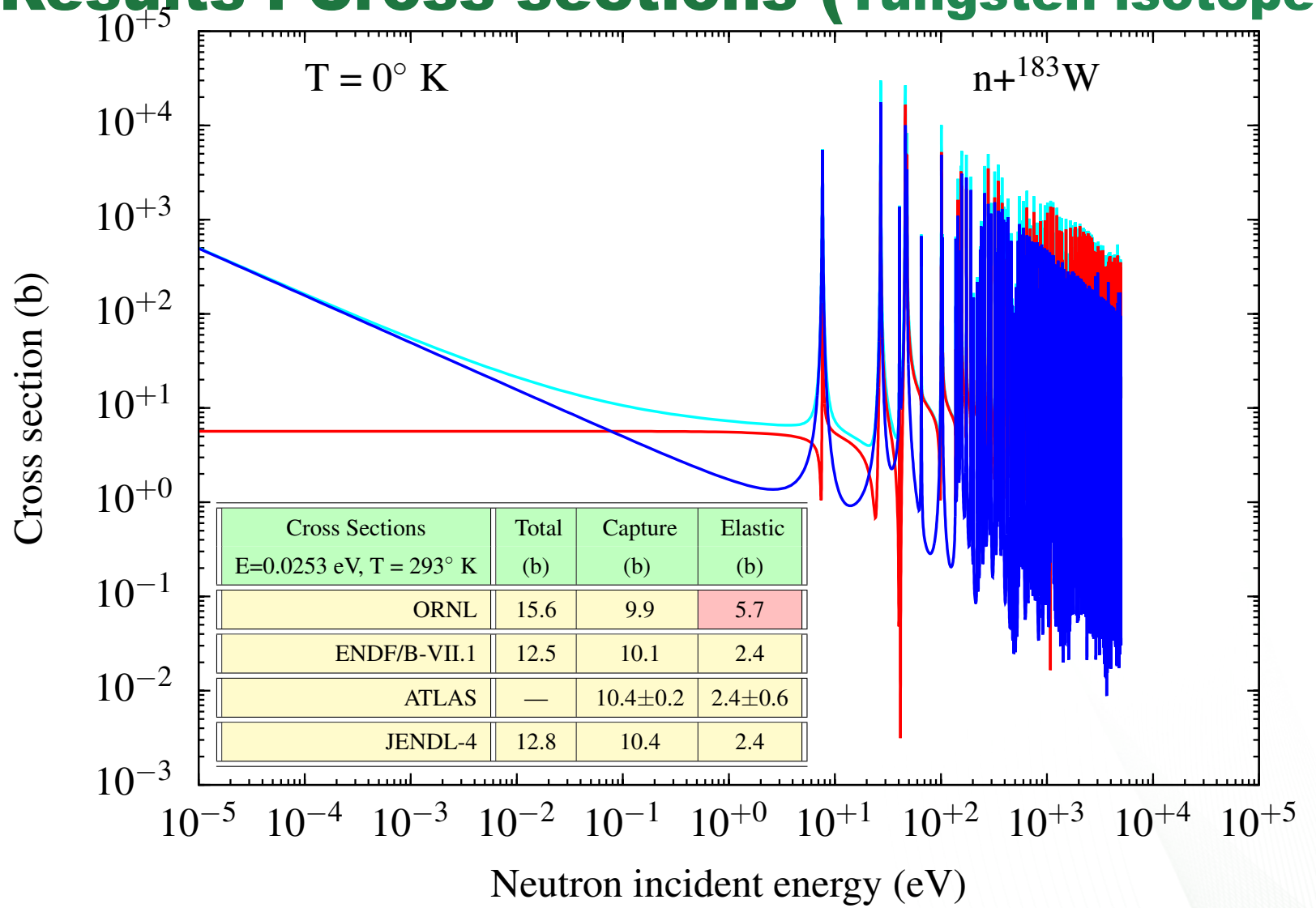
Results : Cross sections (Tungsten isotopes)



Cross Sections E=0.0253 eV, T = 293° K	Total (b)	Capture (b)	Elastic (b)
ORNL	29.1	20.3	8.8
ENDF/B-VII.1	29.5	20.7	8.8
ATLAS	—	19.9±0.3	8.8±0.3
JENDL-4	28.7	19.9	8.8

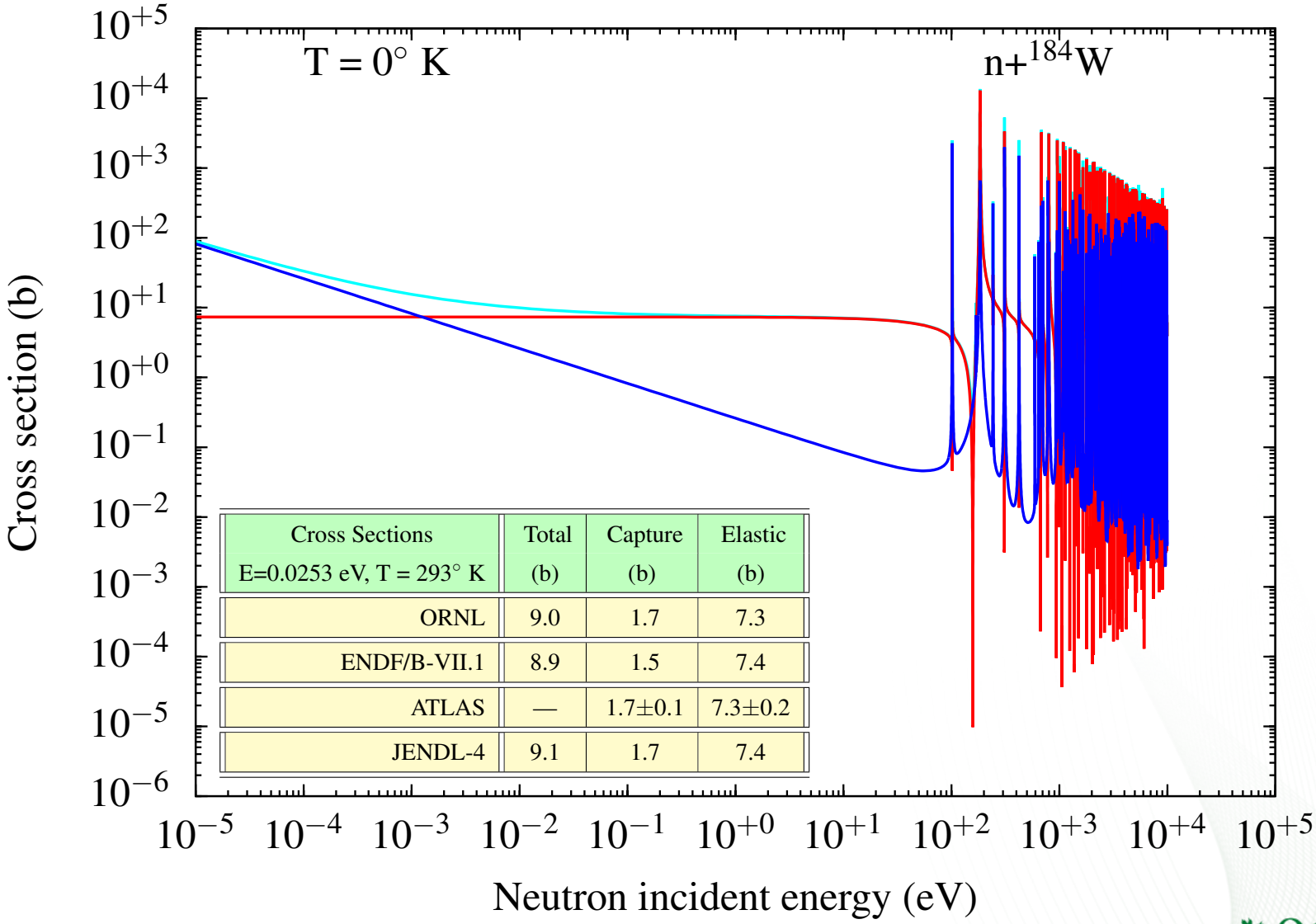
Results : Cross sections (Tungsten isotopes(*))



Cross Sections E=0.0253 eV, T = 293° K	Total (b)	Capture (b)	Elastic (b)
ORNL	15.6	9.9	5.7
ENDF/B-VII.1	12.5	10.1	2.4
ATLAS	—	10.4±0.2	2.4±0.6
JENDL-4	12.8	10.4	2.4

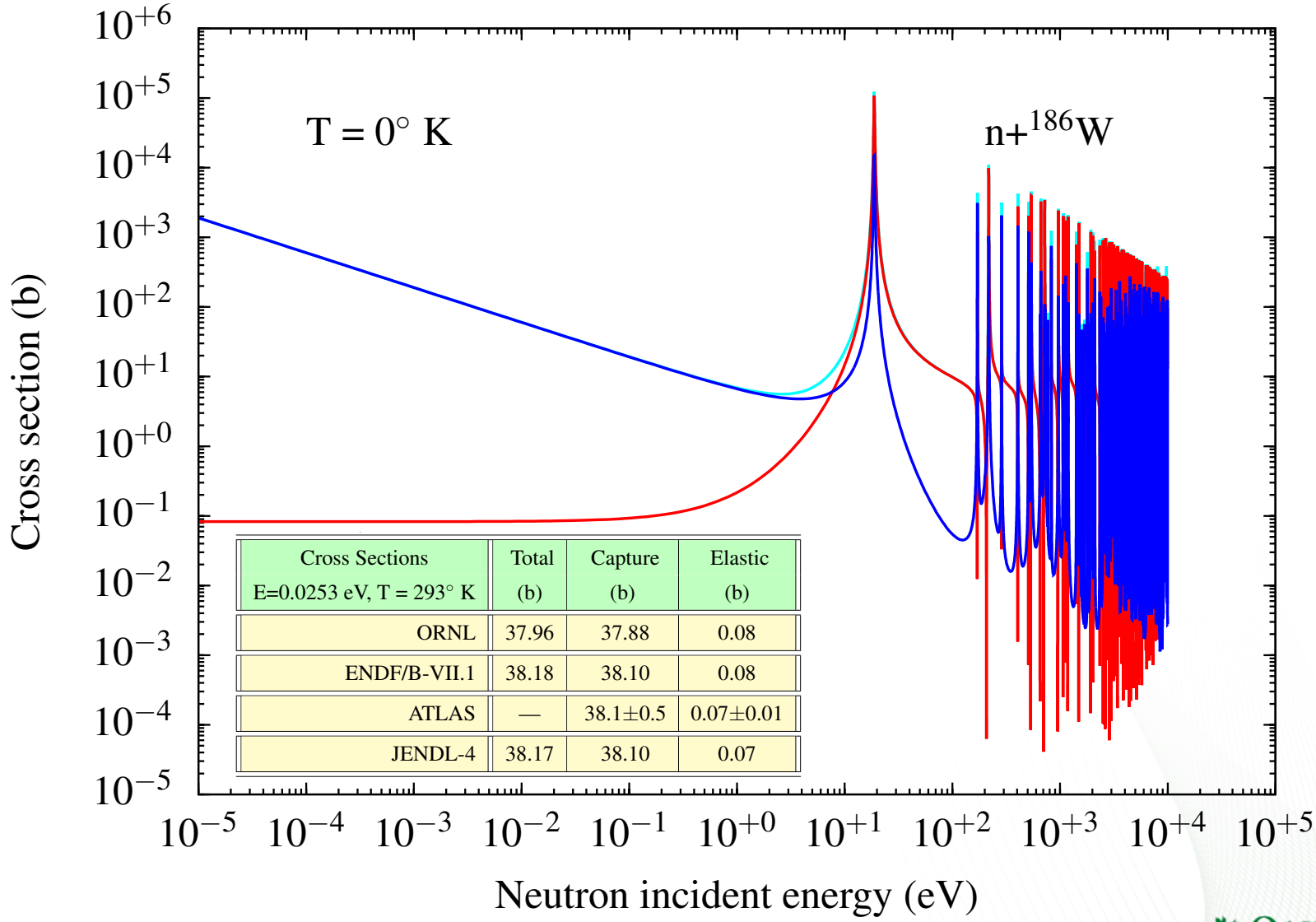
(*) M.T. Pigni et al., PHYSOR 2012 – Advances in Reactor Physics – Knoxville, TN April 15-20 2012 (published)
M.T. Pigni et al., International Conference on Nuclear Data for Science and Technology (ND2013), New York, NY March 4-8 2013 (published)
M.T. Pigni et al., International Conference on Nuclear Criticality Safety (ICNC2015), Charlotte, NC September 13-17, 2015 (accepted)

Results: Cross sections (Tungsten isotopes)



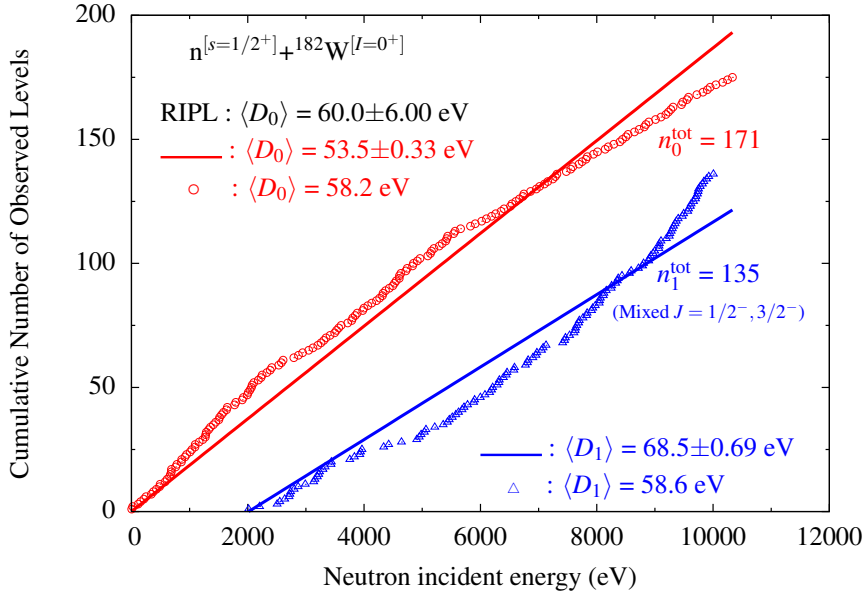
Cross Sections E=0.0253 eV, T = 293° K	Total (b)	Capture (b)	Elastic (b)
ORNL	9.0	1.7	7.3
ENDF/B-VII.1	8.9	1.5	7.4
ATLAS	—	1.7±0.1	7.3±0.2
JENDL-4	9.1	1.7	7.4

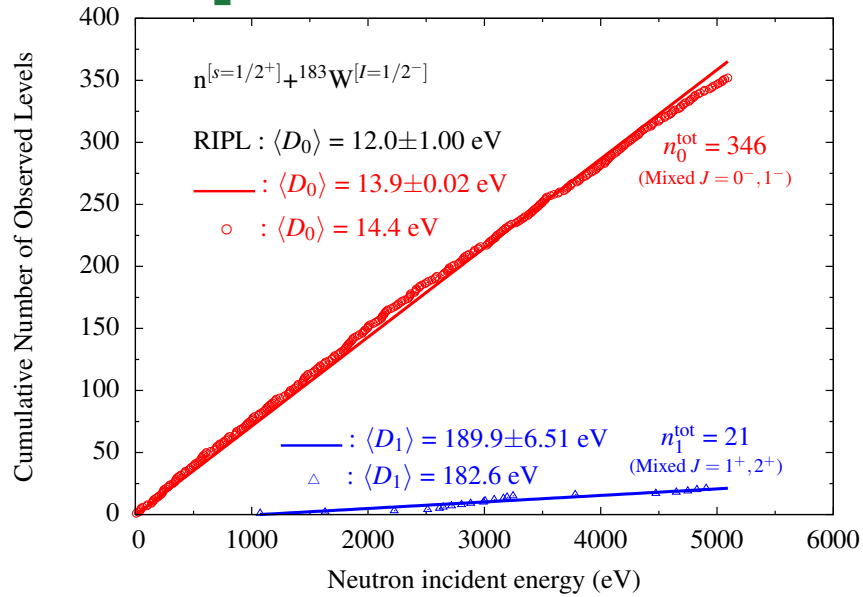
Cross sections (Tungsten)

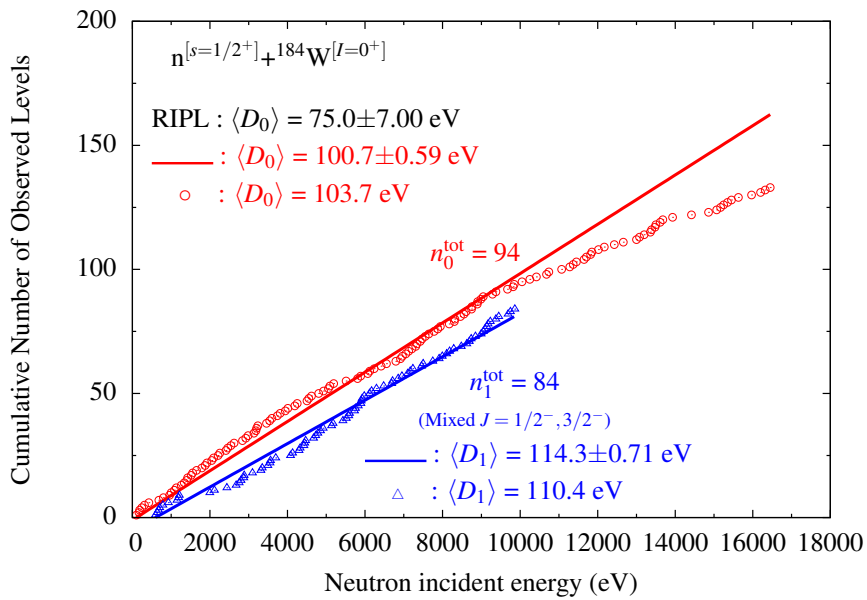


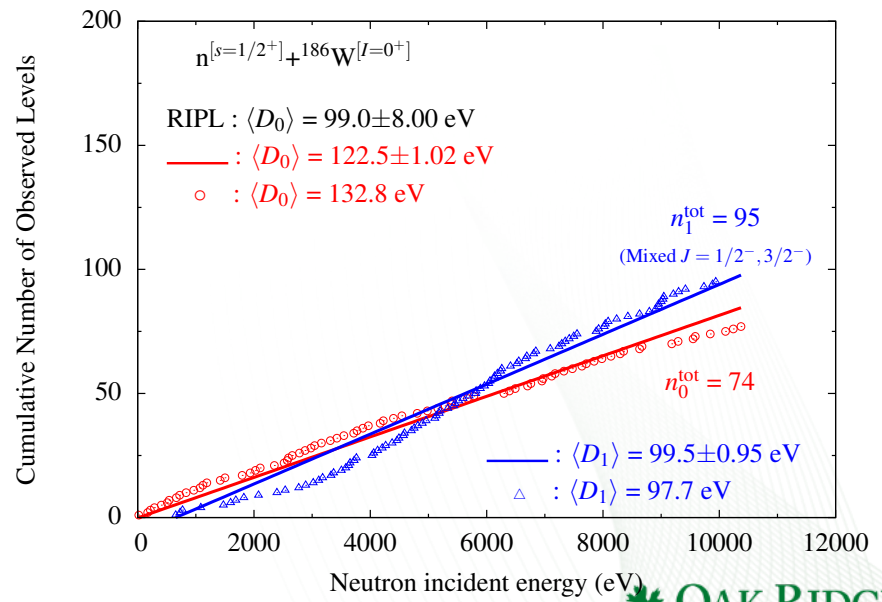
Cross Sections E=0.0253 eV, T = 293° K	Total (b)	Capture (b)	Elastic (b)
ORNL	37.96	37.88	0.08
ENDF/B-VII.1	38.18	38.10	0.08
ATLAS	—	38.1±0.5	0.07±0.01
JENDL-4	38.17	38.10	0.07

Statistics on Resonance parameters

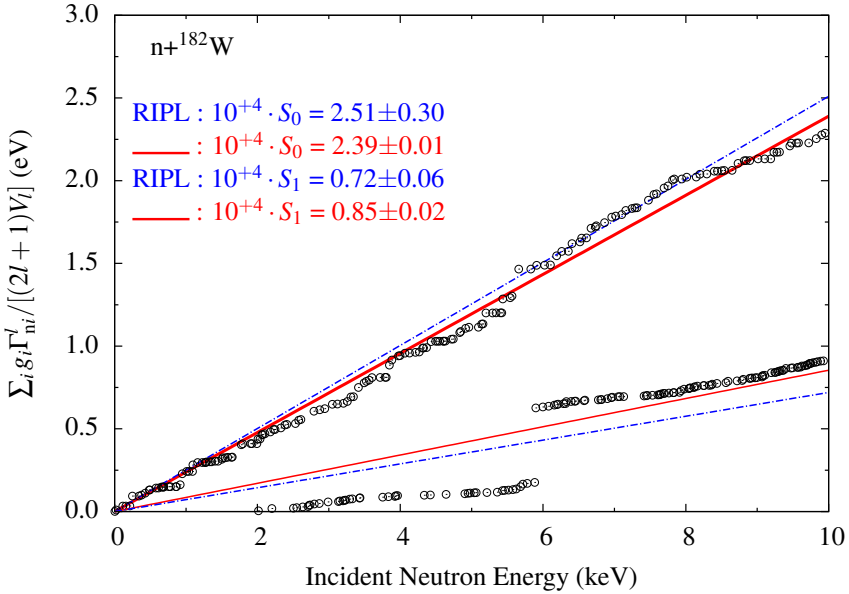


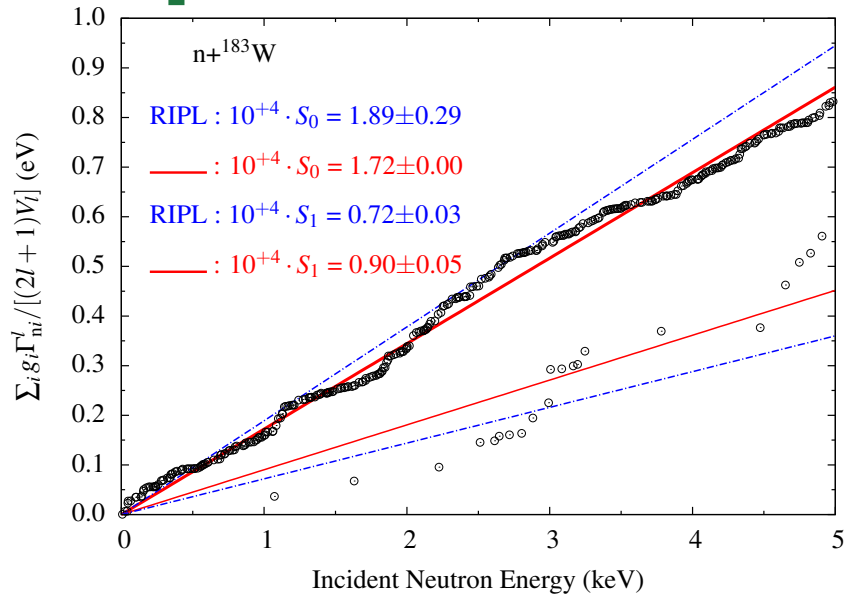


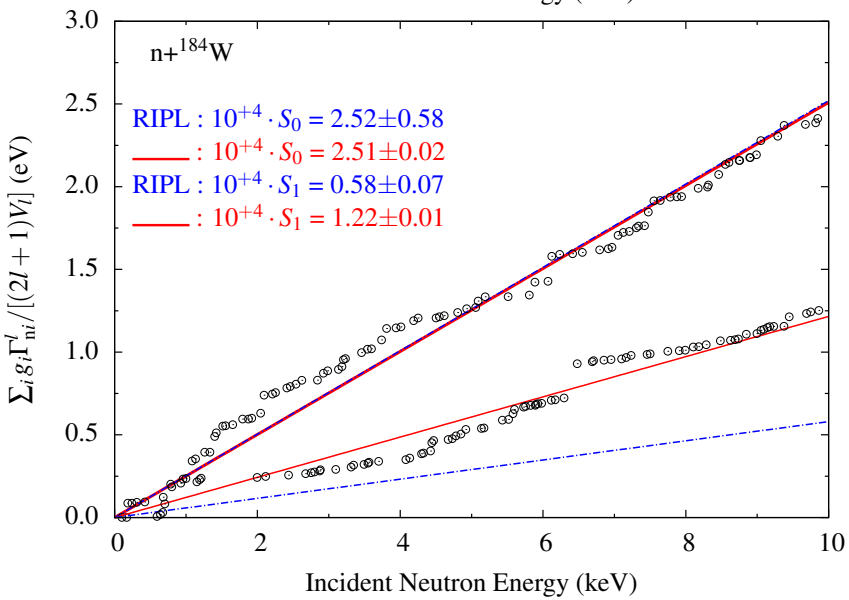


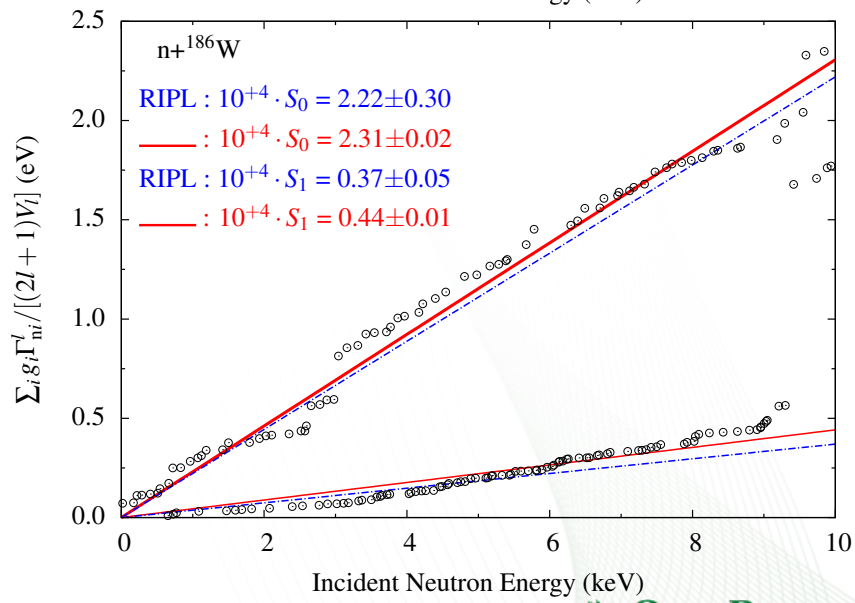


Statistics on Resonance parameters

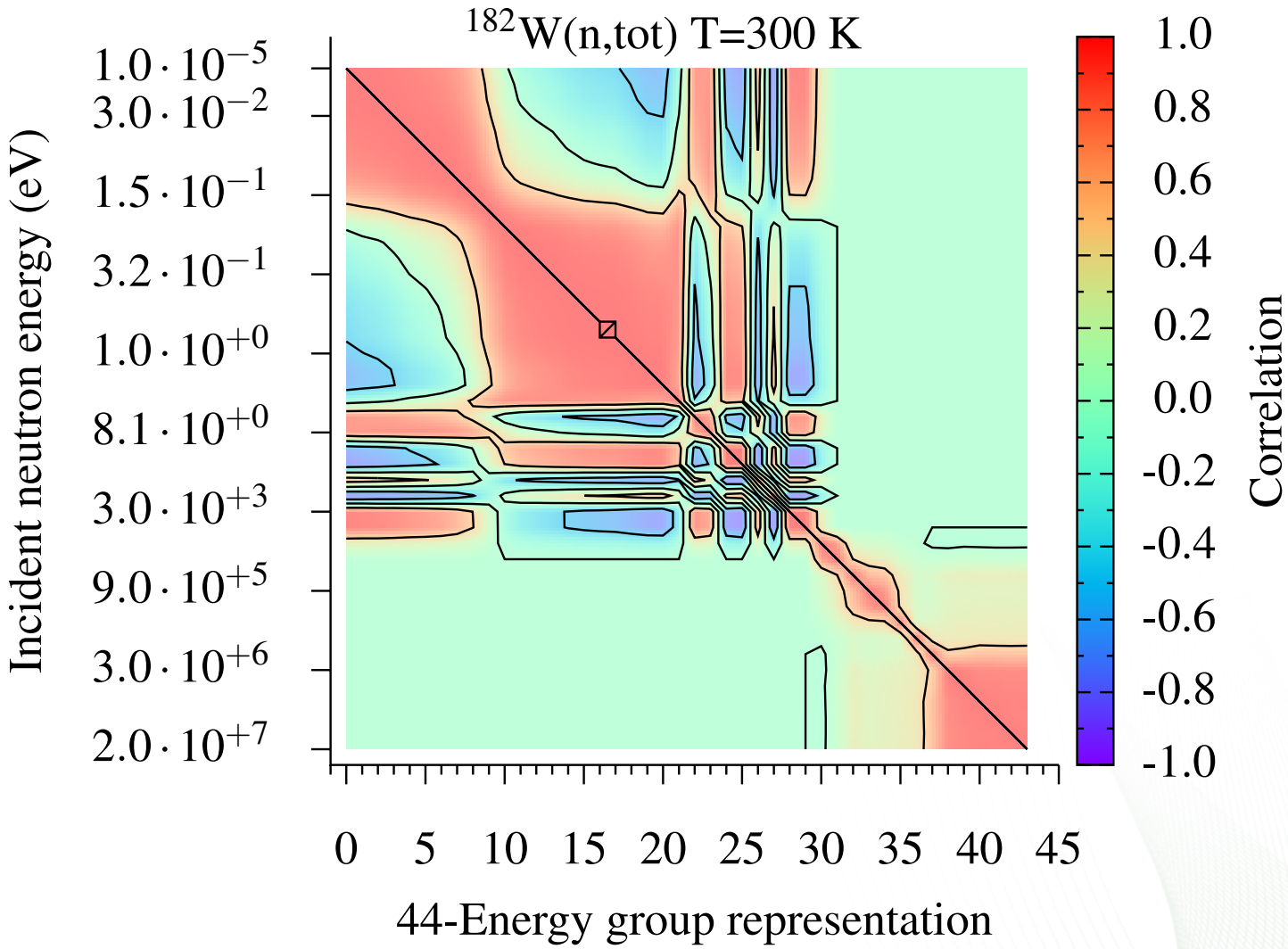








Covariance Evaluations (Total)



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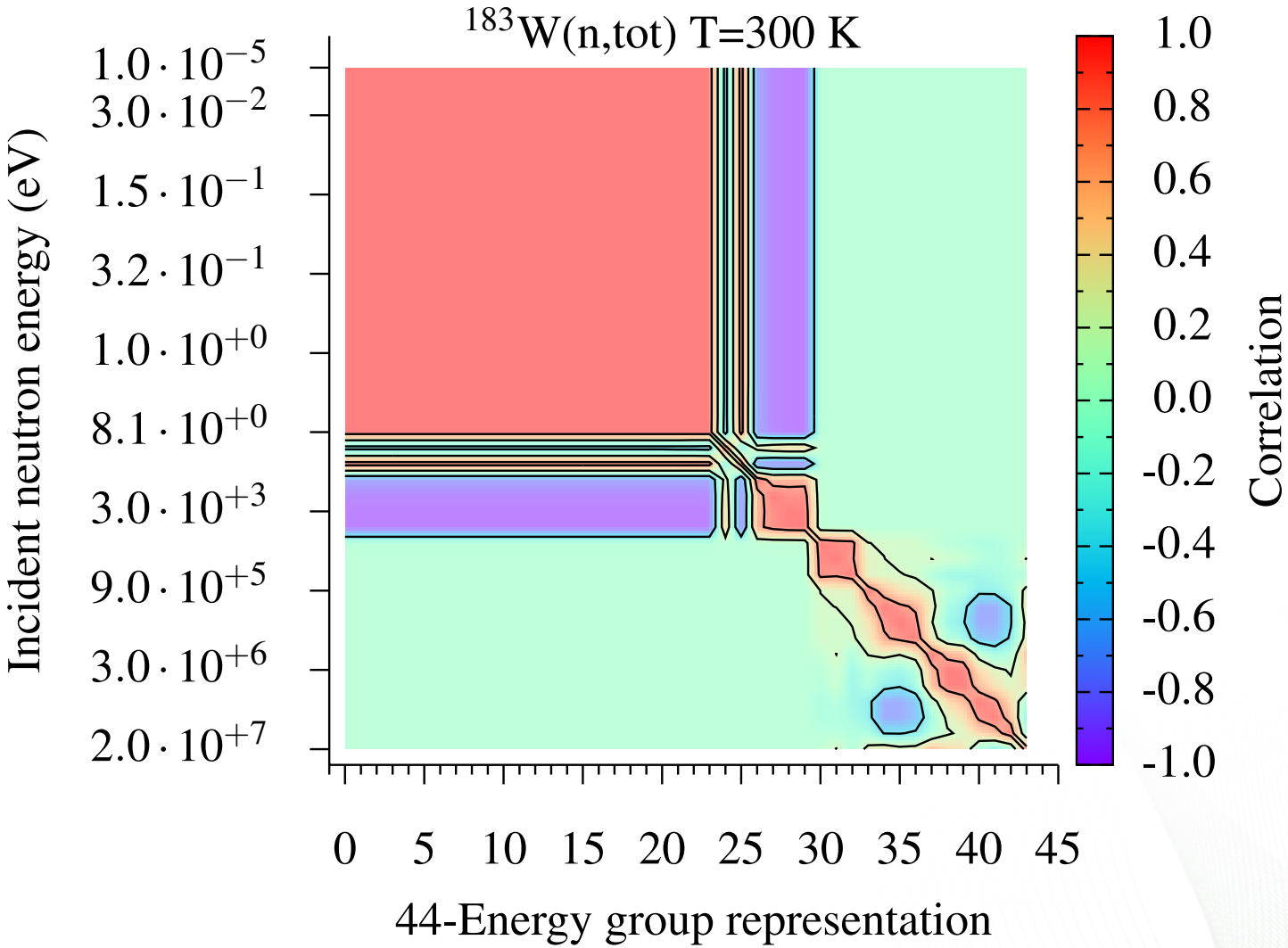
Covariance Evaluations (Total)



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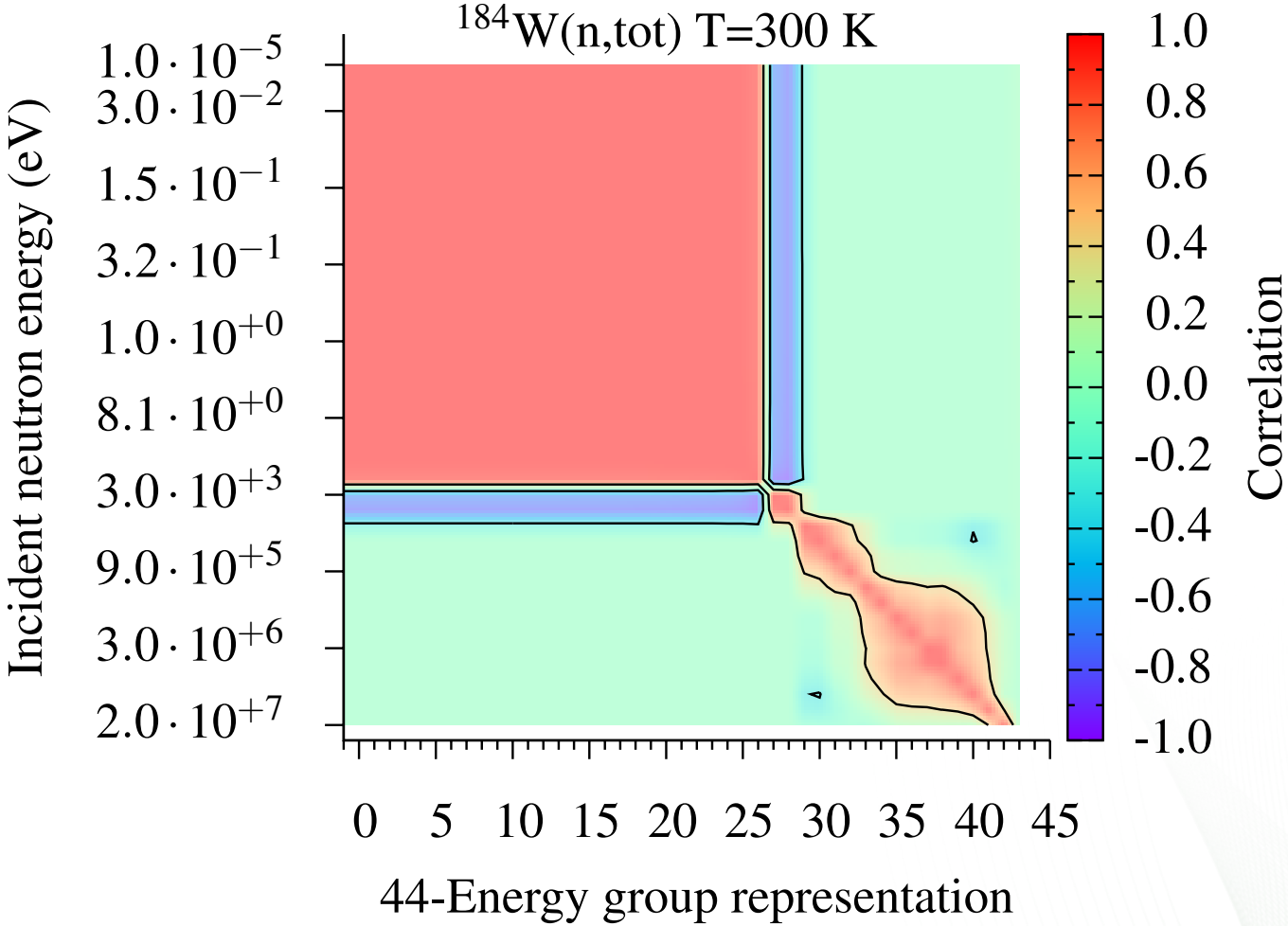
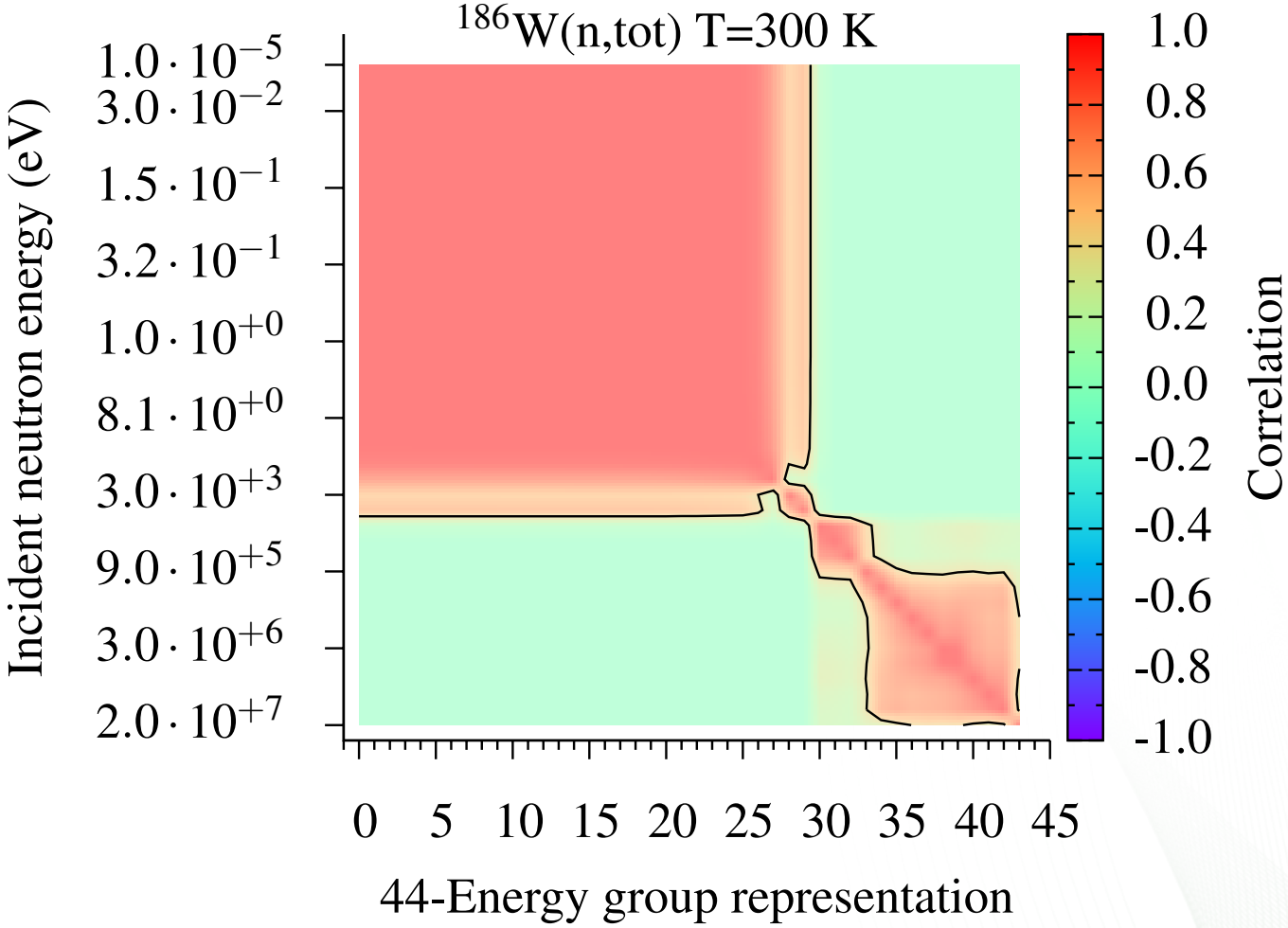
Covariance Evaluations (Total)



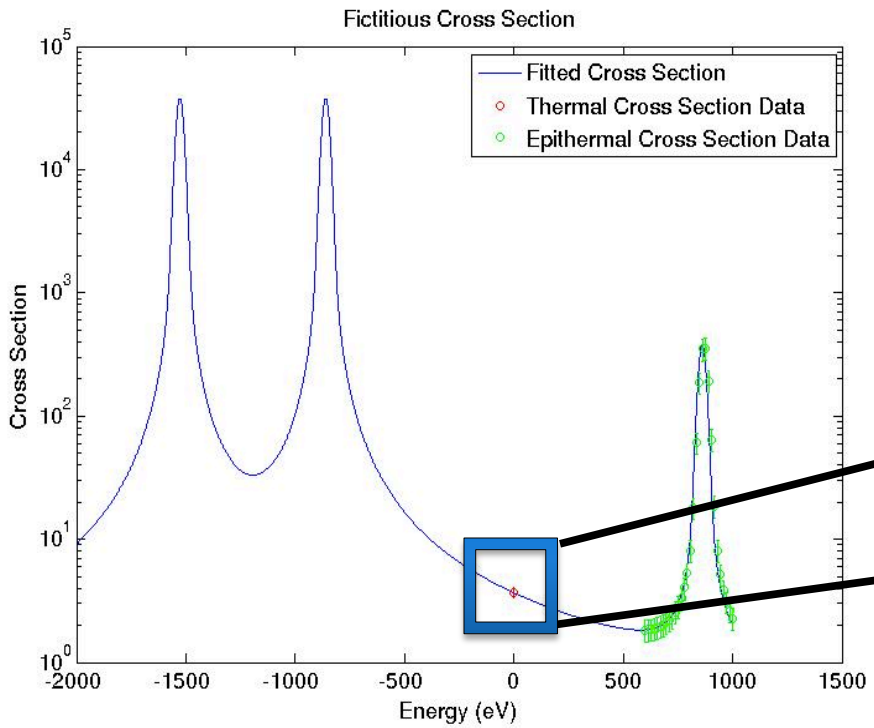
Covariance Evaluations (Total)

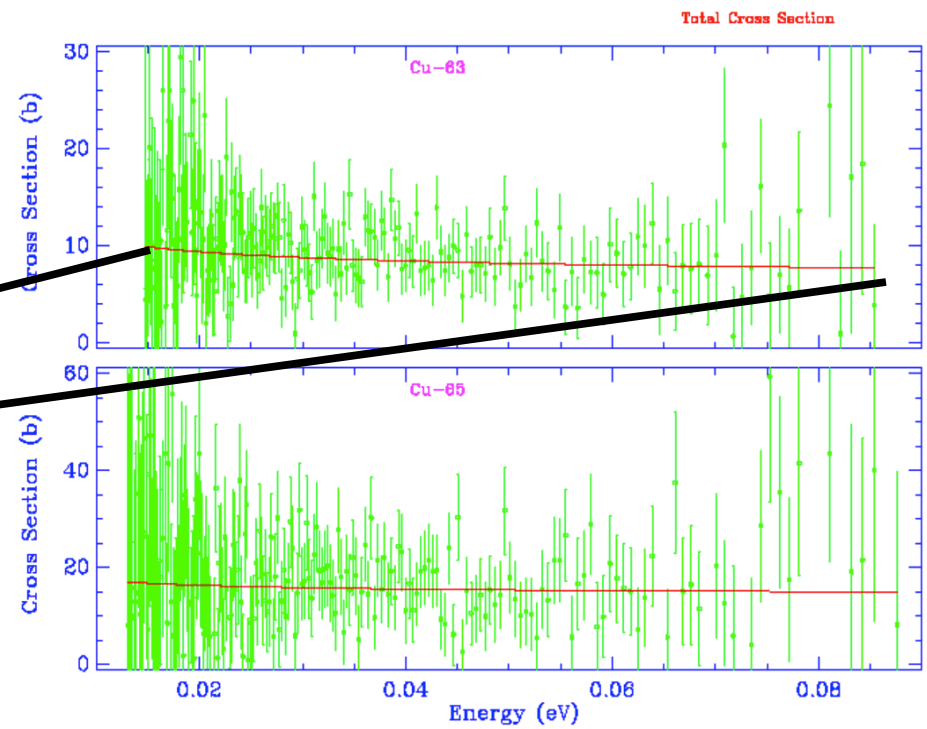


Cu Cross Section Evaluations Thermal (Sobes)

- **Motivation**
  - **Nuclear Data Advisory Group (NDAG) identified Cu-63 and Cu-65 as "IMPORTANT FOR MEASUREMENTS AND EVALUATIONS"**
  - **Purpose of Experiment:**
    - Thermal Cross Section Shape
    - Thermal Cross Section Uncertainty
    - SAMMY Resolved Resonance Analysis

Cu Cross-section Evaluations Thermal (Sobes)





- A better definition of the negative external levels if we fit a differential cross section
- A better definition of the uncertainty and correlations at the thermal energy

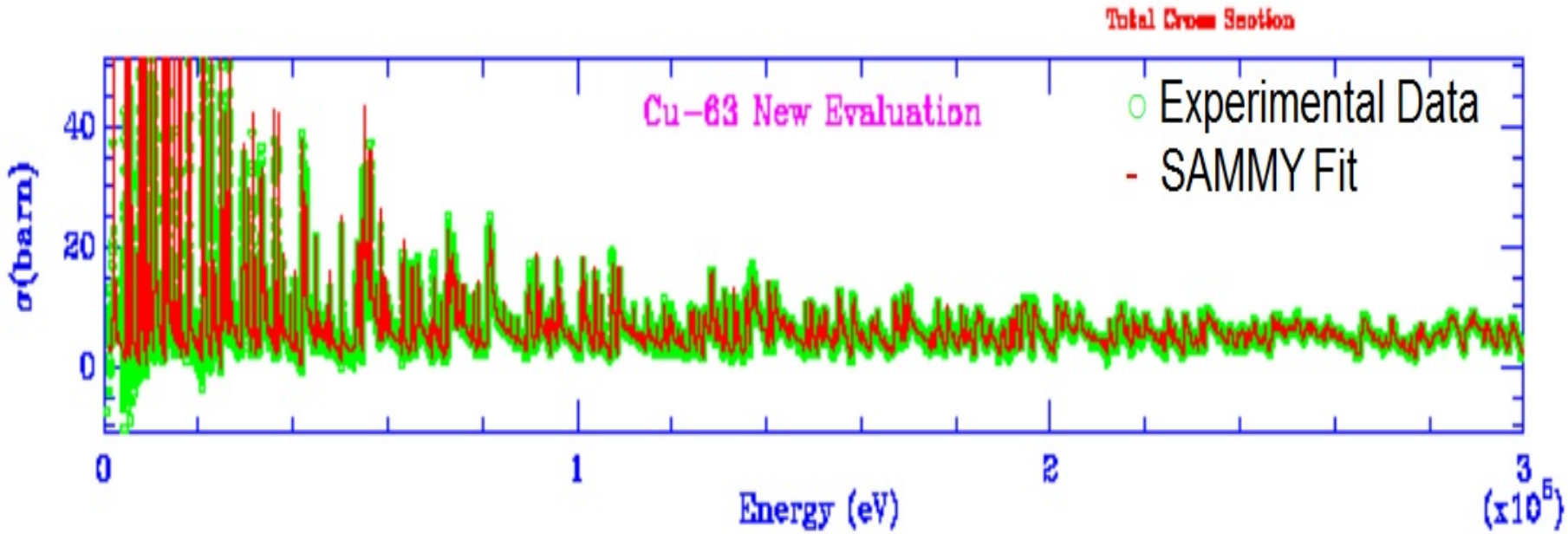
Cu Cross-section Evaluations (Sobes)

- **SAMMY Evaluation of the Transmission Data**
  - **SAMMY analysis of transmission data for Cu-63 and Cu-65**
  - **Measurements made at the Oak Ridge Electron Linear Accelerator (ORELA) by M. S. Pandey, J. B. Garg, and J. A. Harvey (1977)**
  - **Flight-path length: 80 meters**
  - **Thicknesses:**
    - Cu-63 0.07895 at/barns
    - Cu-65 0.07437 at/barns
  - **Energy Range: 0.0001 eV to 300 keV**

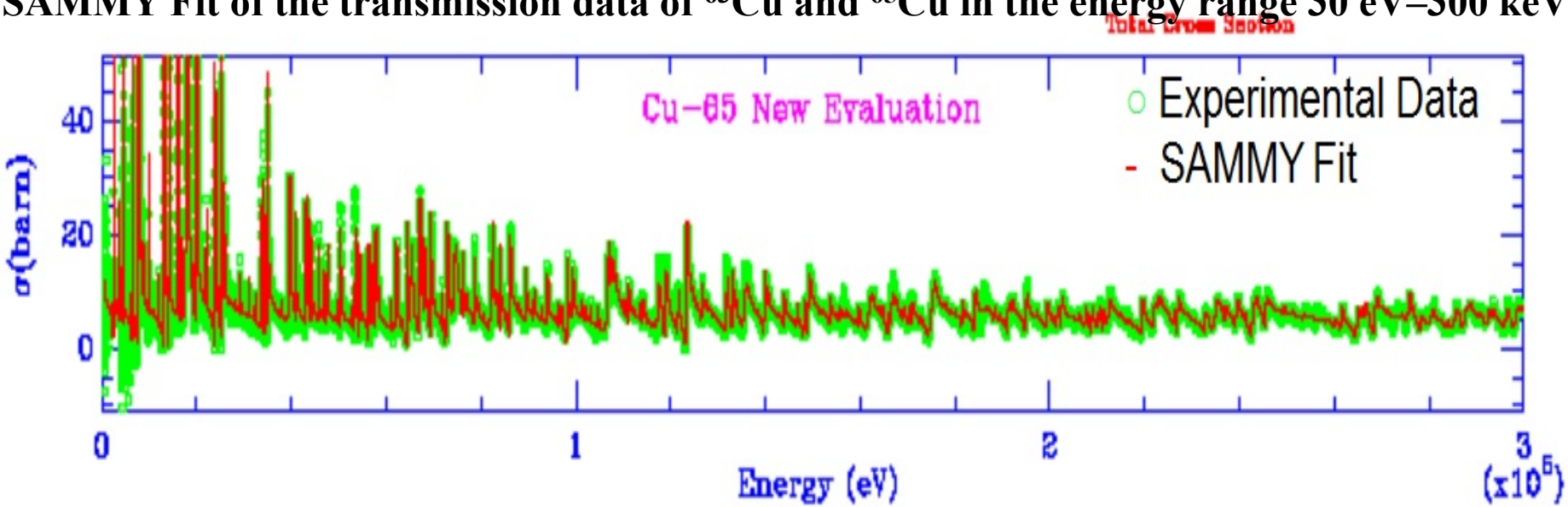
Updated ^{63,65}Cu Evaluations (Sobes)

- **Three major improvements of consequence to the Zeus benchmarks:**
  - **Resolved resonance region expanded three-fold**
  - **Capture cross section evaluated based on experimental measurements**
  - **Detailed angular distributions generated for elastic scattering**

Cu cross section evaluations (Sobes)

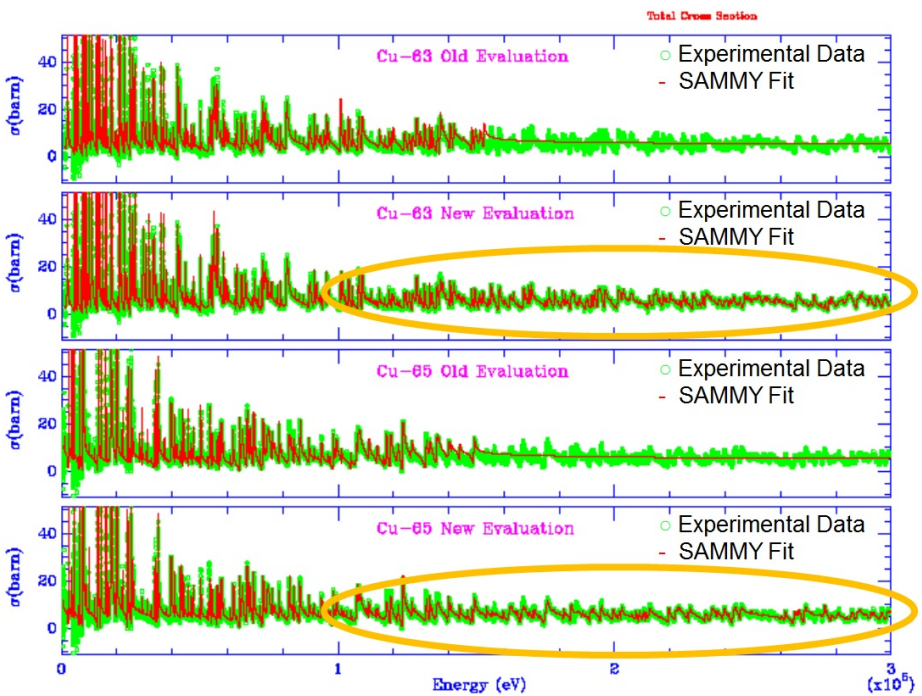


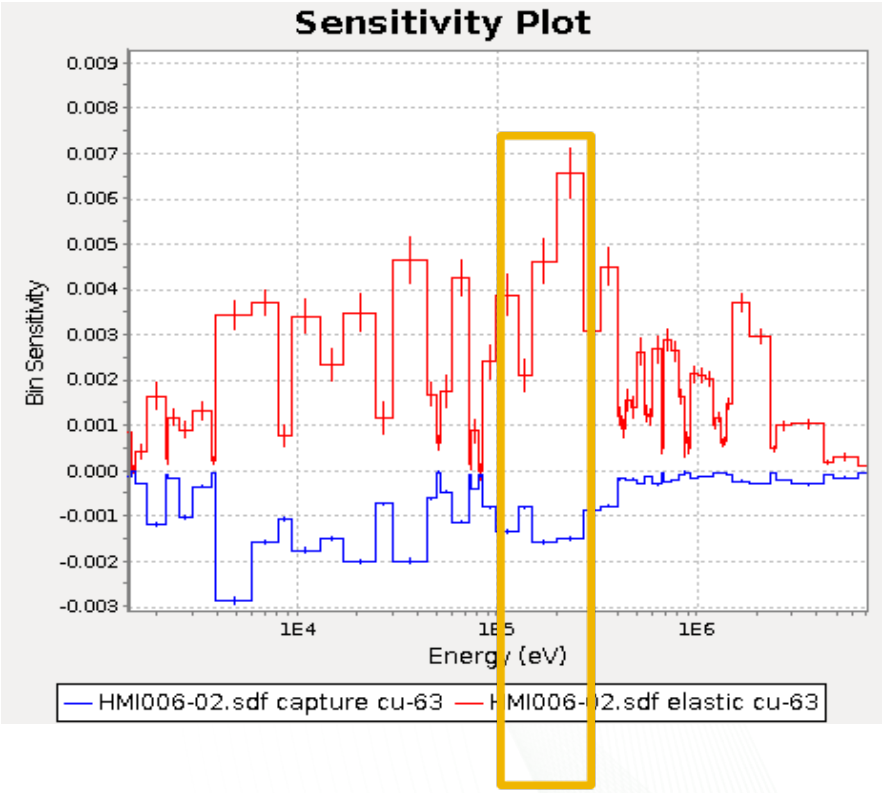
SAMMY Fit of the transmission data of ^{63}Cu and ^{65}Cu in the energy range 30 eV–300 keV



Extending the Resolved Resonance Region

Resolved resonance region of both copper isotopes, has been extended from 99.5 keV to 300 keV.





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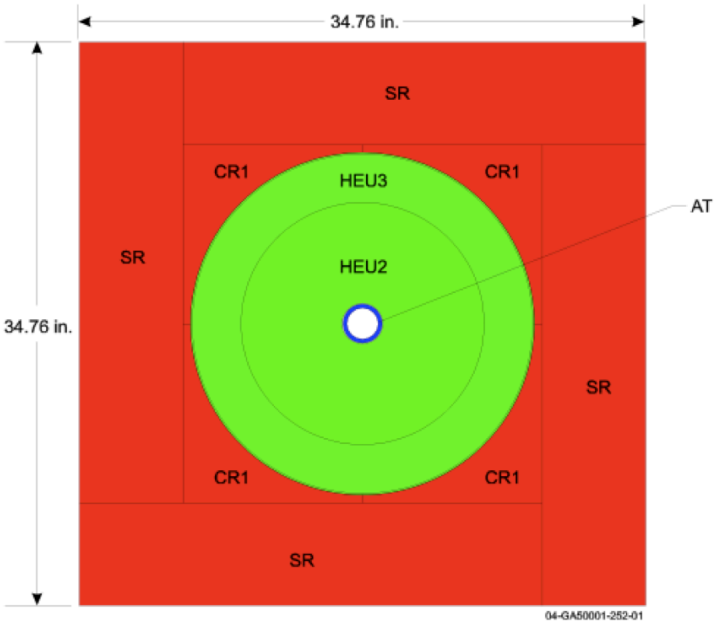
Detailed Angular Distributions

- For the Zeus cases, system k_{eff} is most sensitive to the elastic scattering reaction in copper
- Previous angular distributions came from model calculations
- New angular distributions generated from resonance parameters using Blatt-Biedenharn formalism.
  - Self-consistent with the angle-integrated elastic scattering
  - Display resonance behavior.
- For heavily reflected systems, such as the Zeus cases, the forward/backward component of the angular distribution of elastic scattering determines whether scattered neutrons leak out of the system or return back into the fuel region.



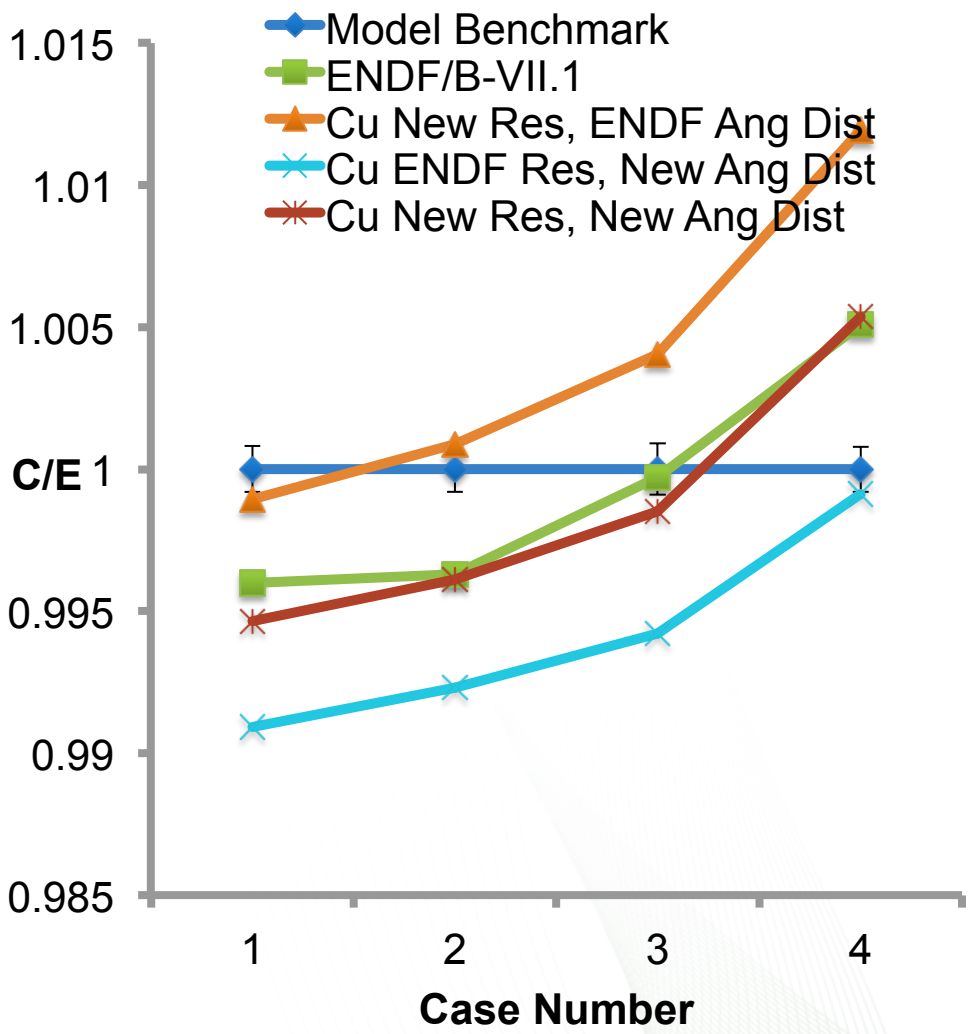
Benchmarking Results: k_{eff}

Case	Model Benchmark	Cu Res. (File 2)	VII.1	ORNL	VII.1	ORNL	ORNL
		Cu Ang. Dist. (File 4-2)	VII.1	VII.1	ORNL	ORNL	ORNL
		^{235}U	VII.1	VII.1	VII.1	VII.1	ORNL
		All other isotopes	VII.1	VII.1	VII.1	VII.1	VII.1
1	0.99770 +/- 0.00080		0.99370	0.99663	0.98864	0.99236	0.99562
2	1.00010 +/- 0.00080		0.99640	1.00097	0.99239	0.99622	0.99903
3	1.00150 +/- 0.00090		1.00120	1.00556	0.99570	1.00001	1.00136
4	1.00160 +/-0.00080		1.00670	1.01355	1.00071	1.00697	1.00423

VII.1 = ENDF/B-VII.1

Updated ^{63,65}Cu Evaluation

- **The capture cross section were updated based on experimental capture measurements.**
- **Updated angular distributions provided the correct balance between forward/backward scattering to give satisfactory benchmark results with the new resonance parameters.**



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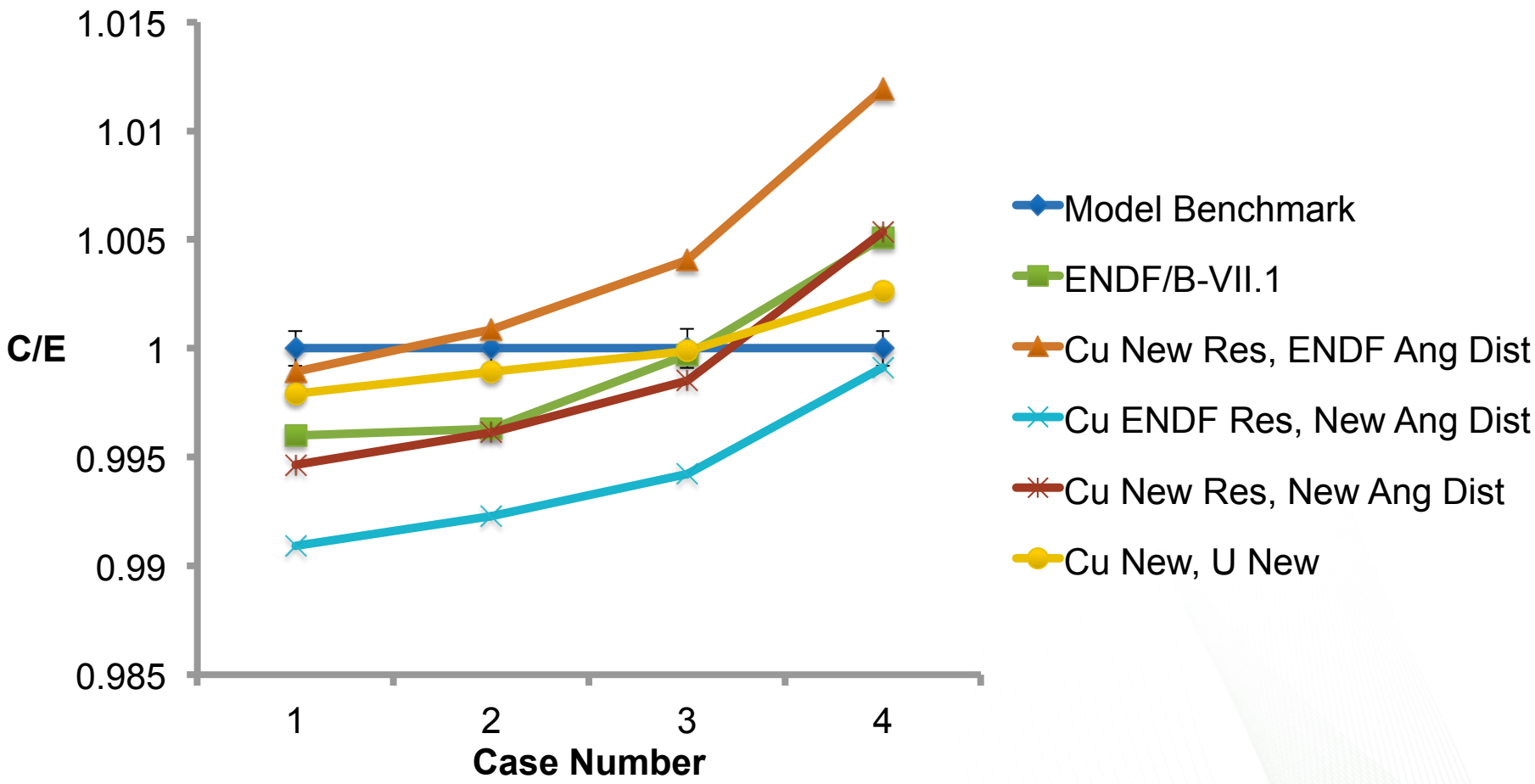
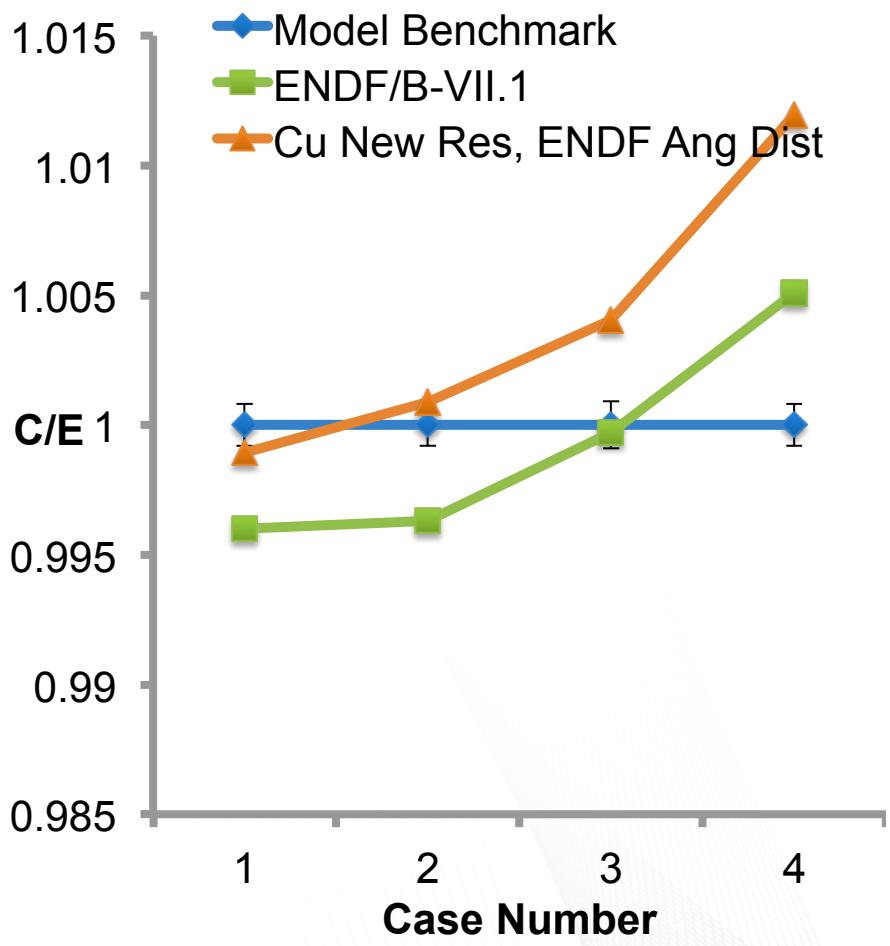
Updated Benchmarking Results

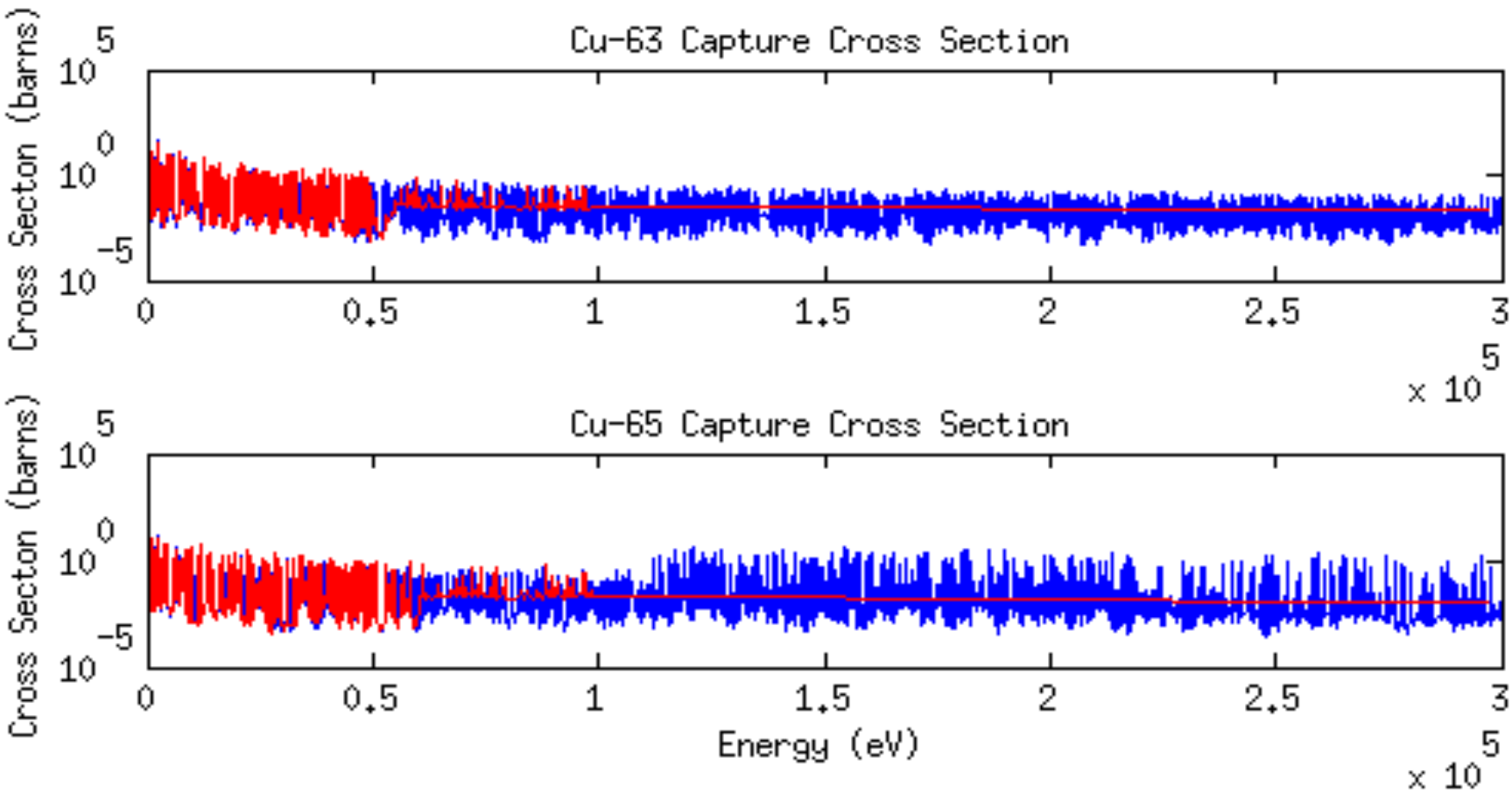


New ^{63,65}Cu Resonance Parameters Only: Smaller Capture Cross Section Found

- **Cu evaluations updated with experimental capture data give smaller capture cross section**
- **Previous evaluation calculated capture from resonance parameters based on experimental transmission data only**



Updated Capture Cross Section



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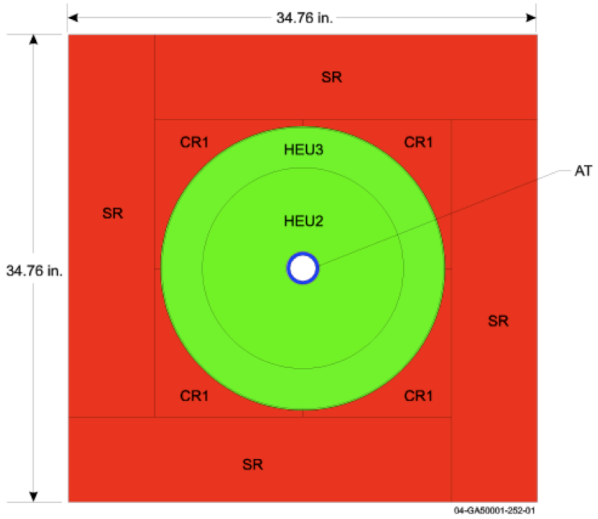
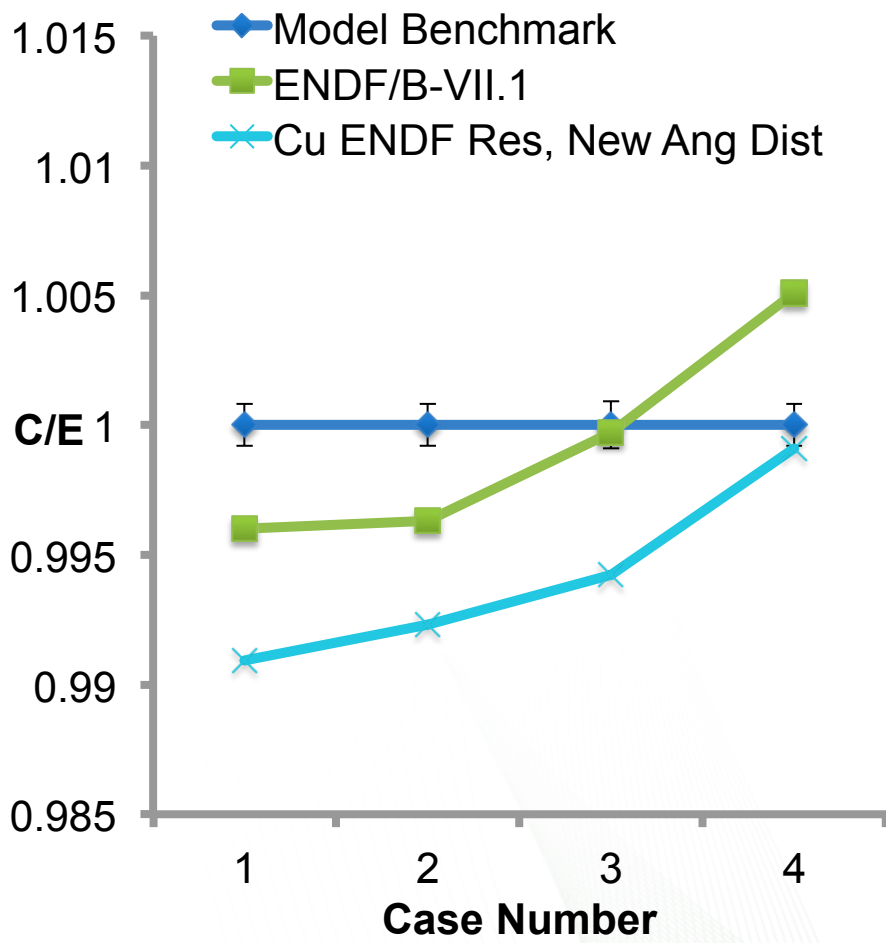
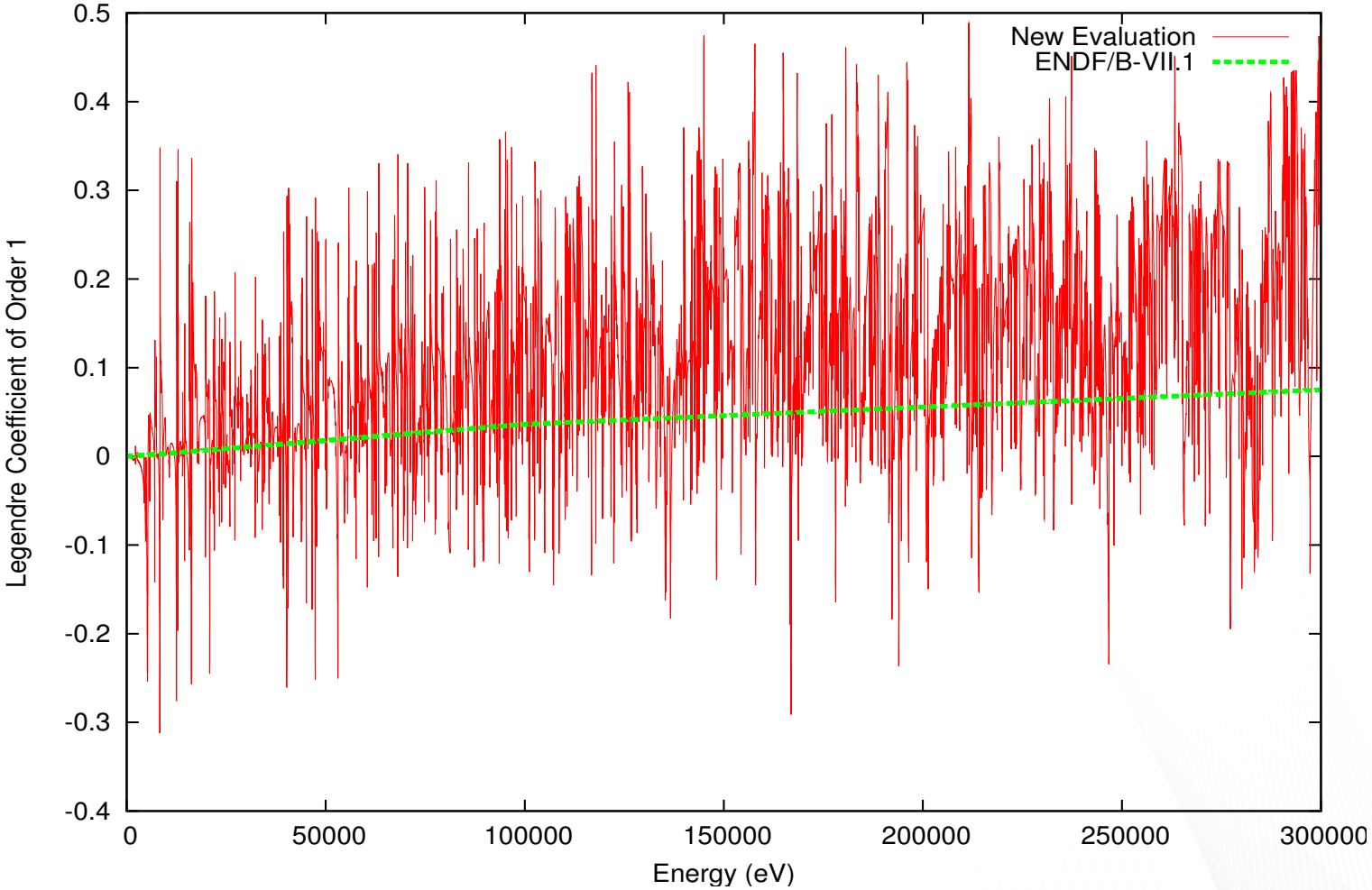
New ^{63,65}Cu Angular Distributions Only

- For the reflected geometry of Zeus a scattering angular distribution plays a significant role in k_{eff}.
- Misrepresentation of the capture cross section in old evaluation was compensated by the angular distributions of elastic scattering.





Detailed Angular Distribution



Summary Tungsten (Pigni/Leal)

- We applied the R-matrix SAMMY method using the Reich-Moore approximation to determine a consistent set of neutron resonance parameters for tungsten isotopes
- In the analyzed energy range, these evaluations double the RRR energy range present in the latest US nuclear data library (ENDF/B-VII.1)
- The experimental data were used sequentially to ensure that the calculated cross sections were in good agreement with multiple transmission data sets
- Results agree with the systematics of the observed s- and p-wave resonances, such as level spacing systematics and strength functions
- Tungsten evaluated files also include cross-section covariance evaluations
- We also evaluated and improved cross sections in the thermal energy range

Summary Copper (Sobes)

- **Concluding Remarks**
  - Measurement of thermal total cross sections at MIT (DOE and NCSP sponsorship)
  - SAMMY analysis of the experimental data was performed for ^{63}Cu and ^{65}Cu in the thermal region and also RRR.
  - The present upper bound energy of the resolved resonance ENDF/B-VII.1 evaluations for ^{63}Cu and ^{65}Cu has been extended from 99 keV to 300 keV (PHYSOR 2012, Knoxville, TN)
  - Benchmark analyses including updated angular distributions and new experimental data on capture cross sections