ORNL EVALUATION REPORT

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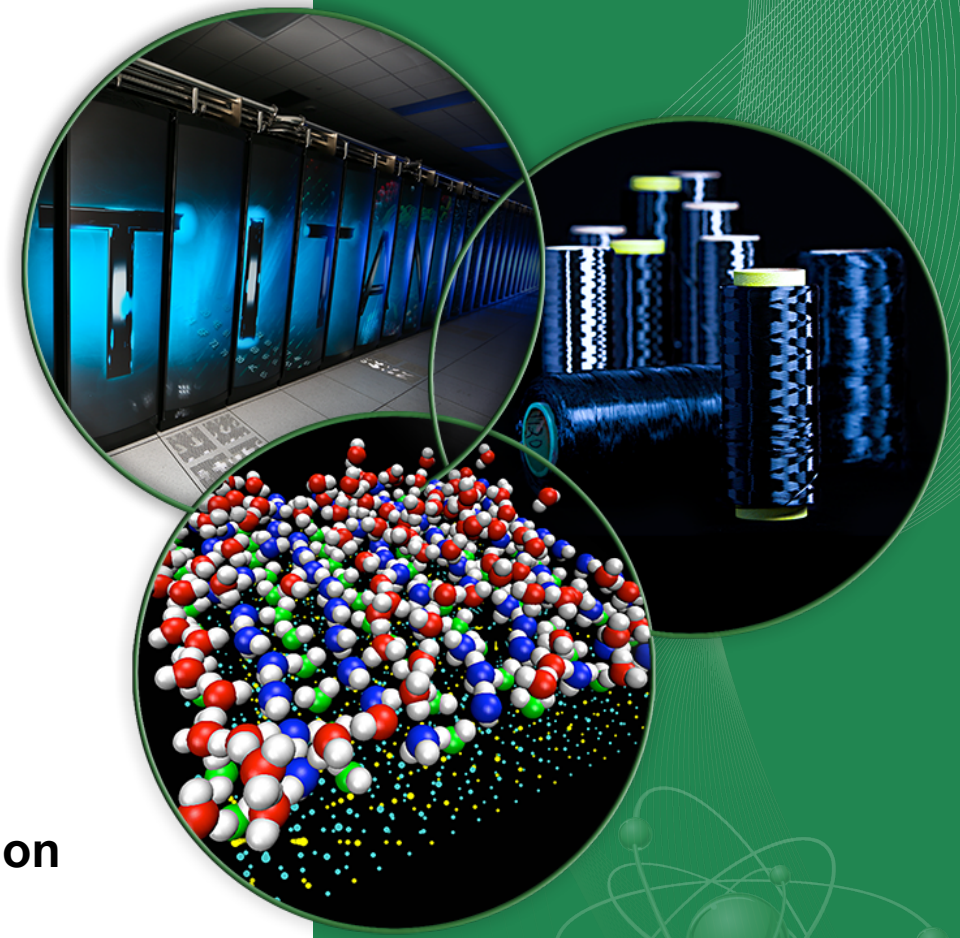

CSEWG Meeting – Cross Section Session
Brookhaven National Laboratory
November 2015

ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory

Outline

- Nuclear Data Evaluation Overview
- $^{183,182,184,186}W$ (Pigni/Leal) : completed
- $^{63,65}Cu$ (Sobes) : completed
- ^{40}Ca (Pigni) : on going
- $^{17,18}O(\alpha,n)$ (Pigni) : on going
- $^{16}O, ^{56}Fe, ^{235}U, ^{239}Pu$ (Leal) : on going

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	1093	545	548	V. Sobes
6 ✓	^{65}Cu ($3/2^-$)	10^{-5} eV-300 (100) keV	RM	952	337	615	V. Sobes

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

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	Evaluator
1 ✗	^{40}Ca (0^+)	10^{-5} eV–1.0 (0.5) MeV	RM	On going	M. T. Pigni
2 ✗	α+^{17}O($5/2^+$)	10^{-5} eV–5.0 MeV	RM	On going	M. T. Pigni
3 ✗	α+^{18}O(0^+)	10^{-5} eV–5.0 MeV	RM	On going	M. T. Pigni
4 ✗	^{16}O (0^+)	10^{-5} eV–6.1 MeV	RM	On going	L. C. Leal
5 ✗	^{56}Fe (0^+)	10^{-5} eV–2 MeV	RM	On going	L. C. Leal
6 ✗	^{235}U ($7/2^-$)	10^{-5} eV–2.25 keV	RM	On going	L. C. Leal
7 ✗	^{239}Pu ($1/2^+$)	10^{-5} eV–4 keV (2)	RM	On going	L. C. Leal

RM – Reich-Moore Approximation

Computer Code SAMMY

- **Used for analysis of *neutron* and *charged-particle* cross section data**
- **Uses Bayes' method to find parameter values**
- **Uses R-matrix formalism in the Reich-Moore approximation**
- **Generates cross section covariance matrix and sensitivity parameters for RRR**

Tungsten Isotope Evaluations

- **Transmission and capture cross section measurements performed at Geel for ^{182,183,184,186}W for energy up to 10 keV and for ^{183}W up to 5 keV**

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- **Early high-resolution total cross section measurements by Harvey at ORELA for natural tungsten**

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- Transmission and capture cross section measurements performed at Geel for ^{182,183,184,186}W for energy up to 10 keV and for ^{183}W up to 5 keV
- Early high-resolution total cross section measurements by Harvey at ORELA for natural tungsten
- **Reich-Moore approximation**

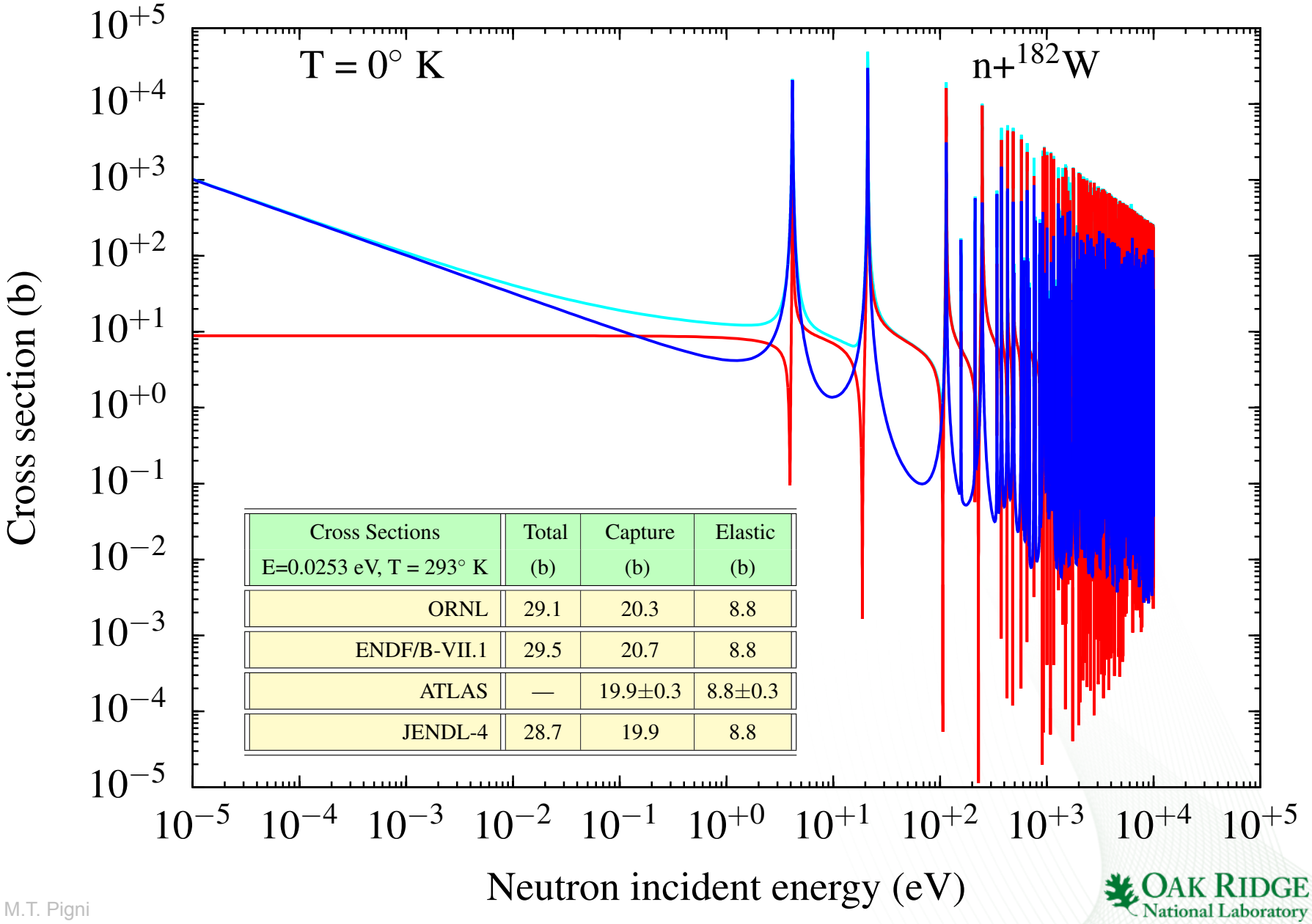
Tungsten Isotope Evaluations

- Transmission and capture cross section measurements performed at Geel for ^{182,183,184,186}W for energy up to 10 keV and for ^{183}W up to 5 keV
- Early high-resolution total cross section measurements by Harvey at ORELA for natural tungsten
- Reich-Moore approximation
- **Cross section covariance matrices (compact format)**

Tungsten Isotope Evaluations

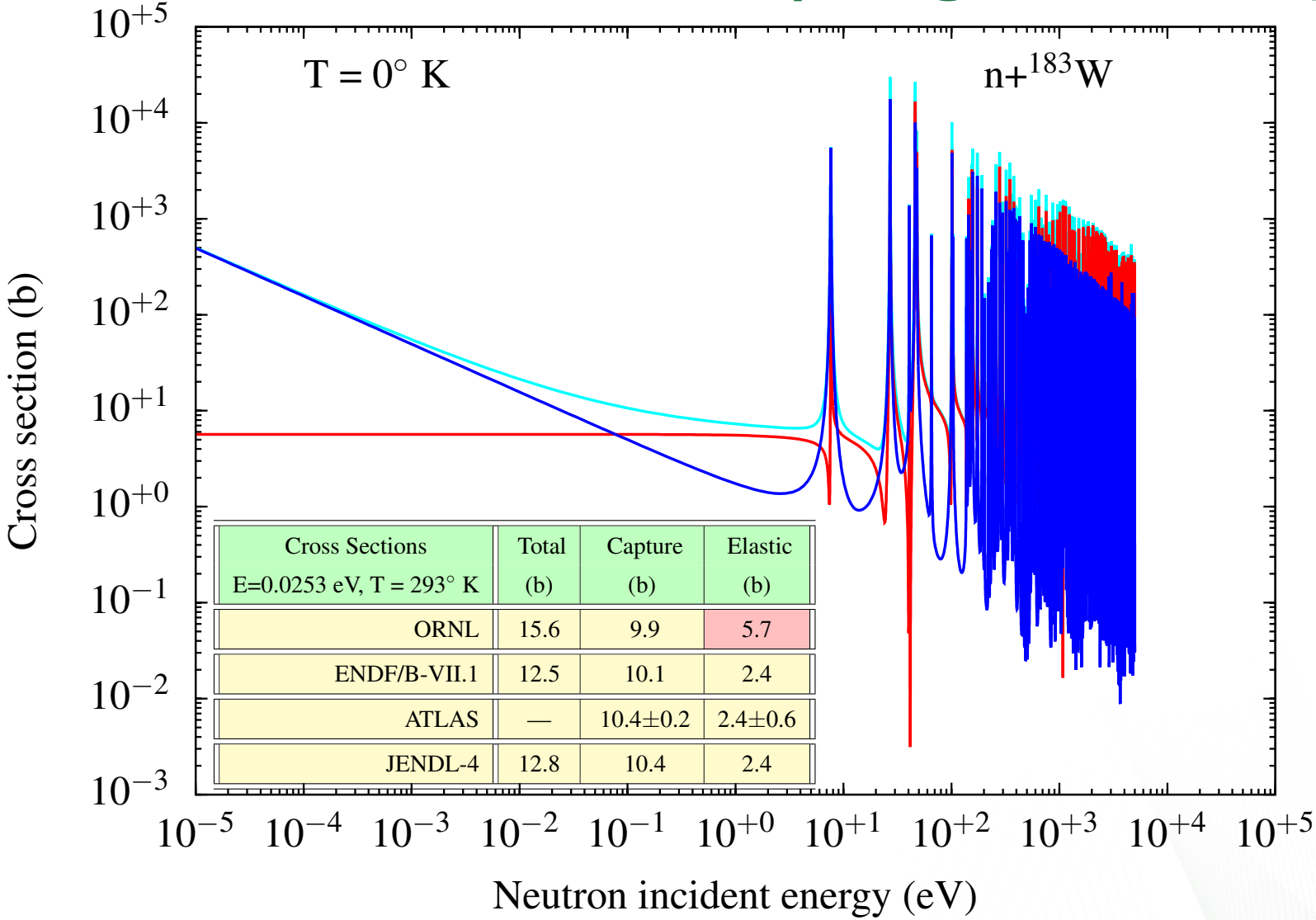
- Transmission and capture cross section measurements performed at Geel for ^{182,183,184,186}W for energy up to 10 keV and for ^{183}W up to 5 keV
- Early high-resolution total cross section measurements by Harvey at ORELA for natural tungsten
- Reich-Moore approximation
- Cross section covariance matrices (compact format)
- **Submitted ENDF files (LRF=7) to NNDC/BNL in August 2014 (revisions 633 to 636 in GFORGE ENDF/A)**

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

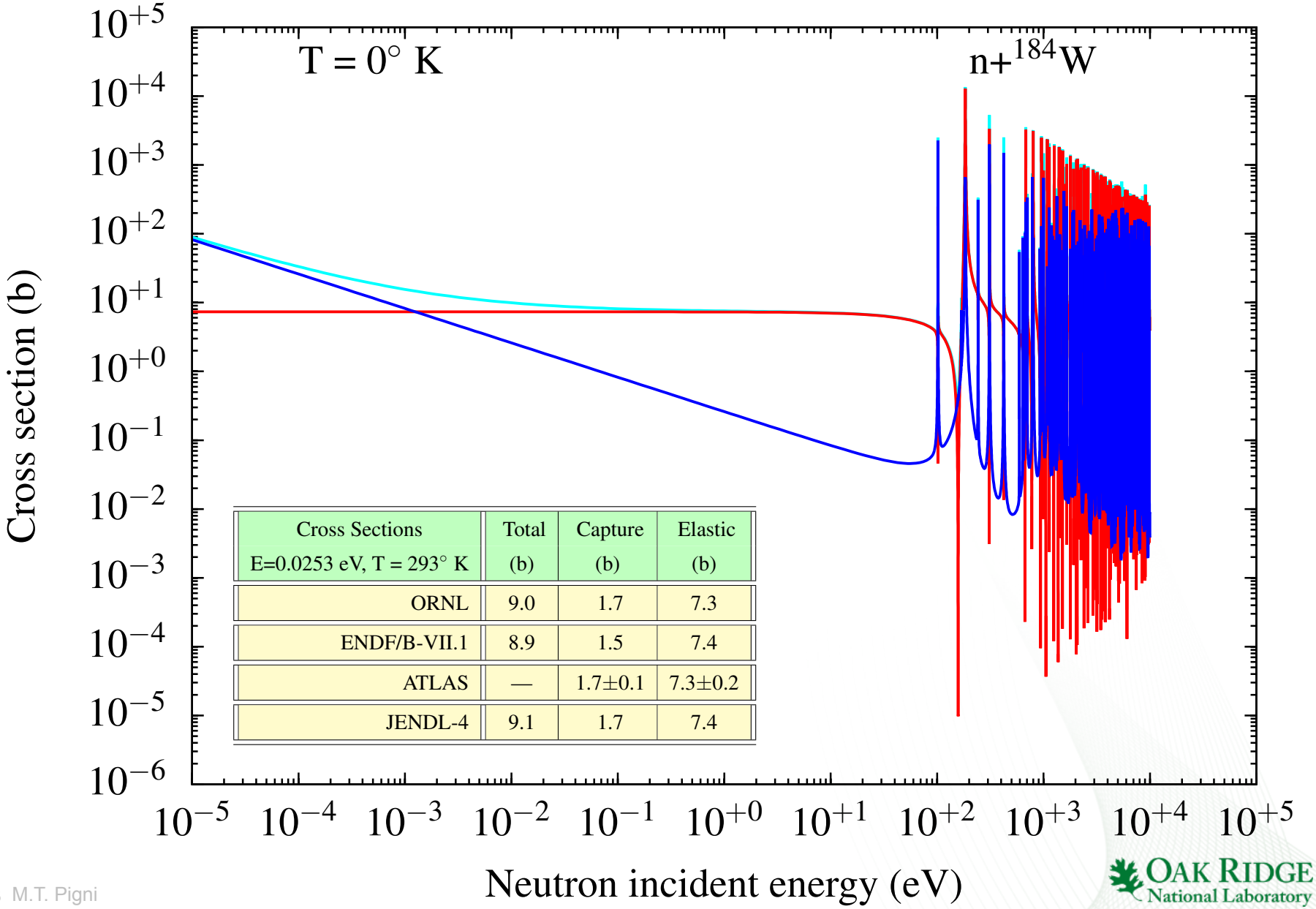
Results: Cross Sections (Tungsten Isotopes(*))



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

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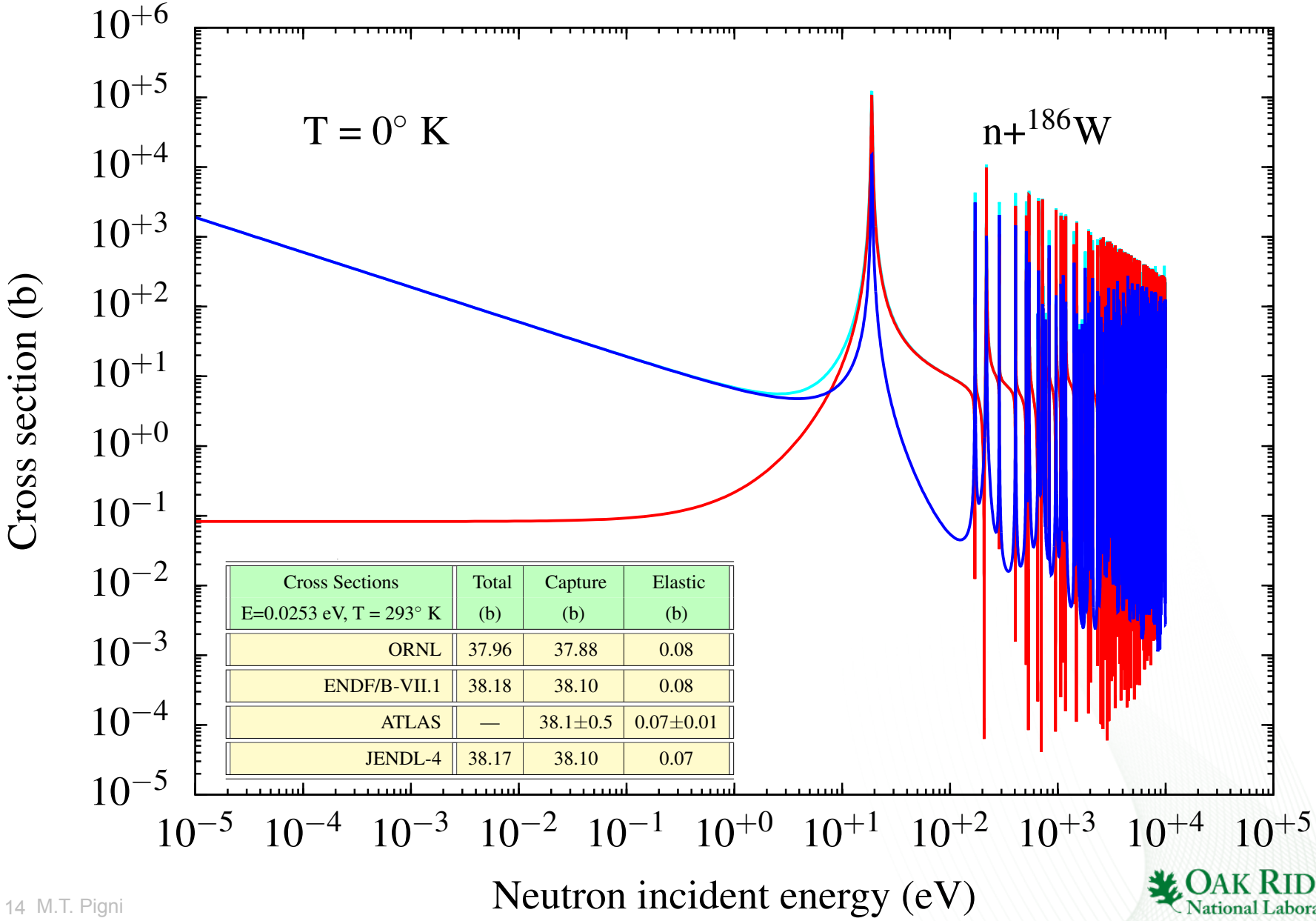
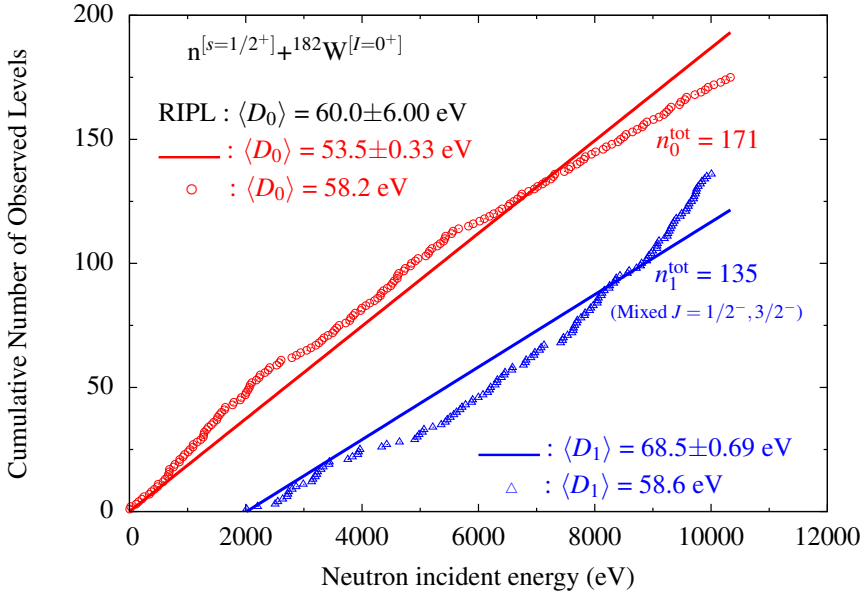
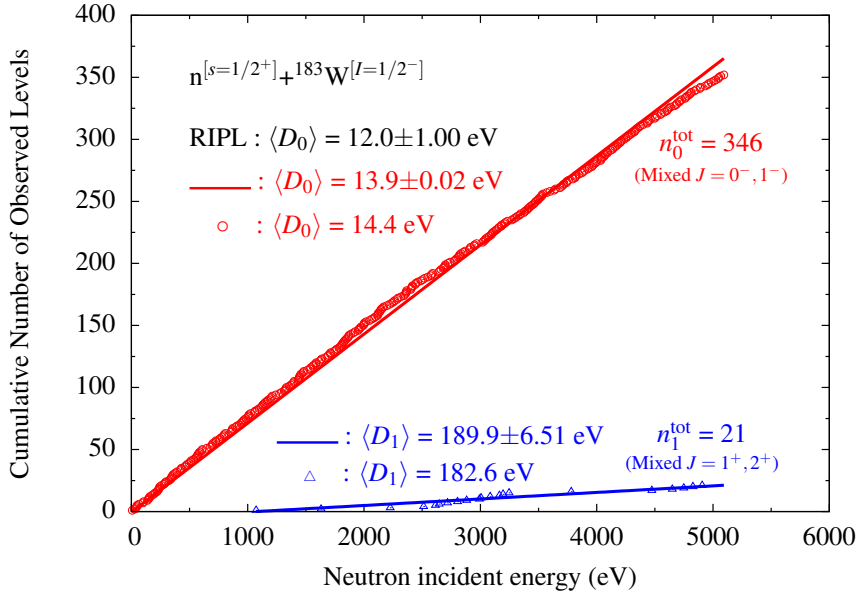
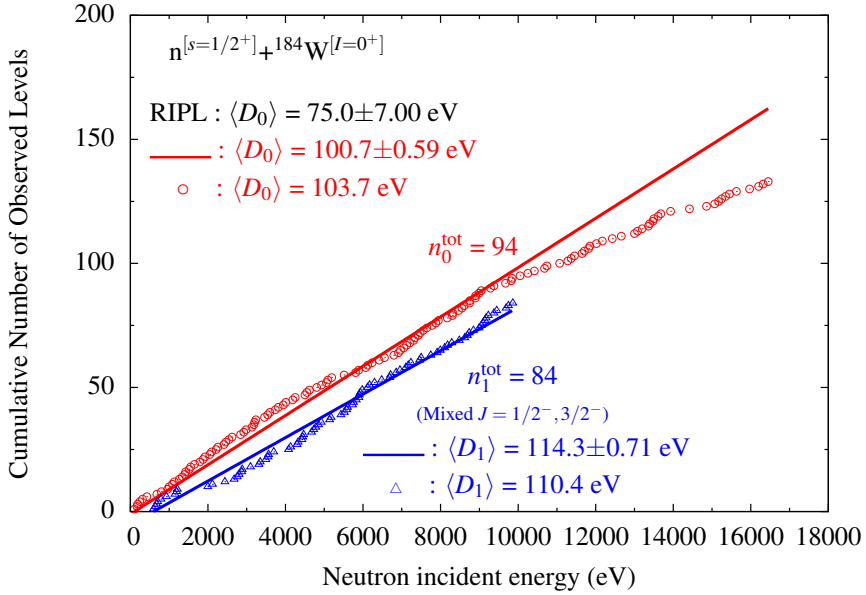


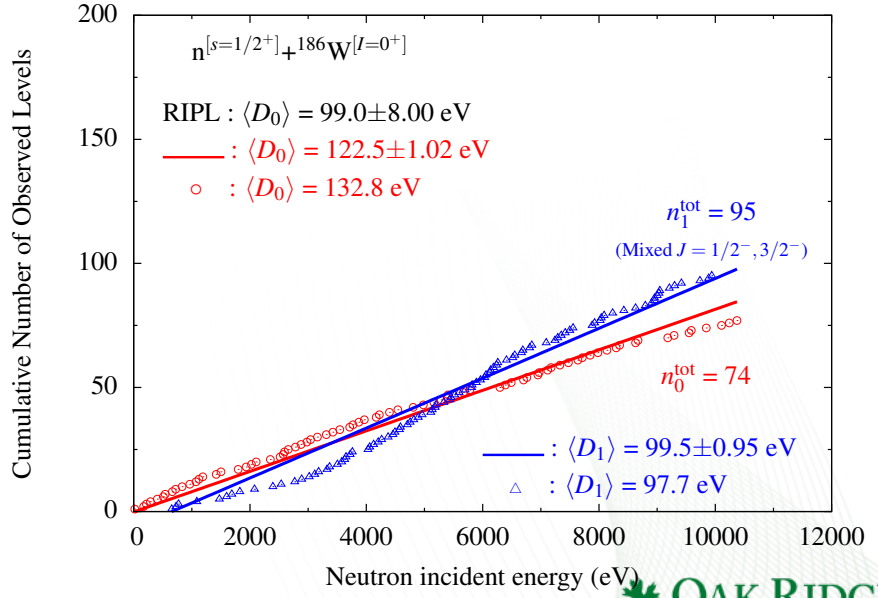
Cross Sections E=0.0253 eV, T = 293° K	Total (b)	Capture (b)	Elastic (b)
ORNL	37.96	37.88	0.08
ENDF/B-VII.1	38.18	38.10	0.08
ATLAS	—	38.1±0.5	0.07±0.01
JENDL-4	38.17	38.10	0.07

Statistics on Resonance Parameters

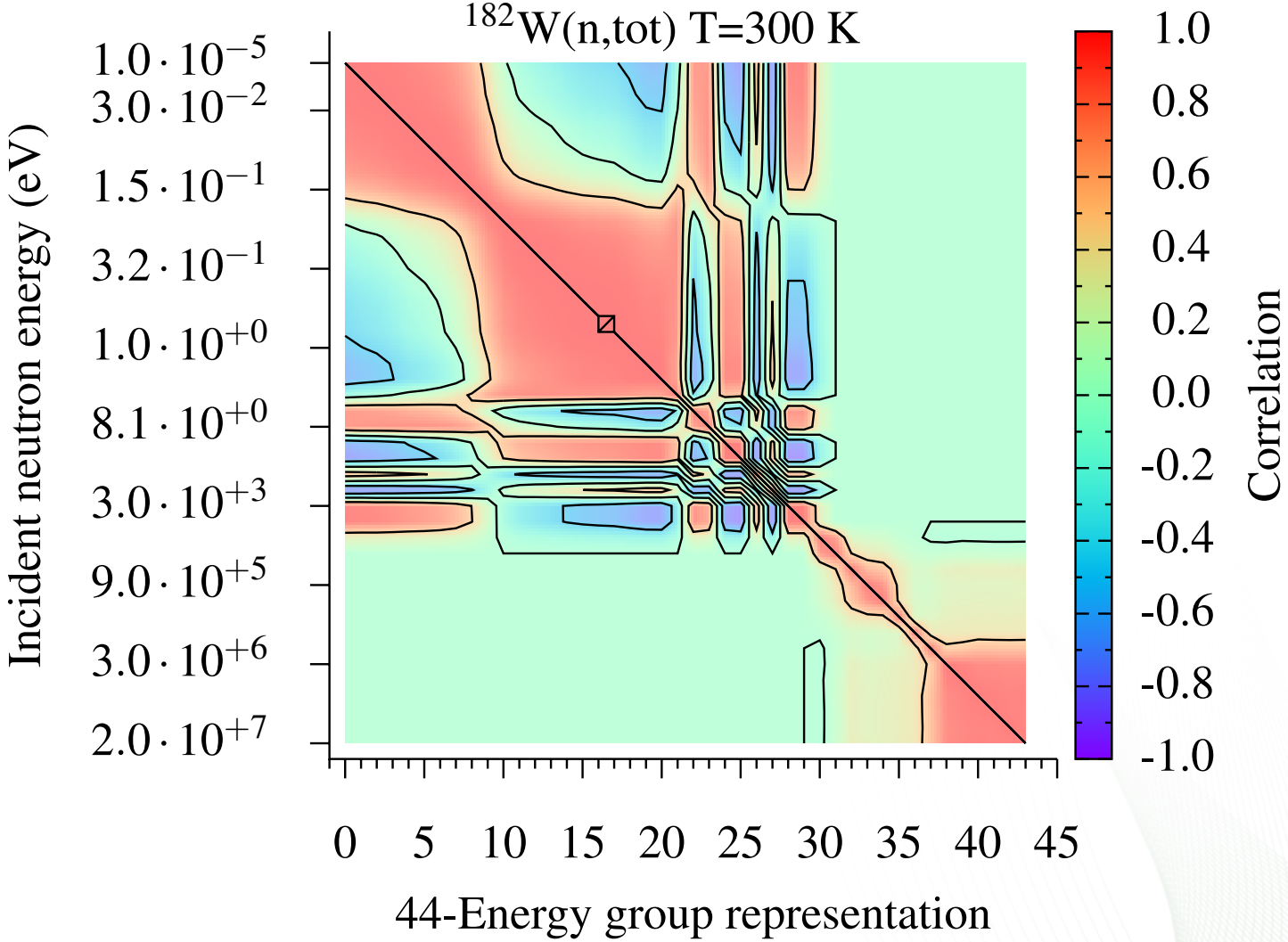








Covariance Evaluations (Total)



Copper Resonance Evaluations

- **Major improvements**
  - **RRR extended (three-fold) up to 300 keV**
    - **Data in the thermal range (Sobes, MIT)**
    - **Transmission data (Pandey, ORELA)**
    - **Capture data (Guber, GELINA)**

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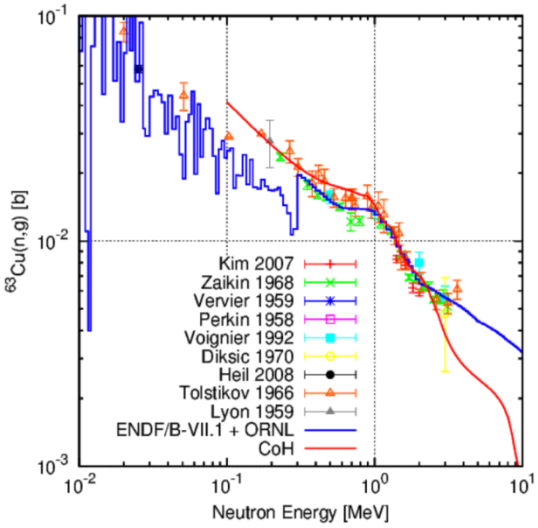
  - **Detailed elastic angular distributions**
    - **Point-wise description of angular distribution reconstructed from resonance parameters**
    - **Test on benchmarks**

Copper Resonance Evaluations

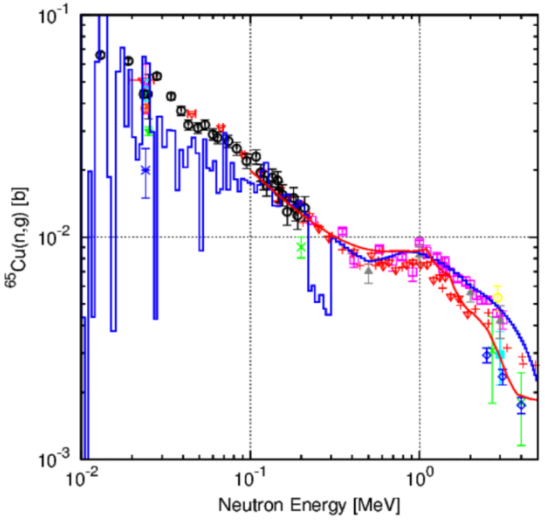
(Capture Cross Sections)

- **From Mini CSEWG 2015 (Kawano)**

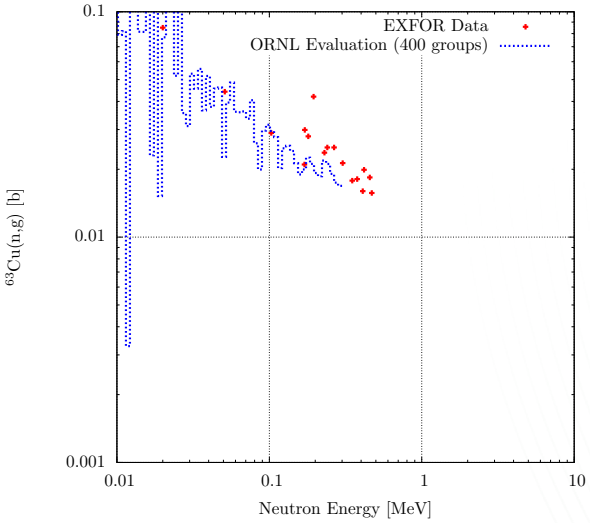
- **Refit of renormalized experimental data matching with high-energy evaluation. On-going work with LANL (Kawano)**

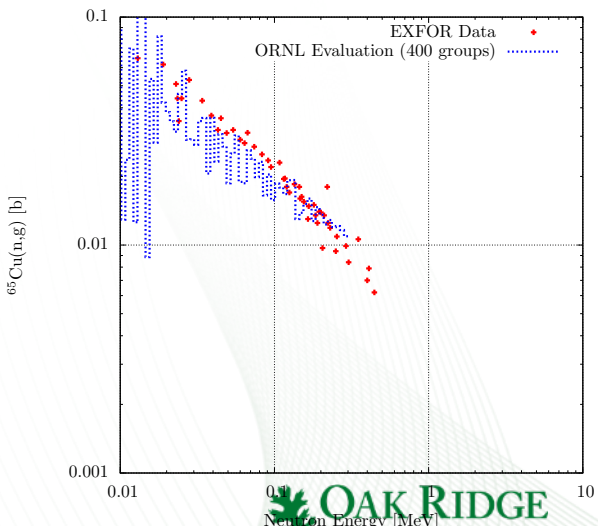


^{63}Cu Capture Cross Section vs. Integral Measurements



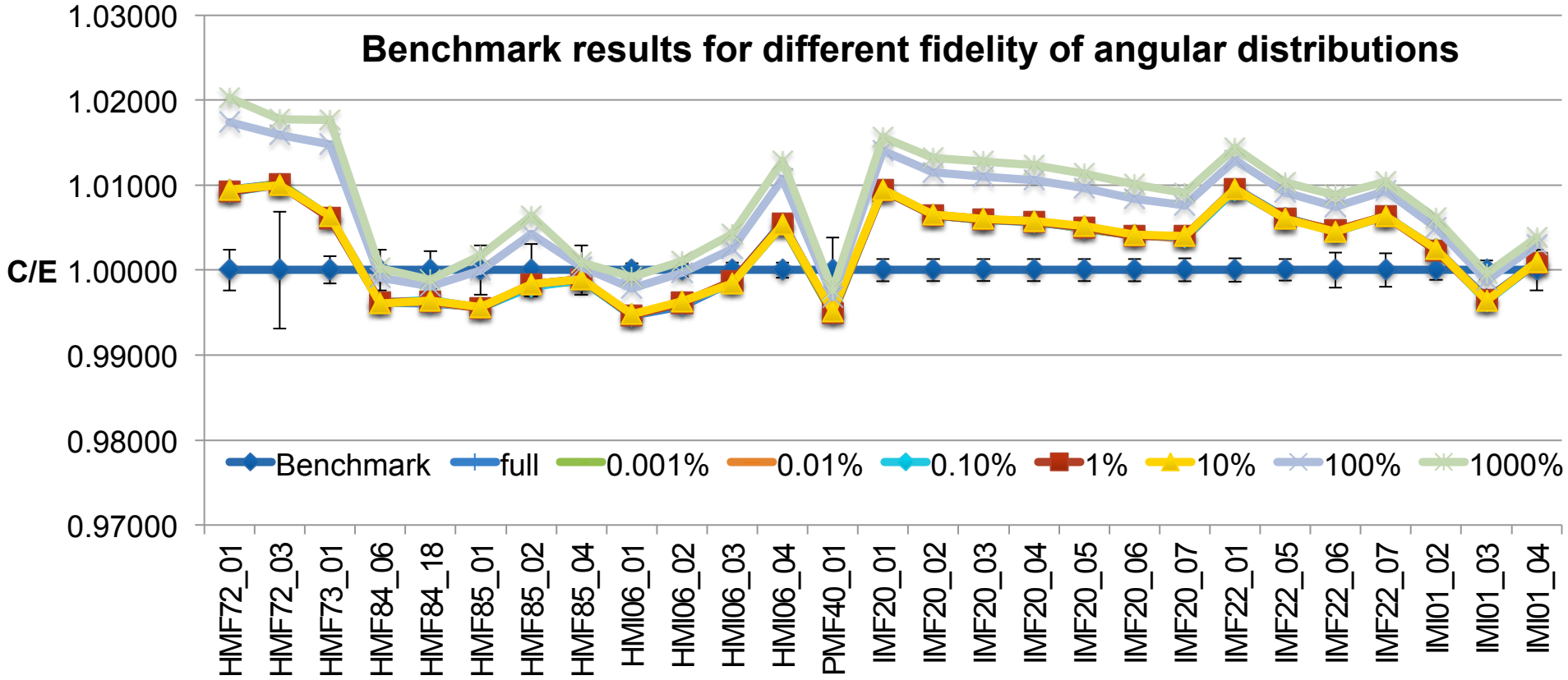
^{65}Cu Capture Cross Section vs. Integral Measurements





Copper Resonance Evaluations

(Benchmark Test on Point-wise Angular Distribution)



Error	0.001%	0.01%	0.1%	1%	10%	100%	1000%
Points	107 000	102 500	94 000	83 000	76 500	17 500	10 000

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^{40}Ca Resonance Evaluation

- **Transmission and capture cross section measurements performed at Geel for ^{nat}Ca in the energy range up to 1 MeV (Guber)**
  - **Measurements of Calcium using metallic samples**
  - **The samples are in Al canning due to reactivity with air**
  - **Transmission experiments w/ different sample thickness (path 50 m)**
  - **Neutron capture using detector system (path 60 m)**

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- **Early high-resolution total cross section measurements by**
  - **Cierjacks (1968, KIC): ^{nat}Ca(n,tot)**
  - **Perey (1972, ORELA): ^{nat}Ca(n,tot)**
  - **Singh (1975): ^{nat}Ca(n,tot)**
  - **Johnson (1978, ORELA): ^{40}Ca(n,tot)**

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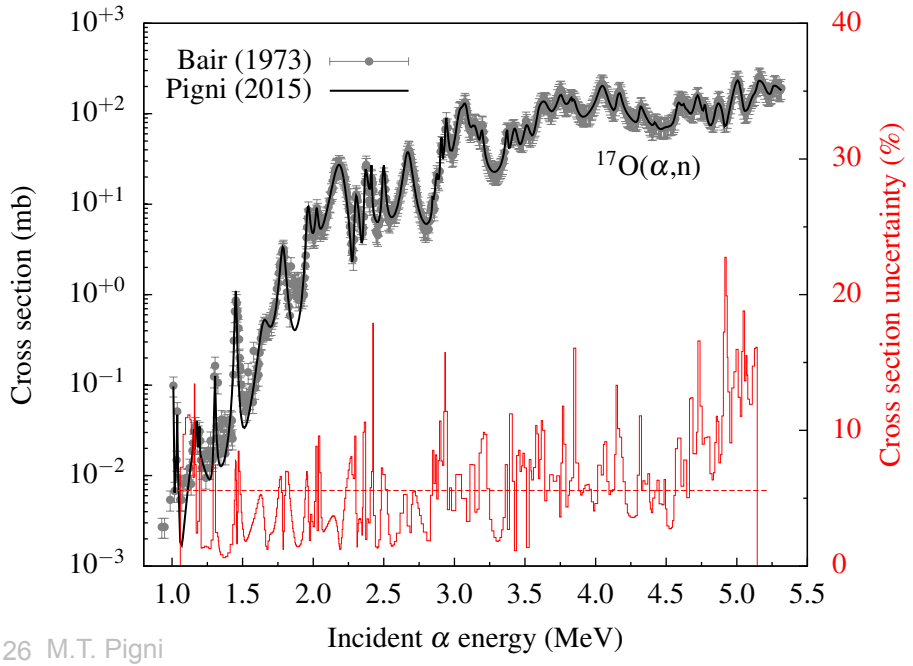
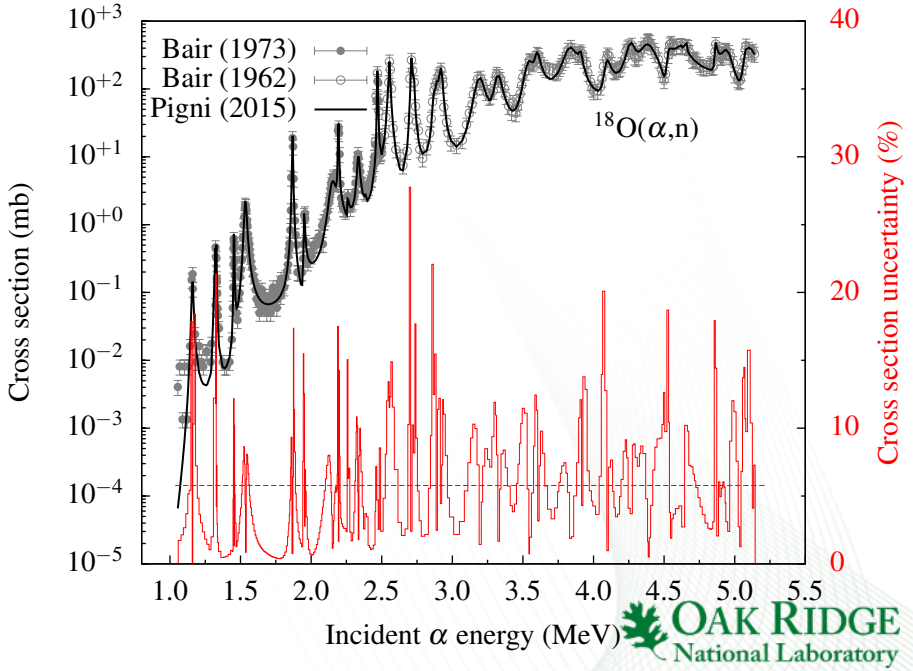
- Used formalism of Reich-Moore approximation
- **Included (n,α) and (n,p) channels**

^{17,18}O(α,n) Cross Sections up to 5 MeV

(…for more details see presentation in the covariance session)

- **R-matrix SAMMY code for lower energy range up to about 5 MeV based on Bair's experimental data**
  - **Reich-Moore parameterization of (α,n) reactions**
    - ^{18}O elastic channel (as well as spin assignment) based on measurement of Goldberg for available excitation energies
    - For ^{17}O up to about 2 MeV see important work of Best

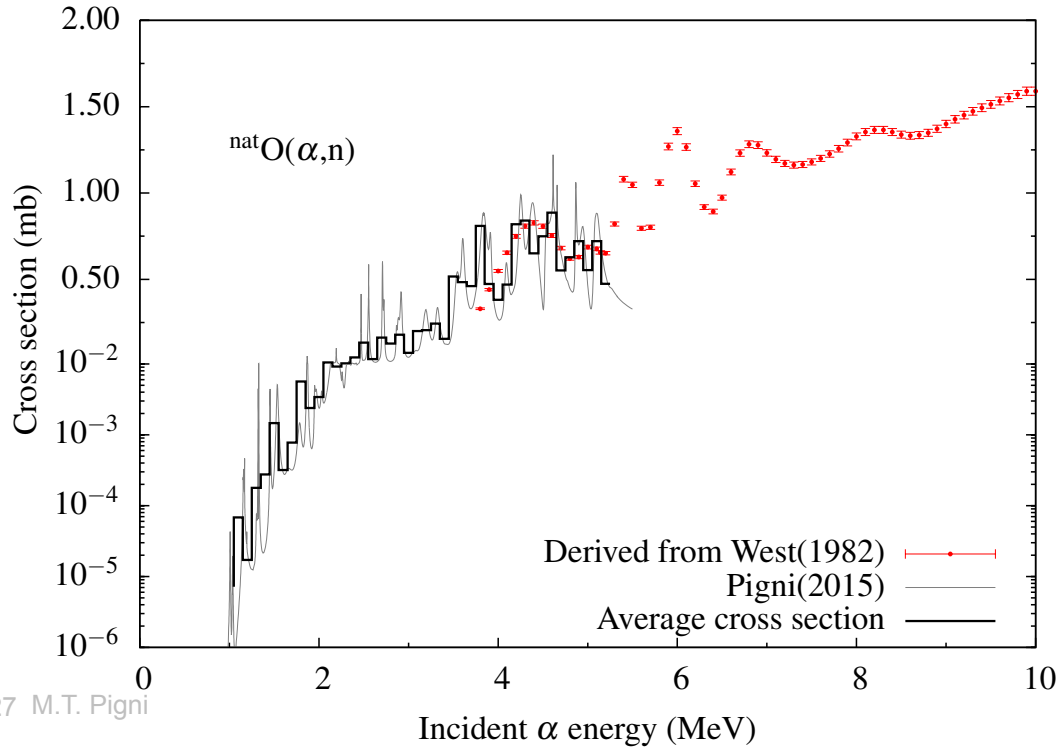




^{17,18}O(α,n) Cross Sections up to 5 MeV

…and above

- **>5 MeV, cross sections based on West's experimental data on natural oxygen**
  - **West's thick target data (1.5% uncertainty)**
- **JENDL cross section data for ^{17}O (0.038%) to determine ^{18}O (0.205%) out of natural oxygen**



Integrating over the energy range 3.8 up to 5 MeV, i.e. the energy range common to both data sets, we found the average cross sections (black line) were 3% lower than the West's cross sections (red dots).

n+^{16}O Resonance Evaluation (ORNL/IRSN)

November 2014:

- ORNL Evaluation (o16ornl1.dat*) in RRR August 2014 (Rev. 629 GF)
- The RRR evaluation up to 6.12 is an update of previous ORNL evaluation (Sayer ORNL/TM-2000/212) up to 6.3 MeV
  - Updated thermal total cross section value: 3.78391 b (T=0° K)
  - (n,n) and (n,α) angular distributions generated by resonance parameters

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November 2015:

- **IRSN/ORNL evaluation***
  - **Updated thermal total cross section value: 3.765 b (T=0° K) (Cielo recommendation)**
  - **Fit of RPI measurements for total cross sections including resolution effects**

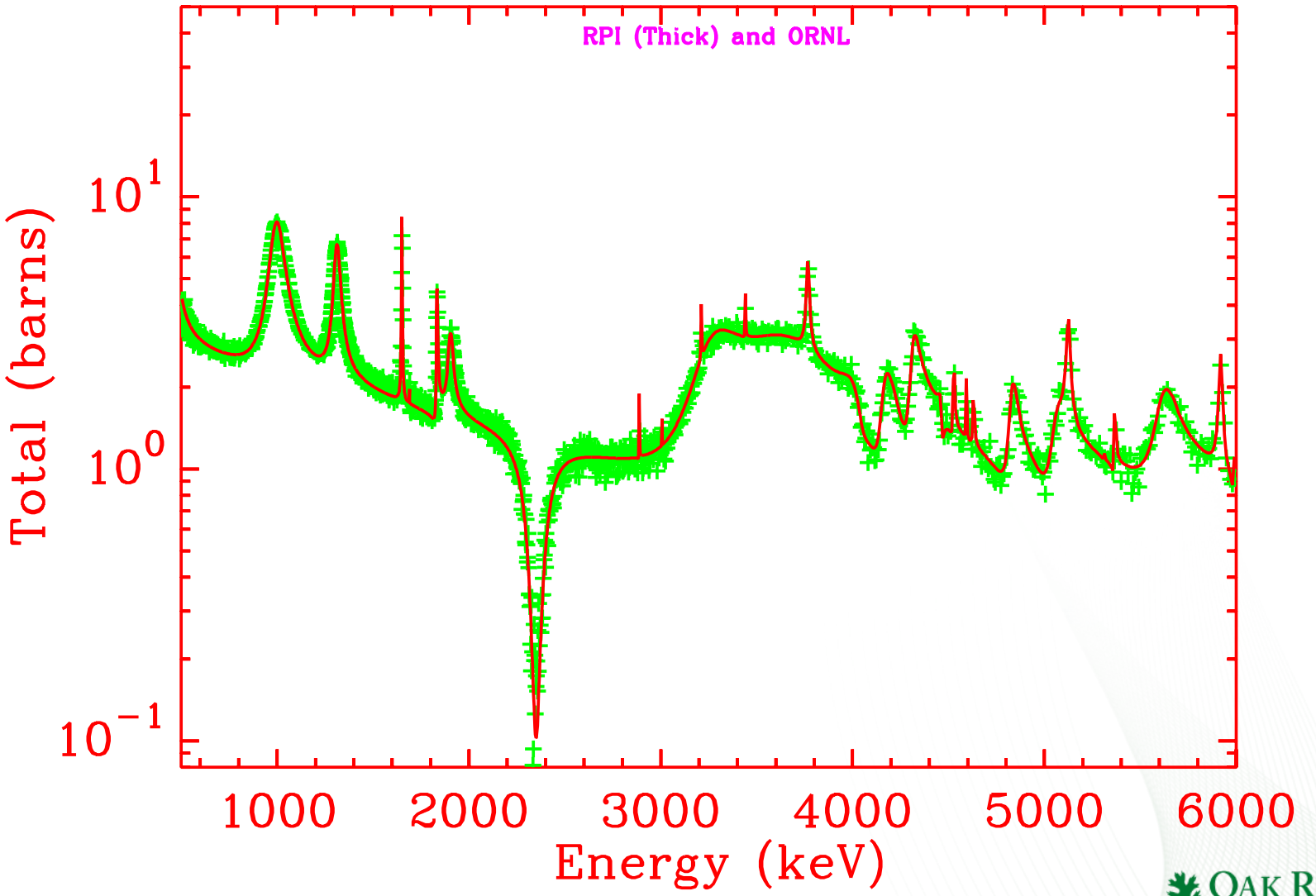
(*) RRR covariance evaluation is not included

n+^{16}O Resonance Evaluation (ORNL/IRSN)

(Experimental Data)

- **^{16}O(n,tot) RPI experimental data, 0.5 – 6 MeV**
- **^{16}O(n,α) experimental data (Giorginis, ND2007, IRMM), 3.95 – 9 MeV with accuracy close 5%**
- **^{13}C(α,n) experimental data (Harissopulos, Phys. Rev. C72, 62801, 2005), 0.8 – 8 MeV with accuracy overall 4%**
- **Giorginis and Harissopulos data give about 30% lower ^{16}O(n,α) cross section data than the Bair-Haas data (Phys. Rev. C7, 1356, 1973), 20% accuracy**

SAMMY Fit with RPI Data



Useful Information on n+^{16}O

(November 2014)

Quantity	ORNL (T = 0° K)	ORNL (T = 293.6° K)	ATLAS
σ_t	3.78391 b	3.90322 b	-
σ_γ	9.58635×10^{-5} b	9.33362×10^{-5} b	$(1.9 +/- 0.19)\ 10^{-4}$ b
σ_s	3.78382 b	3.90313 b	3.761 ± 0.006 b
R’	-	4.15 fm	4.8 ± 0.1 fm
a_{coh}	-	5.646 fm	5.805 ± 0.005 fm
I_γ	-	2.7596×10^{-4}	$(2.7 \pm 0.3) \times 10^{-4}$

Processing performed by NJOY, PREPRO, AMPX, GAIA

Useful Information on n+^{16}O

(Latest Update November 2015)

Quantity	ORNL/IRSN (T = 0° K)	ORNL/IRSN (T = 293.6° K)	ATLAS
σ_t	3.7654 b	3.8841 b	-
σ_γ	1.7153×10^{-4} b	1.6701×10^{-4} b	$(1.9 \pm 0.19)\ 10^{-4}$ b
σ_s	3.7652 b	3.8839 b	3.761 ± 0.006 b
R’	-	4.15 fm	4.8 ± 0.1 fm
a_{coh}	-	5.805 fm	5.805 ± 0.005 fm
I_γ	-	3.0925×10^{-4}	$(2.7 \pm 0.3) \times 10^{-4}$

Processing performed by NJOY, PREPRO, AMPX, GAIA

^{56}Fe Resonance Evaluation

(up to 2 MeV)

- **New experimental data available for ^{56}Fe**
  - **RPI new high resolution transmission data (up to 5 MeV)**
  - **GEEL new inelastic cross section experimental data**

paradigm shift

^{56}Fe Resonance Evaluation

(up to 2 MeV)

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  - RPI new high resolution transmission data (up to 5 MeV)
  - GEEL new inelastic cross section experimental data
- **Use the SAMMY capability to included excited states**

paradigm shift

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(up to 2 MeV)

- New experimental data available for ^{56}Fe
  - RPI new high resolution transmission data (up to 5 MeV)
  - GEEL new inelastic cross section experimental data
- Use the SAMMY capability to included excited states
- **Results**
  - **Transmission data fitted up 1 MeV (Harvey, Perey, RPI)**
  - **Total (RPI) and inelastic (Plompen, Perey) fitted up 2 MeV**
  - **Capture data fitted up 650 keV (Spencer)**
  - **Angular distributions fitted up 1 MeV (Perey), up to 2 MeV (RPI)**
  - **Benchmark ALARM-CF-FE-SHIELD-001 (ICSBEP)**

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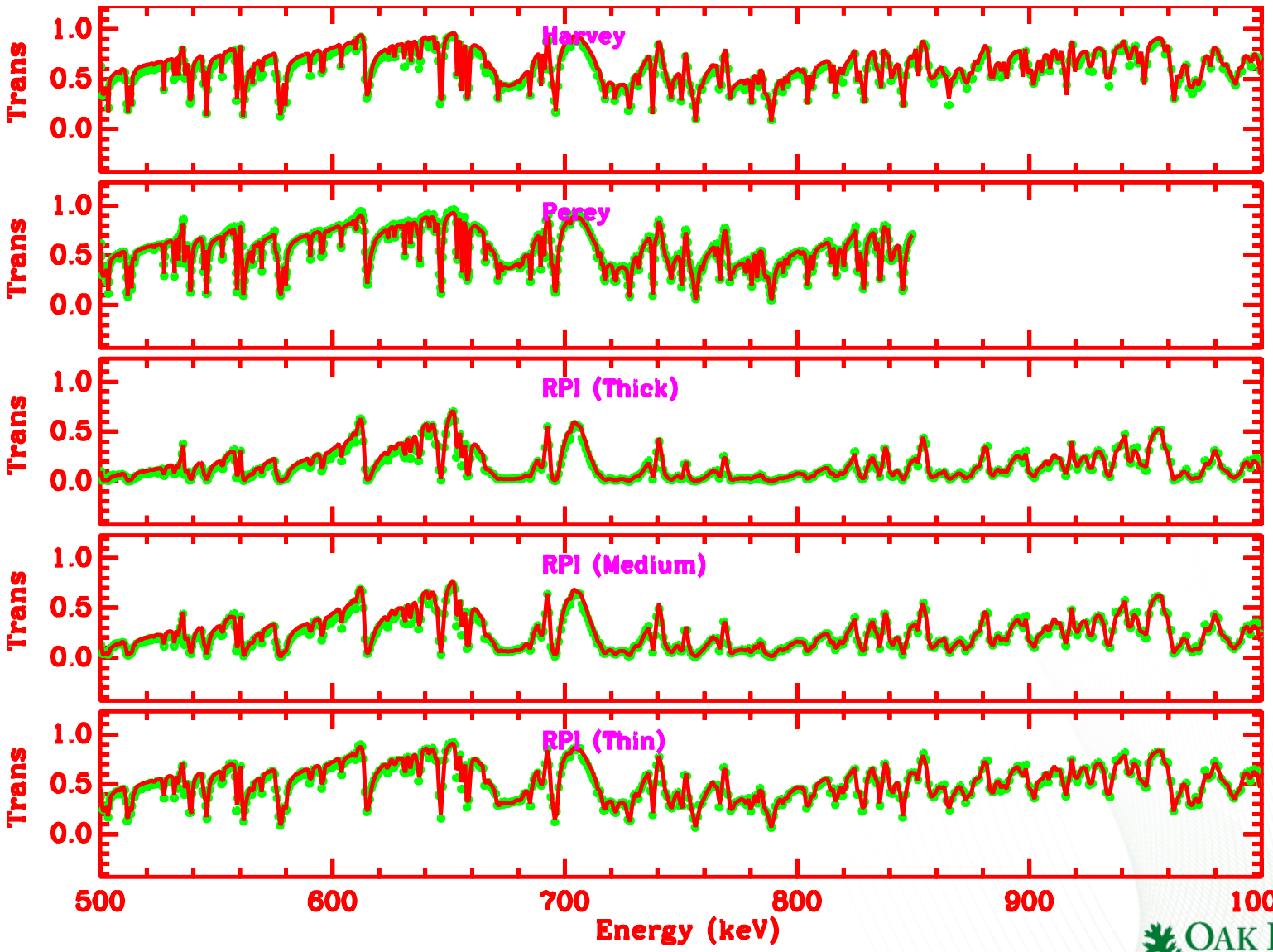
  - Angular distributions fitted up 1 MeV (Perey), up to 2 MeV (RPI)
  - Benchmark ALARM-CF-FE-SHIELD-001 (ICSBEP)
- **On-going work**
  - **Improving benchmarks**

paradigm shift

Experimental Data for ^{56}Fe Evaluation

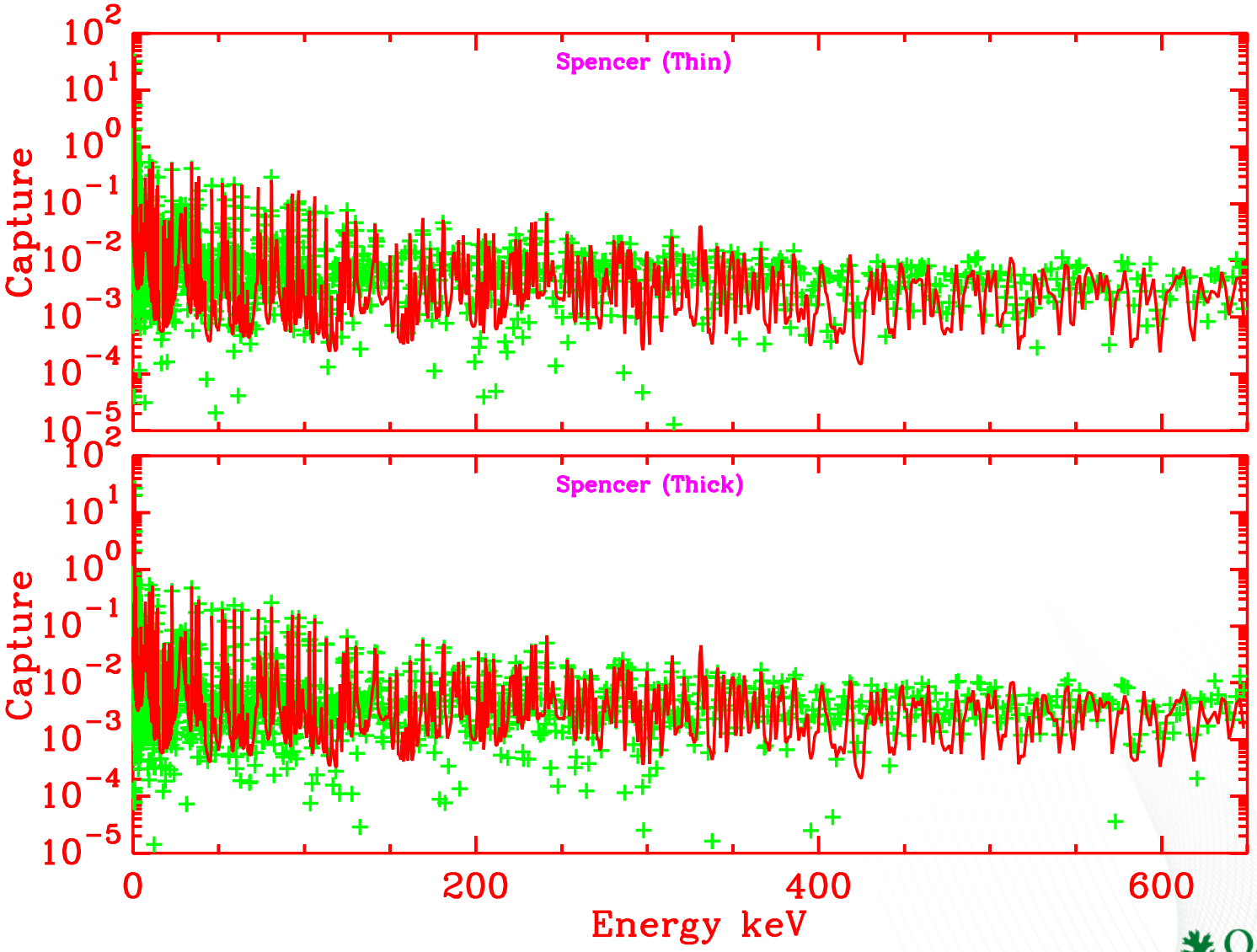
Reference	Energy Range	Facility	TOF (m)	Measurement
Harvey (1987)	0.020 – 2 MeV	ORELA	201.575	Transmission
Perey (1990)	120 – 850 keV	ORELA	201.575	Transmission
Cornelis (1982)	0.5 – 2 MeV	GELINA	387.713	Transmission
Danon et al. (2012) (three thicknesses)	0.5 – 2 MeV	RPI	249.740	Transmission
Danon et al. (2012)	0.5 – 2 MeV	RPI	30.07	Scattering (presentation in the workshop)
Perey (1990)	0.85 – 1.5 MeV	ORELA	201.575	Inelastic
Plompen (2011)	0.85 – 2 MeV	GELINA	198.686	Inelastic
Spencer (1994) (two thicknesses)	0.010 – 650 keV	ORELA	40.0	Capture
Perey (1990)	0.85 – 1.5 MeV	ORELA	200.191	Elastic
Cabé (1967)	0.5 – 1.2 MeV	Université de Louvain (Van de Graaff)	~ 1	Elastic
Shcherbakov (1977)	0.001 – 10 eV	TOF/Russia	9.5	Total
Shcherbakov (1977)	0.001 – 10 eV	TOF/Russia	9.5	Capture

SAMMY Fits to the Transmission Data

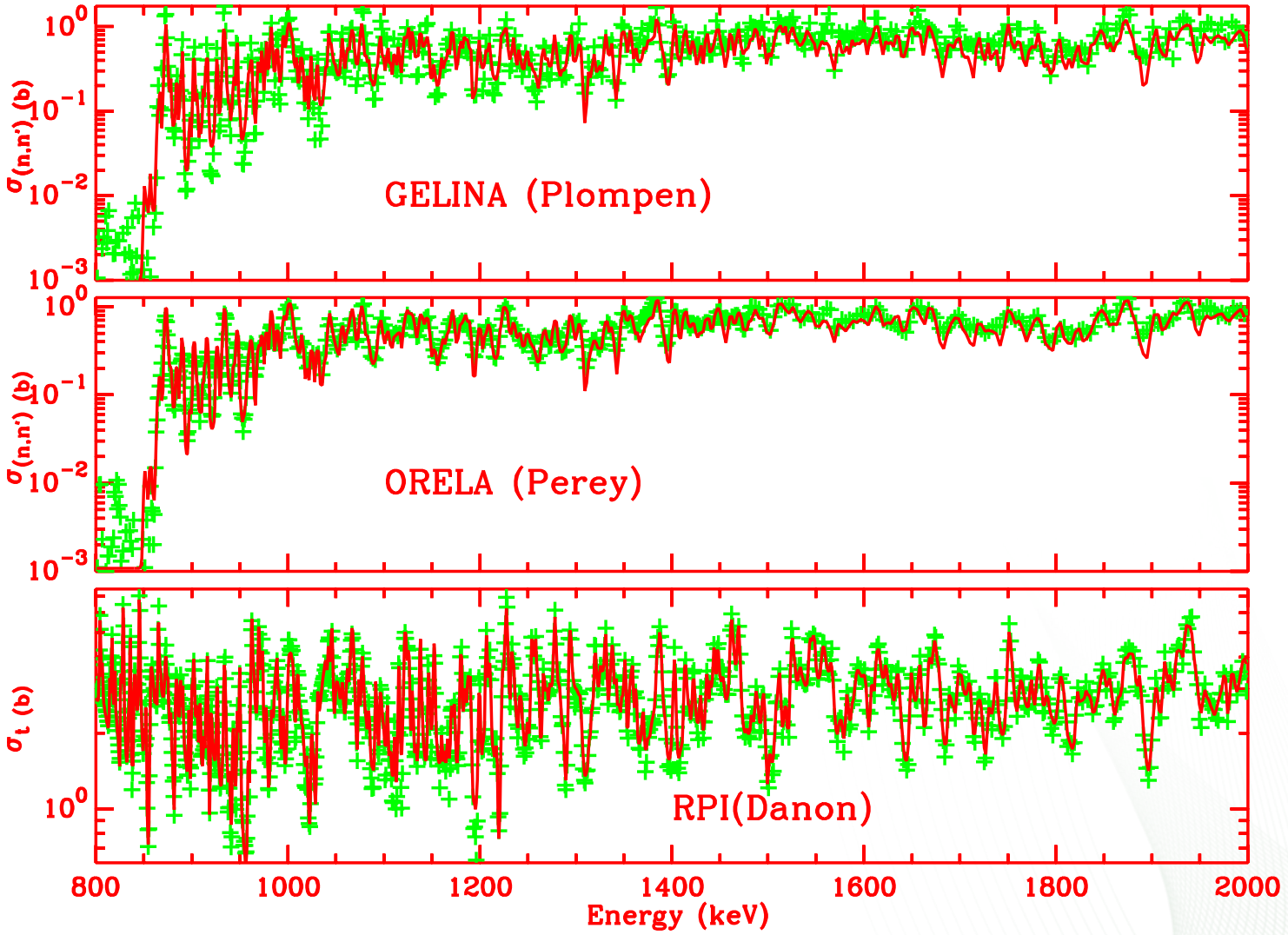


SAMMY Fit to ^{56}Fe Capture Data

(Spencer up to 650 keV)

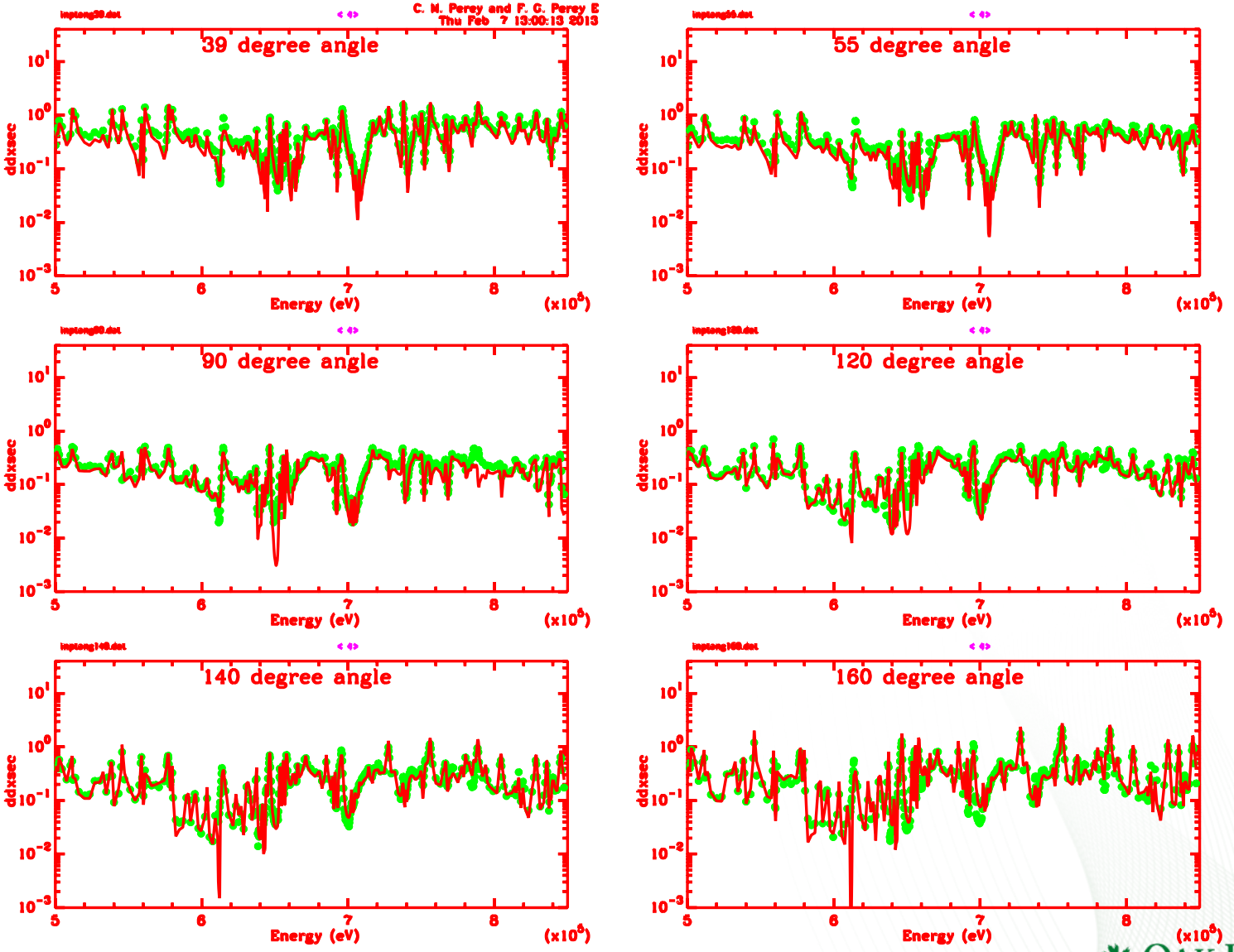


SAMMY Fits to Total/Inelastic ^{56}Fe



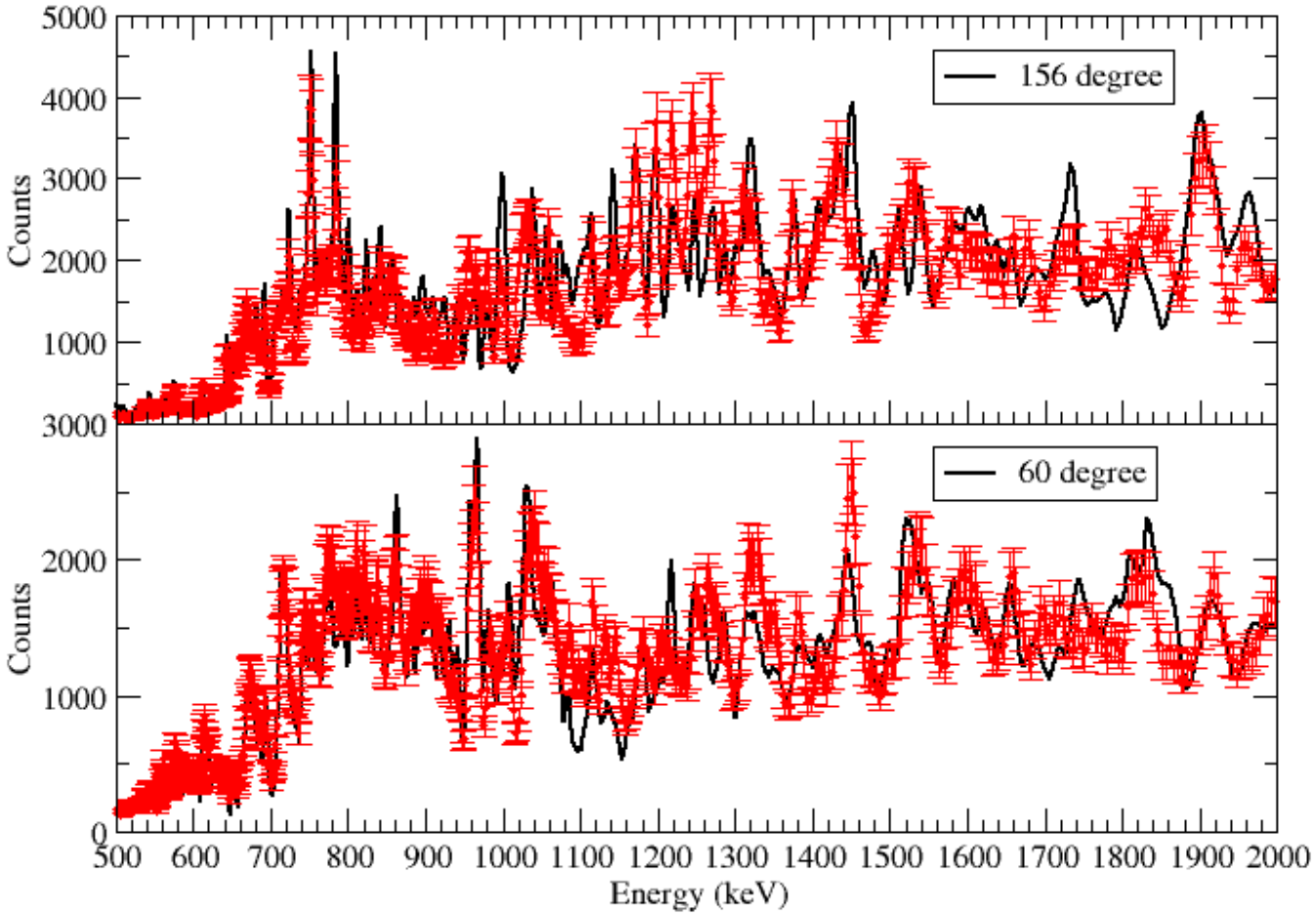
SAMMY Fit to Elastic Angular Distributions ^{56}Fe

(Perey)



SAMMY Fit Angular Distributions

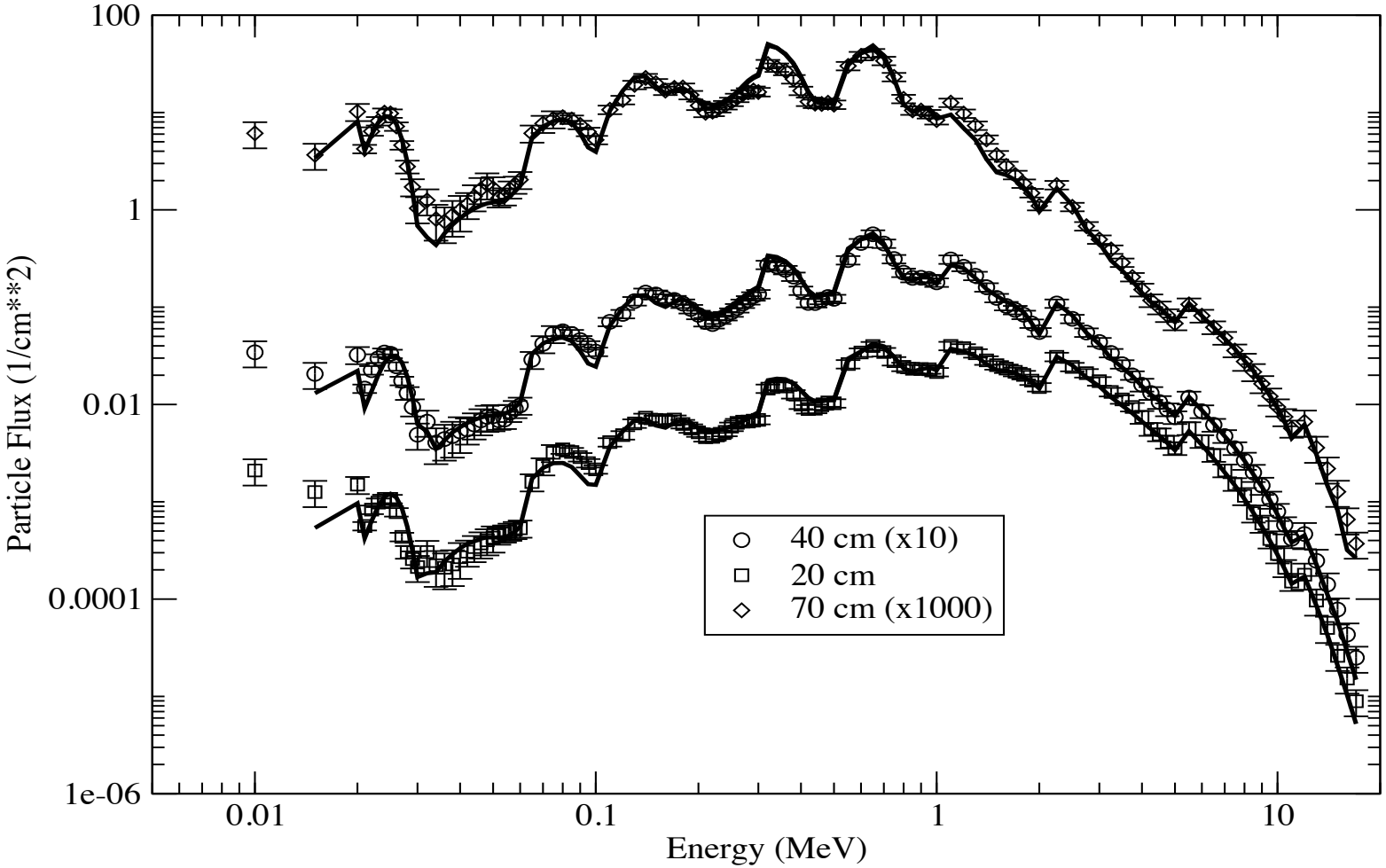
RPI Angular Data



Useful Information on ^{56}Fe

Data (b)	ATLAS	JENDL4	JEFF3.1	ENDF/BVII.1	ORNL/IRSN
σ_t	-	14.78	14.79	14.75	14.78
σ_s	12.69 ± 0.49	12.19	12.21	12.16	12.19
σ_γ	2.59 ± 0.14	2.59	2.58	2.59	2.59
I_γ	(1.36 ± 0.15)*	1.35	1.34	1.35	1.28
*calculated					

^{56}Fe Benchmark Results



ALARM-CF-FE-SHIELD-001 (ICSBEP): Neutron and photon leakage spectra from Cf-252 source at the center of six iron spheres of diameters of 20, 30, 40, 50, 60, and 70 cm (IPPE, Russia)

^{235}U Resonance Evaluation

(issues and resolutions)

- **Overestimated ^{235}U capture cross section in the resonance region range from 0.1 – 2.5 keV**

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Recommendations:

- **New measurements of capture and fission cross sections in the keV region**
  - **Capture and fission data (RPI, alpha measurements)**
  - **Capture data (LANL)**

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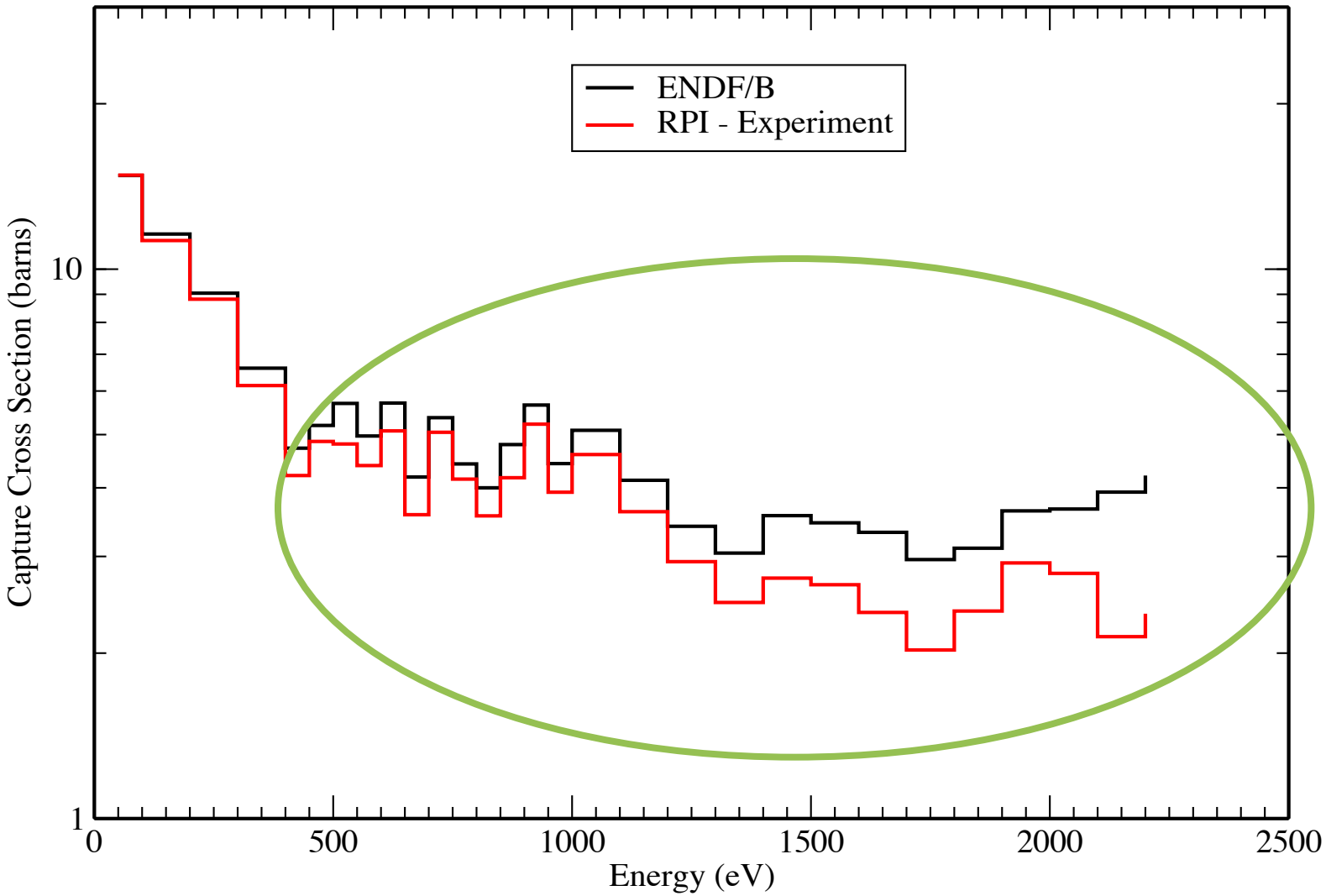
- Perform new resonance analysis in the 0.1 – 2.5 keV region
- **Investigate the reason for the overestimation of criticalities for some benchmarks (ZEUS)**

RPI Capture Data vs ENDF Evaluation



^{235}U Resonance Evaluation

- **Measurements used in evaluation:**
  - **Four transmission**
  - **Eight fission cross section**
  - **Four capture cross section**

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- **Evaluation performed up to 2250 eV:**
  - **3197 total resonances**
  - **29 of which are external resonances**

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- **Reich-Moore approximation**

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  - Four transmission
  - Eight fission cross section
  - Four capture cross section
- Evaluation performed up to 2250 eV:
  - 3197 total resonances
  - 29 of which are external resonances
- Reich-Moore approximation
- **Fitted also integral data such as K1, Westcott factor, capture resonance integral**

Selected Measurements

Author	Energy (eV)	Data
De Saussure (RPI, 1967)	0.01 – 2250	Fission and capture at 25.2 m
Perez (ORNL, 1972)	0.01 – 200	Fission and capture at 39.7 m
Weston (ORNL, 1984)	14.0 – 2250	Fission at 18.9 m
Gwin (ORNL, 1984)	0.01 – 20	Fission at 25.6 m
Spencer (ORNL, 1984)	0.01 – 1	Transmission at 18 m; thickness 0.001468 atom/ barn
Harvey (ORNL, 1986)	0.4 – 68	Transmission at 18 m; thickness 0.03269 atom/barn

Selected Measurements

Author	Energy (eV)	Data
Harvey (ORNL, 1986)	4.0 – 2250	Transmission at 80 m; thickness of 0.00233 atom/ barn cooled to 77 K
Harvey (ORNL, 1986)	4.0 – 2250	Transmission at 80 m; thickness of 0.03269 atom/ barn cooled to 77 K
Wartena (Geel, 1987)	0.0018 – 1	Eta at 8 m
Wagemans (Geel, 1988)	0.001 – 0.4	Fission at 18 m
Schrack (RPI, 1988)	0.02 – 20	Fission at 8.4 m
Weigman (ILL, 1990)	0.0015 – 0.15	Eta (Chopper)

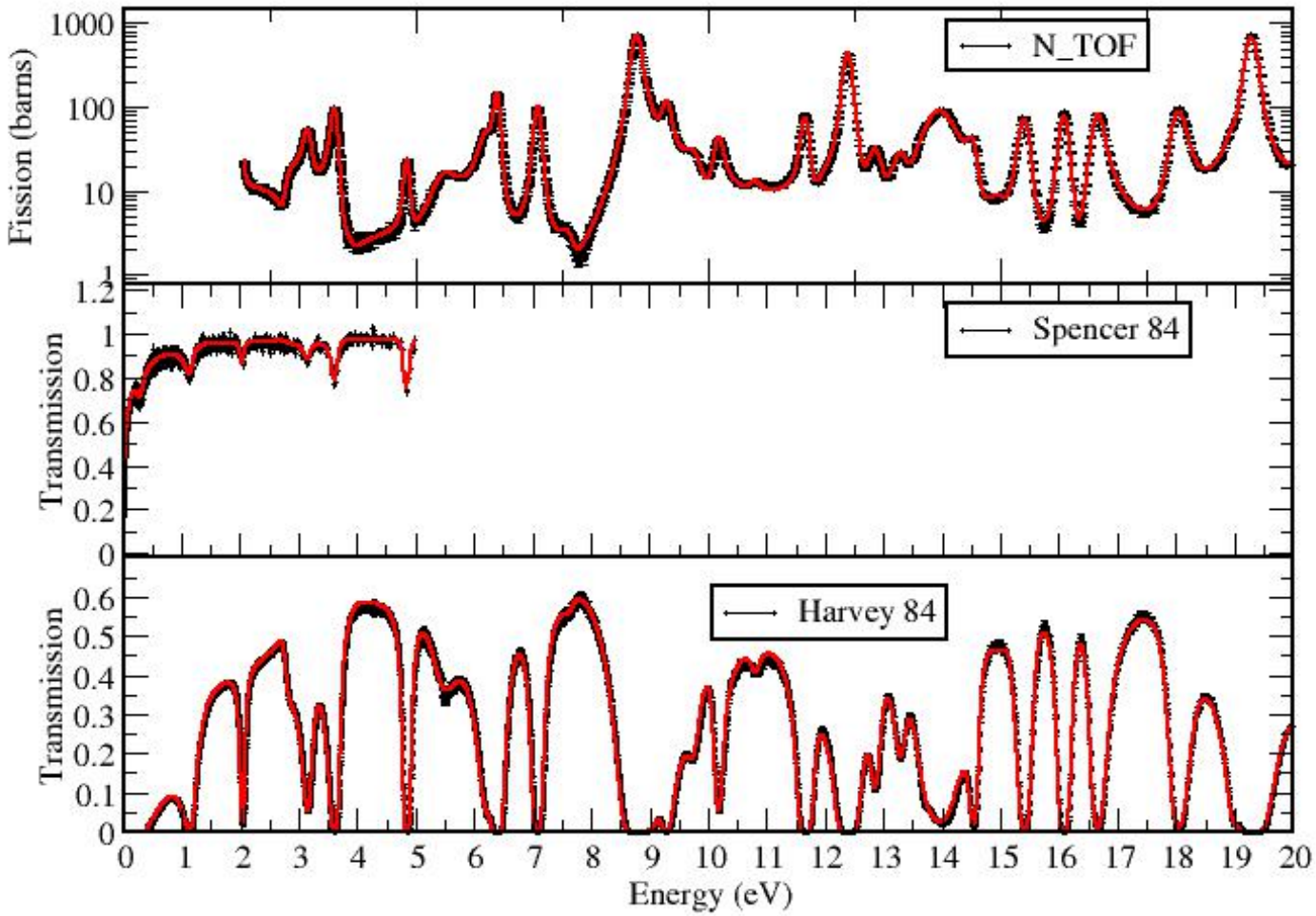
Selected Measurements

Author	Energy (eV)	Data
Weston (ORNL, 1992)	100.0 – 2000	Fission at 86.5 m
Moxon (ORNL, 1992)	0.01 – 50	Fission yield
Gwin (ORNL, 1996)	0.01 – 4	Absorption and fission at 21.68 m
Danon (RPI, 2012)	100 – 5000	Fission and capture yield at 25.56 m (15 ns bursts)
Jandel (LANL, 2012)	100 – 5000	Capture at 25.45 m (125 ns bursts)
n_TOF	2 – 60	Fission

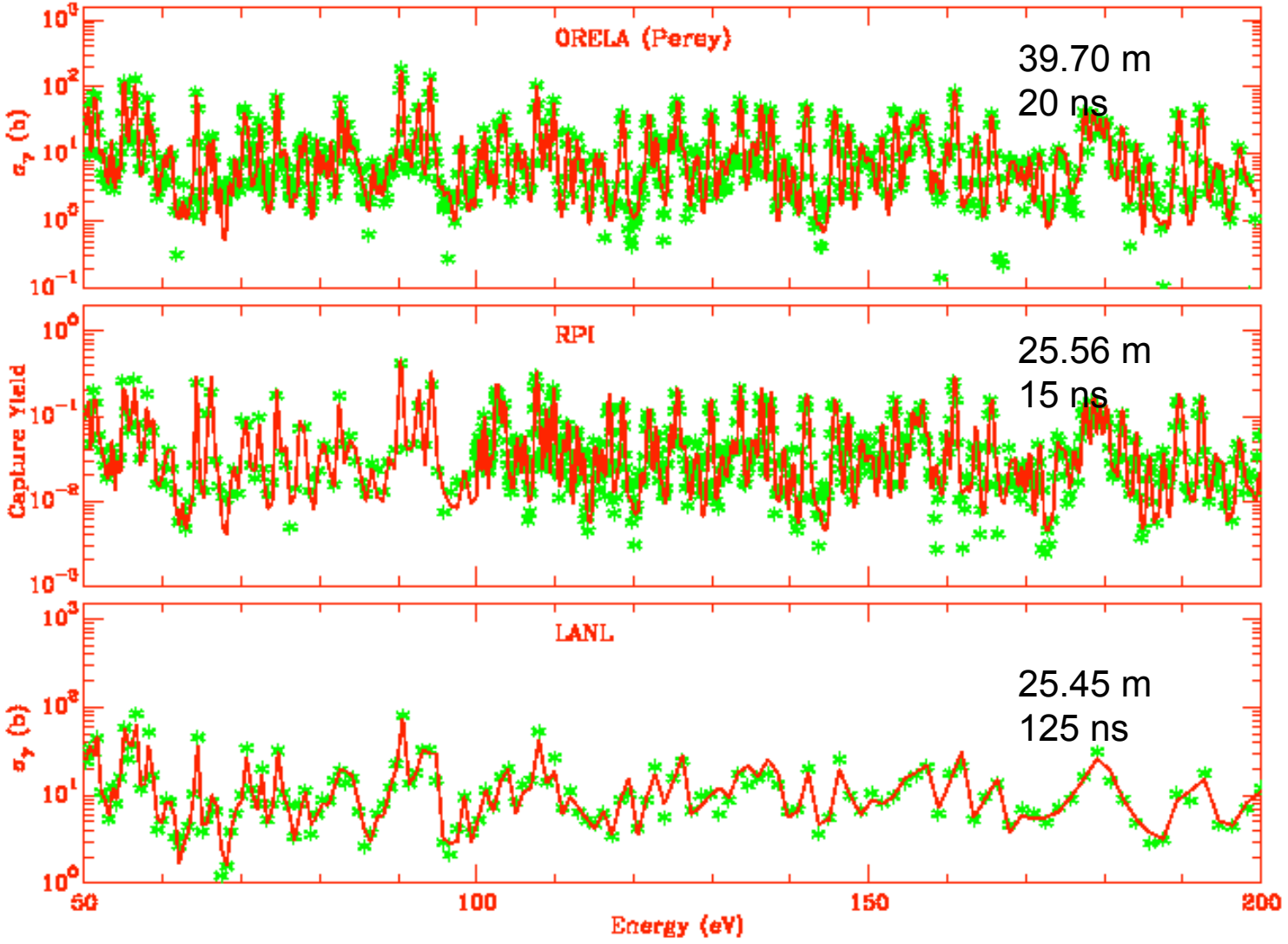
Useful Information on ^{235}U

Quantity	Standard	IRSN
σ_f (b)	584.380 ± 1.030	584.940
σ_γ (b)	99.304 ± 0.725	98.667
σ_s (b)	14.087 ± 0.219	15.465
g_a	0.9789 ± 0.0008	0.9775
g_f	0.9773 ± 0.0008	0.9755
K1	–	722.150
$\int_{0.5MeV}^{20MeV}(\sigma_\gamma/E)dE$	–	0.500

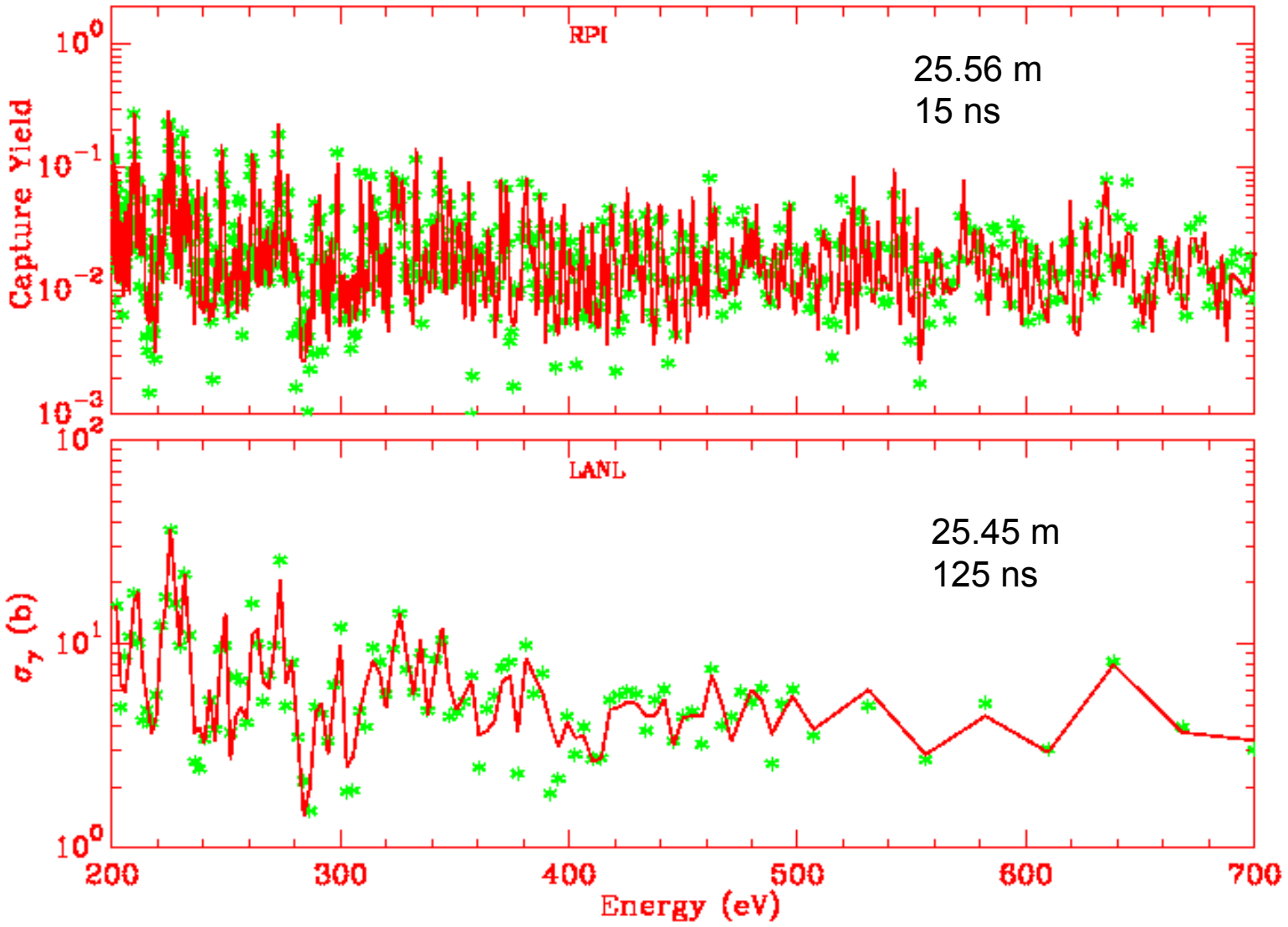
SAMMY Fit



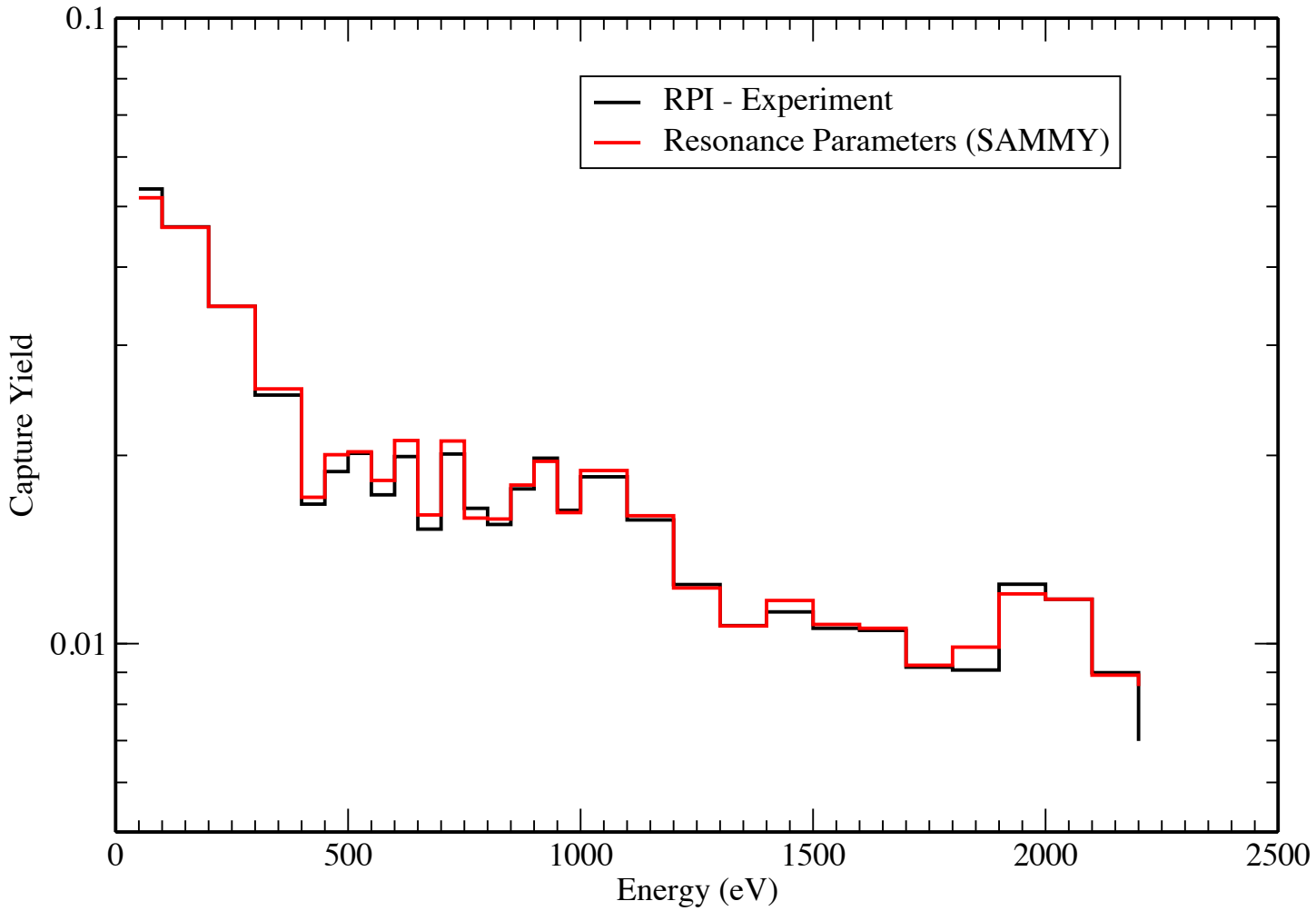
ORNL, RPI, and LANL CAPTURE DATA



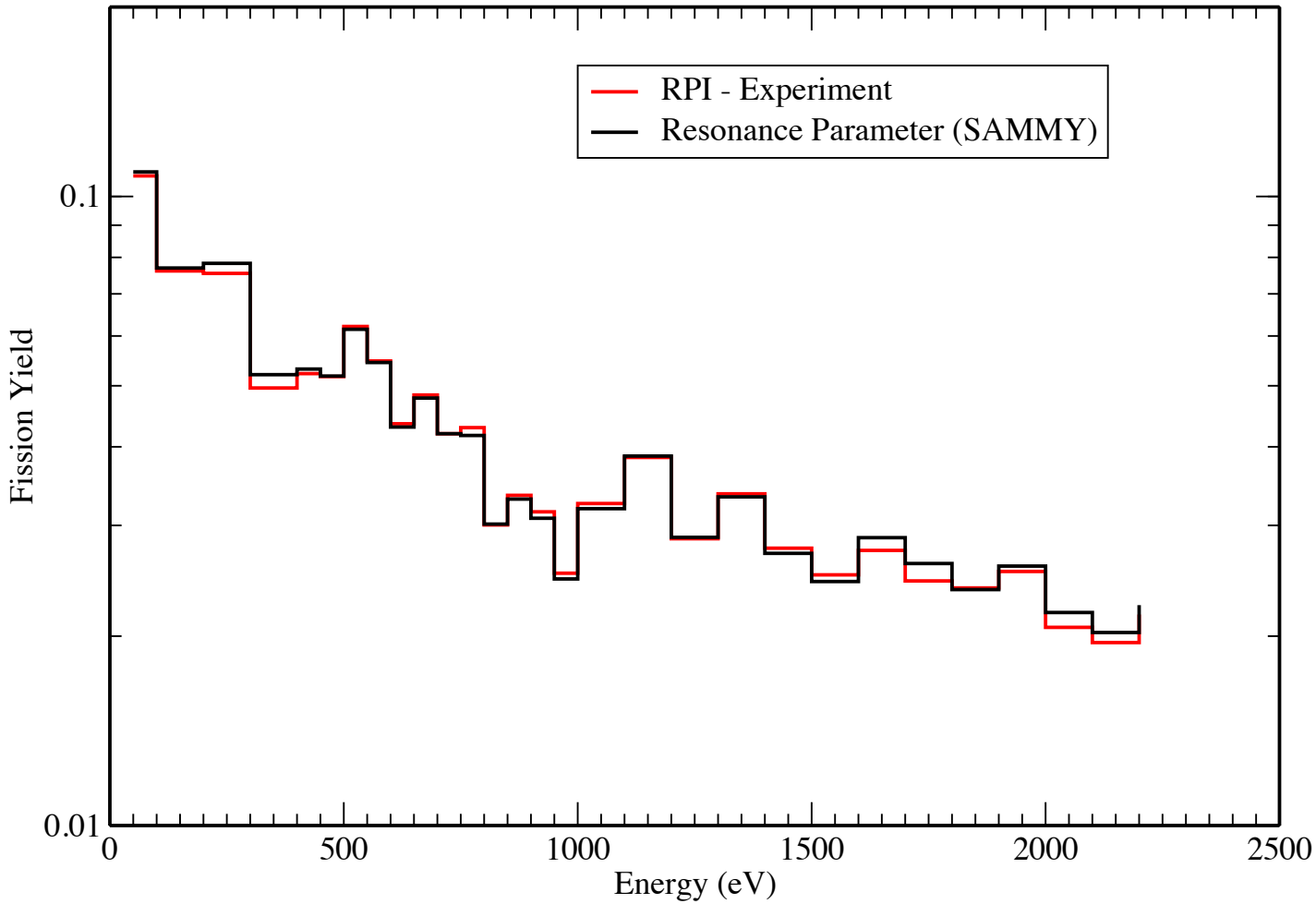
ORNL, RPI, and LANL CAPTURE DATA



Fit to RPI Capture Data



Fit to RPI Fission Data



Improvement of Fission Integral

(using the new fission data)

ΔE (eV)	Standard (b eV)	IRSN (b eV)
0.0206 – 0.0623	19.18 ± 0.11	19.16
7.8 – 11	246.40 ± 1.24	246.021

Improvement of Fission Integral

(using the new fission data)

ΔE (eV)	Standard (b)	IRSN (b)
100 – 200	21.17 (11)	20.21
200 – 300	20.69 (11)	20.57
300 – 400	13.13 (7)	12.93
400 – 500	13.78 (8)	13.30
500 – 600	15.17 (9)	14.95
600 - 700	11.51 (7)	11.30
700 – 800	11.10 (6)	10.86
800 – 900	8.21 (48)	8.00
900 – 1000	7.50 (44)	7.24
1000 – 2000	7.30 (40)	7.14

^{239}Pu Resonance Evaluation

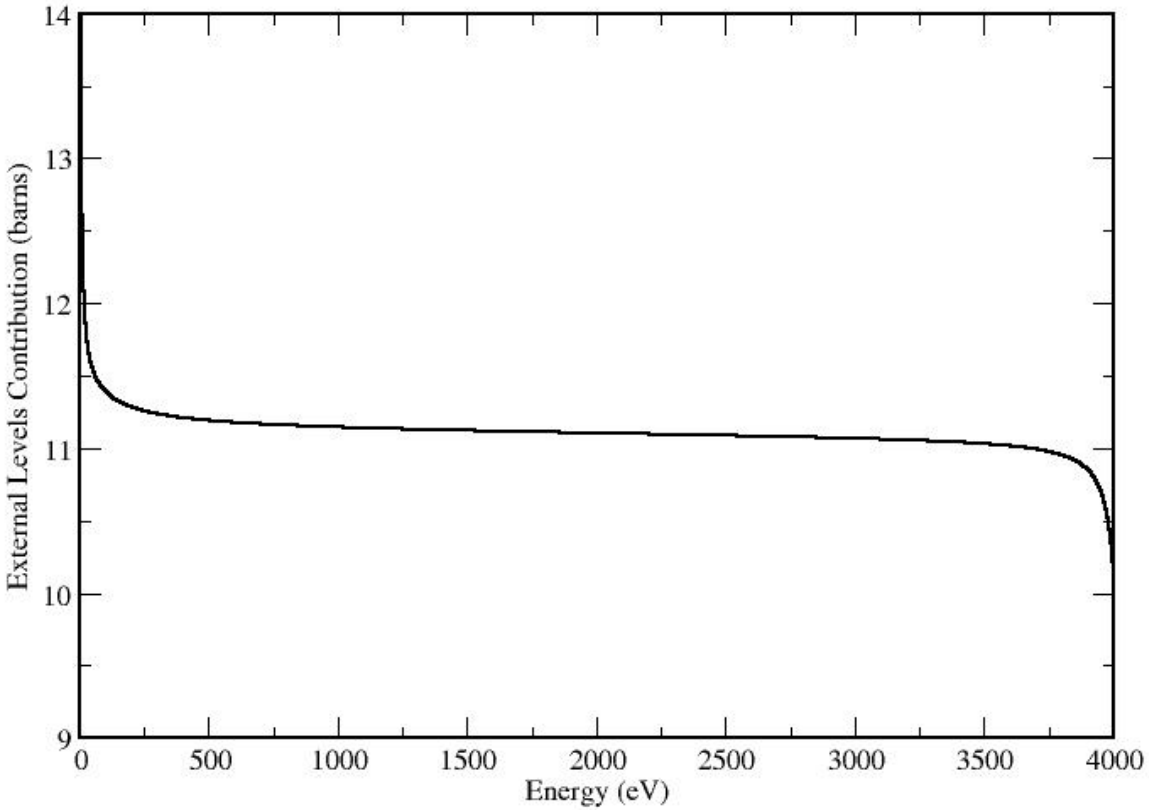
- **RRR extension from 2.5 – 4 keV**
  - **issues with the unresolved resonance representation resolved by using RRR parameters**
- **High-resolution transmission data (Harvey) and fission (Weston) used in the SAMMY fitting**
  - **Fission cross section of Weston (1984) normalized according to the NEA-WPEC-5 subgroup. Recommendation: the fission cross section integral in 100 – 1000 eV is 9275 b eV**

What is Still Needed

- Capture cross section not fitted above 2 keV. New LANL data will help
- Need to know the recommended average values for fission and capture cross sections
- Thermal values far from standards.
- An on-going evaluation (not shared with CIELO yet) indicates the fitted standard values are more consistent with benchmark results
- Would RPI be able to measure capture data as was done for ^{235}U?

External Levels Contribution

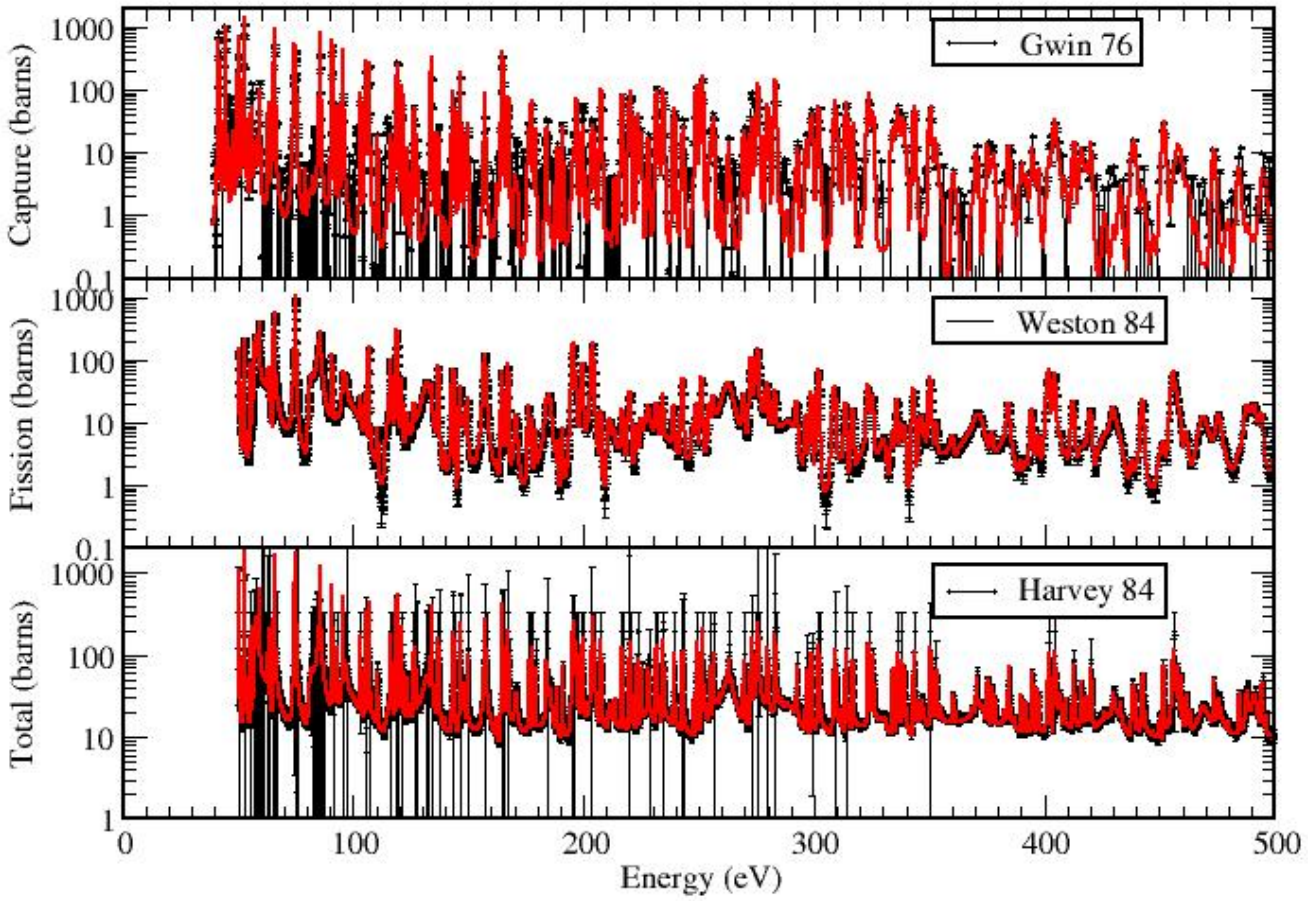
(to include energy bound levels and energies above 4 keV)



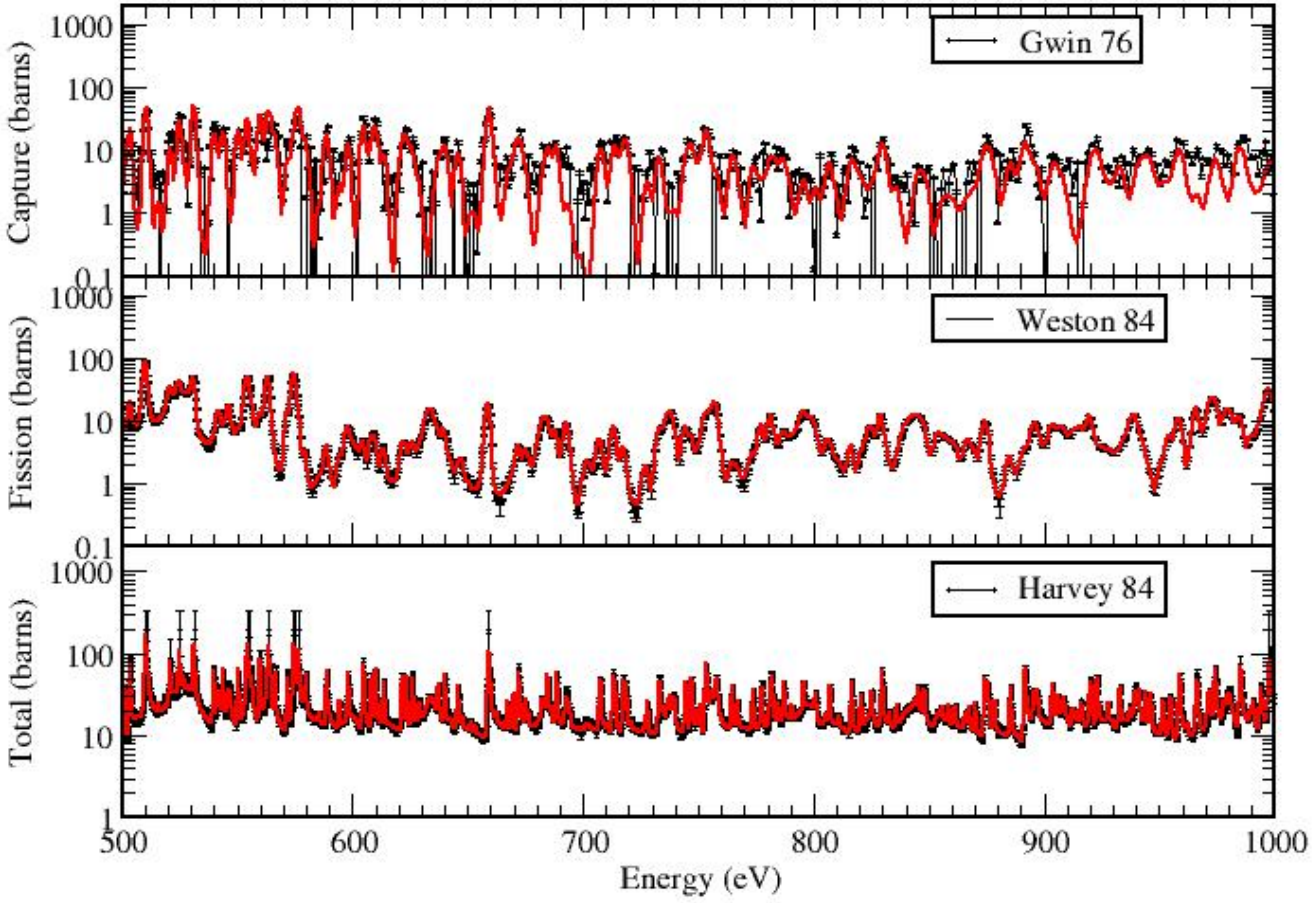
The effective radius R' extracted from the fit of the transmission data is 9.41 fm. This effective radius is used throughout the evaluation

$$R = \lim_{E \to \infty} \left(\frac{\sigma_s}{4\pi} \right)^{1/2} = 9.39 \ fm$$

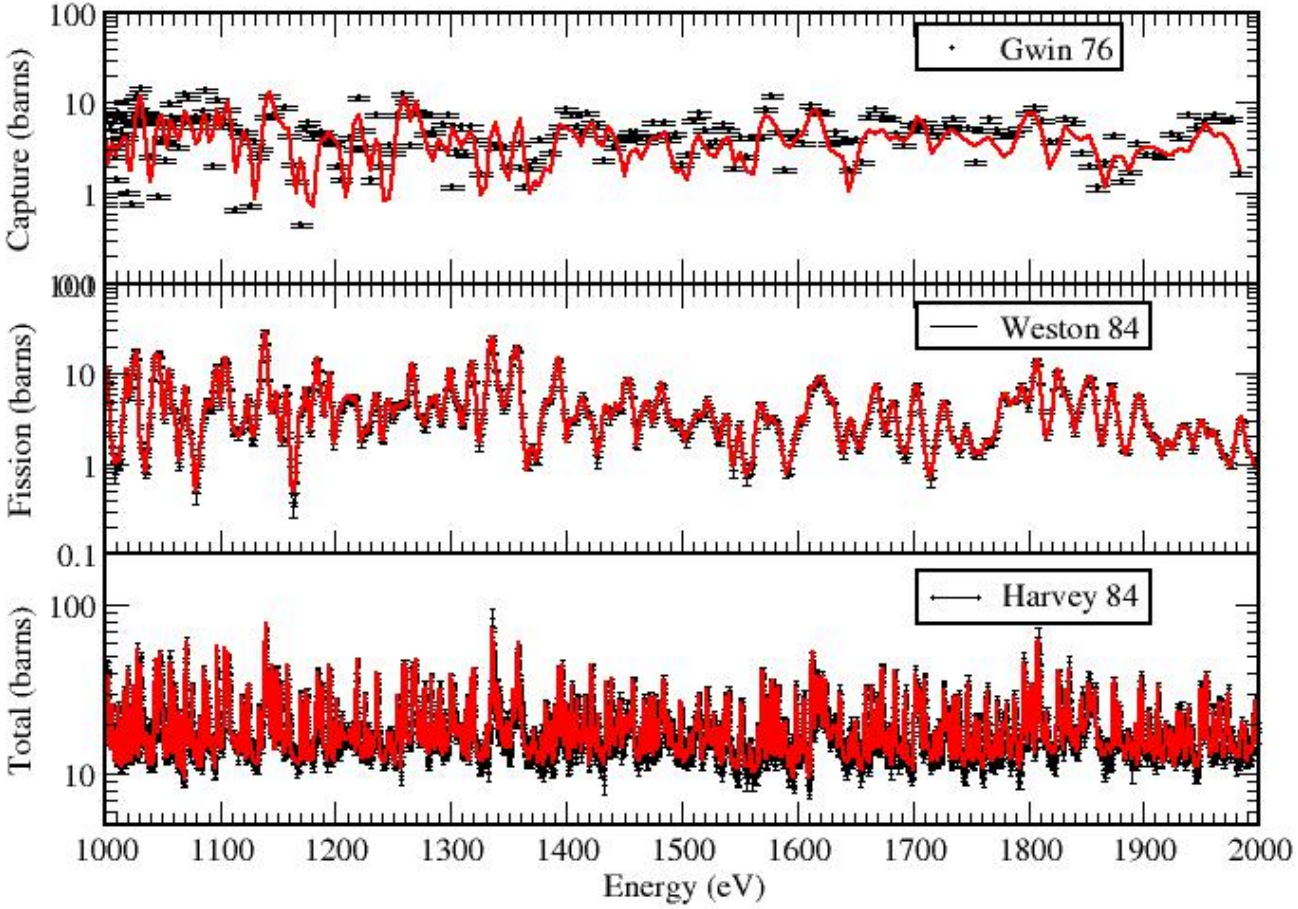
SAMMY Fit to Experimental Data



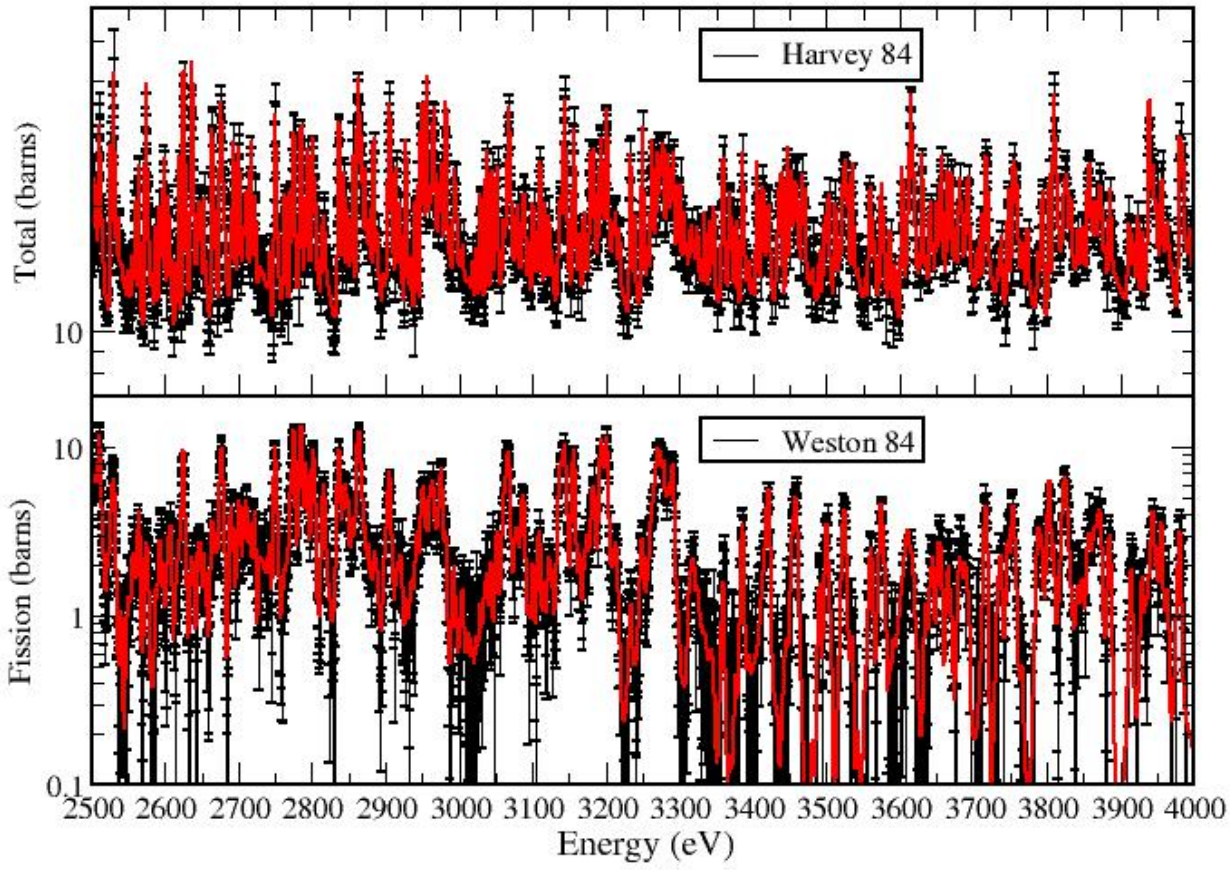
SAMMY Fit to Experimental Data



SAMMY Fit to Experimental Data



SAMMY Fit to Experimental Data



No capture data available in the 2500 – 4000 eV range

Comments

- **Up to 4 keV evaluation can be completed as:**
  - **Adjust the resonance parameter to fit the thermal data to the standard values**
  - **Include capture normalization appropriately in the energy range 2.5 – 4 keV**
  - **Include integral benchmark in addition to the SAMMY fit of the differential data**
  - **The above task can be achieved without adding much burden in the fitting process**

Acknowledgments

This work was supported by the U.S. Department of Energy (DOE) Nuclear Criticality Safety Program (NCSP), National Nuclear Security Administration Office of Defense Nuclear Nonproliferation Research and Development.