ORNL Evaluations Submitted for ENDF/A

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Nuclear Data & Criticality Safety Group

Oak Ridge National Laboratory

CSEWG
Nov 3-5, 2009

Outline

- ^{52}Cr and ^{53}Cr
- ^{58}Ni and ^{60}Ni
- ^{46}Ti, ^{47}Ti, ^{49}Ti, and ^{50}Ti
- ^{239}Pu status (submitted in March 2008; revision in process)
- Comments about Additional ORNL evaluations in ENDF/A
- ^{232}Pa and Hf-isotope evaluations (RQ Wright)

^{52,53}Cr Resonance Evaluation at ORNL

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Computer Code SAMMY

- **Used for analysis of neutron, charged-particle cross-section data.**
- **Uses Bayes' method (generalized least squares) to find parameter values.**
- **Uses R-matrix theory, Reich-Moore approximation (default) or multi- or single-level Breit-Wigner theory.**
- **Generates covariance and sensitivity parameters for resonance region.**

Cr isotope evaluation

- Transmission and capture cross section measurements done at ORELA for ^{52,53}Cr and natural Cr for energy below 500 keV (Guber);
- Early high resolution transmission measurements done by Harvey at ORELA above 100 keV for all Cr isotopes;
- Evaluation performed with SAMMY;
- Preliminary resolved resonance parameters determined for all Cr isotopes;

Cr isotope evaluation

Energy Range for ^{52}Cr

Resolved (OLD):10^{-5} eV – 1.2 MeV

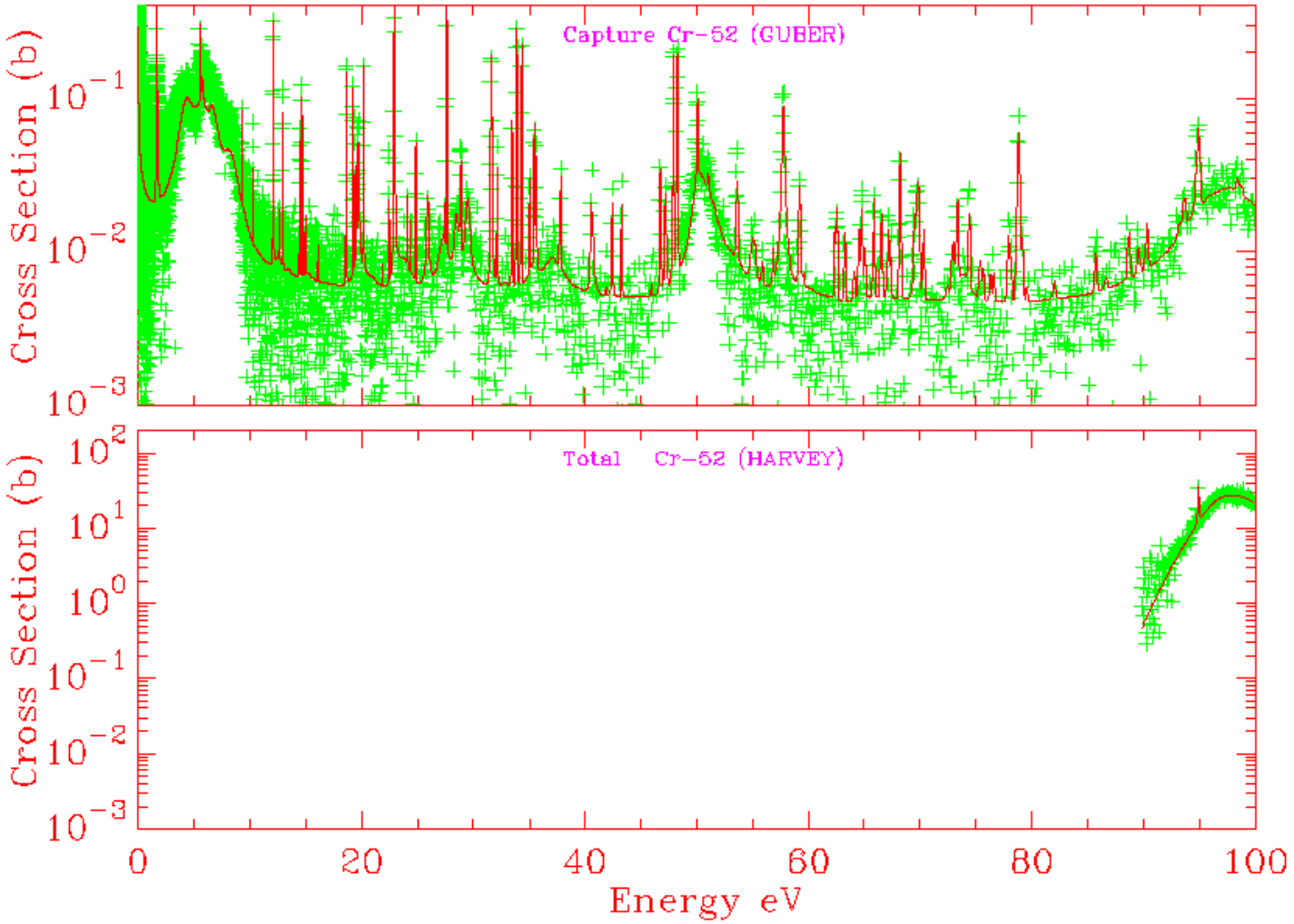
Resolved (ORNL): 10^{-5} eV – 1.43 MeV

Energy Range for ^{53}Cr

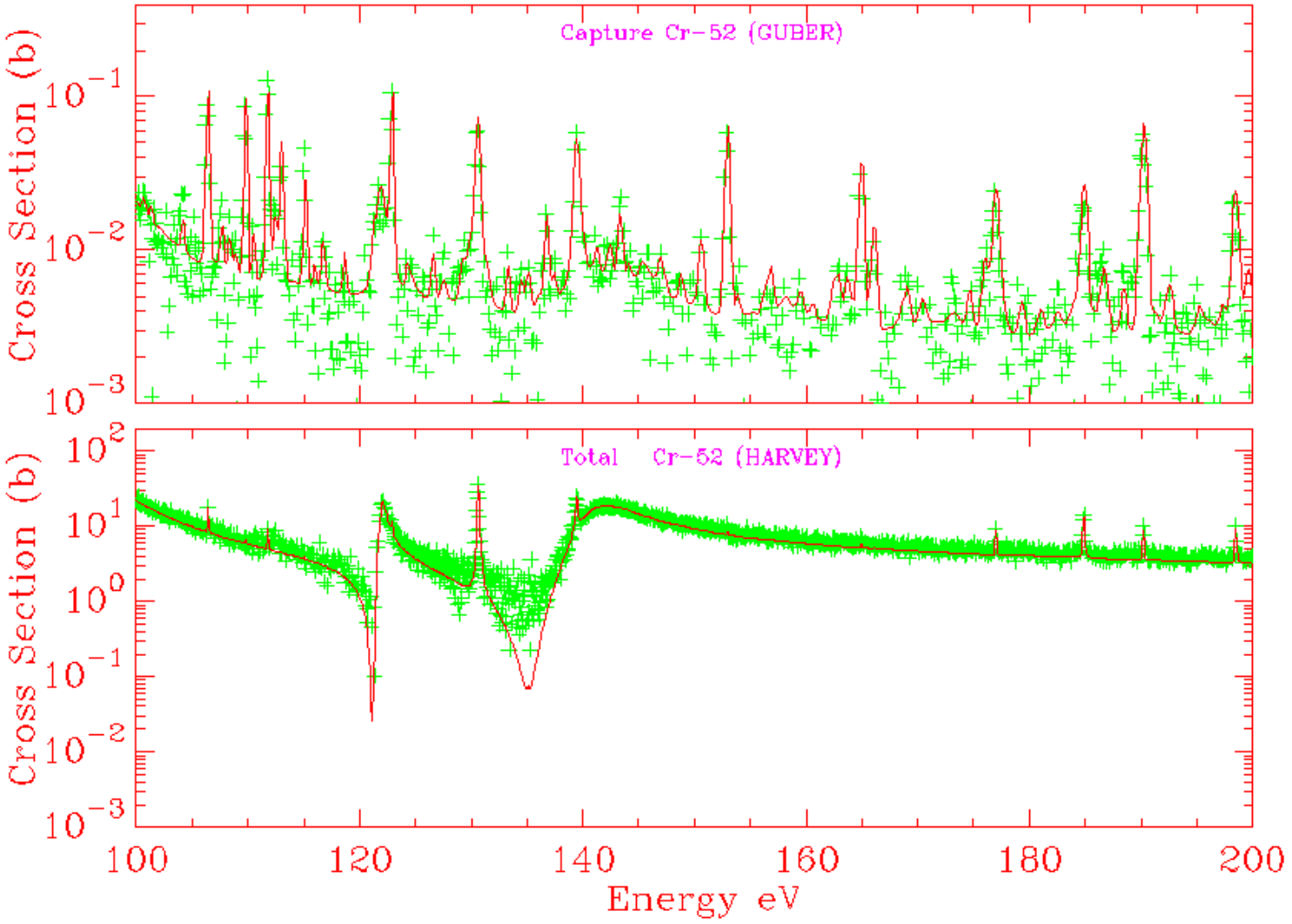
Resolved (OLD): 10-5 eV – 245 keV

Resolved (ORNL): 10^{-5} eV – 564 keV

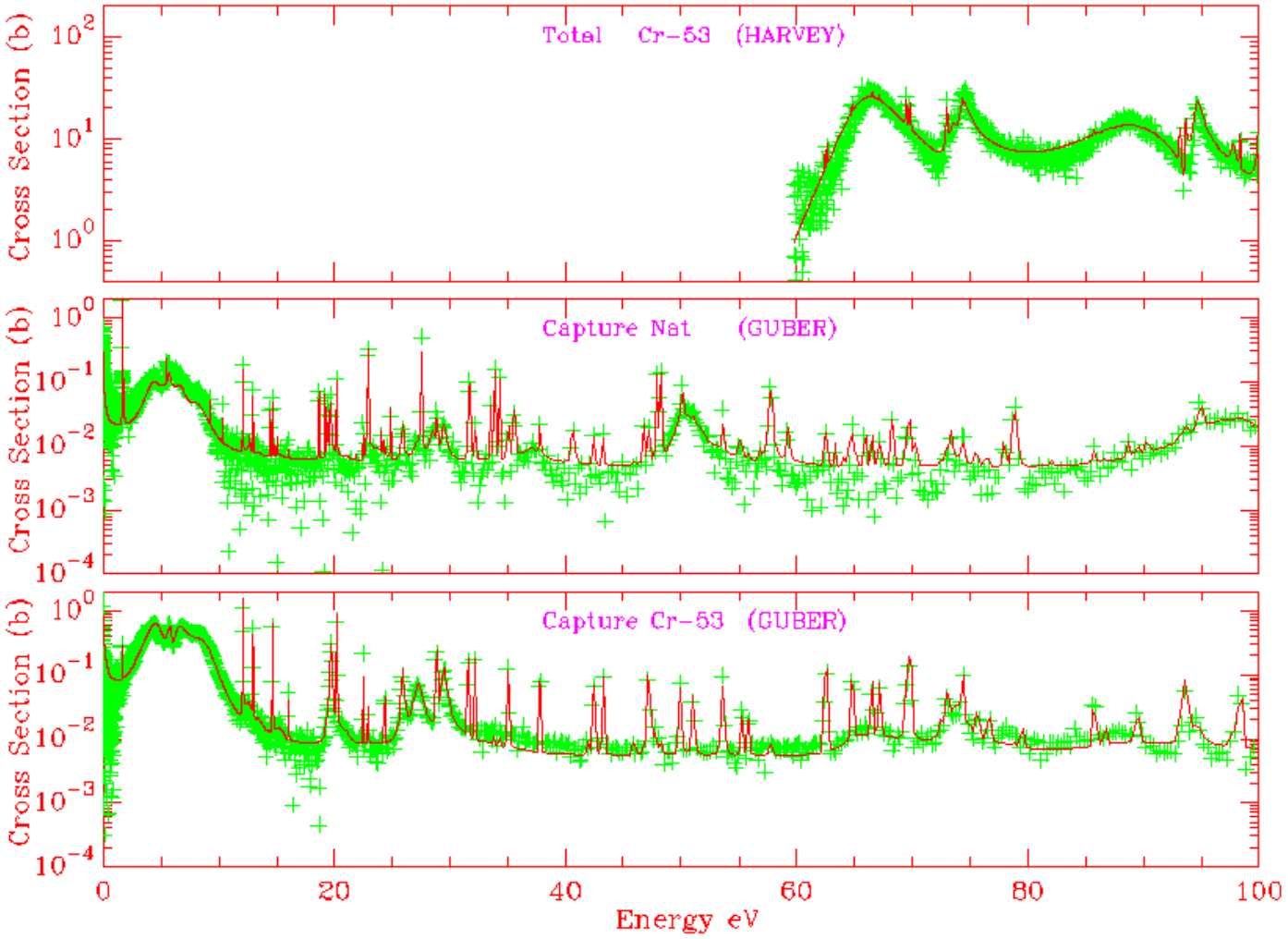
^{52}Cr Resonance Evaluation



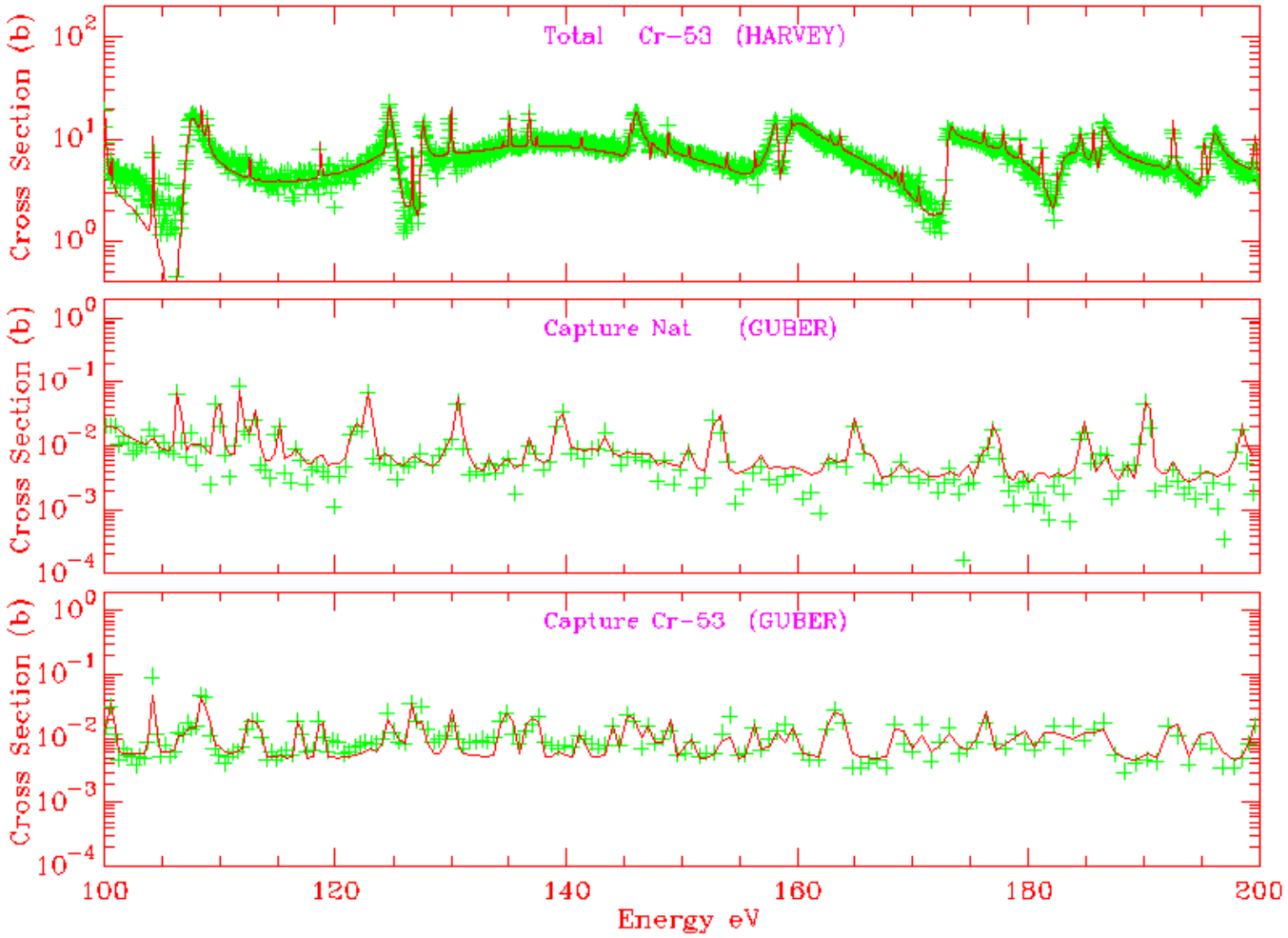
^{52}Cr Resonance Evaluation



^{53}Cr Resonance Evaluation



^{53}Cr Resonance Evaluation



^{52}Cr thermal cross section compared to the values listed in the Atlas of Neutron Resonances

Cross Section	ORNL		Atlas
	Resonance	Direct	
Capture	0.75+/-0.02	0.82	0.86+/-0.02
Total	3.82+/-0.01	3.93	3.82+/-0.03
Scattering	3.07+/-0.07	-	2.96+/-0.02

^{52}Cr uncertainty in the energy group 0.0253 eV - 0.3 eV calculated with covariance data

Cross Section	Average value and uncertainty
Capture	17.32+/-0.48 (2.8%)
Total	26.07+/-0.51 (2.0%)
Scattering	7.89+/-0.28 (4.7%)

^{53}Cr thermal cross section compared to the values listed in the Atlas of Neutron Resonances

Cross Section	ORNL		Atlas
	Resonance	Direct	
Capture	18.09+/-0.42	18.41	18.60+/-0.60
Total	26.07+/-0.51	26.39	26.38+/-0.62
Scattering	7.98+/-0.28	-	7.78+/-0.20

^{53}Cr uncertainty in the energy group 0.0253 eV - 0.3 eV calculated with covariance data

Cross Section	Average value and uncertainty
Capture	0.72+/-0.02 (2.8%)
Total	3.79+/-0.11 (2.9%)
Scattering	3.07+/-0.08 (2.6%)

^{50,54}Cr isotope evaluation (BONUS)

Ready Next Year (~April 2010)

Energy Range for ^{50}Cr

Resolved (OLD):10^{-5} eV – 600 keV

Resolved (ORNL): 10^{-5} eV – 783 keV

Energy Range for ^{54}Cr

Resolved (OLD): 10-5 eV – 750 keV

Resolved (ORNL): 10^{-5} eV – 834 keV

^{58,60}Ni Resonance Evaluation at ORNL

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Nuclear Data & Criticality Safety Group

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INTRODUCTION

- **PREVIOUS EVALUATION by C. M. Perey et al., for ENDF/B-V, VI**
  - **not modified for B-VII-0**
  - **no COVARIANCE DATA available**
  - **^{58}Ni thermal to 800 keV**
  - **^{60}Ni thermal to 450 keV**
- **HIGH RESOLUTION NEUTRON TRANSMISSION at GELINA**
  - **Brusegan, 1994**
- **NEW CAPTURE CROSS SECTION MEASUREMENT at ORELA Guber, 2008**
- **RE-EVALUATION NEEDED by UPDATING THE DATA BASE**
- **RPCM and CSCM CALCULATION**

EXPERIMENTAL DATA BASE

- **OLD ORELA TRANSMISSION DATA by Harvey, Larson, Perey**
  - **^{58}Ni Flight path 78 m, Sample 0.0764 at/b Low Energy**
  - **^{58}Ni Flight path 201 m, Sample 0.172 at/b High Energy**
  - **^{60}Ni Flight path 80 m, Sample 0.029 and 0.084 at/b E < 200 keV**
  - **^{60}Ni Flight path 80 m, Sample 0.0744 at/b E > 200keV**

EXPERIMENTAL DATA BASE

- **GELINA TRANSMISSION DATA by Brusegan et al.**
  - **58Ni Flight path 388 m Sample 0.044 at/b**
  - **60Ni Flight path 388 m Sample 0.0744 at/b**
- **ORELA CAPTURE DATA by Guber**
  - **58Ni Flight path 40 m Samples 0.360 at/b**
  - **60Ni Flight path 40 m Samples 0.364 at/b**

RESULTS

- **Resonance Parameters**

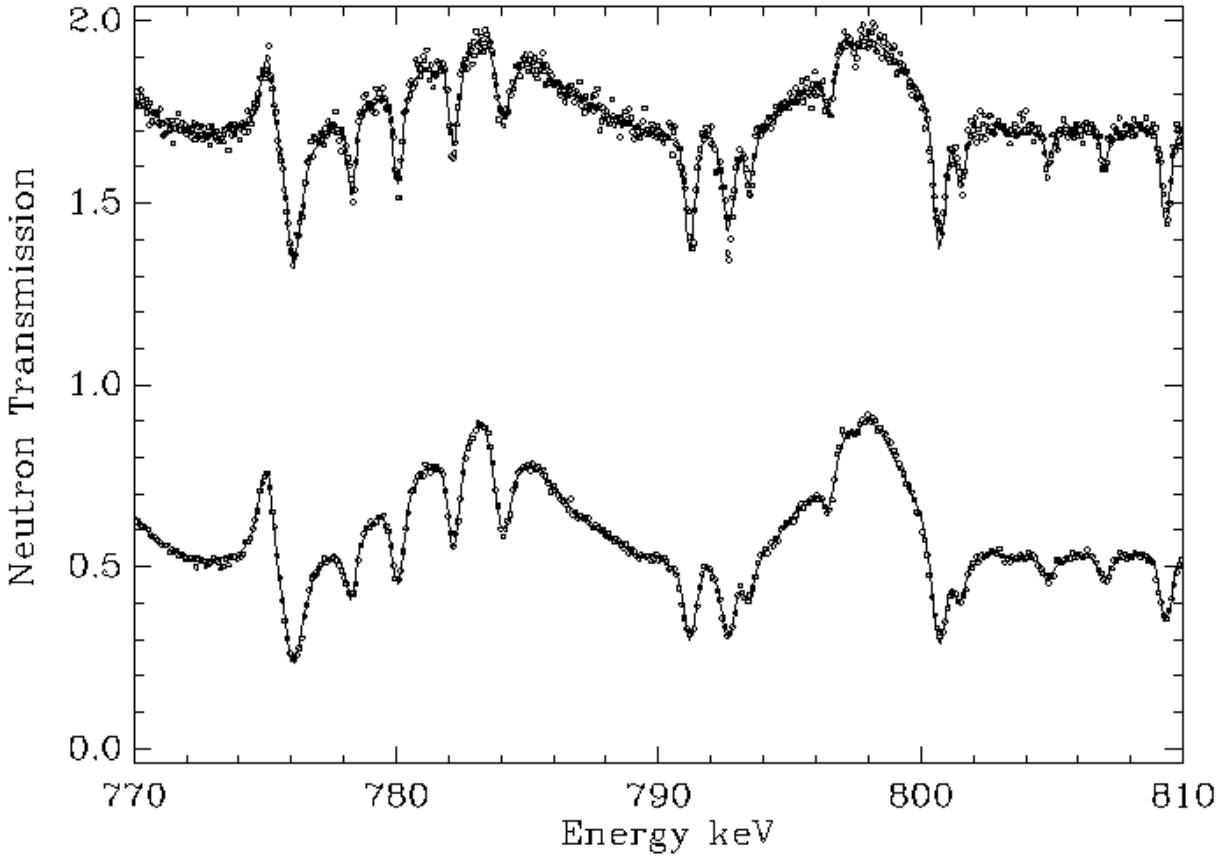
	ENDF/B.VII.0 (keV)	ORNL (keV)
^{58}Ni	10^{-2} – 812.0	10^{-2} – 812.0
^{60}Ni	10^{-2} – 450.0	10^{-2} – **812.0**

RESULTS

- **^{58}Ni Evaluation**
  - **487 resonances from thermal to 812 keV**
  - **61 s-wave; 204 p-wave; 222 d-wave**
  - **Average spacing for s-wave: $D_0 = 12.65 \pm 0.70$ keV**
  - **Neutron Strength Function from fit to PT distribution:**
  - **$S_0 = 3.38 \pm 0.61 \times 10^{-4}$**
  - **$S_1 = 0.48 \pm 0.08 \times 10^{-4}$**
  - **$S_2 = 2.27 \pm 0.30 \times 10^{-4}$**
  - **Thermal Capture : 4.27 ± 0.15 b compared to the ENDF/B-VII 4.62 b**
  - **Capture Integral: 2.095 ± 0.07 b compared to the ENDF 2.20 b**

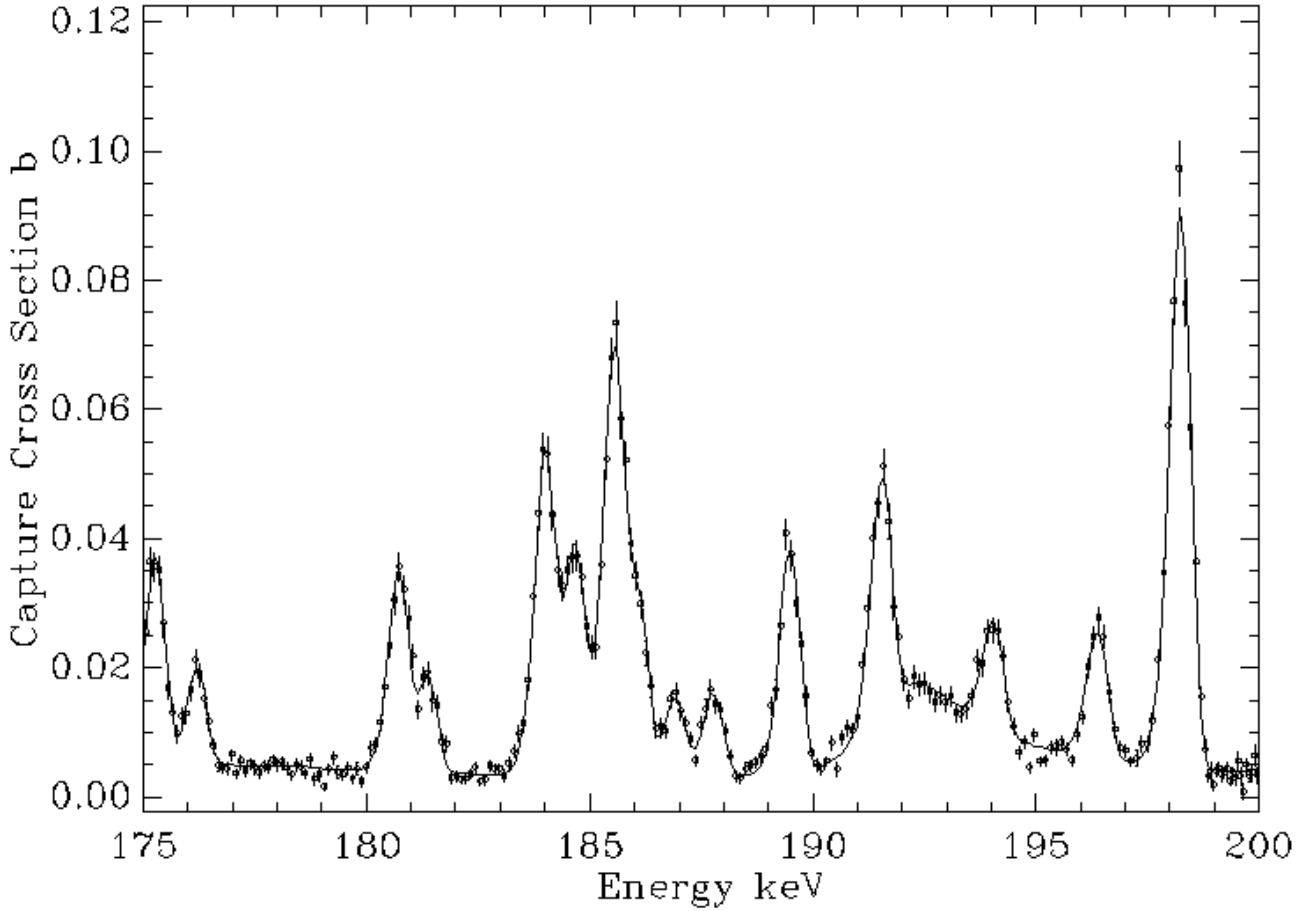
RESULTS

- *^{58}Ni Neutron Transmission in the energy range 770 keV to 810 keV from Brusegan et al. (upper part), and Perey et al. (lower part). The smooth curve represents the transmission calculated by SAMMY. Brusegan data were multiplied by 2 for clarity of the figure*



RESULTS

- *^{58}Ni effective capture cross section in the energy range 175 keV to 200 keV from Guber et al. The smooth curve represents the effective cross section calculated by SAMMY from the resonance parameters*

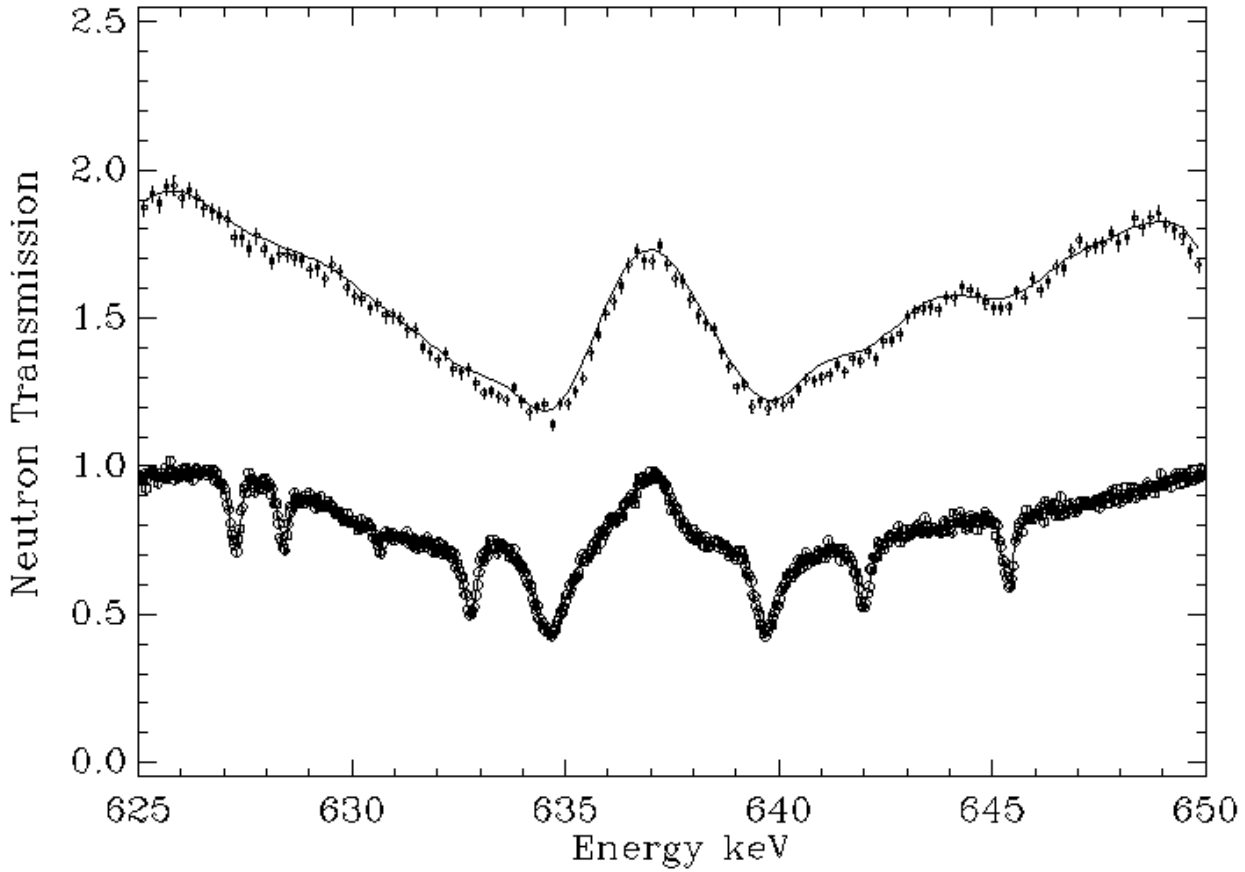


RESULTS

- **^{60}Ni Evaluation**
  - **Extended from 450 keV (ENDF/B-VII) to 812 keV Taking advantage of Brusegan very high resolution transmission**
  - **458 resonances from thermal to 812 keV**
  - **61 s-wave; 236 p-wave; 161 d-wave**
  - **Average spacing for s-wave: $D_0 = 11.94 \pm 0.66$ keV**
  - **Neutron Strength Function from fit to PT distribution:**
  - **$S_0 = 2.64 \pm 0.64 \times 10^{-4}$**
  - **$S_1 = 0.68 \pm 0.09 \times 10^{-4}$**
  - **$S_2 = 0.83 \pm 0.20 \times 10^{-4}$**
  - **Thermal Capture : 2.40 ± 0.06 b compared to the ENDF/B-VII 2.92 b**
  - **Capture Integral: 1.259 ± 0.032 b compared to the ENDF 1.394 b**

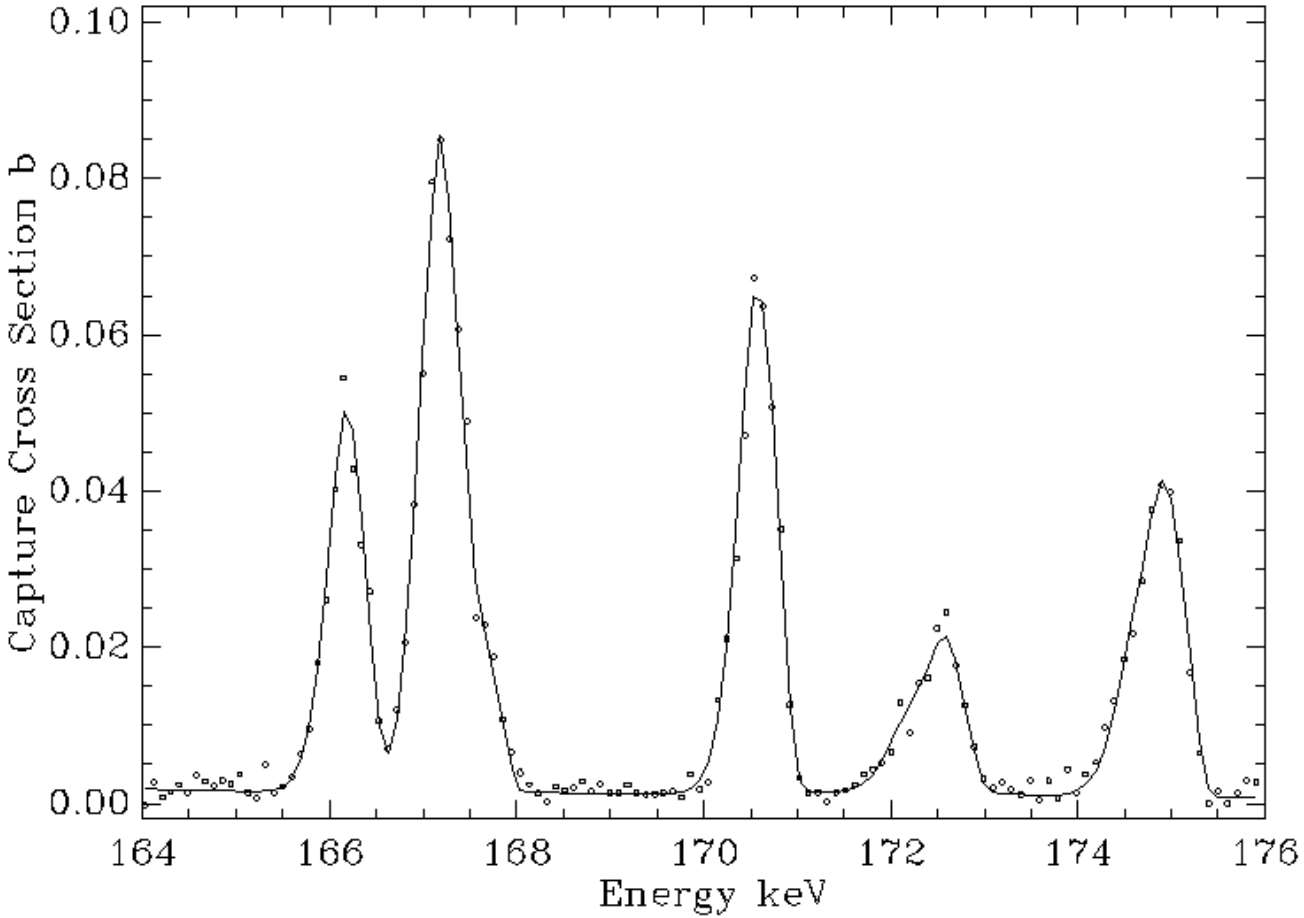
RESULTS

- *^{60}Ni Neutron Transmission in the energy range 826 keV to 850 keV from Brusegan et al. (lower part), and Perey et al. (upper part). The smooth curve represents the transmission calculated by SAMMY. Perey data were multiplied by 2 for clarity of the figure.*



RESULTS

- *^{60}Ni effective capture cross section in the energy range 164 keV to 176 keV from Guber et al. The smooth curve represents the effective cross section calculated by SAMMY from the resonance parameters*



RESULTS

- *^{58}Ni average capture cross sections. The cross sections are given in mb*

Energy keV	Present	B-VII-0	Perey[1]	Froehner[10]
6.31-7.94	13.28±3.17	13.38	13.0±1.0	2.6±0.3
7.94-10.00	6.46±1.34	4.80	3.3±0.6	3.3±3.3
10.00-12.59	8.87±1.51	6.86	6.2±1.6	6.6±1.0
12.59-15.85	179.35±11.5	193.86	196.0±19.	195.0±25.
15.85-20.00	23.63±2.71	21.43	20.9±4.0	26.3±3.2
20.00-25.10	42.08±4.24	42.68	45.8±1.9	35.2±4.4
25.10-31.60	28.83±2.28	33.63	36.3±1.5	26.2±3.9
31.60-39.80	62.13±3.72	75.21	78.6±3.2	55.7±5.0
39.80-50.10	12.75±0.87	13.89	14.5±0.6	10.6±1.3
50.10-63.10	31.01±1.97	39.59	41.7±2.2	31.4±2.3
63.10-79.40	10.79±1.13	13.66	14.2±1.5	9.8±0.7
79.40-100.00	19.93±1.27	24.43	25.5±1.0	17.3±1.7
100.00-125.90	25.82±0.88	34.11	35.2±1.5	22.0±2.1
125.90-158.50	16.35±0.60	20.78	21.3±1.5	12.6±1.0
158.50-199.50	16.80±0.59	22.73	23.6±1.0	16.5±2.4
199,50=251.20	12.36±0.45	18.77	19.3±0.5	13.1±3.3

RESULTS

- *^{60}Ni average capture cross sections. The cross sections are given in mb*

Energy keV	Present mb	Uncertainties	ENDF/B-VII-0	Ratio
1.0-2.0	9.85	5.50	10.57	1.07
2.0-3.0	106.25	7.53	109.58	1.03
3.0-5.0	9.02	4.50	9.57	1.06
5.0-10.0	27.55	3.80	27.24	0.99
10.0-15.0	167.82	9.15	163.60	0.97
15.0-20.0	15.11	2.70	14.17	0.94
20.0-27.0	22.85	2.41	23.70	1.04
27.0-38.0	21.91	2.11	27.06	1.23
38.0-47.0	15.86	2.01	17.22	1.09
47.0-70.0	15.32	1.82	17.52	1.14
70.0-100.0	13.47	1.61	15.56	1.16
100.0-150.0	12.57	1.11	14.35	1.14
150.0-200.0	8.75	0.91	13.66	1.33
200.0-250.0	8.05	0.90	9.61	1.19
250.0-300.0	8.63	0.81	9.55	1.11
300.0-350.0	9.88	0.81	11.27	1.14
350.0-400.0	8.28	0.71	10.37	1.25
600.0-450.0	8.06	0.61	8.86	1.10

Concluding Remarks

- **New experimental data added to the experimental data base**
- **^{60}Ni Resonance Region extended to 812 keV**
- **RPCM and CSCM calculated for both isotope**
- **Average Capture smaller than ENDF/B-VII**

^{46,47,49,50}Ti Resonance Covariance Generation

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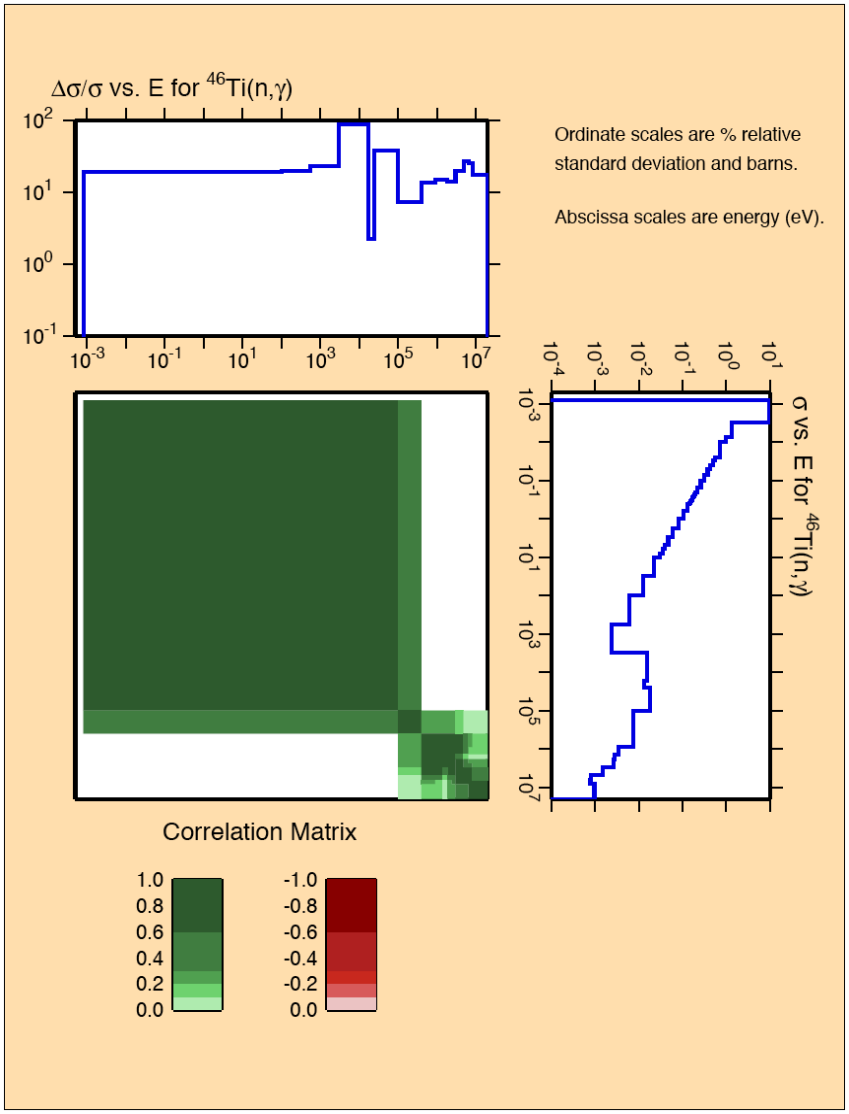
Resonance Parameter Covariance Generation

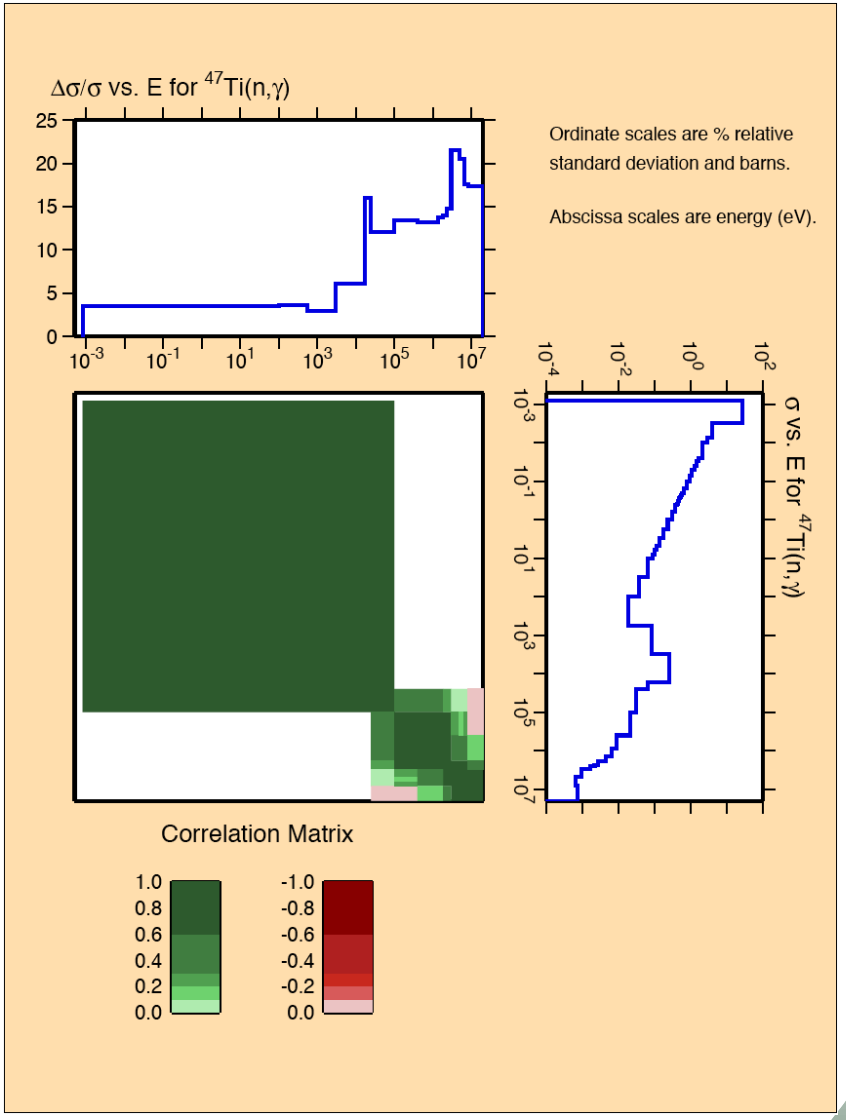
- Resolved resonance parameters of the ENDF/B.VII.0 were converted from MLBW into the RM representation. The resonances were checked against the resonance parameters given in the Atlas of Neutron Resonances.
- For Ti-46 a resonance at 55.67 keV with j=1/2 (l=1) was repeated. According to the Atlas it should be at the energy 56.66 with gt=0.48 eV, gn=0.1 eV and gg=0.38.
- Thermal cross section and resonance integral are unchanged

- COVARIANCE:
  - Resolved resonance covariance data were generate with the SAMMY code for Ti isotopes.
  - SAMMY was run with the option of generating resonance-covariance retroactively using the "propagated uncertainty parameter" option to include systematic data uncertainties.

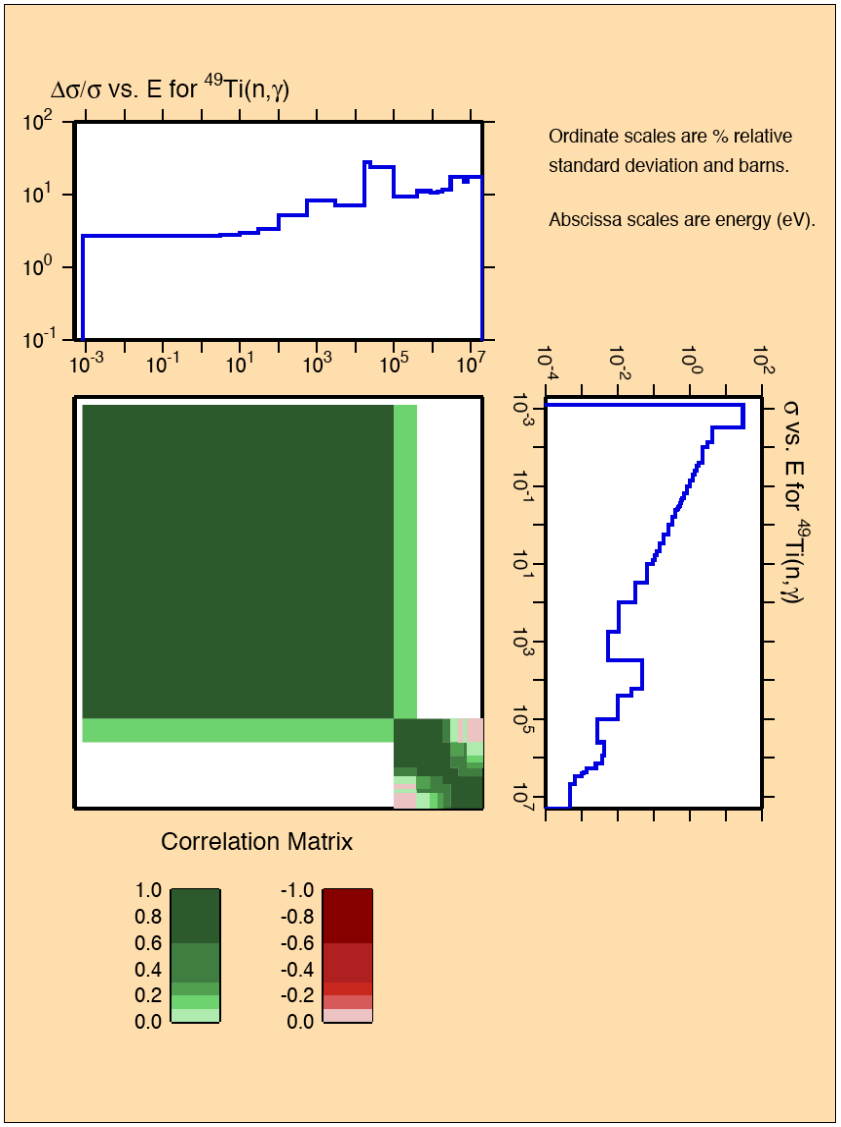
- Combined with LANL ^{46,47,49,50}Ti high-energy evaluations in ENDF/A (submitted March 2009)

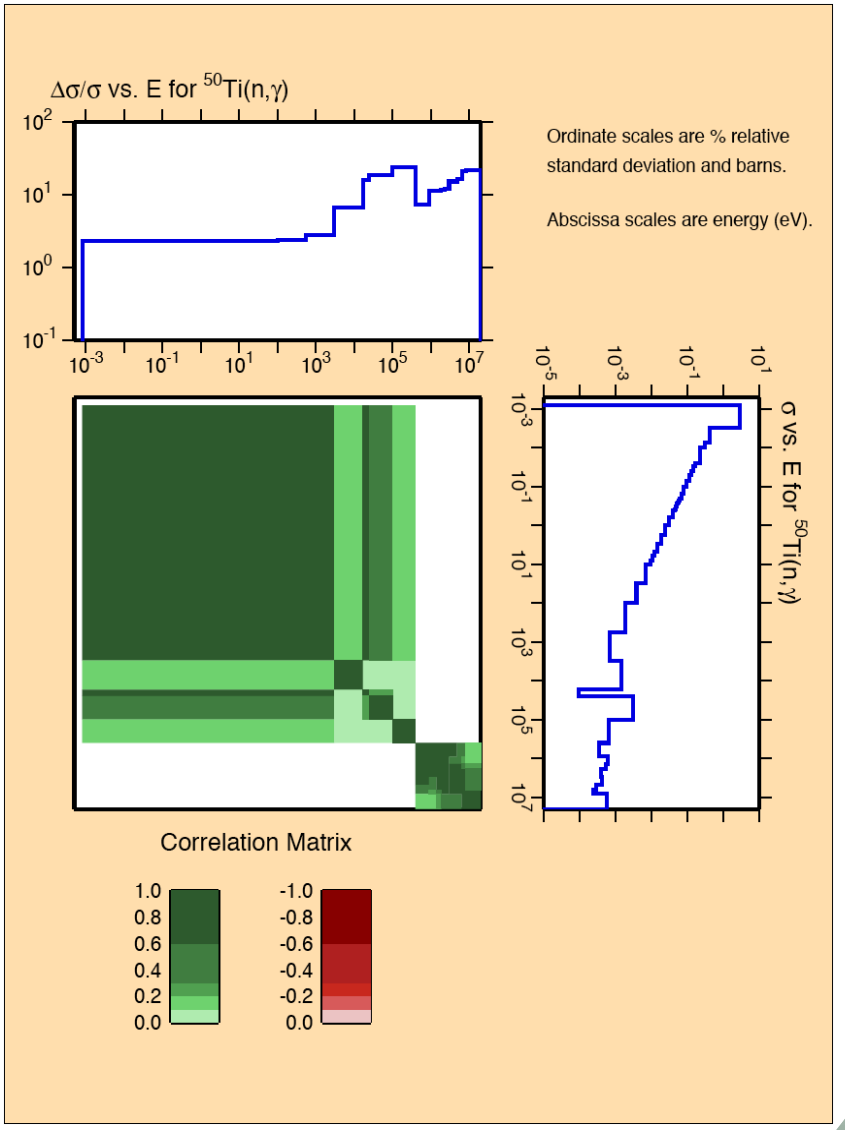
Titanium Resonance Parameter Covariance Generation





Titanium Resonance Parameter Covariance Generation





Summary of Evaluations Submitted by ORNL in 2009

	Resonance Evaluation	Resonance Covariance Evaluation	High Energy Evaluation	High Energy Covariance Evaluation
^{52}Cr	ORNL (new evaluation)	ORNL (new evaluation)	FZK Germany	FZK Germany
^{53}Cr	ORNL (new evaluation)	ORNL (new evaluation)	FZK Germany (?)	FZK Germany (?)
^{58}Ni	ORNL (new evaluation)	ORNL (new evaluation)		
^{60}Ni	ORNL (new evaluation)	ORNL (new evaluation)		
^{46}Ti	ORNL (retroactive)	ORNL (retroactive)	LANL	LANL
^{47}Ti	ORNL (retroactive)	ORNL (retroactive)	LANL	LANL
^{49}Ti	ORNL (retroactive)	ORNL (retroactive)	LANL	LANL
^{50}Ti	ORNL (retroactive)	ORNL (retroactive)	LANL	LANL

^{239}Pu Resonance Evaluation at ORNL (Current Status)

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Motivation for a New Evaluation

- Existing resonance evaluation is divided into three disjoint resonance parameter set as 1.0×10^{-5} eV to 1 keV, 1 keV to 2 keV, 2 keV to 2.5 keV;
- Cross section mismatch at the energy boundaries;
- Not easy to generate uncertainty for the whole energy region (zero correlation);
- Solve long standing problem for thermal benchmark

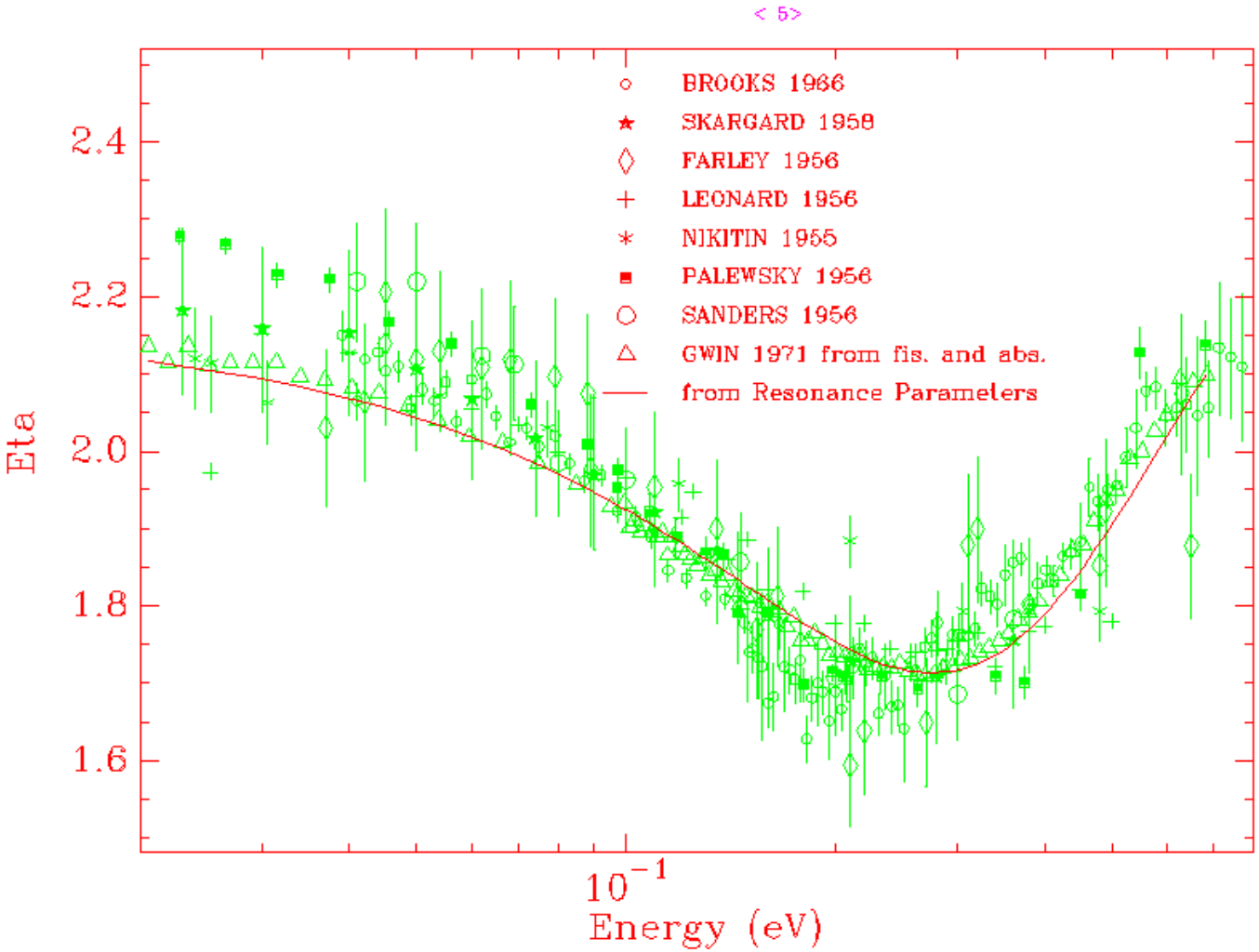
EXPERIMENTAL DATA

Reference	Energy Range (eV)	Facility	Measurement
Bollinger et al. (1956)	0.01 – 1.0		Total Cross Section
Gwin et al. (1971)	0.01 – 0.5	ORELA	Fission and Absorption at 25.6 m
Gwin et al. (1976)	1.0 – 100.0	ORELA	Fission and Absorption at 40.0 m
Gwin et al. (1984)	0.01 – 20.0	ORELA	Fission at 8 m
Weston et al. (1984)	9.0 – 2500.0	ORELA	Fission at 18.9 m
Weston et al. (1988)	100.0 – 2500.0	ORELA	Fission at 86 m
Weston et al. (1993)	0.02 – 40.0	ORELA	Fission at 18.9 m
Wagemans et al. (1988)	0.002 – 20.0	GELINA	Fission at 8 m
Wagemans et al. (1993)	0.01 – 1000.0	GELINA	Fission at 8 m
Harvey et al. (1985)	0.7 – 30.0	ORELA	Transmission at 18 m
Harvey et al. (1985)	30.0 – 2500.0	ORELA	Transmission at 80 m

ORNL Evaluation Status—what needs to be done

- Results of plutonium solution calculations indicate no improvement using ORNL evaluation. Longstanding problem persists!
- In some case the good results from previous ^{239}Pu evaluation deteriorate
- Review of the ^{239}Pu is underway.
  - ORNL, LANL and CEA (WPEC SG)
- Covariance analysis will include differential/integral data from CEA

^{239}Pu Resonance Evaluation



Additional ORNL Evaluations in ENDF/A

- **^{35}Cl and ^{37}Cl:** submitted in 2007—little or no benchmark testing
- **^{39}K and ^{41}K:** submitted Oct 2008—little or no benchmark testing
- **^{55}Mn:** submitted March 2008—ANL noted improved performance for benchmark testing
- **^{19}F:** submitted Oct 2008
  - New inelastic scattering data incorporated in resonance analysis
  - New evaluation has not improved benchmark performance—but has not made benchmark calculations worse either
- **^{233}U, ^{235}U, and ^{238}U** covariance evaluations: submitted March 2008
  - ORNL (resonance parameter covariance data) and LANL (High energy covariance data)
  - Covariance data utilized in SG33 analyses and also distributed with SCALE 6 by ORNL

Minor Actinide Evaluations

Richard Q. Wright

CSEWG Meeting

November 3−5, 2009

Pa–232 Evaluation

- Thermal cross sections from other evaluations: (JENDL−3.3 does not have resonance parameters).

	ENDF/B−VI.8	JENDL−3.3
Total	1762.2	1176.2
Elastic	32.8	12.2
Fission	1517.3	700.0
Capture	212.1	464.0

Pa–232 Evaluation

- ENDF/B-VII Background Information

  Pa–232 was revised in Oct, 2005 starting from ENDF/B-VI.8; the MLBW formalism was used for the resolved resonance range, 0 to 10 eV (RQW). The thermal cross sections were not in agreement with with the Atlas of Neutron Resonances.

	ENDF/B−VII	ANR
Fission	977.3	1502 ± 28
Capture	651.2	246 ± 30

Pa–232 Evaluation

- Changes to MF = 2 (MLBW) are as follows:

  Bound level at –5.0 eV from ANR

  28 positive levels from ANR

  EHIR = 21.2 eV

- Minor changes to MF = 3 below 100 eV

Pa–232 Evaluation

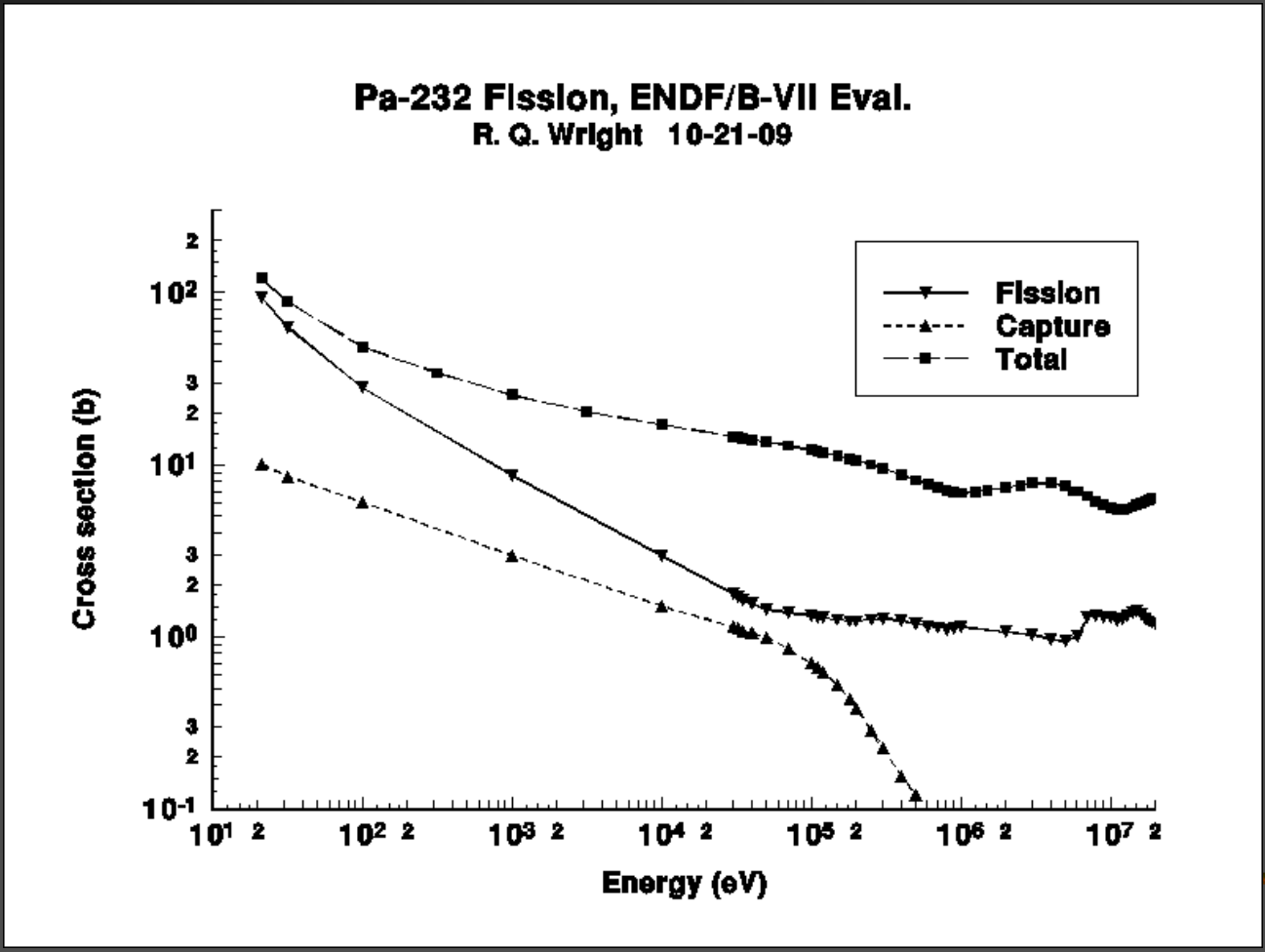
- Impact is to change cross sections in the resolved resonance region (< 21.2 eV).

The thermal cross sections are:

	ENDF/B–VII	Revised
Total	1672.4	1752.1
Elastic	43.9	12.8
Fission	977.3	1493.9
Capture	651.2	245.4

Pa-232 Revised Evaluation

- Figure 1



Impact on applications

- Pa–232 decays (1.31 days) to U–232.

  A change in the low energy fission or capture cross section will impact the amount of Pa–232. This will affect the amount of U–232 produced from Pa–232.

  This is turn affects the quantity of U–232 and the amount of U–232 daughter nuclides.

Hafnium Evaluations

Richard Q. Wright

CSEWG Meeting

November 3−5, 2009

Introduction

- The original ENDF/B-VII evaluations were done in 1976. In 1991/1992 the resonance region (resolved and unresolved) below 90 keV was revised (RQW). These evaluations are now quite old and in need of revision.

  The JENDL−3.3 evaluations were done in 2001. Gamma−ray production files are included.

More discussion

- In 2005 the JENDL files were revised in JEFF−3.1 to include new resonance parameters up to 200 eV. The current revisions start from these JENDL/JEFF−3.1 evaluations with minor changes.

The most significant change is to increase the upper limits of the resolved resonance range for Hf-177, Hf-178, Hf-179, and Hf-180. This may not make much difference for multigroup libraries but could be of some importance for pointwise libraries.

Continued

- We observed in 1991 that several of the hafnium resonances are at very nearly the same energies as U-238 resonances. There may be some impact on the scattering and absorption in a pointwise calculation.

- Hf-174 resolved resonance parameters are taken from the Atlas of Neutron Resonances (2006). Two bound levels and the first positive level of Hf-180 were also modified.

Hafnium Evaluations

- Thermal Capture Cross Sections

Nuclide	Orig.	Mod.	ANR
Hf-174	549.5	549.1	549 ± 7
Hf-176	21.3	21.4	23.5 ± 3.1
Hf-177	373.5	373.5	375 ± 10
Hf-178	83.9	83.9	84 ± 4
Hf-179	42.8	42.8	41 ± 3
Hf-180	13.10	13.06	13.04 ± 0.07

- Increasing the upper limit of the resolved resonance range for Hf-177, Hf-178, Hf-179, and Hf-180 did not significantly change the capture resonance integrals.

This implies almost no change in the average capture cross section (for 1/E weighting). See the next slide for the capture resonance integrals.

Hafnium Evaluations

- Capture Resonance Integrals

Nuclide	Orig.	Mod.	ANR
Hf-174	442.3	345.0	307 ± 15
Hf-176	694.3	691.3	708 ± 15
Hf-177	7197	7197	7200 ± 200
Hf-178	1872	1879	1882 ± 20
Hf-179	522	523	527 ± 30
Hf-180	29.7	33.5	33 ± 1

Comparison with Previous Eval.

- Capture Cross Sections

Nuclide	ENDF/B-VII	Mod.	% diff.
Hf-174	561.8	549.1	-2.3
Hf-176	13.8	21.4	55
Hf-177	373.5	373.5	0
Hf-178	84.0	83.9	-1.2
Hf-179	43.6	42.8	-1.8
Hf-180	13.01	13.06	0.4

Comparison with Previous Eval.

- Capture Resonance Integrals

Nuclide	ENDF/B-VII	Mod.	% diff.
Hf-174	355.0	345.0	-2.8
Hf-176	401.3	691.3	72.3
Hf-177	7175	7197	0.3
Hf-178	1905	1879	-1.4
Hf-179	548	523	-4.6
Hf-180	34.5	33.5	-2.9

Impact on Natural Hafnium

- Compared to ENDF/B-VII the thermal capture is 0.3% higher and the capture resonance integral is 0.4% higher. We do not expect a large impact for thermal systems.

For fast systems the impact may be significant relative to ENDF/B-VII but should be small compared to the JENDL/JEFF evaluations. The revised evaluation has gamma-ray production data; ENDF/B-VII does not.