Cross Section Uncertainties in the Thermal and Resonance Regions

S. F. Mughabghab and P. Oblozinsky*

National Nuclear Data Center
Brookhaven National Laboratory

**Email: mugabgab@bnl.gov*

Background

- Increasing interest in uncertainties of neutron resonances required for advanced reactor systems.

- This information is available in the Atlas of Neutron Resonances.

- In the Atlas, resonance information reproduces the cross sections and resonance integrals, but not their uncertainties.

- Present study initiated to achieve consistencies between measured and calculated uncertainties.

Background

- The Subgroup 26 of the International Working Party on evaluation cooperation is interested in 53 materials comprising 19 actinides and 34 structural, coolant and moderator materials.
- Out of these NNDC produced covariances for 35 materials.
- In the present project, emphasis is placed on the uncertainties of the thermal capture (fission) cross sections for the following.
- ^{19}F, ^{23}Na, ^{28}Si, ^{52}Cr, ^{55}Mn, ^{56}Fe, ^{57}Fe, ^{58}Ni, ^{90}Zr, ^{91}Zr, ^{92}Zr, ^{94}Zr, ^{166}Er, ^{167}Er, ^{168}Er, ^{170}Er, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{209}Bi, ^{233}U, ^{234}U, ^{236}U, ^{237}Np, ^{238}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am ^{242m}Am, ^{243}Am, ^{242}Cm, ^{243}Cm, ^{244}Cm, ^{245}Cm.

Methodology

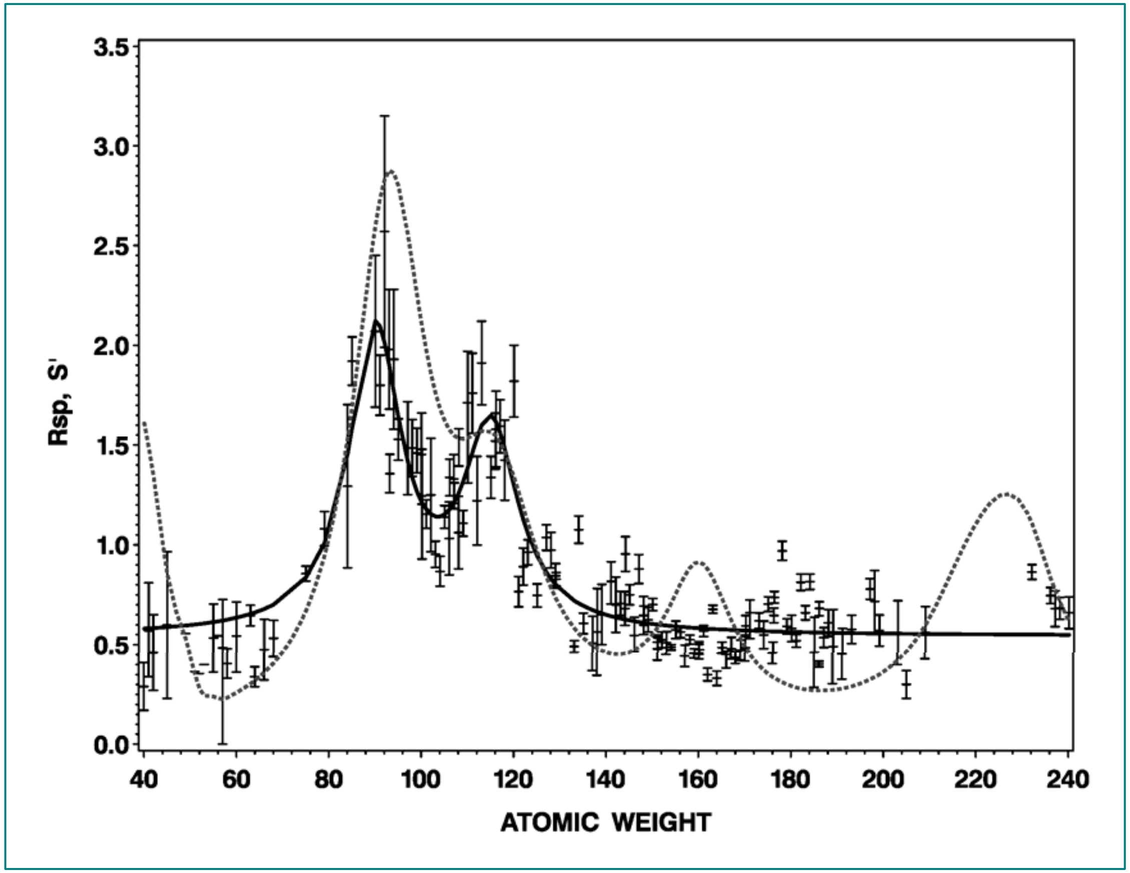
- Inspect the Atlas electronic files . Fill in the missing information, such as Γ_γ for s- and p-wave resonances and estimated uncertainties.
- Convert the Atlas file to ENDF format by applying PTANAL program; Random assignments of spins to follow (2J+1) law.
- Run PSY325 to calculate the contributions from the various resonances to the thermal cross section and resonance integral with their uncertainties read from the Atlas file.
- Compare with the uncertainty of the measured thermal cross section. Carry out changes in the uncertainties of RP, iterate the procedure until conversion is achieved.

Methodology

- Attribute reported uncertainty to that of bound levels and/or low-lying positive energy resonances.

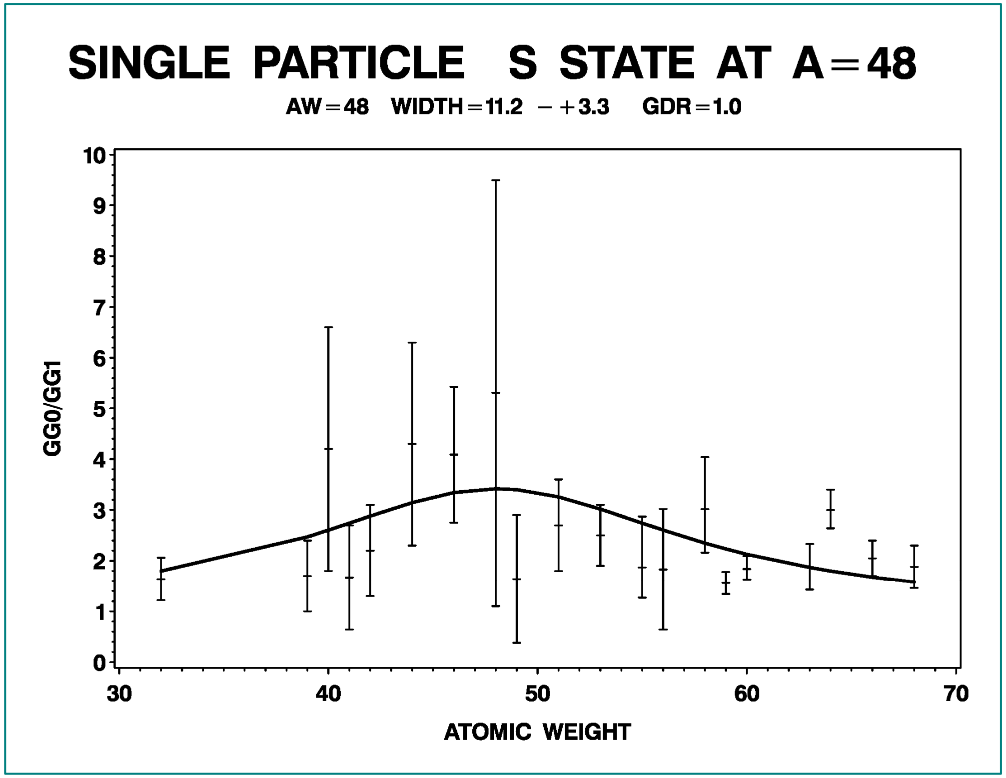
$\Gamma_{\gamma 1} / \Gamma_{\gamma 0}$ and S_1 Versus Mass Number

Systematics



$\Gamma_{\gamma 0} / \Gamma_{\gamma 1}$ Versus Mass Number

Systematics



Methodology

$$(\Delta\sigma_\gamma)^2 = \left(\frac{\partial\sigma_\gamma}{\partial\Gamma_n}\Delta\Gamma_n\right)^2 + \left(\frac{\partial\sigma_\gamma}{\partial\Gamma_\gamma}\Delta\Gamma_\gamma\right)^2 + \left(\frac{\partial\sigma_\gamma}{\partial\Gamma_f}\Delta\Gamma_f\right)^2 + \left(\frac{\partial\sigma_\gamma}{\partial E_o}\Delta E_0\right)^2$$

$$(\Delta\sigma_f)^2 = \left(\frac{\partial\sigma_f}{\partial\Gamma_n}\Delta\Gamma_n\right)^2 + \left(\frac{\partial\sigma_f}{\partial\Gamma_\gamma}\Delta\Gamma_\gamma\right)^2 + \left(\frac{\partial\sigma_f}{\partial\Gamma_f}\Delta\Gamma_f\right)^2 + \left(\frac{\partial\sigma_f}{\partial E_o}\Delta E_0\right)^2$$

Methodology

$$\left(\Gamma_\gamma, \Gamma_n\right) = 2\left(\frac{\partial \sigma_\gamma}{\partial \Gamma_n} \Delta\Gamma_n\right)\left(\frac{\partial \sigma_\gamma}{\partial \Gamma_\gamma} \Delta\Gamma_\gamma\right)\rho\left(\Gamma_\gamma, \Gamma_n\right)$$

$$\left(\Gamma_f, \Gamma_\gamma\right) = 2\left(\frac{\partial \sigma_f}{\partial \Gamma_f} \Delta\Gamma_f\right)\left(\frac{\partial \sigma_f}{\partial \Gamma_\gamma} \Delta\Gamma_\gamma\right)\rho\left(\Gamma_f, \Gamma_\gamma\right)$$

^{55}Mn Thermal Cross Sections and Resonance Properties

$^{55}_{25}$Mn $^{55}_{25}$Mn

THERMAL CROSS SECTIONS

σ_γ^0=13.36±0.05 b
σ_s=2.06±0.03 b
σ_{coh}=1.734±0.017 b
σ_{incoh}=0.6±0.2 b
b_{coh}=−3.750±0.018 fm
$b_{coh(+)}$=−2.36±0.03 fm
$b_{coh(-)}$=−5.69±0.03 fm
R'= 4.5±0.4 fm

RESONANCE PROPERTIES

D_0=2.42±0.15 keV
D_1=1.1±0.1 keV
S_0=4.2±0.8
S_1=0.31±0.05
$\langle\Gamma_{\gamma 0}\rangle$=0.75±0.15 eV
$\langle\Gamma_{\gamma 1}\rangle$=0.40±0.10 eV
I_γ=13.4±0.5 b

^{55}Mn Resonance Parameters

RESONANCE PARAMETERS

I^{π} = 5/2− %Abn = 100 Sn = 7270.45±0.13 keV

$\sigma_{\gamma}(+)$ = 1.75 b $\sigma_{\gamma}(-)$ = 8.28 b $\sigma_{\gamma}(B)$ = 3.33 b

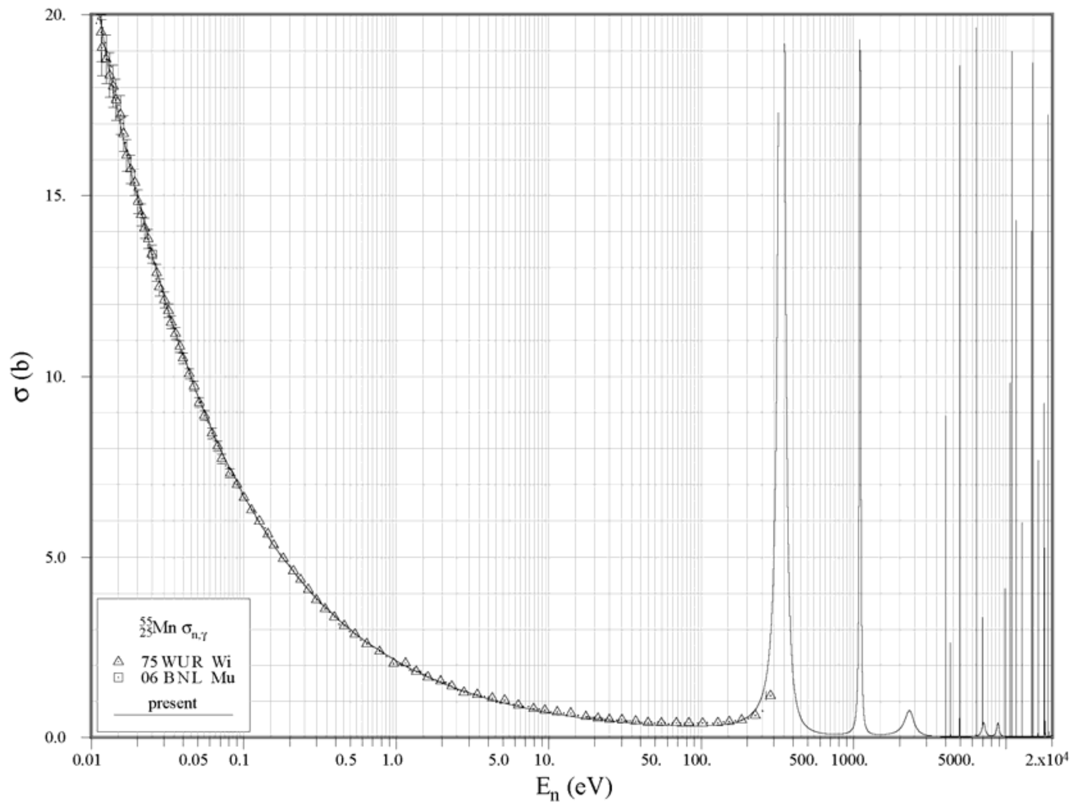
E_0 (keV)	J	l	$2g\Gamma_n$ (eV)	Γ_{γ} (eV)	$2g\Gamma_n^0$ (eV)	$2g\Gamma_n^1$ (eV)
−1.615	3	0		(0.75)	49.217	
−0.2028	2	0		(0.75)	0.0805	
0.3373±0.0010	2	0	18.3 ± 0.4	0.31 ±0.02	0.998 ±0.022	
1.099 ±0.002	3	0	18.0 ± 0.8	[a]0.435±0.100	0.543 ±0.024	
2.327 ±0.005	3	0	460 ±24	0.34 ±0.13	9.45 ±0.49	
4.000 ±0.008		[2]	0.00124± 0.00014			0.00387±0.00044
4.302 ±0.009		1	0.00384± 0.00024			0.0108 ±0.0007
4.939 ±0.010		1	0.932	0.290±0.013		2.12
6.330 ±0.006		1	0.232 ± 0.011			0.365 ±0.017
6.960 ±0.006		1	0.0073 ± 0.0011			0.0100 ±0.0015
7.102 ±0.006	2	0	332 ± 8	1.03 ±0.08	3.94 ±0.09	
8.815 ±0.007	3	0	432 ±12	0.82 ±0.08	4.60 ±0.13	
9.789 ±0.008		1	0.014 ± 0.001			0.0115 ±0.0008
10.615 ±0.009		1	0.0432 ± 0.0018			0.0315 ±0.0013
10.895 ±0.009		1	0.24 ± 0.02			0.17 ±0.01
11.629 ±0.010		1	0.067 ± 0.003			0.043 ±0.002
12.688 ±0.010		1	1.1 ± 0.1	0.323±0.035		0.61 ±0.06
14.705 ±0.012		1	0.096 ± 0.003			0.043 ±0.001
14.948 ±0.012		1	0.358 ± 0.020			0.157 ±0.009
16.167 ±0.013		1	0.704 ± 0.056			0.275 ±0.022
17.725 ±0.015		1	0.0700 ± 0.0048			0.0238 ±0.0016
17.802 ±0.015	3	0	12.8 ± 2.3	0.740±0.032	0.096 ±0.017	
17.990 ±0.015	2	0	54 ± 5	0.47 ±0.02	0.40 ±0.04	
18.812 ±0.016		1	1.43 ± 0.24			0.447 ±0.075
19.127 ±0.016		[2]	0.0113 ± 0.0017			0.00344±0.00052
20.225 ±0.017		1	0.36 ± 0.02			0.101 ±0.006
20.488 ±0.017		[2]	0.0038 ± 0.0020			0.0010 ±0.0006

Note: on basis of the present resonance parameters, 85% of thermal neutron capture takes place in channel spin J=2.

[a] A measured radiative width of 310 meV results in a calculated resonance capture integral of 11.7 barns, which is at variance with a measured weighted average value of 13.4−+0.5 b.

^{55}Mn Capture Cross Section

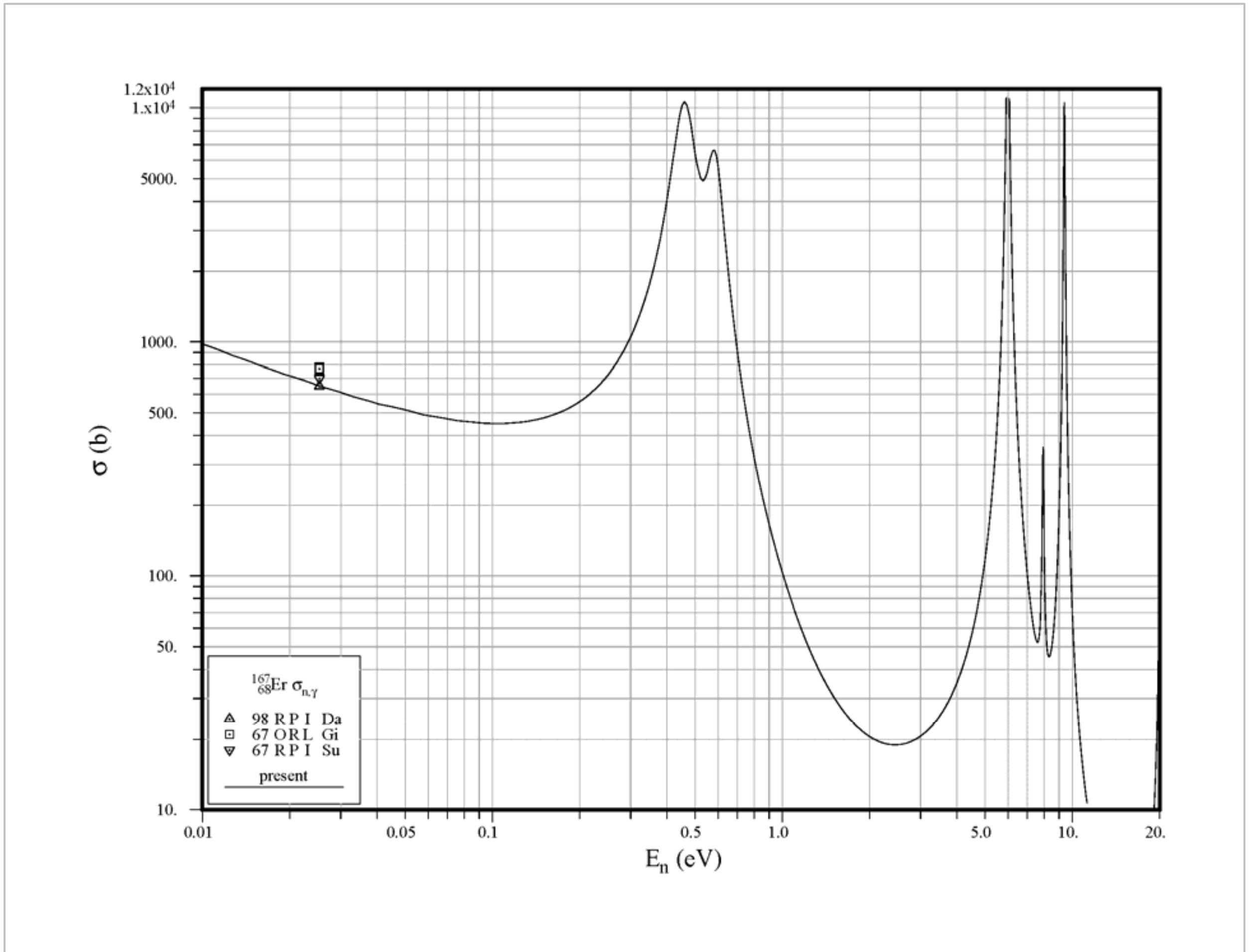
σ_γ =13.36 ± 0.05 (0.37%) b



^{55}Mn Uncertainty Adjustments

E_0(keV)	$2g\Gamma_n$(eV)	Γ_γ(eV)	σ_γ-b
-16.15	6255(0, 0)	0.790, 0.75(0, 0)	0.32
-0.202	1.15(0, 0)	0.790, 0.75(0, 0)	3.28
0.337	18.3(0.2, 2.2)	0.400, 0.31(0, 6.5)	7.44
1.099	18(0.4, 4)	0.488,0.435(0, 23)	1.50
2.327	460(0.02, 5.2)	0.340, 0.40(0, 38)	0.17

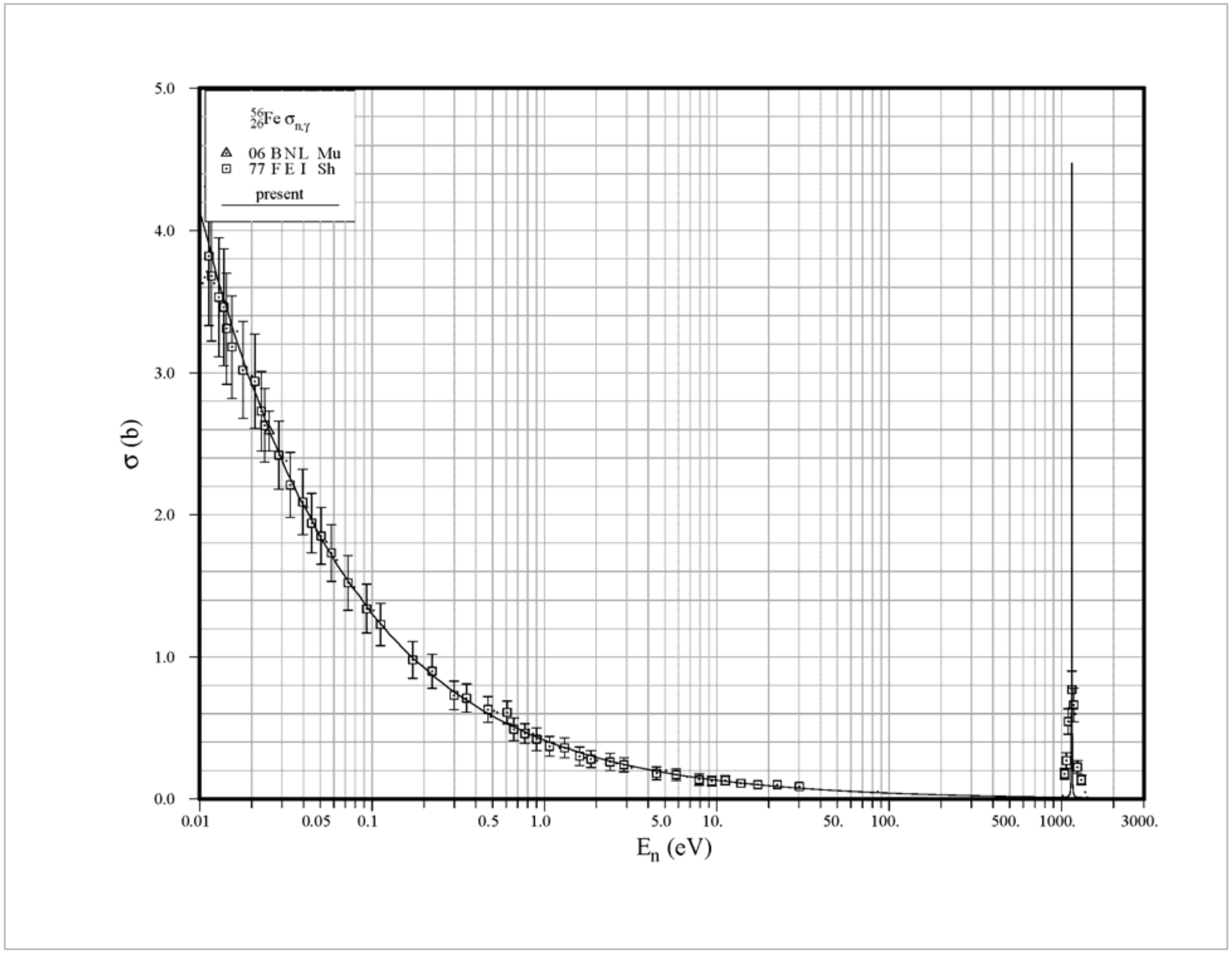
^{167}Er Capture Cross Section



^{167}Er $\sigma_\gamma = 649 \pm 8$ b

E_0(eV)	$2g\Gamma_n$ (mV)	Γ_γ (mV)	σ_γ (b)
-23.6	117 (3.3, 0)%	88.0 (11, 0)%	7.9
0.460	0.3031 (3.3, 3.3)%	87.12 (0.4, 0.2)%	423
0.584	0.2163 (4.6)%	86.20 (0.4, 0.4)%	161

^{56}Fe Capture Cross Section



Some Sources of Correlations

- Capture Kernel $\frac{g\Gamma_n\Gamma_\gamma}{\Gamma}$: $\rho(\Gamma_n, \Gamma_\gamma)$ is Negative.
- Capture and Fission Kernels: Γ_f / Γ_γ is Determined.
  Hence, $\rho(\Gamma_f, \Gamma_\gamma)$ is Positive.
- Neutron Sensitivity Correction to Capture Measurements:
  $\Gamma_\gamma(\text{exp.}) = \Gamma_\gamma + k\Gamma_n$
  Hence, $\rho(\Gamma_n, \Gamma_\gamma)$ is Positive.
- However, This May Be Signature of Valence Capture.

Effect of $\rho(\Gamma_n, \Gamma_\gamma)$ on Uncertainties

nucleus	σ_γ (b)	$\rho = 0$ Δ(b)	$\rho = -1$ Δ(b)	$\rho = +1$ Δ(b)
^{52}Cr	0.86±0.02	0.020	0.018	0.023
^{55}Mn	13.36±0.05	0.047	0.044	0.049
^{237}Np	178.7±3.0	3.0	1.6	4.0

Conclusions

- Internal consistency between calculated and estimated uncertainties is achieved for 15 actinides and 21 coolant and structural materials.
- This was realized by re-assigning uncertainties to the parameters of the bound levels and low-energy resonances.
- If the major contribution to the thermal cross section is due to the positive energy resonances, then their uncertainties are drastically changed.
- In few cases, where the thermal cross sections are dominated by bound levels, the uncertainties of the positive energy resonances are unaffected.
- The correlations between parameters are studied and their effects on the uncertainties is determined for some cases.

Conclusions

- Outstanding issue:
  - In certain cases, uncertainty of positive energy resonances drastically reduced.
  - Possible solution to invoke negative correlation between the bound levels and positive energy resonances.