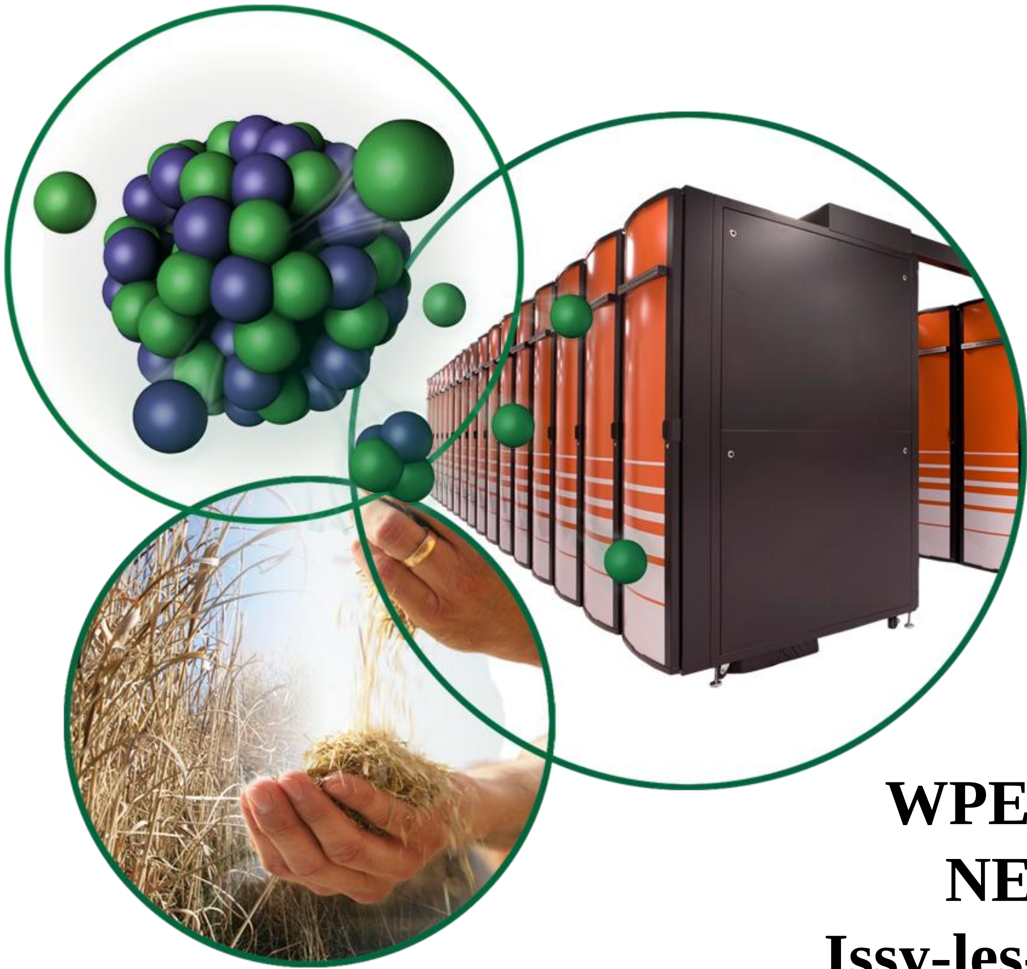
Resonance Region of ^{56}Fe for the CIELO Project



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^{56}Fe Resolved Resonance Evaluation up to 2.0 MeV and Unresolved Resonance in the Energy Range 2-4 MeV

- Motivation for evaluating ^{56}Fe;
- Evaluation description;
- Use RML option of the SAMMY code (R-matrix Limited Format);
- Experimental Data;
- Combination of differential and integral data in the SAMMY fitting procedure;
- Results and Conclusions;

Motivation for evaluating ^{56}Fe

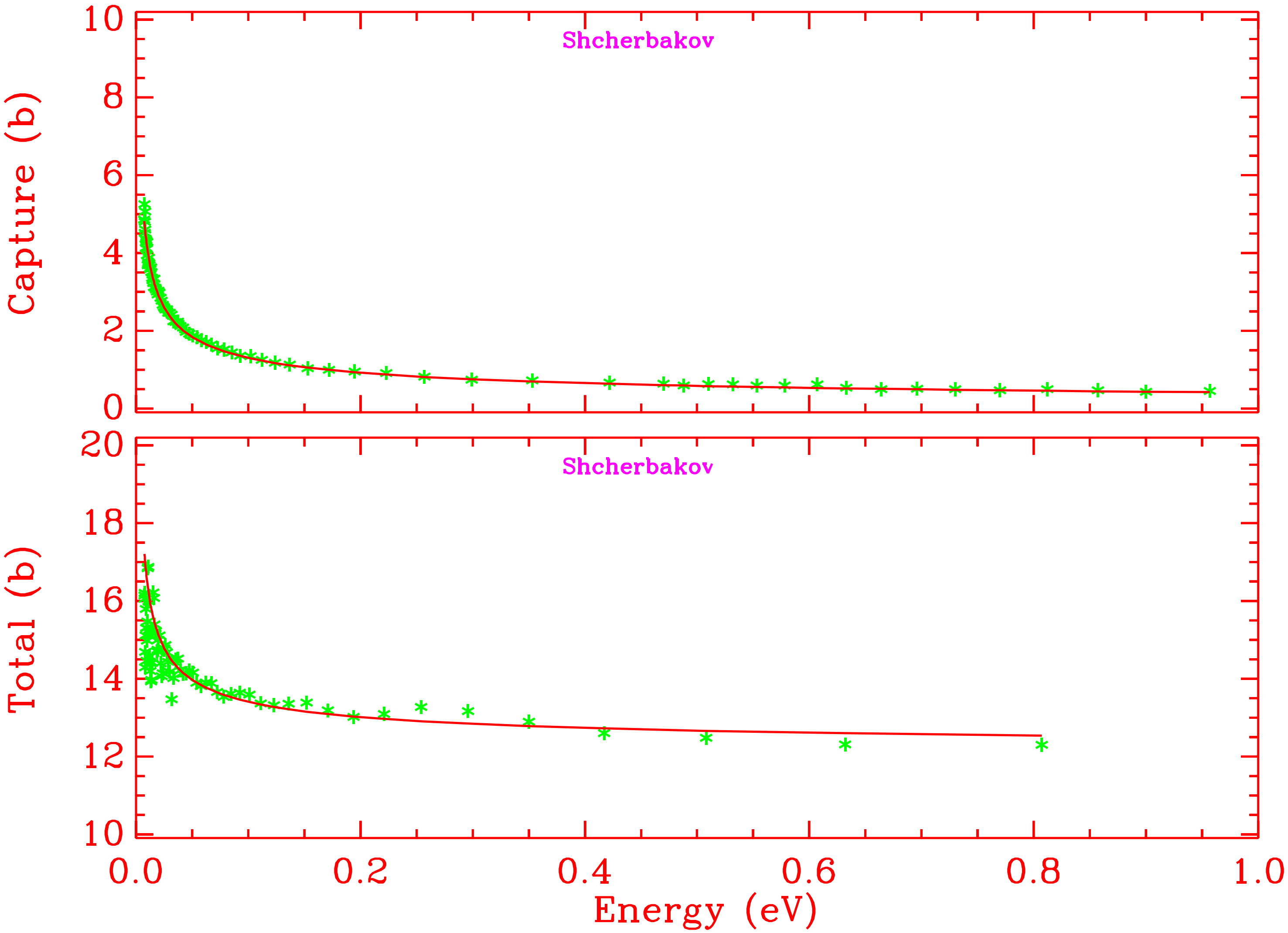
- High resolution transmission measurements done at the RPI extending the resonance region up to 5 MeV (Danon);
- Inelastic cross section measurements done at GEEL (Plompen);
- Use of the SAMMY/RML feature to include inelastic channel in the R-matrix analysis;
- Additional data:
  - Low energy capture and total cross section;
  - Differential elastic cross section;
- Improve benchmark results for Iron benchmark calculations;

Evaluation Features

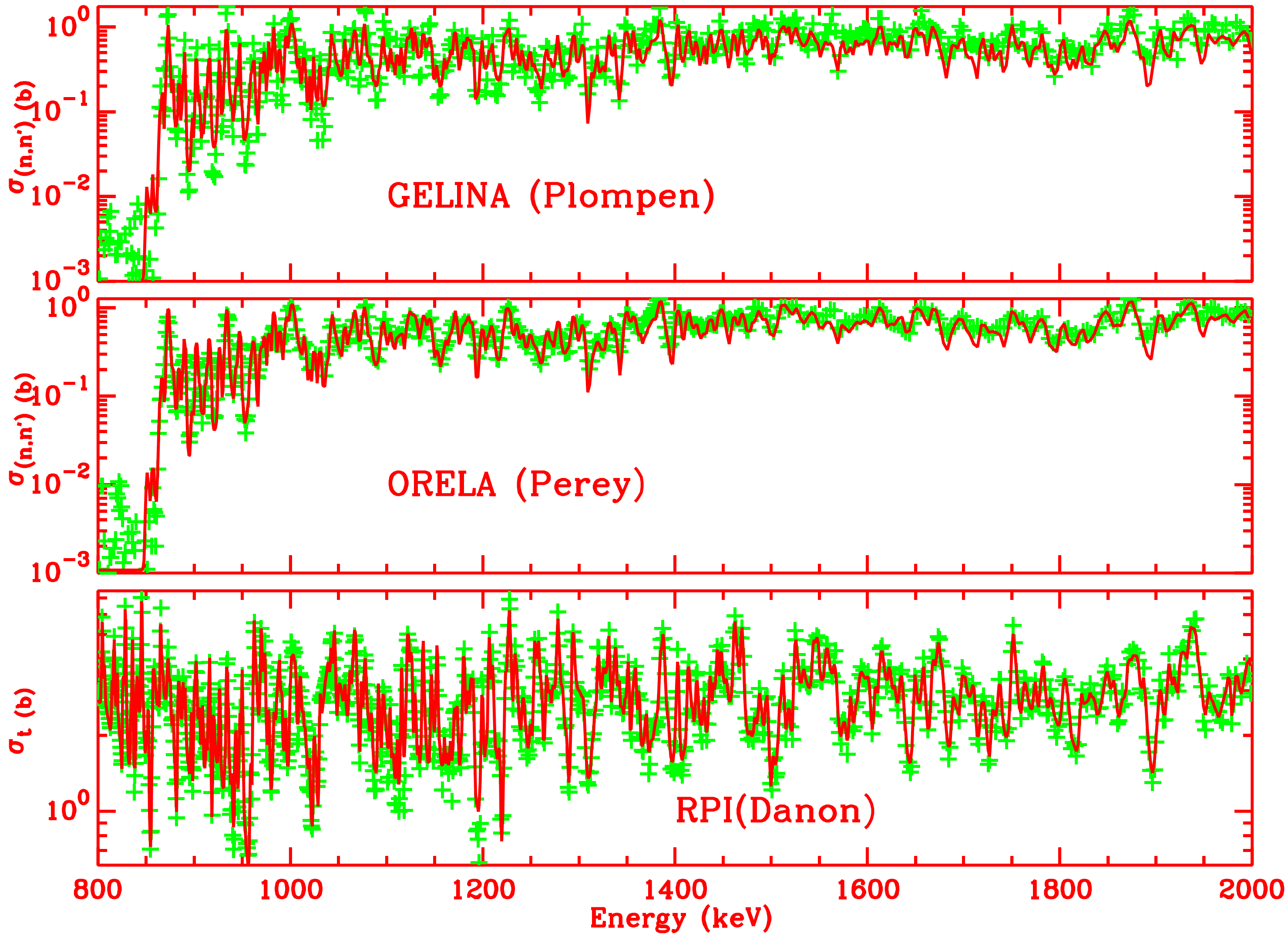
- Extend the resolved resonance region from 850 keV to 2.0 MeV;
- Fit RPI transmission data in the energy range 2-4 MeV;
- Include new transmission measurements and inelastic cross section data
- Use the extended R-matrix formalism in the SAMMY code for fitting the experimental data
- Fit differential scattering cross section using Blatt and Biedenharn formalism in SAMMY;
- Process and compare the cross sections processed with SAMMY, NJOY, AMPX and PREPRO using the evaluated iron resonance parameters;
- Generate covariance data using the compact formalism;
- Inclusion of integral data together with the SAMMY (SAMINT) fitting of the differential data;

Experimental Data for the n+^{56}Fe Interaction

Reference	Energy Range	Facility	TOF (meters)	Measurement
Harvey (1987)	20 keV – 2 MeV	ORELA	201.575	Transmission
Perey (1990)	120 keV – 850 keV	ORELA	201.575	Transmission
Cornelis (1982)	500 keV – 2 MeV	GELINA	387.713	Transmission
Danon (2012) (three thicknesses)	500 keV – 2 MeV	RPI	249.740	Transmission
Perey (1990)	850 keV – 1.5 MeV	ORELA	201.575	Inelastic
Plompen (2011)	850 keV – 2 MeV	GELINA	198.686	Inelastic
Spencer (1994)) (two thicknesses)	10 eV – 650 KeV	ORELA	40.0	Capture
Perey (1990)	850 keV – 1.5 MeV	ORELA	200.191	elastic
Cabé (1967)	500 keV – 1.2 MeV	Université de Louvain (Van de Graaff)	~ 1	elastic
O.A.Shcherbakov (1977)	0.001 eV – 10 eV	TOF/Russia	9.5	Total
O.A.Shcherbakov (1977)	0.001 eV – 10 eV	TOF/Russia	9.5	Capture

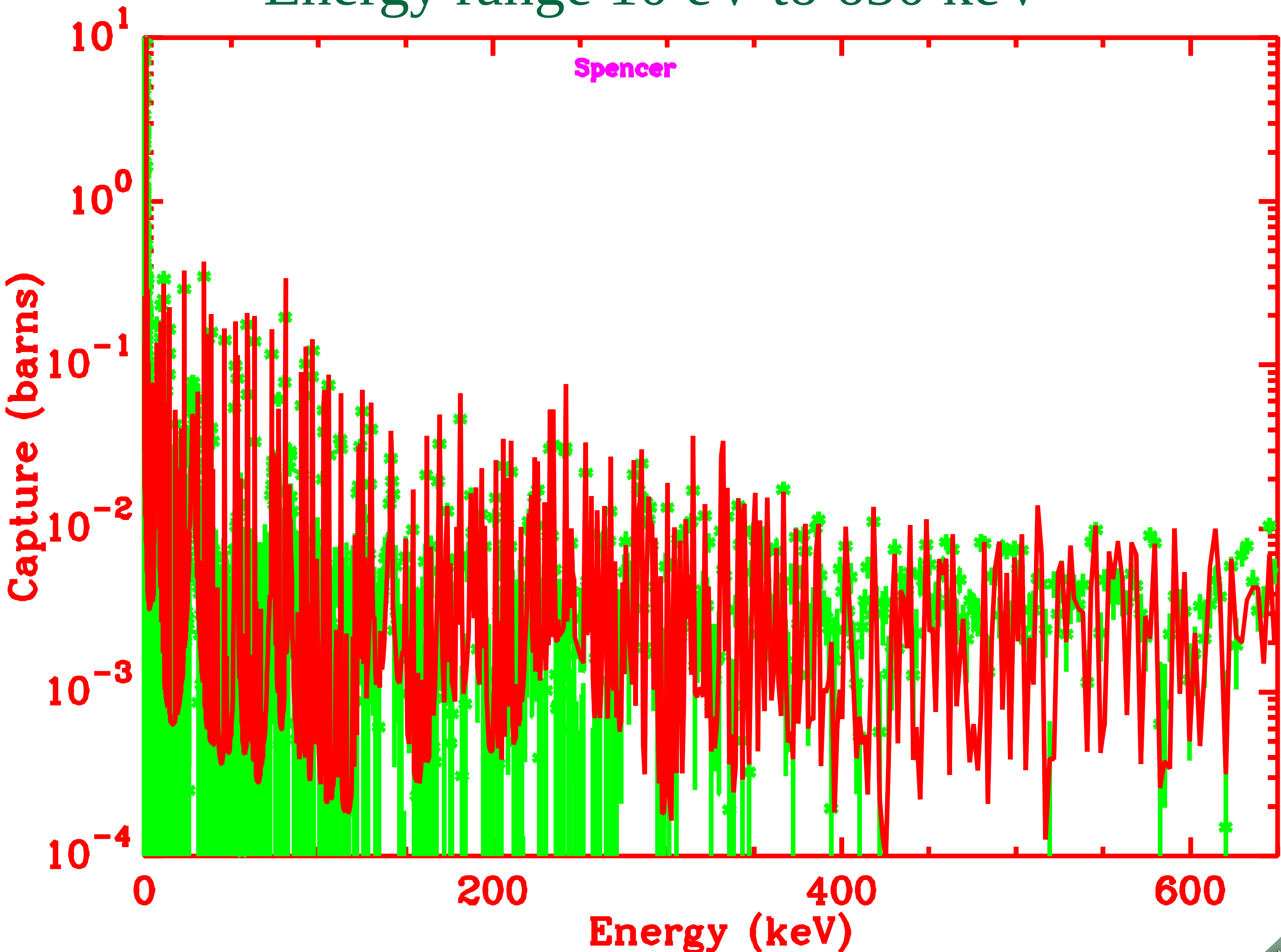


Comparison of SAMMY predictions to total and capture data of Shcherbakov.

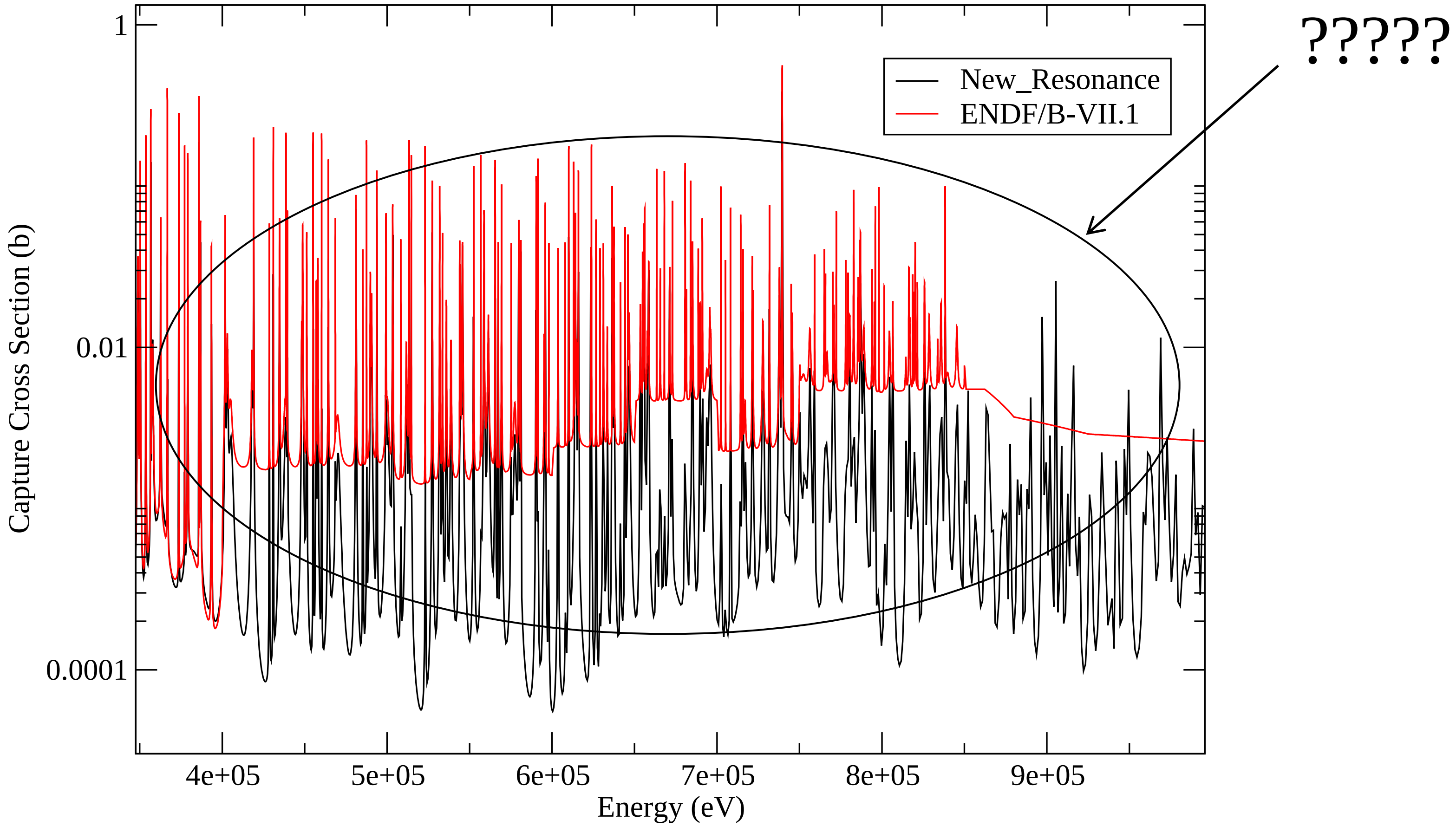


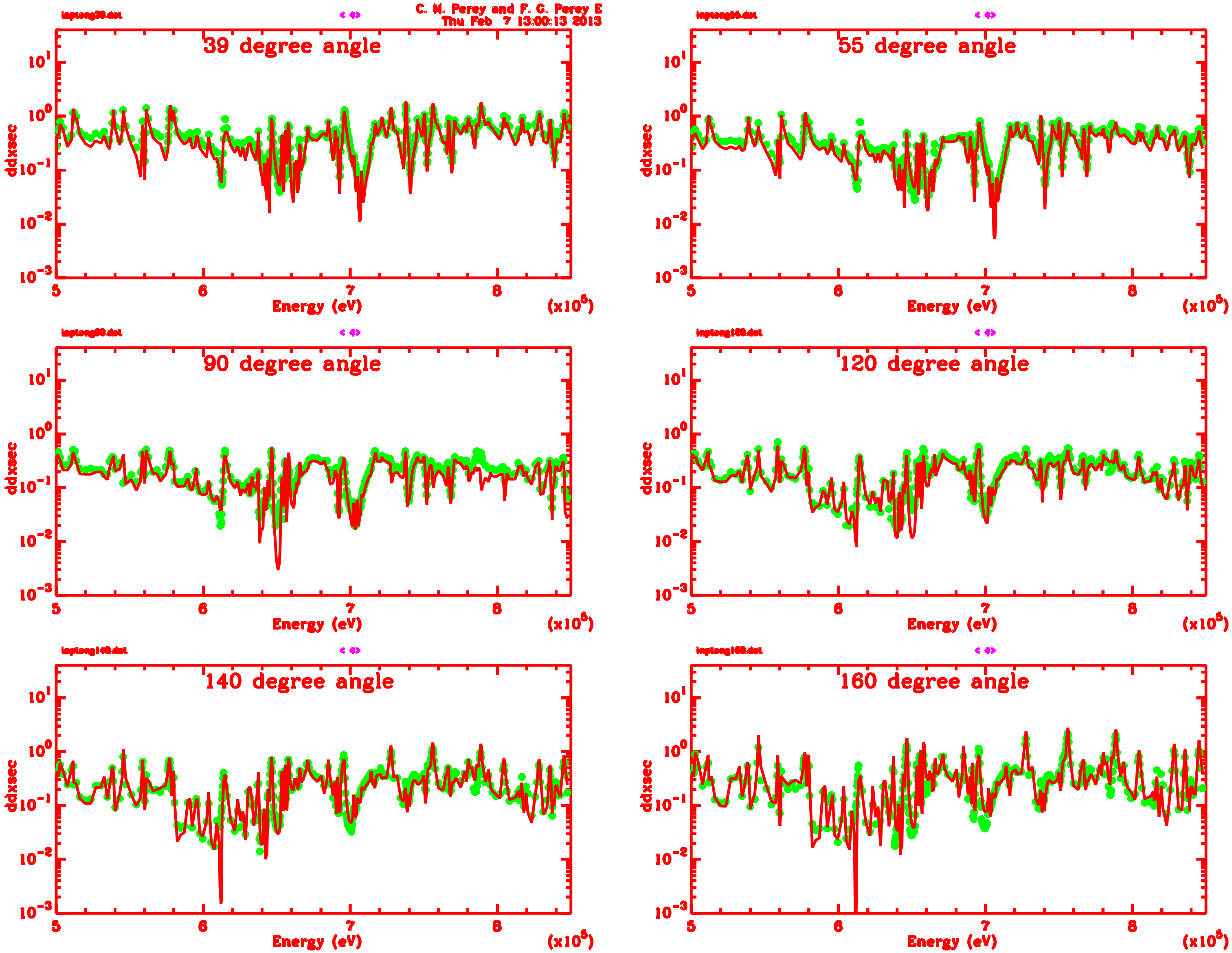
Comparison of SAMMY predictions of Total and inelastic data.

SAMMY fit to the experimental capture data of Spencer. Energy range 10 eV to 650 keV

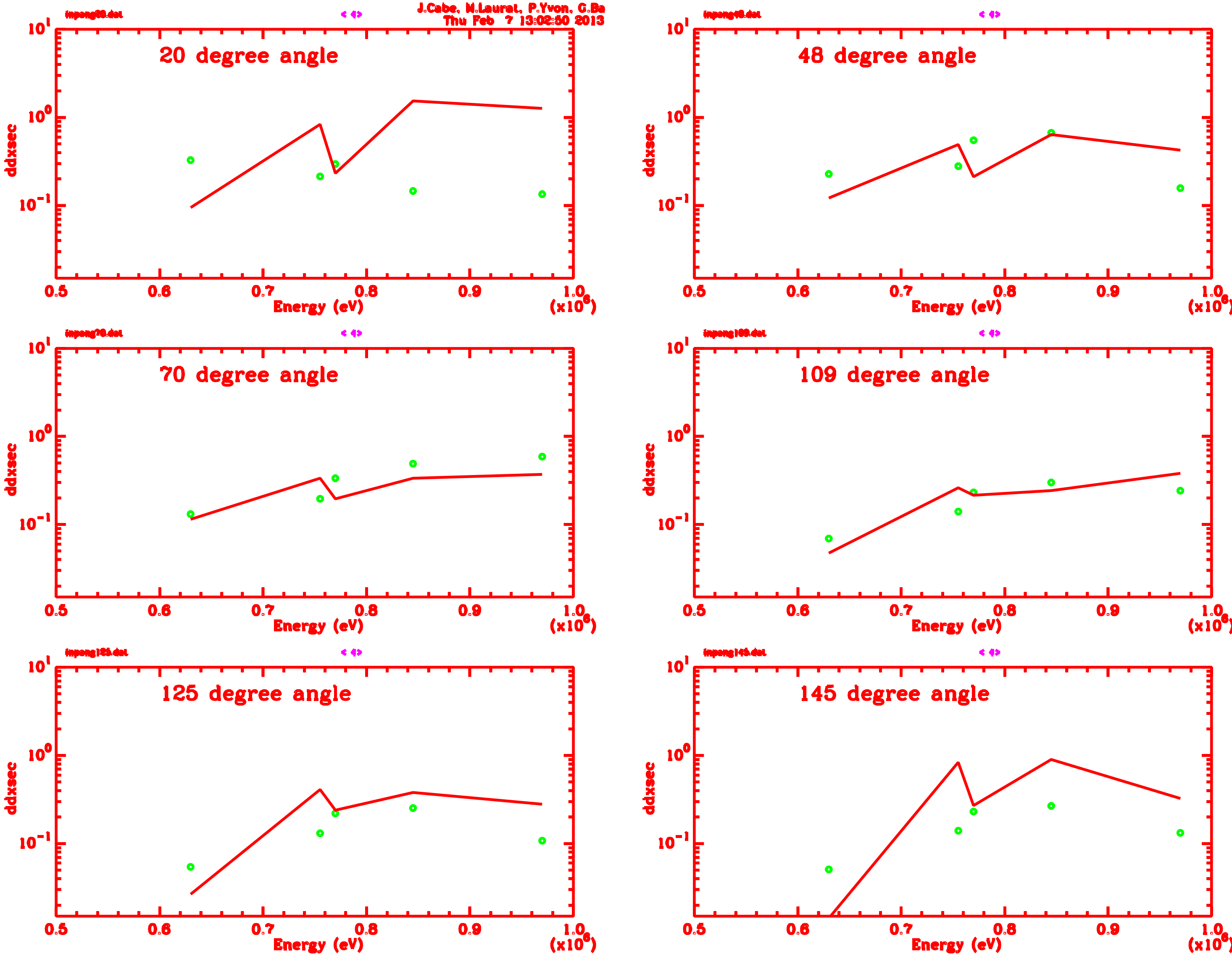


Issues with Fe-56 capture cross-section data identified through collaborative work with IRSN



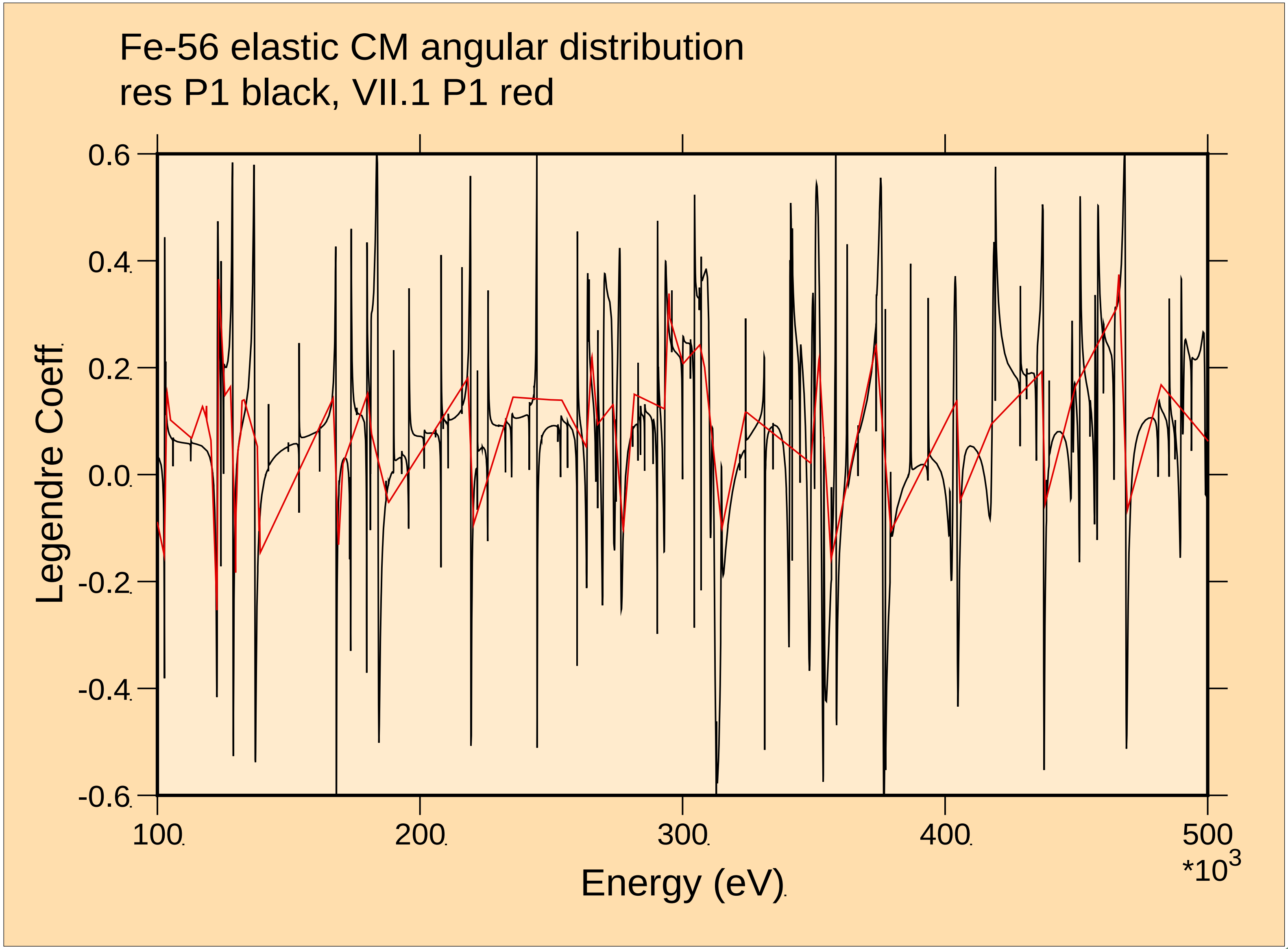


Comparison of SAMMY predictions to differential elastic data of Perey.

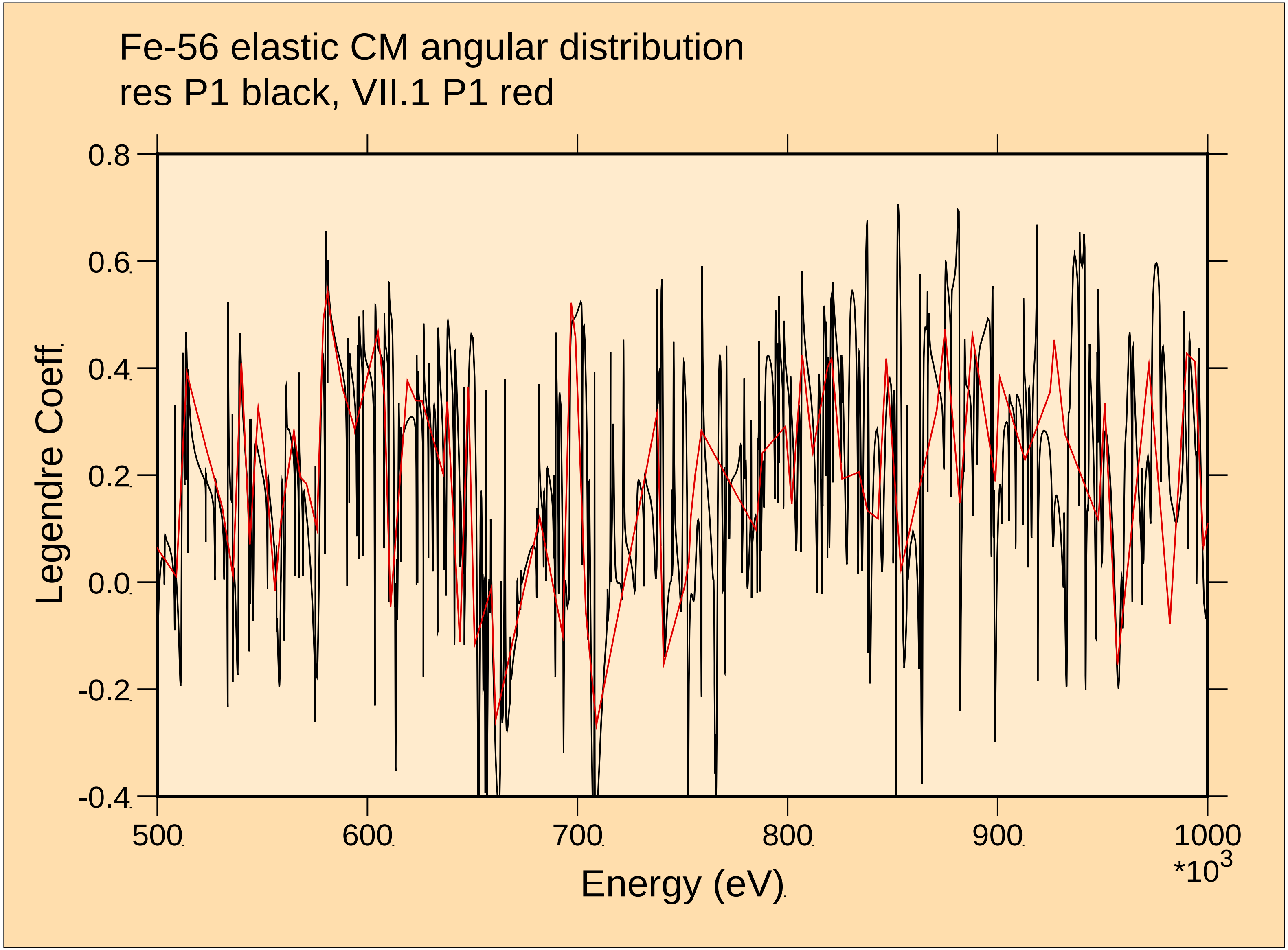


Comparison of SAMMY predictions to differential elastic data of Cabé .

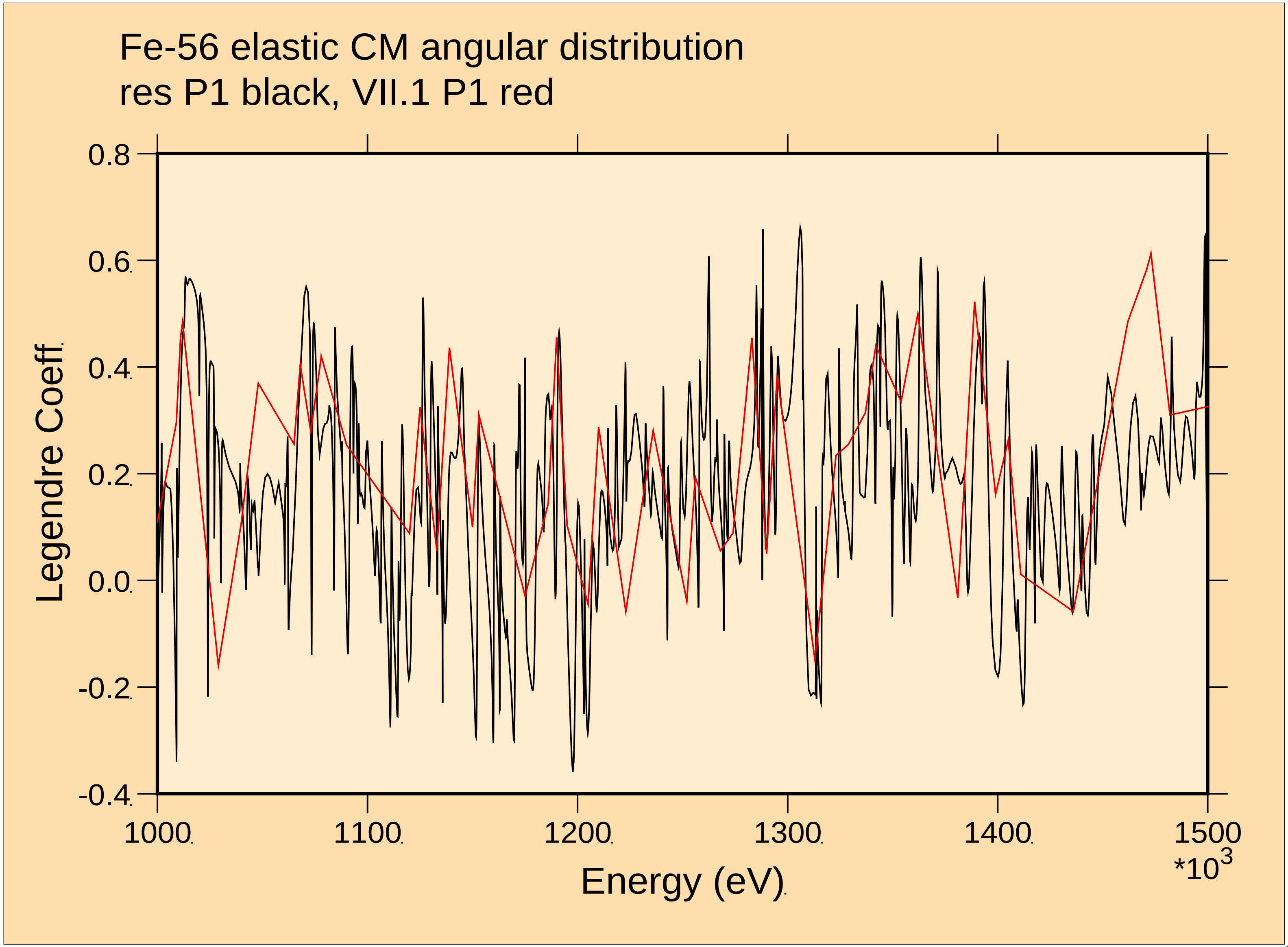
Legendre coefficient calculated by NJOY



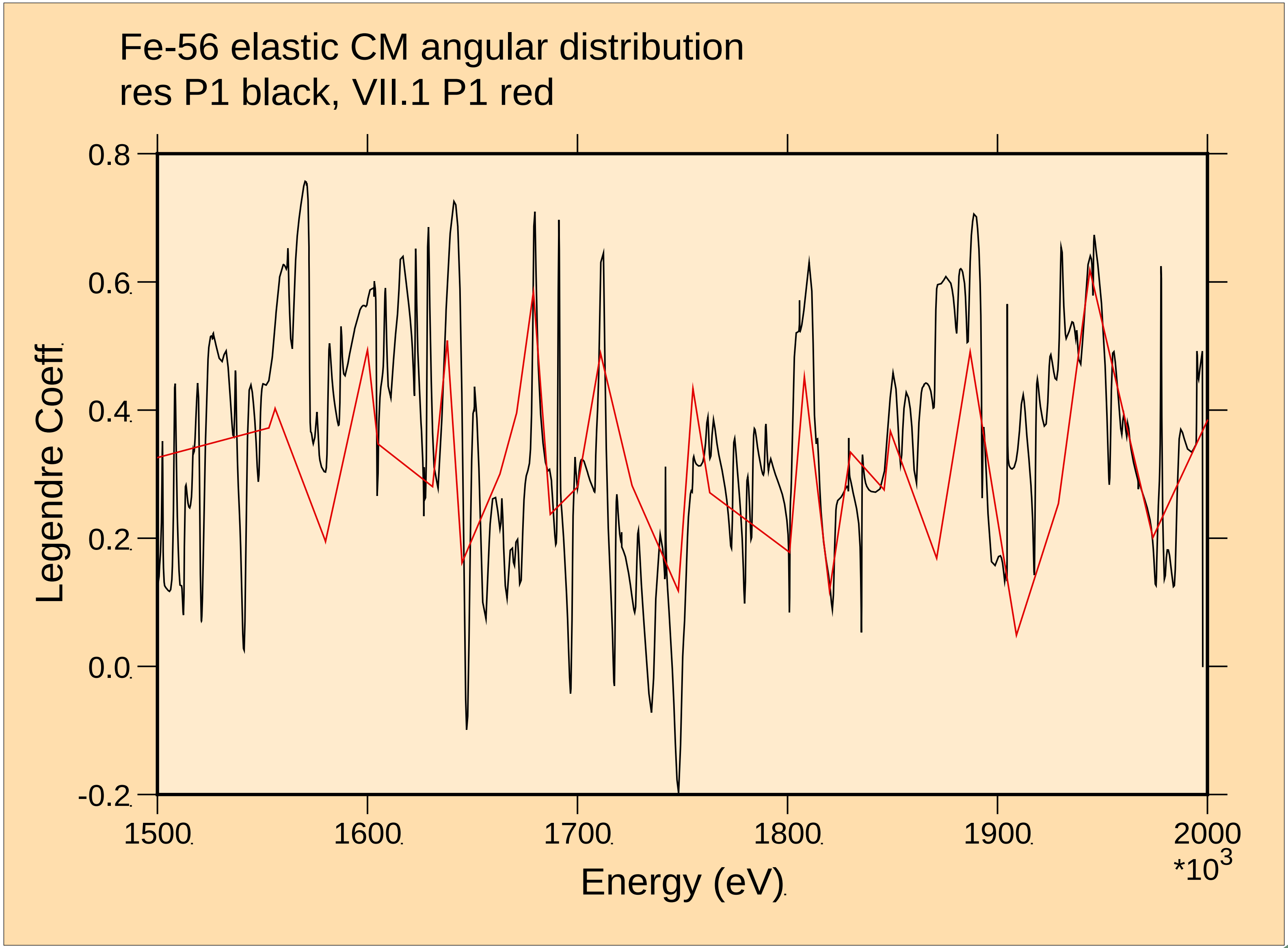
Legendre coefficient calculated by NJOY



Legendre coefficient calculated by NJOY



Legendre coefficient calculated by NJOY



Thermal and Resonance Integral (T=293.6 K)

Data (barns)	Mughabghab	JENDL4	JEFF3.1	ENDF/BVII.1	ORNL4
σ_t	15.21	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	1.34
*calculated					

Coherent Scattering

Scattering length in terms of a^+ and a^- for spin states $I + 1/2$ and $I - 1/2$

$$a^2 = \left[\frac{I+1}{2I+1} a^+ + \frac{I}{2I+1} a^- \right]^2 + \frac{I(I+1)}{(2I+1)^2} (a^+ - a^-)^2$$

with

$$a_{coh} = \frac{I+1}{2I+1} a^+ + \frac{I}{2I+1} a^-$$

and

$$a_{inch} = \frac{[I(I+1)]^{1/2}}{2I+1} (a^+ - a^-)$$

Coherent Scattering

For nuclei with $I = 0$ $a_{coh} = a^{+}$ *and* $a_{inch}=0$
that is:

$$a = a_{coh}$$

$$a_{coh} = \lim_{E \to 0} \left(\frac{s_s}{4p} \right)^{1/2}$$

Data (fm)	Mughabghab	JENDL4	JEFF3.1	ENDF/BVII.1	This Evaluation
a_{coh}	10.1 ± 0.2	9.8	9.8	9.6	9.7

Covariance Generation

1. Compact format used together with the LRF=7 option;

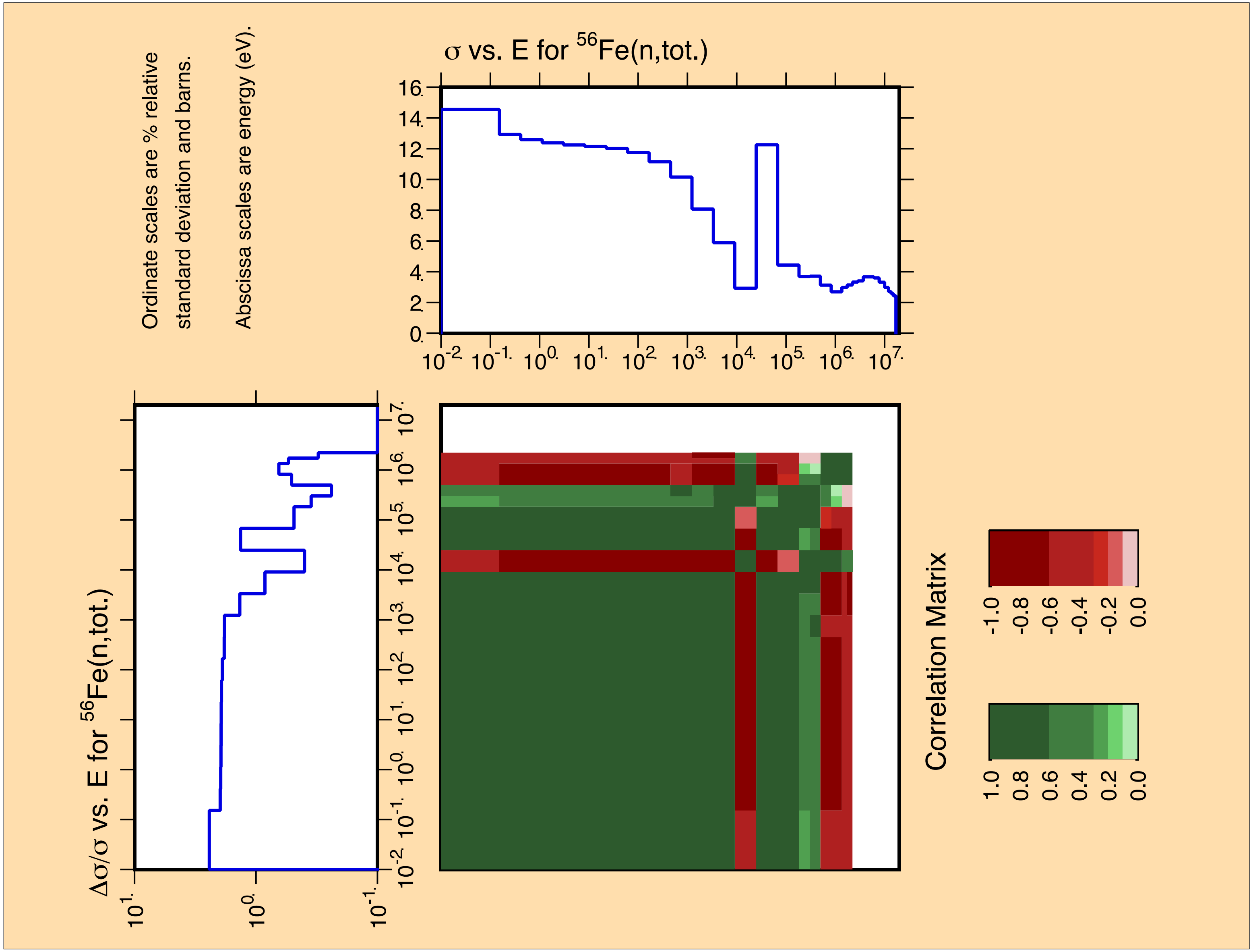
1. Data processed with NJOY(ERROR) and AMPX(PUFF);

3. Uncertainties calculated with NJOY, AMPX agree well with calculations with SAMMY;

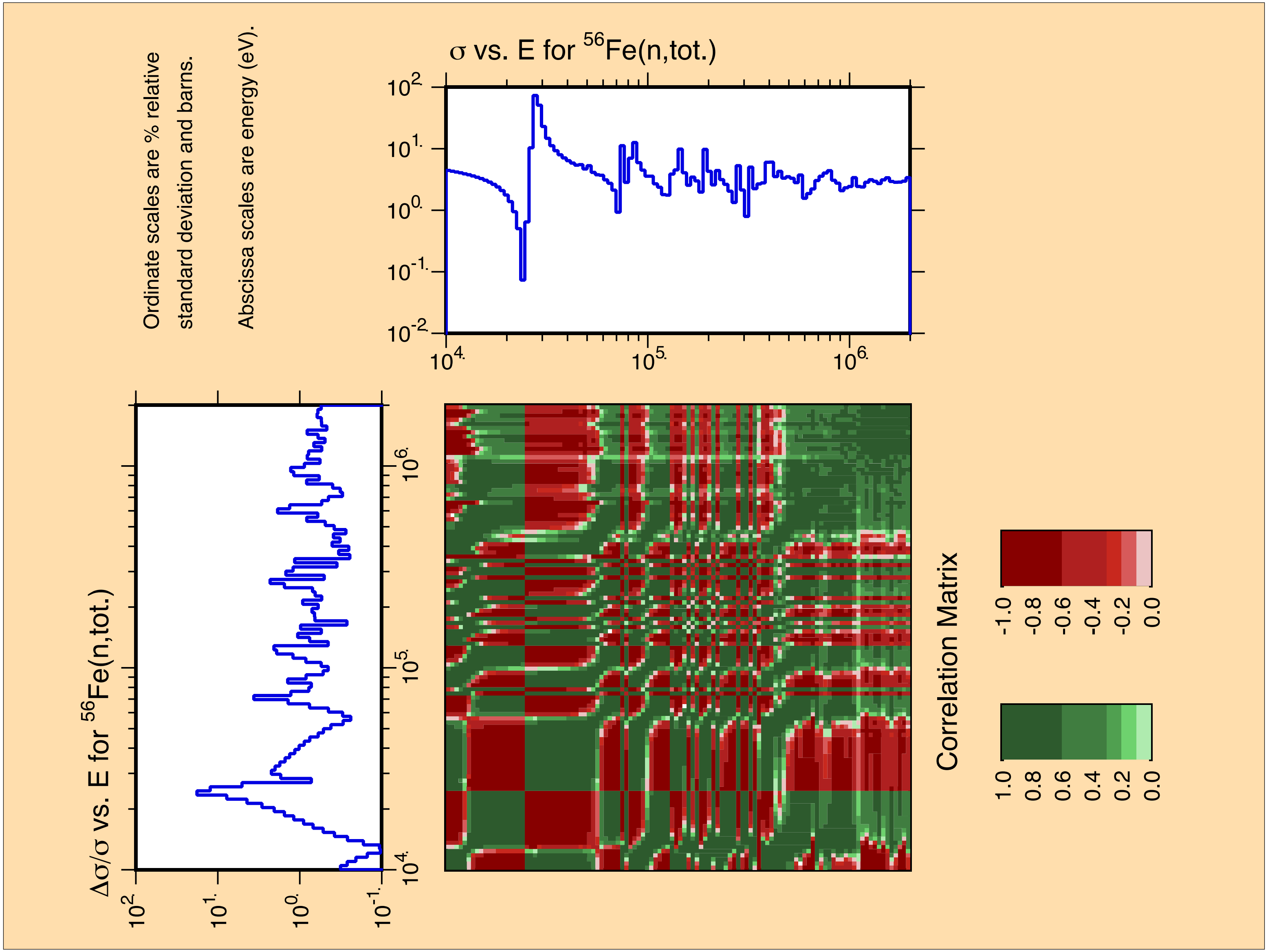
Thermal and Resonance Integral and uncertainties calculated with covariance data at T=293.6 K

Data (barns)	Mughabghab	ORNL4
σ_t	15.21	14.78 ± 0.32
σ_s	12.69 ± 0.49	12.19 ± 0.23
σ_γ	2.59 ± 0.14	2.59 ± 0.16
I_γ	(1.36 ± 0.15)*	1.34 ± 0.22
*calculated		

44-group covariance from thermal to 2 MeV



112 log-spaced groups between 10 keV and 2 MeV



Benchmark Results

1. Californium-Iron shielding benchmark: Six iron spheres of diameters of 20, 30, 40, 50, 60, and 70 cm. Experiments done at IPPE, Russia.

1. ICSBEP benchmarks:
   a) Highly Enriched Uranium Metal Fast benchmark (HMF013 and HMF021);
   b) Plutonium Metal Fast benchmark (PMF025 and PMF032)

3. Highly Enriched Uranium Metal Intermediate benchmark (HMI-001)

1. 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)

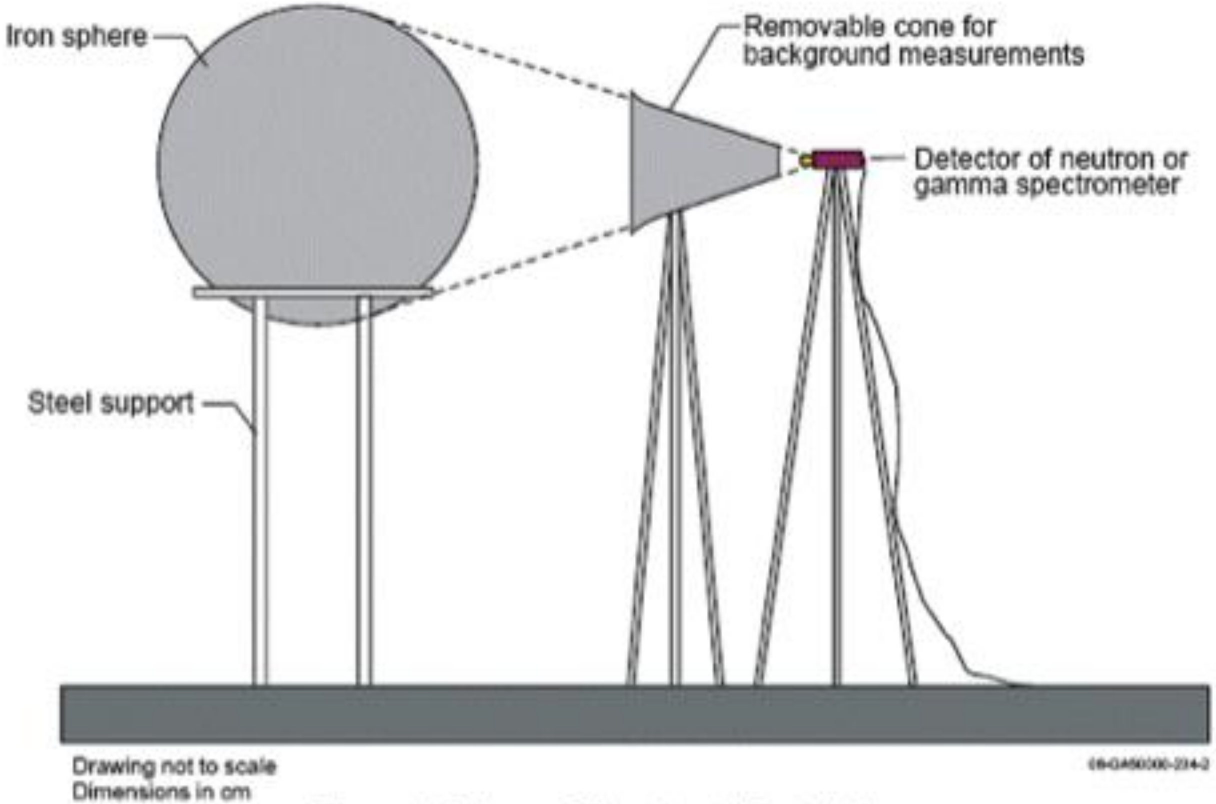
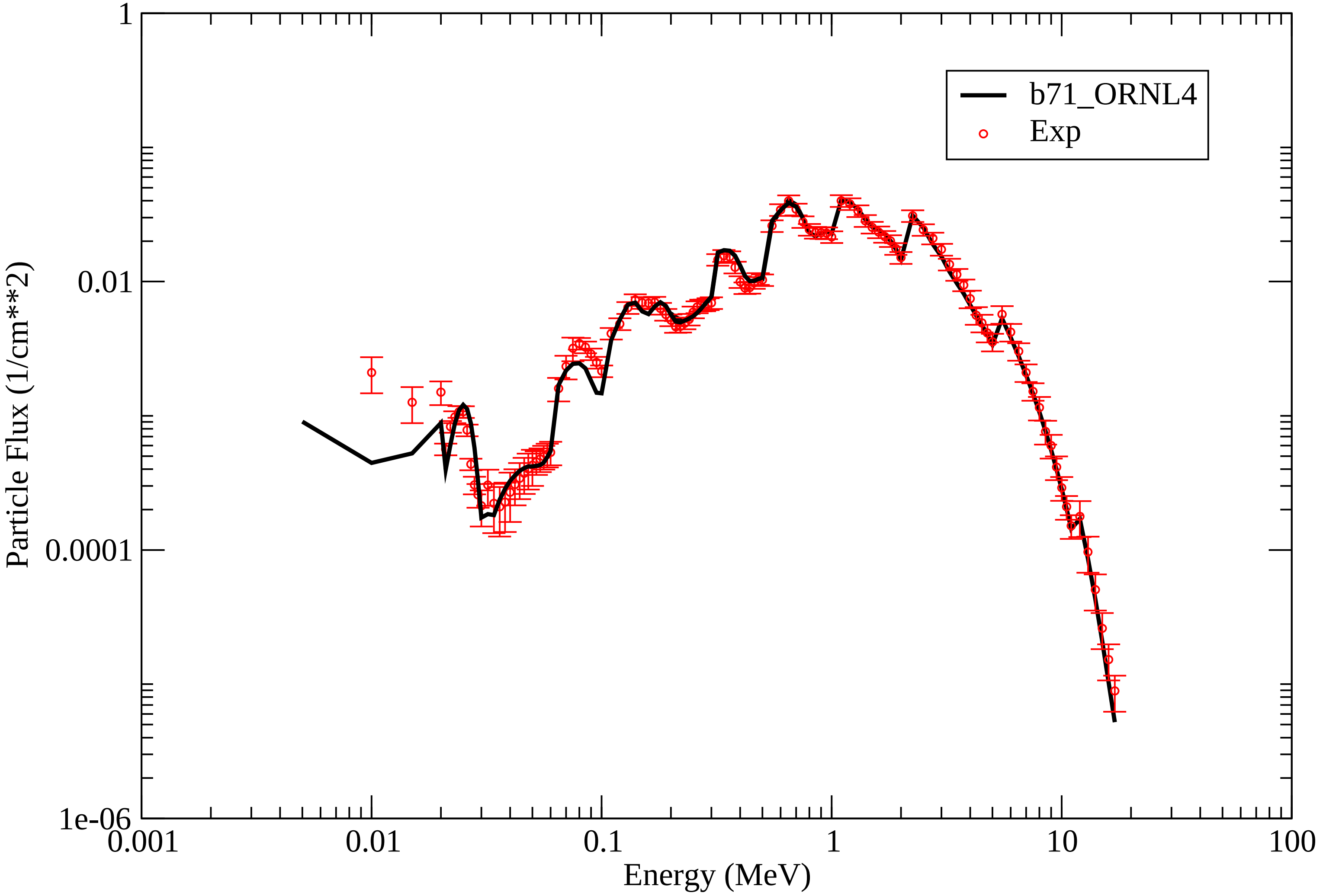


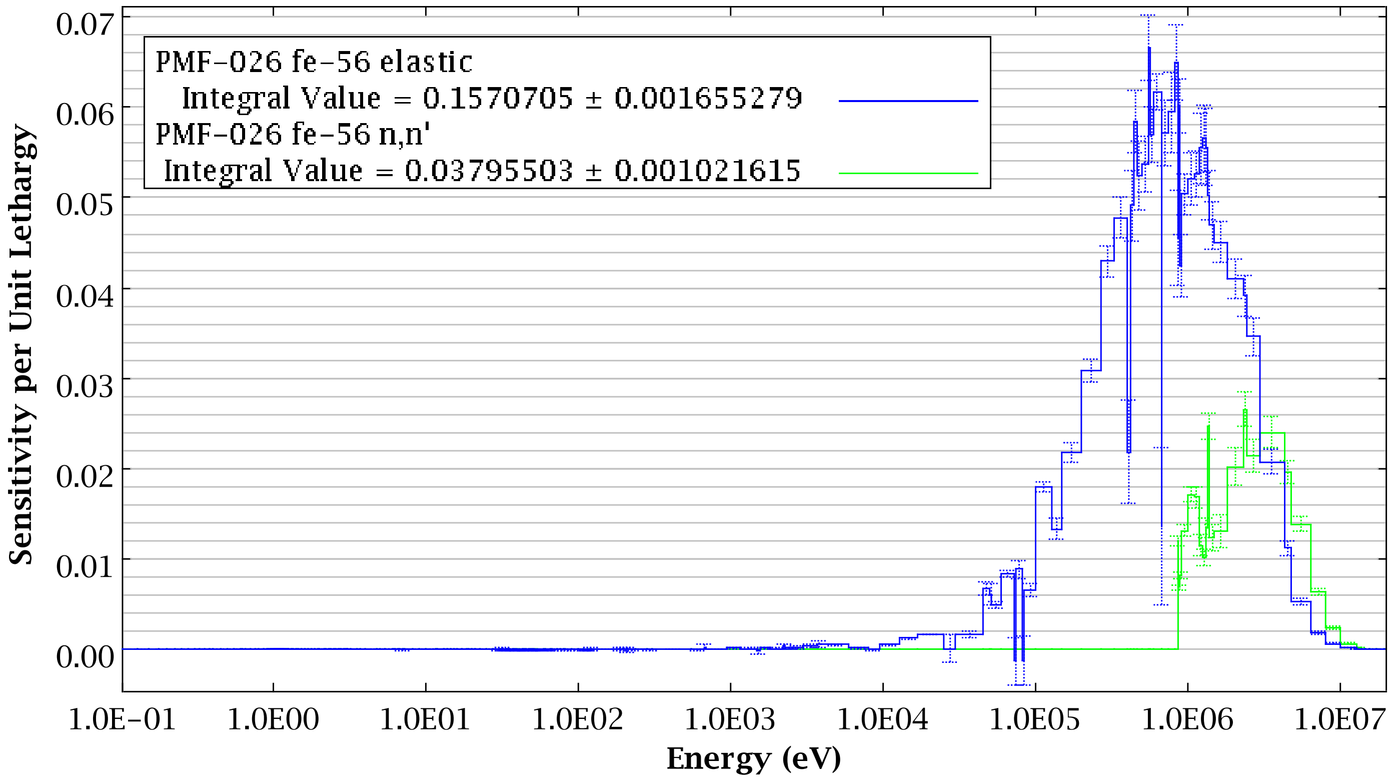
Figure 1. Scheme of Experimental Installation.

Case: 20 cm (Cf-252 neutron source)



2. K_eff for HMF and PMF

Sensitivity of k_eff to the elastic and inelastic cross section For PMF-026



K_eff for HMF and PMF

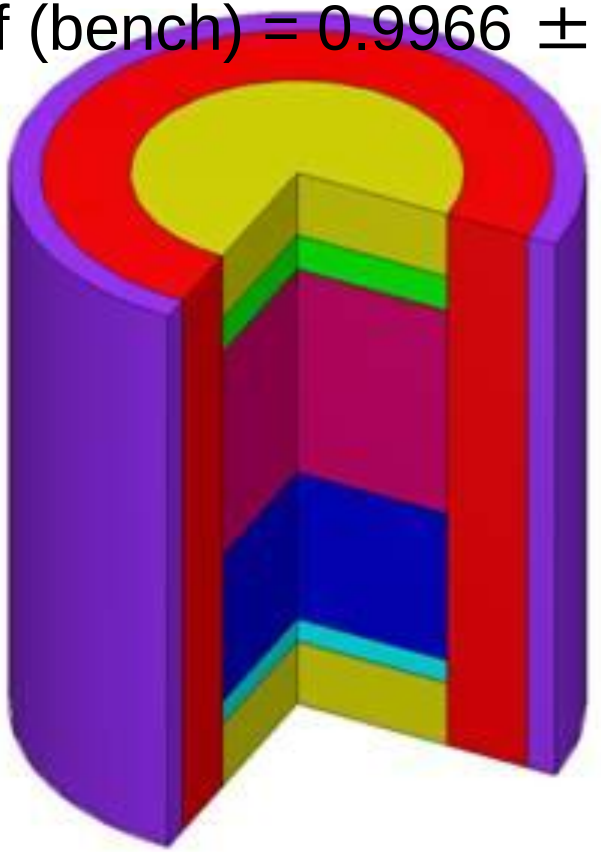
C/E		
benchmark	**ORNL4**	**ENDF/BVII.1**
HMF013	0.99850	0.99841
HMF021	0.99633	0.99720
PMF025	0.99892	0.99890
PMF032	0.99792	0.99877

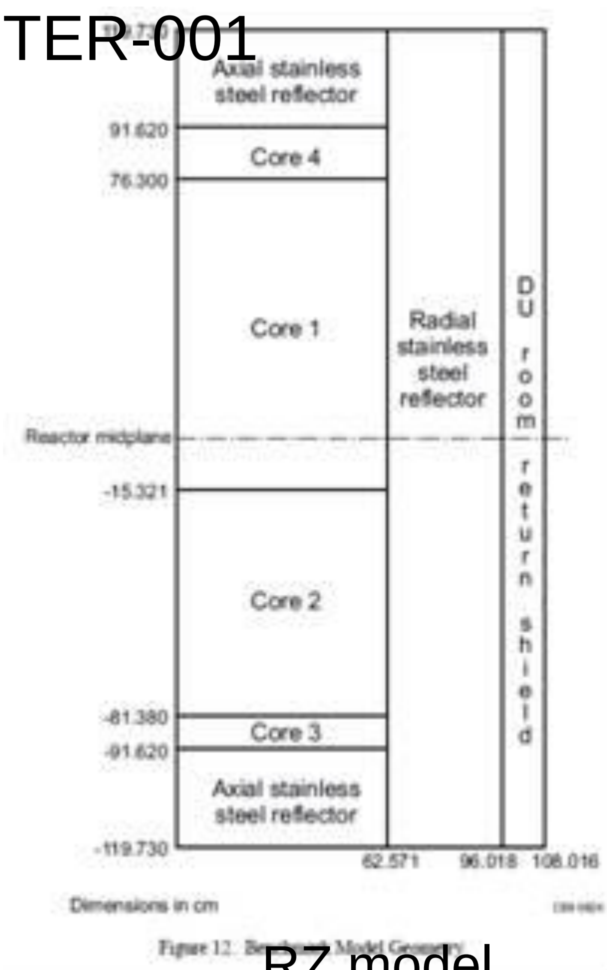
3. ZPR 9/34 loading 303

1. Highly enriched uranium/ iron benchmark, reflected by steel.

2. ICSBEP identification: HEU-MET-INTER-001

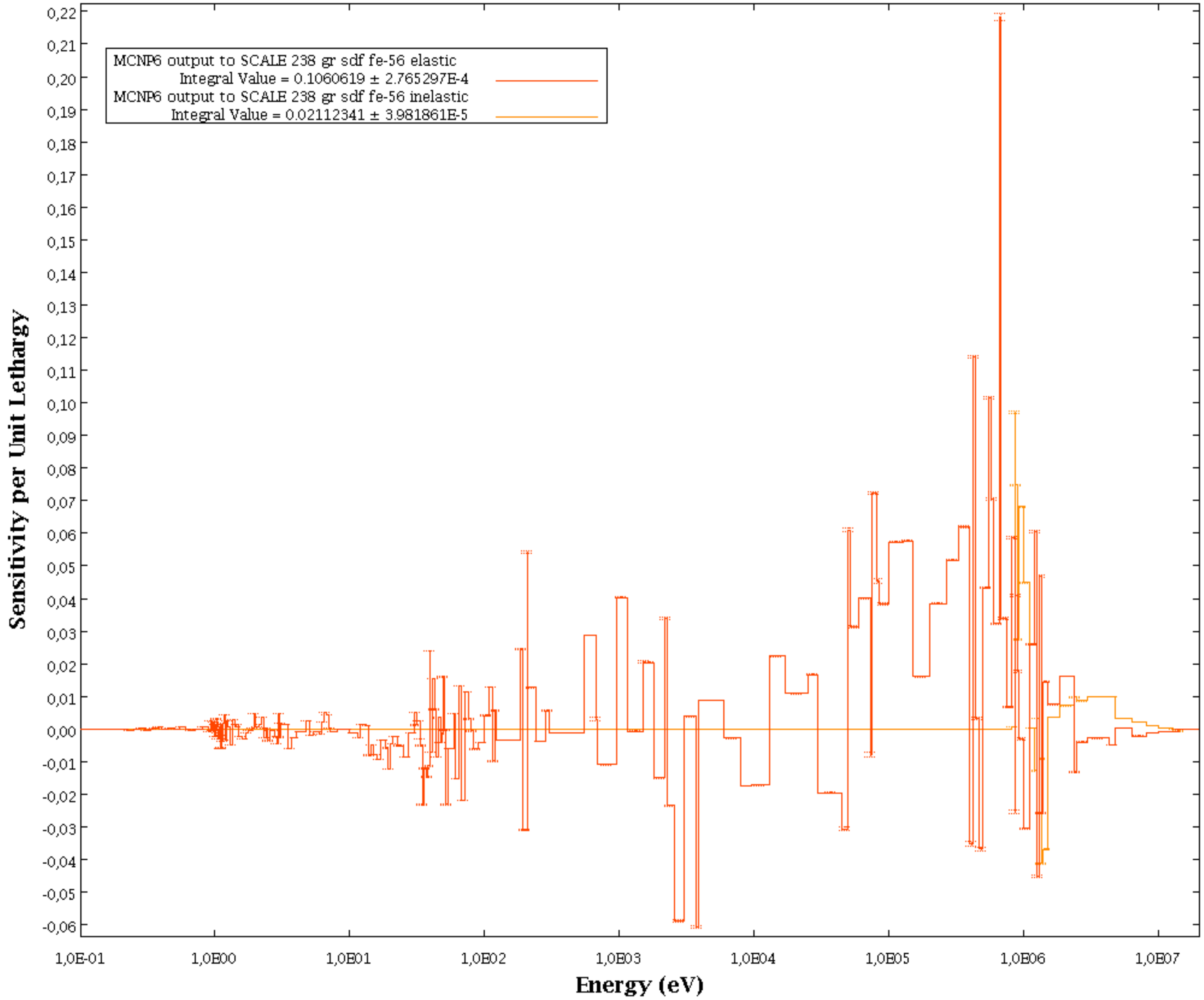
3. K_eff (bench) = 0.9966 ± 0.0026





RZ model

Sensitivity of k_eff to elastic and inelastic calculated with MCNP6



K_eff for HMF and PMF

HMI-001 K_eff=0.9966 ± 0.0026		
B7.1	1.00157(21)	-
U-235 (CIELO)	0.99907(21)	Fe-56 (B7.1)
Fe-56 (CIELO)	0.99759(21)	U-235 (B7.1)
U-235 + Fe-56 (CIELO)	0.99574(22)	With Fe-56 and U-235

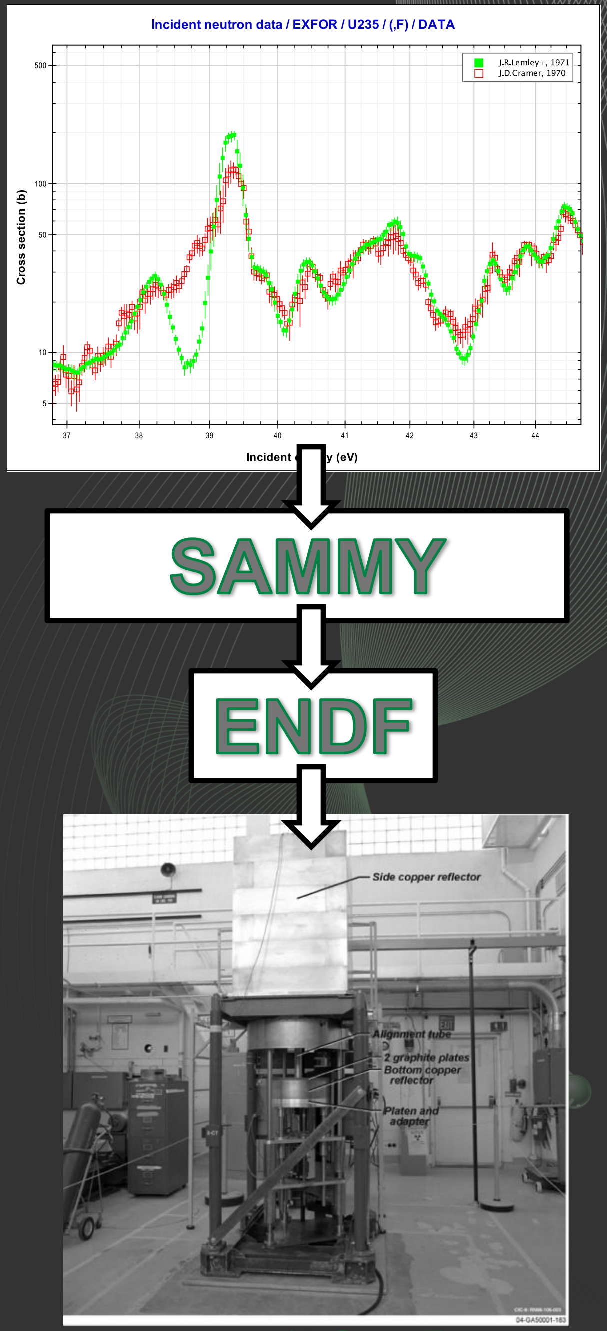
SAMINT

V. Sobes and L. Leal

SAMINT is an auxiliary program designed to allow SAMMY to adjust nuclear data parameters based on integral data

Traditional SAMMY Evaluation

- **Traditionally SAMMY has used differential experimental data ($\sigma(E_i)$ vs E_i) to adjust nuclear data parameters:**
  - **Resonance energies**
  - **Resonance widths**
  - **Number of prompt neutrons per fission**
  - **Etc…**
- **Integral experimental data, such as ICSBEP benchmarks, have remained only a tool validation of completed nuclear data evaluations.**



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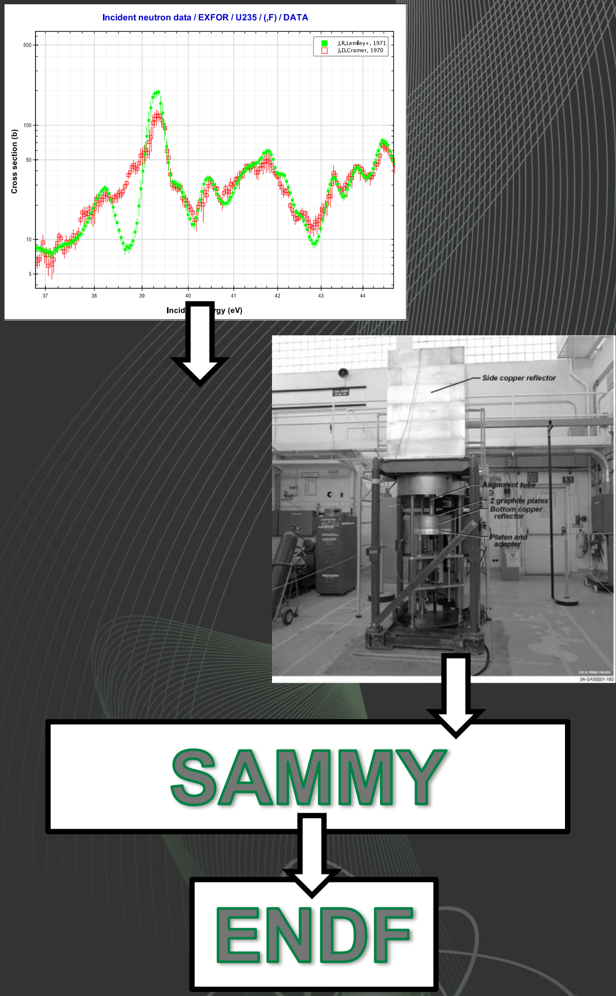
Integral Experiments to Aid Nuclear Data Evaluation

- **SAMINT can be used to extract information from integral benchmarks to aid the nuclear data evaluation process.**
- **Near the end of the evaluation based on differential experimental data, integral data can be used to:**
  - **Resolve remaining ambiguity between differential data sets**
  - **Guide the evaluator to troublesome energy regions**
  - **Inform the evaluator of the most important nuclear data parameters to integral benchmark calculations**
  - **Improve the nuclear data covariance matrix evaluation**



SAMINT Methodology

Generalized Linear Least Squares (GLLS)

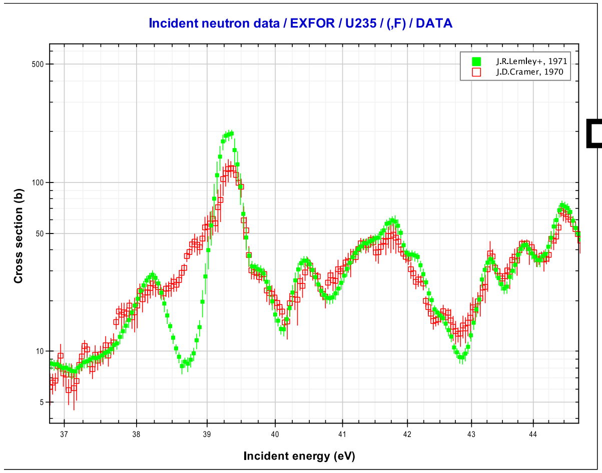
- **SAMMY fits nuclear data parameters to experimental cross-section data utilizing the first derivative of the continuous energy cross section**
  - **$d\sigma(E)/d\Gamma_\lambda$**
- **SAMINT provides SAMMY with the first derivative of the k-eigenvalue**
  - **$dk/d\Gamma_\lambda$**

k-Eigenvalue Sensitivity Analysis

- **Codes such as CE-TSUNAMI and MCNP-6 have the capability to generate k-eigenvalue sensitivity to continuous energy cross sections**
  - **$dk/d\sigma(E)$**
- **SAMINT multiplies the two derivatives**
  - **$dk/d\sigma(E) \times d\sigma(E)/d\Gamma_\lambda = dk/d\Gamma_\lambda$**

Using SAMINT with SAMMY

Differential Experimental Data



Integral Experimental Data

SAMMY

$d\sigma(E)/d\Gamma_\lambda$

SAMINT

$dk/d\sigma(E)$

CE-TSUNAMI or MCNP-6

$dk/d\Gamma_\lambda$

SAMMY

Updated Γ_λ and $\delta\Gamma$

ENDF

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SAMINT Proper Use:

- **SAMINT is not intended to bias the nuclear data towards fitting a certain set of integral experiments**
- **SAMINT should be used to supplement evaluation of differential experimental data**
- **Using the GLLS methodology ensures that the update nuclear data parameters respect the original fit of the differential data**

SAMINT Today and Tomorrow

Current Capabilities

- Adjusting resolved resonance parameters and associated covariance
- Adjusting number of prompt neutrons per fission
- Calculating continuous energy cross sections, K1, eta values (reactor physics), etc to satisfy integral benchmarks
- Works with both CE-TSUNAMI and MCNP-6 k-eigenvalue sensitivities
- Limited to constraints of the linearity assumptions of GLLS

Future Developments

- Near term:
  - Addition of iteration for non-linearity
  - Expansion to the unresolved resonance region
- Long term:
  - Expansion to high energy region
  - Adjustment of angular distribution data and associated covariance
  - Support for future TSUNAMI generalized sensitivity theory developments

K_eff for HMF and PMF

K_eff			
benchmark	**ORNL5**	**benchmark**	**C/E**
HMF013	0.99935(9)	0.9990(15)	1.00035
HMF021	1.00005 (10)	1.0000(24)	1.00005
PMF025	1.00001 (9)	1.0000(20)	1.00001
PMF032	1.00017(9)	1.0000(20)	1.00017

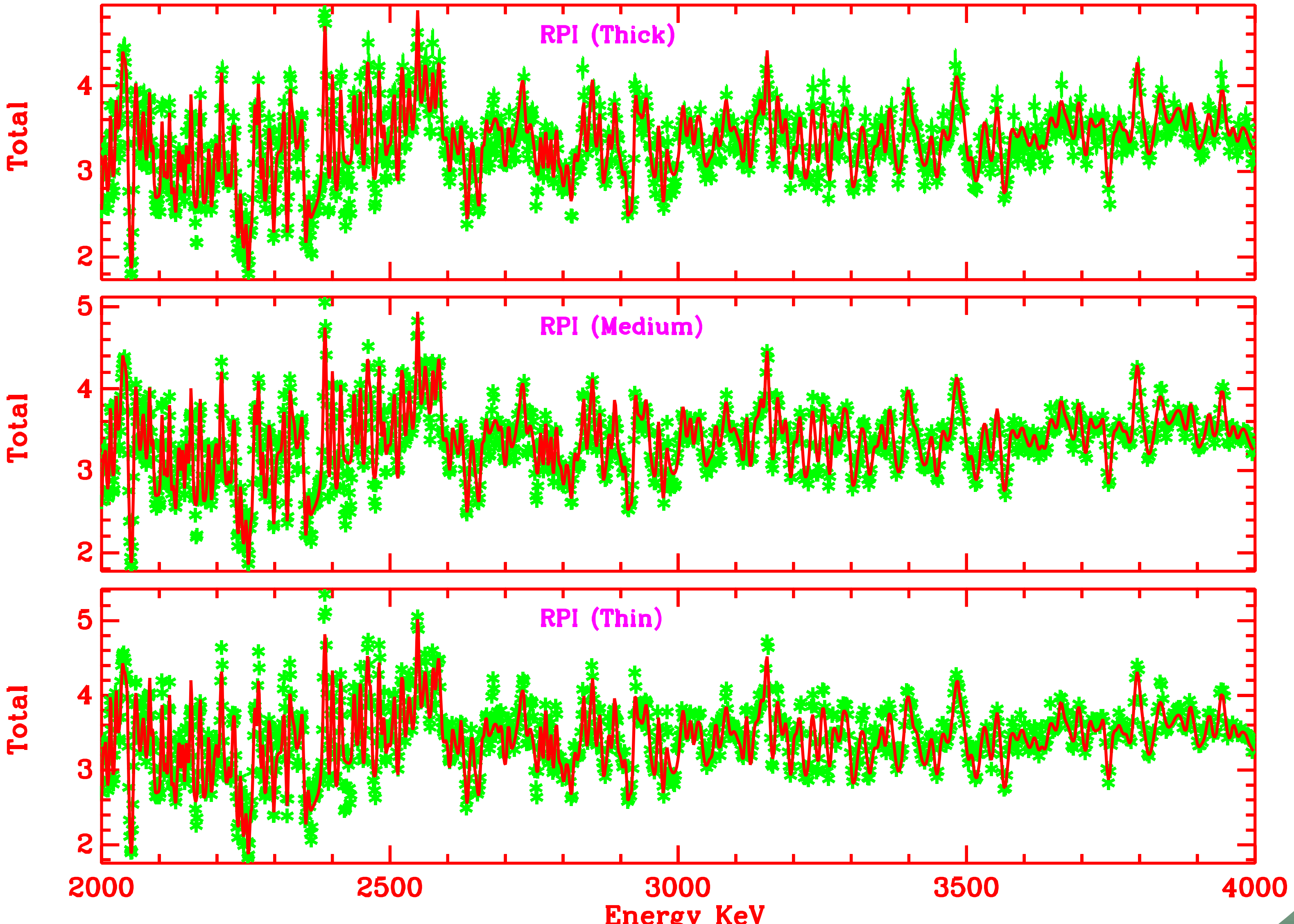
K_eff for HMF and PMF using SAMINT

C/E			
benchmark	**ORNL4**	**ORNL5**	**ENDF/BVII.1**
HMF013	0.99850	1.00035	0.99841
HMF021	0.99633	1.00005	0.99720
PMF025	0.99892	1.00001	0.99890
PMF032	0.99792	1.00017	0.99877

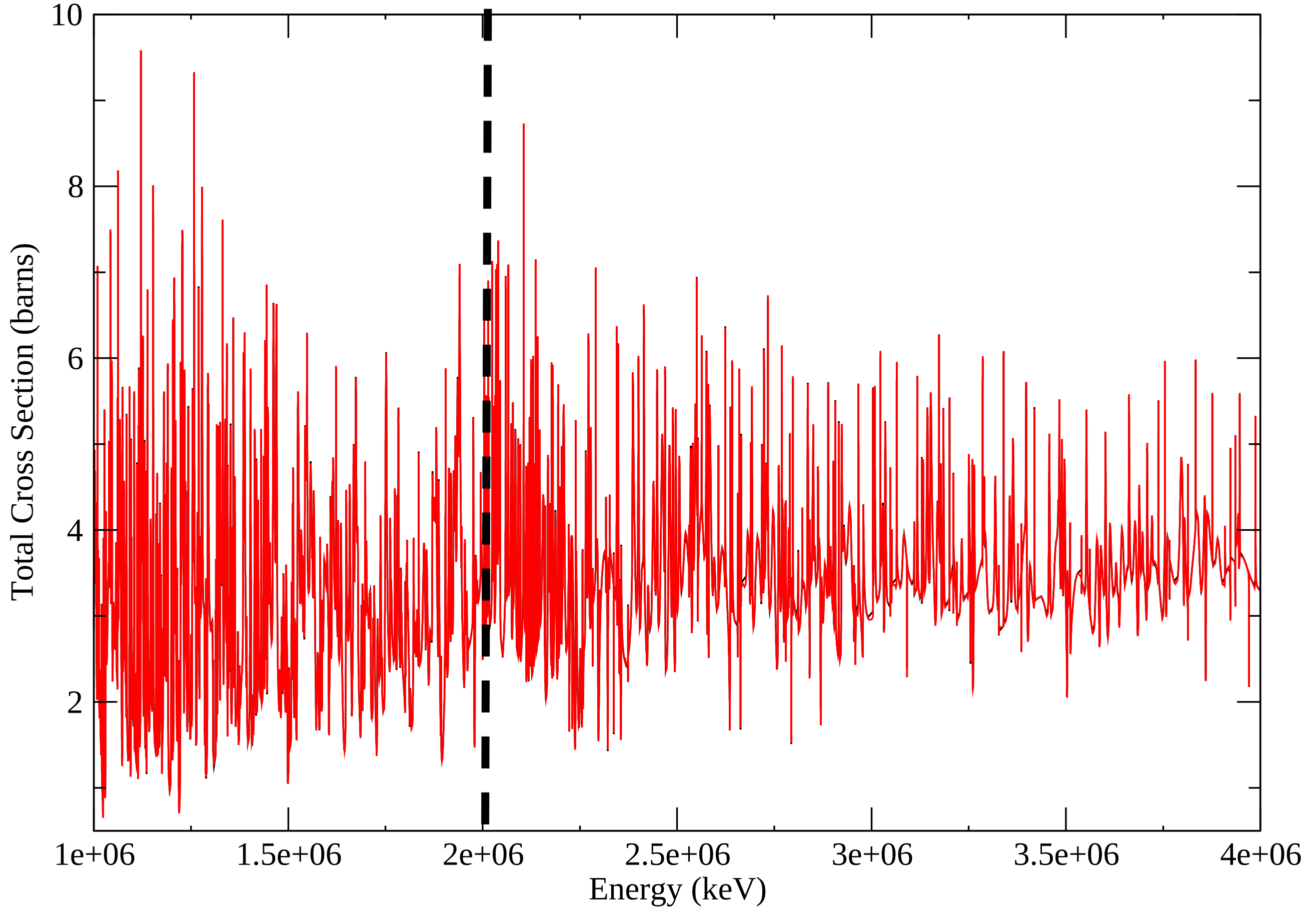
Unresolved Resonance in the Energy Range 2-4 MeV

- High-resolution experimental data allows the extension of the resonance region to higher energy;
- Any R-matrix derived formalism can be used as opposed to the use of the SLBW;
- Use of the RML option is a perfect fit;
- Angular data can represented with the resonance parameters;
- Combination of differential and integral data in the SAMMY (SAMINT) can be done;

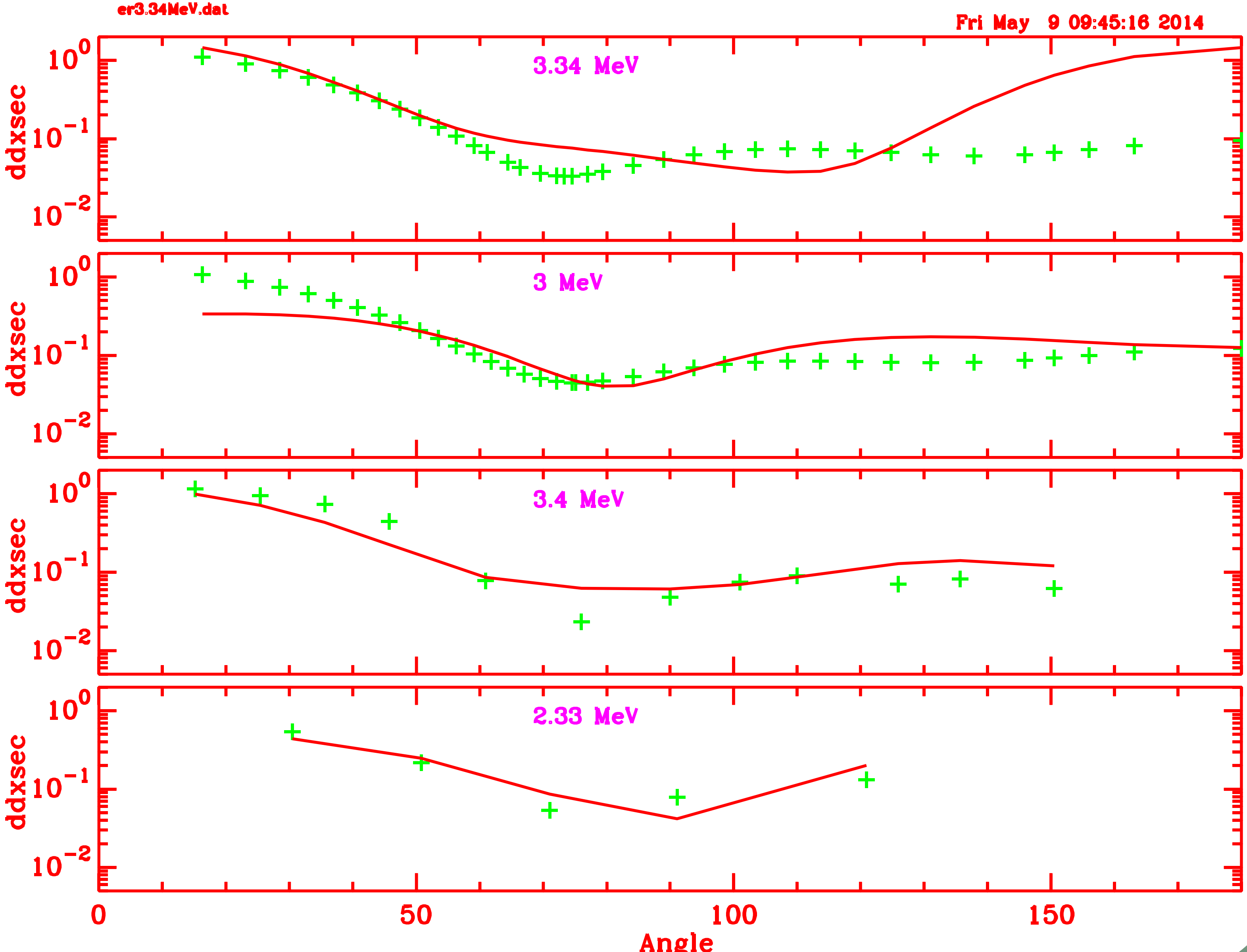
SAMMY fit to the RPI data in the energy range 2-4 MeV



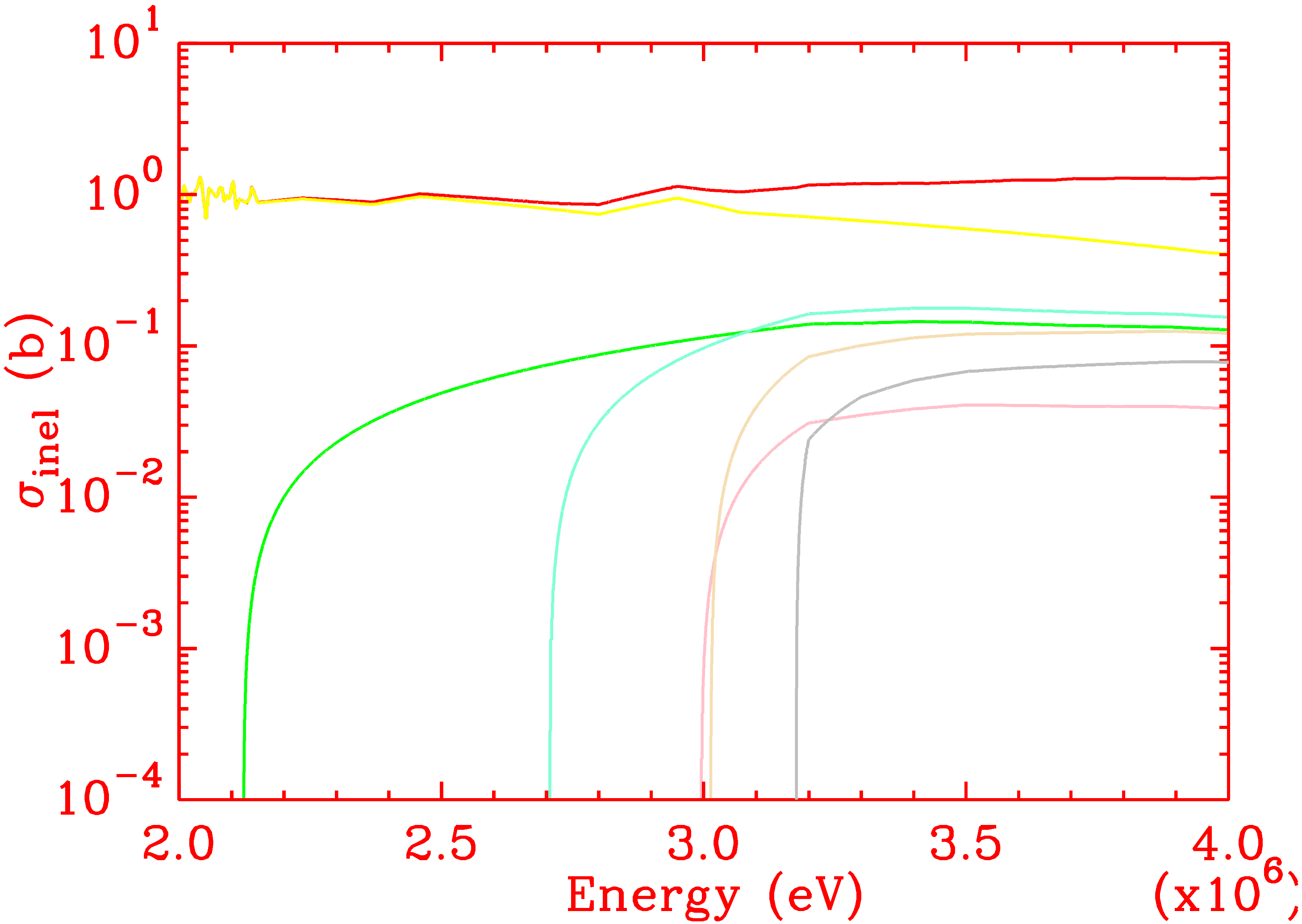
Total cross section processed with NJOY. Two disjoint resonance parameters set



SAMMY fit to angular in the energy range 2-4 MeV



Inelastic levels in the energy range 2-4 MeV



CONCLUSIONS

- SAMMY fit of the experimental data up to 2 MeV have been performed;
- The new preliminary CIELO Fe-56 library seems to perform well;
- NJOY, AMPX and PREPRO able to process the LRF=7, angular data;
- NJOY (ERROR), AMPX(PUFF) processed the compact formalism;
- Use of sensitivity data for benchmark processed with MCNP6/CE_TSUNAMI can be used to adjust the resonance parameters without compromising the differential data;
- Pseudo-resonance parameters in the range 2-4 MeV can be an option for better calculation of the self-shielding effects;