Evaluation for ^{16}O from Thermal to 6 MeV

IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Faire avancer la sûreté nucléaire

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WPEC
9-13 May 2016,
OECD Headquarters Conference Centre,
Paris, France.

IRSN
Date 1 à 5 Mai 2016
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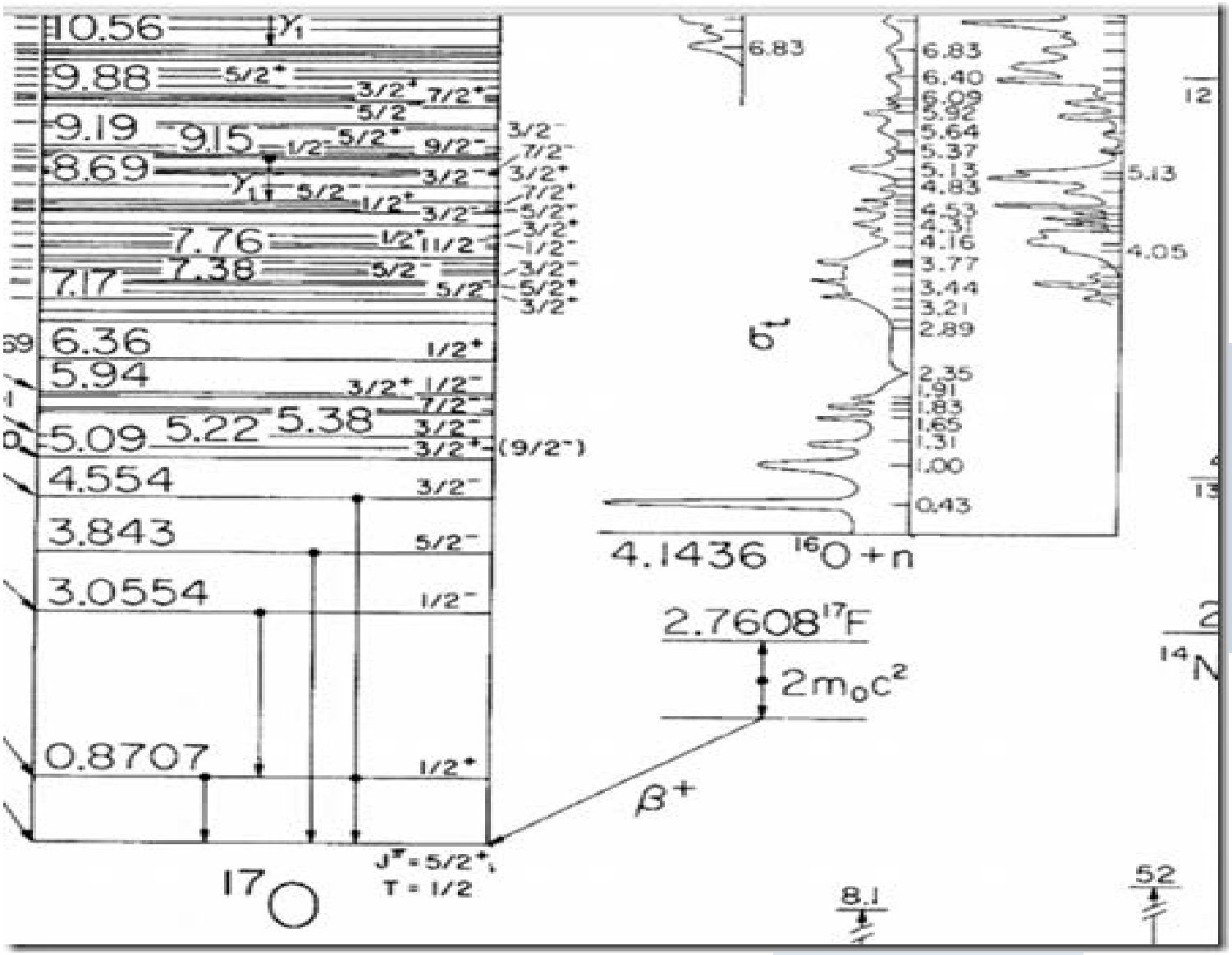
Outline

- SAMMY code and the ENDF LRF=7 option for resonance parameter representation;
- Experimental data base;
- (n, total), (n, n), (n, γ), scattering, (n,α), angular distributions are calculated from resonance parameters;
- Resonance parameter covariance description;
- Updated thermal scattering cross section according to suggested value of 3.765 b at 0K;
- Experimental (n,α) cross section can differ by as much as 30 %;
- Concluding Remarks;

Tool For Data Evaluation: Computer Code SAMMY Used for Resonance Evaluation

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

Bound Energy Levels for ^{16}O



Bound Energy Levels for ^{16}O

S* - separation energy
E* - compound nucleus energy
COM to Lab conversion – (A + 1) / A
E – resonance energy for ^{16}O + n
E = {(A +1) / A} * {E* - S*}

S* = 4.1436 MeV
A = 16

a) For E* = 0.8707 MeV
E={17/16}*{0.8707 - 4.1436}
E = -3.47746 MeV

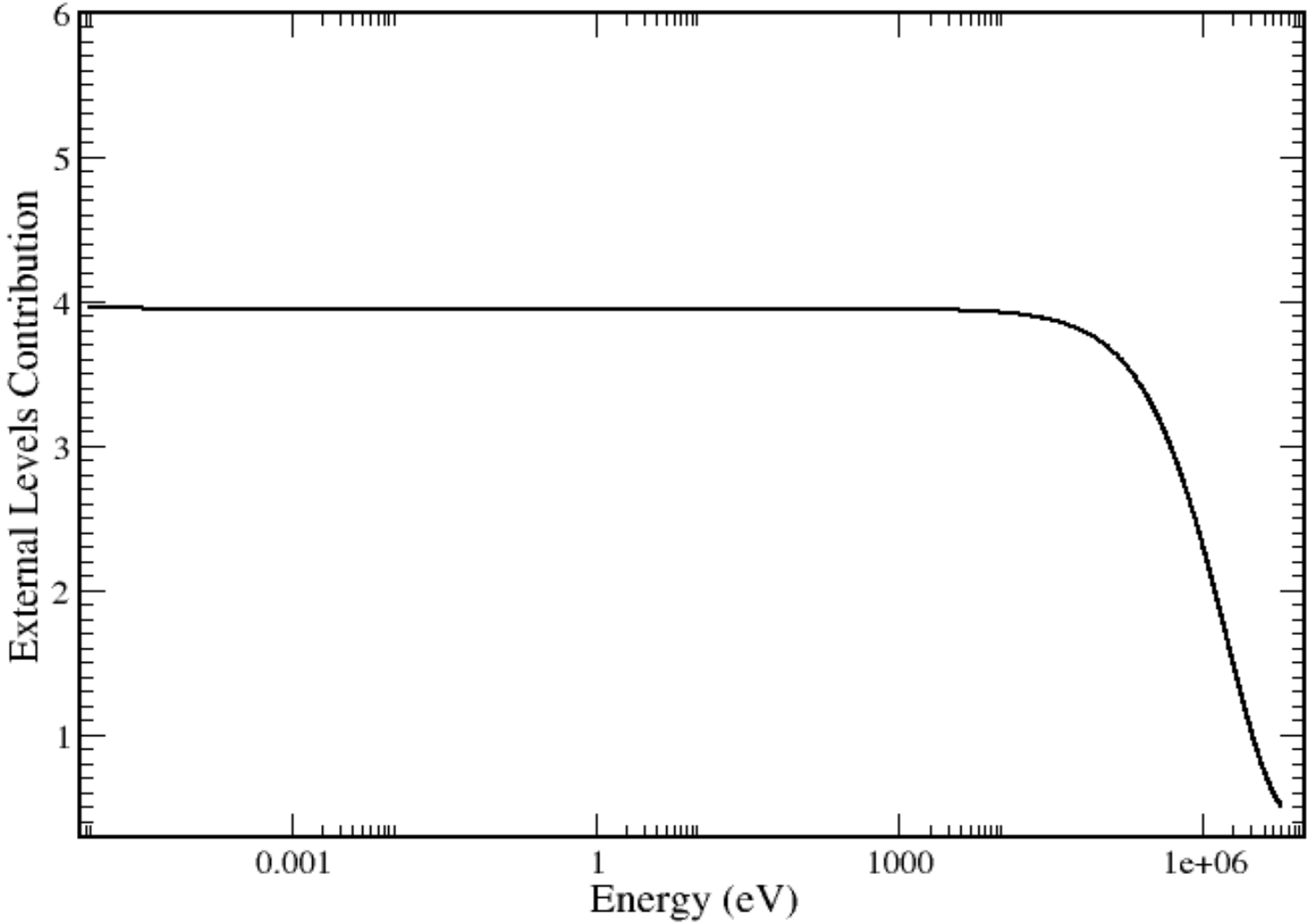
b) For E* = 3.0554 MeV
E = {17/16}*{3.0554 - 4.1436}
E = -1.1562 MeV

c) For E* = 3.843 MeV
E = {17/16}*{3.843 - 4.1436}
E = -0.3194 MeV

SAMMY resonance parameters: Negative Energy Levels

E_r	Γ_γ	Γ_n	Γ_p	Spin Group
-3477456.00	184.305000	3923179.+3	0.0000	0 0 0 0 1
-1157275.00	261.434100	13305730.0	0.0000	0 0 0 0 3
-319387.500	297.301600	92559.3200	0.0000	0 0 0 0 6
434103.9867	2700.00000	44216370.0	0.0000	0 0 0 0 3
999687.6127	250.000000	95884120.0	0.0000	0 0 0 0 4

Bound Energy Levels for ^{16}O



Experimental data Base

Experimental Data	Flight-Path (meters)	Energy Range (MeV)	Data Reference	Year
Capture Cross Section	-	Thermal	Firestone	2015
Coherent Scattering Length	-	-	Sears	1992
Total Cross Section	79.46	2.0 – 6.3	ORELA (Larson)	1980
Total Cross Section	249.75	2.0 – 6.3	RPI (Danon) [14]	2015
Total Cross Section	41.0 and 47.0	0.6 – 4.3	ORNL Van de Graaff (Fowler, Johnson, and Feezel)	1973
Total Cross Section	189.25	3.14 – 6.3	KFK cyclotron (Cierjacks)	1980
(n,alpha) extracted from (alpha,n)	-	3.2 – 6.3	ORNL Van de Graaff (Bair and Hass)	1973
(n,alpha) extracted from (alpha,n)	-	3.0 – 6.3	Tandem Accelerator Universtät Bochum (Harissopulos)	2005

Thermal Cross Section

Coherent Scattering Length includes potential and resonance parts defined as

$$a_{coh} = a_{pot} + a_{res}$$ where

$$a_{pot} = \lim_{E \to 0} \left(\frac{\sigma_s}{4\pi} \right)^{1/2}$$ For T = 0 K

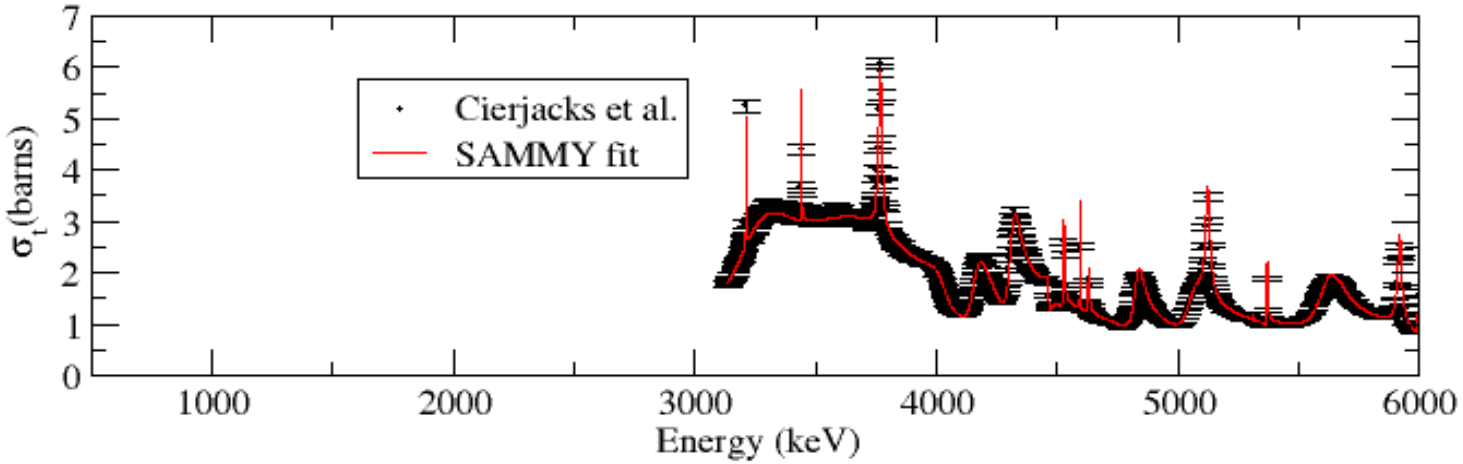
For s-wave based on the SLBW formalism

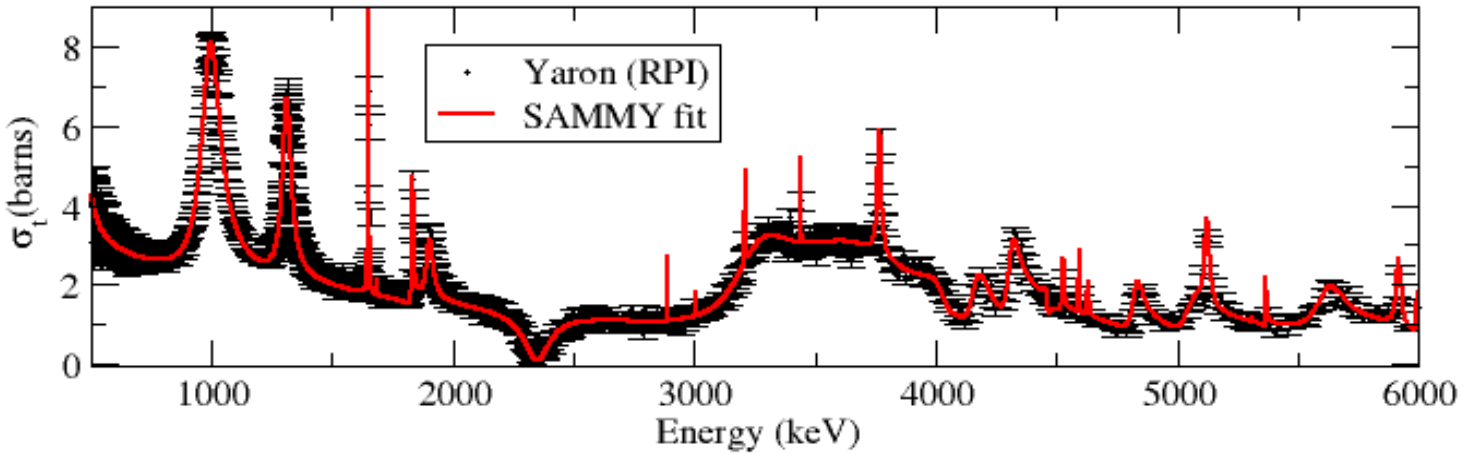
$$a_{res} = \sum_r \frac{\Gamma_n^r}{2k_r \left[(E - E_r) + \frac{i\Gamma}{2} \right]}$$

Results calculated with NJOY

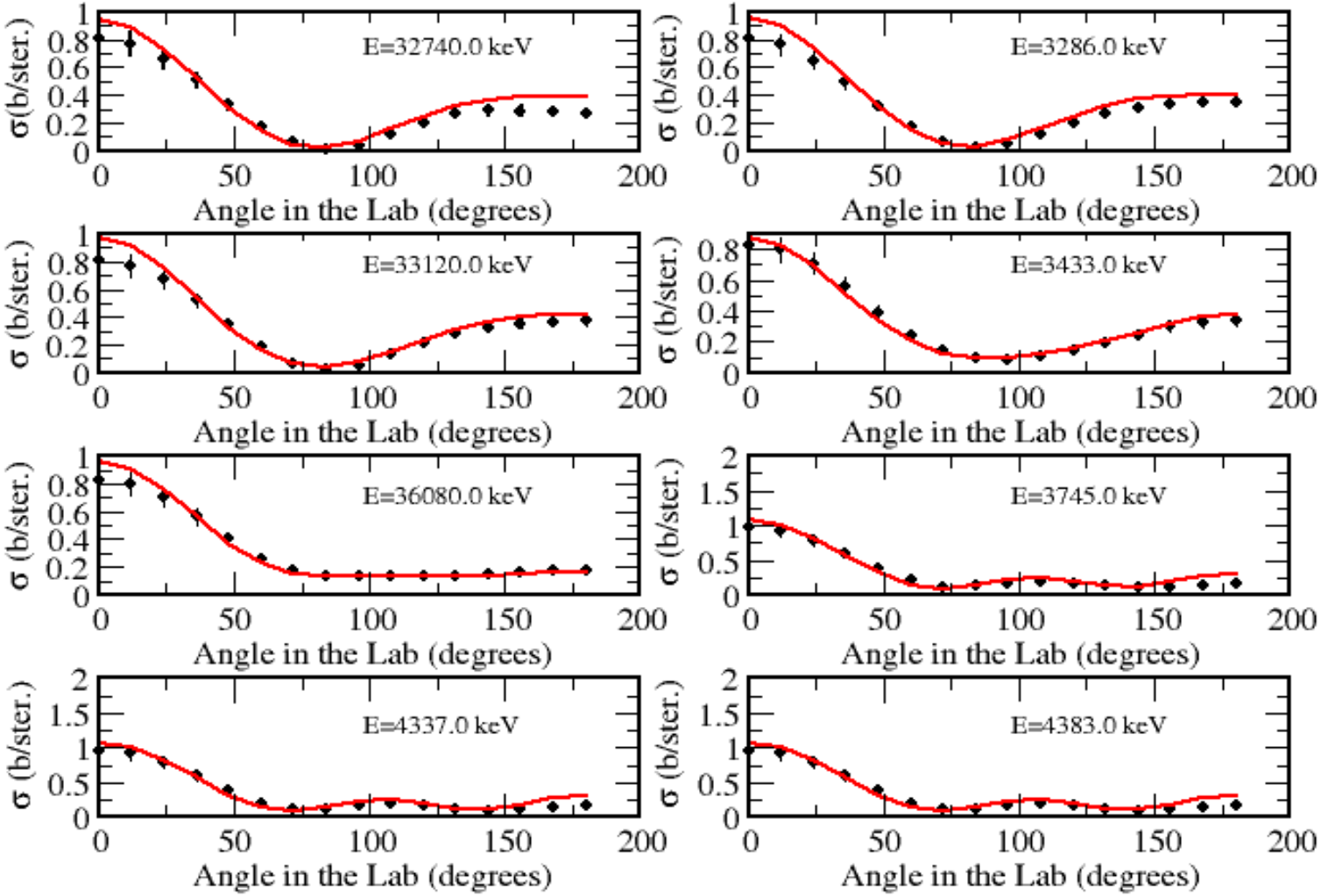
Quantity	IRSN1 (barns) (T=0K)	IRSN1 (barns) (T=293.6K)	Mughabghab (barns)
σ_t	3.7654	3.8841	
σ_γ	1.7153×10^{-4}	1.6701×10^{-4}	$(1.9 +/- 0.19) \times 10^{-4}$
σ_s	3.7652	3.8839	3.761 ± 0.006
R’	4.15 fm		4.8 ± 0.1 fm
a_{coh}	5.805 fm		5.805 ± 0.005 fm
I_γ	-	3.0925×10^{-4}	$(2.7 \pm 0.3) \times 10^{-4}$

Total cross section measurements.
SAMMY comparison including resolution effects



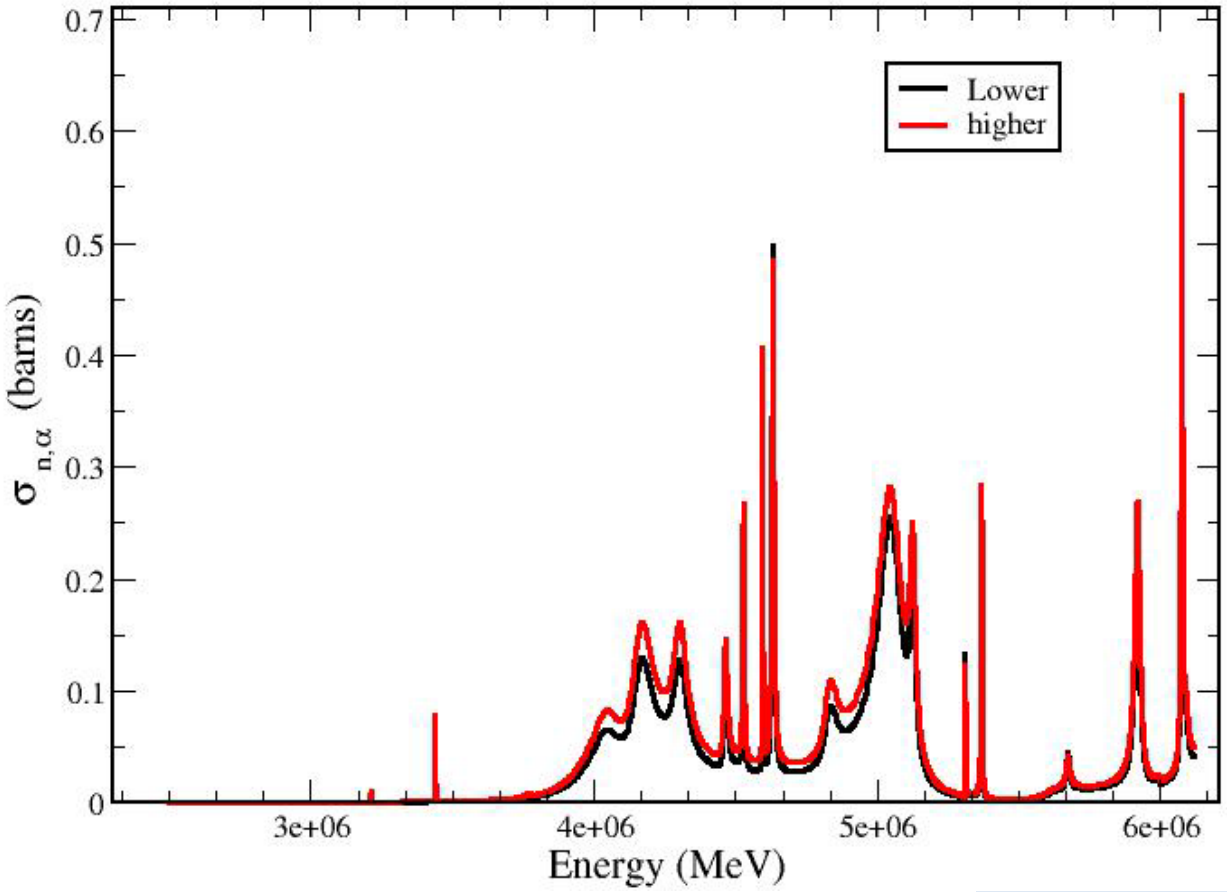


SAMMY fits for the ^{16}O differential elastic cross section of Lister and Savers

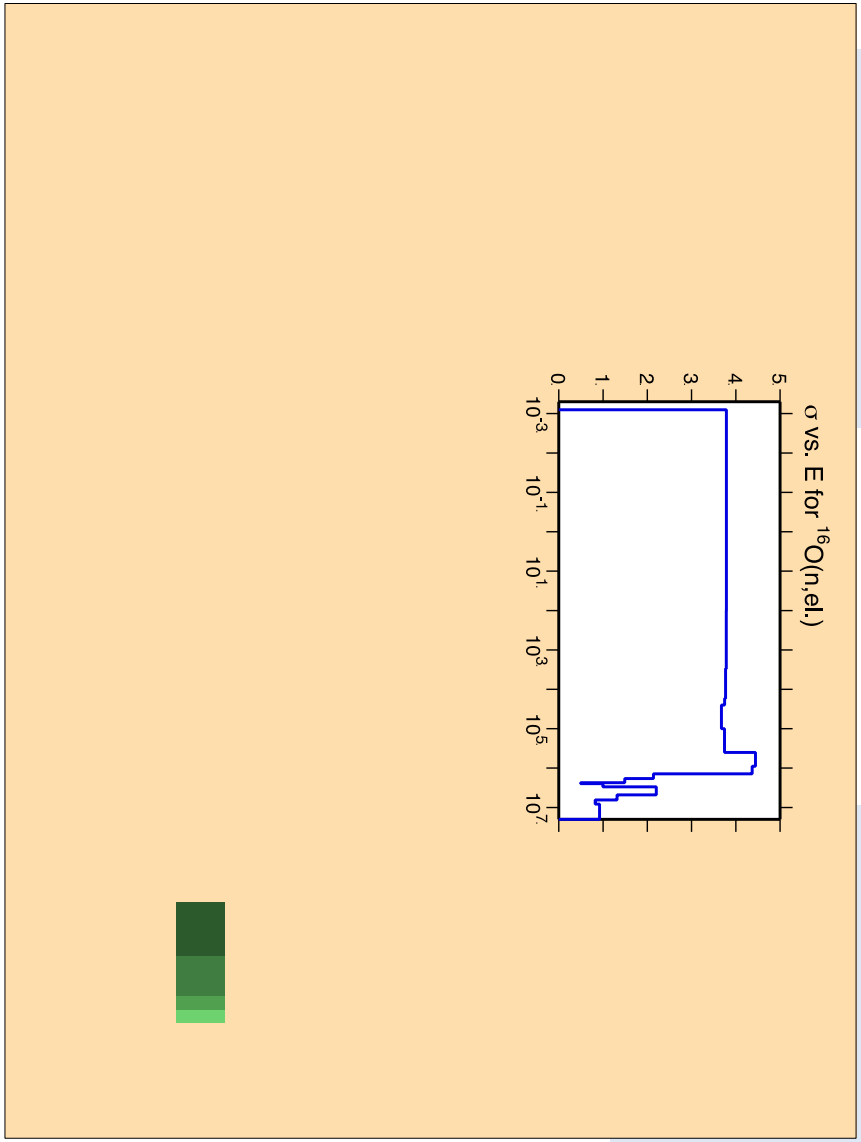


Issues with the experimental (n,α) cros-section

^{16}O(n, a) data (Giorginis, et al., IRMM) and ^{13}C(a, n) data (Harissopulos, et al.) give about 30% lower ^{16}O (n, a) cross section values than the Bair-Haas



RRP Covariance for the Scattering Cross Section



Impact on Benchmark Results

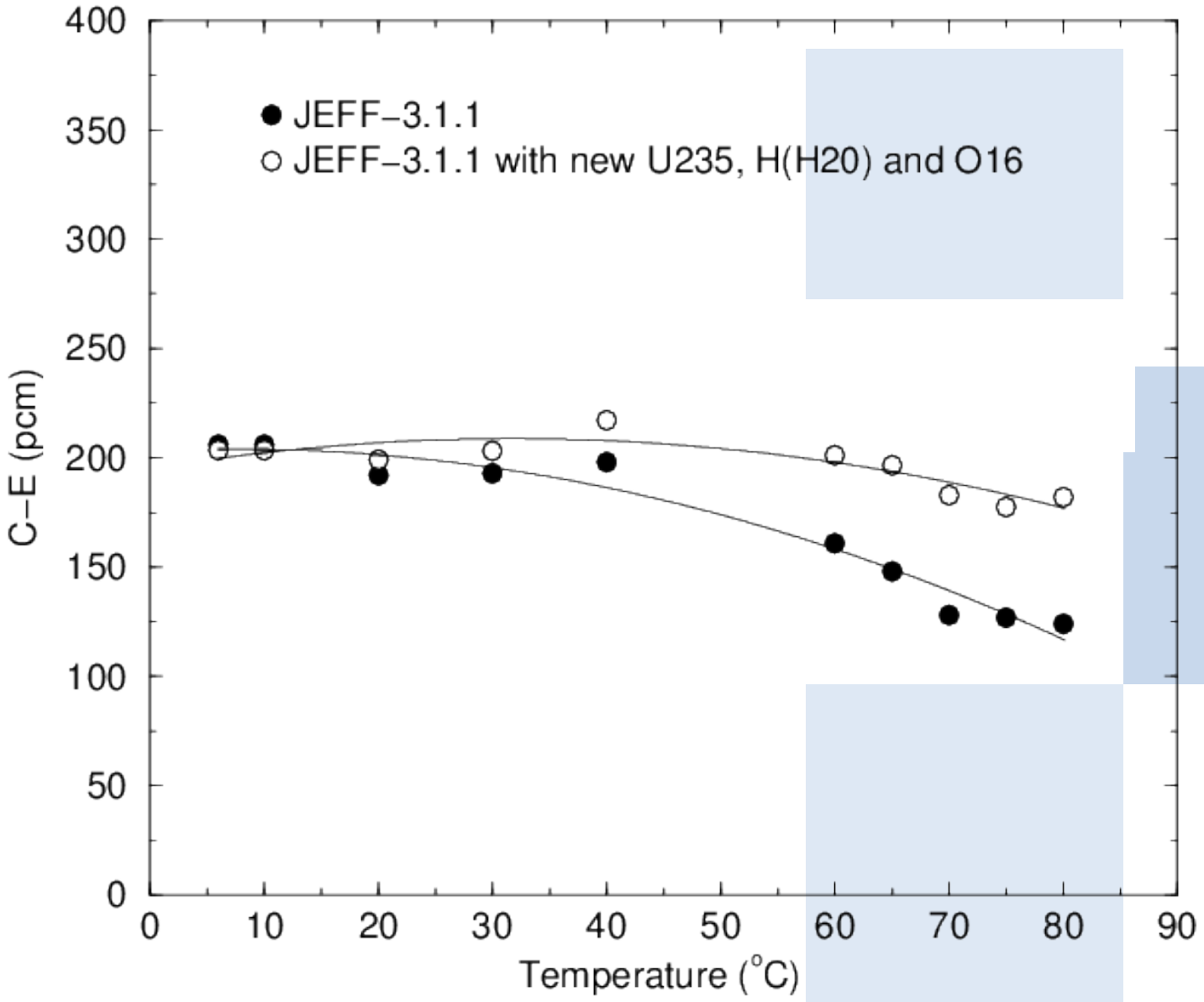
Three low-enriched ^{235}U and heavy-water moderated benchmark systems:

- **Two from the ICSBEP: LEU-MET-THERM-015 cases 15 and 16**
- **One from the IRPhE: ZED-2**

	A	B	C
Benchmark	**ENDF/B-VII.1**	**LOW**	**HIGH**
LEU-MET-THERM-015-15	**1.00533 ± 0.00052**	**1.00351 ± 0.00050**	**1.00311 ± 0.00052**
LEU-MET-THERM-015-16	**1.00549 ± 0.00052**	**1.00344 ± 0.00052**	**1.00242 ± 0.00052**
ZED-2	**0.99866 ± 0.00018**	**0.99833 ± 0.00019**	**0.99772 ± 0.00019**

*Calculations performed with MCNP

Doppler Reactivity Coefficient



Concluding Remarks

- ✓Good fit of experimental total cross section and angular data obtained with the SAMMY code;
- ✓New updated thermal scattering cross-section value lowers k_{eff} of about ~200 pcm;
- ✓Benchmark results seem to favor higher value of the (n,α) cross section;
- ✓Covariance data reproduces reasonably well the experimental data uncertainty;

Evaluation of ^{56}Fe from Thermal to 2 MeV

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^{56}Fe Evaluation Features

- New high resolution transmission measurements done at the RPI extending the resonance region up to 5 MeV;
- New inelastic cross-section measurements done at IRMM/GELINA;
- New RPI angular scattering data (presented in this meeting);
- Use the SAMMY/RML feature to include inelastic channel in the R-matrix analysis and evaluation;
- Elastic and Inelastic angular data derived from resonance parameters

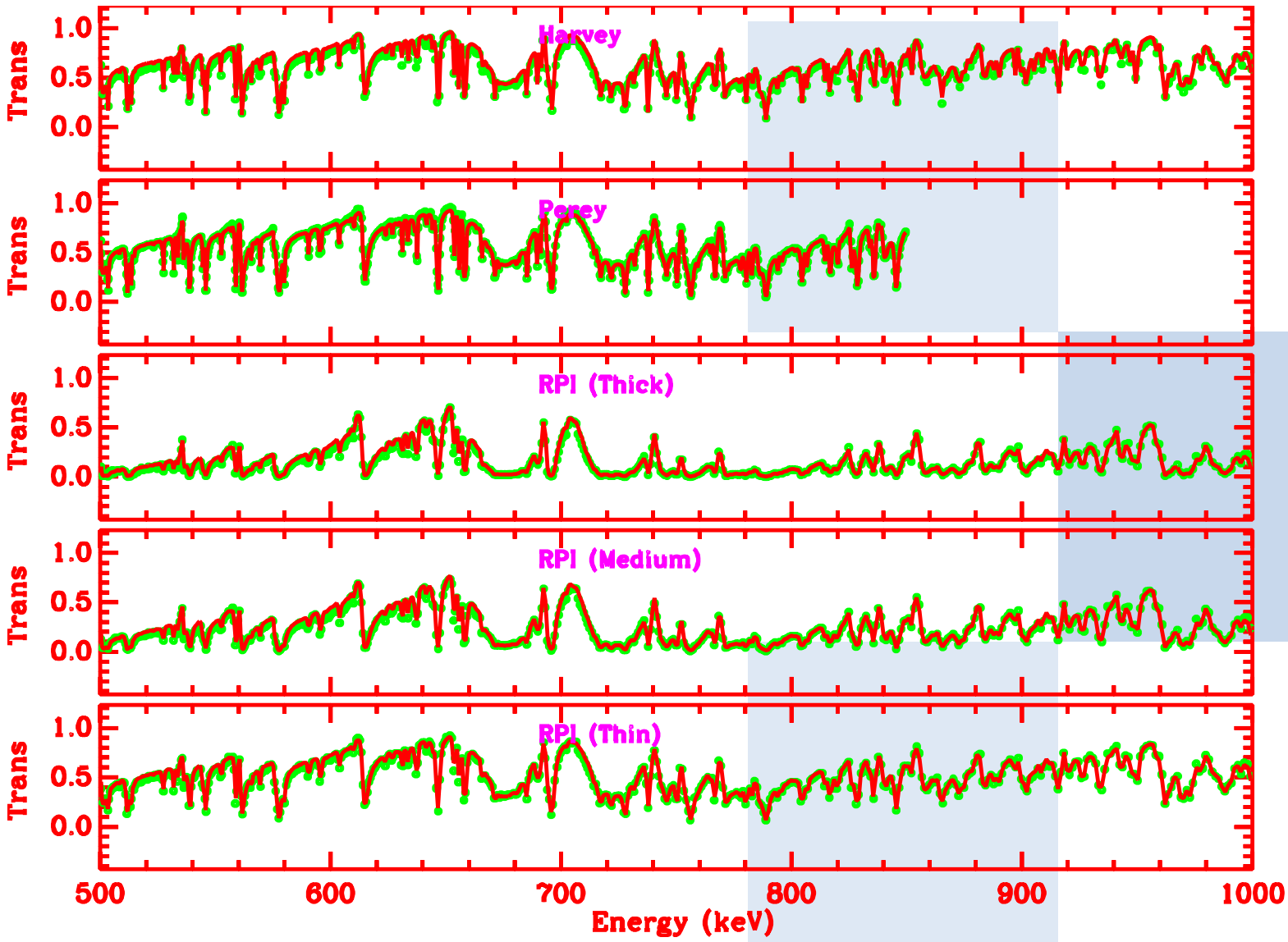
Experimental Data

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
Danon, Rapp et al. (2012) (three thicknesses)	500 keV – 2 MeV	RPI	249.740	Transmission
Danon et al. (2016) (enriched and natural)	100 keV – 2 MeV	RPI	45.277	Capture
Danon, Daskalakis et al. (2012)	500 keV – 2 MeV	RPI	30.07	Scattering (presentation in the workshop)
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

Experimental Data

Reference	Energy Range	Facility	TOF (meters)	Measurement
Bertold et al (natural) (1994)	700 keV – 2 MeV	GELINA	387.739	Total
Cornelis et al (enriched) (1982)	200 keV – 2 MeV	GELINA	387.713	Total

Comparison of SAMMY Fits to the Data



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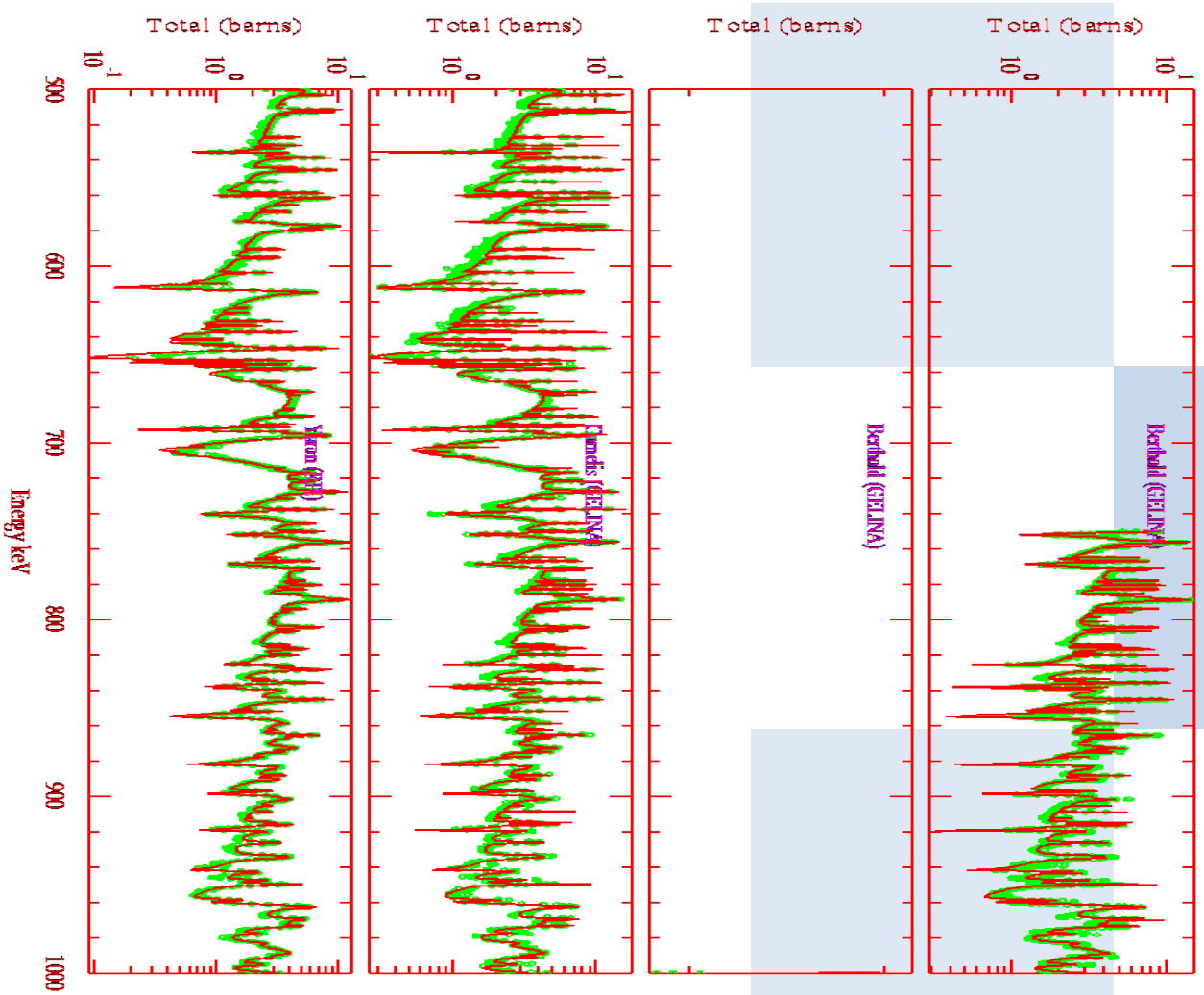

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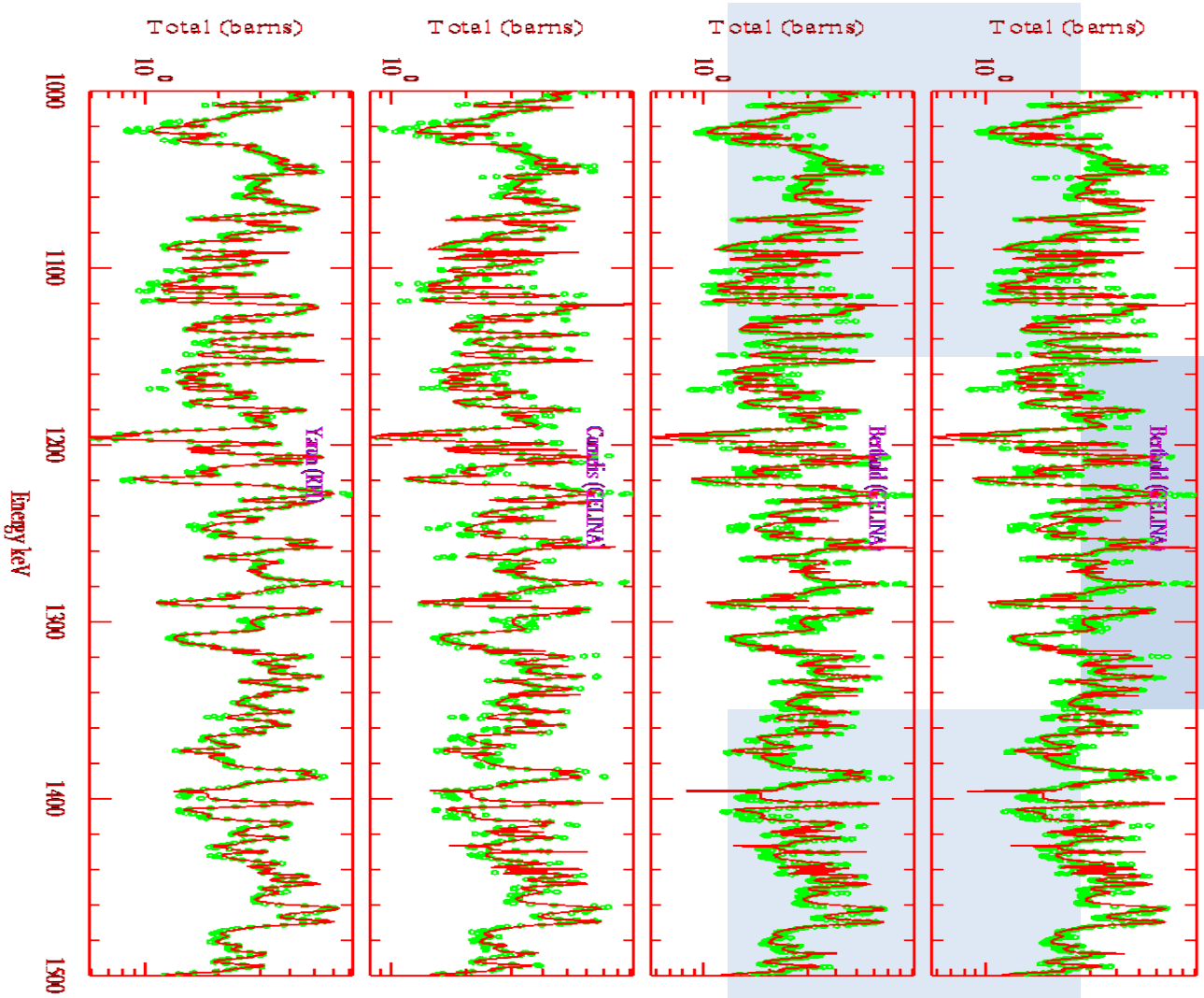

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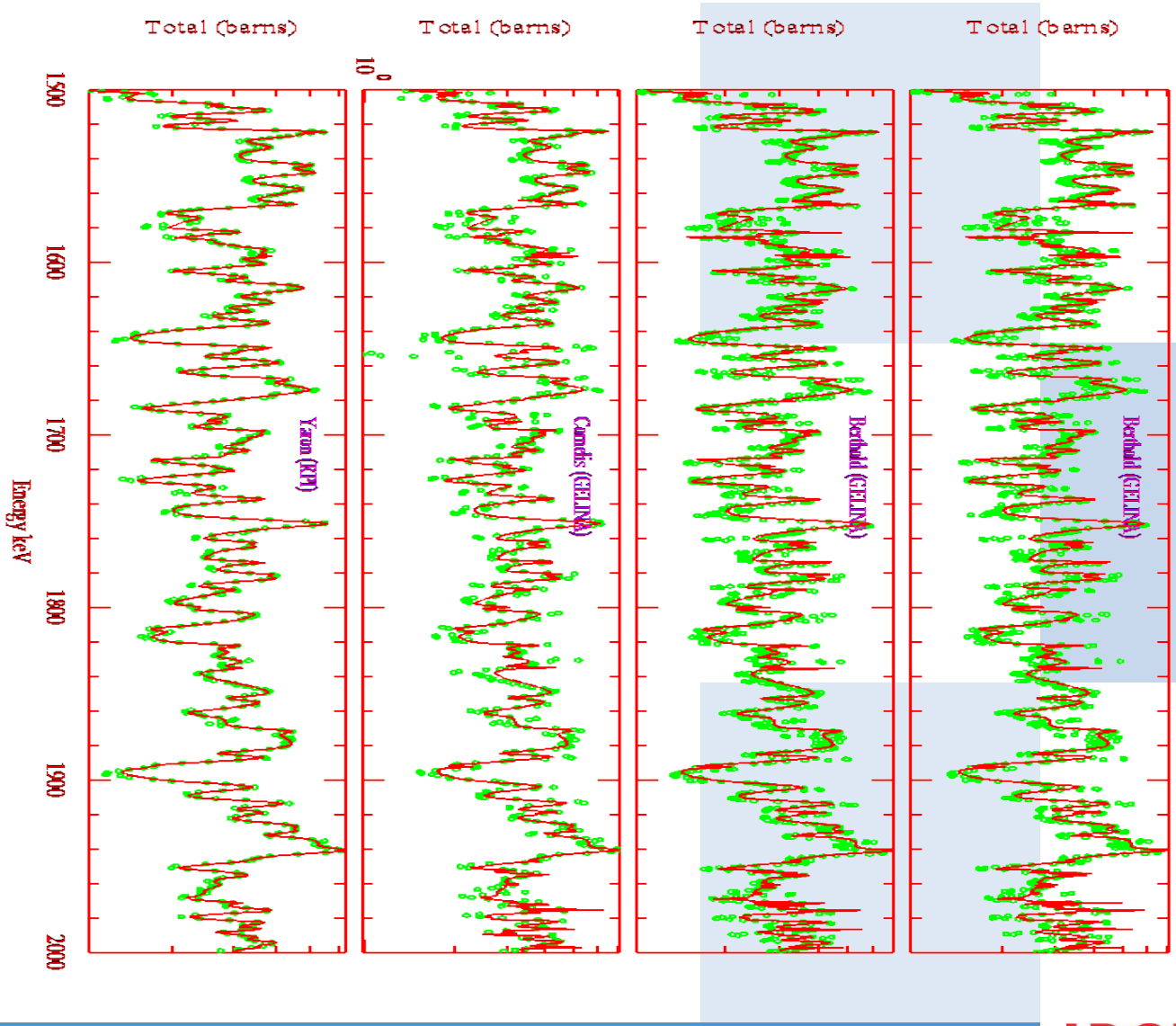
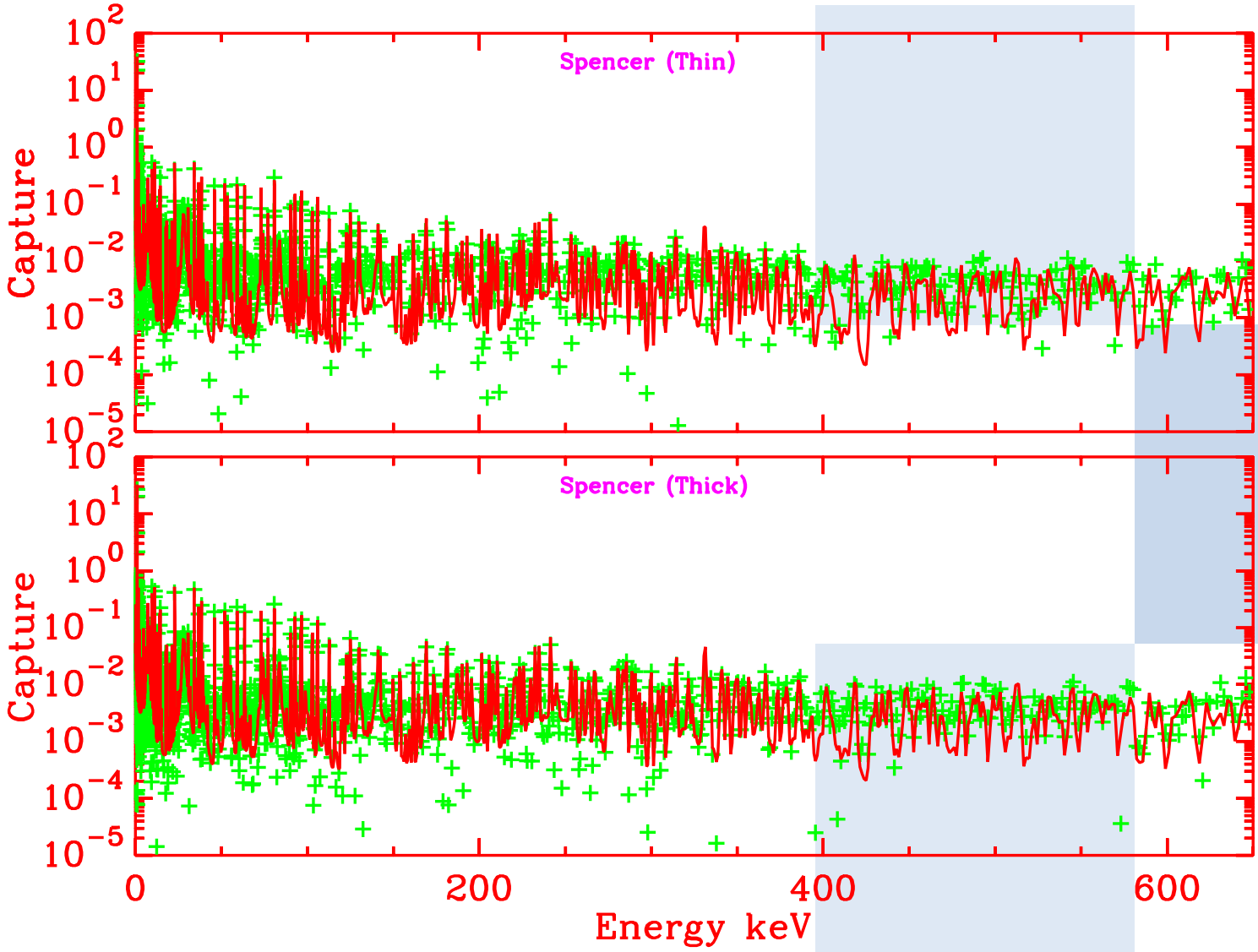
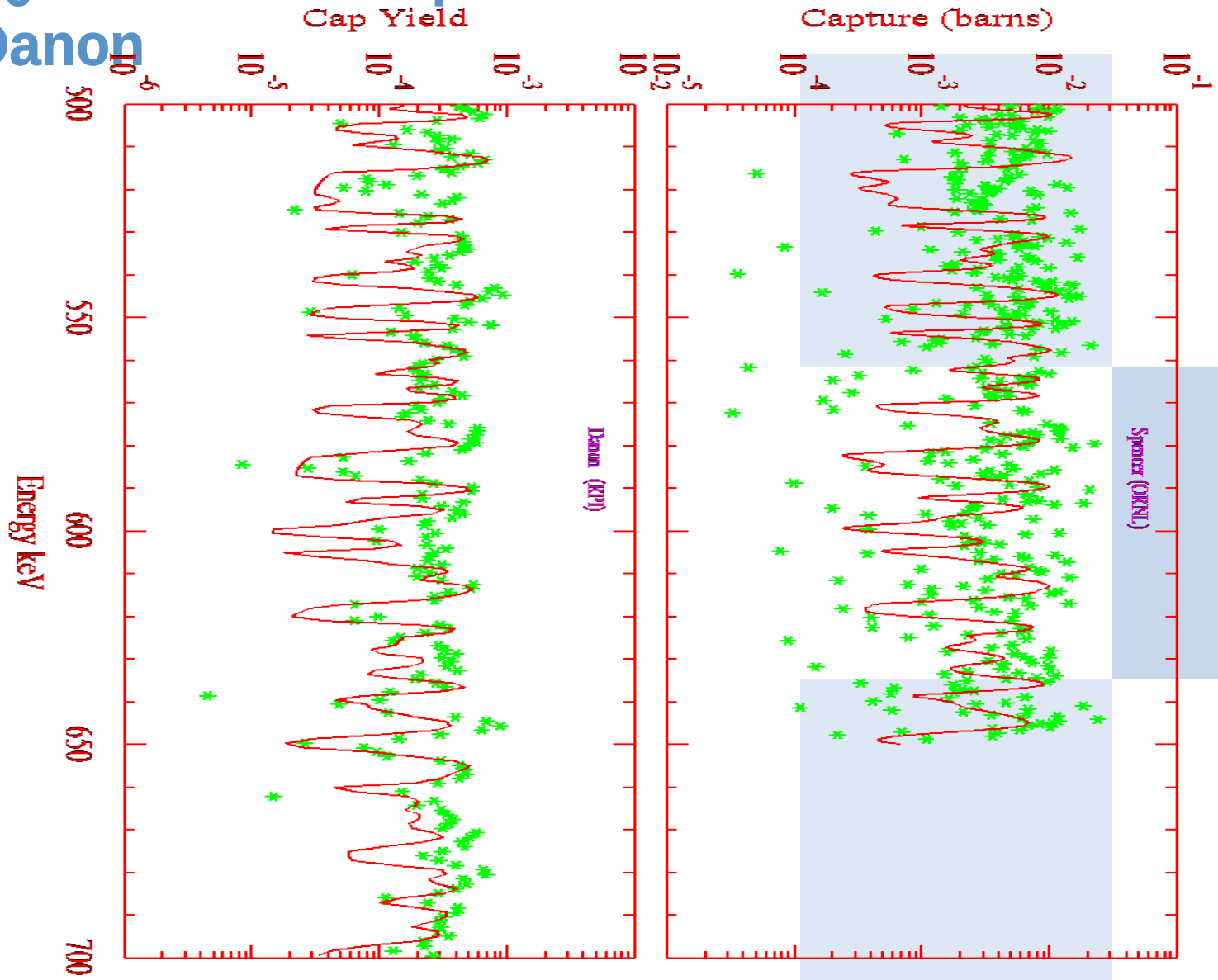


Fitting of the ^{56}Fe capture cross-section data of Spencer



Fitting of the ^{56}Fe capture cross-section data of Spencer and Danon



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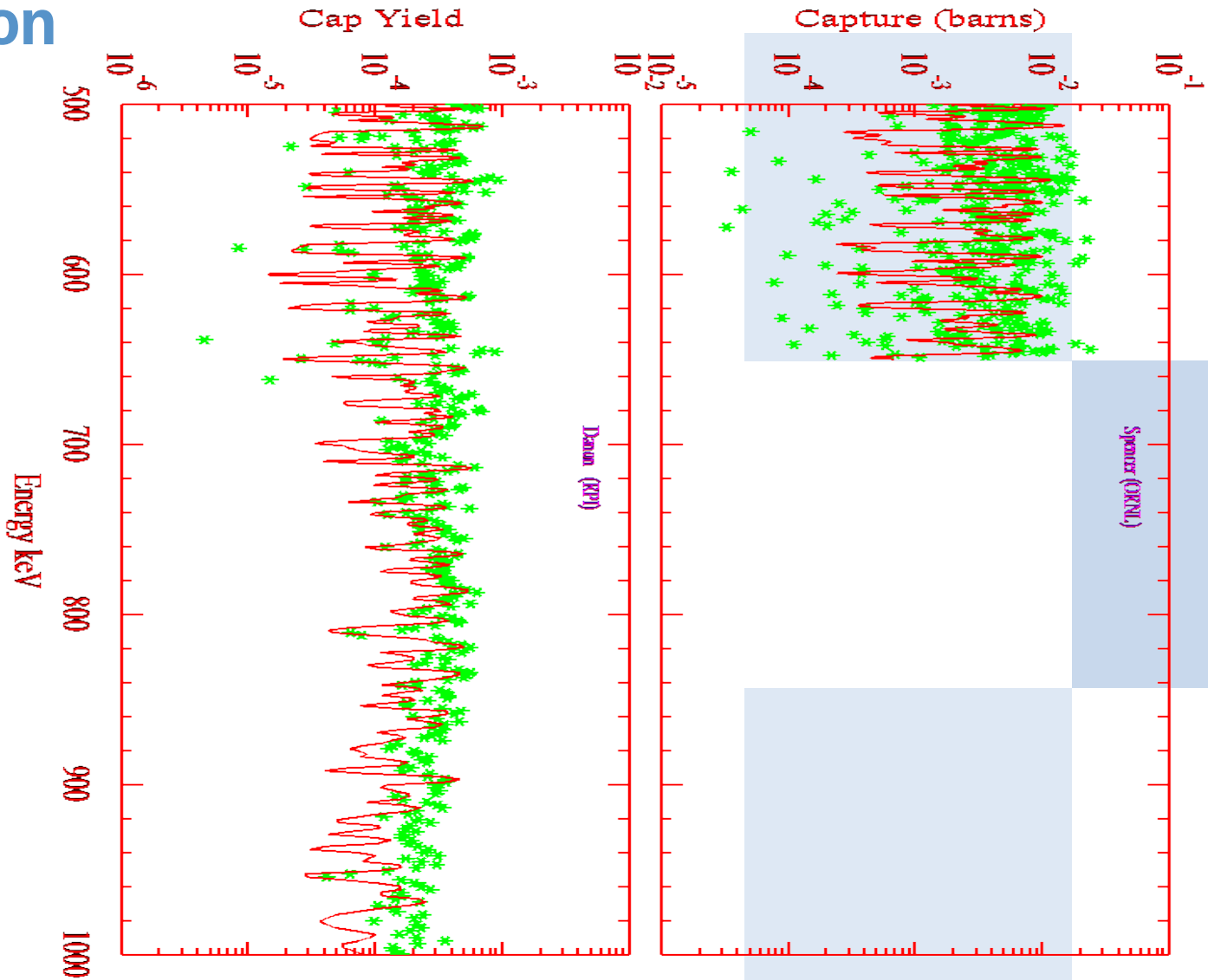
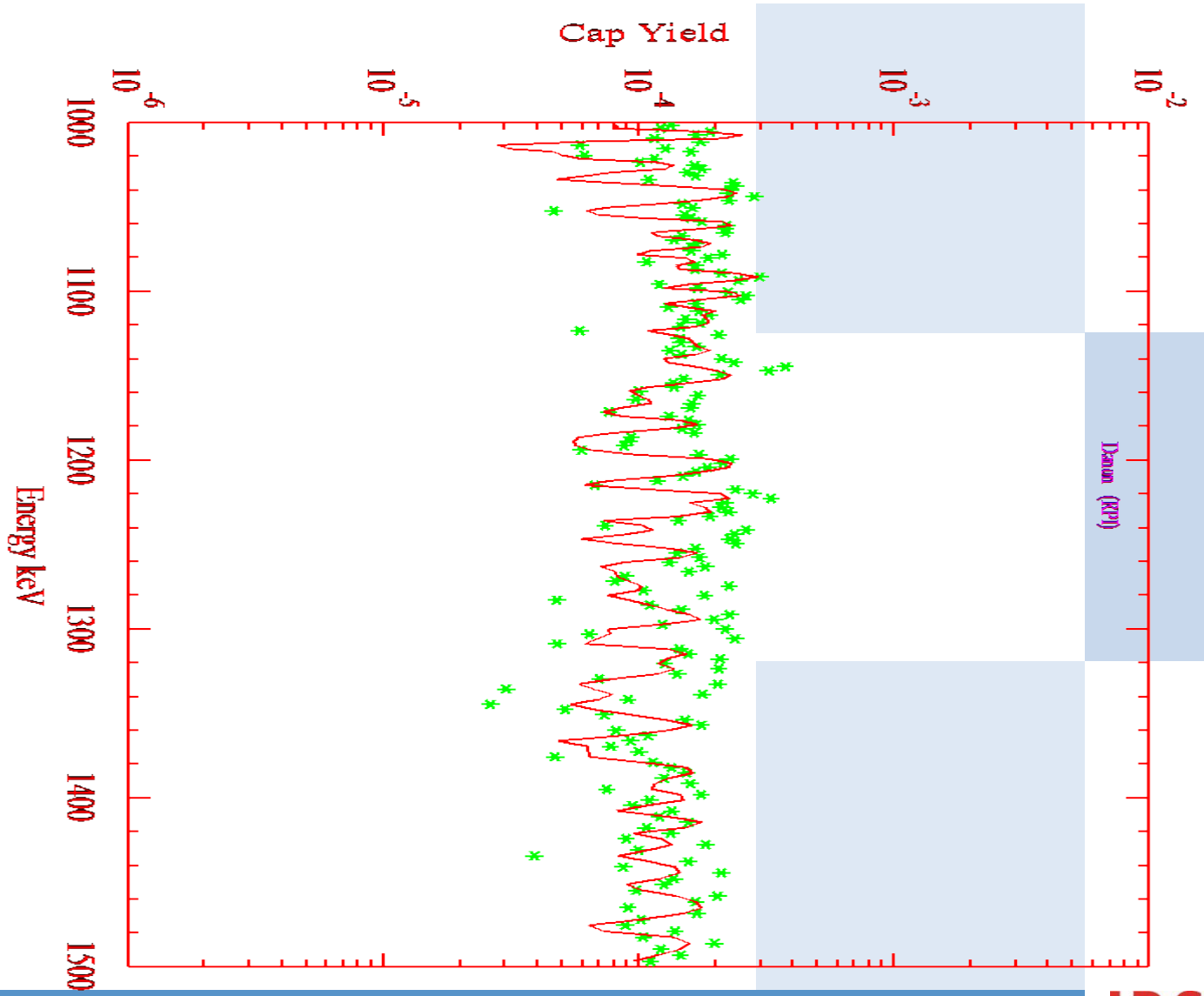


Fitting of the ^{56}Fe capture cross-section data of Danon



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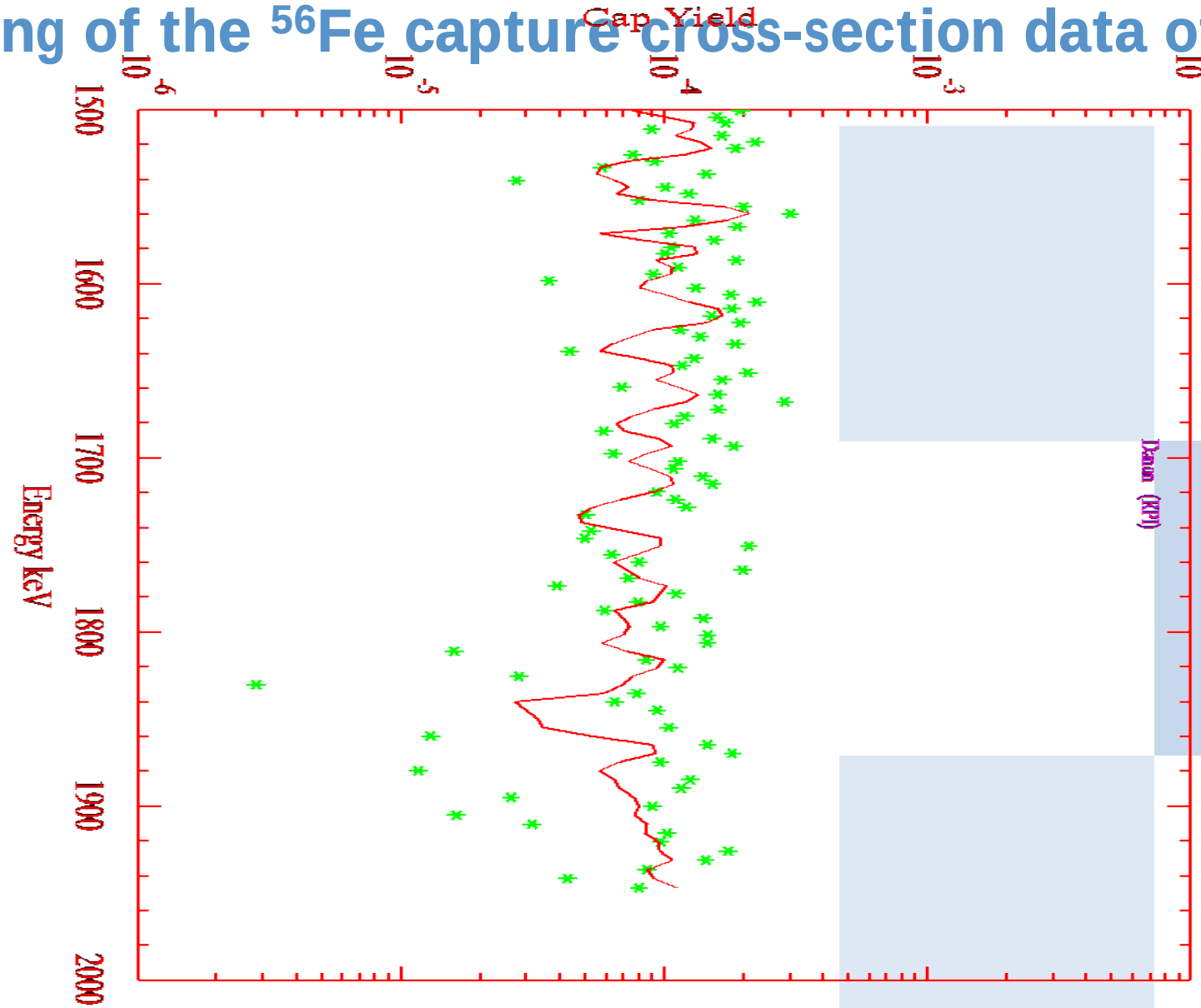
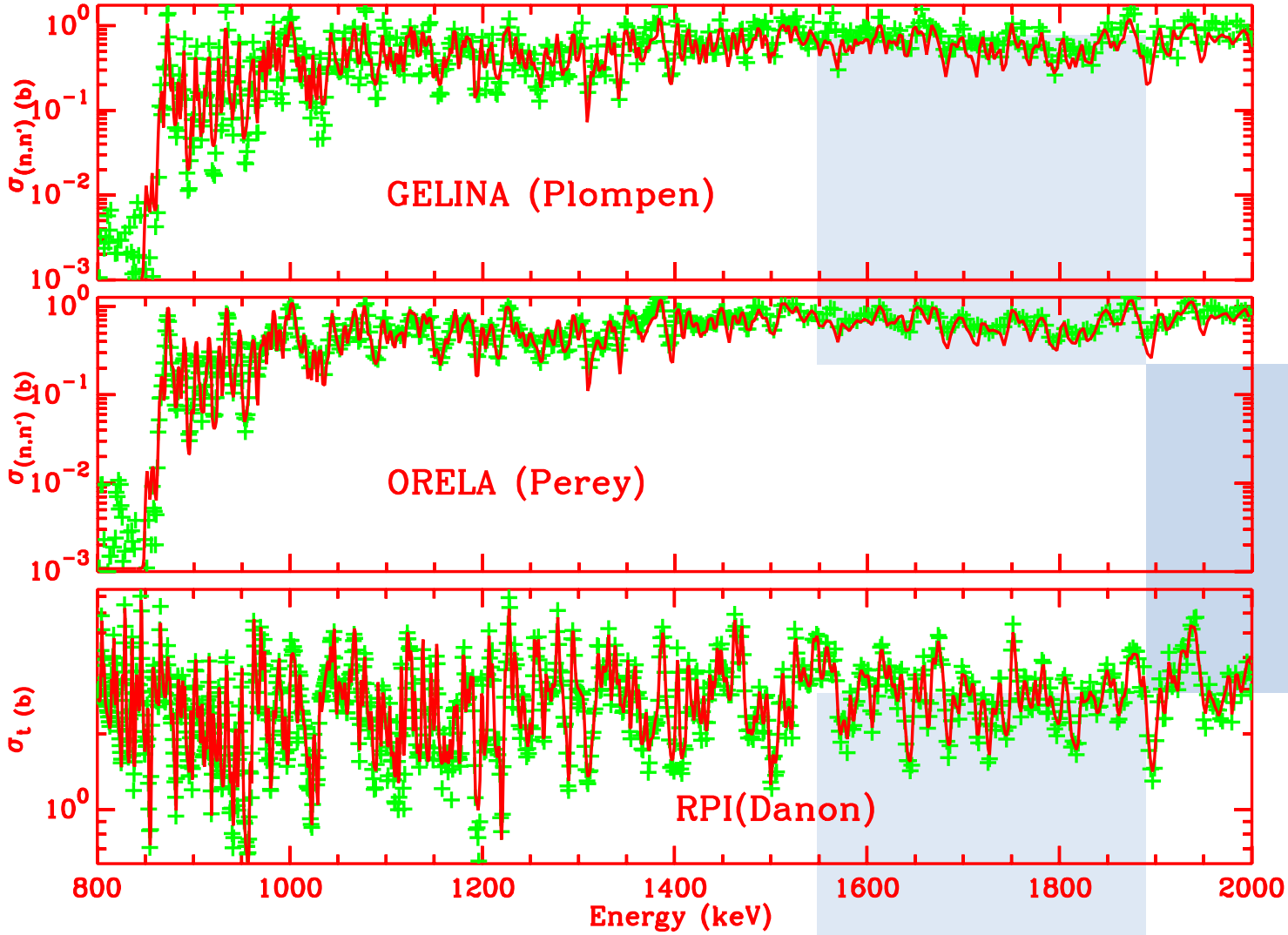
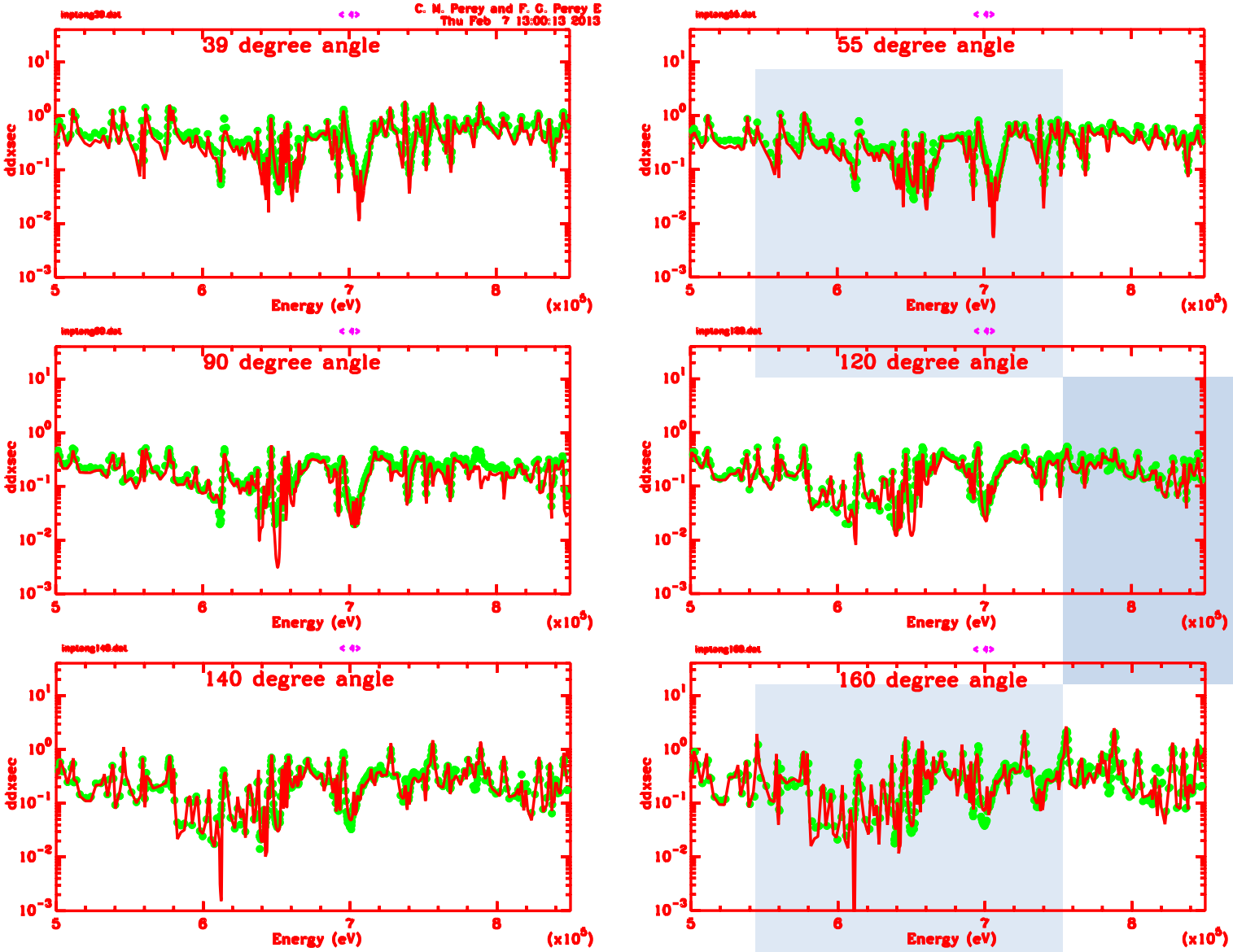


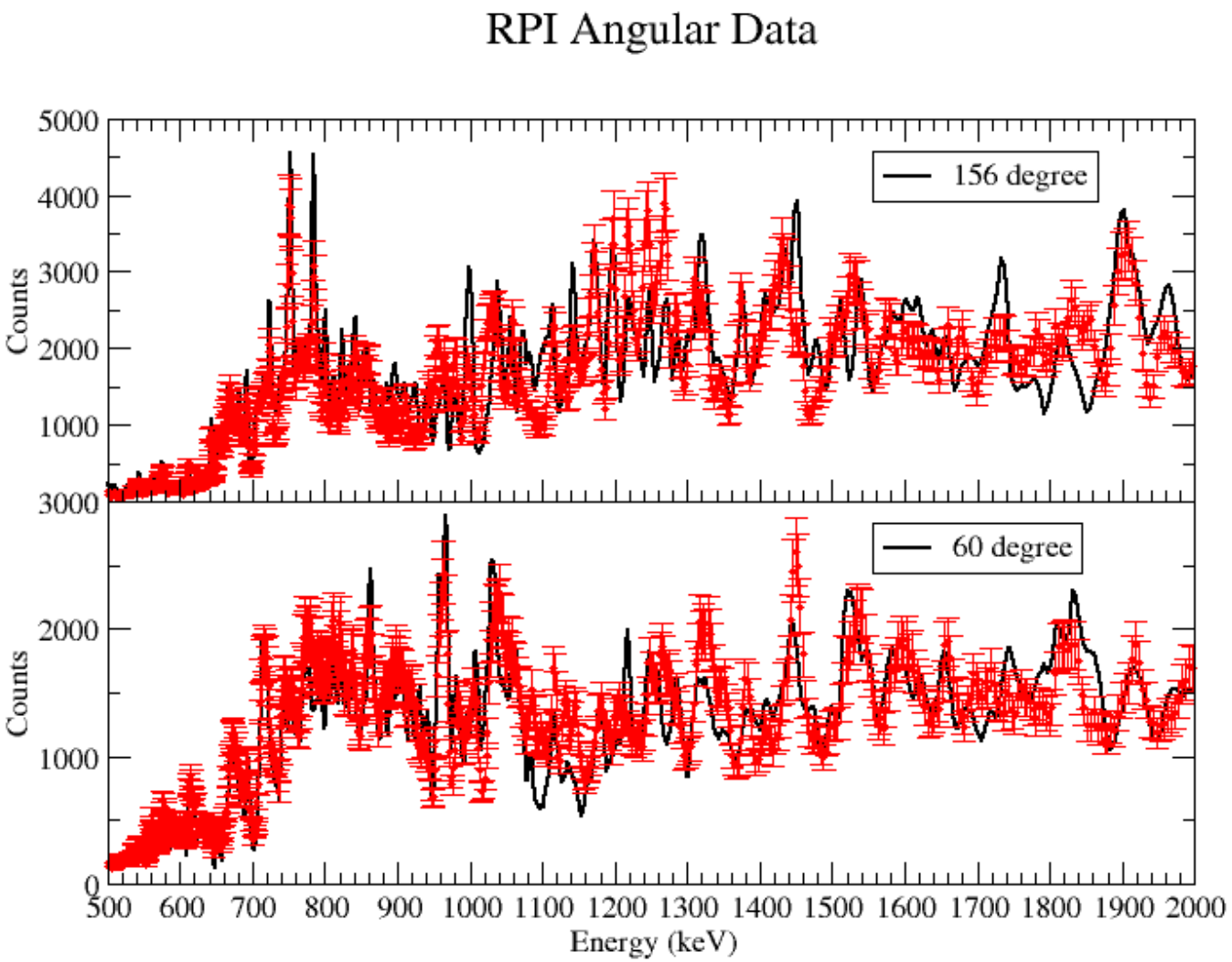
Comparison of SAMMY Fits for Total and Inelastic ^{56}Fe data



Comparison of SAMMY Fits to Perey Differential Elastic ^{56}Fe data



SAMMY calculations and RPI Experimental data

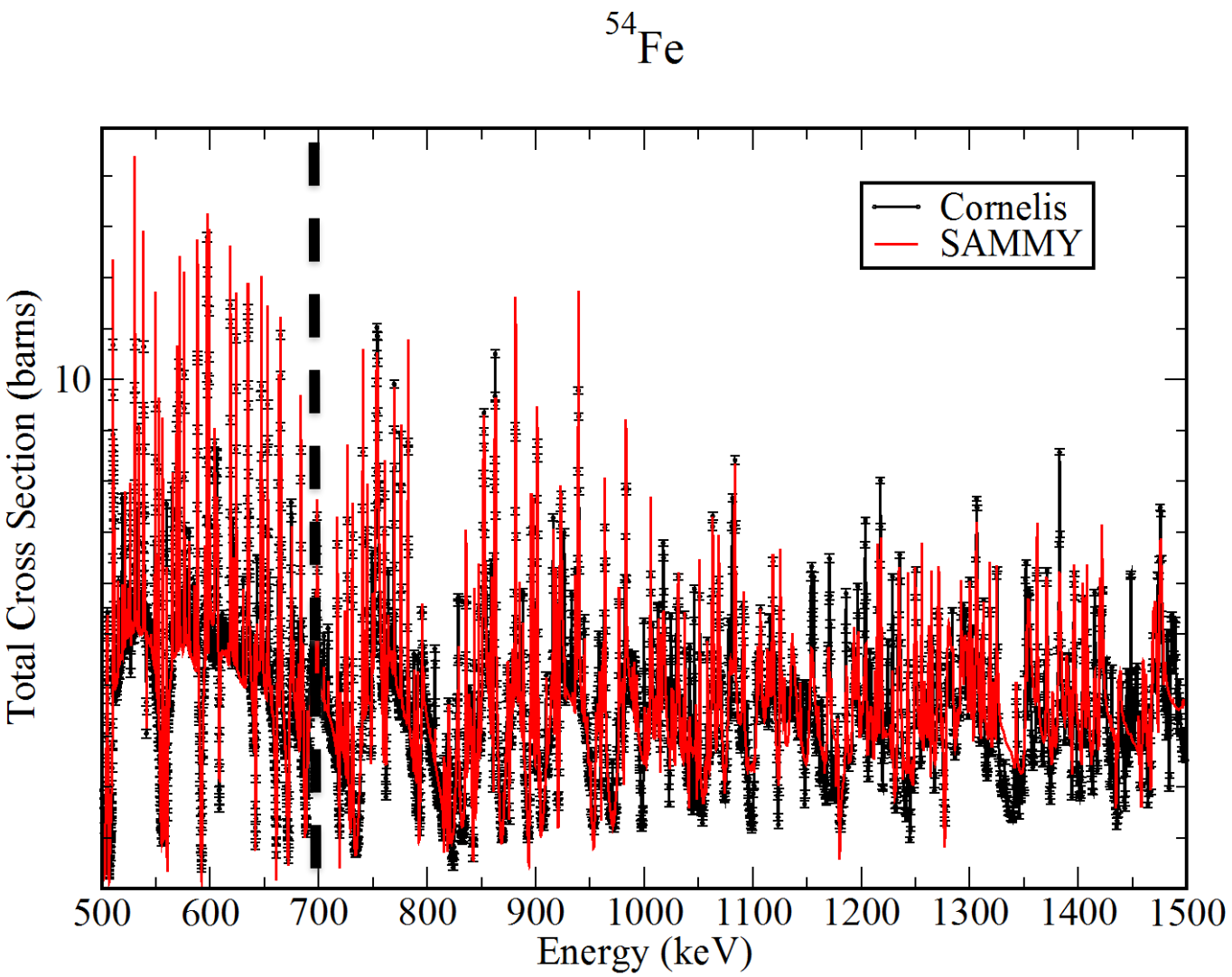


Data (barns)	Mughabghab	JENDL4	JEFF3.1	ENDF/BVII.1	This Evaluation
σ_t	-	14.78	14.79	14.75	14.78
σ_s	12.69 ± 0.49	12.19	12.21	12.16	12.19
σ_γ	2.59 ± 0.14	2.59	2.58	2.59	2.59
I_γ	(1.36 ± 0.15)*	1.35	1.34	1.35	1.28
*calculated					

^{54}Fe Evaluation in the Resolved Resonance

- Natural Iron: ^{56}Fe(91.75 %), ^{54}Fe(5.85 %) and ^{57}Fe(2.12 %);
- Resonance region in existing nuclear data libraries is 10^{-5} eV to 700 keV;
- Transmission, capture data needed to extend the evaluation up to 2 MeV;
- DDX Scattering cross section needed;
- First inelastic channel opens 1.434 MeV;
- Inelastic cross section data needed;

^{54}Fe Evaluation in the Resolved Resonance



Concluding Remarks

- Fitting so far seem acceptable;
- Some work are need to close on the evaluation effort;