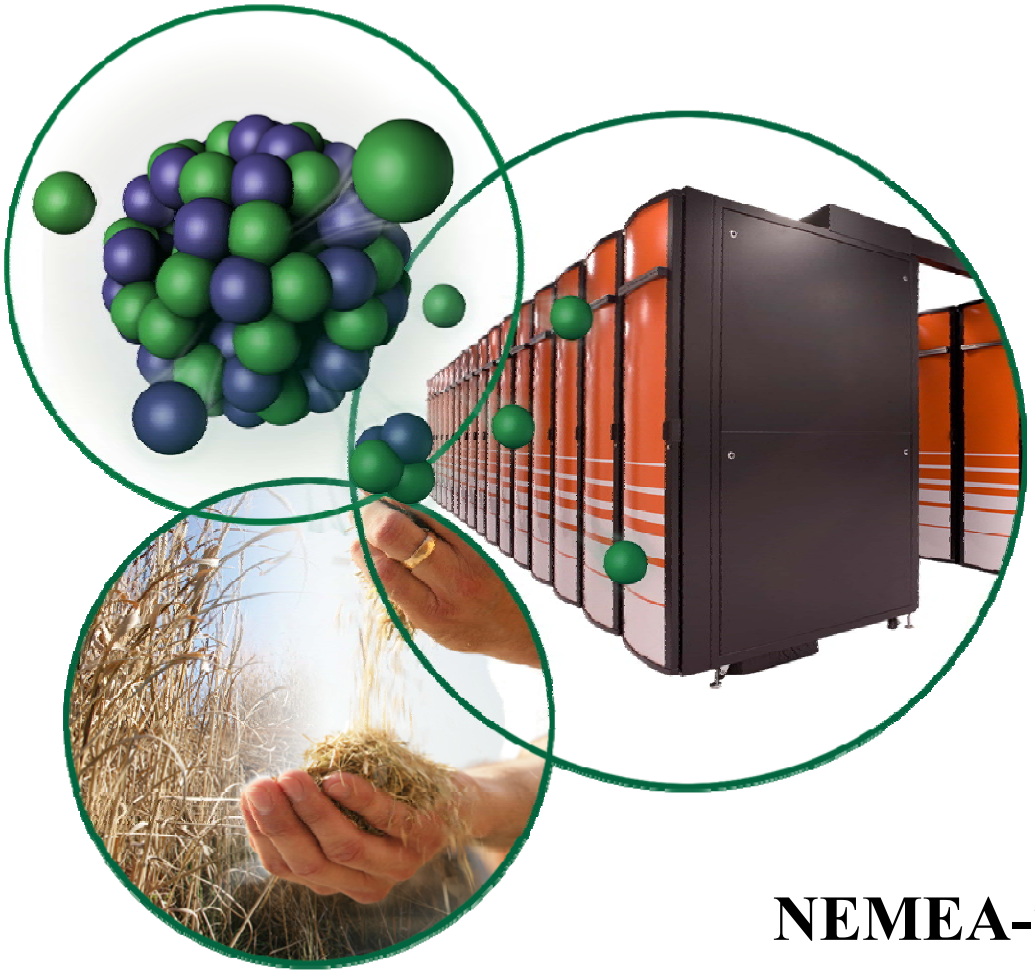
Resonance Evaluations for ^{56}Fe and ^{16}O for the CIELO Project



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2) **Los Alamos National Laboratory**

3) **IRSN**

NEMEA-7/CIELO Workshop
November 5-8, 2013

OAK RIDGE National Laboratory

^{56}Fe Resonance Evaluation up to 2.0 MeV

- Motivation for evaluating ^{56}Fe in the resolved resonance Region;
- Evaluation description;
- Use RML option of the SAMMY code (R-matrix Limited Format);
- Experimental Data;
- Preliminary results;

paradigm shift

Motivation for evaluating ^{56}Fe in the Resolved Resonance Region

- New high resolution transmission measurements done at the RPI extending the resonance region up to 5 MeV (Yaron Danon);
- New inelastic cross-section measurements done at GEEL (Arjan Plompen);
- Use the SAMMY/RML feature to include inelastic channel in the R-matrix analysis;
- Improve the results of benchmark systems calculations;

Evaluation Features

- Extend the resolved resonance region from 850 keV to 2.0 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
- Compare the cross section processed with SAMMY, NJOY, AMPX and PREPRO using the evaluated iron resonance parameters;

paradigm shift

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
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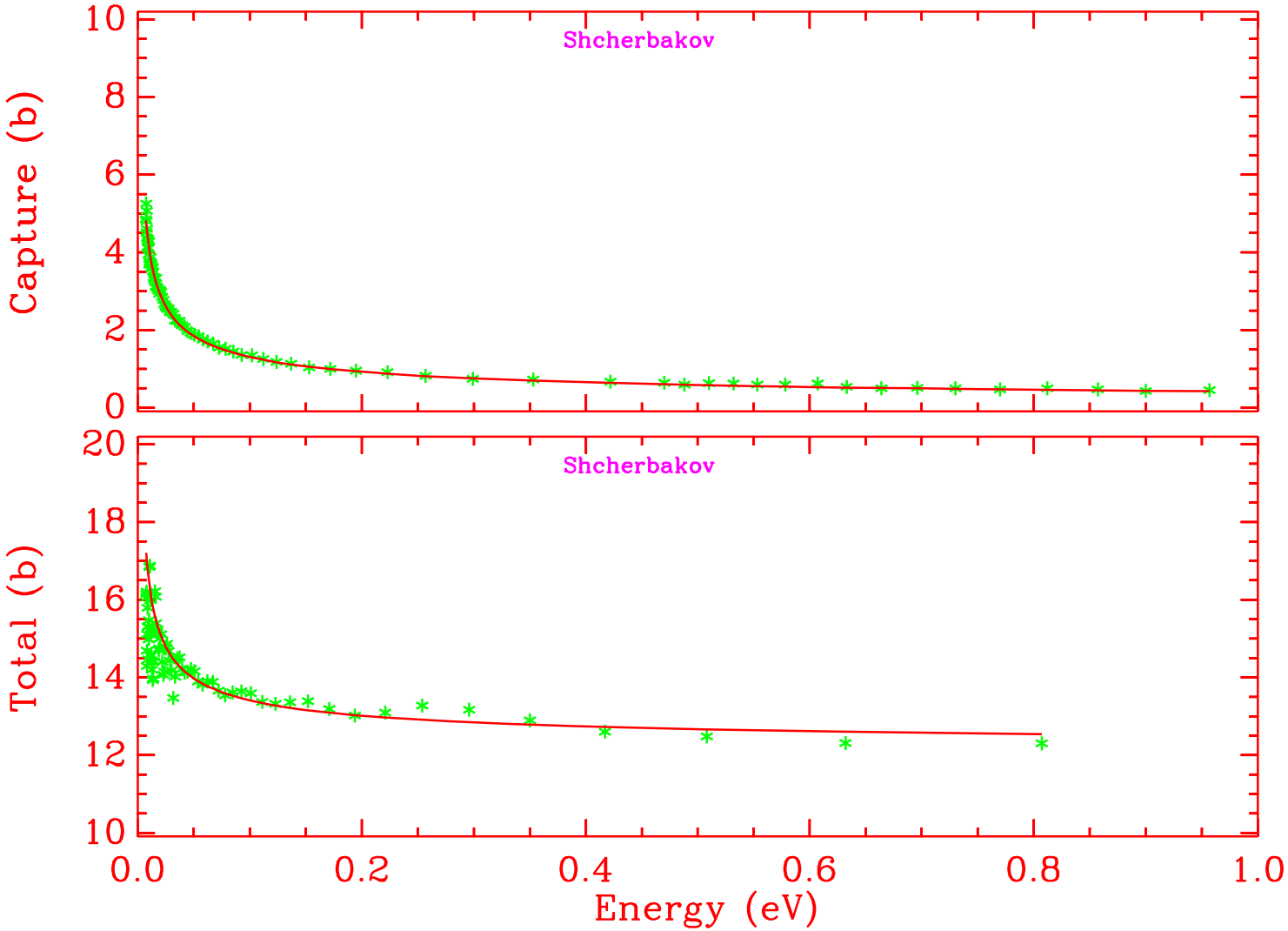
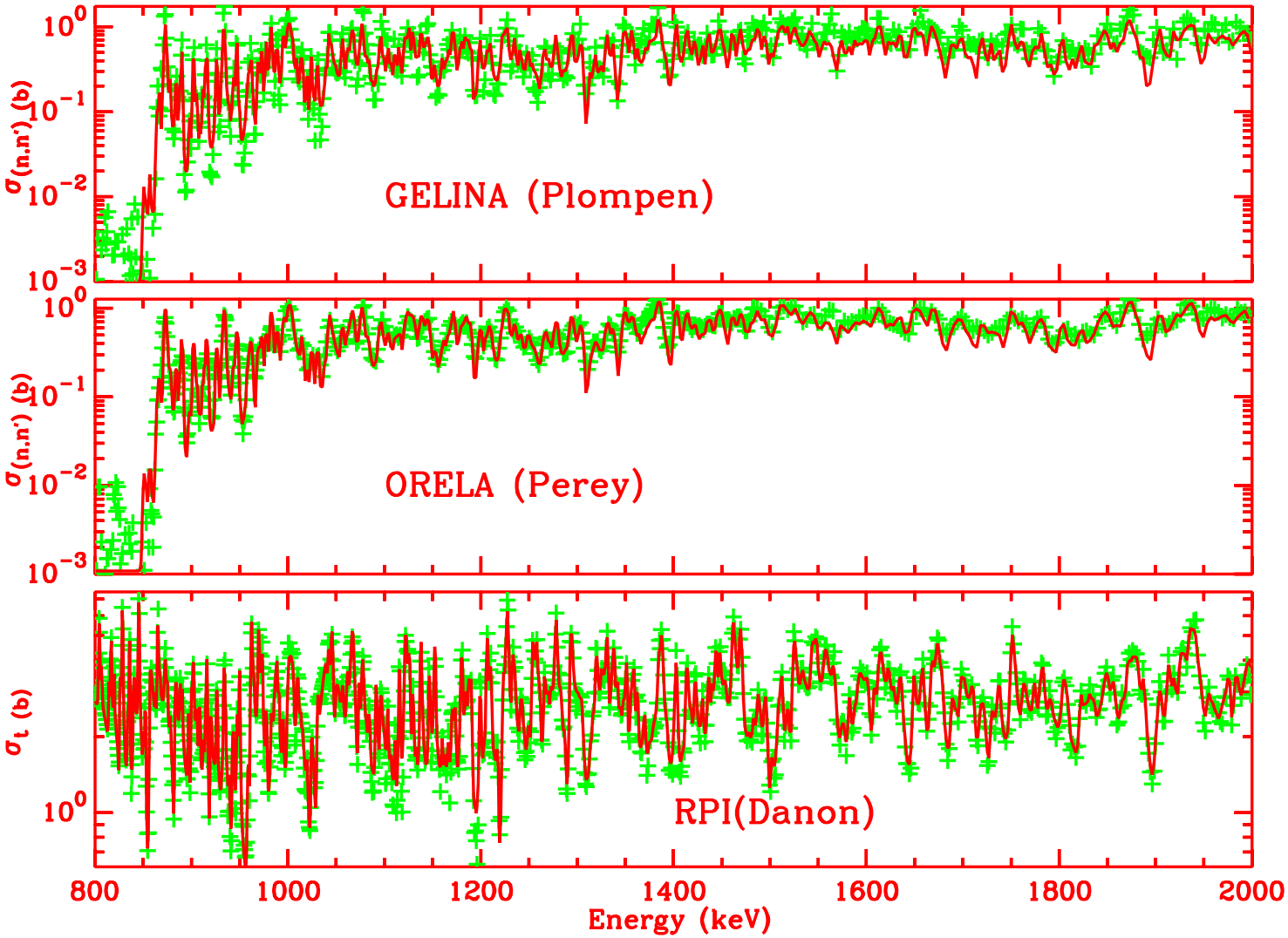


Comparison of SAMMY predictions to total and capture data of Shcherbakov.



Comparison of SAMMY predictions of Total and inelastic data.

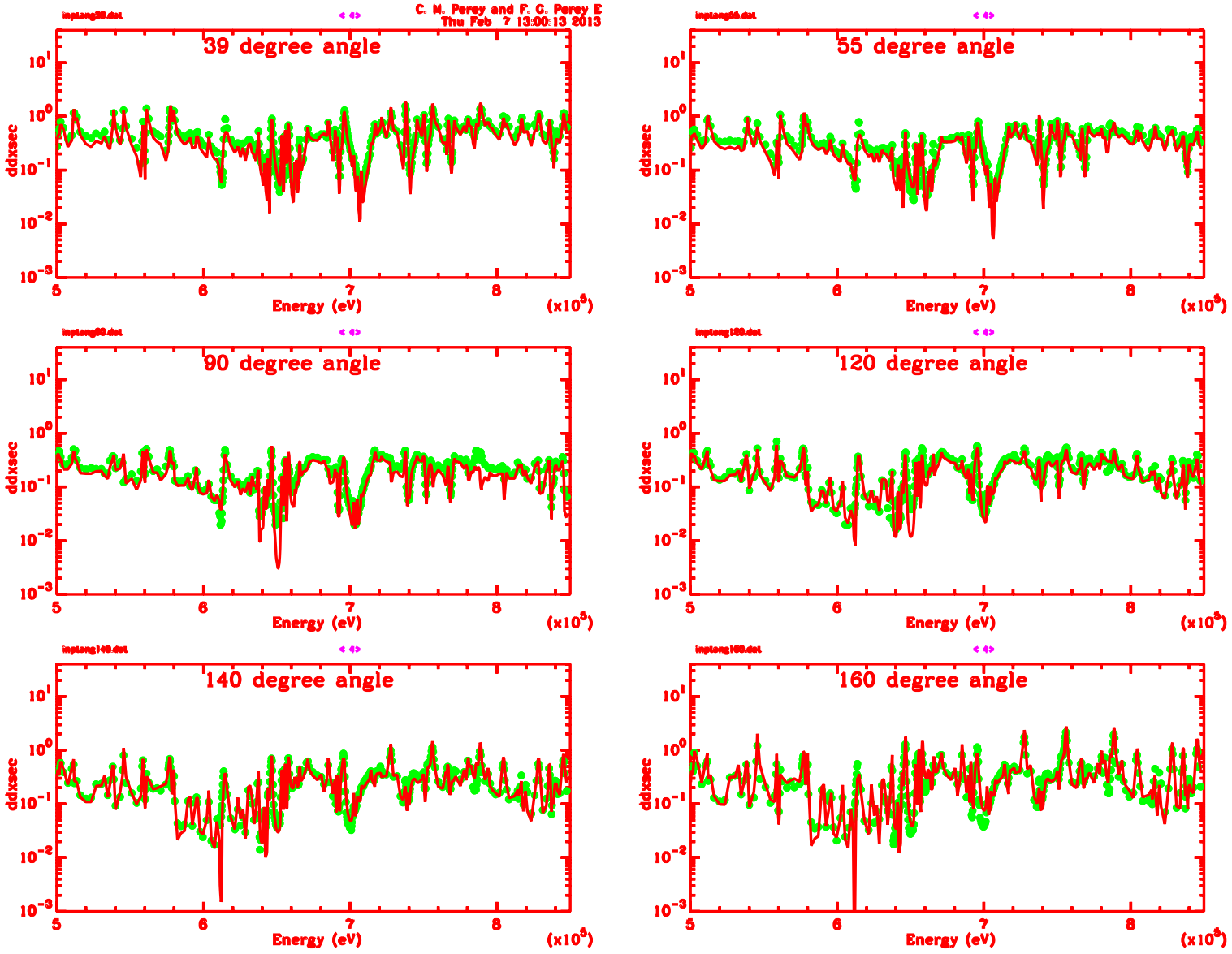
$$\sigma_s(E,\mu) = \frac{\sigma_s(E)}{2\pi} \sum_{l=1}^{NL} \frac{2l+1}{2} a_l(E)\, p_l(\mu)$$

$$a_0(E) = 1$$

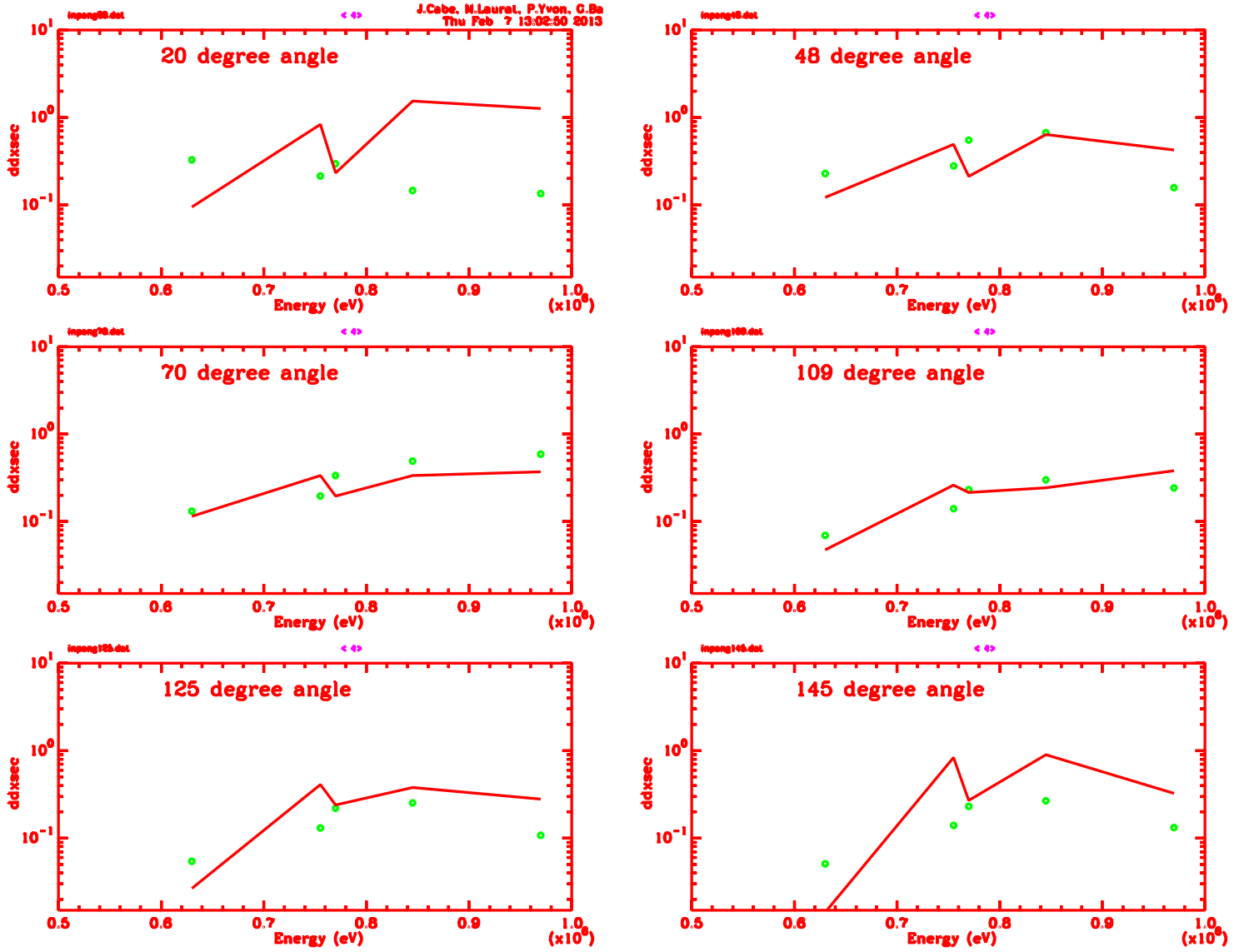
$\sigma_s(E)$

$a_l(E)$

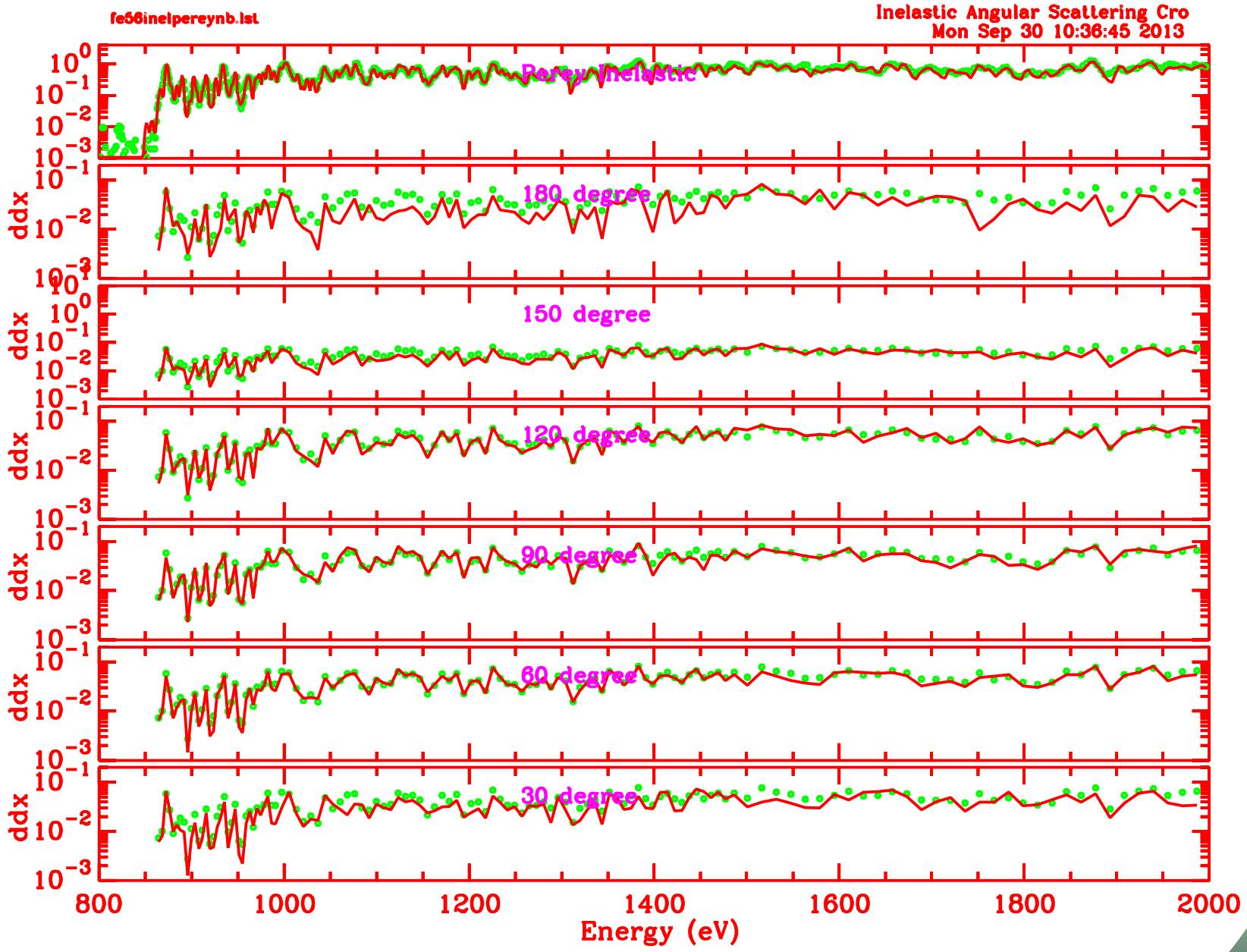
} calculated from resonance parameters



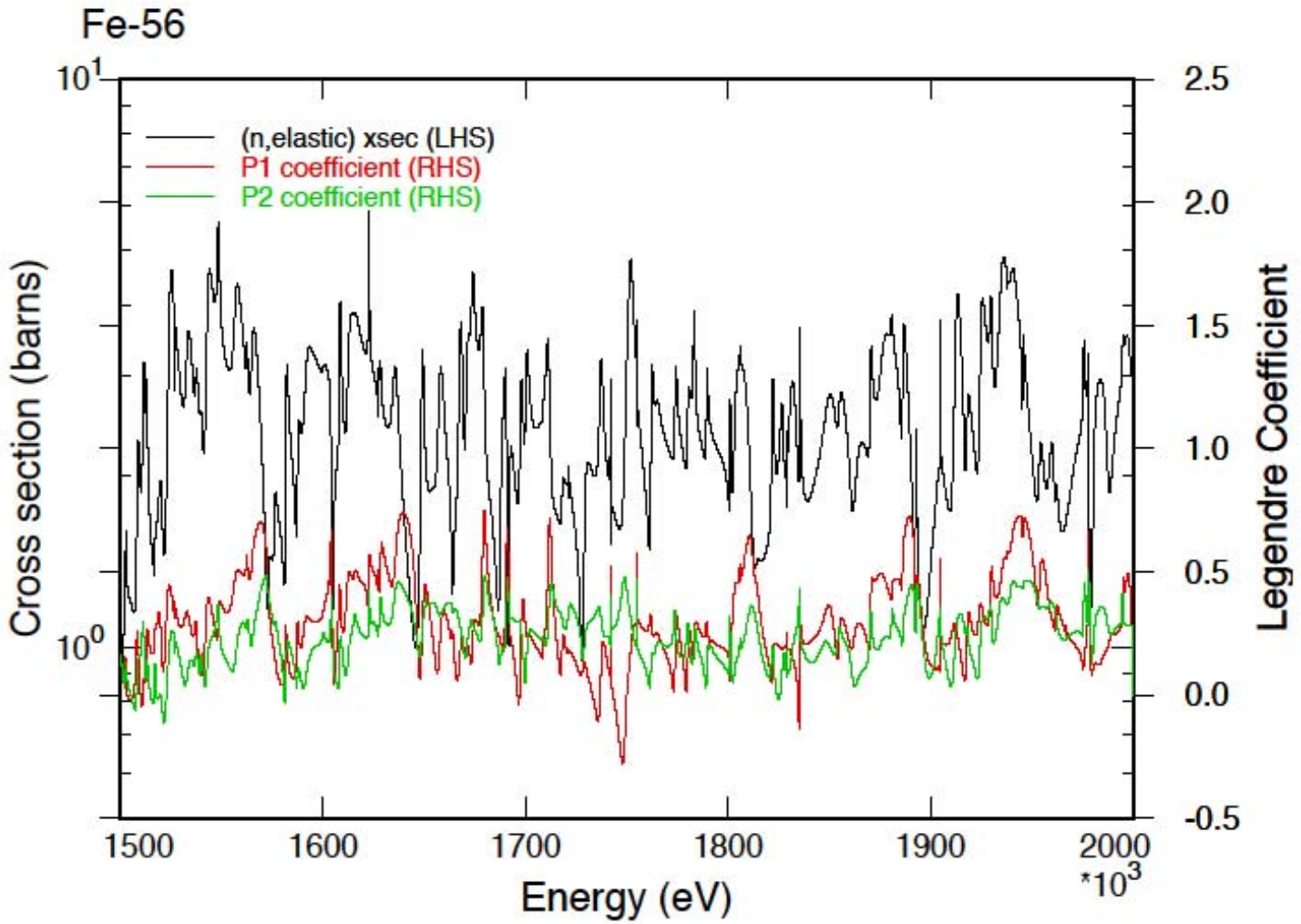
Comparison of SAMMY predictions to differential elastic data of Perey.



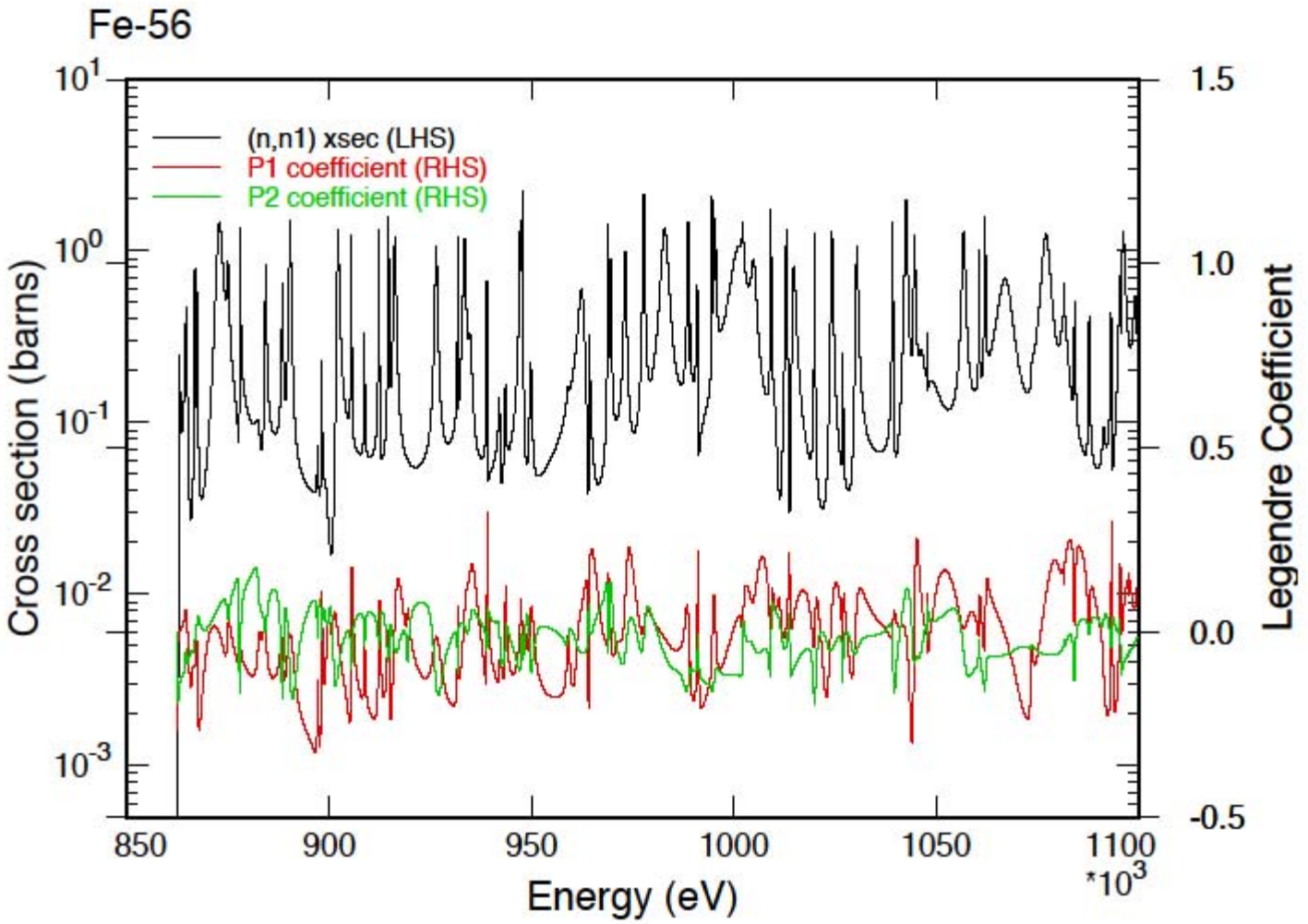
Comparison of SAMMY predictions to differential elastic data of Cabé .



Comparison of SAMMY predictions to differential inelastic with ENDF



NJOY2012 calculation of the inelastic cross section



NJOY2012 calculation of the inelastic cross section

Thermal and Resonance Integral

Data (barns)	Mughabghab	JENDL4	JEFF3.1	ENDF/BVII.1	This Evaluation
σ_t	-	14.78	14.79	14.75	14.77
σ_s	12.69 ± 0.49	12.19	12.21	12.16	12.18
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					

paradigm shift

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:

$$a = a_{coh}$$

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

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

^{16}O Resonance Evaluation

Starting from an evaluation done at ORNL using SAMMY R-matrix limited (RML) format (ORNL/TM-2000/212) with charge particle penetrability included in SAMMY.

- **New, lower thermal cross section (3.773 b at 0K).**

- **New $^{16}O(n, \alpha)$ data (Giorginis, et al., IRMM) and $^{13}C(\alpha, n)$ data (Harissopulos, et al.) give about 30% lower ^{16}O (n, α) cross section values than the Bair-Haas values used in the 2000 ORNL evaluation.**

- **Few-parameter RML resonance parameter representation is advantageous:**

  - **Cross section details are well-represented.**

  - **Avoids excessive number of point-wise values.**

^{16}O Evaluation - Data

Table 1. Total and Reaction Cross Section Data Sets for ^{16}O Evaluation

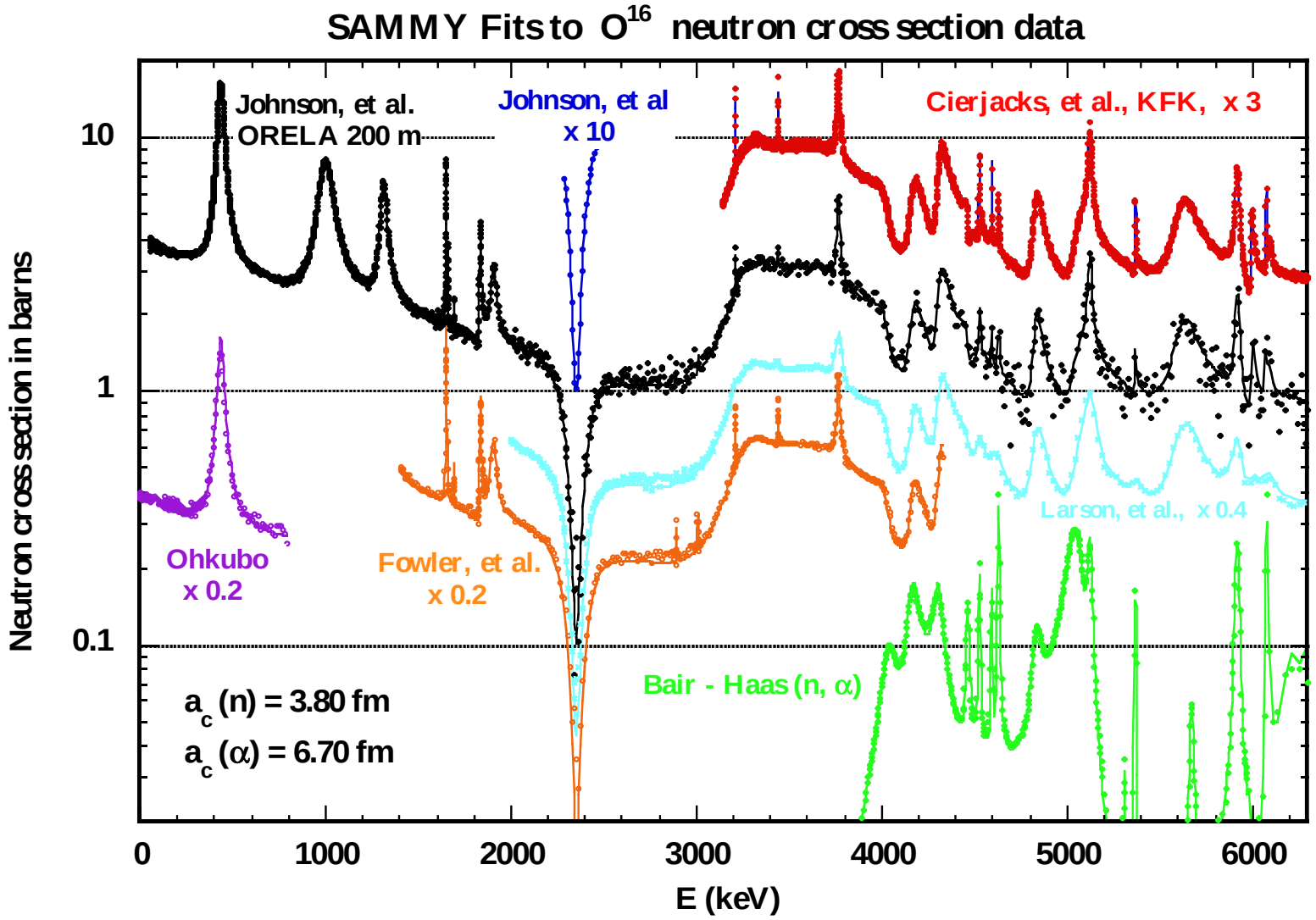
Type	Authors	Facility (Flight path)	Energy Analysis Range (MeV)	Atoms/barn	Normalization *
Total	Johnson, et al [JO74]	ORELA 198.731 m	0.2 – 6.3	0.183	(1.000)
Total	Larson [LA80]	ORELA 79.46 m	2.0 – 6.3	0.5485	0.9998
Total	Cierjacks, et al [CI80]	KFK cyclotron 189.25 m	3.14 – 6.3	1.201	0.9663
Total	Fowler, Johnson, and Feezel [FJF73]	ORNL Van de Graaff 41 and 47 m	0.6 – 4.3	0.488	0.9997
Total (2.35 MeV)	Johnson, et al [JO80]	ORELA 198.731 m	2.25 – 2.49	6.7	
Total	Ohkubo	JAERI 47 m	0.00079 - 0.935		
(n, !) [from (! ,n)]	Bair and Haas [BH73]	ORNL Van de Graaff	3.2 – 6.3		
(n, !) [from (! ,n)]	Drotleff, et al [DR93]	Stuttgart Dynamitron	2.87 – 3.48		

* Normalization obtained by integrating the total cross section from 3.45 to 3.72 MeV.

^{16}O Evaluation – Angular Distribution Data

Table 2. Angular Distribution Data Sets for ^{16}O Cross Section Evaluation

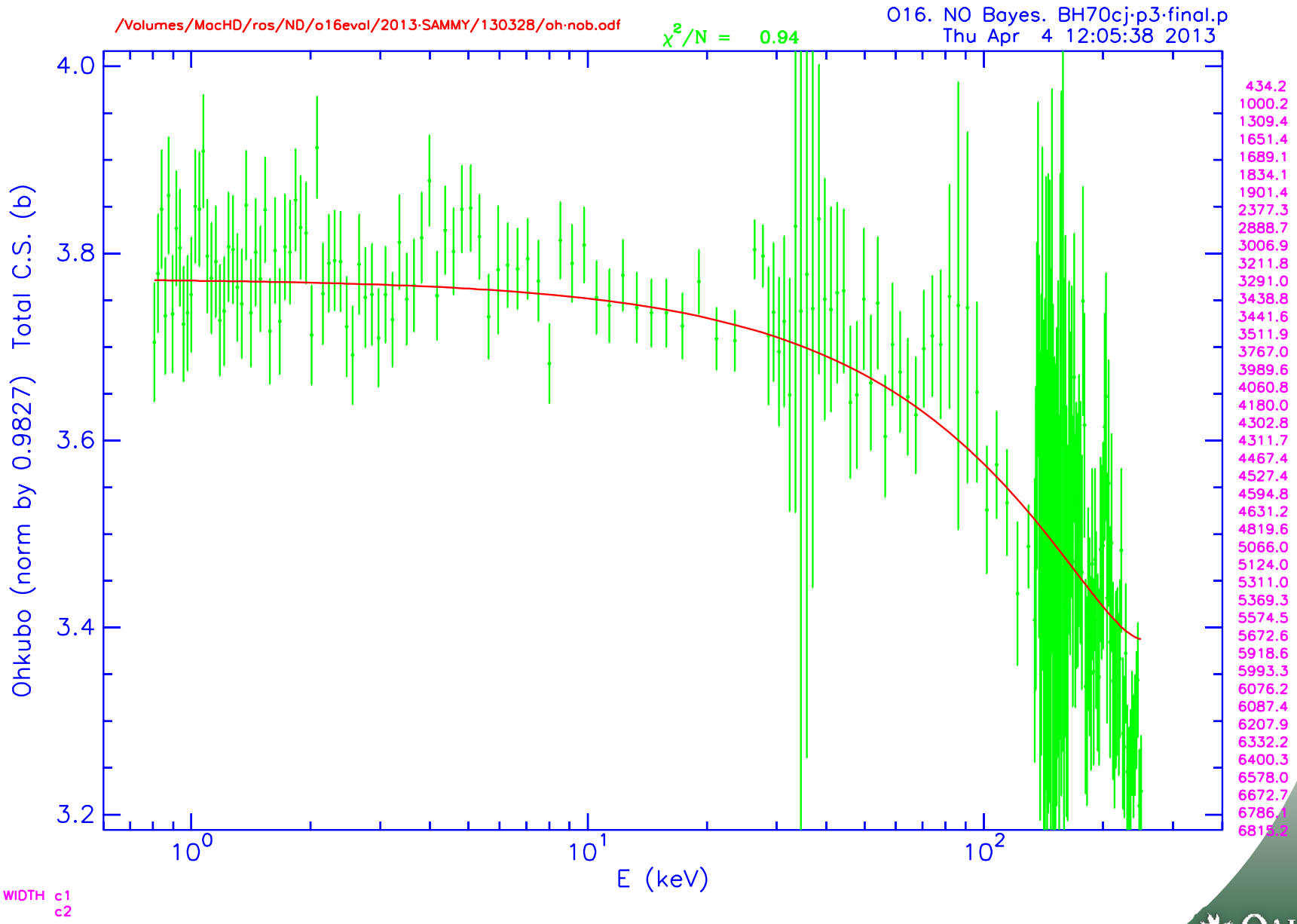
Authors	Facility	Energies (MeV)	FWHM ! E (keV)	CM Angles (degrees)
Okazaki 1955	University of Wisconsin	.410 – .493	16	46 - 133
Fowler and Cohn 1958	ORNL Van de Graaff	0.73 – 2.15	50	32 - 138
Phillips 1960	LANL	3.0 – 6.0	30	22 - 152
Martin and Zucker 1962	BNL	1.51 – 2.25	33 - 63	21 - 166
Hunzinger and Huber 1962	University of Basel Cockcroft-Walton	2.00 – 4.11	10 – 51	41 - 147
Lister and Sayres 1966	Columbia University Van de Graaff	3.1 – 4.7	18 - 25	Legendre Coefficients
Johnson and Fowler 1967	ORNL Van de Graaff	3.266 – 4.200	14 - 33	20 - 147
Fowler and Johnson 1970	ORNL Van de Graaff	1.833 – 3.441	5 – 13	20 - 146
Kinney and Perey 1972	ORNL Van de Graaff	4.34 – 6.44	60 – 80	16 - 139
L. Drigo, et al. 1976	Lignaro Van de Graaff	2.56, 2.76	30	26 - 156



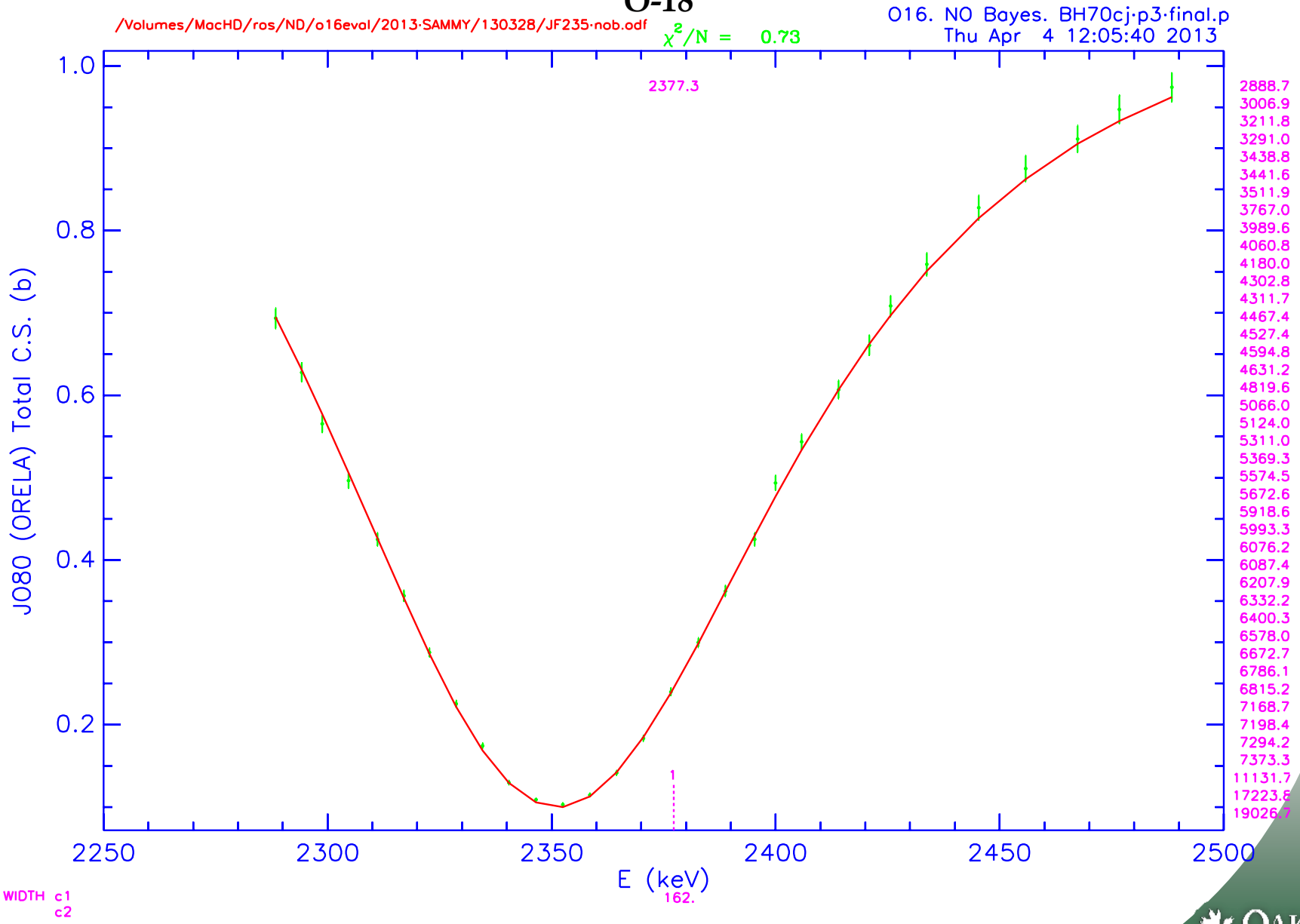
^{16}O Re-Evaluation – Preliminary Results

- **Thermal to 3.0 MeV.**
  - **Resonance parameters were adjusted to fit :**
    - **Thermal 0K cross section value: 3.773 b**
    - **Accurate Johnson-Fowler 2.35 MeV window data corrected for O-17 and O-18**
    - **JO74 ORELA data**
  - **New resonance parameters used to fit data of Ohkubo to obtain a normalization of 0.9827**
- **3.0 to 6.3 MeV.**
  - **Bair-Haas normalized by 0.70 and Cierjacks (KFK) normalized by 1.035 were simultaneously fit to obtain new resonance parameters**
    - **Good fits up to 4.7 MeV. At minima in the total cross section near 4.75 (5.0) MeV, the fit is about 3 (6) percent lower than the KFK data**

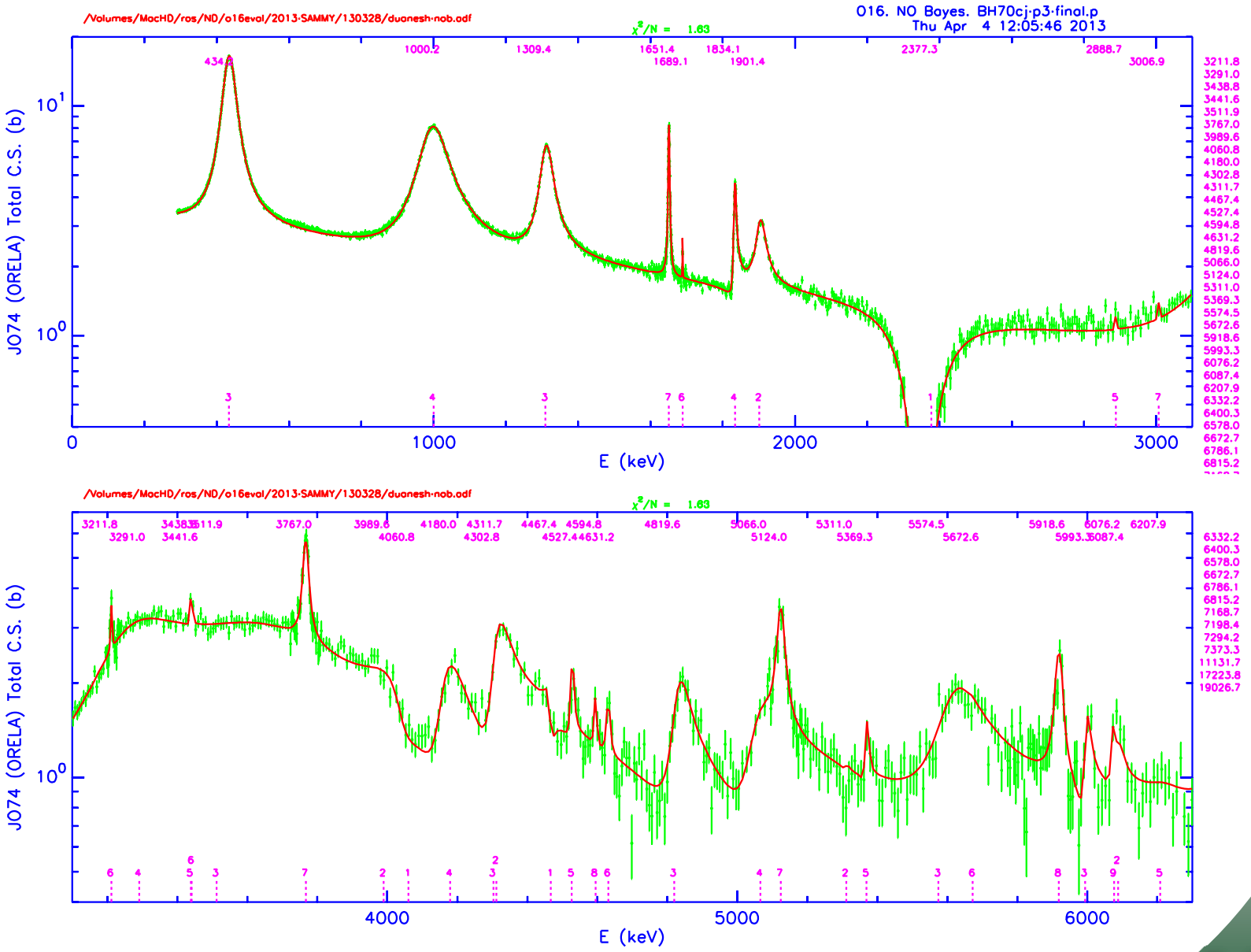
SAMMY Fit to Ohkubo Data normalized by 0.9827



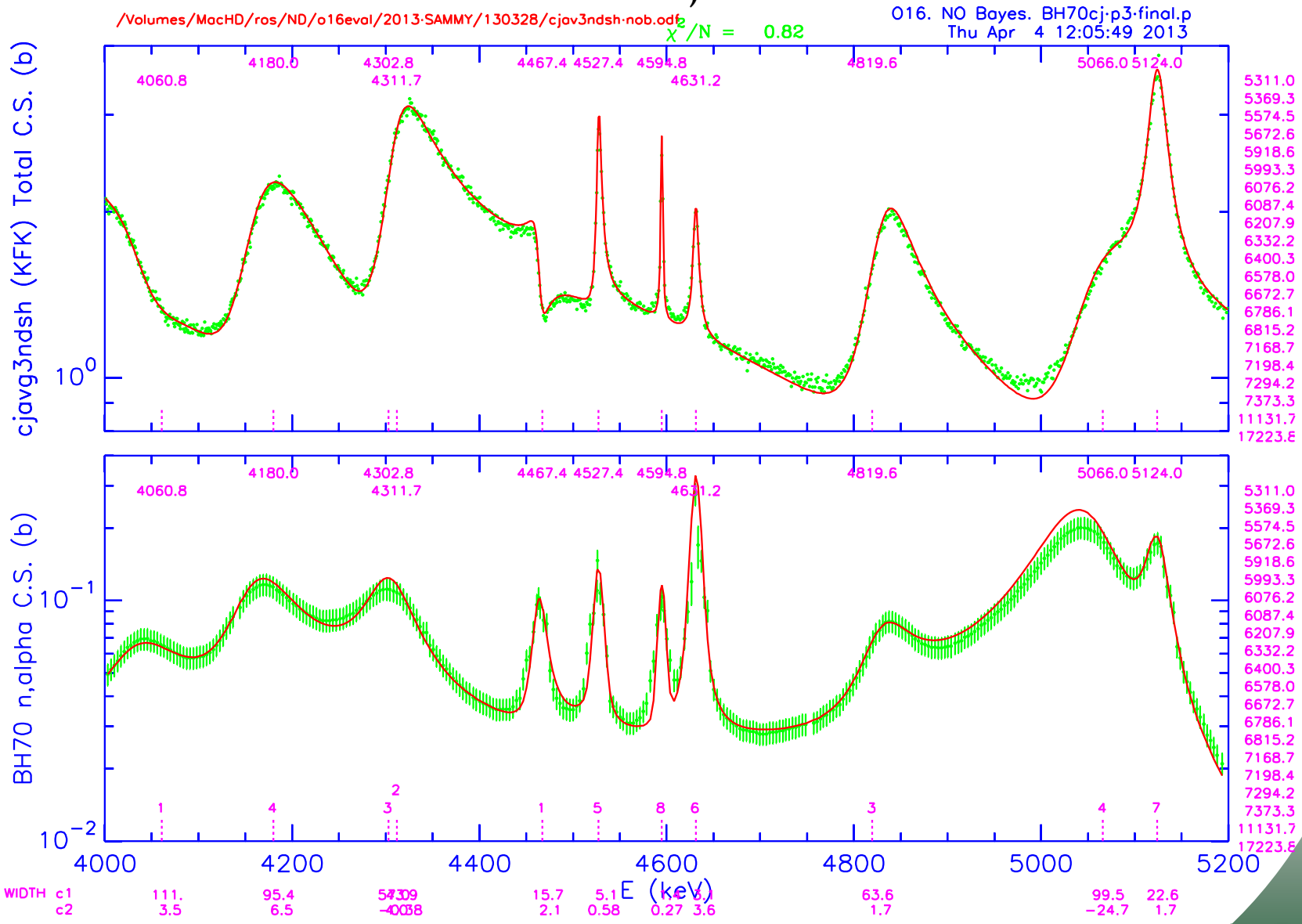
SAMMY Fit to 2.35 MeV Window data of Johnson and Fowler (corrected for O-17 and O-18



SAMMY Fit to JO74 ORELA total cross section data



SAMMY Fit to 1.035 * (Cierjacks total cross section data) and 0.70 * (Bair-Haas (n,α) data)



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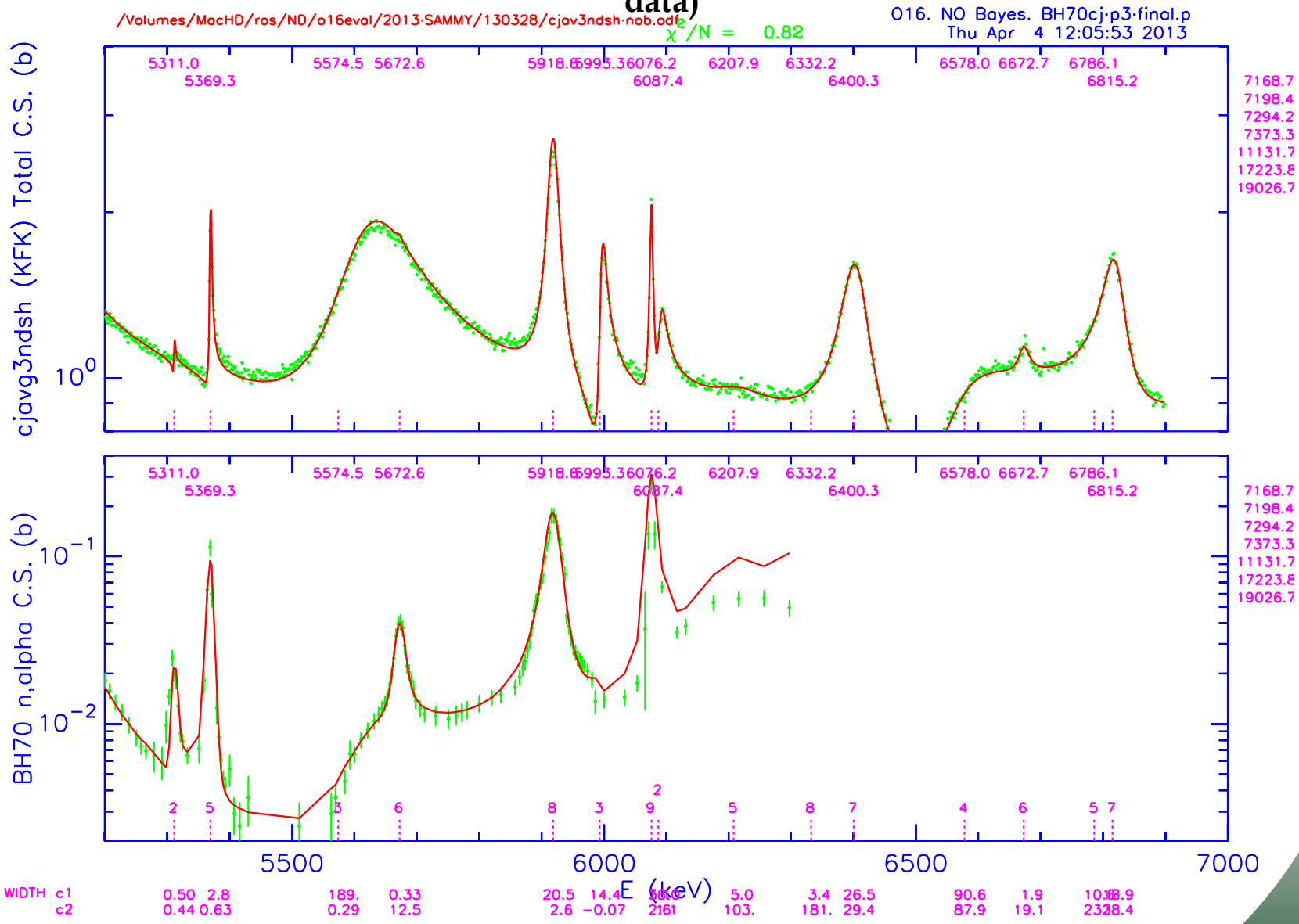

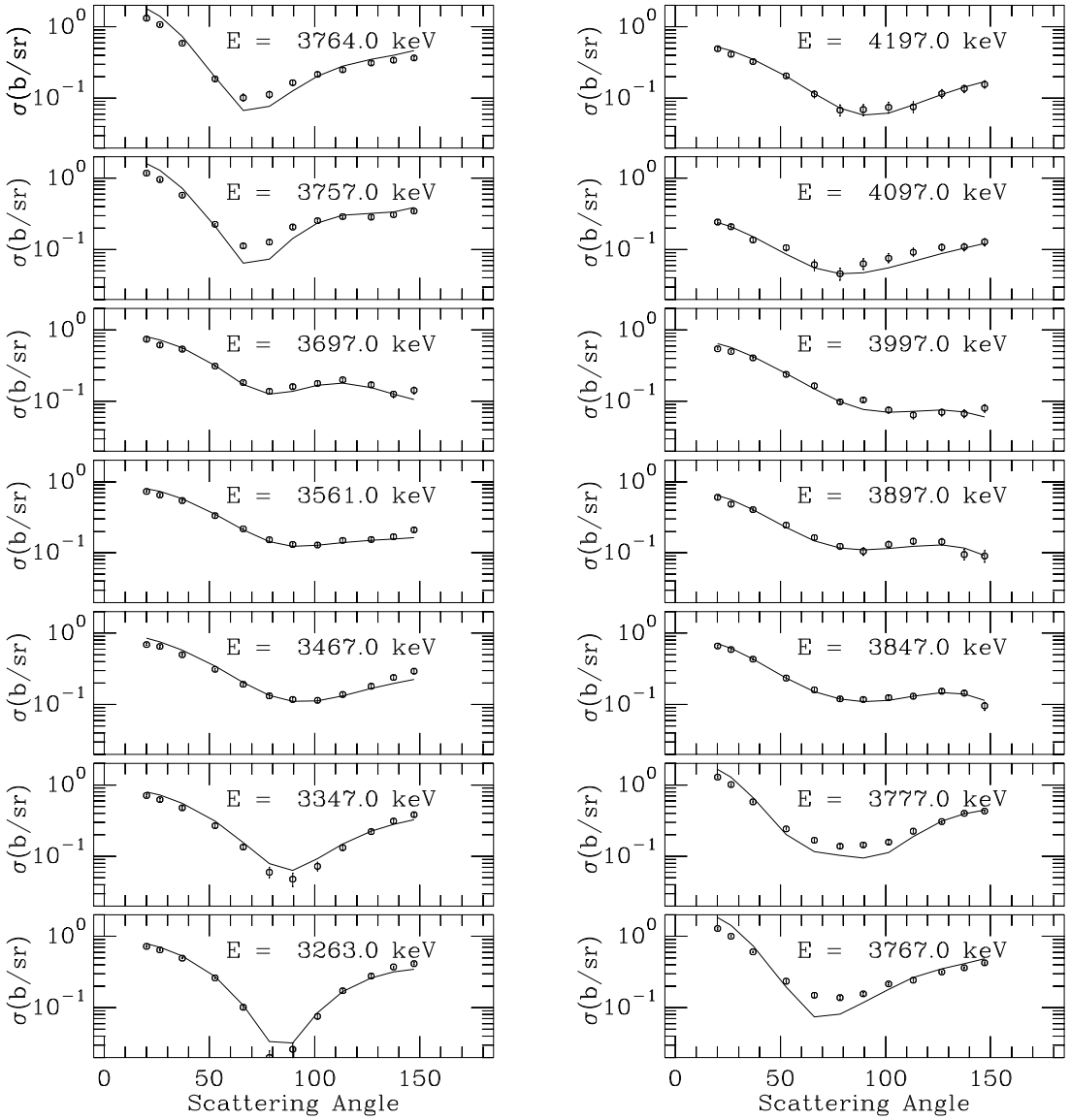

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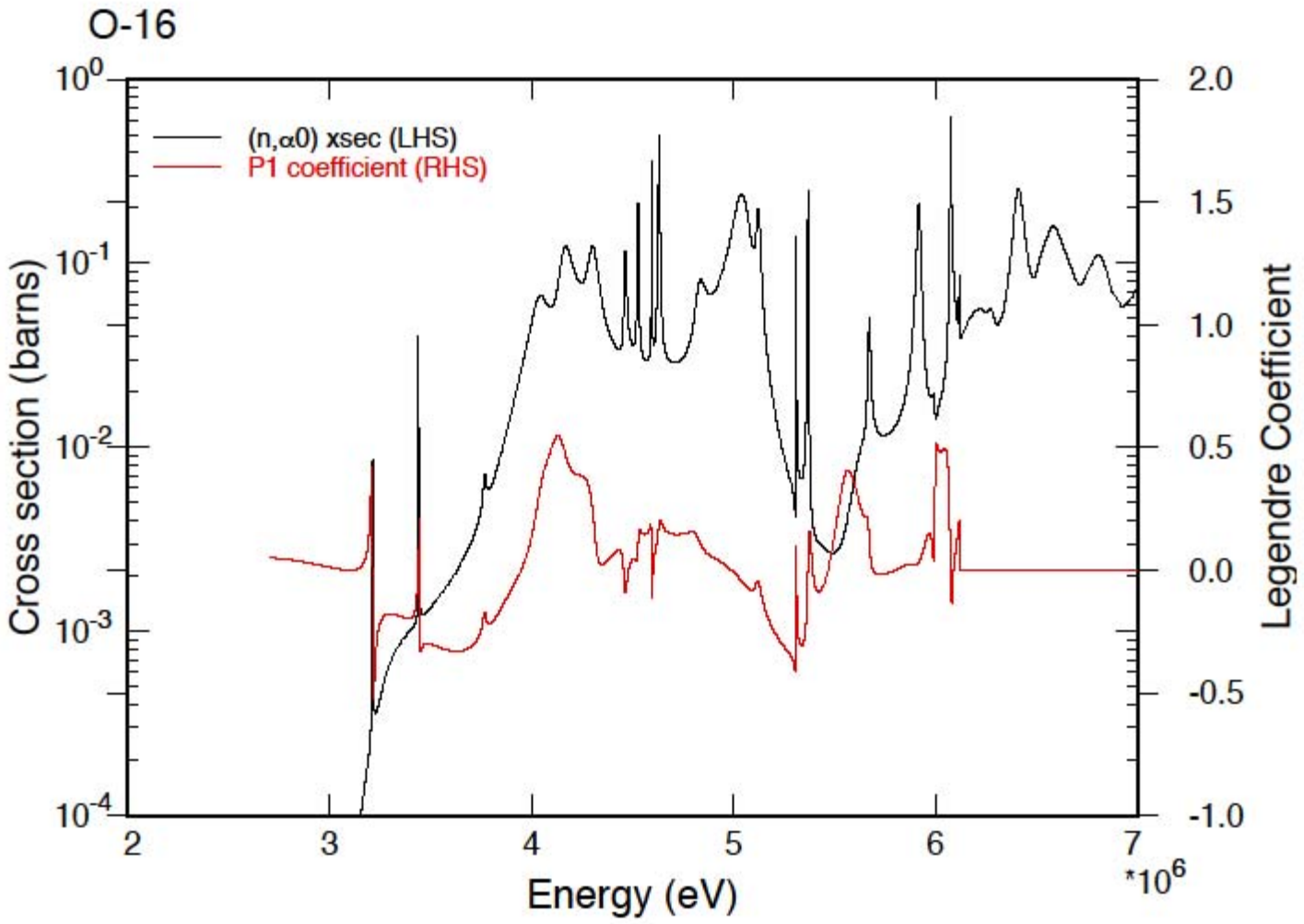


NJOY2012 calculation of the (n,α) cross section

Next Phase:

- **To Do**
  - **Simultaneous fits of all data with variable normalizations for the KFK, JO74, and Bair-Haas data**
  - **Angular distribution fits**
  - **Integral Benchmark calculations with new resonance parameter representation**

General Conclusions

✓**Differential data and benchmark tests are crucial to define whether the evaluation is acceptable;**

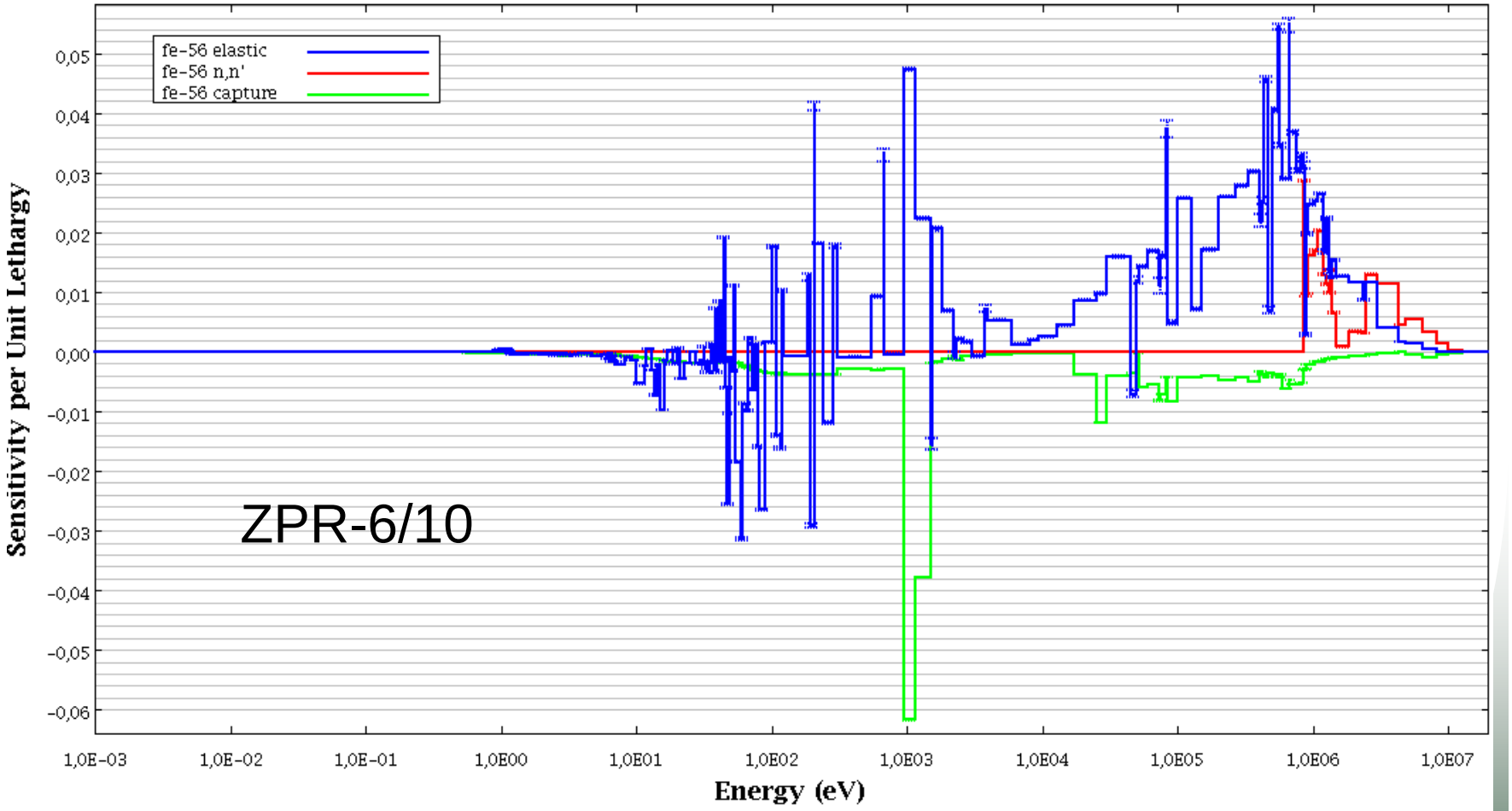
✓**Results of nuclear data processing codes, nuclear data evaluation codes must be checked;**

✓**Continue work under the CIELO project;**

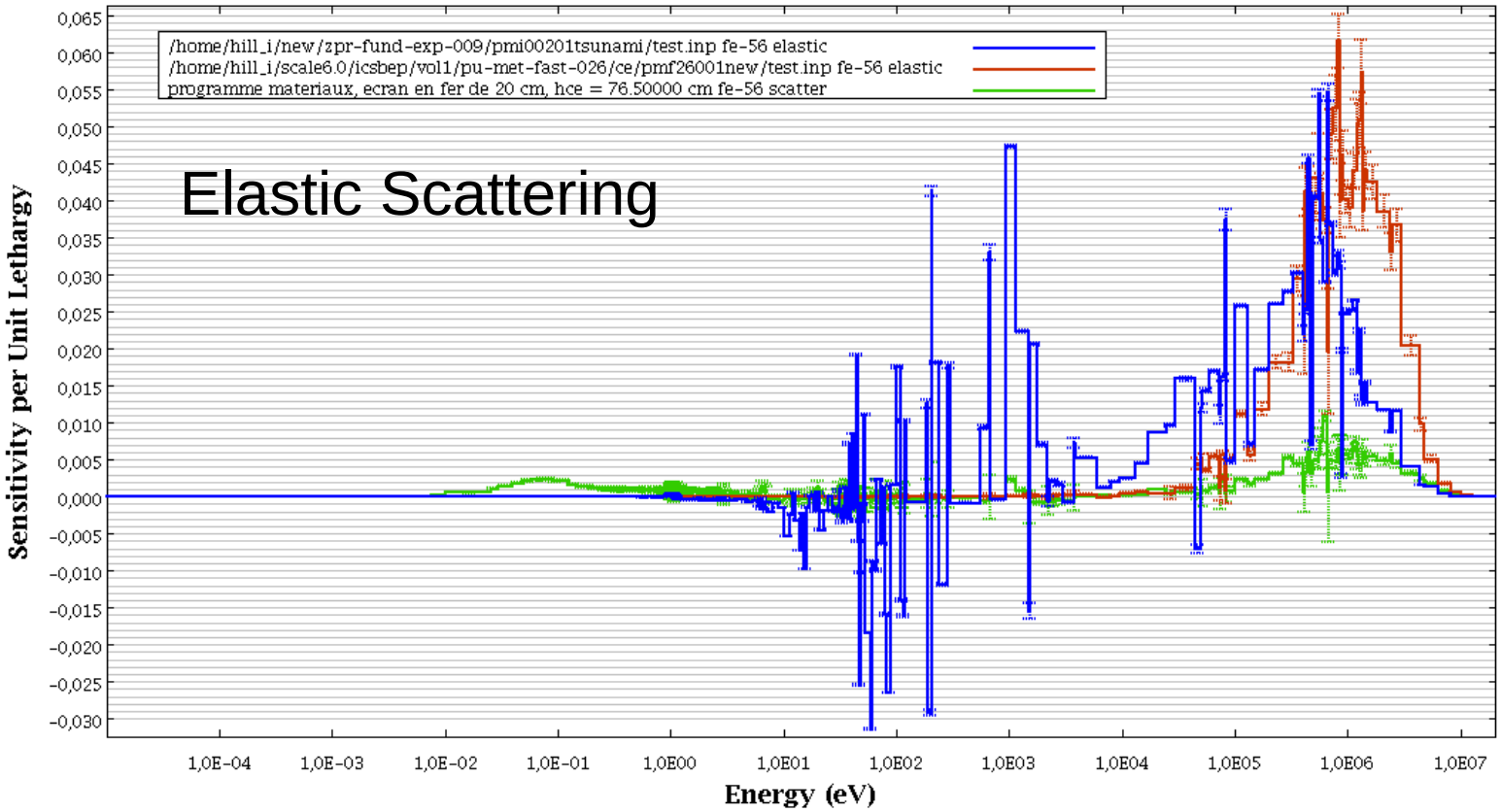
Integral Experiments for Validation of ^{56}Fe

IRSN experiments +									
LCT010	LCT040	LCT017	PMF028	PMF026	HMF084	HMF085	IMF005	PMF016	PMF032
HMF072	PMF-025	HMF013	HMF021	PMI002	HMI001	LCT043	LCM002	HMM006	HMM018
HCI005	MMIO003	PMF015	PMF042	PMF045	PCF004	HMF024	HMF043	HMI001	HST038
HCI003	LCF001	LCT036	LCT066	LCT068	MMF006	MMI003	MCF006		

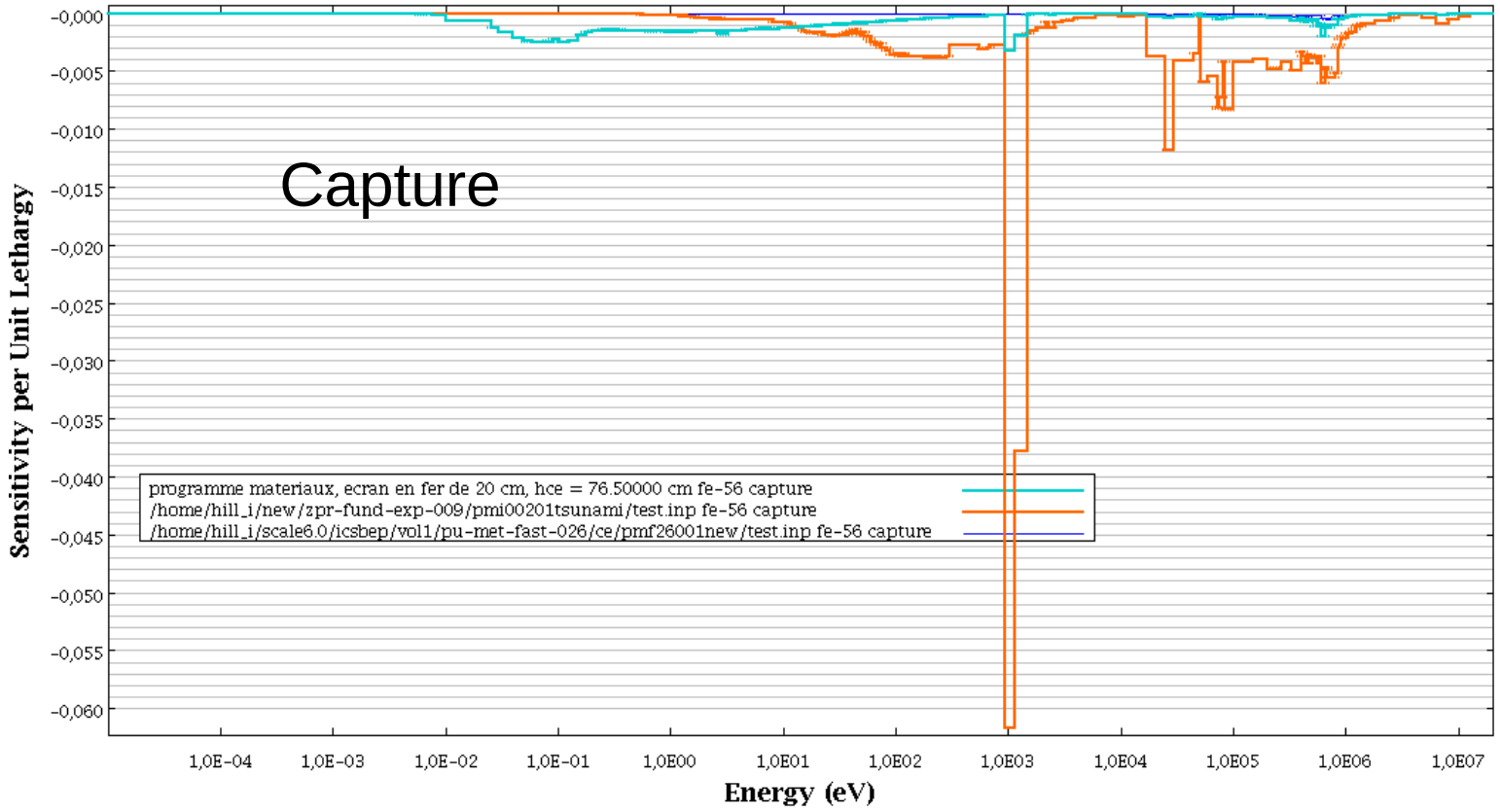
Integral Experiments for Validation of ^{56}Fe



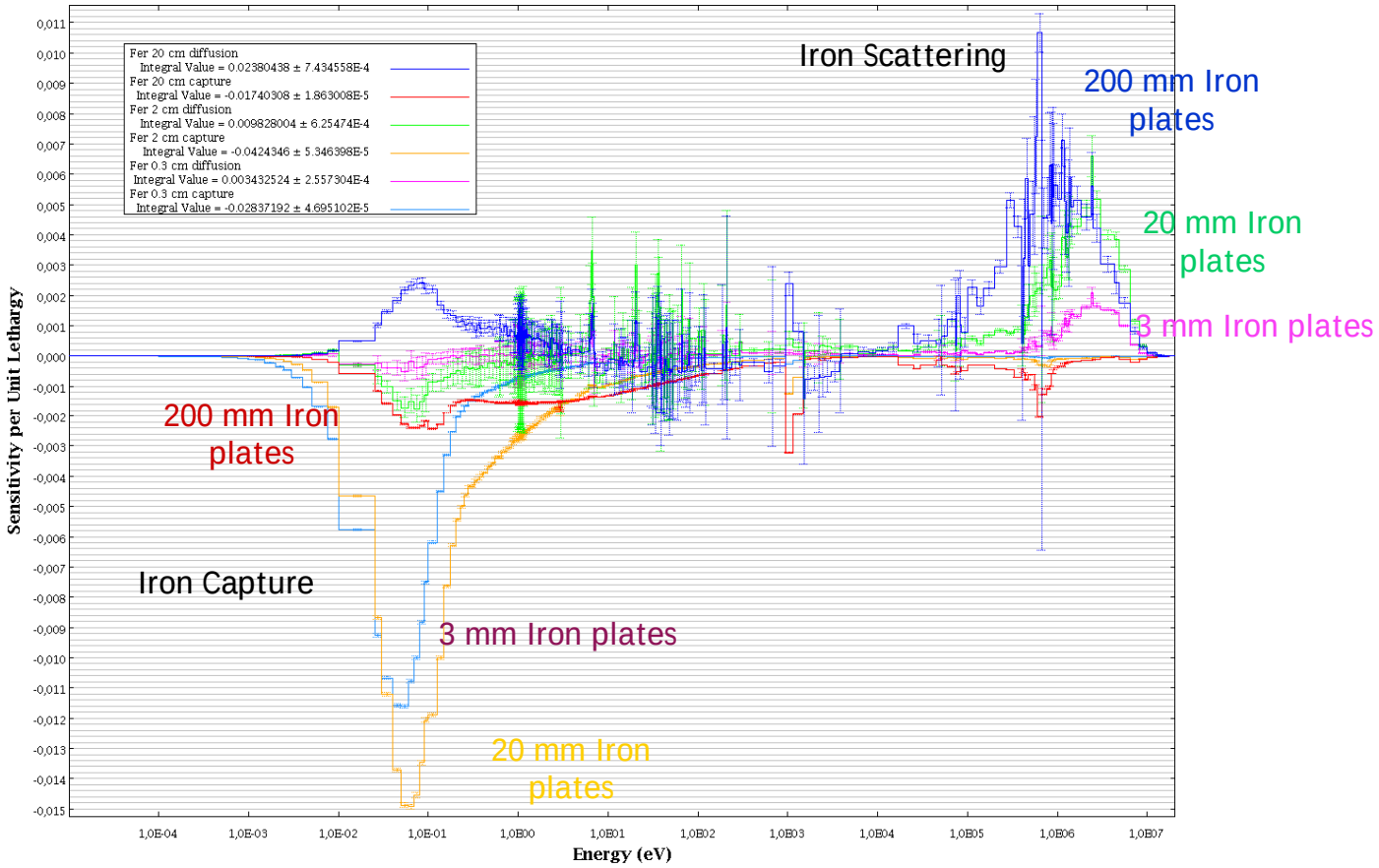
Integral Experiments for Validation of ^{56}Fe



Integral Experiments for Validation of ^{56}Fe

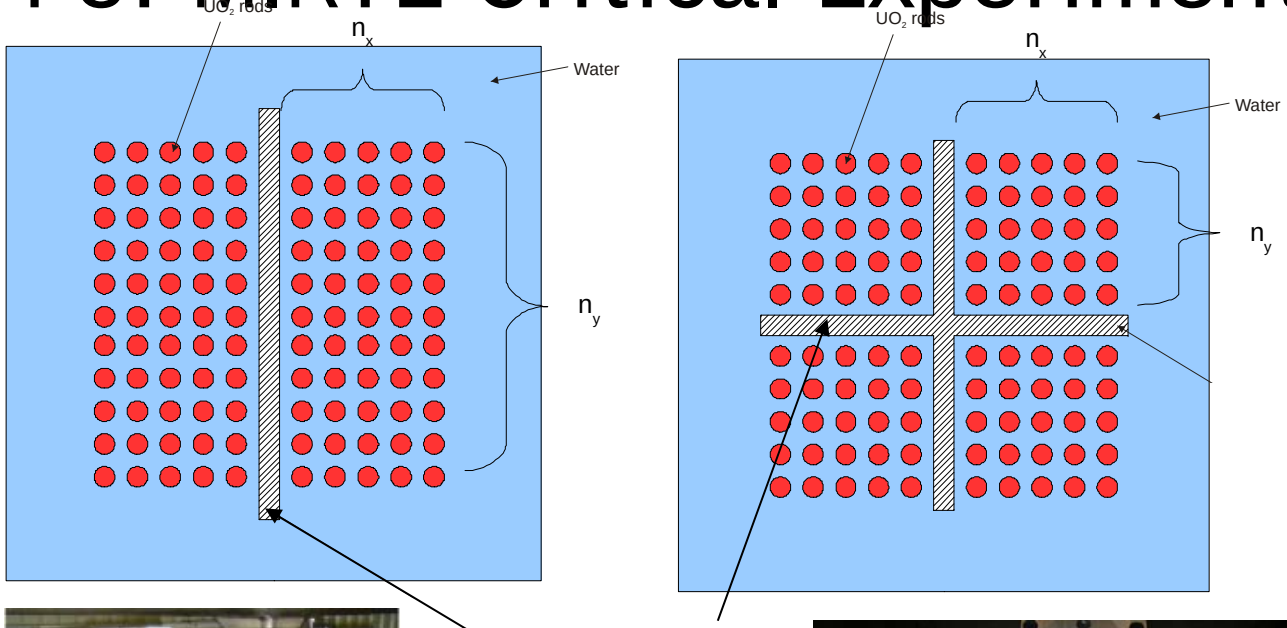


Integral Experiments for Validation of ^{56}Fe: MIRTE Critical Experiments*

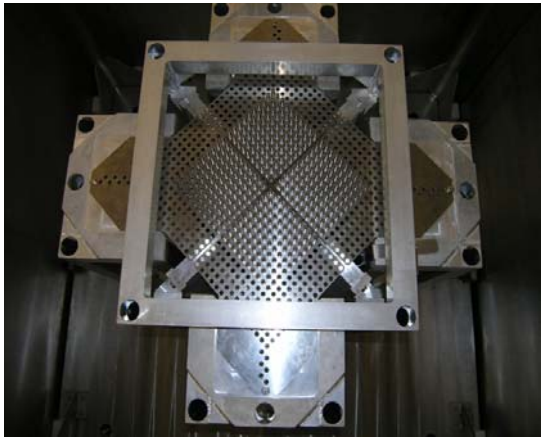


*Performed at Valduc facility, CEA, France. Not openly available

Integral Experiments for Validation of ^{56}Fe: MIRTE Critical Experiments*



Fe screen of different thicknesses



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Software Tools Available

Cross-section Processing

NJOY, AMPX GAIA

Integral Parameters Calculations

SCALE/KENO CE, 238-gr. MORET CE, 172 gr.

MCNP CE

Sensitivity Calculations

SCALE/TSUNAMI 238-gr.

Data Assimilation

SCALE/TSURFER BERING

GAIA

- **New nuclear data processing software prototype under development at the IRSN**
- **Reconstruct cross sections in the new R-Matrix Limited (RML) format of ENDF-6**
- **Generate angular distributions from R-matrix resonance parameters**
- **Uses Fourier transforms for cross-section Doppler broadening**
- **Demonstrated good agreement with NJOY and SAMMY for ^{56}Fe, ^{16}O and ^{35}Cl**

Further Work

- **Further development of GAIA**
- **Work on other isotopes of mutual interest (Cu, Gd, Ca, and others)**
- **Establishment of experimental correlations for the selected benchmarks**
- **Add reaction rates and reactivity worth into data assimilation**
- **Use of BERING together with TSURFER for data assimilation**