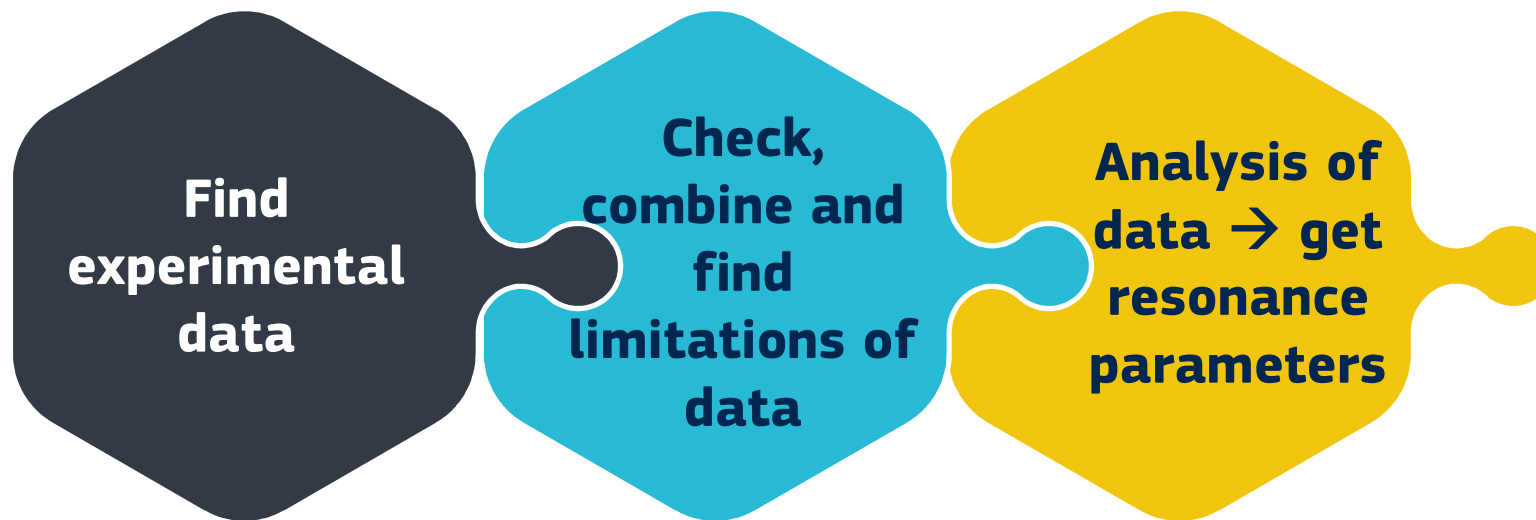


JRC contribution to the JEFF project

S. Kopecky, A. Oprea, C. Paradela, P. Shillebeeckx, R. Mucciola, C. Massimi, M. Hursin, D. Rochman

6th International Workshop On Nuclear Data Evaluation for Reactor applications WONDER 2023, Aix-en Provence, 05-09/May/2023

Steps of an evaluation in the RRR

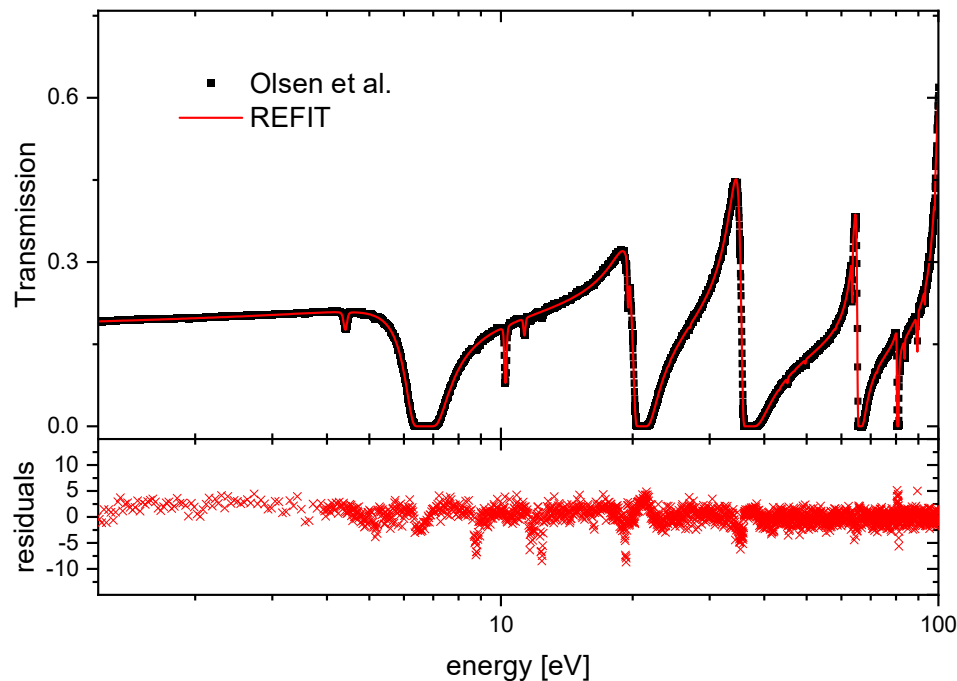


Find all useful experimental data (EXFOR) and publications e .g
Energy dependent data, scattering length, integral benchmark.....

Identify the limitations of data, the use of data from publications without data in EXFOR, data discrepancies and possible explanations

Resonance shape analyses
→ Ensure file is “complete”,
→ Isotopes are consistent with each other,.....

“Ideal” situation



- Well documented TOF experimental data available in EXFOR
- Measurements with isotopically enriched samples for consistent resonance assignment
- Resonance parameters obtained by a combined RSA, including facility TOF response

The molybdenum case

Current situation in the RRR

- Two independent evaluations: JENDL-3.3 and JENDL-4.0
- No transmission or capture data sets are available in EXFOR
- Evaluations do not exploit all available experimental data sets

Experimental data used for JENDL-3.3

	Transmission	Capture	Spin
⁹² Mo	Wasson (ORELA)	Weigmann (GELINA) Musgrove (ORELA)	Musgrove (ORELA)
⁹⁴ Mo		Weigmann (GELINA) Musgrove (ORELA)	
⁹⁵ Mo	Shwe and Coté (ARGONNE)	Weigmann (GELINA)	
⁹⁶ Mo		Musgrove (ORELA) Wiegmann (GELINA)	
⁹⁷ Mo		Weigmann (GELINA)	
⁹⁸ Mo	Chrien (ORELA)	Musgrove (ORELA) Weigmann (GELINA)	Musgrove (ORELA)
¹⁰⁰ Mo	Weigmann (ORELA)	Musgrove (ORELA) Weigmann (GELINA)	Musgrove (ORELA)

Experimental data used for JENDL-4.0

	Transmission	Capture	Spin
^{92}Mo	Wasson (ORELA)	Wiegmann (GELINA) Musgrove (ORELA)	Musgrove (ORELA)
^{94}Mo	Wang (POHANG)	Wiegmann (GELINA) Musgrove (ORELA)	
^{95}Mo	Shwe and Coté (ARGONNE) Wang (POHANG)	Wiegmann (GELINA)	
^{96}Mo	Wang (POHANG)	Musgrove (ORELA) Wiegmann (GELINA)	
^{97}Mo	Wang (POHANG)	Wiegmann (GELINA)	
^{98}Mo	Chrien (ORELA) Wang (POHANG) Babich and Anufriev	Musgrove (ORELA) Wiegmann (GELINA)	Musgrove (ORELA)
^{100}Mo	Wiegmann (ORELA) Wang (POHANG)	Musgrove (ORELA) Wiegmann (GELINA)	Musgrove (ORELA)

Study of Molybdenum in RRR

- 1) Search in literature
- 2) Study of transmission and capture data reported in the literature:
 - compilation of resonance parameters based on these data
- 3) Transmission cross section measurements using ^{nat}Mo samples at 50m GELINA:
 - adjust the compiled resonance parameter file by RSA with REFIT

Experimental data available

	Transmission	Capture	Spin
⁹² Mo	Wasson (ORELA)	Wiegmann (GELINA) Musgrove (ORELA)	Musgrove (ORELA)
⁹⁴ Mo	Wang (POHANG)	Wiegmann (GELINA) Musgrove (ORELA)	Sheets (LANL)
⁹⁵ Mo	Shwe and Coté (ARGONNE) Wang (POHANG)	Wiegmann (GELINA)	Sheets (LANL)
⁹⁶ Mo	Wang (POHANG)	Musgrove (ORELA) Wiegmann (GELINA)	
⁹⁷ Mo	Shwe and Coté (ARGONNE) Wang (POHANG)	Wiegmann (GELINA)	Walker (LANL)
⁹⁸ Mo	Chrien (ORELA) Wang (POHANG) Babich and Anufriev	Musgrove (ORELA) Wiegmann (GELINA)	Musgrove (ORELA)
¹⁰⁰ Mo	Wiegmann (ORELA) Wang (POHANG)	Musgrove (ORELA) Wiegmann (GELINA)	Musgrove (ORELA)
natMo	Leinweber (RPI), Pevzner (DUBNA), Wynchank (Columbia)		

Compilation of resonance parameters

- 1) Resonance energies from Weigmann as reference, adjusting the other data sets
- 2) Combination of Weigmann and Musgrove capture kernels up to 5 keV
- 3) Combine capture with transmission data, including transmission of natural samples (Leinweber, Wynchank)

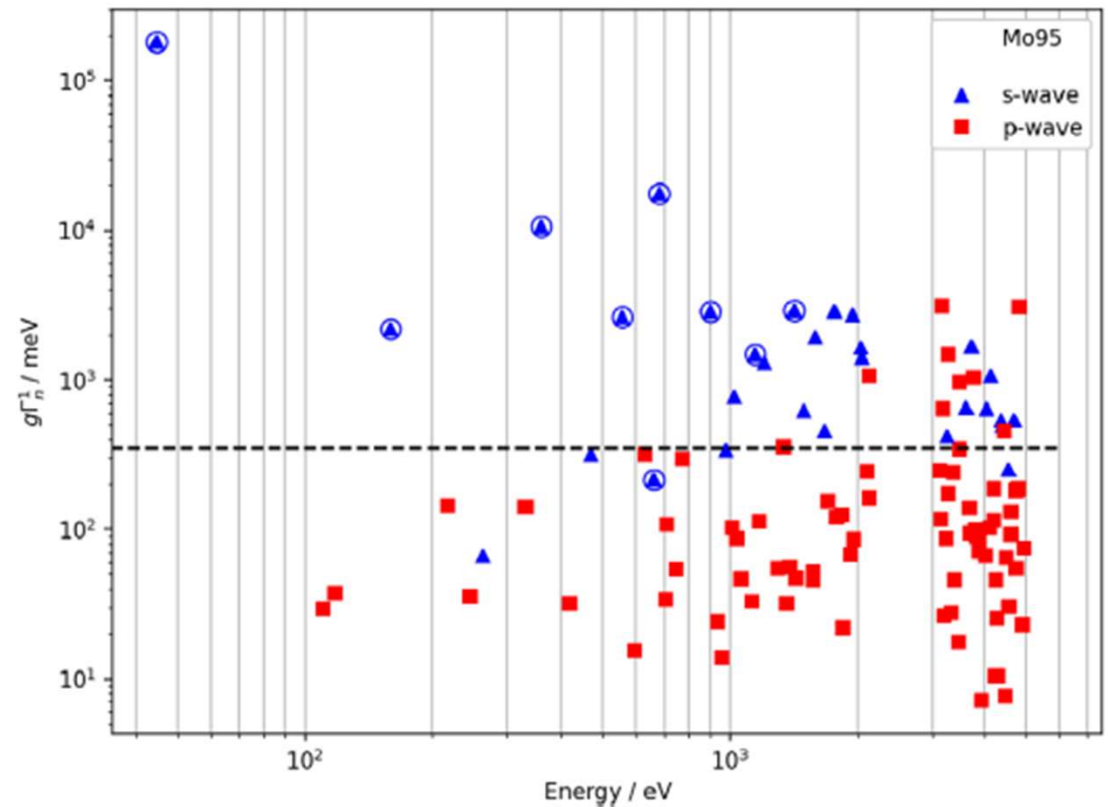
$$K_{\gamma} = g\Gamma_n\Gamma_{\gamma}/\Gamma$$

$$K_t = g\Gamma_n$$

- 4) Check spin and parity assignments for g calculation

Spin assignment

- Parity and spin assignments using full literature available
- Verified based on values of the reduced neutron width supposing all p-waves
- S-wave assignment based on asymmetry resonance profile in transmission (circles)



Compilation of resonance parameters

- 5) If capture kernel K_γ and resonance strength K_t available, capture width obtained

$$\Gamma_\gamma = \frac{1}{g} \frac{K_t K_\gamma}{K_t - K_\gamma}$$

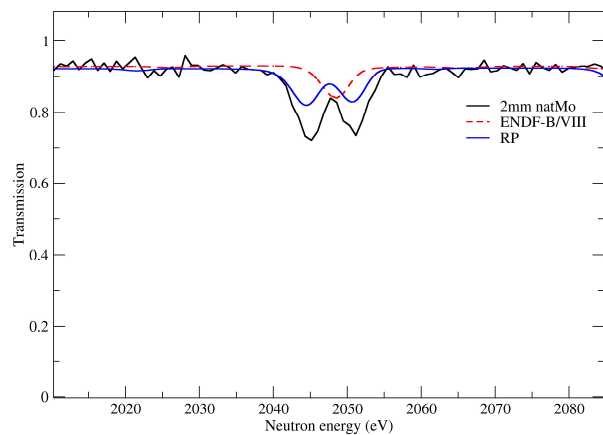
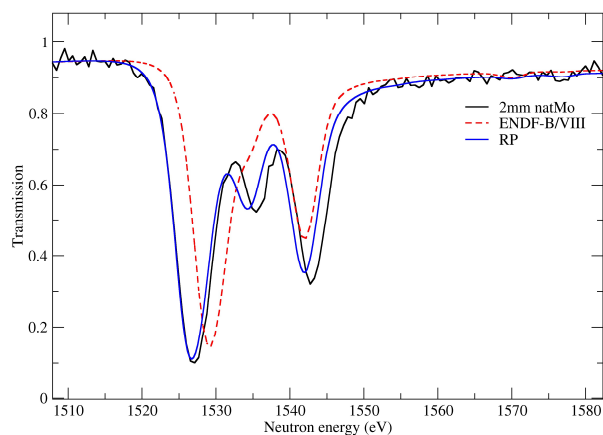
- 6) Γ_γ adopted if <50% deviation from average radiation width

- 7) If only capture kernel available, average radiation width adopted and Γ_n obtained from

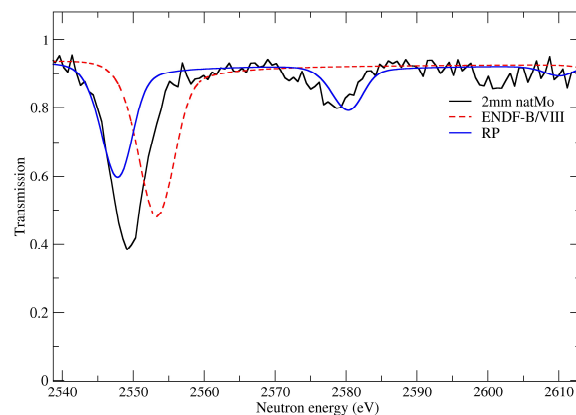
$$\Gamma_n = \frac{\bar{\Gamma}_\gamma K_\gamma}{g \bar{\Gamma}_\gamma - K_\gamma}$$

- 8) Initial set of parameters verified by comparison with experimental transmission

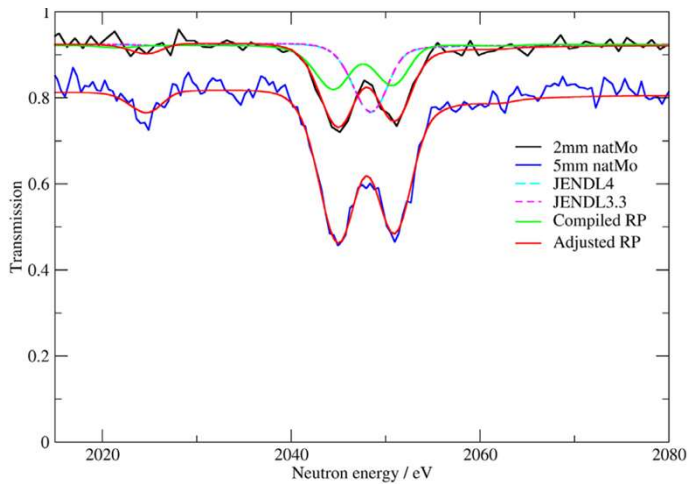
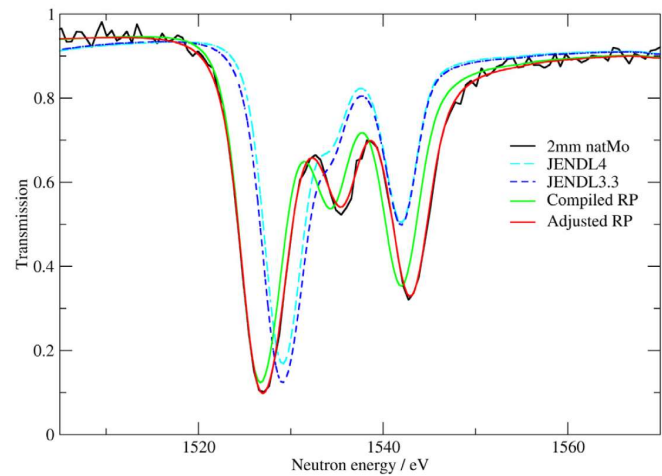
Verification of proposed RP



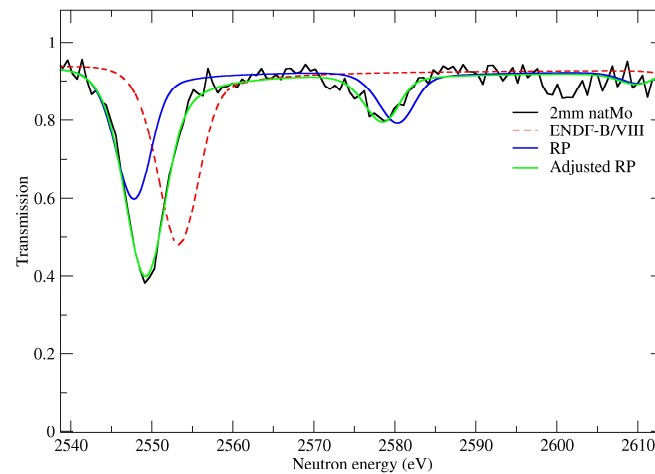
- RP file verified by transmission data (50 m) of 2 mm and 5 mm thick ^{nat}Mo samples
- Inconsistency for various resonance parameters in ENDF/B-VIII.0 (JENDL-3.3) library
- Missing resonances in ENDF/B-VIII.0 added to compilation using literature data
- **New RP file improve data description.**



Adjusted RP



- RP file improved by an adjustment to transmission data using REFIT
- Fit of resonances up to 5 keV



Reporting new resonance parameters

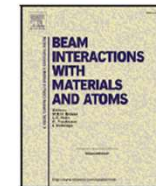
Nuclear Instruments and Methods in Physics Research B 531 (2022) 100–108



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Evaluation of resonance parameters for neutron interactions with molybdenum

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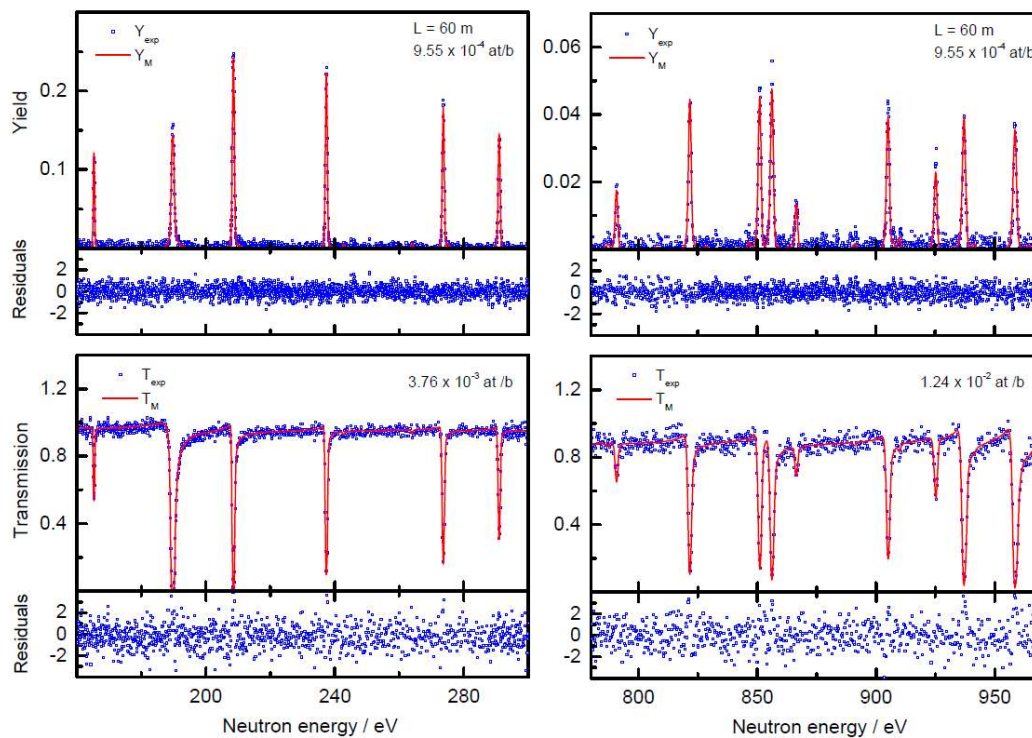
Neutron resonance parameters
Transmission measurements
R-matrix analysis
Evaluation
GELINA
Molybdenum

ABSTRACT

Resonance parameters for neutron interactions with ^{92,94,95,96,97,98,100}Mo in the energy region below 5 keV were evaluated. The parameters are the result of a compilation of experimental data available in the literature together with a least squares adjustment to transmission data obtained at the time-of-flight facility GELINA. The experiments were performed at a 50 m transmission station using a ⁶Li glass scintillator as neutron detector and metallic samples of natural Mo with a thickness of 2 mm and 5 mm. The REFIT code was used to adjust the resonance parameters, i.e. resonance energy and strength.

Evaluation of $^{238}\text{U}+n$ in RRR in JEFF-4.0

New evaluations in ENDF/B-VIII and JEFF-4.0



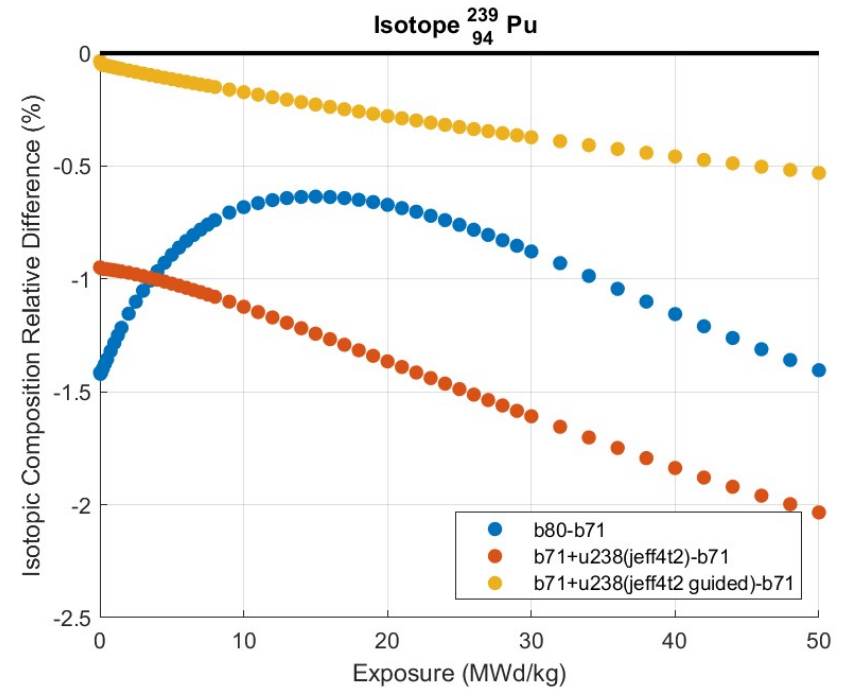
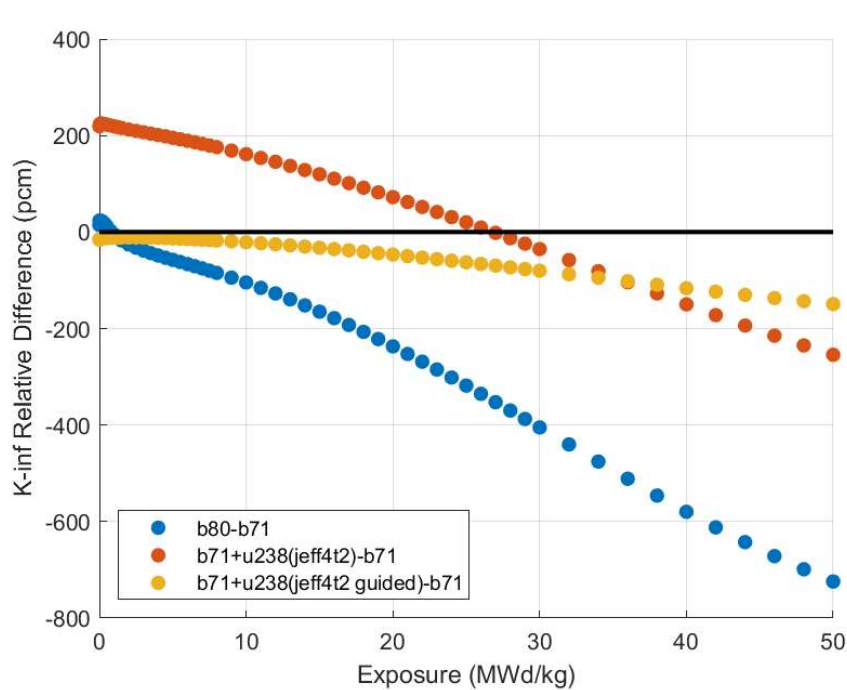
Y_{exp} (GELINA) and T_{exp} (ORELA):

fully consistent,
without any additional
renormalisation
or background correction

- $\langle \Gamma_{\gamma} \rangle$
 - This work : 22.5 meV
 - Derrien et al. : 23.0 meV

BUT...

U-238 observed problem with JEFF-4.0



Trend of K_{inf} overprediction with increasing burn-up, partially due to U-238

Test: $+1\% \langle \Gamma_{\gamma} \rangle \rightarrow$ trend almost disappear

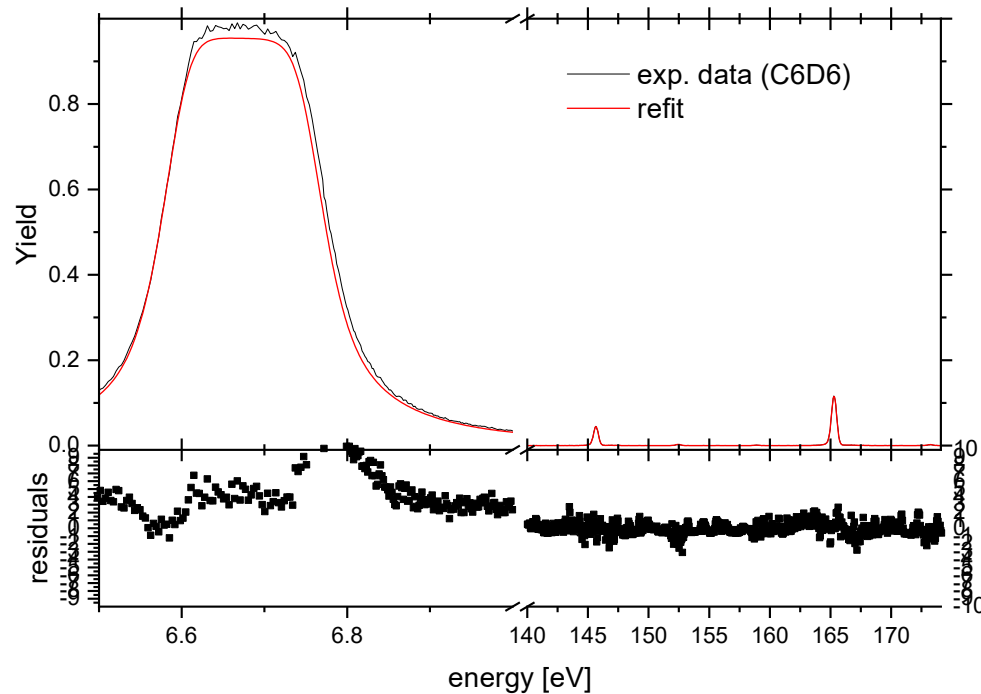
Average Γ_γ

Year	author	$\langle \Gamma_\gamma \rangle$	
1988	Sowerby	23.5	From energy dependent data
1994	Sowerby and Moxon	23	From energy dependent data
2004	Courcelle	22.7	Derived from integral benchmark LEU-MET-THERM-006
2005	Derrien	23.24	Kept 23.0 assigned to resonances
2016	JEFF-3.3	22.5	From energy dependent data Assigned to all resonances

Available experimental data

Energy range	reference	measurement	samples	FP	
6 eV – 10 keV	De Saussure ORELA (1973)	Capture	2 samples	40 m	Energy dependent normalization
0.25 keV – 20 keV	Macklin ORELA (1988)	Capture	2 samples	150 m	Energy dependent normalization
0.5 eV- 1.2 keV	Kim GELINA (2016)	Capture	2	12.5 m	
0.1 keV- keV	Kim GELINA (2016)	Capture	1	60 m	
1eV-80keV	Wright n_TOF (2017)	Capture (TAC)	1	185 m	No – resolution
1eV-710keV	Mingrone n_TOF (2017)	Capture (C6D6)	1	185 m	No – normalization
10 eV- keV	GELINA (no ref)	Transmission	1	50 m	Calibration
0.5 eV – 1 keV	Olsen ORELA (1979)	Transmission	7 samples	42 m	

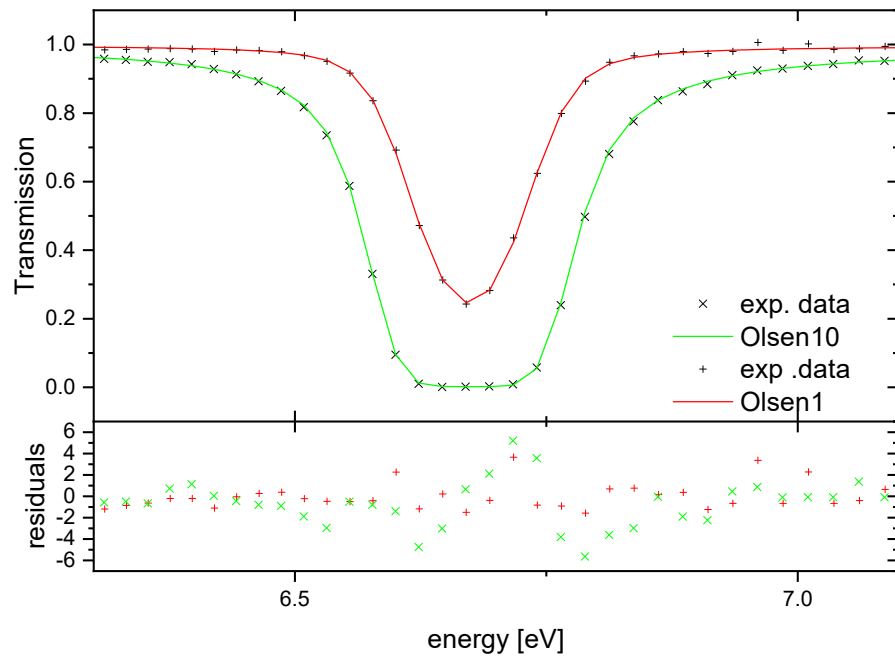
N_TOF (C6D6)



$$\Gamma_n \ll \Gamma_\gamma$$

- RP from transmission and normalisation from capture
- 5% difference in normalisation between resonances
- Background correction not complete
- Reason/solution not clear, so data not used (at least for the moment)

Fitting first resonance

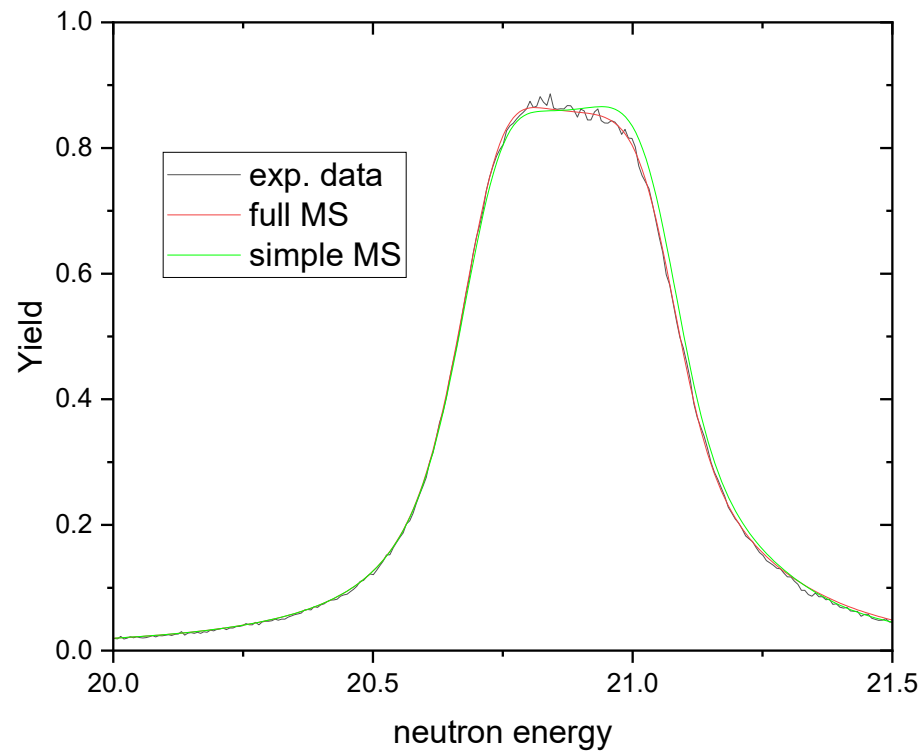


$$\Gamma_n = 1.49 \text{ meV}$$
$$\Gamma_\gamma = 22.71 \text{ meV}$$

RSA of transmission data only!

Doppler broadening FWHM 90 meV
Resolution FWHM 3 meV

Fitting second resonance



$$\Gamma_n = 10.08 \text{ meV}$$

$$\Gamma_\gamma = 22.75 \text{ meV}$$

Saturated capture yield $\Gamma_\gamma / (\Gamma_n + \Gamma_\gamma)$

multiple scattering

Gamma attenuation correction

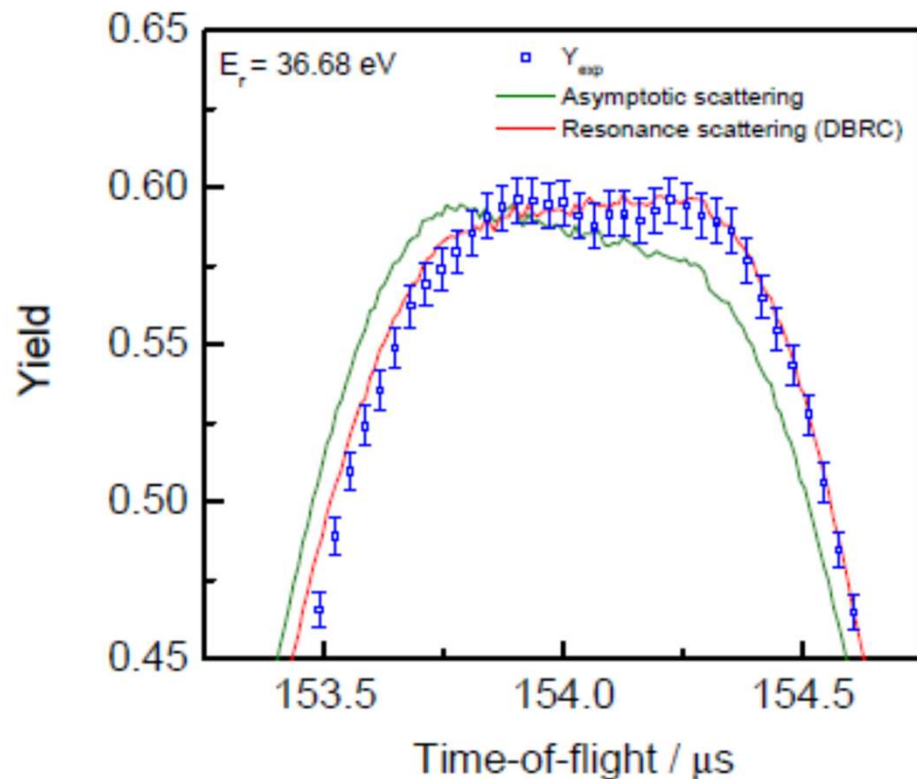
→ Moderate correction

Transmission data Γ_n , Γ_γ , RSA

Doppler FWHM 157 meV

Resolution FWHM 35 meV

Fitting third resonance



$$\Gamma_n = 33.59 \text{ meV}$$

$$\Gamma_\gamma = 22.26 \text{ meV}$$

Saturated capture yield $\Gamma_\gamma / (\Gamma_n + \Gamma_\gamma)$

multiple scattering

Gamma attenuation correction

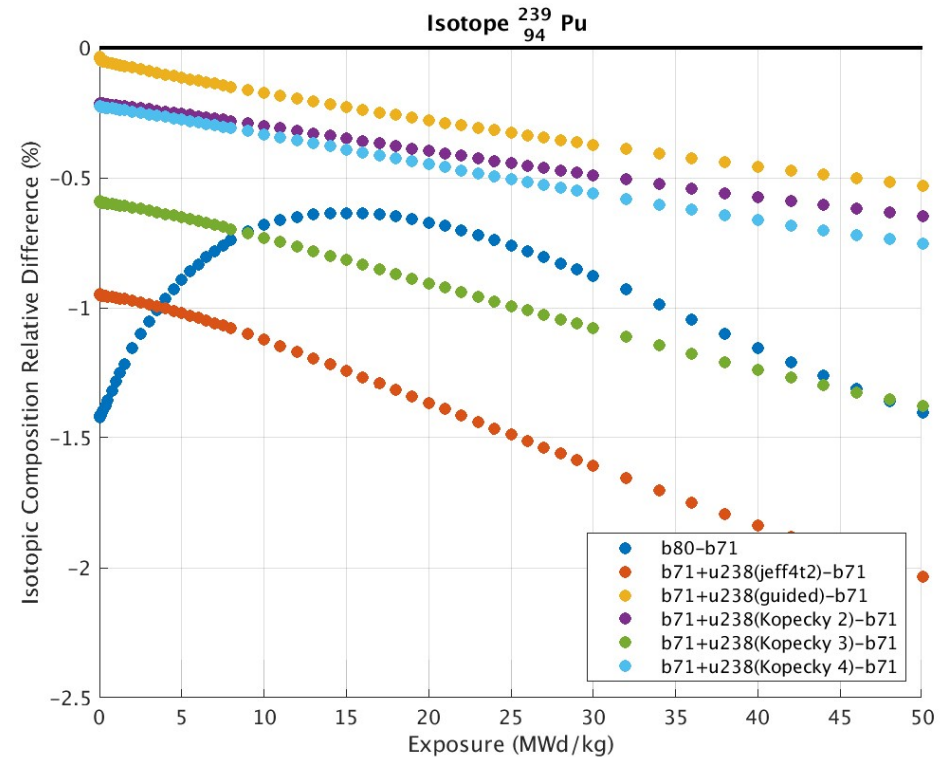
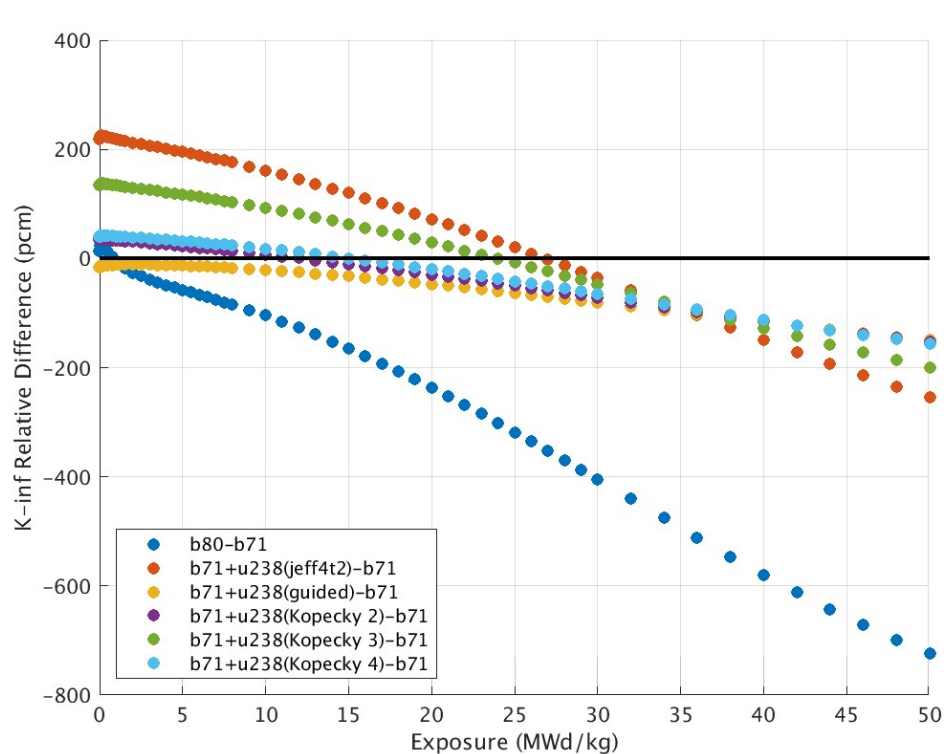
→ Significant corrections (DBRC)

Transmission data Γ_n , Γ_γ , RSA

Doppler FWHM 200 meV

Resolution FWHM 51 meV (Olsen)

Impact of new U-238 evaluation



JEFF-4.t2 $\langle \Gamma_\gamma \rangle = 22.75$ meV (Consistent with fitted two first resonances)

Trend with burnup largely reduced, but work still in progress

Conclusion

For reliable evaluation in the resolved resonance region (especially when the experimental database is limited)

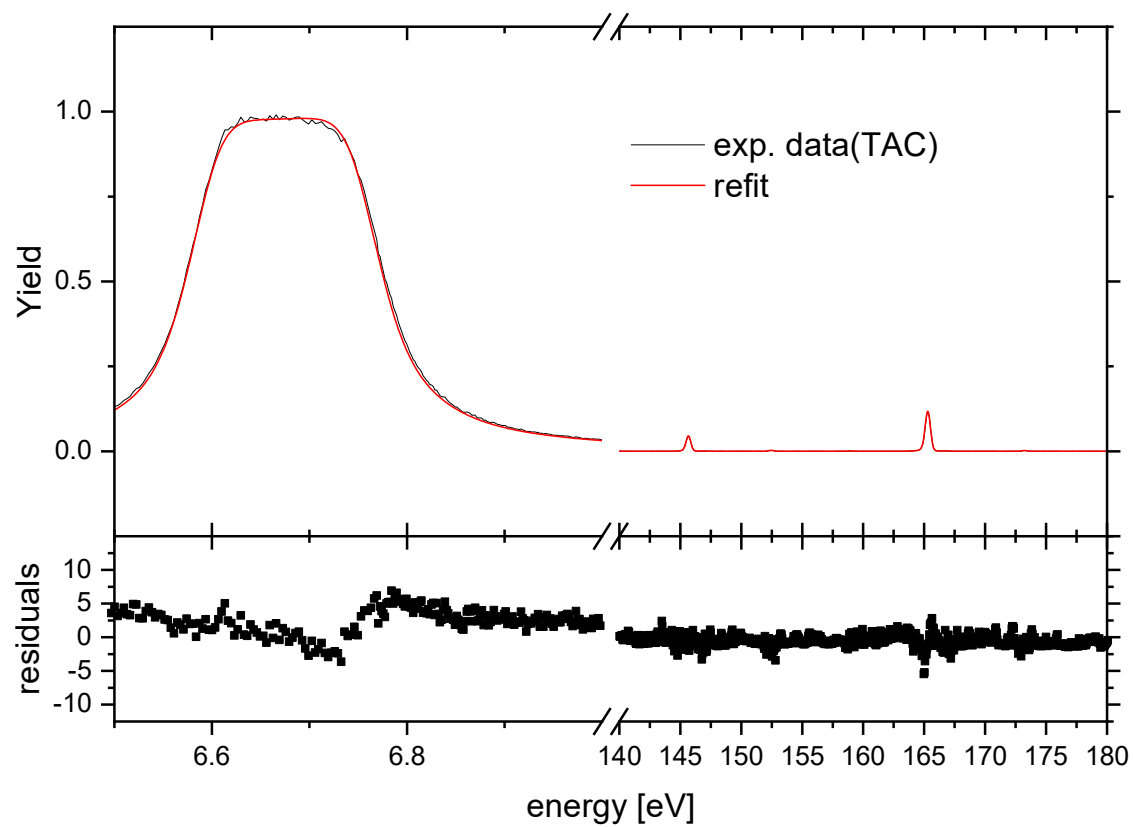
- Find **all** available experimental data (EXFOR and publications)
- **Assessment** of data (read papers.....)
 - Find limitations of data
- **Account** for all relevant information
- Derive a consistent set of resonance parameters
- Always **check consistency** with (thick) transmission on natural samples
- New U-238 evaluated file for test in JEFF4.t2. New capture data would help

Thank you

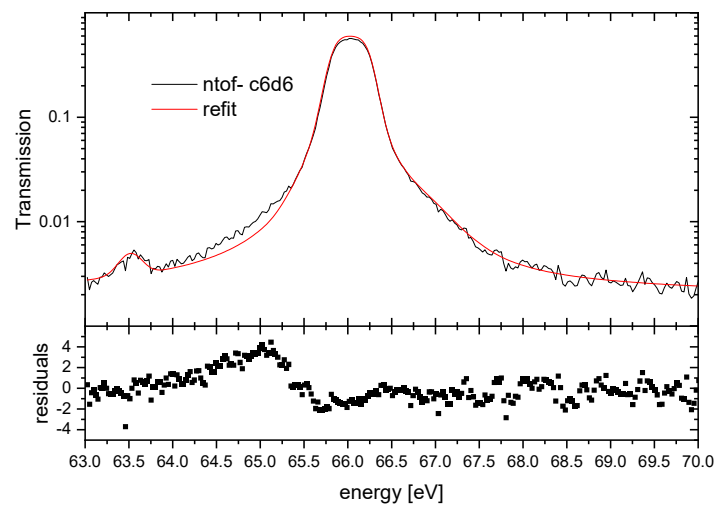
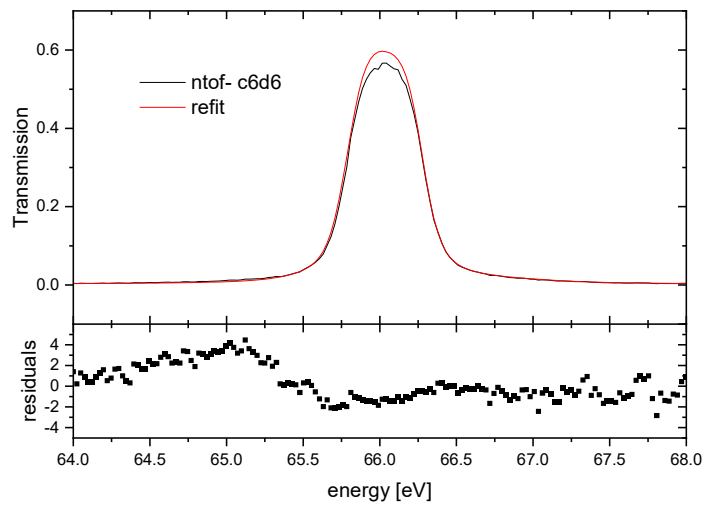
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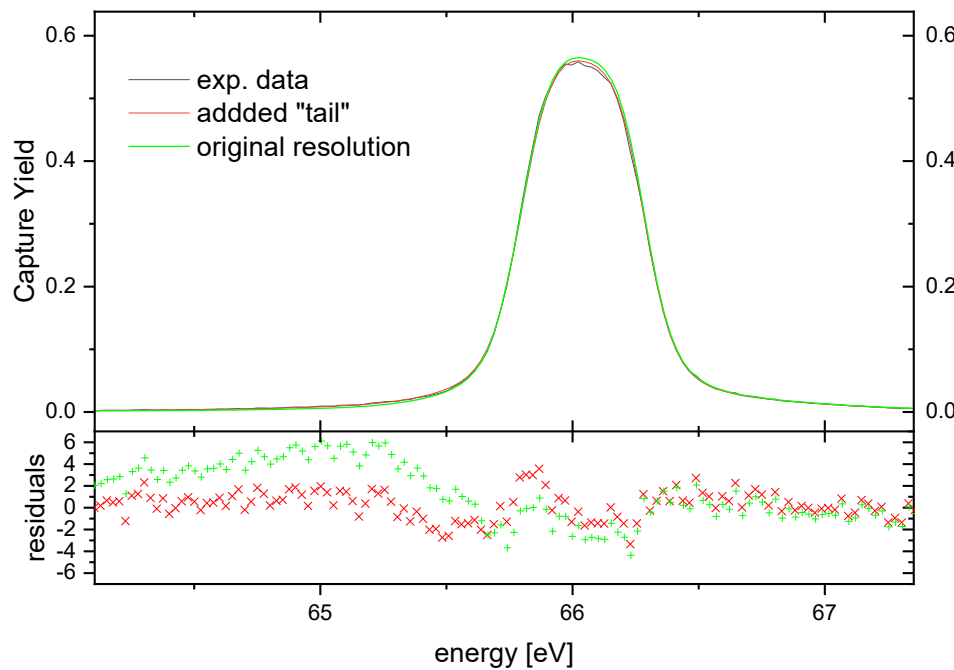
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Slide xx: [element concerned](#), source: [e.g. Fotolia.com](#); Slide xx: [element concerned](#), source: [e.g. iStock.com](#)



- Consistency checks of normalisation at three resonances
- Resolution function (Gunsing)





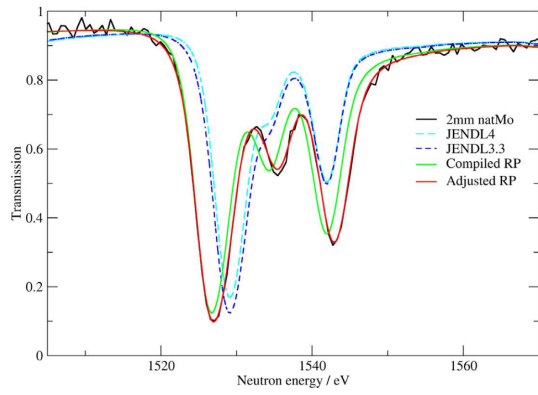
Additional “tail” in resolution function

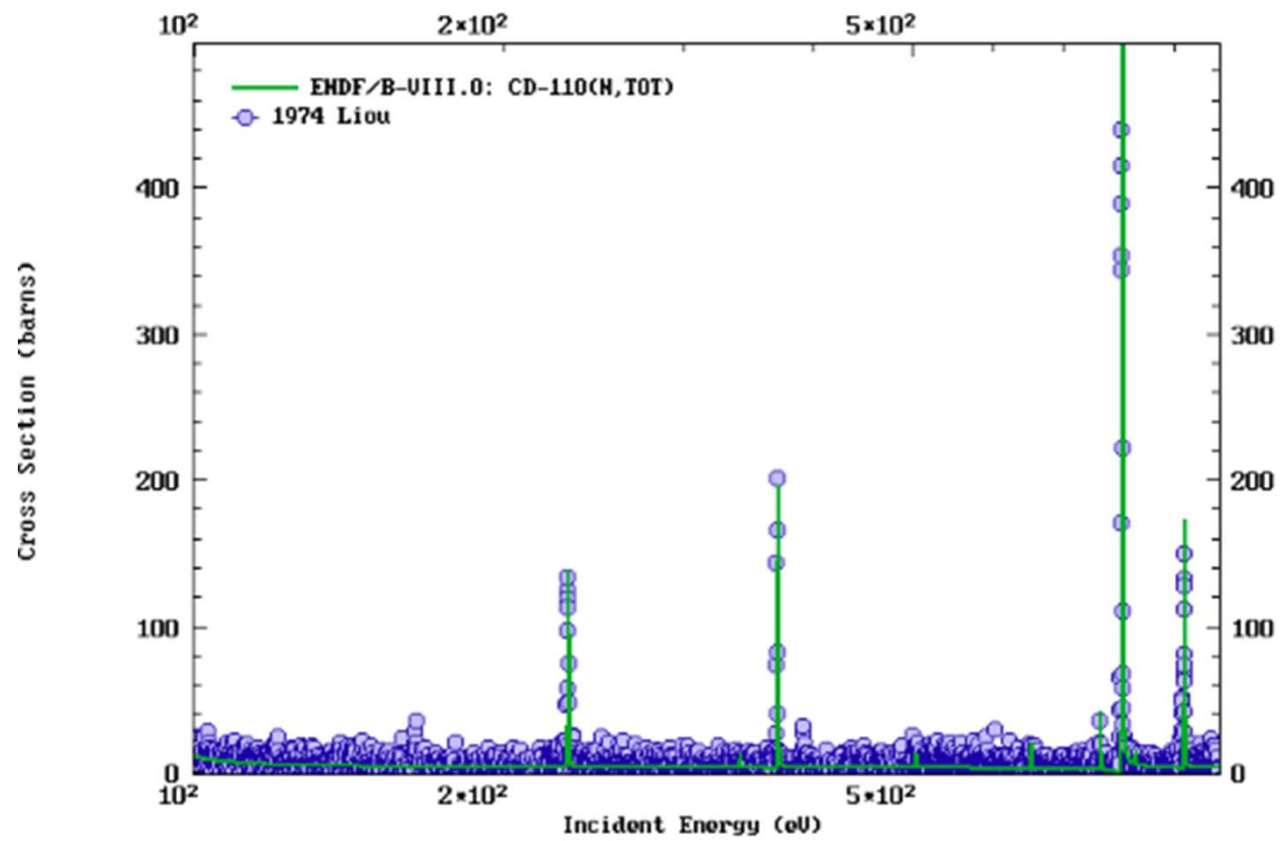
Amplitude a few percent

Exponential decay with time constant equivalent to approx. 60 cm equivalent distance

Simultaneous fit of TAC and GELINA data not possible
 Gg TAC 5-6 % higher than GELINA data
 Gg higher than JEFF-3.2 and JEFF-3.3

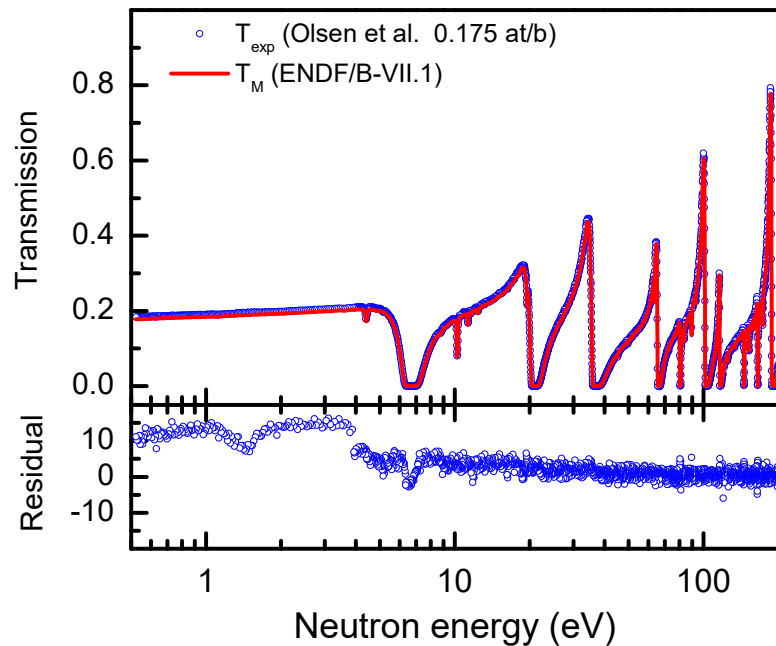
resolution or neutron sensitivity/multiple scattering?



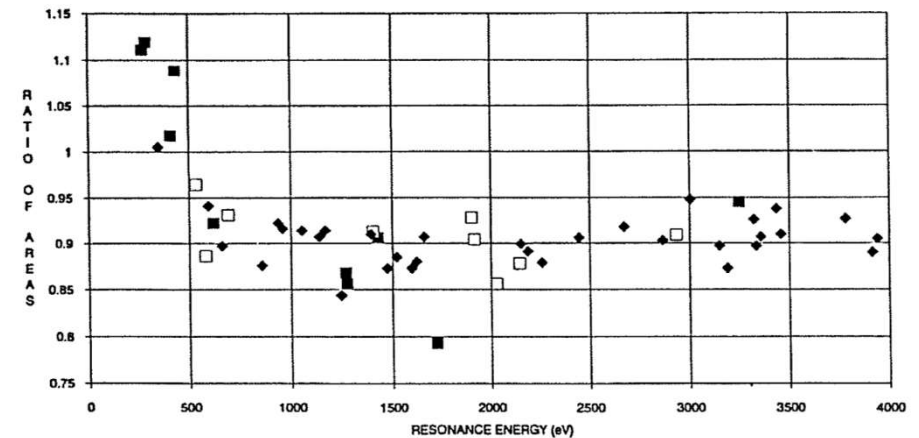


Evaluation of $^{238}\text{U}+n$ in RRR in ENDF/B-VII

- Transmission data
 - Not consistent with evaluated resonance parameters
 - Data were re-normalised



- Capture data
 - All data included in evaluation require a substantial renormalisation
 - de Saussure et al. x 0.85
 - Macklin et al. x 1.10
- See Moxon et al., PHYSOR 90



The ratio of the measured to calculated capture areas for a selection of resolved resonances in the data of Macklin et al. The solid squares, open squares and solid diamonds are for resonances with Γ_n values <40 , $40-80$ and >80 meV respectively.