OAK RIDGE National Laboratory

ORNL Contribution to the Cross Section Evaluation Working Group

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Nuclear Data Criticality Safety
Oak Ridge National Laboratory, USA

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for the US Department of Energy

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U.S. DEPARTMENT OF ENERGY

Outline

- n+^{16}O (Pigni)
- α+^{17,18}O (Pigni/Croft/Gauld)
- n+^{28,29,30}Si (Pigni/Arbanas/Guber[1]/Capote[2]/Trkov[2])
- n+^{35}Cl (Pigni/Guber[1])
- n+^{40}Ca (Pigni/Guber[1])
- n+^{63,65}Cu (Guber/Sobes/Leal[3])
- n+^{140,142}Ce (Chapman/Pigni/Guber[1])
- n+^{155,156,157,158,160}Gd (Leal[3]/Sobes)
- n+^{156,158,160,161,162,163,164}Dy (Pigni)
- n+^{180,182,183,184,186}W (Pigni/Leal/Guber[1])
- n+^{233}U (Pigni/Guber[1])
- n+^{235}U (Pigni/Leal[3]/Capote[2]/Trkov[2])
- n+^{239}Pu (Pigni/Guber[1])
- n+^{51}V, ^{139}La, ^{181}Ta (Guber[1]/Pigni/Barry[4])

(1) For experimental contribution
(2) IAEA
(3) IRSN
(4) RPI

n+^{233}U evaluation – Status

- Precise ^{233}U(n,f) and ^{233}U(n,tot) cross section measurements performed at ORELA (1997–2000) built the basis of the ORNL evaluation (2001) included in ENDF/B-VII.1 library (2006). However, **only the shape of the ORELA fission cross sections was used**
  - The newly measured fission data were normalized to consistently fit the total cross section and the existing capture measurements
  - A recent ^{233}U(n,f) cross section measurement performed at the nTOF facility (*Phys. Rev.* C80, 044604 (2009)) shows agreement (within 2%) with the ORELA fission data

- Poor performance in benchmarks calculations
- In ENDF/B-VIII.0 library resonance parameter evaluation (file 2) is up to 600 eV but the related covariance file (32) is only up 300 eV!!!!

Detailed report on the status of ^{233}U was prepared within NDAG/NCSP (Guber 2018)

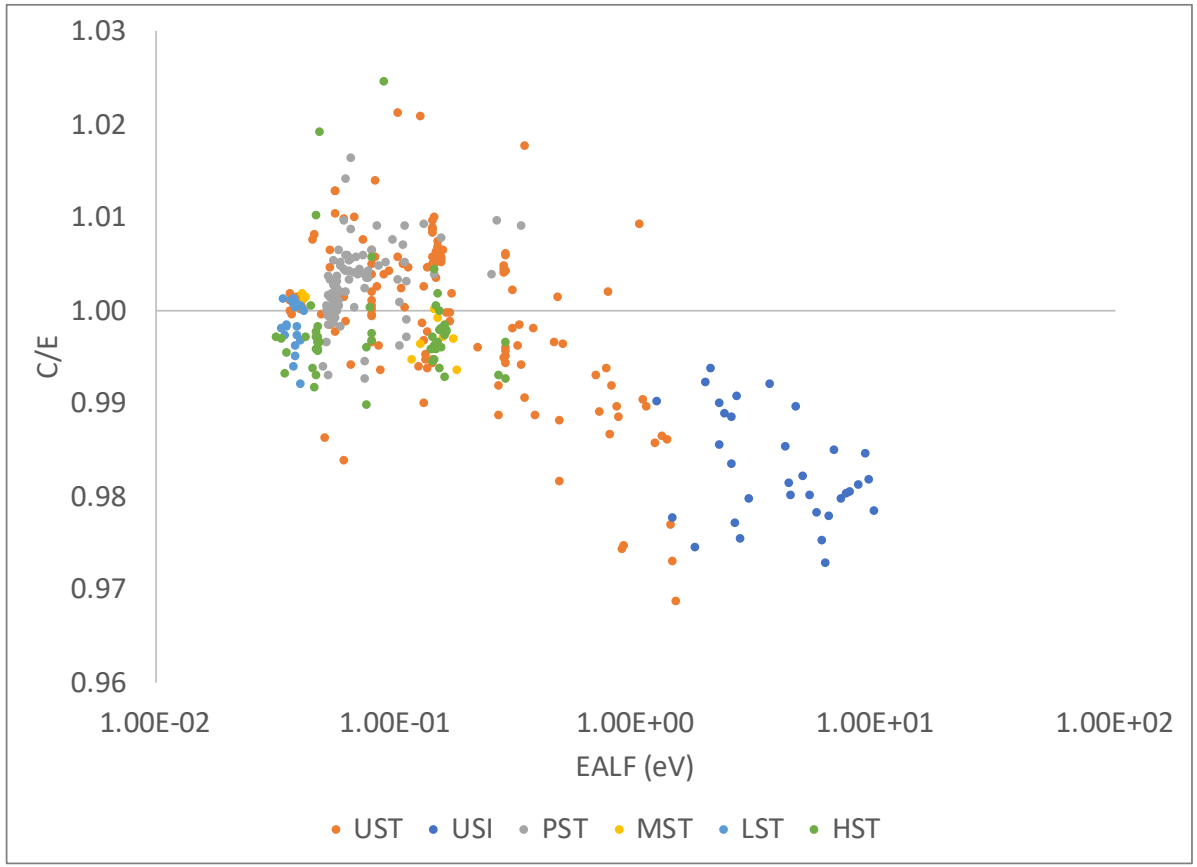
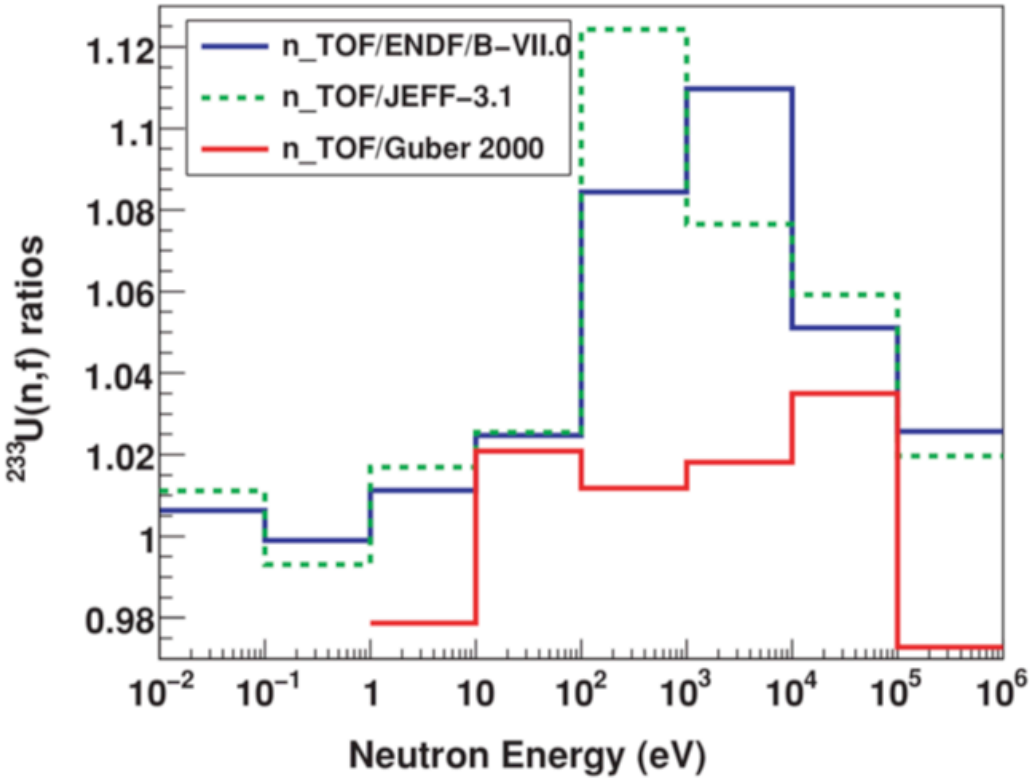


Figure from B.J. Marshall

n+^{233}U evaluation – Plan

- To generate an updated RRR evaluation fitting the ORELA measured fission data
  - Deviations up 8% between 0.1—1 keV between theoretical and measured data (see figure taken from Phys. Rev C 80 44604). However, the **real deviation** needs to be determined due to the large uncertainties obtained in the integration over energy bins.
- To check the consistency and normalization of the measured capture data to accordingly fit the fission and transmission data
- To improve the poor performance in benchmark calculations



n+^{28,29,30}Si evaluations – Status

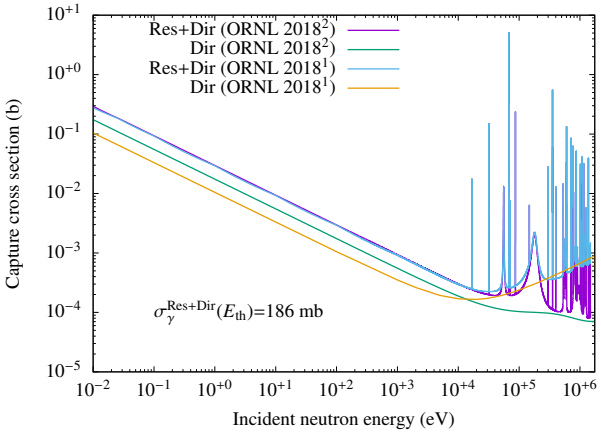
- The set of RM resonance parameter evaluations of ^{28,29,30}Si was restored from the archives (ORNL/TM-2001/271)
  - These evaluations were never included in the ENDF/B-VII.0 release because of the difficulty, at that time, of processing ENDF files containing direct neutron capture contributions
- In the thermal energy range the direct capture contribution is not negligible (about 40%)
- The ^{28}Si(n_{th},γ) cross was controversial due to the discrepant experimental values
- Although ENDF/B-VIII.0 library for silicon evaluations was not updated, the overall agreement with integral measurements improved but not for measurements sensitive to the thermal range

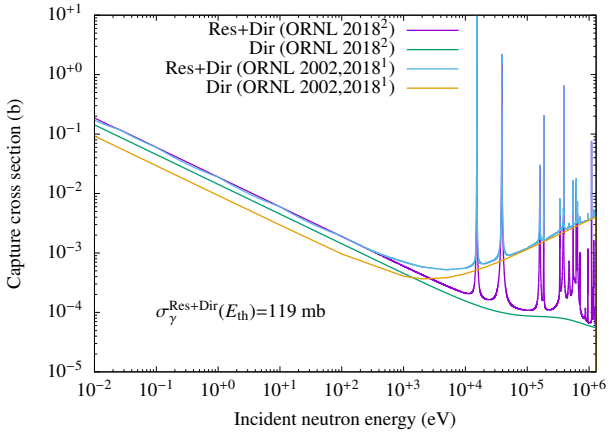
Author (Year)	Value (mb)	σ_γ(res)	σ_γ(dir)
Islam (1990)	207±4		
Kennett (1992)	171±3		
Raman (1992)	169±3		
Mughabghab (2006)	177±4		
ORNL (2002)	168.9	103.1	65.8
IAEA (2007)	186±3	N/A	N/A
ENDF/B-VIII.0 (2018)	169.1	169.1	0
ORNL (20181)	184.5	131.9	52.6
ORNL (20182)	186.01	76	110

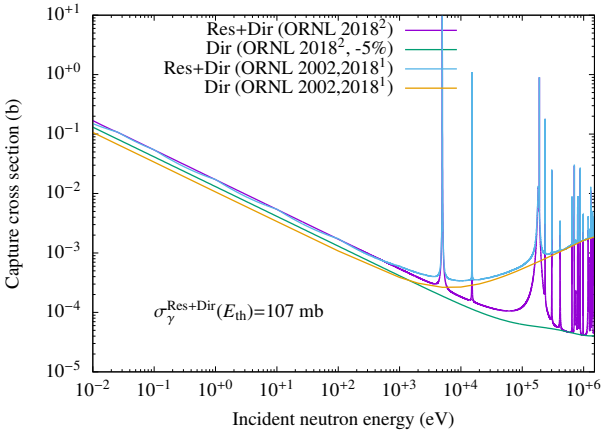
- Two sets of silicon evaluations were produced. The first set of evaluations (ORNL I) used the original TEDCA calculations for the direct contribution. The second set (ORNL II) relied on updated calculations performed by CUPIDO code

n+^{28,29,30}Si evaluations – Plans

- The goal is to correct the unfavorable behavior of the TEDCA calculations for neutron energy above 10 keV
- New calculations with the CUPIDO code were performed (G. Arbanas) by using a complex optical potential to consistently account for the absorption cross sections







- CUPIDO calculations needed to be decreased by 5% to match the $\sigma_\gamma(E_{th}) = 107$ mb
- Tests on ORNL II gave improved results on benchmark calculations over ORNL I and ENDF/B-VIII.0
- Inclusion of a **complex** component for the **channel radii** (new feature) can be used to describe the direct capture component within R-matrix formalism. This allows to produce resonance parameters and related reconstructed cross sections in full unitary regime

^{28,29,30}Si evaluations - Status

^{28}*Si* **Thermal capture increased by ~10% following Firestone et al, IAEA EGAF**

Direct capture considered by CUPIDO (ORNL) and new consistent ORNL evaluations

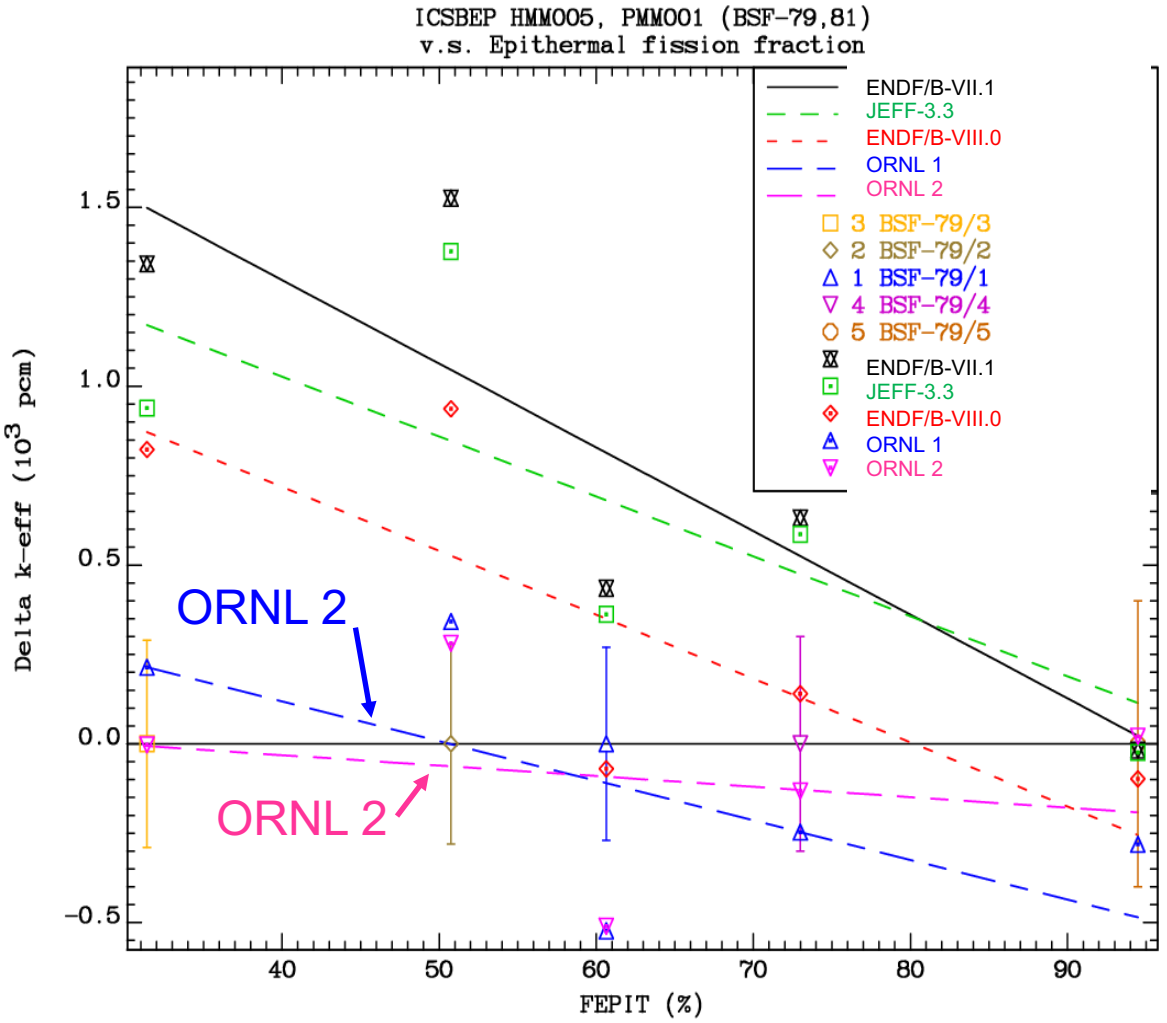
-> Criticality impact ~ -800 pcm in thermal assemblies (e.g., hmm005.3)

Criticality is independent of the epithermal fraction in spectra (~zero slope) !!

Better physics & criticality performance improved in new evaluations

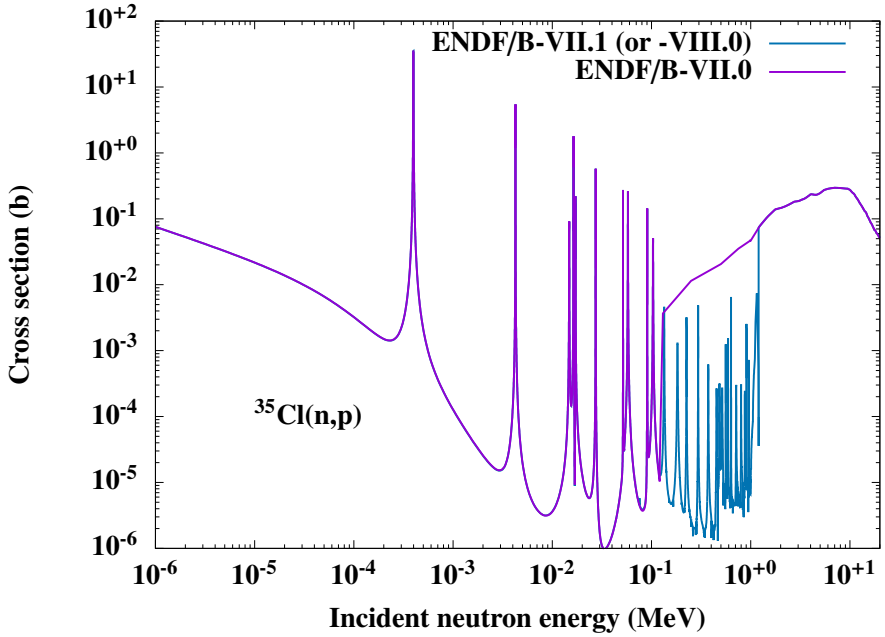
Consistent unitarity in R-matrix treatment

New evaluations READY !



n+^{35}Cl evaluations – Status

- The n+^{35}Cl evaluation in the RRR up to 1.2 MeV was performed at ORNL for the release of the ENDF/BVII.0 nuclear data library in 2006
  - Due to the limited energy range of the (n,p) measured data, in that evaluation the R-matrix analysis of (n,p) reaction channel included resonance parameters only up to 100 keV
- In a revision of the ENDF/B-VII.1 library in 2011 (adopted by the ENDF/B-VIII.0), the energy range of the ^{35}Cl(n,p) cross sections was extended up to 1.2 MeV by using the average proton width obtained from the measured data previously used in the ENDF/B-VII.0 evaluation
- A proposal to measure high-resolution n+^{35}Cl cross sections and generate an updated evaluation/validation was submitted to LAB18-903
  - At the nTOF facility, measurements of ^{35}Cl(n,p) cross sections are in progress



n+^{35}Cl evaluations – Plans

- The changes in the average (n,p) cross sections in the neutron energy range of 100 keV up to 1 MeV between the ENDF/B-VII.0 and ENDF/B-VIII.0 (or ENDF/B-VII.1) releases lead to significantly different reactivities in nuclear reactor simulations
- The ^{35}Cl evaluation is currently part of the NCSP appendix B plan. The resonance parameter evaluation will be performed by
  - including newly measured (n,p) cross sections, e.g. nTOF data.
  - updating the set of RP in $B_c = -l$ basis
  - including an estimate of the minor (n,α) reaction channel to preserve unitary of collision matrix
  - including the direct capture component (about 400 mb at thermal energy) by using a complex channel radius
- The n+^{35}Cl evaluation will be validated with particular emphasis on fast reactor applications

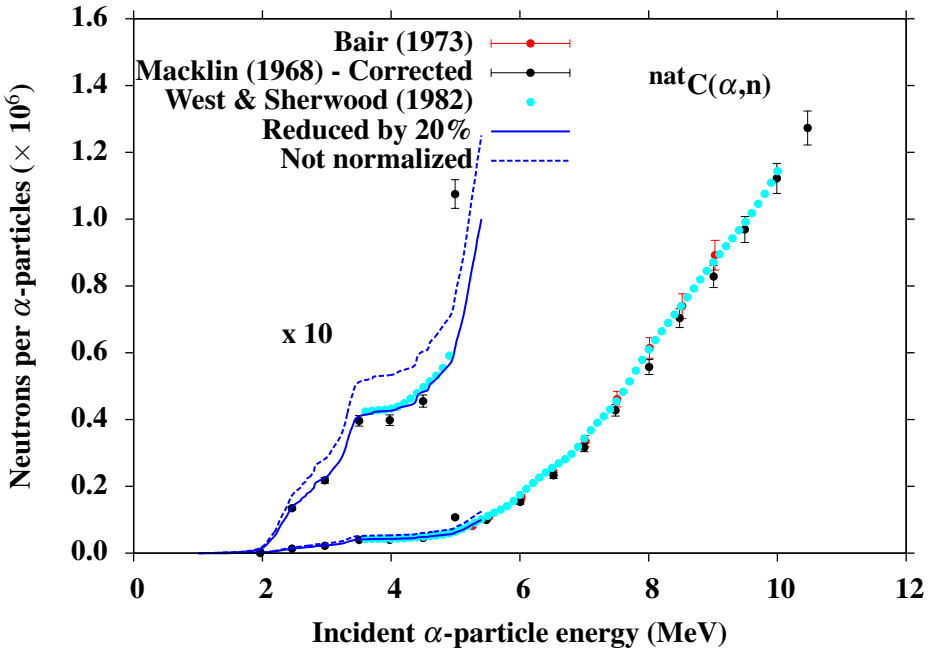
n+^{16}O evaluation – Status

- The R-matrix code SAMMY was used to generate a set of resonance parameters for n+^{16}O reactions in the energy range of thermal up to about 6 MeV
- Three advanced major features of the present evaluation are as follows
  - a) The use of the $B_c = -l$ boundary condition commonly used in the formal R-matrix theory but rarely used in SAMMY evaluation work.
  - b) The capture channel was treated as particle channels whose penetrability factor is set to be unitary in SAMMY input file
  - c) Closed-channel effects[1] were included for the (n,α) reaction channel (new feature in SAMMY)
- The evaluation work builds on a comprehensive resonance analysis that was initiated in FY16 a),b)[2] and updated through FY17 c)[3]
- This work did NOT follow on CIELO recommendations on the (n,α) cross sections. The normalization factor applied on this reaction channel based on the (corrected) Macklin's thick target measured data as explained in (2)
- This evaluation work is currently part of the series of INDEN meetings on light nuclei evaluations

(1) For threshold reaction channel as ^{16}O(n, α)^{13}C the RPs are sensitive to the cross sections also below E_{thr}
(2) Notes on the consistency of ^{16}O(n, α)^{13}C cross sections
(3) ORNL contribution to ENDF/B-VIII.0 and progress on the light nuclei evaluations

n+^{16}O evaluation – Plans

- The aim of this work is to provide a set of resonance parameters (RP)s as an alternative to the extant point-wise evaluation of oxygen in the ENDF/B-VIII.0 library
- Longstanding issues from measured ^{13}C(α,n)^{16}O cross sections due to the discrepancies between Bair (1973) and Harissopulos (2005) data sets are understood but additional thick target measurements for $E_a \leq 3$ MeV may be helpful



- Are the (n,α) yield data measured at LANL available?
- RPs are important in nuclear data evaluation analyses in which measurements were performed on oxide samples or liquid samples that have been dissolved or diluted with solutions containing light nuclei

n+^{239}Pu – Status/Plans

Status

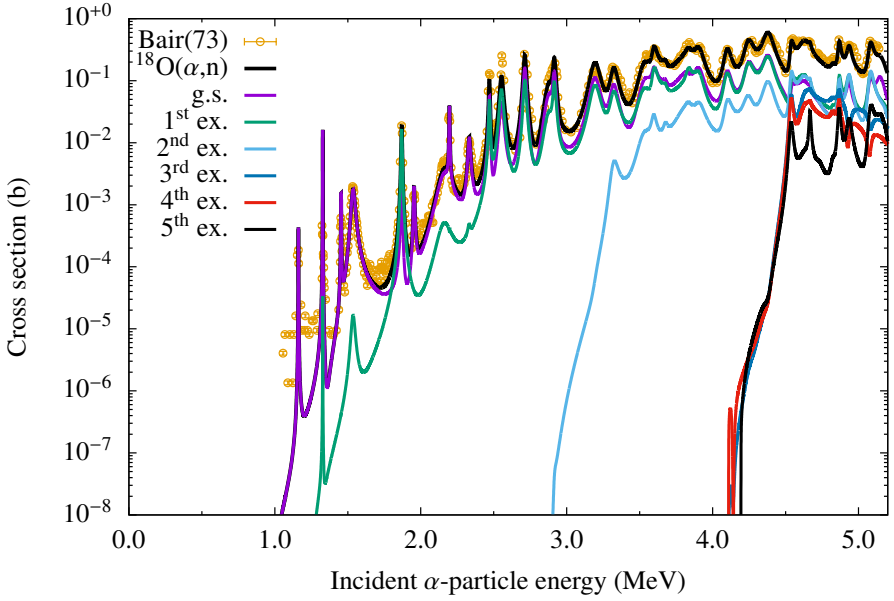
- In the ENDF/B-VIII.0 library the ^{239}Pu evaluated RP + covariances adopted from WPEC/SG42
  - This WPEC/SG42 work mainly consists on merging three independent sets of resonance parameters into a single set of parameters by keeping unchanged the performances of the evaluated data on PST benchmarks and MOX fuel calculations
  - No updates in the RRR performed within CIELO collaboration
- The URR parameters are the same as ENDF/B-VI library (1993)
- Post-fission observables, such as Prompt Fission Neutron Spectrum and neutron multiplicity, were updated by LANL evaluations

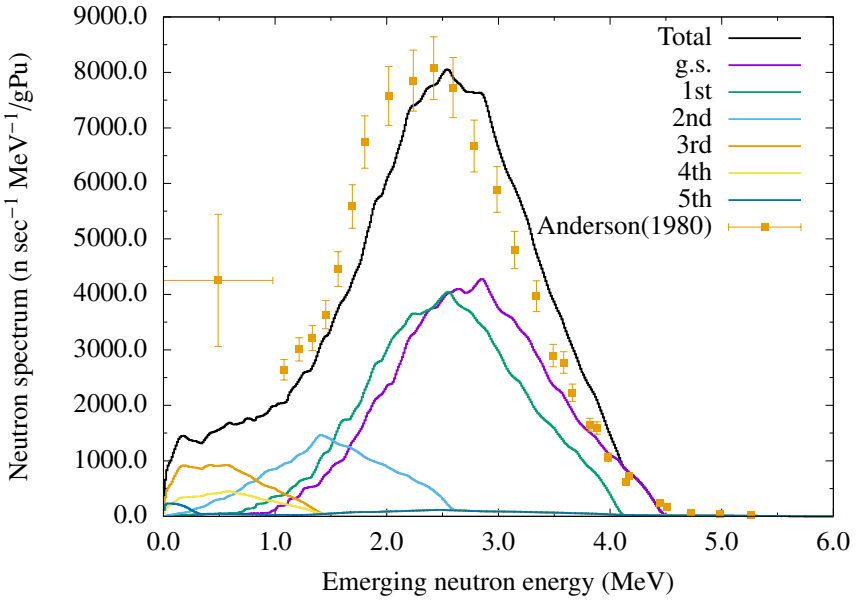
Plan

- To include new thermal neutron constants
- To include latest ^{239}Pu(n,γ) measured data starting from 1 eV
- The first resonances at 0.3 eV are based on old measurements (1958). New transmission experimental data are needed to improve the R-matrix parameterization
- The treatment of the two-step process, i.e., (n,f) + (n,γf), for the fission channel preserving the unitary of the collision matrix (S-matrix)
  - To investigate the possibility to extract experimental information on the (n,γf) process
- To improve URR by including an improved description of the broad intermediate structures

α+^{17,18}O evaluation – Plans

- Submittal of the α +^{17,18}O evaluations to ENDF repository
- Production of a suite of integral measurements is in progress and will be used to validate the oxygen cross sections
  - Example: Anderson et al. (1980) measured the energy-dependent neutron spectrum from (α ,n) reactions and spontaneous fission performed within a series of measurements from a moderated and unmoderated ^{238}Pu–^{18}O source
- Some information on the proper distribution of the excited states may be obtained from integral measurements
- Inclusion of Hauser-Feshbach calculations (new capability) for incident $E_a \geq 5$ MeV





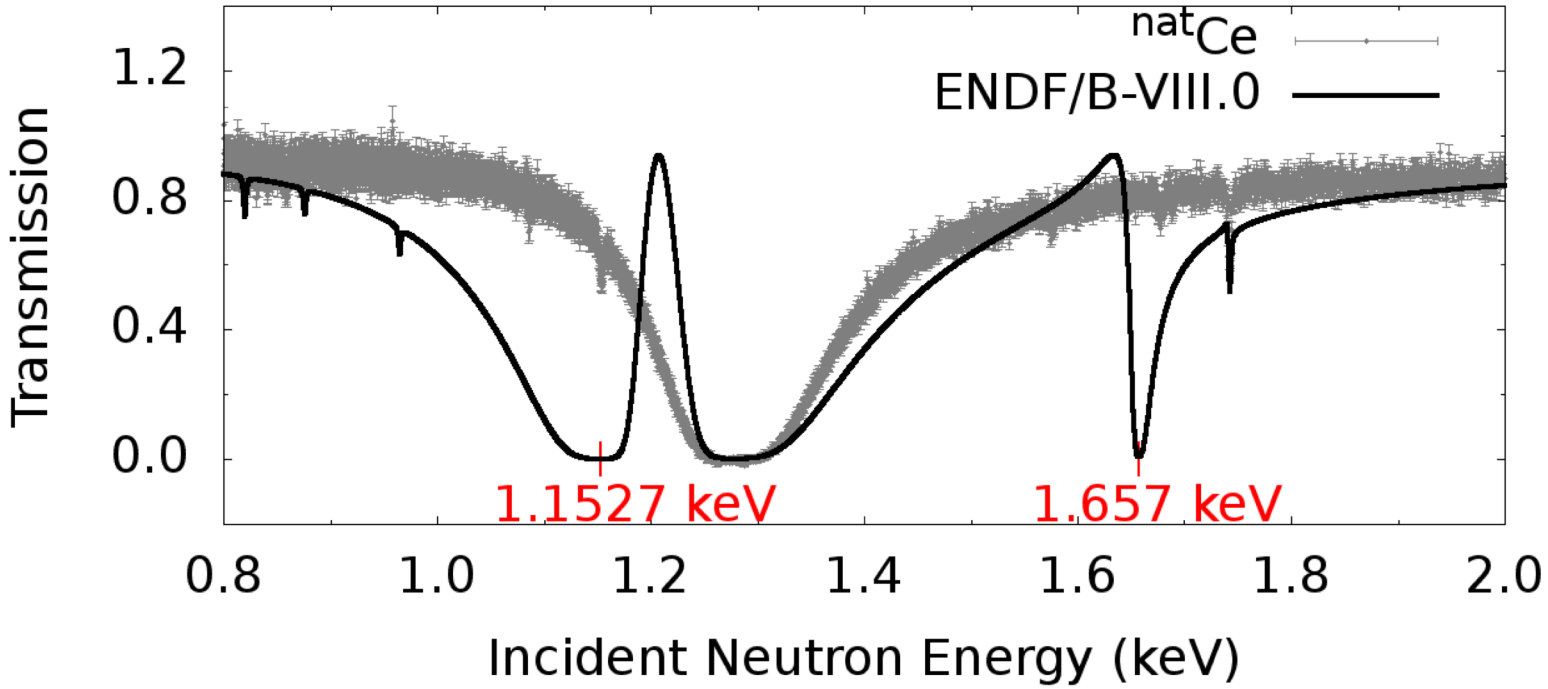
α+^{17,18}O evaluation – Status

- NA22 program recently funded α +^{17,18}O evaluations to improve the state of the art in modeling neutron emission processes needed for defense nuclear nonproliferation
- This work follows another project (*Prog. Nuclear Energy*, **91**, 147 (2016)) to quantitatively assess nuclear data uncertainties for safeguards and nonproliferation where ORNL focused on cross section covariance data for light nuclei used for neutron source calculations
- In the RRR up to 5 MeV, the evaluations will be represented by a set of RM resonance parameters in ENDF and GND format
- R-matrix analysis of (α,α) and (α,n) reaction channels up to about 5 MeV is based on available experimental data sets
  - (α,n) experimental data are based on Bair's measurements for both nuclei, however, these data are convoluted and it is impossible to quantify accurately the partial cross sections related to each excited states
  - In JENDL-AN (2002) the partial cross sections were based on HF calculations
  - In Sources4C the calculations of the partial cross section related to each excited states are also based on HF calculations performed by the GNASH code
- For ^{18}O Elastic channel, the spin assignment was based on measurement and the resonance analysis of Goldberg (*Phys. Rev.* C**69**, 24602, 2004) for available excitation energies
  - Goldberg's elastic angular excitation functions and angular distributions are not possible to fit together with (α,n) data sets
- Preliminary results published in proceedings of 2nd Advances in Nuclear Nonproliferation Technology and Policy Conference (ANTPC) 2018

n+^{140,142}Ce evaluations – Status/Plan

- Includes s-, p-wave resonances
- Energy range of RRR evaluation
  - ^{140}Ce: 0-200 keV
  - ^{142}Ce : 0-13 keV
- Formalism is in MLBW and no covariance data
- RP taken from ATLAS (approved by SG23, 2009)

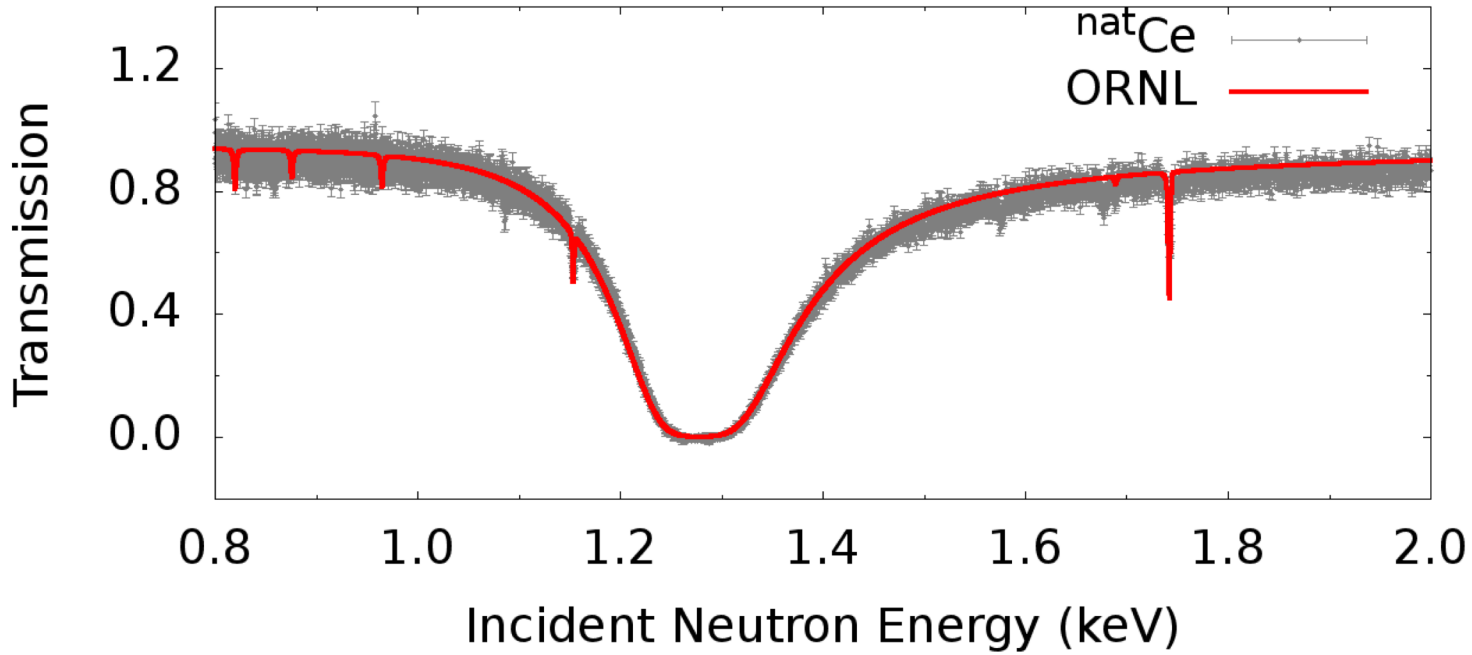
ATLAS reported wrong neutron resonances widths of ^{142}Ce at E_n=1.1527 and 1.657 keV



n+^{140,142}Ce evaluations – Status/Plan

- Strength Functions
  - External levels calculated using strength function
  - 4 resonances used to include edge effects
- Preliminary Fit
  - Corrected neutron resonance widths

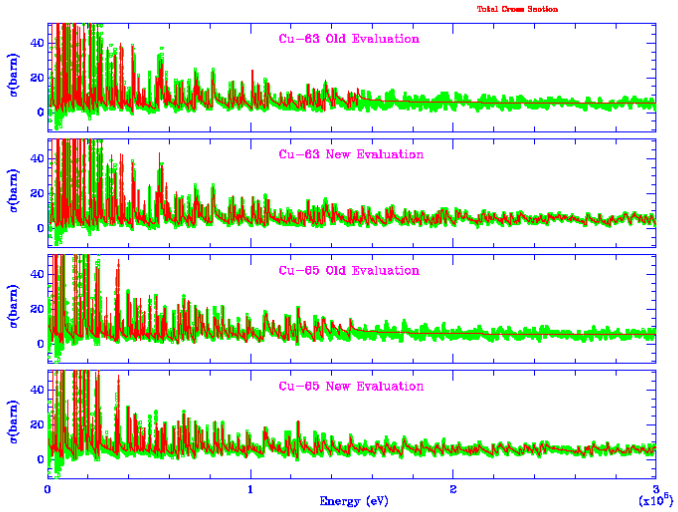
Energy (keV)	1.1527	1.657
Old spin group	s-wave	s-wave
New spin group	p-wave	p-wave
Old width (meV)	50000	10000
New width (meV)	50	10

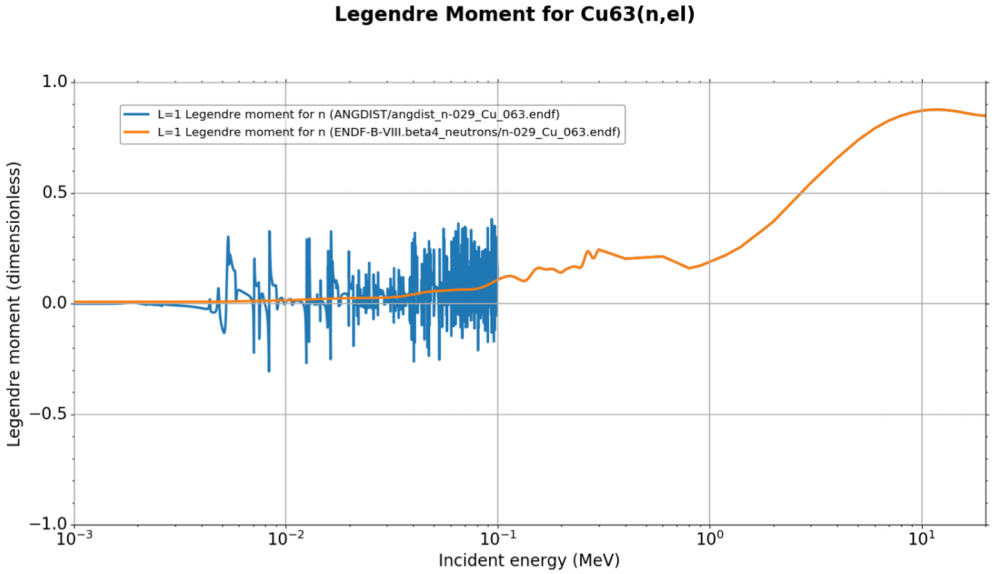


n+^{63,65}Cu evaluations – Status

A new evaluation for copper was proposed for ENDF/B-VIII.0

1. Resolved resonance region was extended above 100 keV based on experimental cross section measurements (left bottom)
2. New experimental capture data was evaluated
3. Detailed resonance behavior of angular distributions were provided (right bottom)
4. A full resonance parameter covariance matrix was provided





n+^{63,65}Cu evaluations – Plan

In ENDF/B-VIII.0 to achieve a better χ^2 value of fit to integral benchmarks (red versus purple curve below)

1. Resonance behavior above 100 keV was discarded

2. Capture widths reset to constant values

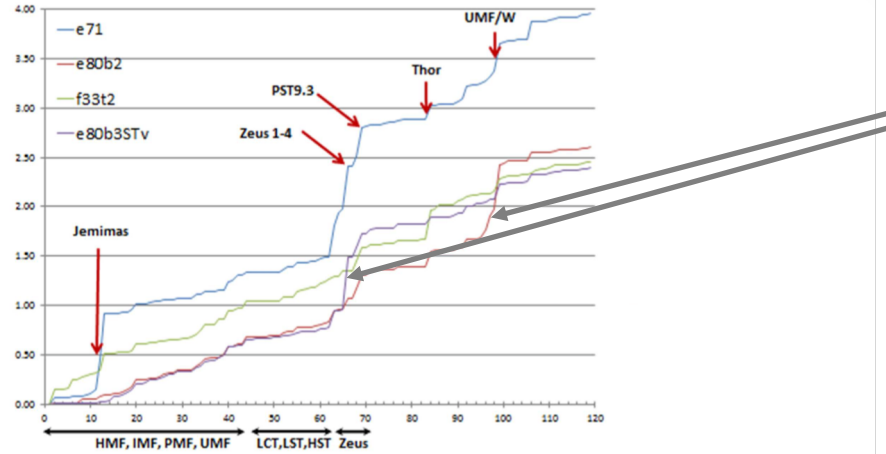


Figure 1: Cumulative Chi^2/DoF for the LANL suite of 119 benchmarks with different libraries.

Swapping "beta2" evaluations for copper in "e80b2STv" alone resulted in a decrease of Chi^2/Dof from 2.39 to 2.12, compared to Chi-square of 4 for the ENDF-B/VII.1 and of 2.46 for the JEFF3.3T2.

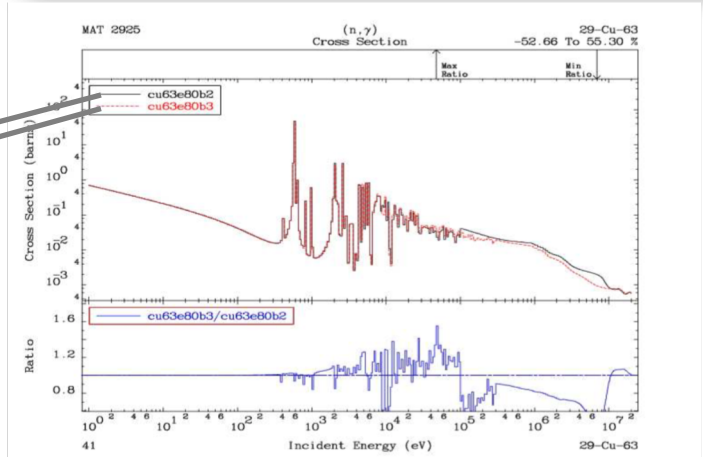


Figure 2: Comparison of the capture cross sections between "beta2" and "beta3" evaluations.

3. Angular distributions were smoothed and adjusted

4. The new file 32 was kept with resonance parameters from new proposed evaluation

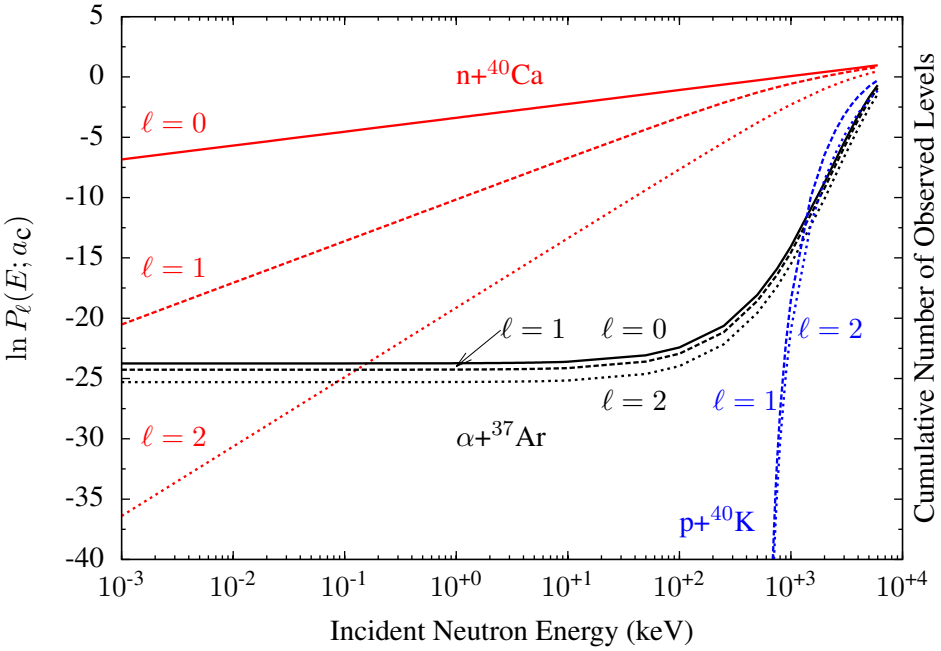
Conclusions

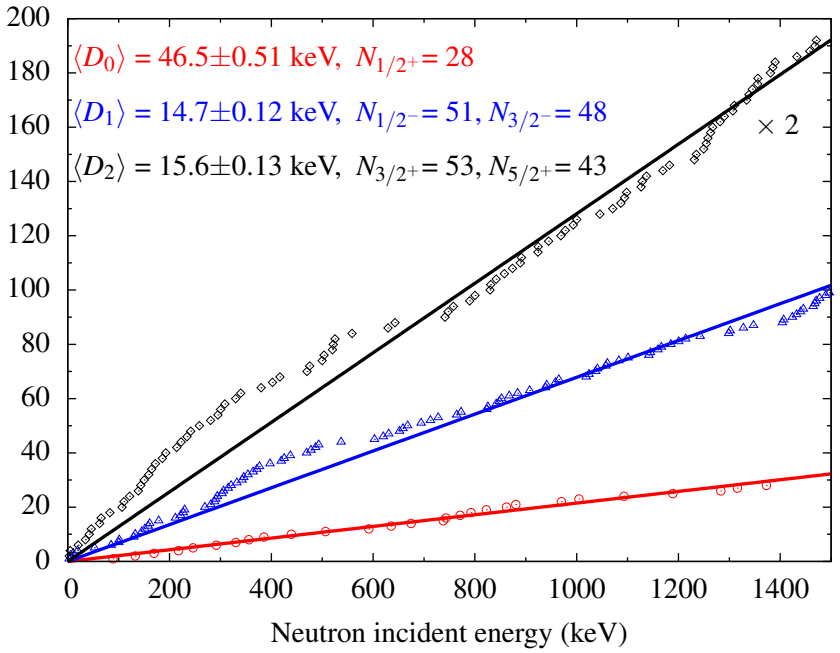
The current pair of copper evaluations in the "beta3" library is causing poor performance. It is recommended to go back to copper beta2 files. Further work is needed to improve copper nuclear data.

Copper resonance evaluation will be revised by ORNL high energy evaluation will be developed by BNL to achieve better agreement with integral experiments. Validation will be done in collaboration with IAEA under the INDEN project for structural materials.

n+^{40}Ca evaluations – Status

- Evaluated RP and related covariance matrix in RM formalism up to 1 MeV performed within NCSP and included in the ENDF/B-VIII.0 library
- RRR evaluation based on recent measurements performed at Geel for ^{nat}Ca in the energy range up to 1 MeV (Guber) and available total cross section high-resolution measurements (Cierjacks/Perey/Singh/Johnson)
- Although very small, (n,α) and (n,p) reaction channels were included to preserve unitary in R-matrix calculations. In ENDF/B-VII.1 library, (n,α) reaction channel was added as background





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n+^{40}Ca evaluations – Plans

- To test the evaluation with the updated Coulomb calculations implemented in the SAMMY-8.2 release
  - Penetrability factors for (n,p) reaction channels can be very small at threshold
- In the low energy range, (n,α) and (n,p) are very small and there is lack of experimental data. It is difficult to estimate the resonance widths accurately.
- Minor isotopes, ^{43,48}Ca, should be updated for completeness

^{155,156,157,158,160}Gd - Status

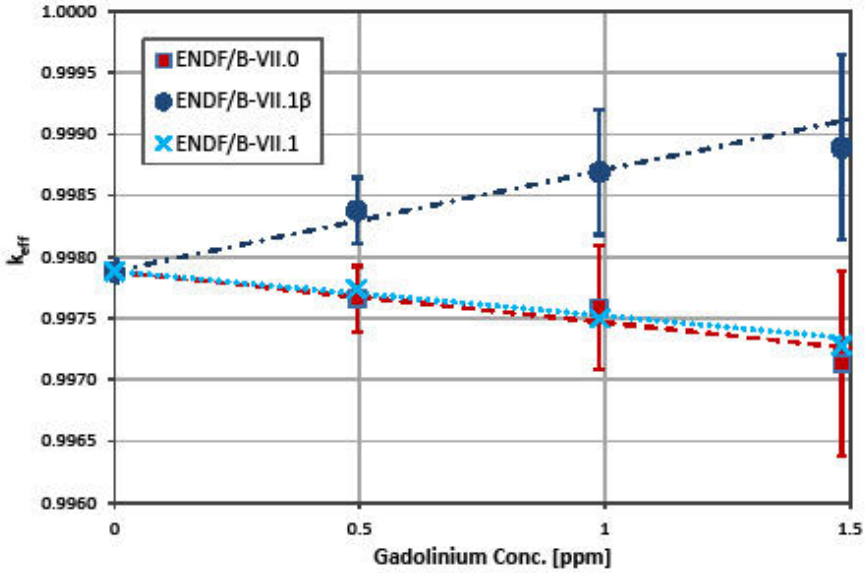
ENDF/B-VIII.0 adopted from ENDF/B-VII.0 evaluations (produced by WPEC SG23)

Status – Differential measurements

- Current evaluation is discrepant with average cross section measurements from Karlsruhe
- Experimental measurements from the RPI Gaerttner LINAC Center suggest **discrepancies of up to 9%** in the thermal cross section values

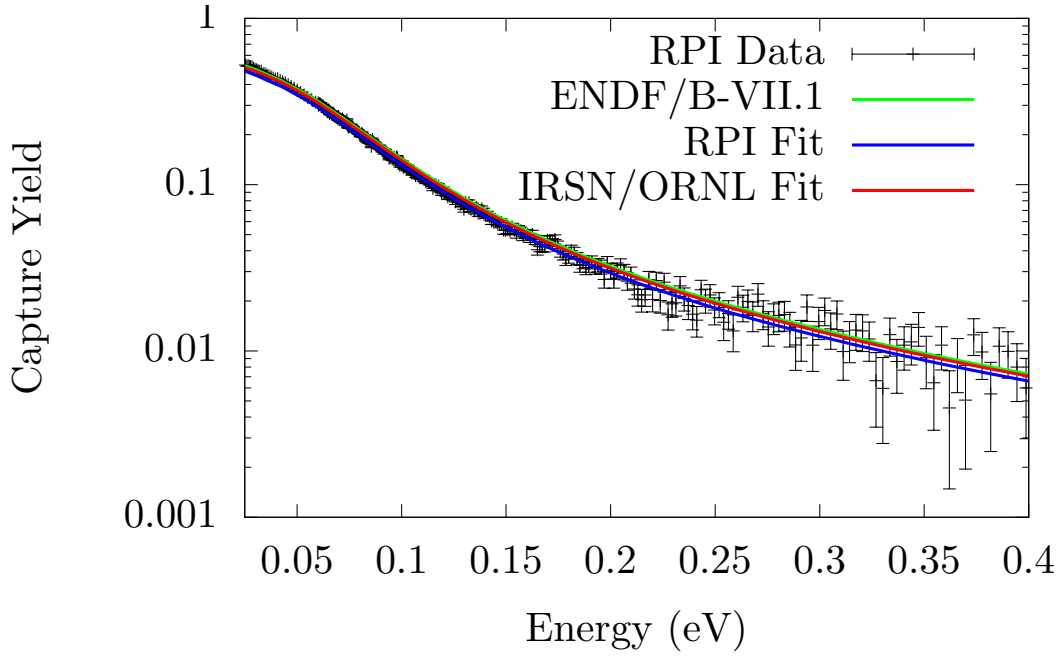
Status – Integral measurements

- BJ Marshal, "**The Case For and Against a Gadolinium Bias in SCALE**: Opening Arguments," ANS Annual Meeting, June 20, 2018, Philadelphia, PA – a lack of a clear validation case in ICSBEP for Gadolinium
- AECL ZED-2 critical facility measured k_{eff} vs Gd concentration: **under-prediction** of the capture cross section in the **ENDF/B-VII.1β** release and **over-prediction** in **ENDF/B-VII.1.** (Not part of ICSBEP)



^{155,156,157,158,160}Gd – On-going evaluation

- IRSN (Leal) and ORNL (Sobes) are partnering to complete a new evaluation for the five major isotopes of Gadolinium
- The new evaluation seeks to resolve some of the discrepancies between the experimentally measured data
- The new evaluation will deliver a covariance matrix with cross-isotope covariances that are a natural byproduct of the analysis of natural samples of gadolinium
- Beta-testing release expected in Fall of 2019.
- Full evaluation planned to be complete by end of FY19.



n+^{156,158,160,161,162,163,164}Dy evaluations – Status

Isotope	Nat. Abnd. (%)	E_{max} (eV)	l	Levels	Trans	(n,γ)
^{156}Dy	0.056	100	s	19		
^{158}Dy	0.095	90	s	3		
^{160}Dy	2.329	2000	p	65	X	
^{161}Dy	18.889	1000	s	253	X	X
^{162}Dy	25.475	5000	p	75	X	X
^{163}Dy	24.896	1000	s	114	X	X
^{164}Dy	28.26	7000	p	69	X	X
^{nat}Dy	100	N/A	s,p	all	X	X

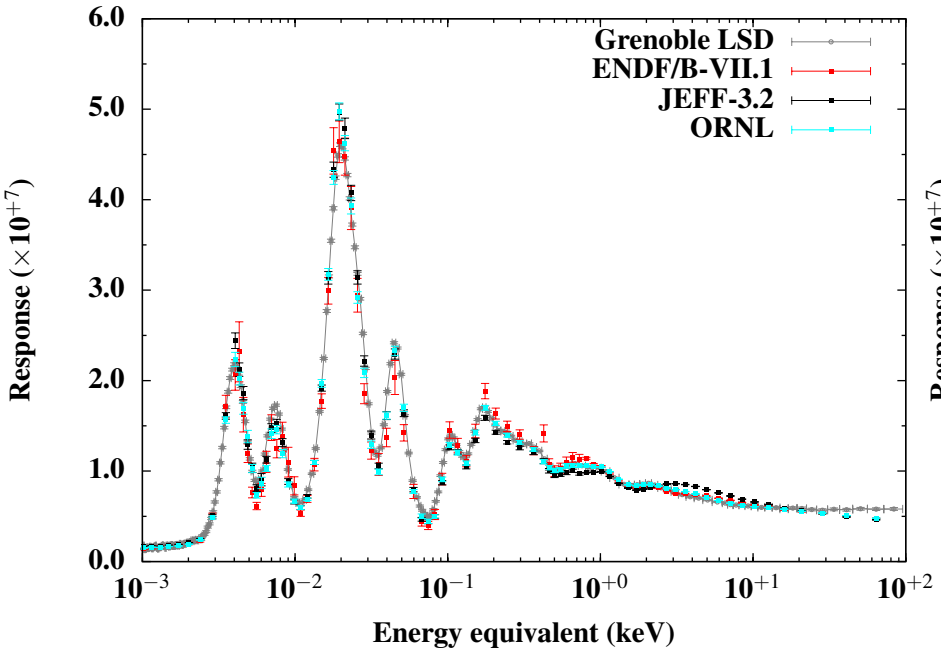
- Review of old existing Liou's transmission data (1975) sets showed several issues
  - The large number and magnitude of negative values found in the ^{160,163,164}Dy total cross sections imply an over correction of the background contribution
  - The measurements were performed on oxide samples (Dy_2O_3), but the number of atoms/barn reported seems related to the specific enriched isotope. This affected our ability to correctly calculate the total number of atoms/barn of the sample
  - Several "black" resonances were reported and no uncertainty analysis was reported
- Recent measurements performed at RPI facility: transmission of ^{nat}Dy up to 20 eV and capture measurements on enriched samples up to a few keVs.
- **Newly evaluated RP evaluations and related covariance matrices were completed within the NCSP**

n+^{156,158,160,161,162,163,164}Dy evaluations – Plans

- In the ENDF/B-VIII.0 library, the URR the average resonance parameters were adjusted to reproduce the measured data of Voss et al. (*Phys. Rev.* C**59**, 1154 (1999))
- New measured data on 197Au(n,γ) (*Phys. Rev.* C**83**, 0346608 (2011)) showed about 4.7% higher MACS than the MACS data used by Voss et al. Therefore the capture cross section in the URR should be renormalized
- The URR and fast neutron region has no covariance information
- Liou's transmission data are comprehensive but poorly documented. Are transmission measurements for Dy isotopes needed?

n+^{180,182,183,184,186}W – Status/(Plans?)

No.	Nucleus (I^π)	E_{max} $\left(E_{max}^{ENDF/B-VII.1}\right)$	Method	No. Levels	J_0	J_1
1	^{183}W (1/2$^-$)	5 (2.2) keV	RM	387	346	21
2	^{182}W (0$^+$)	10 (5.0) keV	RM	306	141	135
3	^{184}W (0$^+$)	10 (4.0) keV	RM	178	94	84
4	^{186}W (0$^+$)	10 (8.3) keV	RM	169	95	74



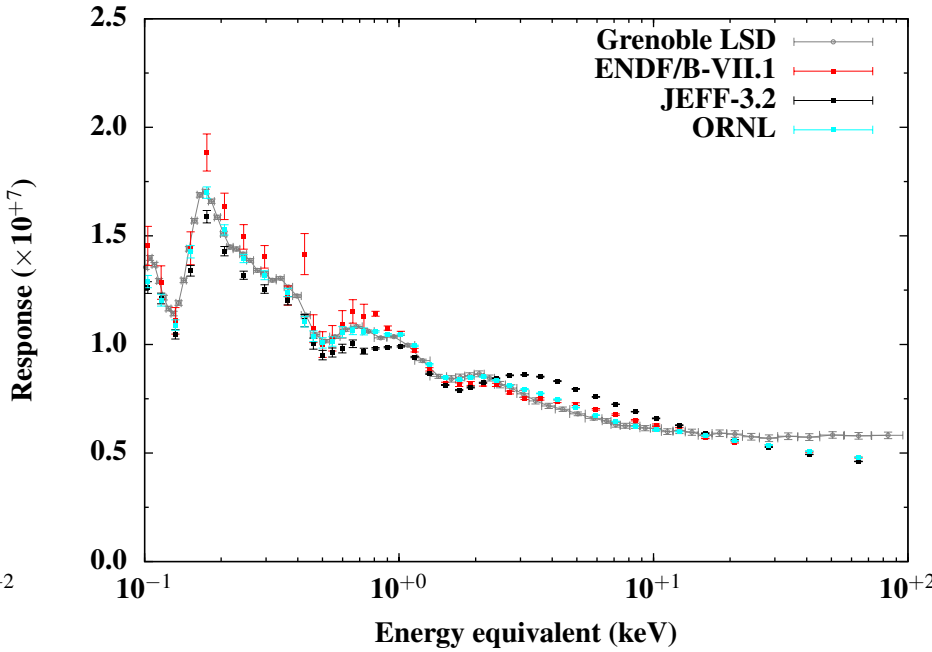
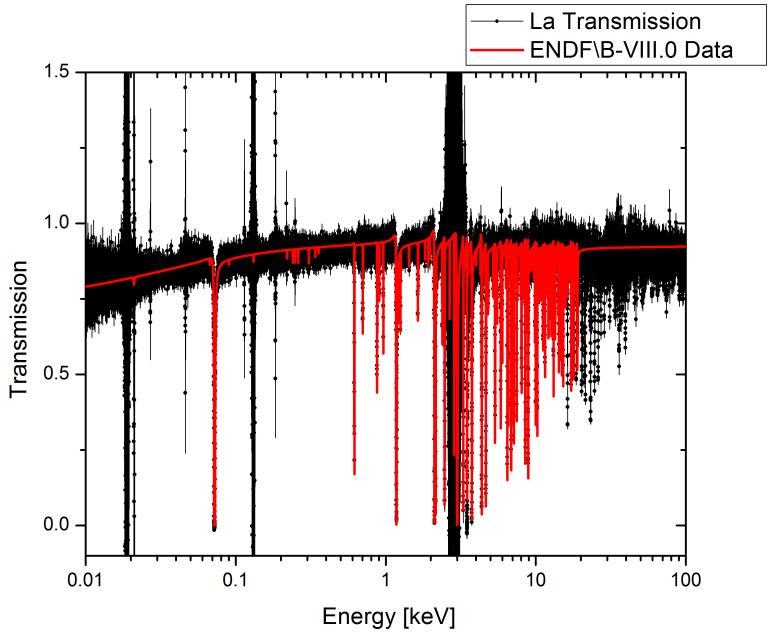
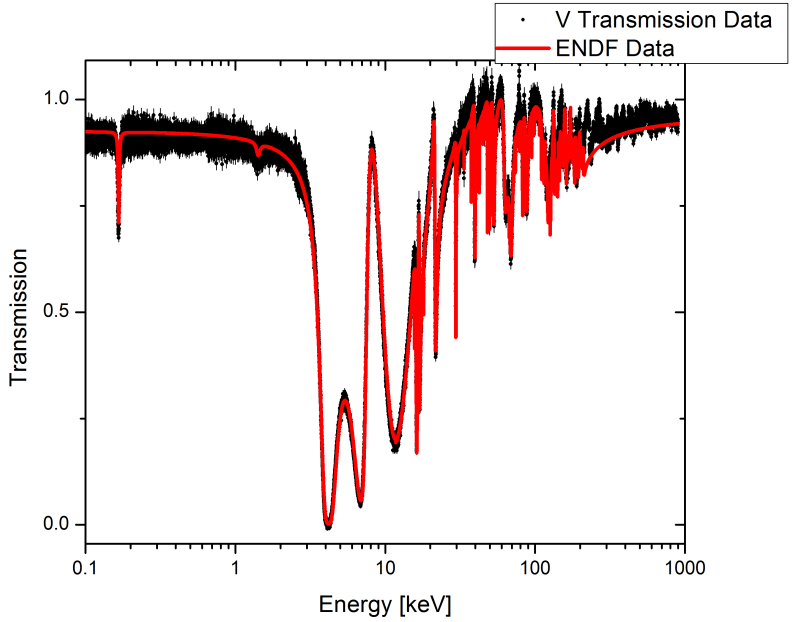


Figure 1: Experimental spectrum of the Grenoble Lead Slowing Down benchmark (gray dots) in the energy range of 1 eV up to 100 keV compared with the spectra obtained with the ENDF/B-VII.1 (red dots), JEFF-3.2 (black dots) and the set of tungsten ORNL evaluations (cyan dots). ND2016 EPJ Web of Conferences 146, 06010 (2017).

n+^{51}V, ^{139}La, ^{181}Ta – Status / Plans

- ^{51}V, ^{139}La, and ^{181}Ta measurements completed within the NDCS program (APPENDIX B five years plan)
- RRR (and URR for ^{181}Ta) evaluations are planned to start in FY19
- Transmission and capture measurements on ^{51}V and ^{139}La samples were performed at the GELINA facility (about ^{139}La see Guber's presentation for details)
- Transmission and capture measurements on ^{181}Ta sample were performed in the RRR/URR at RPI. Evaluation work in the RRR was recently initiated by D. Barry by using high resolution data measured at ORELA by J. Harvey.





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Thank you!