LAUR-10-02501

Nuclear Data Evaluation Upgrades for ENDF/B-VII.1

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P.G. Young, T. Kawano, P. Talou, S. Kahler, S. Holloway

Principle Upgrades Planned for ENDF/B-VII.1

- Covariances – See tomorrow
- Light nuclei based on R matrix work (6Li(n,t), 9Be, 16O …)
- Structural materials (ORNL lead) – supported by criticality safety
- Fission products (Pu FPYs & delayed neutron, gamma data)
- Actinides – minor actinide improvements to fission, capture, n2n including much usage of feedback from critical assembly reaction rate data, and data from LANSCE, CERN *etc*

  -*And much use of new JENDL data for MA*

- Actinides – major (for future release):
  - Big issues in fission neutron spectra will take longer to resolve
  - 239Pu resonance evaluation (ORNL +Cadarache/CEA)
  - We're interested in WPEC/Iwamoto conclusions re. 235U capture.
  - Need to fix DN problems reported

LANL Submissions for VII.1
(This does not include all the covariance work)

- Little's ACE library –based fixes
- Hale: n+ alpha, 6Li, 9Be, 16O – see Gerry's talk
- Kawano: 48Ti (+other Ti isotopes)
- Holloway: 58Ni, using LANSCE alpha-production - with a tweak coming
- 89Y – fix by Little; more fixes by Kawano made….
- 233U DN fix?
- Talou: 233,5U and 239Pu VII.0 fiss neutron spectra on finer grid
- Talou: 239Pu VI.0 resonance info put back in
- Kawano/Chadwick 236U improved capture; (but 237U was submitted but not issued in beta-0 – impr. fiss)
- Holloway/Chadwick: 237Np (n,2n), thermal, .. improvements (from Maslov)
- Talou, Young: 238Pu and 240Pu
- Kawano/Chadwick: 241Am capture, fission
- Chadwick/Kwano: New FPY evaluation for fast neutrons on 239Pu, at 0.5 & 2 MeV

Fission Product Yields for 0.5 MeV Fission Spectrum Neutrons on 239Pu

- Results and conclusions endorsed by an Expert Panel, led by LANL and LLNL with external scientists, eg from NIST(Gilliam), CEA, AWE, .. Discussed with Robert Mills too.
- Experimental and evaluation paper will be published in Dec Nucl. Data Sheets
- Used LANL-ILRR measured data for the first time in ENDF
- 4-5% changes for 99Mo, 147Nd, and 1-2% changes for 95Zr, 144Ce, at 0.5 MeV
- Accounted for energy dependence between 0.5-2 MeV for the first time - created a new set of data at 2 MeV as well as .5 MeV

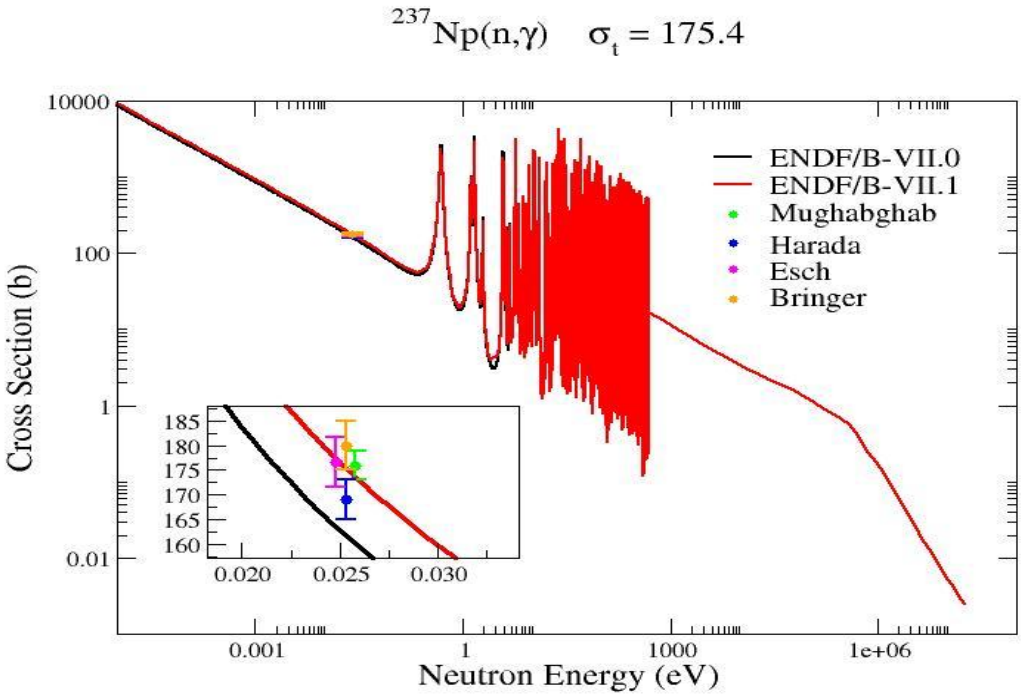
Future tasks:

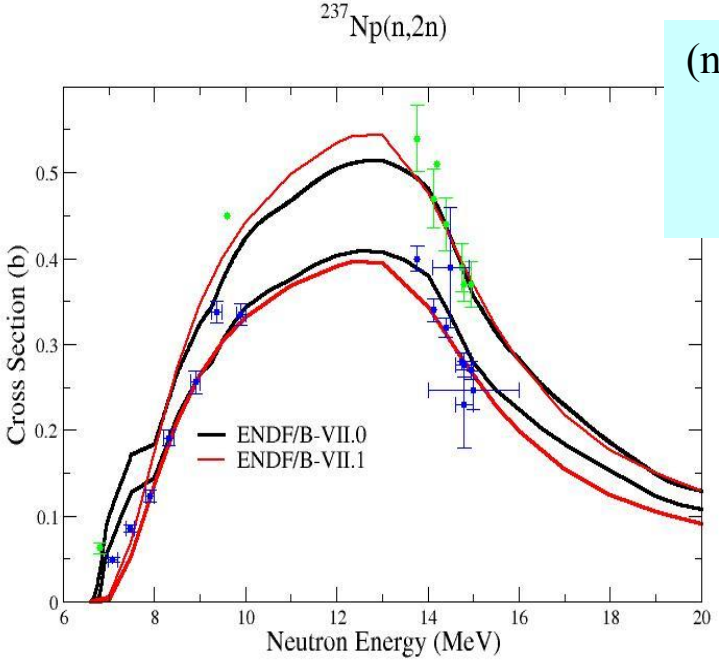
- implement in ENDF file for cumulative & individual yields
- Make changes at 14 MeV too - updating the key LANL and LLNL measurements that influence the 14 MeV data to use modern 239Pu fiss xs
- Consider similar extensions for 235,8U

^{237}Np

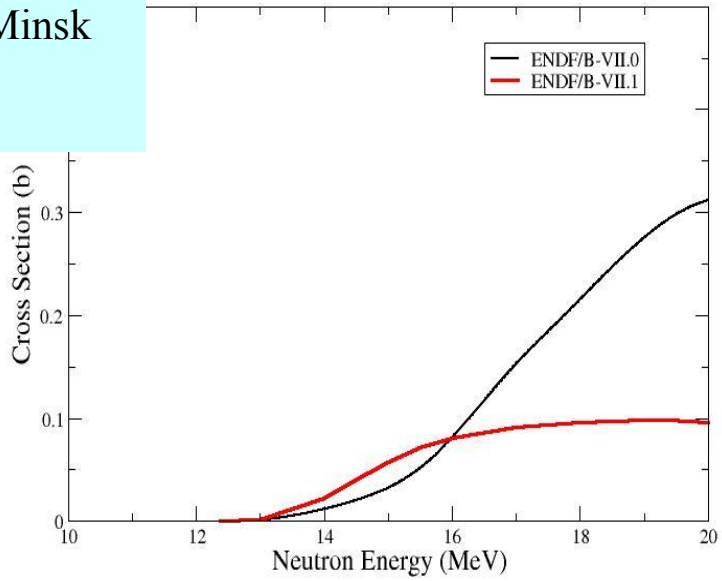
Resonance parameters adjusted to bring thermal capture cross section into agree with average value

$\blacklozenge_t$ =175.4 b



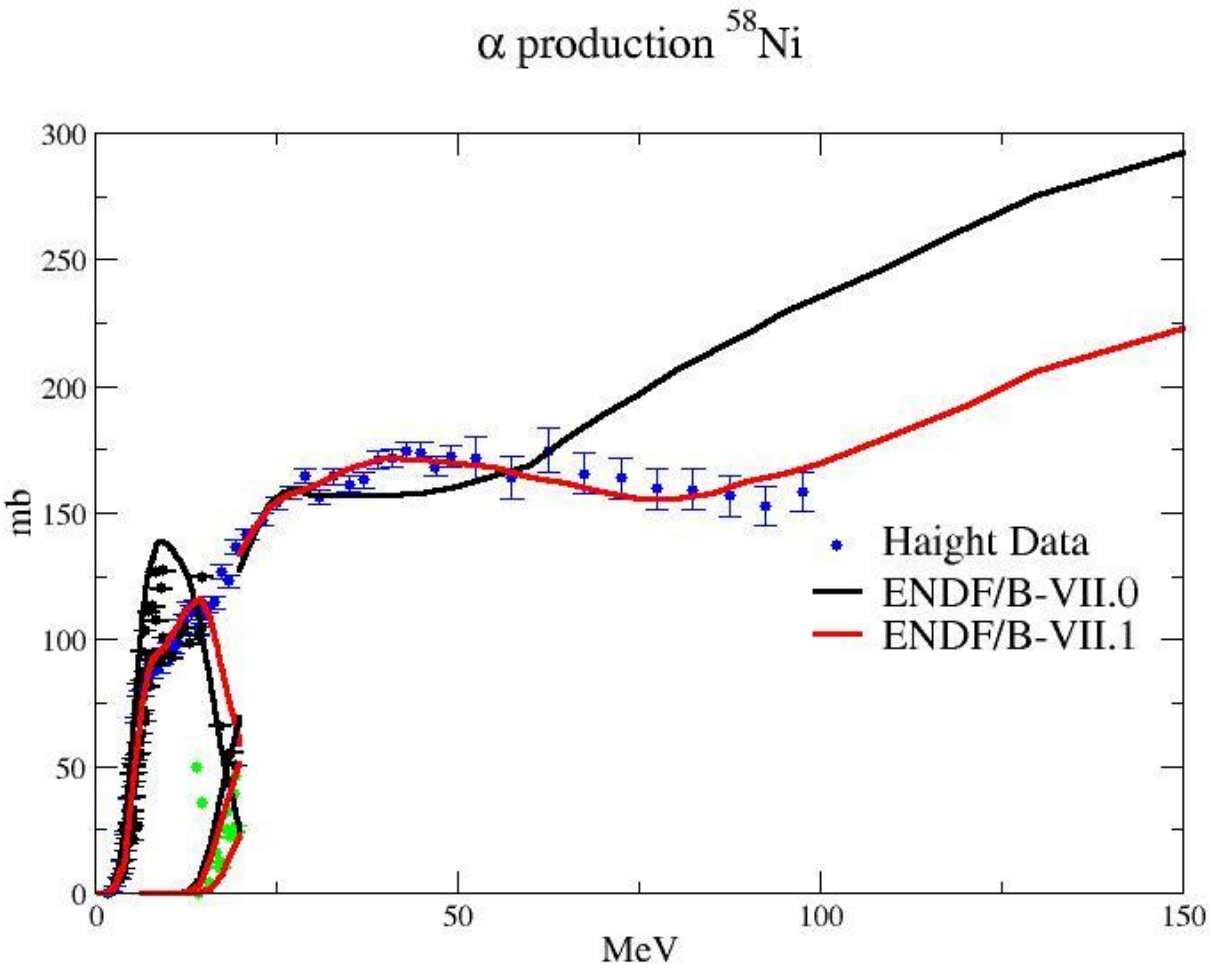


(n,2n) and (n,3n) adopted From Maslov, Minsk evaluation

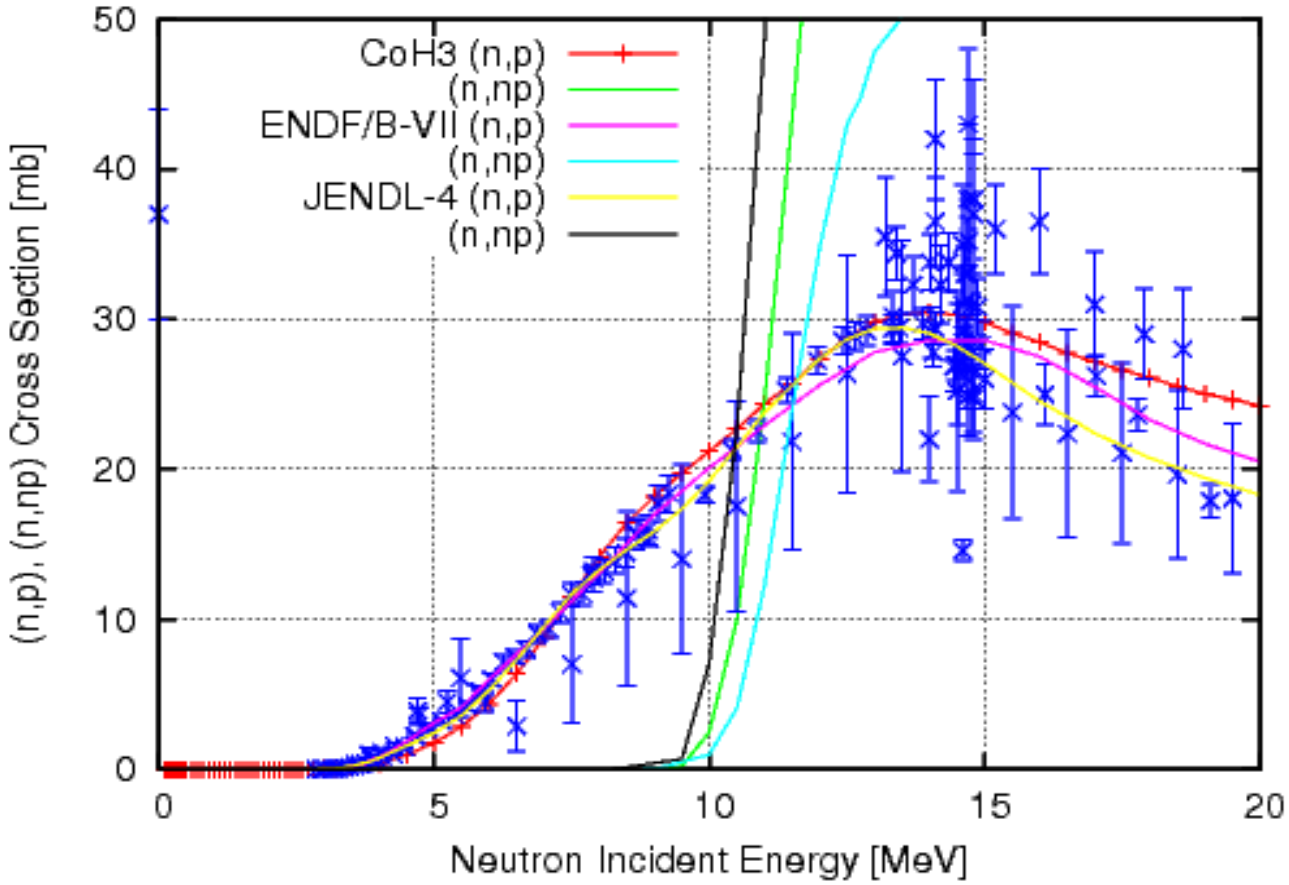


^{58}Ni

- Updated low energy (n,α), (n,nα), (n,pα) cross sections.
- Statistical fit to low energy (n,α) data (< 11 MeV)
- High energy α production ratio updated.



CoH3 Calculations for V51(n,p) Reactions



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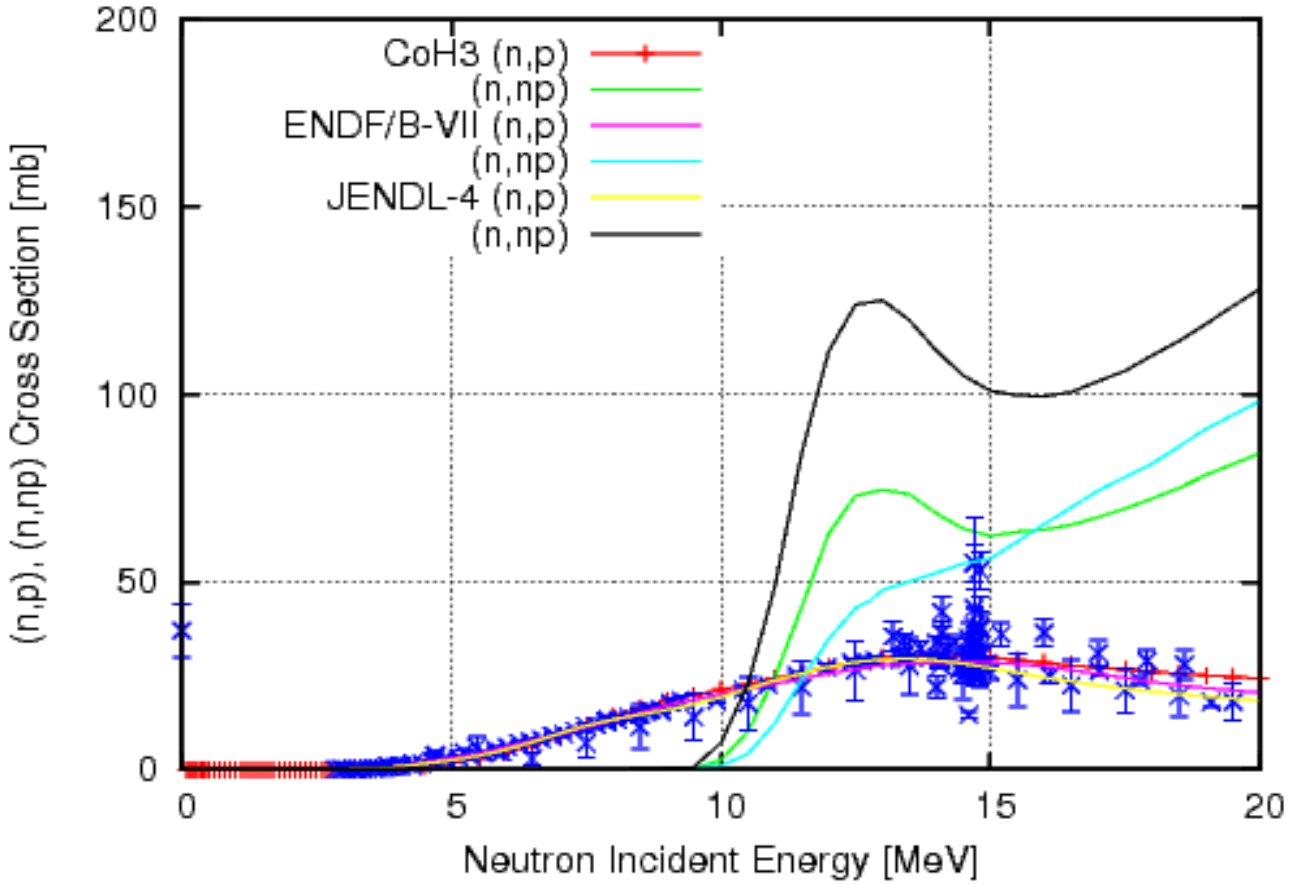
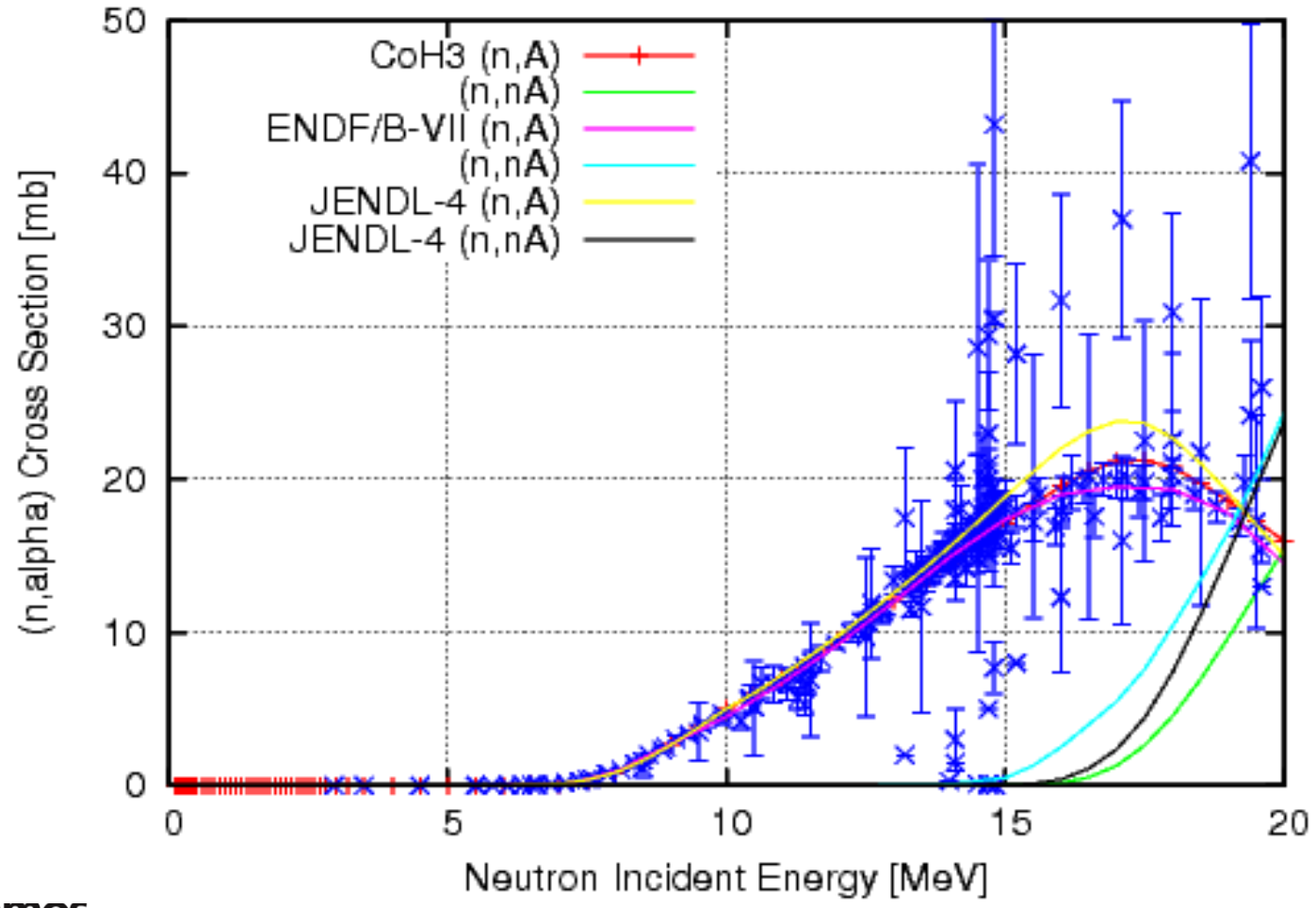
CoH3 Calculations for V51(n,np) Reactions



CoH3 Calculations for V51(n,alpha) Reactions



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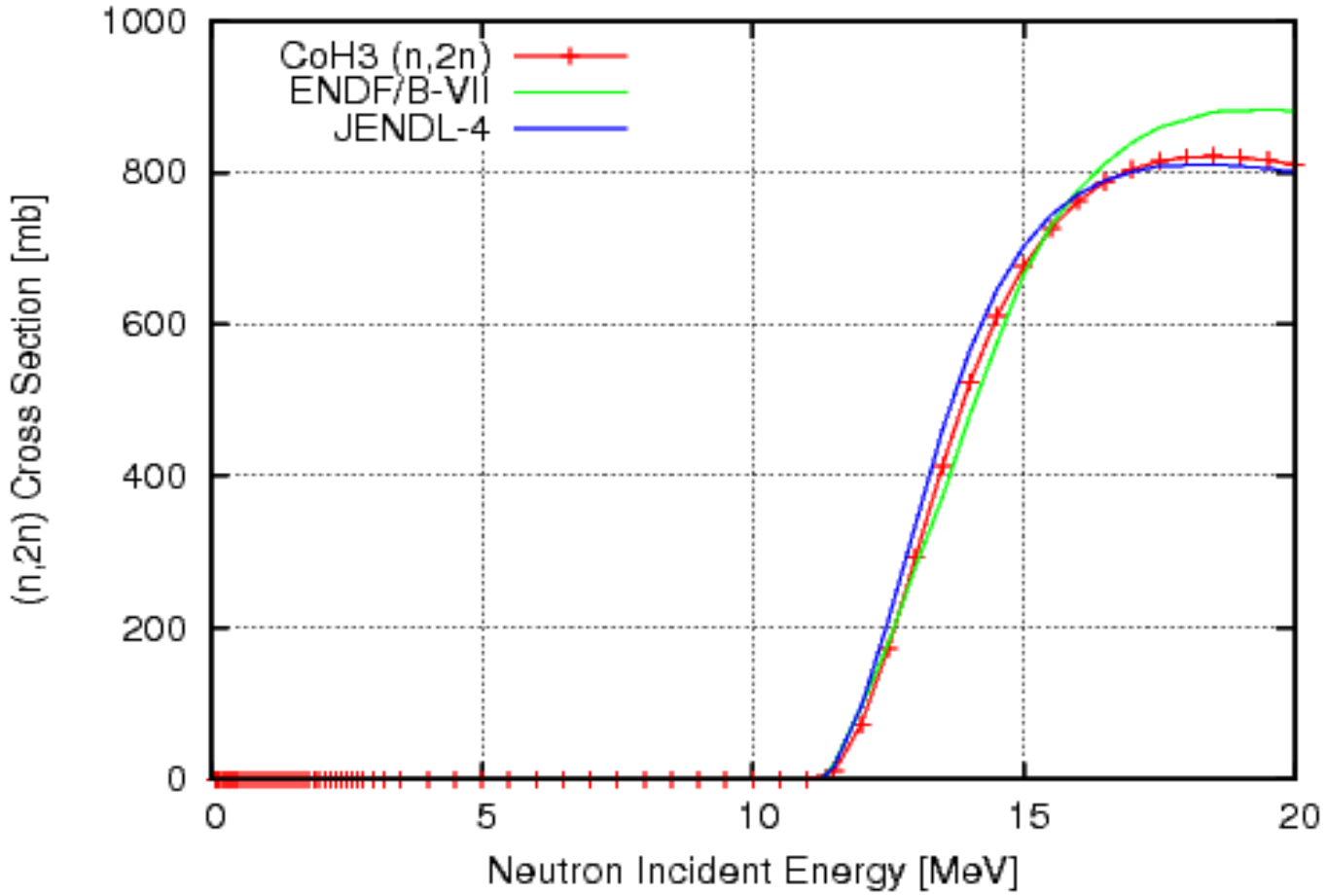
CoH3 Calculations for V51(n,2n) Reactions



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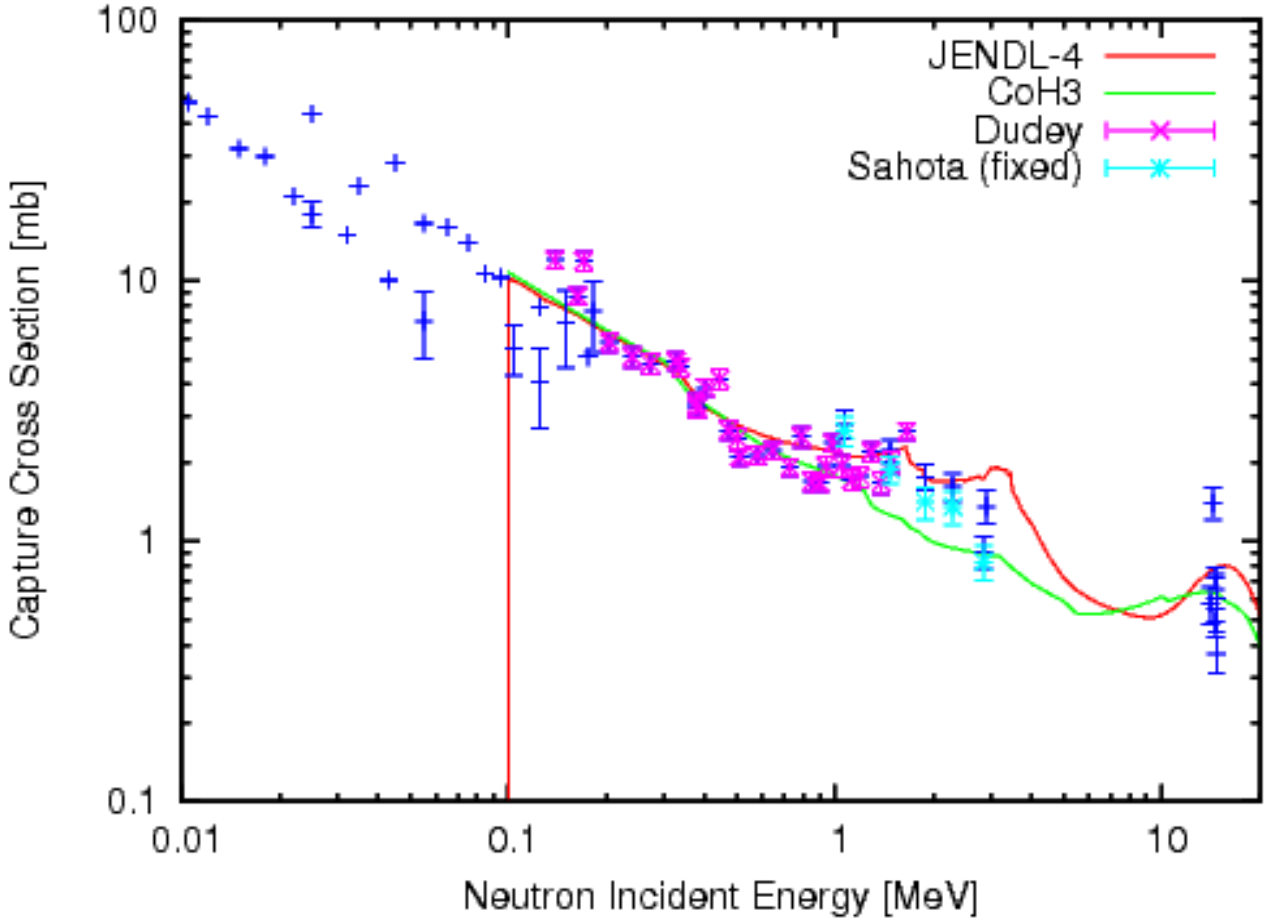
CoH3 Calculations for V51 Neutron Capture



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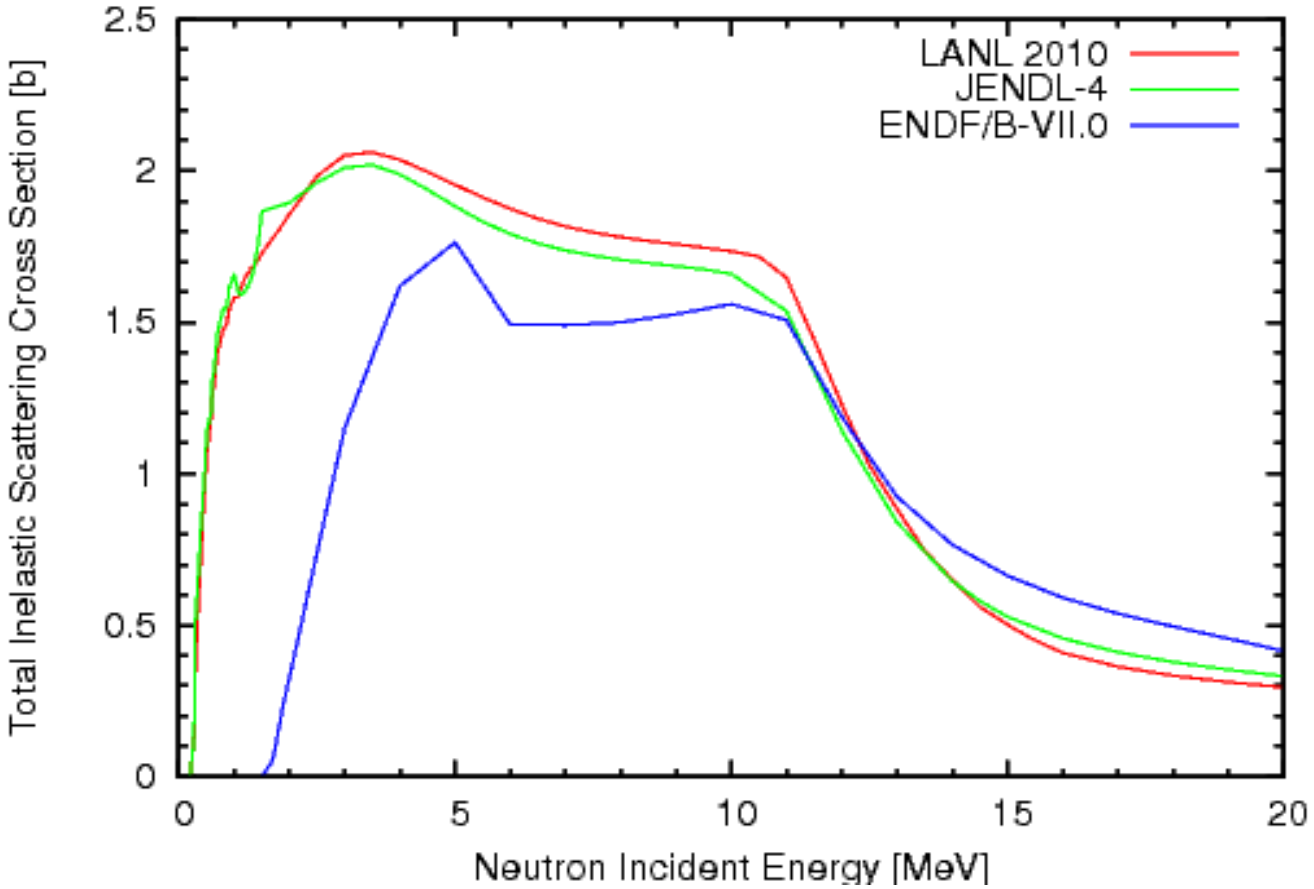
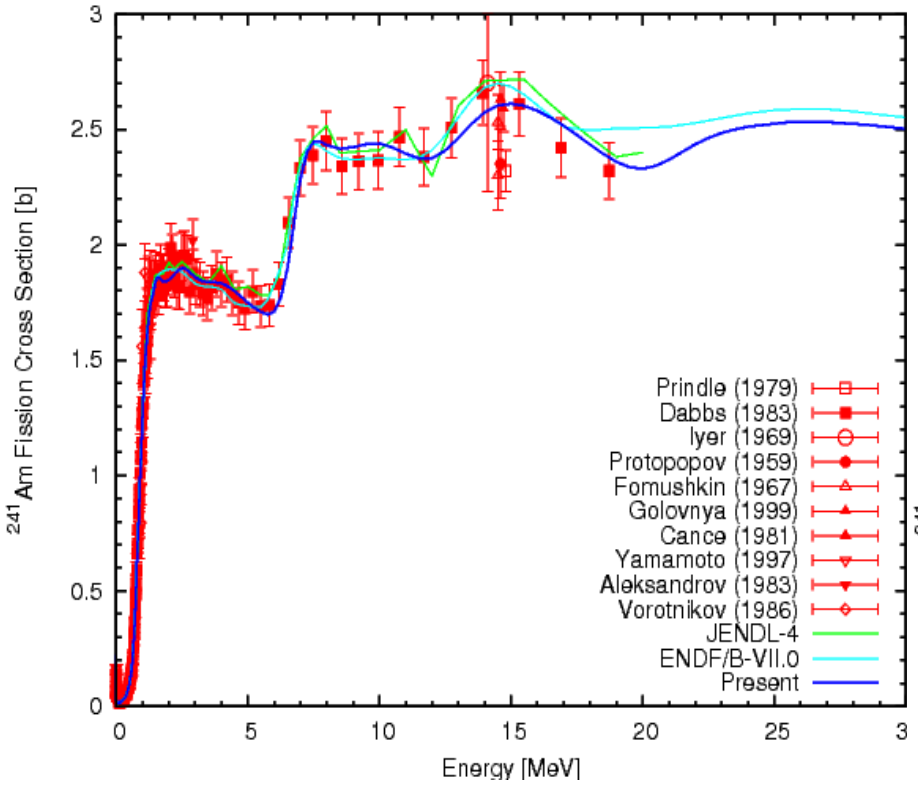
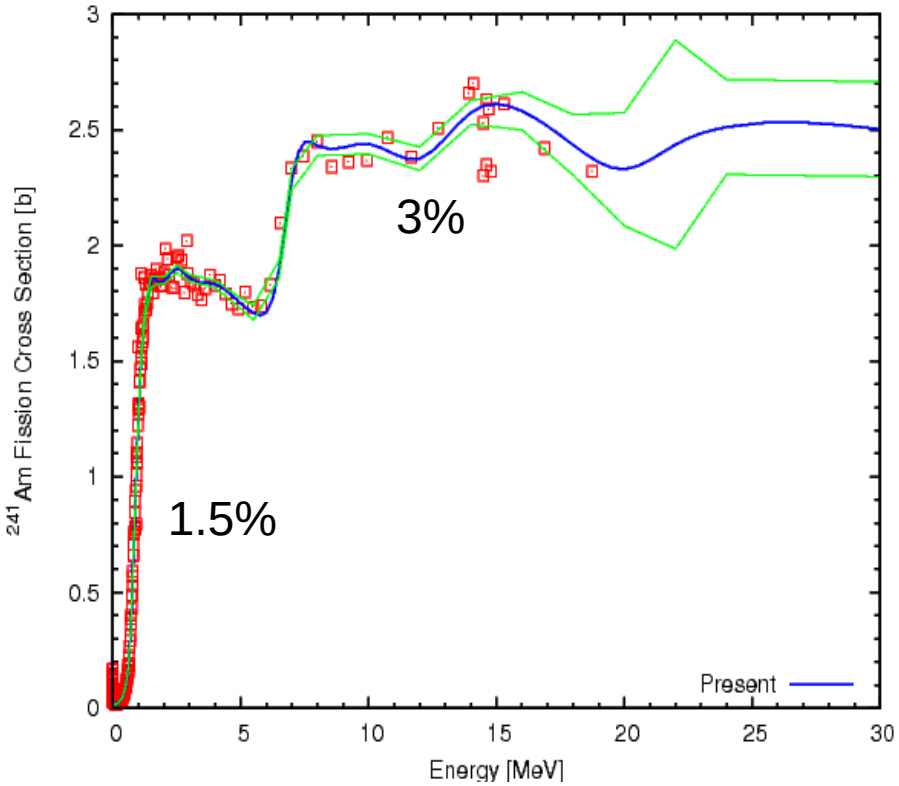
CoH3 Calculations for As75 Total Inelastic



Covariance Evaluation for Am241 Fission





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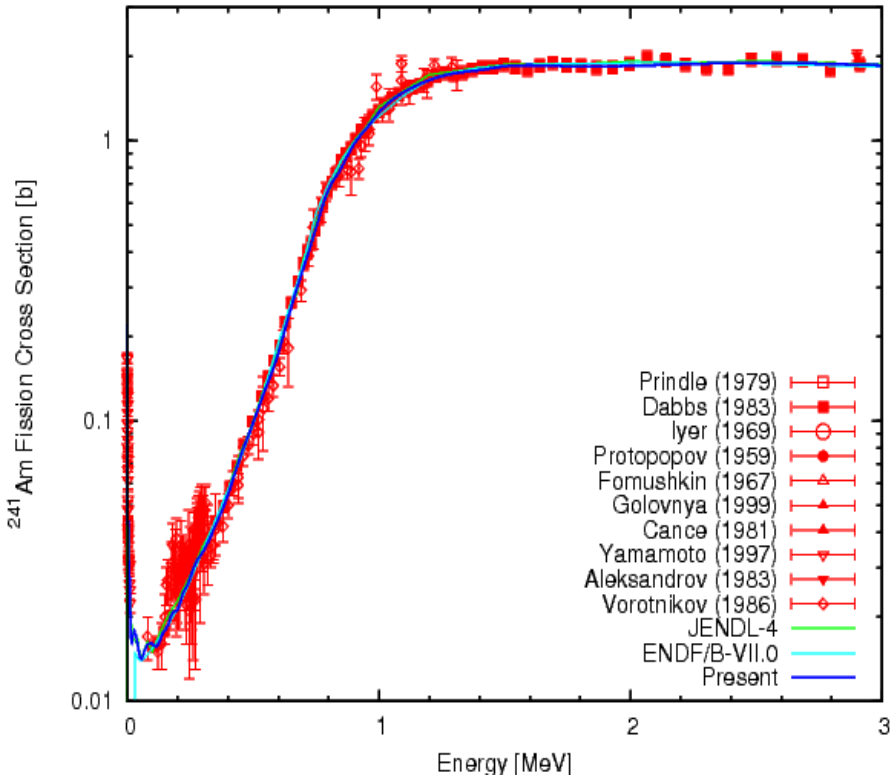
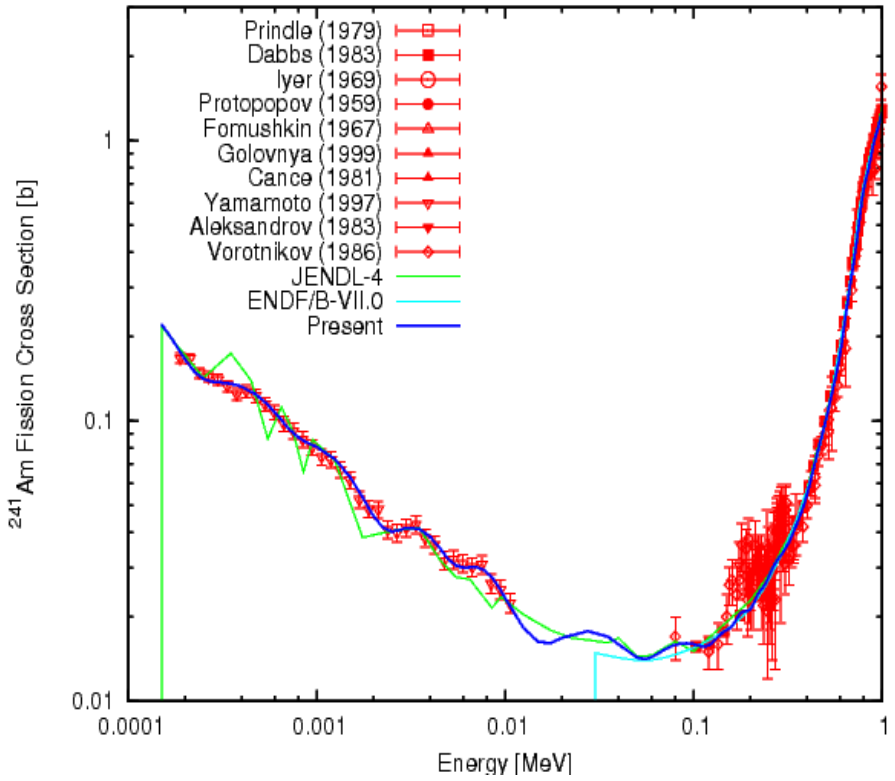
Am241 Fission Cross Section in Fast Range





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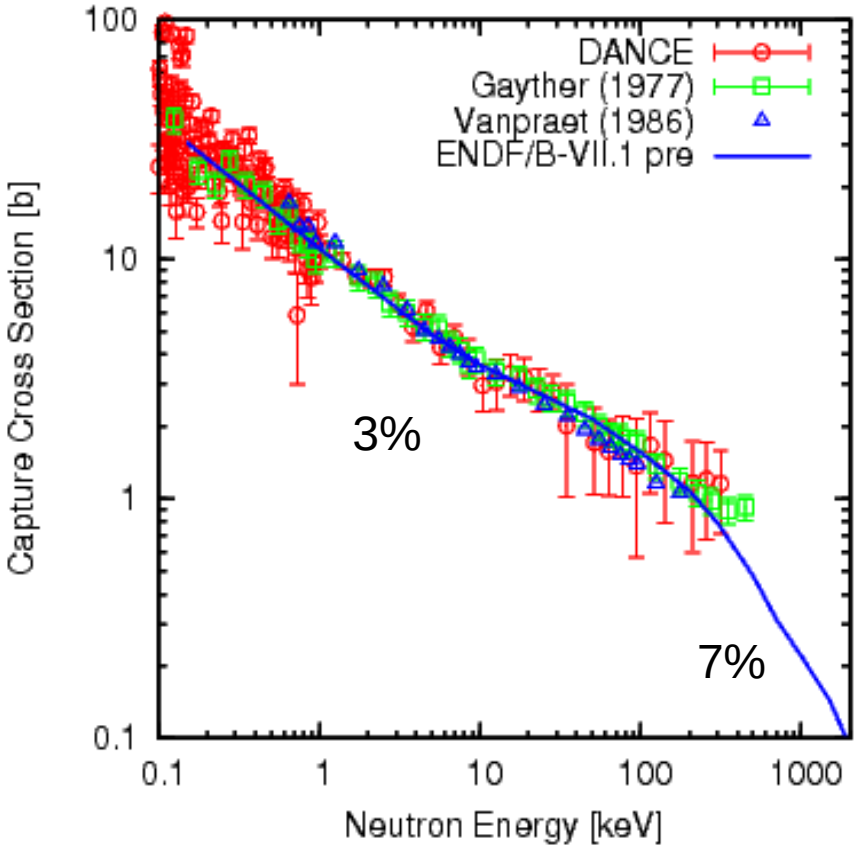
Am241 Capture Cross Section



- Statistical model calculation
  - DANCE experimental data
- Benchmark Calculations
  - LANL reaction rate measurements in the critical assemblies
- Resonance Range
  - LSSF=1 Used
  - JENDL-4 Resolved/unresolved resonance parameters adopted

Update on ACTI Gamma Ray Emission Data In ENDF/B

LA-UR-10-7231

CSEWG

November 1-3, 2010

Morgan C White

XCP-5

Los Alamos National Laboratory

Abstract

- During the late 1990's, there was considerable effort placed on updating the gamma-ray production data for a suite of isotopes important for oil-well logging. This work was performed as part of a CRADA at LANL. It is documented in S.C. Frankle, R.C. Reedy, and P.G. Young, "Improved Photon-Production Data for Thermal Neutron Capture in the ENDF/B-VI Evaluations," Los Alamos National Laboratory report LA-13812 (2001). The updated evaluations were included in ENDF/B-VI releases 6 and 8. During the ENDF/B-VII work, some of these data have been overwritten. Many of these highly detailed spectra are considerably better than the generic work that has replaced them and should be put back into the database. A general discussion of the data involved is presented herein.

The ACTI Data
Enhanced Thermal Gamma-Ray Emission Data

H1 OK

He4 OK

Be9 OK

N14 OK (VI.8 -> VII.0)

O16 OK

F19 OK *

Na23 OK (VI.8 -> VII.0)

Mg ->Isotopic

Al27 Replaced

Si28-30 OK

S, S32 ->Isotopic

Cl35,37 OK

K ->Isotopic

Ca ->Isotopic

Sc45 OK

Ti ->Isotopic

V OK

Cr50,52-54 OK *

Mn55 Replaced

Fe54,56-58 OK

Ni58-62,64 OK *

Cu63,65 OK

W182-184,186 Replaced *

Some Notes & Recommendations

- F19 – thermal spectrum carried to 2.000001+5 eV VI.8 versus 2.000100+5 VII.0
  - Makes gamma-ray yield values consistent with emission line data
  - Kudos to ORNL for catching and updating this!
- Cr52 – continuum emission distribution data has been updated
- Ni59 – incomplete evaluation replaced; no discrete gammas given
- W – no discrete lines given for any of the isotopes but…
  - W180 - first time this minor isotope has been given

- For the isotopes where discrete data were replaced, recommend putting the ACTI data back into evaluation
- For the elementals that are now isotopics, recommend reformulating discrete data by isotope and putting ACTI data into evaluation

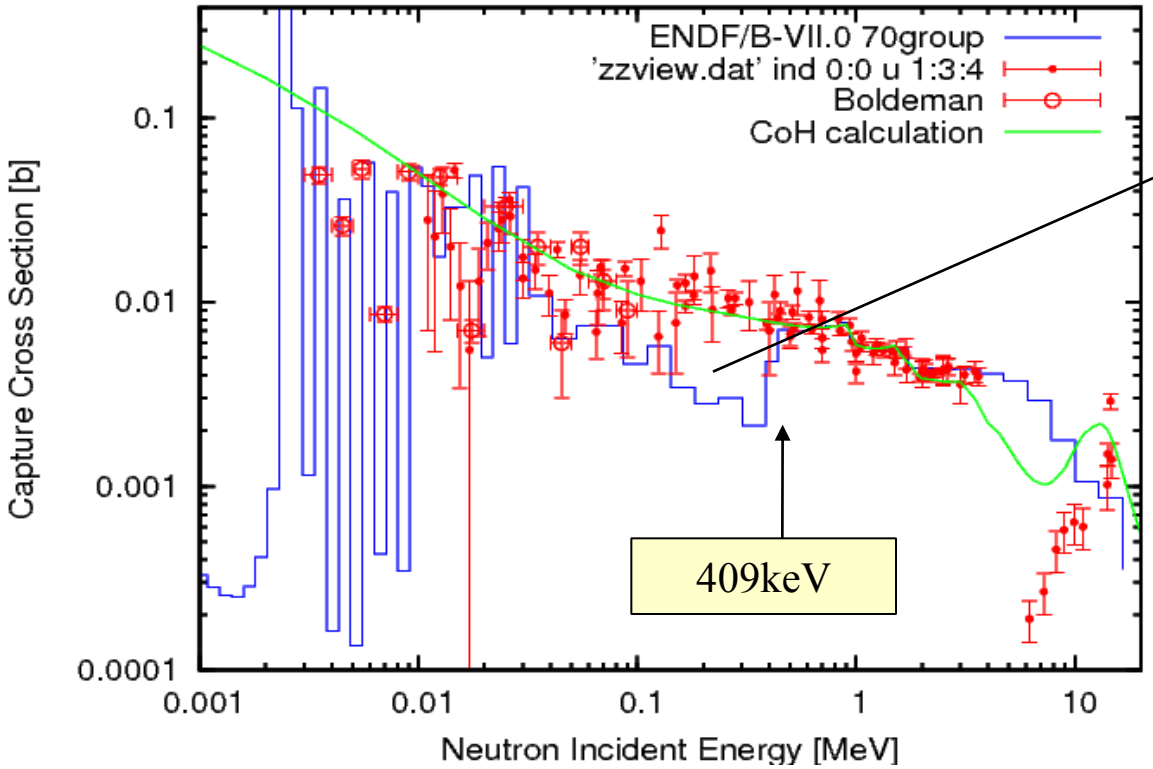
To Do

- ^{9}Be neutron angular distribution
- ^{16}O higher energy (7-20 MeV) upgrade?
- Alpha production ^{60}Ni, ^{56}Fe – use Haight data
- ^{243}Am (n,2n) isomer production
- Delayed Neutron: Reconsider changes made for VII.0
- Evaluations (^{55}Mn), ^{51}V, ^{73,74,75}As isotopes

Elements in Medium Mass Range

- Ti isotopes
  - New evaluations from LANL and ORNL
    - I think we are waiting to include new resonance parameter covariances from ORNL (retroactive, using LANL resonances)
    - γ-production for some isotopes (^{47}Ti fixed by LLNL)
- ^{58}Ni(n,α),^{56}Fe(n,α) < 20 MeV
  - work in progress (Holloway, Kawano) using LANSCE data
  - Goal – do by next CSEWG.
- ^{63,65}Cu
  - Mosteller tested new CENDL-3 data, and new JENDL data
    - Zeus benchmark testing not so satisfactory – like B-.VII.0, but perhaps this is a 235U(n,g) issue instead near 1 keV – more testing needed
- ^{89}Y
  - capture data fixed at low energies (Kawano)

Y-89 Capture 70 Group Cross Section: Thanks to Ignatyuk for noting a problem!



d- f-wave contributions are missing ?

Gamma width
ENDF 134meV
RIPL-3 130meV
D0
ENDF 4.4keV (approx)
RIPL-3 3.7keV

Change the upper limit to 30keV or so, or
Increase the radiative width to match the Hauser-Feshbach calculation

Minor Actinides

- ^{233}U
  - delayed neutron typo, E-02 -> E-03, confirmed
- ^{236}U ^{241}Am
  - small adjustment of fission cross sections in the sub-threshold region
  - capture calculated for better production of integral data
- ^{240}Pu
  - adopt LANL new evaluation
    - comparison of resonance region reported by R. Cullen
    - P. Young and O. Bouland will review this again
- ^{237}U
  - new evaluation – work esp. on fission cross section (crits perform well)
- ^{237}Np
  - (n,2n) new evaluation by Holloway underway, taking account of isomeric state production cross section – adopting insights by Maslov. New data testing of (n,f) and (n,g) against crit data (Bigten, as well as hotter) good.
- ^{238}Pu
  - New work underway and will be completed soon. But our calculations overpredict new LANSCE/CEA fission data, and agree well with new LLNL surrogate data (not yet understood way recent CEA calculations differ). (n,3n) at 14 MeV is 85 times smaller than VII.0!
  - We also plan to fix 243Am(n,2n) – Maslov feedback

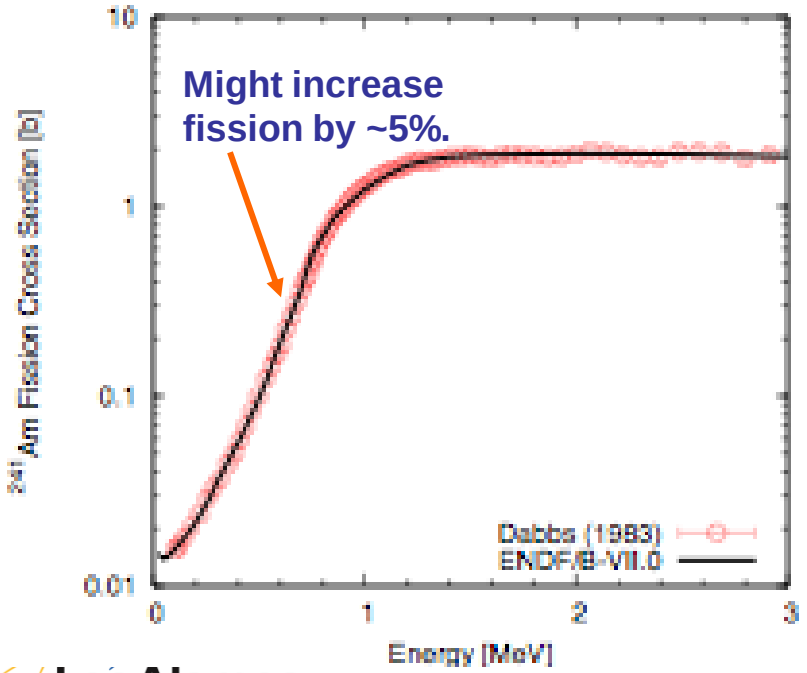
FPY : Fast neutrons on 239Pu, 235U, 238U

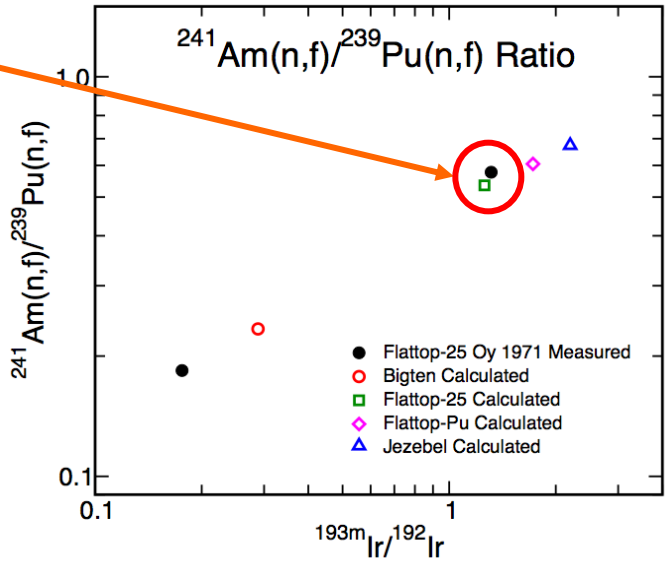
- The longstanding discrepancy between LANL and LLNL has been resolved, for the few key FPs using for monitoring fissions. LLNL estimates now agree with LANL.
- Our results are supported by an external “Expert Panel” review
- 3 papers being finalized for NDS Dec 2010
- To do – finalize evaluated numbers, and include in upgraded FPY evaluation. Extend work to include energy deposition for all FPY in fast region. E.g. augment current fast ENDF FPY data (at ~”0.5 MeV”) with another suite at 2.0 MeV, Will require some work (Kawano, Lestone, MBC,… + BNL).

241Am fission: ~5% increase near 500 keV?

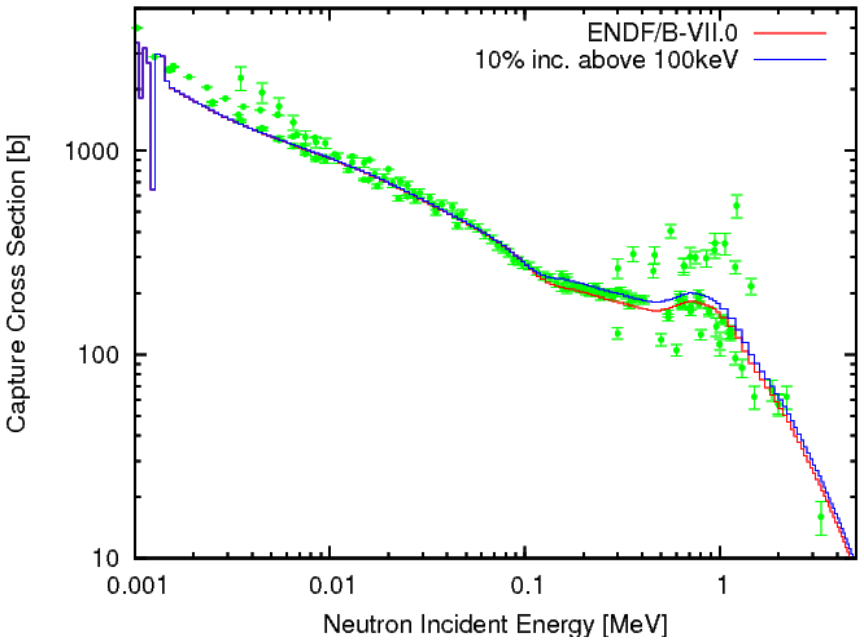
Japanese FCA data testing suggest that B-VII needs increasing 3-6% in the ~ 500 keV region

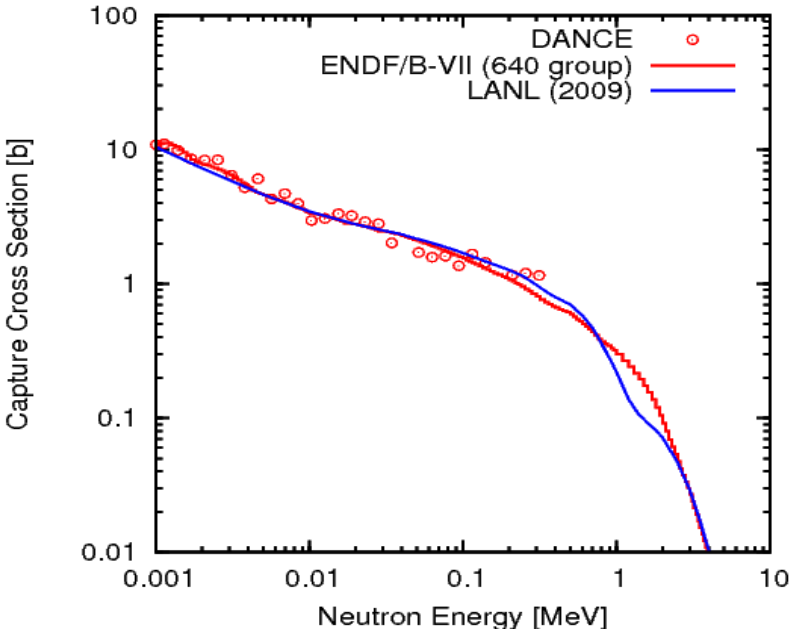
~ Similar to LANL results





U-236 and Am-241 Capture Cross Section



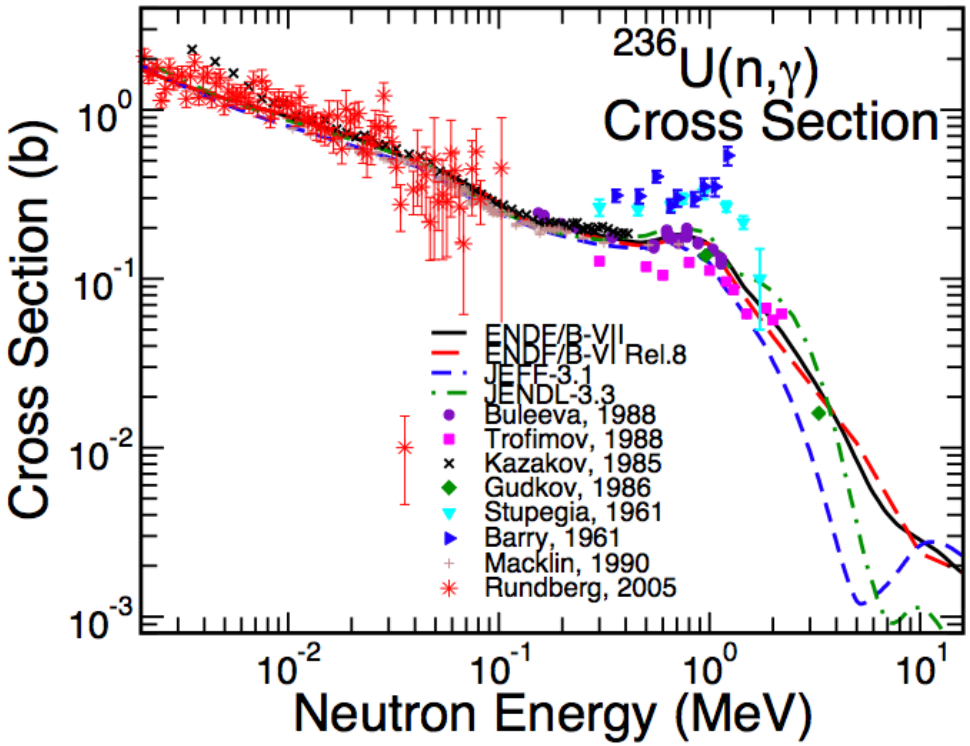


M. Jandel et al.
Phys. Rev. C, 78 034609 (2008)

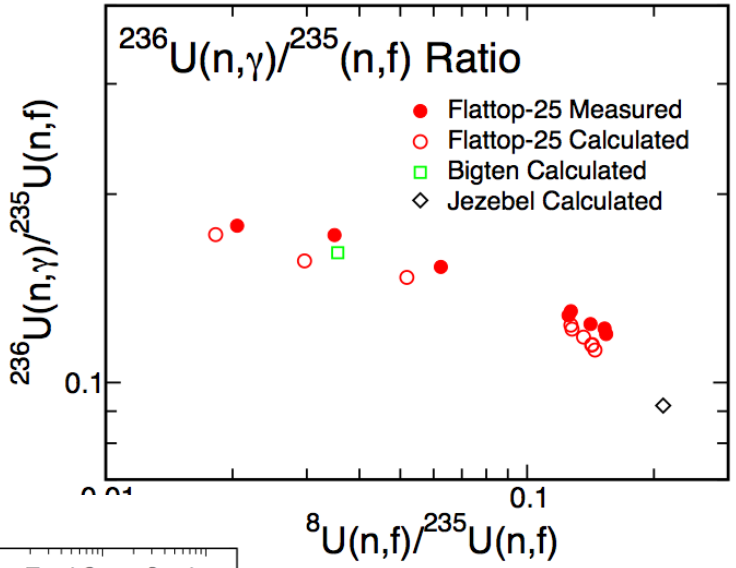
Increase capture cross sections slightly for better reproduction of critical assembly data (See Kahler's talk)

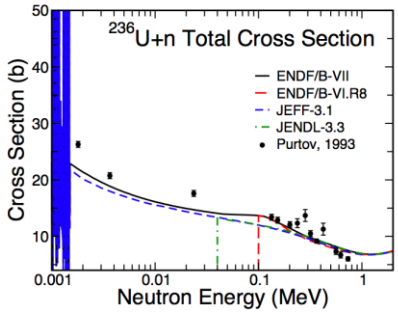
236U - Possible ~10% increase to capture

Spread in measured data would allow an increase in capture



Testing of capture cross section suggests ~ 10% increase needed in 10kev - 1-2 MeV region. (critical assemblies here have most neutrons >10 keV)





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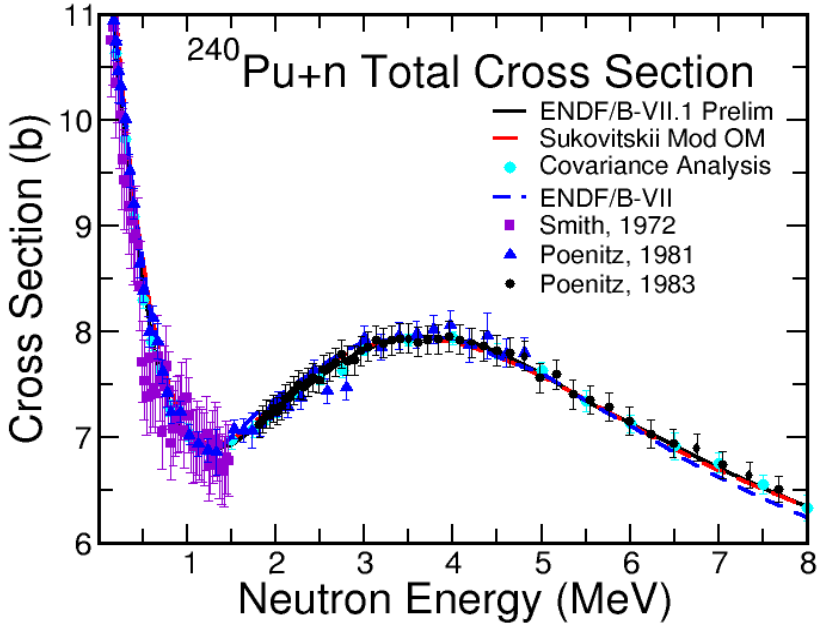
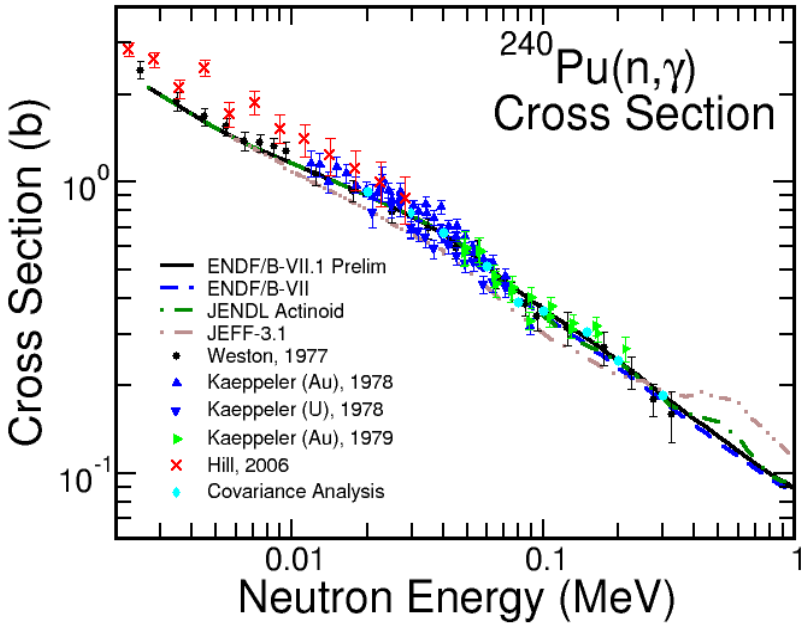
Pu-240 LANL Evaluation - Total and Capture,



Total Cross Section
modified Sukovitskii optical potential

Fission Cross Section
GLUCS analysis
and JENDL/AC (up to 30keV)



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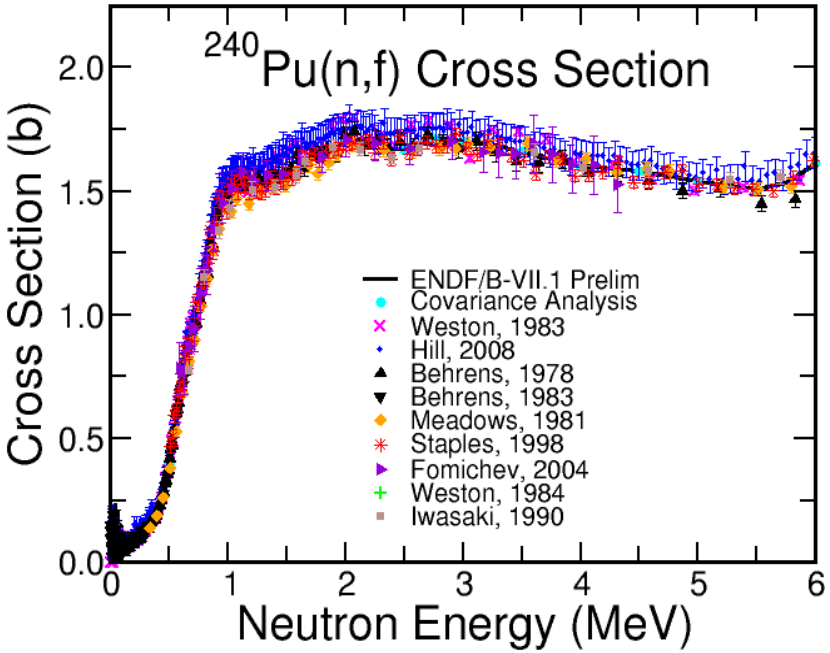
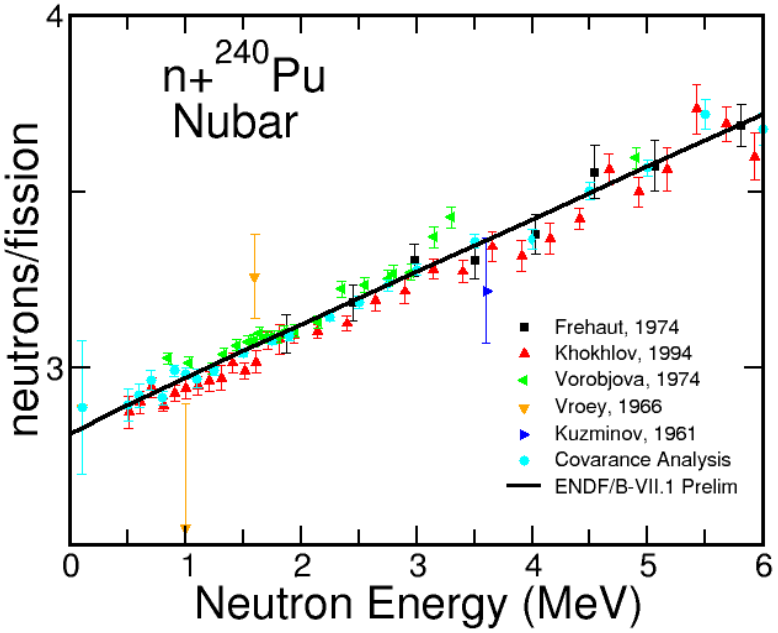
Pu-240 LANL Evaluation, Fission

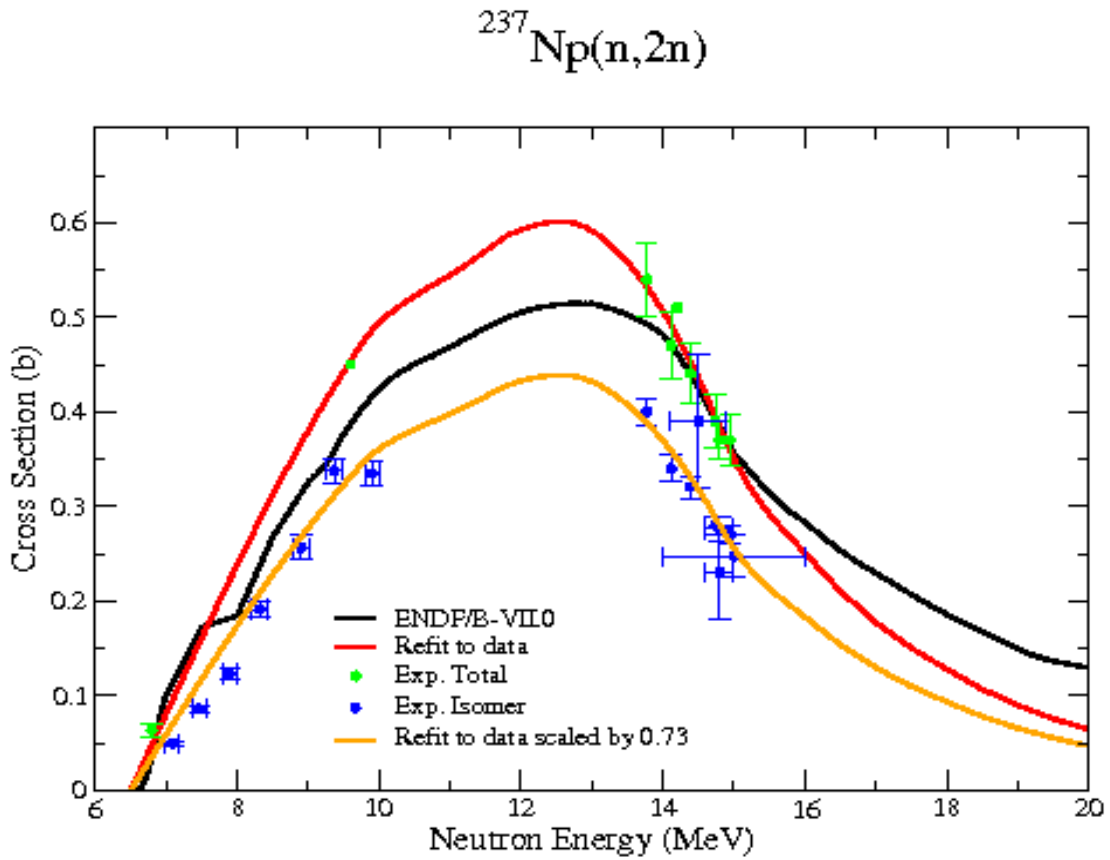
When we model Pu crits with high 240Pu content,
we now believe we get the right answer for the right reason!





Covariance data are also provided

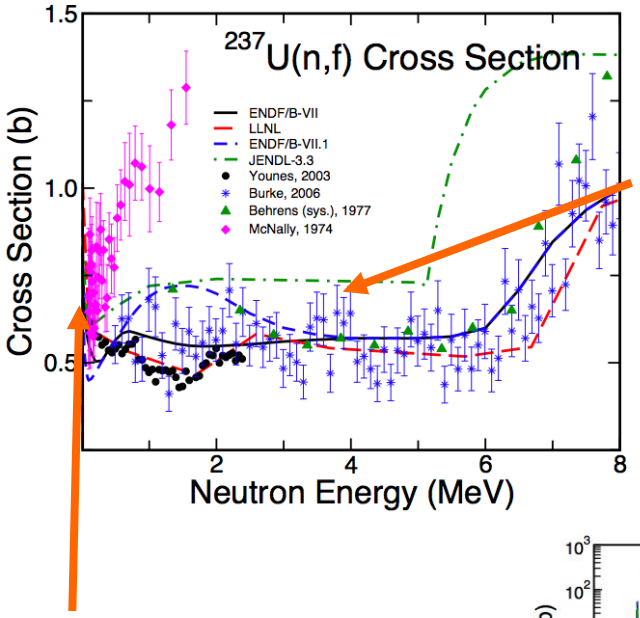
Np-237 – Focus on (n,2n) Improvements. We use Maslov's predicted m/tot isomer ratio



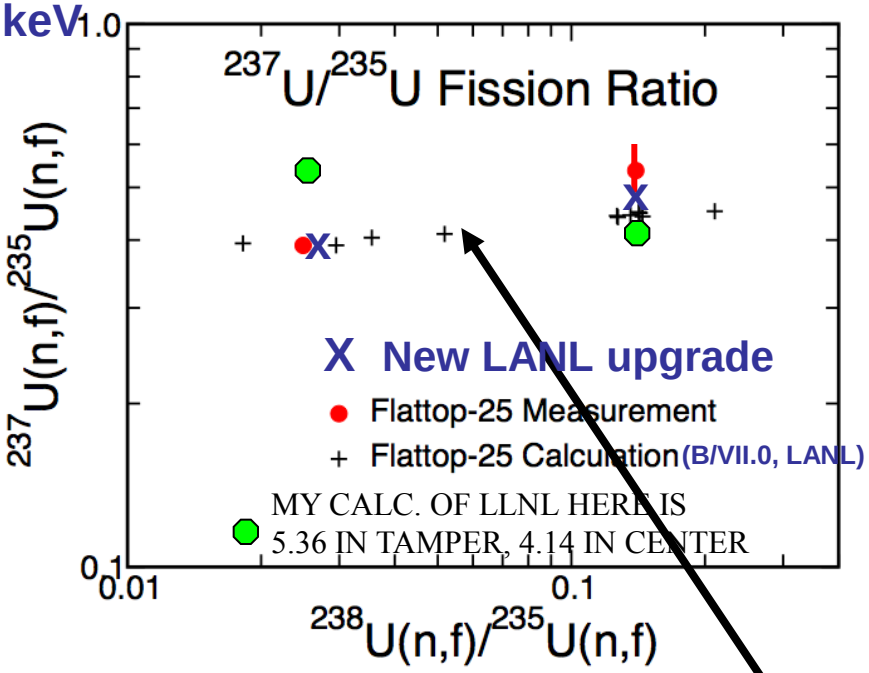
(n,2n) upgraded based on total and isomer production data

237U - LANL new evaluation

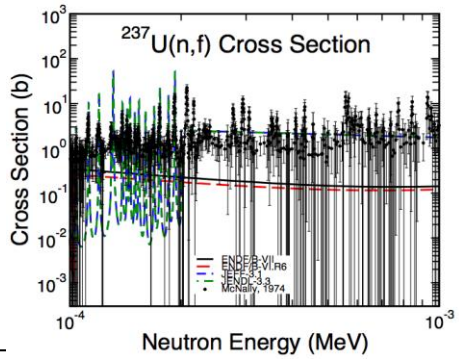
LANL/ENDF 237 fission ~ poor below 10 keV (used old ENDF res. Parameters). We propose:
-LANL + JENDL3.3 at lower energies for B-VII.1
-LANL - longer term, use LANL/LSD expt ~ 1 keV

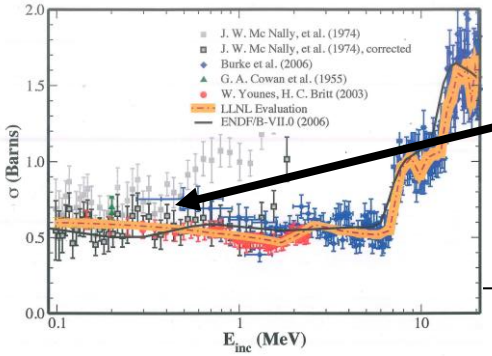


LANL VII.1 proposal
Higher here to better match:
a) Crit assembly data
b) Behrens systematcis
c) Lynn-Hayes calc.



Experiment at LANSCE being planned below 1 keV





Slope dictated by fission x/s slope

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Okajima Physor08 FCA data testing of fission

Japanese testing of ENDF/B-VII.0 fission:

237Np - good
241Am, 243Am - C/E is 3-6% low
238Pu - good, maybe 2% low
242Pu - 4-8% too high
244Cm - 0-7% too high

Table 2
C/E values of CFRRs for TRU in FCA cores

$^{237}Np/^{239}Pu$

Core	Nuclear data libraries		
	JENDL-3.3	ENDF/B-7.0	JEFF-3.1
IX-1	1.05 ±2%	1.03 ±3%	1.00 ±5%
IX-2	1.00 ±2%	1.03 ±2%	1.01 ±2%
IX-3	1.02 ±1%	1.00 ±1%	1.01 ±1%
IX-4	1.03 ±2%	1.03 ±2%	1.03 ±2%
IX-5	1.02 ±1%	1.01 ±1%	1.02 ±1%
IX-6	1.00 ±1%	1.01 ±2%	1.00 ±1%
IX-7	1.01 ±1%	1.00 ±1%	1.00 ±1%
X-1	1.00 ±2%	0.98 ±2%	1.00 ±2%

$^{241}Am/^{239}Pu$

Core	Nuclear data libraries		
	JENDL-3.3	ENDF/B-7.0	JEFF-3.1
IX-1	1.00 ±2%	0.97 ±3%	0.95 ±5%
IX-2	0.94 ±2%	0.96 ±2%	0.95 ±2%
IX-3	0.98 ±1%	0.96 ±1%	0.97 ±1%
IX-4	0.97 ±2%	0.96 ±2%	0.97 ±2%
IX-5	0.97 ±1%	0.96 ±1%	0.97 ±1%
IX-6	0.96 ±2%	0.97 ±2%	0.95 ±2%
IX-7	0.95 ±1%	0.94 ±1%	0.93 ±1%
X-1	0.94 ±2%	0.91 ±2%	0.94 ±2%

$^{238}Pu/^{239}Pu$

Core	Nuclear data libraries		
	JENDL-3.3	ENDF/B-7.0	JEFF-3.1
IX-1	1.00 ±2%	1.00 ±3%	1.15 ±5%
IX-2	-	-	-
IX-3	1.00 ±1%	0.99 ±1%	1.04 ±1%
IX-4	0.99 ±1%	0.98 ±1%	1.01 ±1%
IX-5	0.99 ±1%	0.98 ±1%	1.00 ±1%
IX-6	0.98 ±1%	0.97 ±1%	0.99 ±1%
IX-7	0.98 ±1%	0.97 ±1%	0.99 ±1%
X-1	0.97 ±1%	0.97 ±1%	1.01 ±1%

$^{243}Am/^{239}Pu$

Core	Nuclear data libraries		
	JENDL-3.3	ENDF/B-7.0	JEFF-3.1
IX-1	0.98 ±2%	0.95 ±3%	0.92 ±5%
IX-2	0.93 ±2%	0.96 ±2%	0.94 ±2%
IX-3	0.97 ±1%	0.95 ±1%	0.96 ±1%
IX-4	0.95 ±2%	0.94 ±2%	0.95 ±2%
IX-5	0.96 ±1%	0.94 ±2%	0.96 ±1%
IX-6	0.95 ±2%	0.95 ±2%	0.93 ±2%
IX-7	0.95 ±1%	0.94 ±1%	0.93 ±1%
X-1	0.92 ±2%	0.89 ±2%	0.92 ±2%

$^{242}Pu/^{239}Pu$

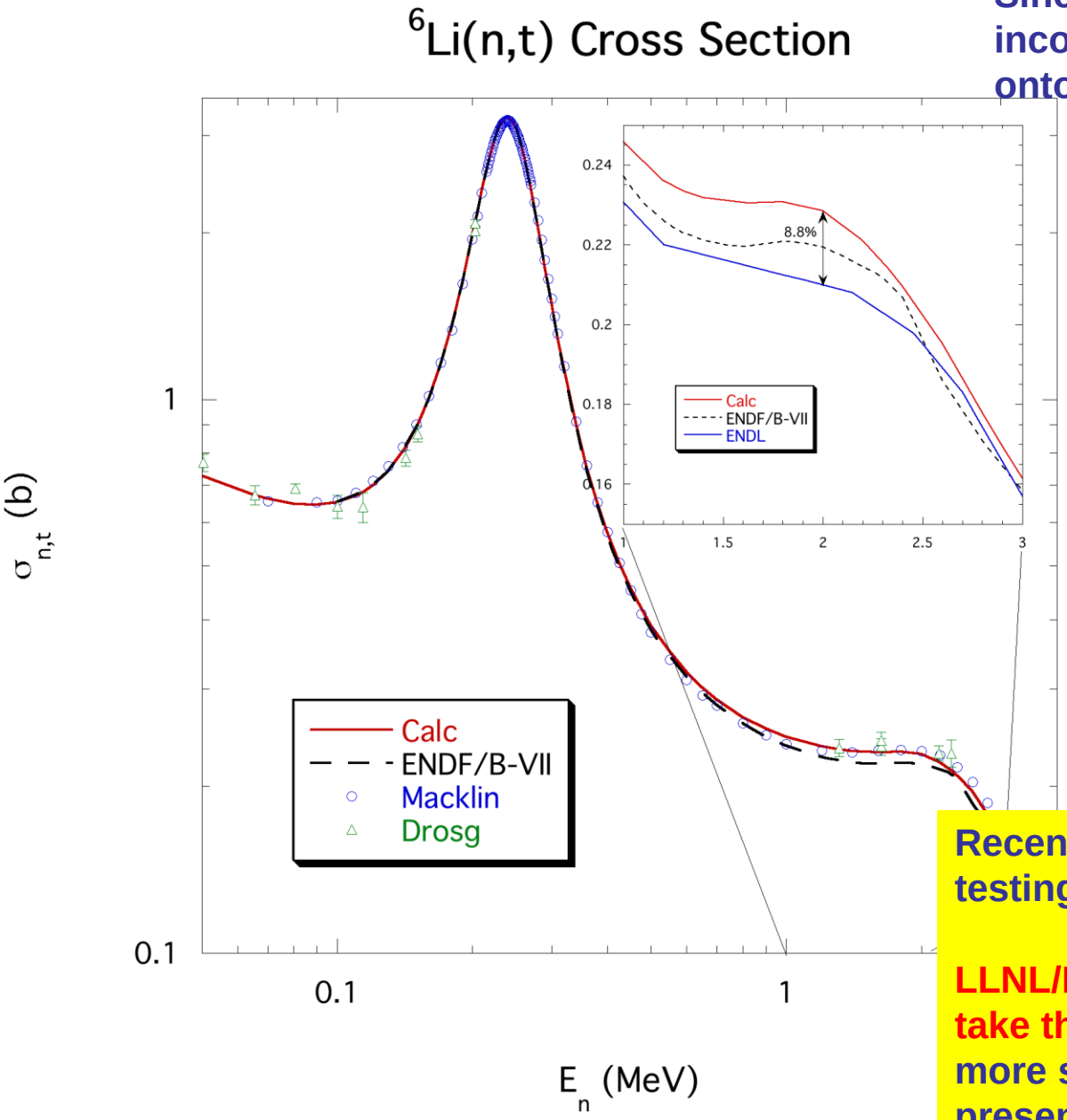
Core	Nuclear data libraries		
	JENDL-3.3	ENDF/B-7.0	JEFF-3.1
IX-1	1.10 ±2%	1.08 ±3%	1.08 ±5%
IX-2	1.05 ±2%	1.08 ±2%	1.10 ±2%
IX-3	1.08 ±1%	1.06 ±1%	1.11 ±1%
IX-4	1.07 ±2%	1.08 ±2%	1.12 ±2%
IX-5	1.08 ±1%	1.08 ±1%	1.12 ±1%
IX-6	1.06 ±2%	1.07 ±2%	1.09 ±2%
IX-7	1.06 ±1%	1.05 ±1%	1.09 ±1%
X-1	1.05 ±2%	1.04 ±2%	1.09 ±2%

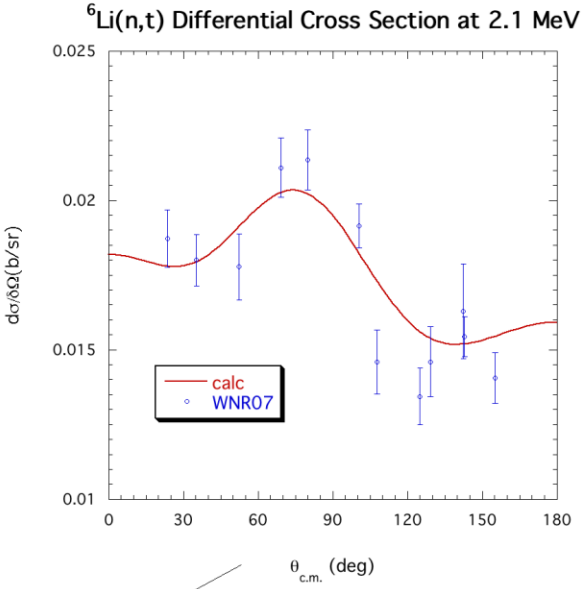
$^{244}Cm/^{239}Pu$

Core	Nuclear data libraries		
	JENDL-3.3	ENDF/B-7.0	JEFF-3.1
IX-1	1.02 ±2%	1.00 ±3%	0.99 ±5%
IX-2	1.01 ±2%	1.04 ±2%	1.03 ±2%
IX-3	1.05 ±1%	1.03 ±1%	1.06 ±1%
IX-4	1.05 ±2%	1.06 ±2%	1.07 ±2%
IX-5	1.05 ±1%	1.05 ±1%	1.07 ±1%
IX-6	1.05 ±1%	1.07 ±1%	1.07 ±1%
IX-7	1.04 ±1%	1.03 ±1%	1.04 ±1%
X-1	1.01 ±2%	1.00 ±2%	1.02 ±2%

^{6}Li(n,t) Reaction - LANSCE data gives increase in 1-3 MeV range

Since this is a standard <1 MeV, we incorporate new results >1 MeV onto existing file.





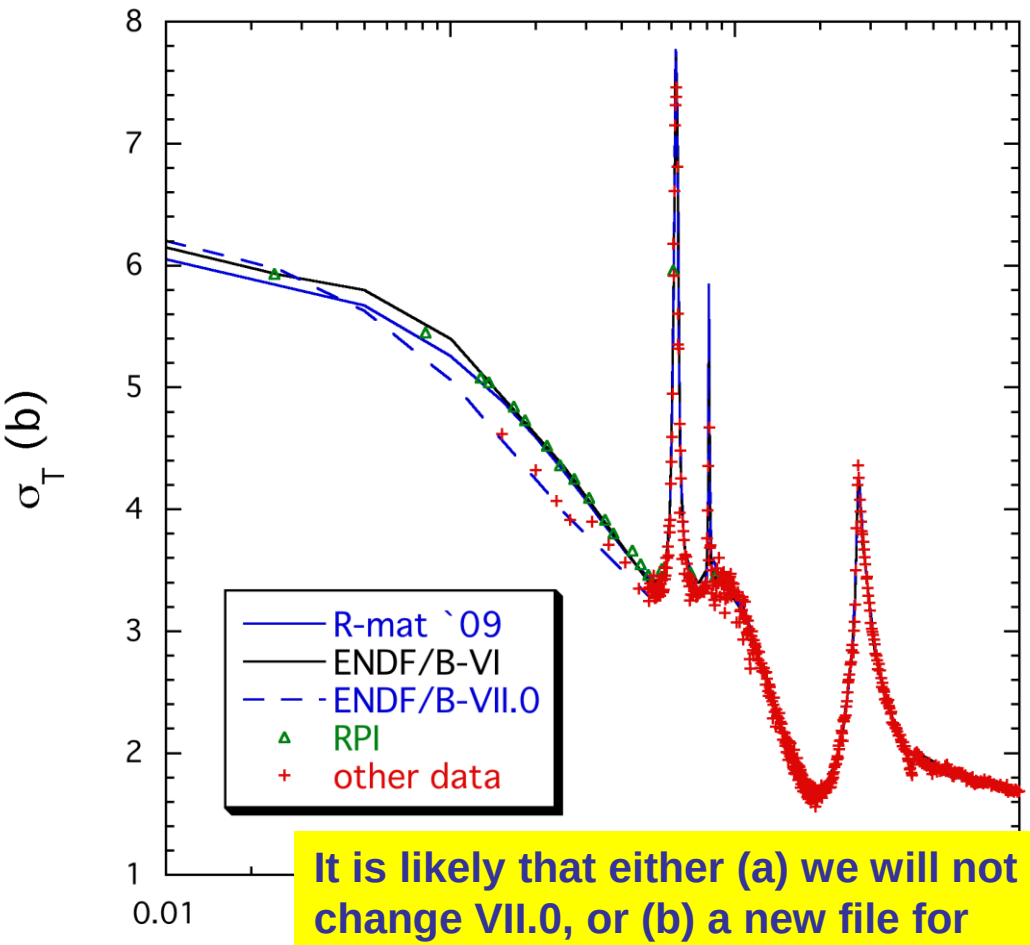
Recent Bethe sphere integral testing successful

LLNL/David Brown has offered to take this file and reformat using more standard formats (though the present file does process OK)

n+^{9}Be Total Cross Section – New RPI Data

Shown is Hale's latest 9Be evaluation - different to B-VII because RPI data included (looks more like B-VI at low energies, but now higher than most other data there).

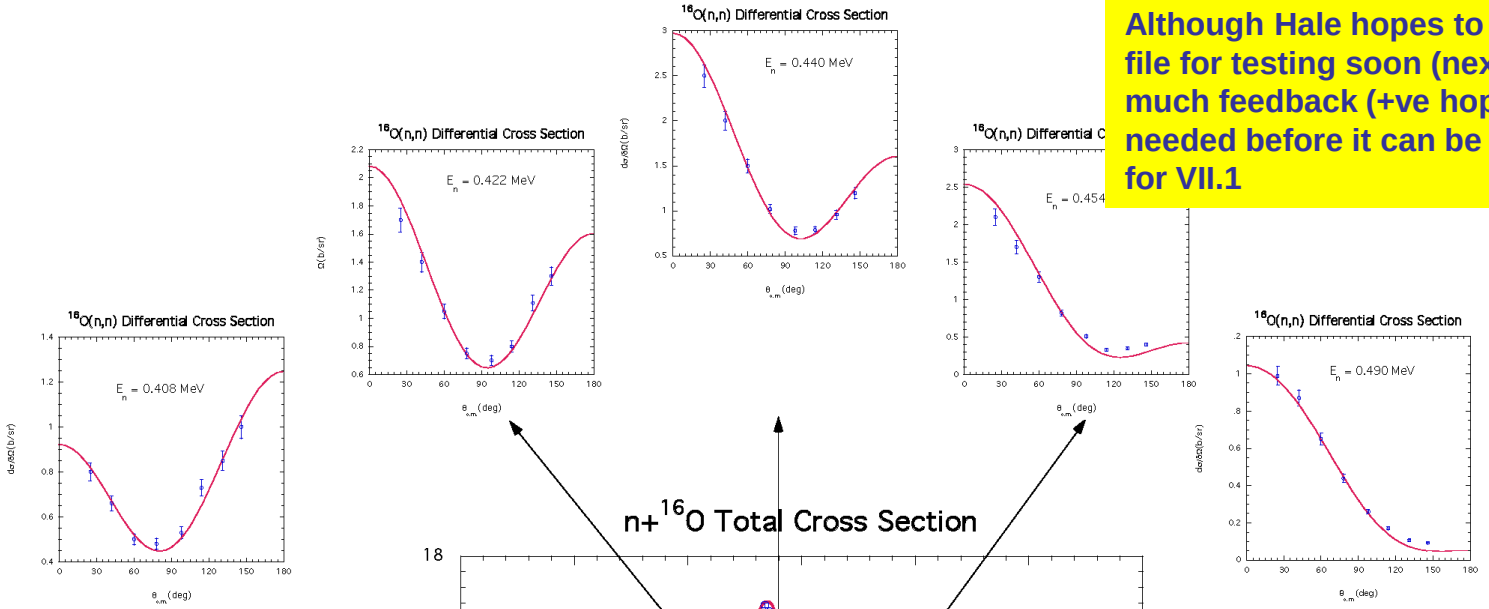
To do:
Test performance in critical assemblies:
-try to resolve discrepant info on feedback from LANL and LLNL Be reflected crits
- study what is the problem with the 233U Be reflected crits (ENDF/B/VII.0 performed better!)

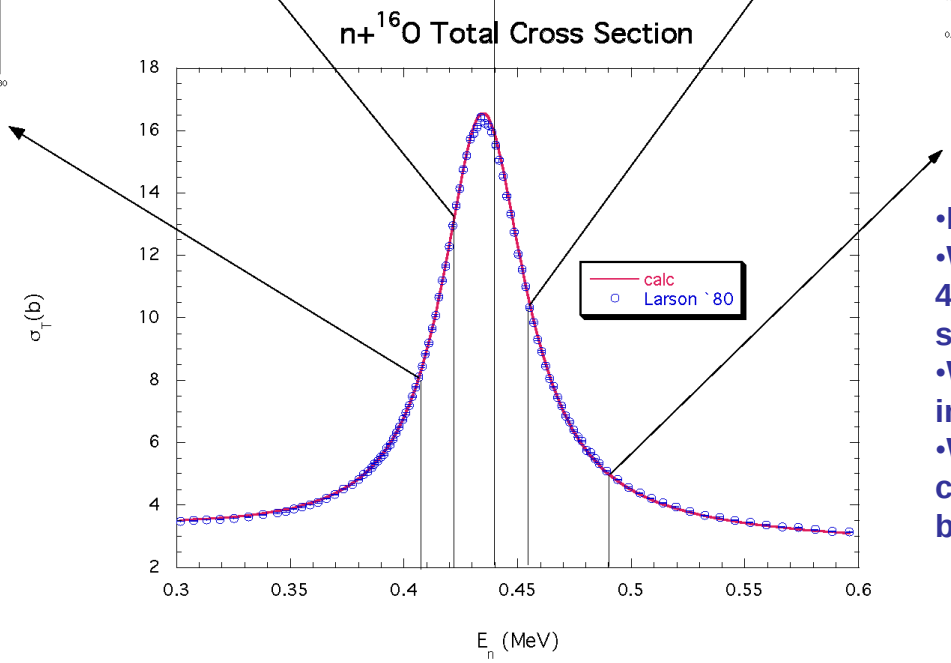


It is likely that either (a) we will not change VII.0, or (b) a new file for VII.1 will still hav problems comparable to VII.0 in its prediction of Be-reflected crits

n+^{16}O Cross Sections Across the 440-keV Resonance: Important Data for Studies Quantifying Reactor Criticality Uncertainty

Although Hale hopes to have a new file for testing soon (next week!), much feedback (+ve hopefully) is needed before it can be considered for VII.1





But we note the R-matrix uncertainties obtained by Hale are very small (<1%) – realistic?

- New R-matrix analysis begun
- Will provide covariances, eg for 440 keV resonance (for reactor simulations)
- Will use lots of new data, including (n,alpha)
- Will need to test against many crits, including LCTs, and broomstick etc

Major Actinides

- ^{238}U: New Wallner capture data validates VII.0 evaluation.
- 235U: We are monitoring the WPEC/Iwamoto work, and may want to adopt their result (lower capture in the 0.5-4 keV region). Some may view the lower energy boundary for the resonance region a drawback. Much validation testing will be needed.
- ^{239}Pu. Inelastics – VII.0 based on old evaluation. Maslov argues that total inelastic is too high in the fast region. Kawano will assess and initiate a new effort to model and evaluate inelastic reactions – but for an ENDF upgrade beyond VII.1. Kahler continues to test ORNL/CEA new resonance region work, including interplay of fission spectrum shape and other data in solution criticals.

Patrick has refined the grids for the major actinide fiss spec > 10 MeV out; He is also using the LANL model to create fiss spec for minor actinides, some of which we could use for VII.1.

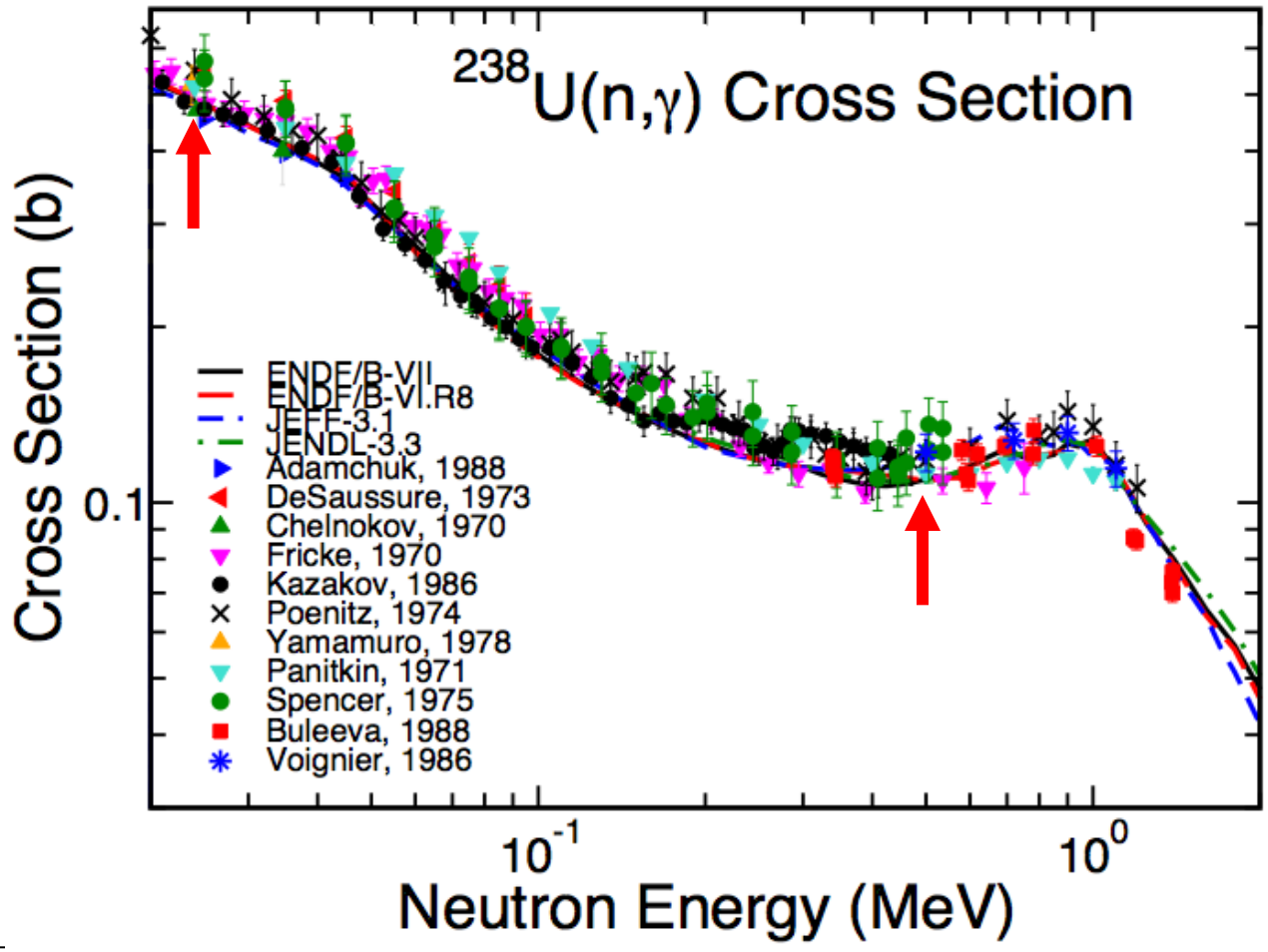
238U capture: ~ We're Monitoring Wallner expt.

As part of an IAEA CRP, Toni Wallner (Vienna) is measuring 238U(n,γ)

Irradiation at Karsruhe, at ~25 and ~500 keV. with acc. mass spectrometry.

First results now available – CONFIRM B-VII.0 (and JEFF differs by ~ 10%!)

IAEA/CSEWG standard, in line with earlier WPEC group, concluded that most measurements suffer from multiple scattering & are too high. Evaluation unc. claimed to be small (~2% or less)



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