Light element evaluation updates for neutrons on ^{6}Li, ^{9}Be for ENDF/B-VIII.1β2

mini-CSEWG

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2023-04-23

LA-UR-23-24421

2023 R-matrix Workshop on Methods & Applications

Ohio University June 20-23

- Overview
- First Circular
- Important Dates
- Call for Abstracts
- Registration
- Registration Payment
- Invited Speakers
- Accommodations
- Travel Information
- Participant List
- Code of Conduct

Contact

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We would like to invite you to participate in the 2023 R-matrix Workshop on Methods and Applications to be held from June 20 - 23, 2023 at Ohio University. Please note that this workshop will be **in-person only**, no remote participation will be accepted.

The aim of this meeting is to bring together a diverse group of researchers with representatives from experiment and theory who utilize the R-matrix formalism for a variety of purposes. Talks will span a wide range of topics covering experimental, theoretical, evaluation developments using R-matrix.

Organizing committee:

Carl Brune (OU)
James deBoer (UND)
Gerry Hale (LANL)
Marco La Cognata (INFN)
Mark Paris (LANL)
Marco Pigni (ORNL)
Ian Thompson (LLNL)

We acknowledge support from IReNA, the University of Notre Dame, and the Institute of Nuclear and Particle Physics at Ohio University.

IReNA

INSTITUTE OF NUCLEAR & PARTICLE PHYSICS INPP @OHIO UNIVERSITY

UNIVERSITY OF NOTRE DAME

- Abstracts by May 7
- Support available, esp. for students/early-career
- Not just R-matrix!
  - *Nucl. Data*
  - *Nucl. Astro*
  - *Nucl. Reactions*
    - *Theory*
    - *Expt*
  - *Atomic systems*

Outline

- Evaluation updates: ENDF/B-VIII.1β1 → ENDF/B-VIII.1β2
  - n+^{6}Li
  - n+^{9}Be

- *Caveat Emptor*: beta version naming not same as NNDC's git
  - β0 = β1.0, β1 = β1.1 etc.

Versions of `n-003_Li_006.endf`

- ENDF/B-VII.1 (2008-09)
  - R-matrix to 4.0 MeV; Legendre above
  - (n,n'd): *not* in MT=32 but
    - *pseudo-level* description: MT=51,52,54-56,58-81
- CP2011 (2011)
  - R-matrix to 4.3 MeV
  - (n,n'd): MT=32 in this version
  - BUT: LCT=2 (LAB) (should have been → LCT=1 (CM))
- ENDF/B-VIII.0
  - MT=105 (n,t) updated
  - But MT=32 from CP2011 was not adopted
    - (n,n'd) from pseudo-level of ENDF/B-VII.1
- ENDF/B-VIII.1
  - β1: CP2020
    - With corrections for MF=6 MT=32 for energy conservation
    - Higher energy R-matrix to 8.0 MeV
      - Inelastic (n,n') MT=52
  - β2:
    - MF=6 MT=2 moved to MF=4 MT=2
    - Other incidental changes (see git.nndc)
    - **(n,t) STANDARD restored to ENDF/B-VIII.0**

MT=105 standard region:

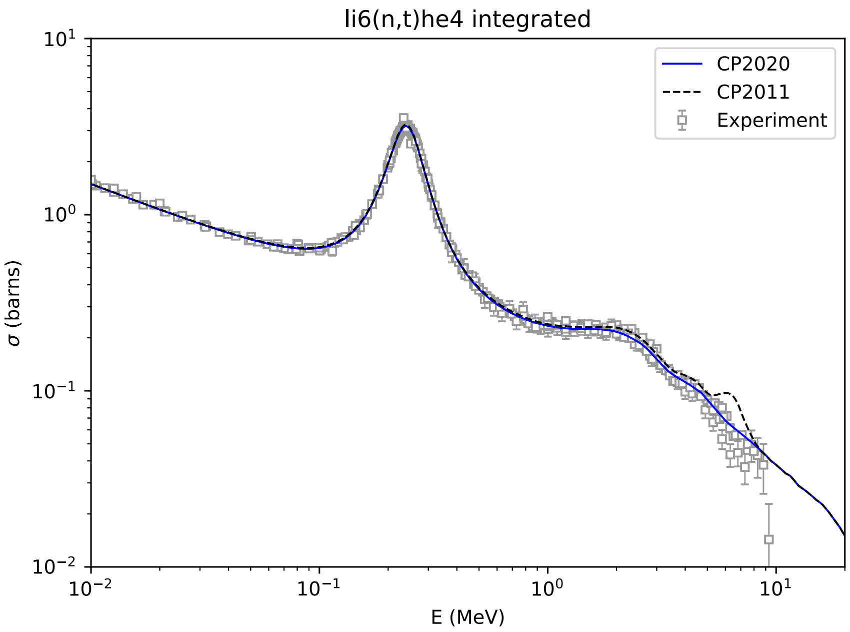
^{6}Li(n,t) 0.0253 eV to 1 MeV

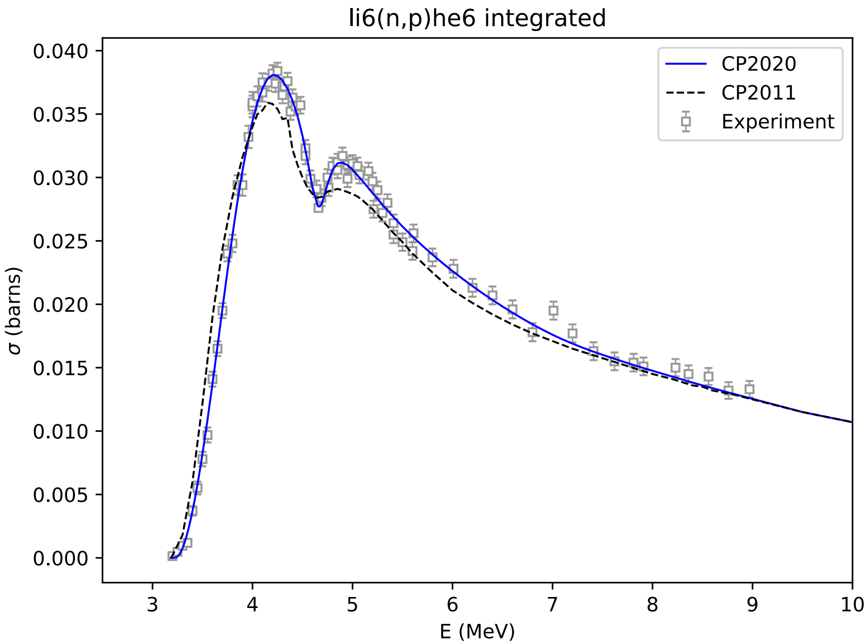
RESTORED in ENDF/B-VIII.1β2

n+^{6}Li

R-matrix evaluation update/extension ENDF/B-VIII.1β1

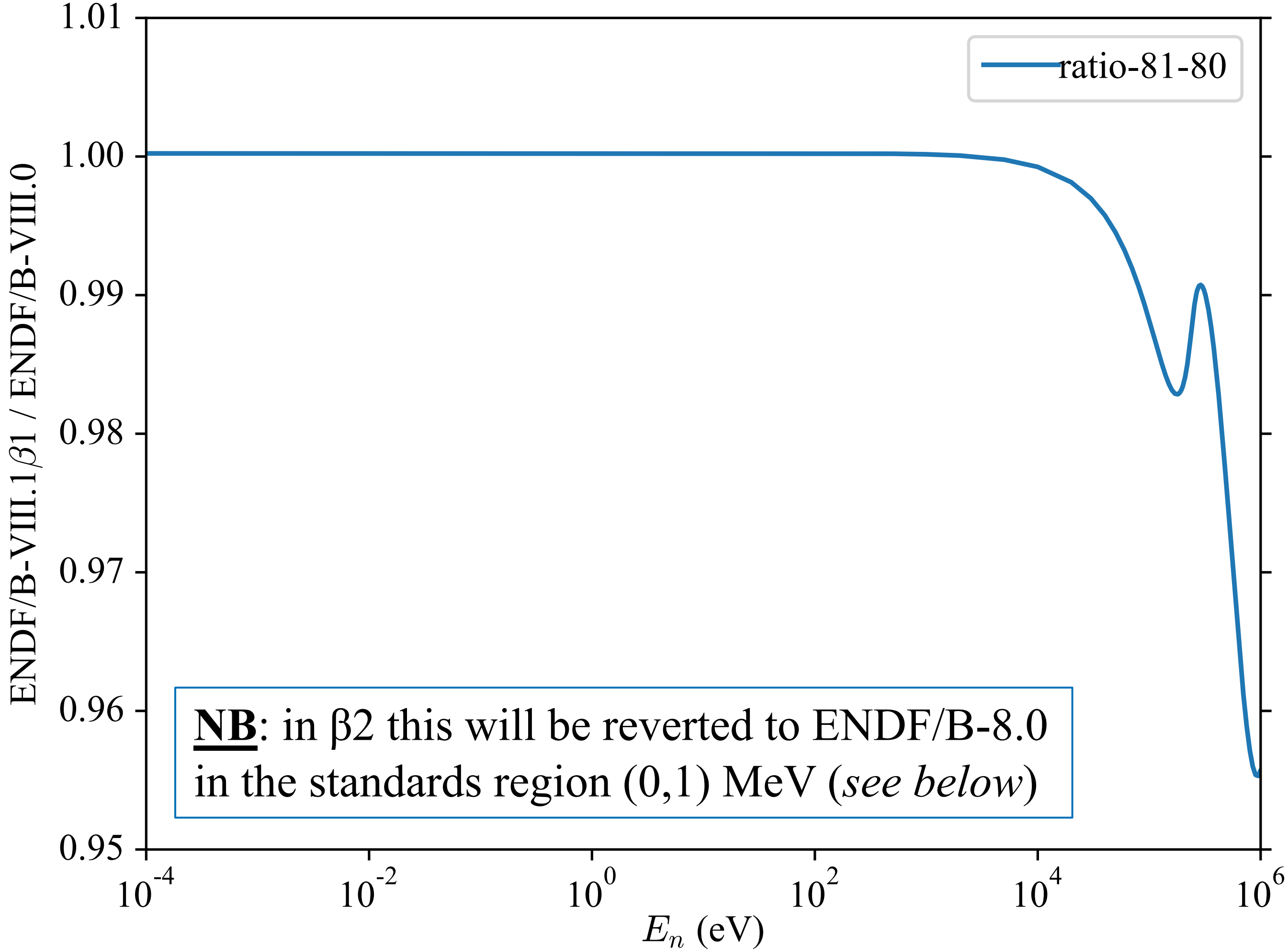
- Previous evaluation ENDF/B-VII.1 (LANL internal "CP2011")
  - upper energy limit $E_n \leq 4.3$ MeV
  - configuration: t+^{4}He, n+^{6}Li, n+^{6}Li*(3^+; 2.19 MeV), d+^{5}He*($3/2^-$)
  - ~3,800 data points; $\chi^2/dof \approx 1.36$
  - formatting changes: MF=4→MF=6; MT=24→41 (n,2np)
    - β2: AND BACK TO MF=4! (N. Gibson: "NJOY/ENDF-102 req'd")
- Updated evaluation (submitted for ENDF/B-VIII.1β1)
  - upper energy limit $E_n \leq 8.0$ MeV
  - new configuration = old config + inelastic: n_2+^{6}Li(0^+; 3.56 MeV)
  - new data covering all channels
  - corrected ^{6}Li(n,n'd)^{4}He spectra





n+^{6}Li: *β1*

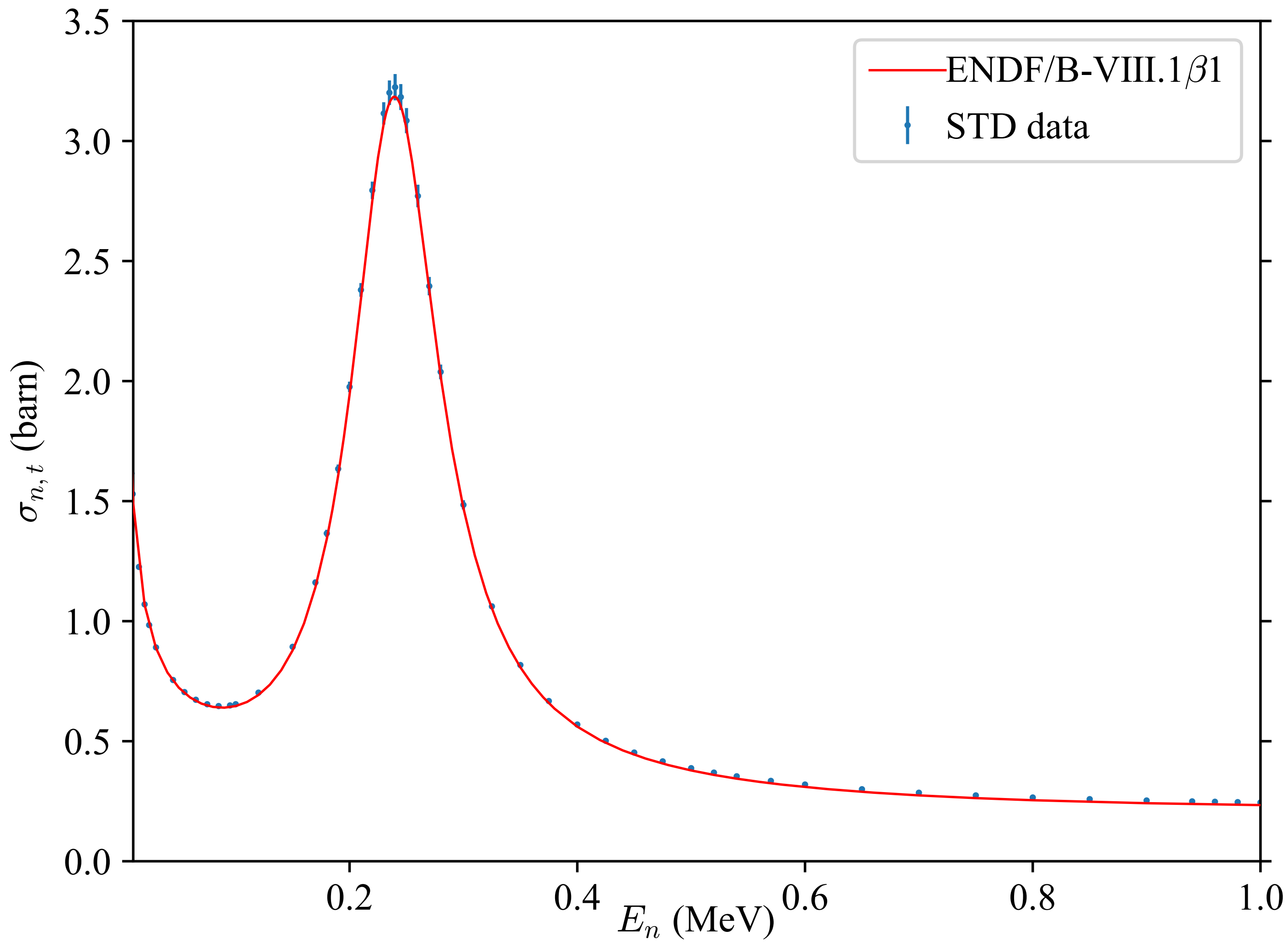
- Ratio comparison
  - 8.1β1 (`n-003_Li_006.endf`) to ENDF/B-VIII.0 (`std-003_Li_006.endf`)
  - Standard region (0, 1 MeV) was changed for β1 (for testing, looking ahead to 9.0)



NB: in β2 this will be reverted to ENDF/B-8.0 in the standards region (0,1) MeV (*see below*)

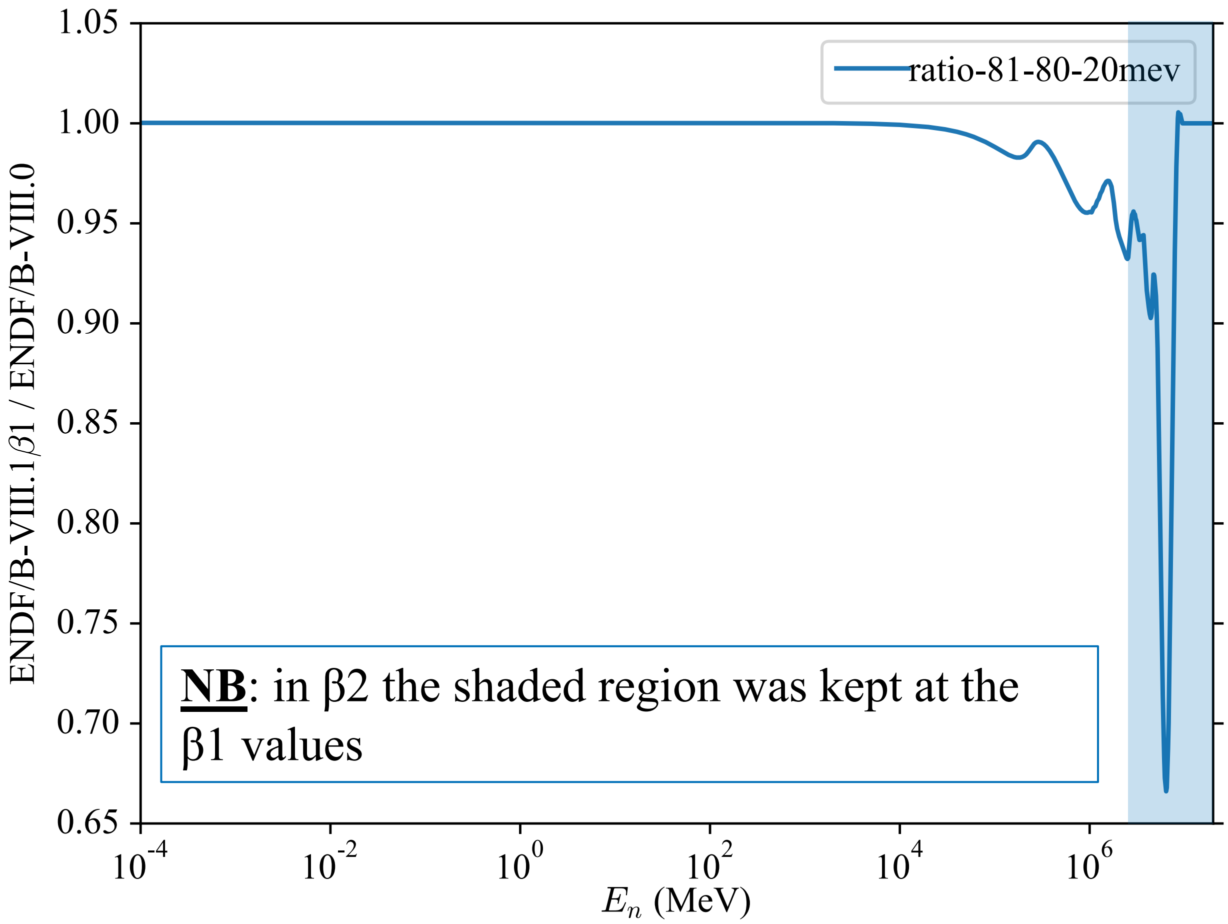
n+^{6}Li: *β1*

- Absolute comparison
  - 8.1β1 (`n-003_Li_006.endf`) to standards ***data***
  - Lower in $J^{\pi} = \frac{5}{2}^{-}$ resonance at 245 keV ($E_x \approx 7.5$ MeV) by ~ 1.5%



n+^{6}Li: *β1*

- 8.1β1 (`n-003_Li_006.endf`) to ENDF/B-VIII.0 (`std-003_Li_006.endf`)
- Full ENDF/B region (0, 20 MeV)

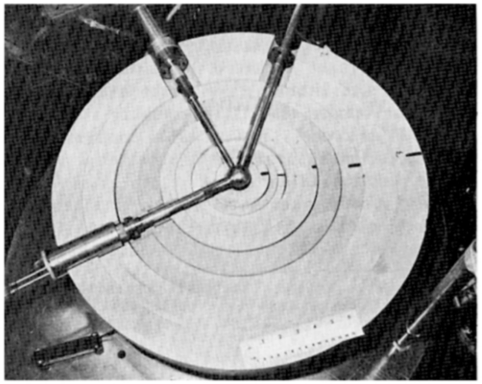


n+^{6}Li(*β1*) integral testing [preliminary]

Kleedtke (LANL/XCP-5)

Experiment	Measured k_{eff}	Calculated k_{eff} (ENDF/B-VIII.0 XSDIR)		Calculated k_{eff} (ENDF/B-VIII.1 XSDIR)	
		ENDF/B-VIII.0	New	ENDF/B-VIII.0	New
HMF63, Case 1	0.99930(400)	1.00340(9)	1.00364(9)	1.00317(9)	1.00357(9)
HMF63, Case 2	0.99880(470)	1.00365(9)	1.00368(9)	1.00349(9)	1.00361(9)
PMF33	0.99670(260)	0.99505(10)	0.99529(10)	0.99538(10)	0.99535(10)

- Nominally worse on HMF/PMF
  - HMF/PMF config: cyl. assy. of U5 & P9 with LiD
  - HEU-MET-FAST-063 driven away from a calculated/experimental value of unity; changes are small compared to the measured k_{eff} uncertainty



Bethe Sphere Ampule Number	Measured H_3 Production	Calculated H_3 Production (ENDF/B-VIII.0 XSDIR)	
		ENDF/B-VIII.0	New
137	2.4317(1459)E-29	2.34223(5621)E-29	2.34626(5866)E-29
139	1.5917(955)E-28	1.58785(1524)E-28	1.59146(1512)E-28
141	3.9896(2394)E-28	3.96243(3051)E-28	4.07348(3096)E-28
111	6.9235(4154)E-28	6.88907(7165)E-28	7.33917(7266)E-28

Bethe Sphere Ampule Number	Measured H_3 Production	Calculated H_3 Production (ENDF/B-VIII.1 XSDIR)	
		ENDF/B-VIII.1	New
137	2.4317(1459)E-29	2.31806(5401)E-29	2.33955(5662)E-29
139	1.5917(955)E-28	1.58332(1536)E-28	1.58512(1506)E-28
141	3.9896(2394)E-28	3.96881(3056)E-28	4.06523(3090)E-28
111	6.9235(4154)E-28	6.92023(7197)E-28	7.36749(7367)E-28

- Bethe spheres
  - Better for outer ampules
  - Markedly worse (overshooting) for inner ampules
  - **Puzzle: no change for 8.1b1 above 9 MeV**

n+^{6}Li(*β1)* integral testing [preliminary]

Kleedtke (LANL/XCP-5)

		Calculated k_{eff} (ENDF/B-VIII.0 XSDIR)		Calculated k_{eff} (ENDF/B-VIII.1 XSDIR)	
Experiment	**Measured k_{eff}**	**ENDF/B-VIII.0**	**New**	**ENDF/B-VIII.0**	**New**
HMF63, Case 1	0.99930(400)	1.00340(9)	1.00364(9)	1.00317(9)	1.00357(9)
HMF63, Case 2	0.99880(470)	1.00365(9)	1.00368(9)	1.00349(9)	1.00361(9)
PMF33	0.99670(260)	0.99505(10)	0.99529(10)	0.99538(10)	0.99535(10)

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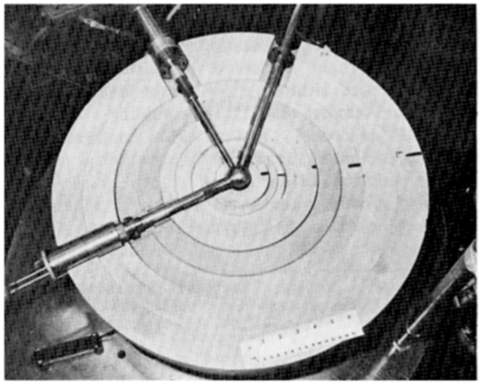
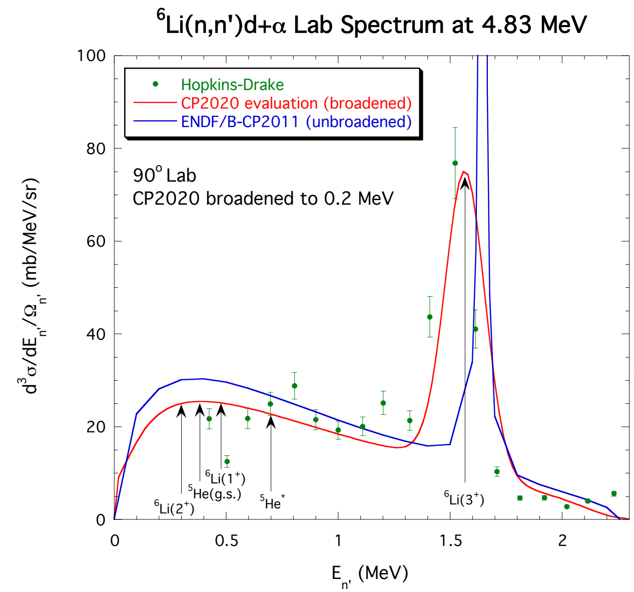


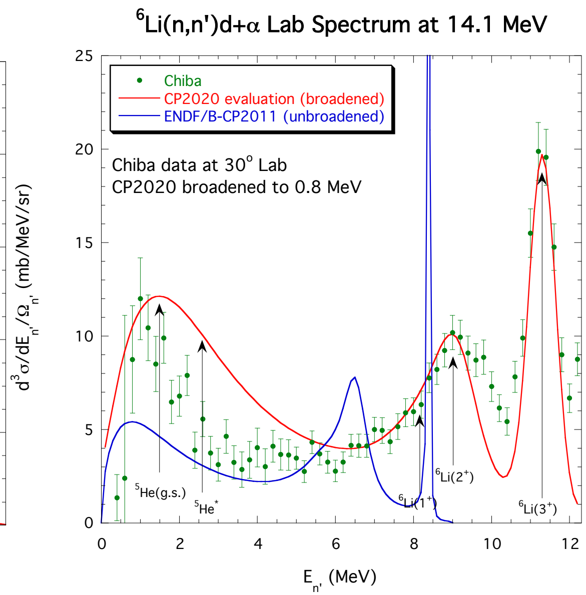
	ENDF/B-VIII.0 XSDIR		ENDF/B-VIII.1 XSDIR	
Ampule	ENDF/B-VIII.0	new ^{6}Li	ENDF/B-VIII.1	new ^{6}Li
111	0.99503	1.06004	0.99953	1.06413
137	0.96321	0.96486	0.95327	0.96210
139	0.99758	0.99985	0.99474	0.99587
141	0.99319	1.02102	0.99479	1.01896

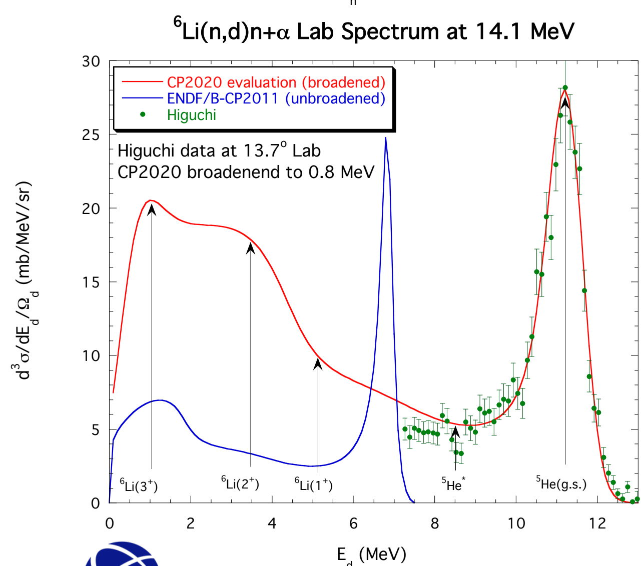
- Bethe spheres
  - ~same for *middle* ampules
  - Markedly worse (overshooting) for inner ampules
  - **Puzzle: no change for 8.1b1 above 9 MeV**

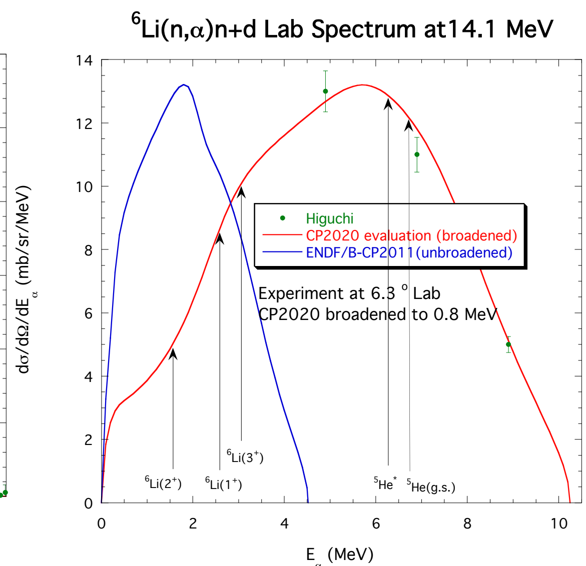
^{6}Li(n,n'd)^{4}He laboratory spectra

Correction of <u>error</u> in CP2011: LAB→CM (LCT=1 →2)









CP2020 ≡ ENDF/B-VIII.1β1

<u>Panels</u>

- **Upper-left**: incident n low-energy (4.83 MeV) neutron spectrum
- **Upper-right**: 14.1 MeV neutron spectrum
- **Lower-left**: 14.1 MeV deuteron spectrum
- **Lower-right**: 14.1 MeV ^{4}He spectrum

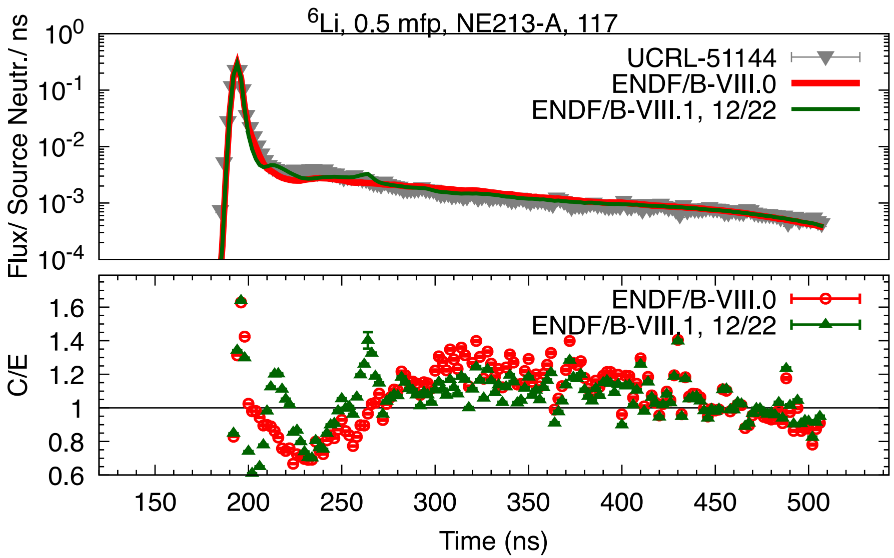
***Note the significant "heating" of 14.1 MeV spectra**

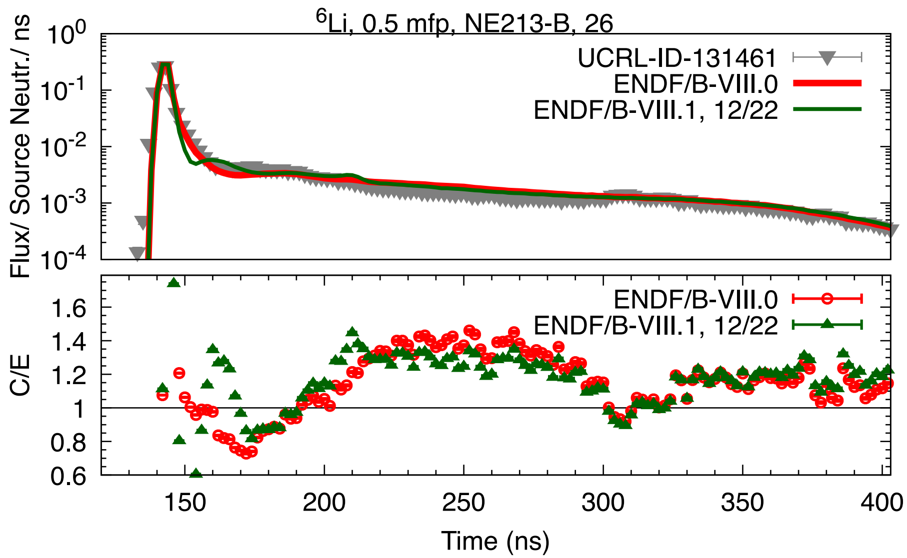
***Perhaps explains significant effect on Bethe and pulsed spheres (if 8.0 is "like" LCT=1 in CP2011)**

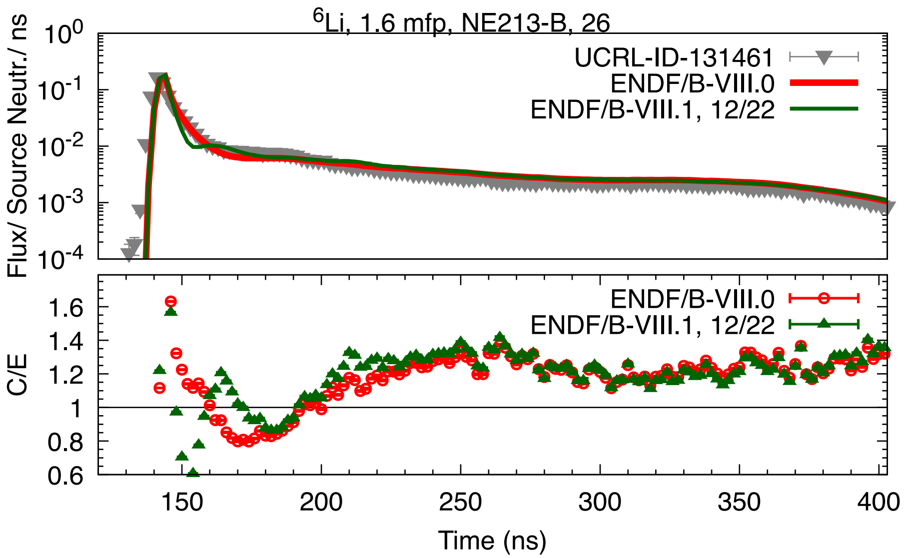
***No other change from 8.0 is significant enough to cause**

n+^{6}Li(*β1*) integral testing [preliminary]

LLNL pulsed spheres—Neudecker (LANL)

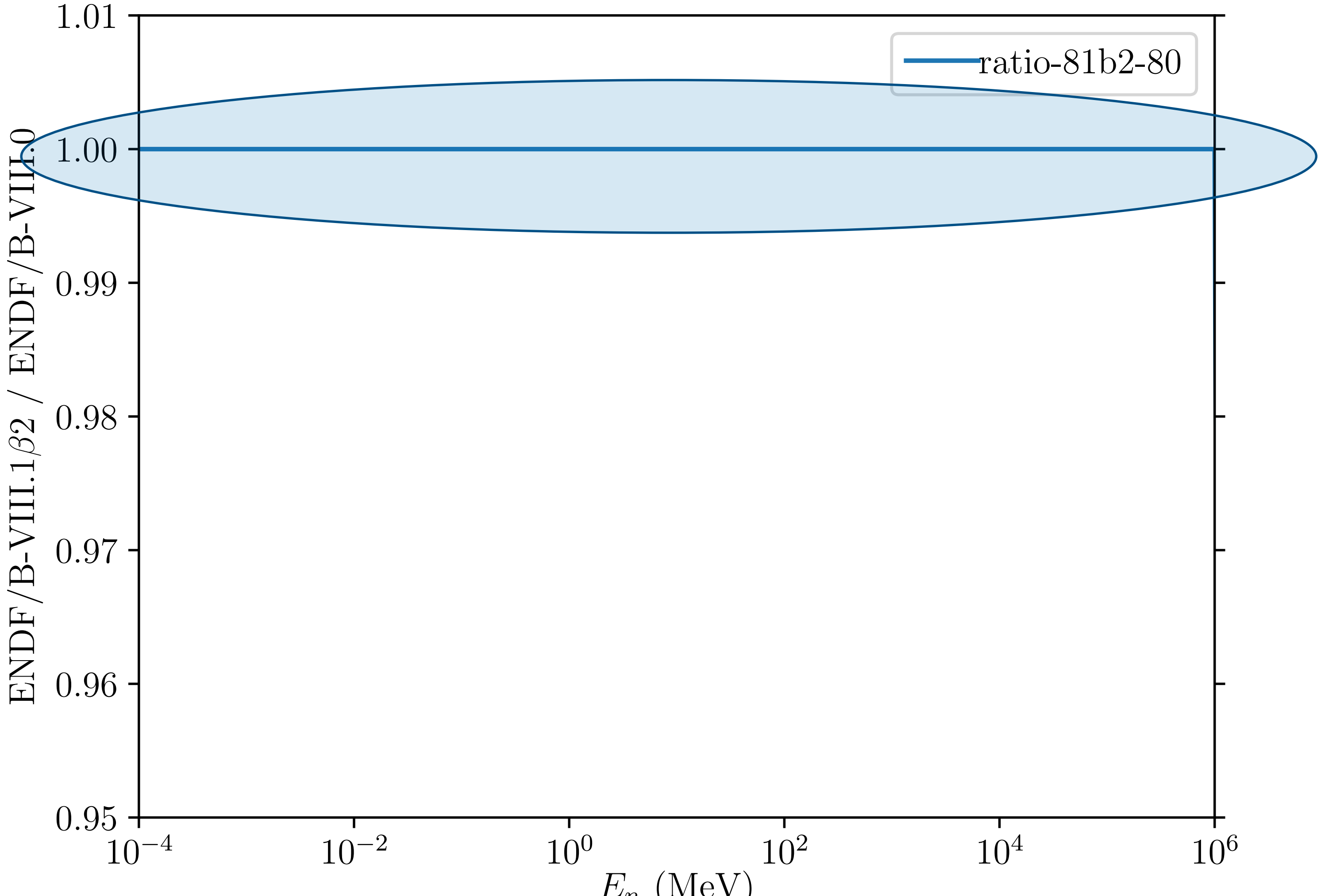






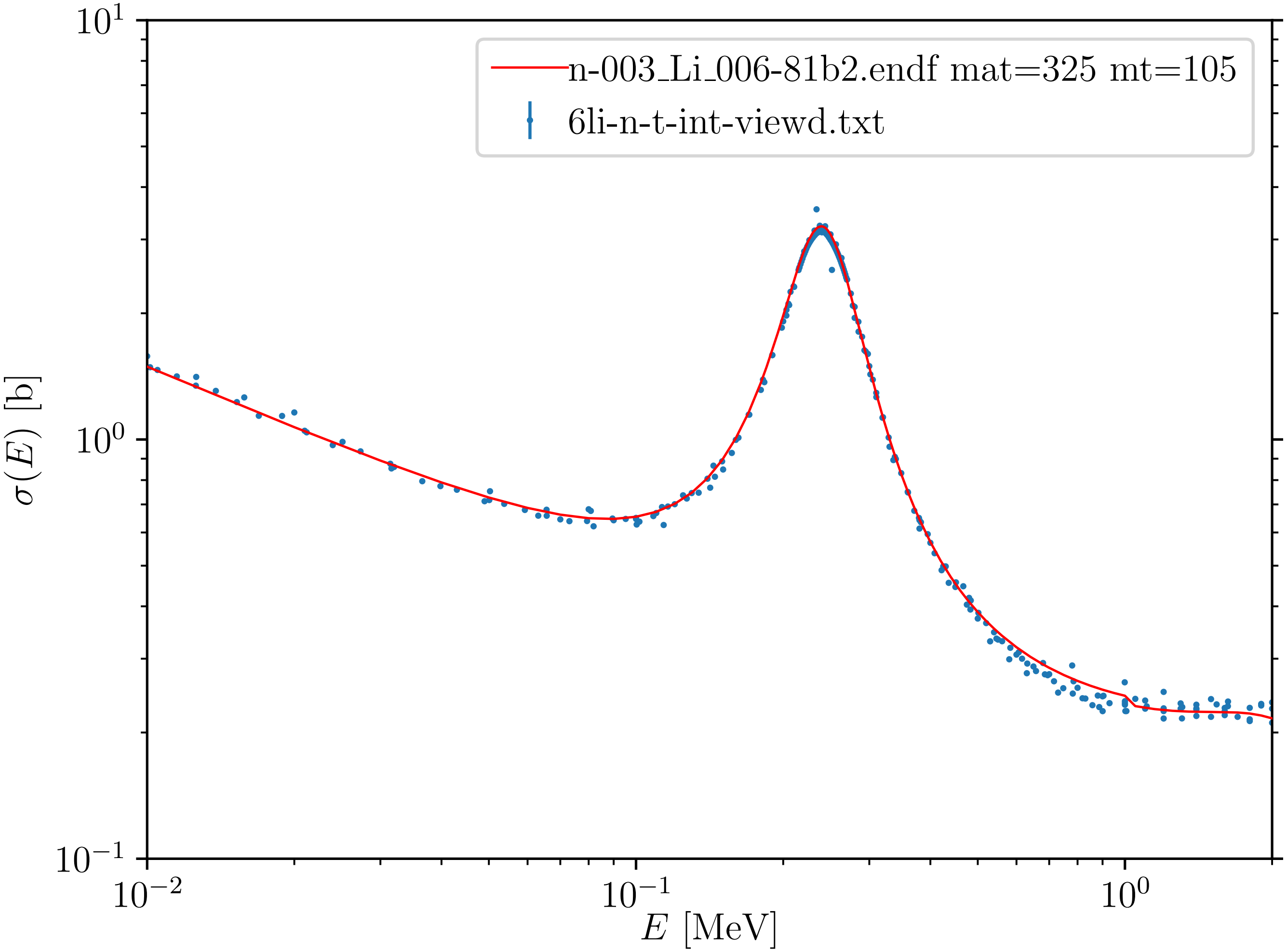
New n+^{6}Li (*β2*)

- Ratio comparison
  - 8.1β2 (`n-003_Li_006.endf`) to ENDF/B-VIII.0 (`std-003_Li_006.endf`)
  - Standard region unchanged from ENDF/B-VIII.0



New n+^{6}Li (β2)

- Absolute comparison
  - 8.1β2 (`n-003_Li_006.endf`) to world data



^{9}Be

n+^{9}Be

R-matrix configuration

Channel	a_c(fm)	$\ell_{\max}$
n+^{9}Be($\frac{3}{2}^-$)	4.67	3
^{4}He+^{6}He(0^+)	5.00	4
$(nn)_0$+^{8}Be(2^+)	5.20	3
n +^{9}Be*($\frac{5}{2}^-$)	5.20	1

Process	E_n range	Observables	N_{dat}	χ^2/N_{dat}
^{9}Be$(n,n_0)^9$Be	(1.25 eV, 15.4 MeV)	$\sigma_{\text{tot}}, \sigma, \sigma(\theta), A_y(\theta)$	5782	1.65
^{9}Be$(n,{}^4\text{He})^6$He	(0.63, 8.5) MeV	$\sigma, \sigma(\theta)$	178	1.40
^{9}Be$(n,2n)^8$Be	(1.8, 14.7) MeV	σ	40	NA
^{9}Be$(n,n_1)^9$Be*	(2.7, 5.0) MeV	$\sigma(\theta)$	83	1.65
Total			6083	1.75

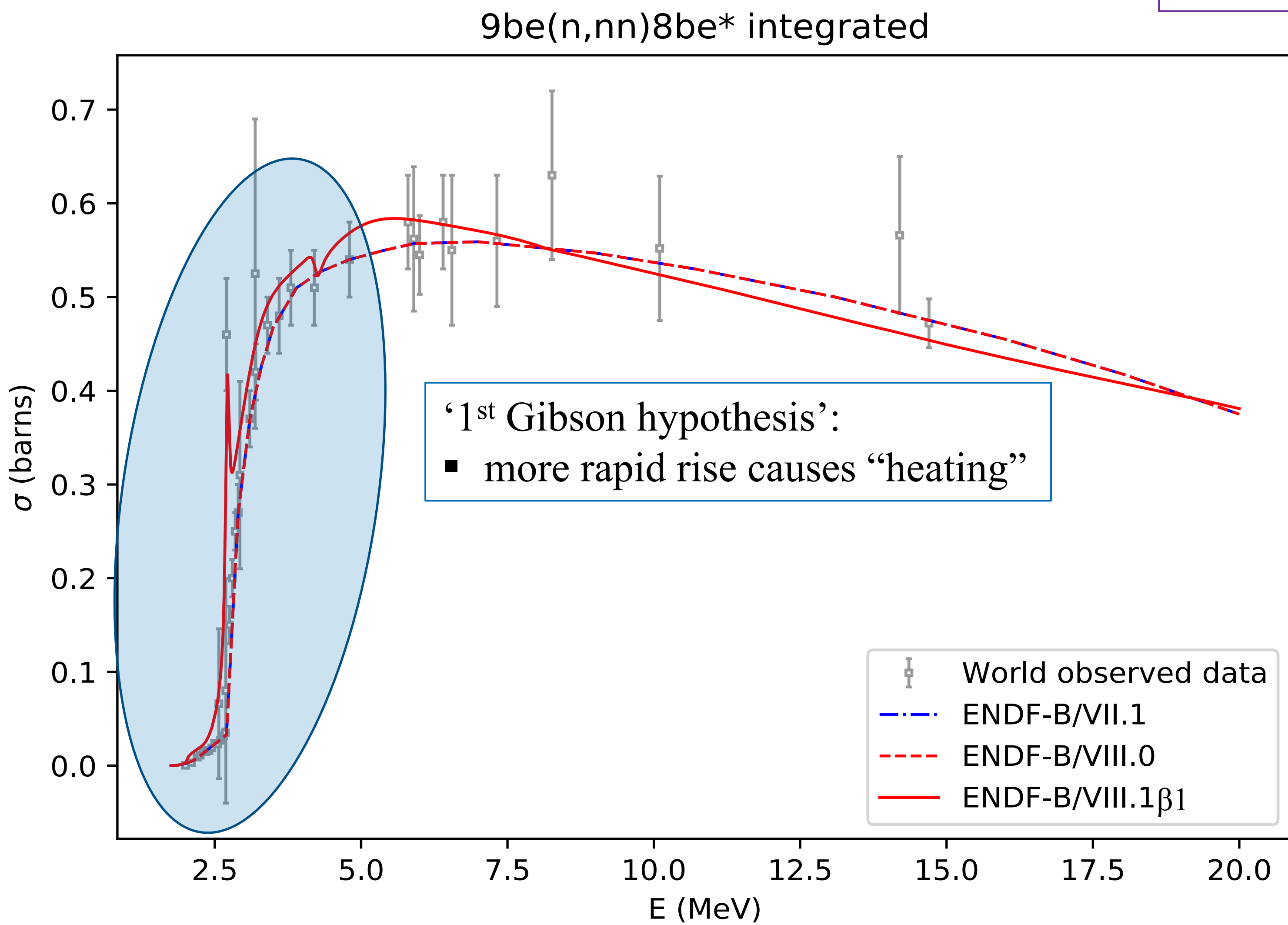
- Added data: elastic, (n,α), (n,n_1)
- Extended upper energy from 1.6 MeV to 5.0 MeV

^{9}Be(n,2n)

(n,2n) changes: MT=16 VII.1 → MT=24 VIII.1β2

MT=16 (n,2n):
- Residual = ^{8}Be

MT=24 (n,2nα):
- Residual = ^{4}He



'1st Gibson hypothesis':
- more rapid rise causes "heating"

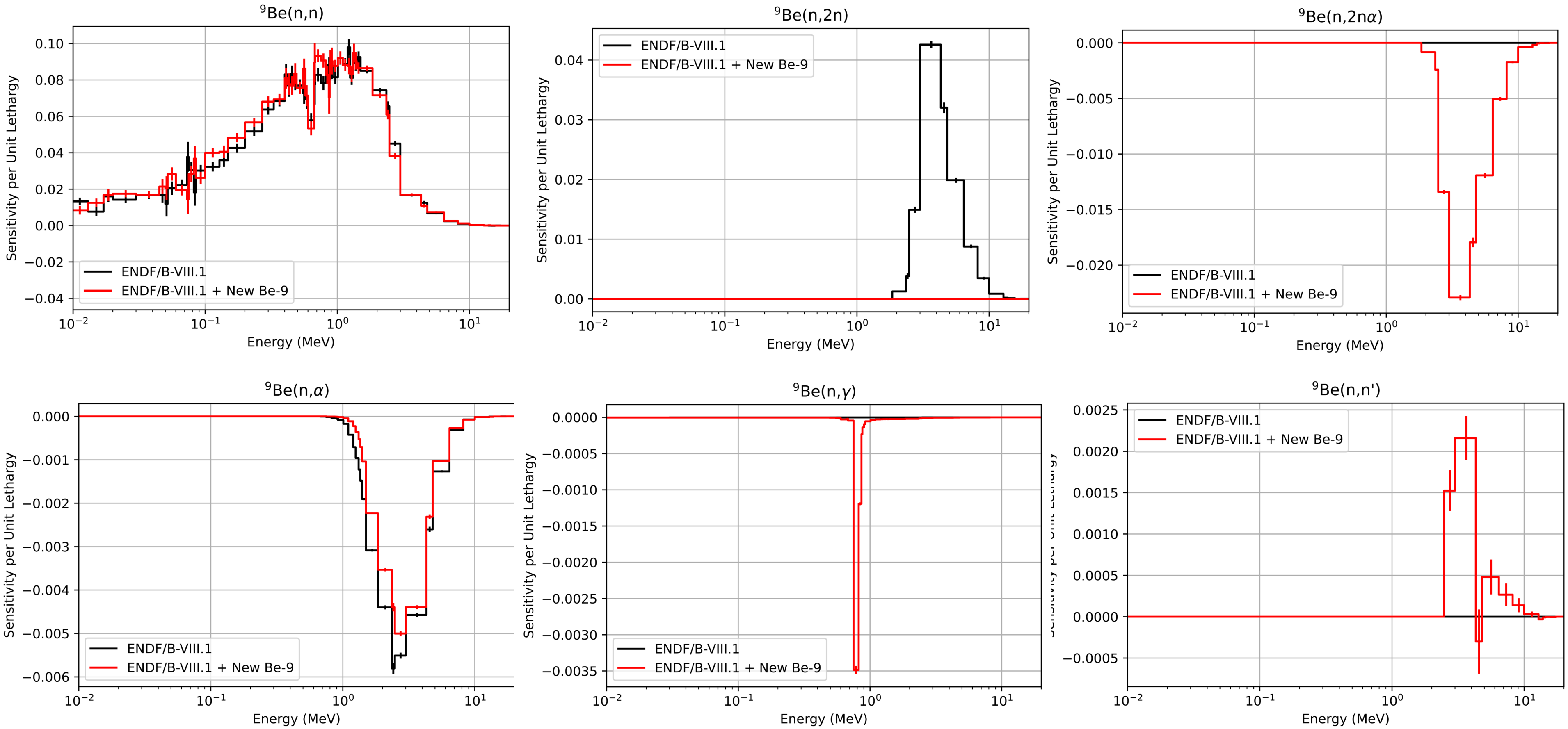
n+^{9}Be integral testing [preliminary]

Kleedtke (LANL/XCP-5)

		Calculated k_{eff} (ENDF/B-VIII.0 XSDIR)		Calculated k_{eff} (ENDF/B-VIII.1 XSDIR)	
Experiment	Measured k_{eff}	ENDF/B-VIII.0	New	ENDF/B-VIII.0	New
HMF75	0.9985(27)	1.00172(9)	1.00229(9)	1.00107(9)	1.00164(9)
HMF101, Case 1	1.00065(+78/-62)	1.00036(4)	1.00231(4)	1.00012(5)	1.00203(5)
HMF101, Case 2	1.00345(+79/-62)	1.00321(5)	1.00514(5)	1.00282(5)	1.00488(5)
HMF101, Case 3	1.00017(+81/-62)	1.00028(4)	1.00217(5)	0.99990(5)	1.00174(4)
HMF101, Case 4	1.00048(+76/-60)	1.00030(5)	1.00215(5)	0.99999(5)	1.00183(5)
HMF101, Case 5	1.00189(+76/-59)	1.00181(5)	1.00372(5)	1.00139(4)	1.00329(5)
MMF7, Case 1	1.0000(45)	1.00094(11)	1.00301(11)	1.00088(11)	1.00318(11)
MMF7, Case 2	1.0000(23)	1.00566(11)	1.00734(11)	1.00580(11)	1.00732(11)
MMF7, Case 3	1.0000(28)	1.00414(10)	1.00464(10)	1.00442(10)	1.00450(10)
MMF7, Case 4	1.0000(28)	1.00339(10)	1.00308(10)	1.00339(10)	1.00320(10)
PMF38	1.0007(19)	1.00092(10)	1.00186(10)	1.00054(10)	1.00173(10)

- Nominally worse on HMF/MMF
  - HMF/MMF/PMF config: cyl. assys. of U5 or P9+HEU hemishells & P9 with ^{9}Be reflectors
  - Generally hotter by 100-200 pcm
  - **β2 will explore reversion to ENDF/B-VIII.0 (n,2n) (but in MT=24)**
    - **This should reduce/cool k_{eff}**

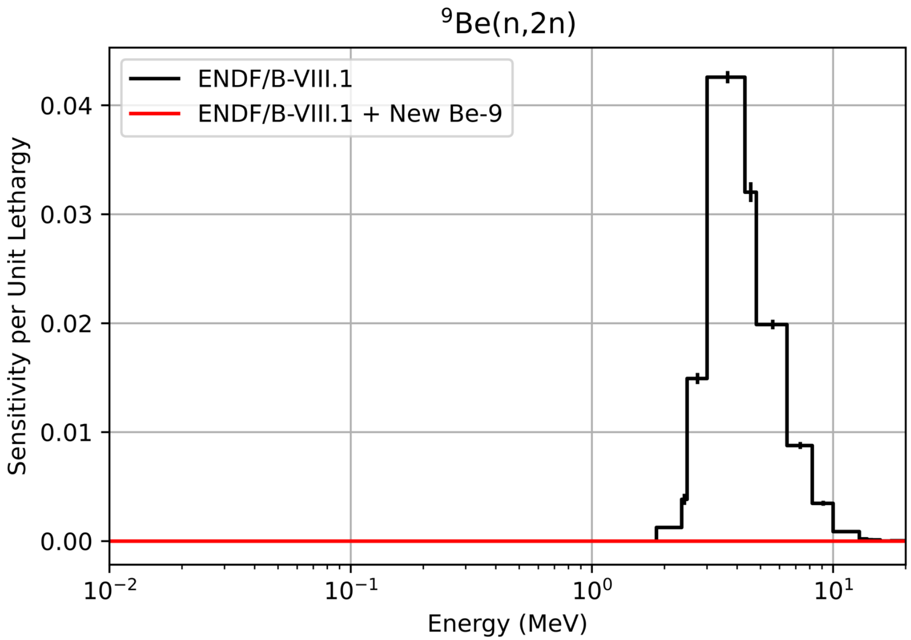
MMF7 Sensitivies
N. Kleedtke's KSEN runs

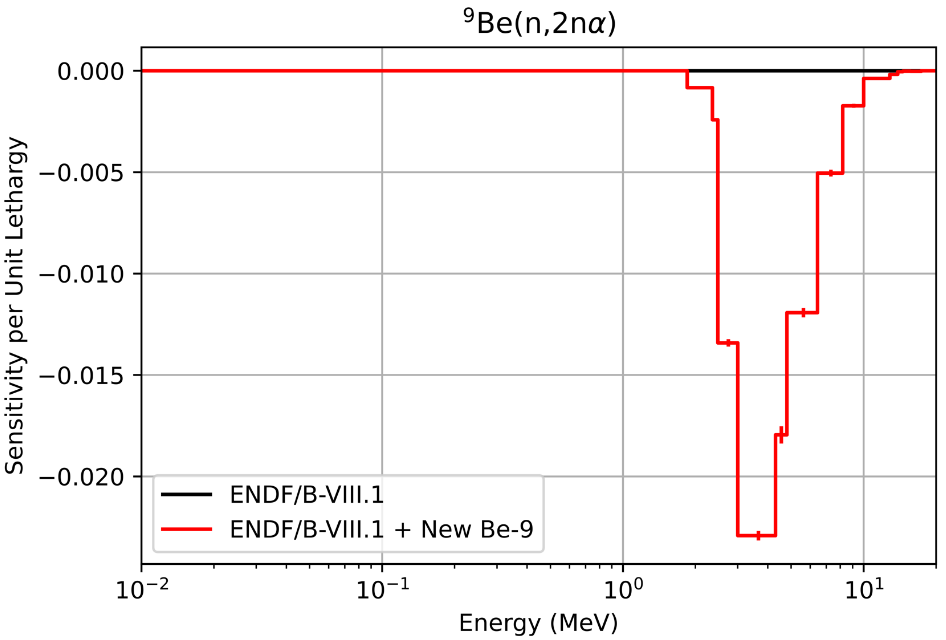


- Decreasing sensitivity from left → right, top → bottom

MMF7 Sensitivies

N. Kleedtke's KSEN runs (n,2n) MT=16 (left) MT=24 (right)

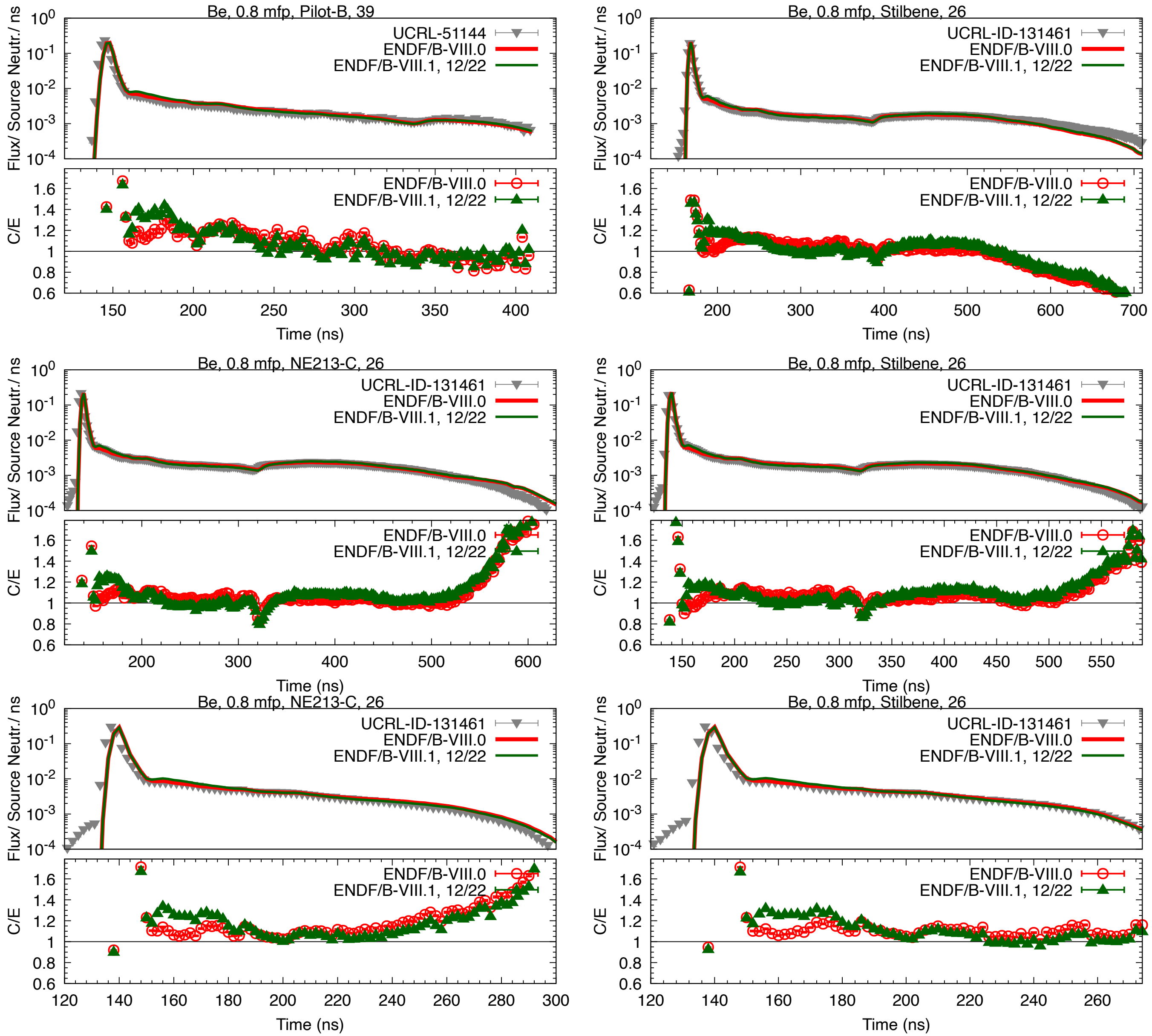




- Opposite sign – why?
- Size – factor of 2 larger magnitude in MT=16
- '2nd Gibson Hypothesis':
  - NJOY is MT16/24 agnostic
  - What about MCNP? (ACE and/or KSEN?)

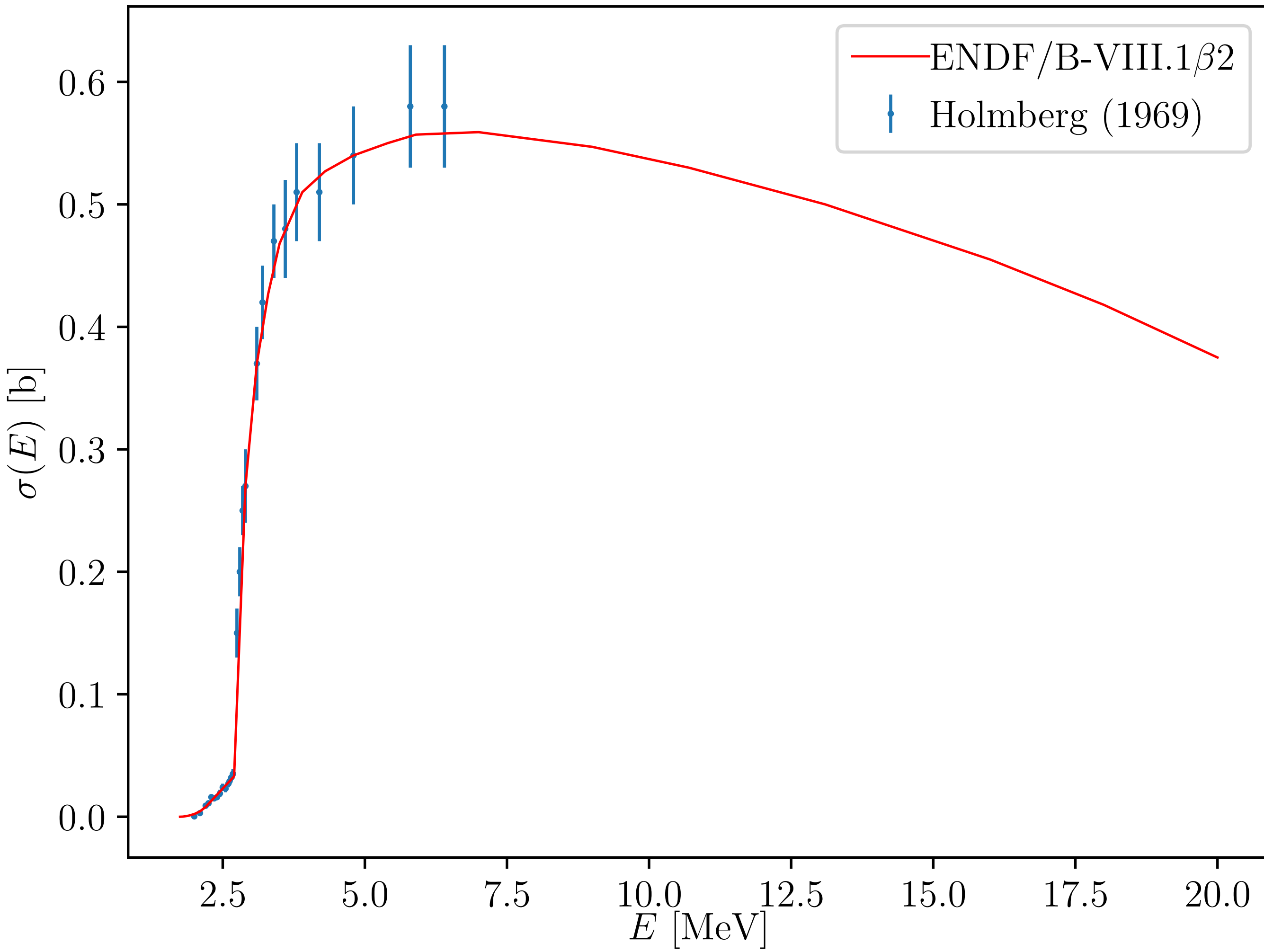
n+^{9}Be integral testing [preliminary]

LLNL Pulsed spheres—Neudecker (LANL)



New $^{9}Be(n,2n)$

MT=24 VIII.1β2 from MT=16 VIII.0



= ENDF/B-VIII.0

Further testing

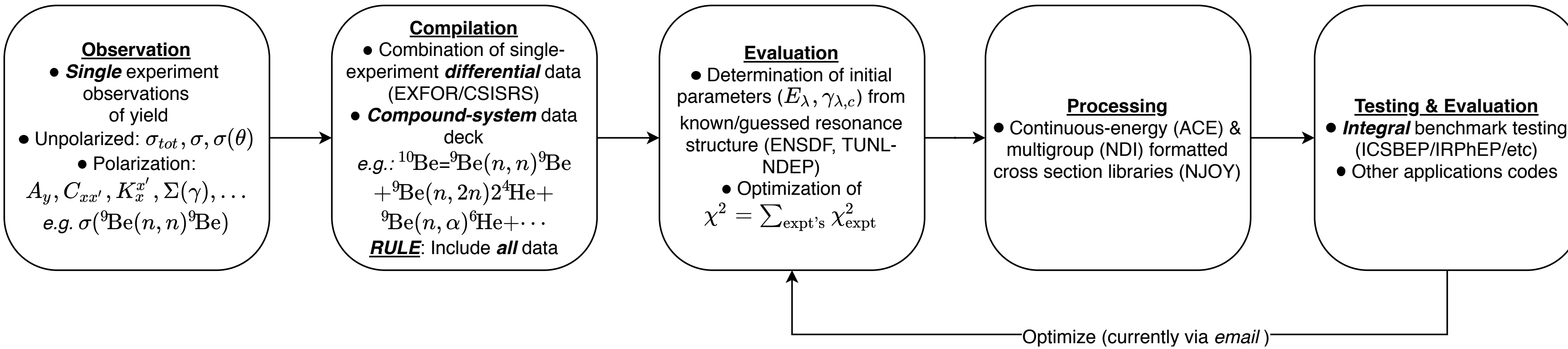
- ^{6}Li
  - Change LCT=1 (LAB) → LCT=2 (CM) in CP2011 and re-run Bethe Sphere, MMF7 *et al.*
  - Others?
  - Evaluation check
    - How did (n,n') spectra change between 8.0 and 8.1?
      - Plot pseudo-level (MT=51, …) representation against MT=32
      - …

- ^{9}Be
  - Change ENDF/B-VIII.0 MT=16 to MT=24 (no other change)
  - Check the 2nd Gibson Hypothesis
    - For ACE (NJOY16): processing agnostic
    - For crits (MCNP): transport agnostic
  - Evaluation checks
    - Can this all be angular distribution changes?
      - Restore MF=4 MT=2 from ENDF/B-III.0

Thank you!

Evaluation pipeline
EDA R-matrix procedure

Nuclear Data Pipeline
EDA cross section evaluation



1. **`EDAf90`** code handles all types of data [*EXFOR/CSISRS; publications; priv. comm.*]
   - total, integrated, diff'l, polarized, unpolarized; neutron- and CP-induced: (n,X), (p,X), (d,X), (t,X),...
2. **`EDAf90`** handles all the compound system (here: ^{10}**Be**) data ***simultaneously***
3. Optimization over parameters simultaneously fits all the data with the same parameters
4. **`EDAf90`** → ENDF-6 formatted ENDF/B libraries for processing to CE & MG libraries
5. Testing & evaluation by hand; future: automate

R-matrix

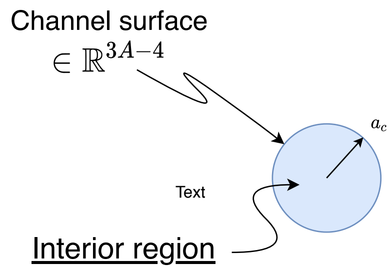
Overview of evaluation framework

Exterior region

$$|\Psi_c^{(+)}\rangle = |\mathscr{I}_c\rangle - \sum_{c'} S_{cc'} |\mathscr{O}_{c'}\rangle$$

$$S_{cc'} = \delta_{cc'} - 2\pi i \rho_c T_{cc'}$$

$r \to \infty$



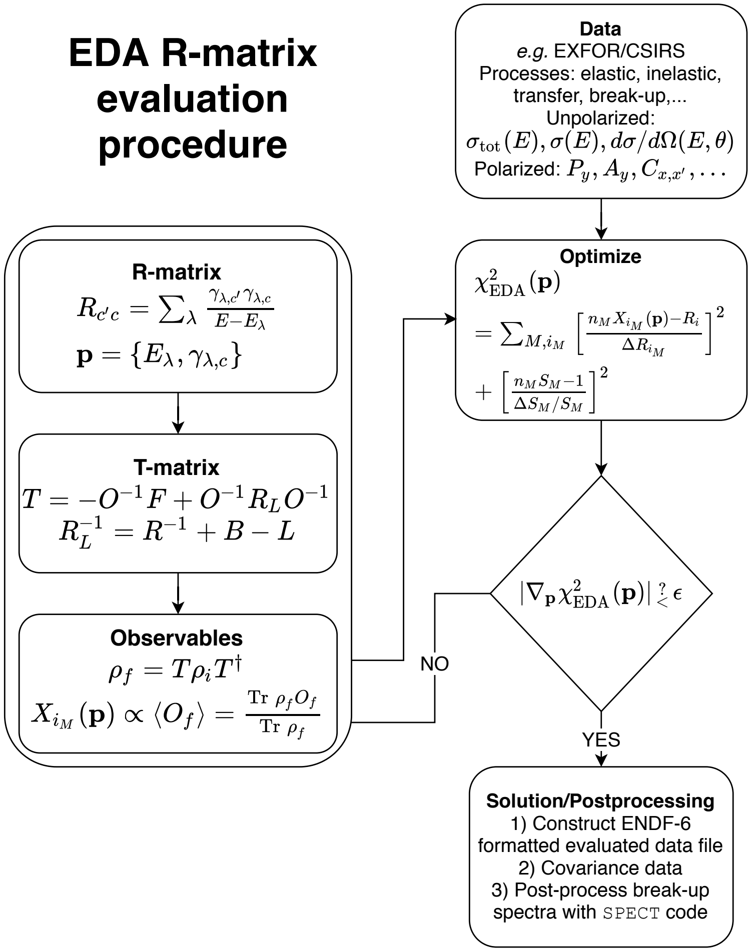
Interior region

$$[H + \mathscr{L}_B] |\lambda\rangle = E_\lambda |\lambda\rangle$$

$$|\Psi^{(+)}\rangle = [H + \mathscr{L}_B - E]^{-1} \mathscr{L}_B |\Psi^{(+)}\rangle$$

$$\mathscr{L}_B = \sum_c \frac{i a_c}{2 m_c} |a_c\rangle\langle a_c| (\hat{p}_r + i B_c)$$

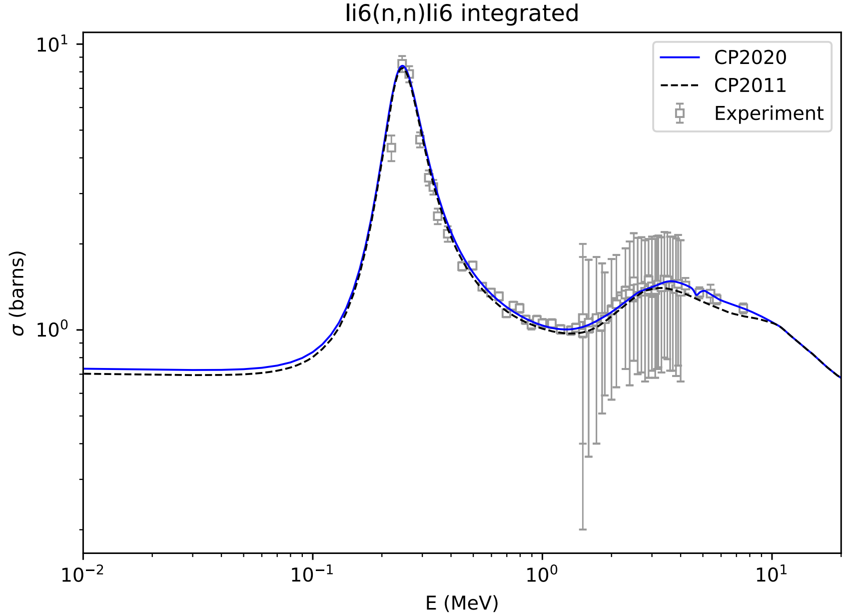
$$R_{B,c'c} = \langle c' | [H + \mathscr{L}_B - E]^{-1} | c\rangle = \sum_\lambda \frac{\langle c'|\lambda\rangle\langle\lambda|c\rangle}{E_\lambda - E}$$

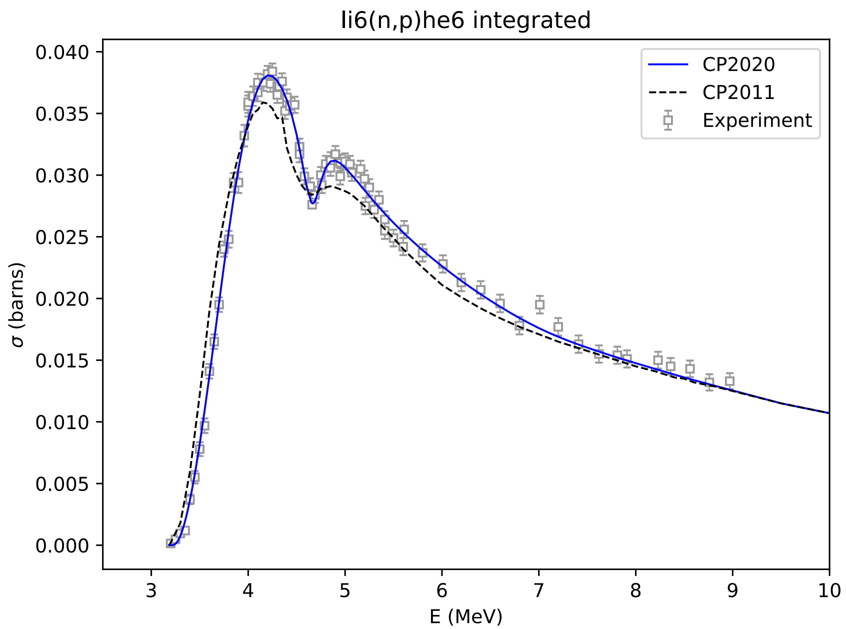


n+^{6}Li

R-matrix evaluation update/extension

- Previous evaluation ENDF/B-VII.1 (LANL internal “CP2011”)
  - upper energy limit $E_n \leq 4.3$ MeV
  - configuration: t+^{4}He, n+^{6}Li, n+^{6}Li*(3^+; 2.19 MeV), d+^{5}He*($3/2^-$)
  - ~3,800 data points; $\chi^2/dof \approx 1.36$
  - formatting changes: MF=4→MF=6; MT=24→41 (n,2np)
- Updated evaluation (submitted for ENDF/B-VIII.1β1)
  - upper energy limit $E_n \leq 8.0$ MeV
  - new configuration = old config + inelastic: n_2+^{6}Li(0^+; 3.56 MeV)
  - new data covering all channels
  - corrected ^{6}Li(n,n’d)^{4}He spectra





n+^{6}Li

R-matrix evaluation update/extension

- Previous evaluation ENDF/B-VII.1 (LANL internal "CP2011")
  - upper energy limit $E_n \leq 4.3$ MeV
  - configuration: t+^{4}He, n+^{6}Li, n+^{6}Li*(3^+; 2.19 MeV), d+^{5}He*($3/2^-$)
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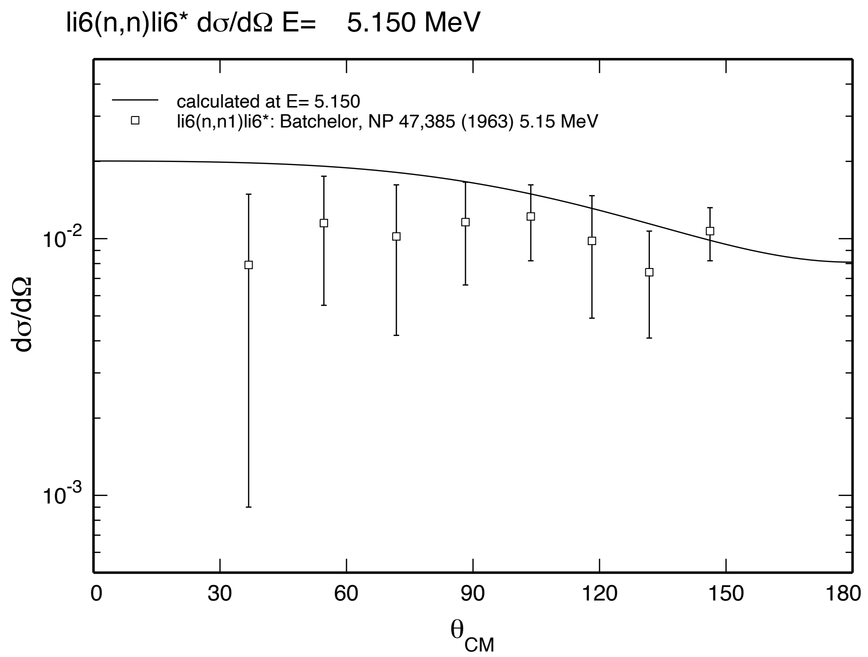

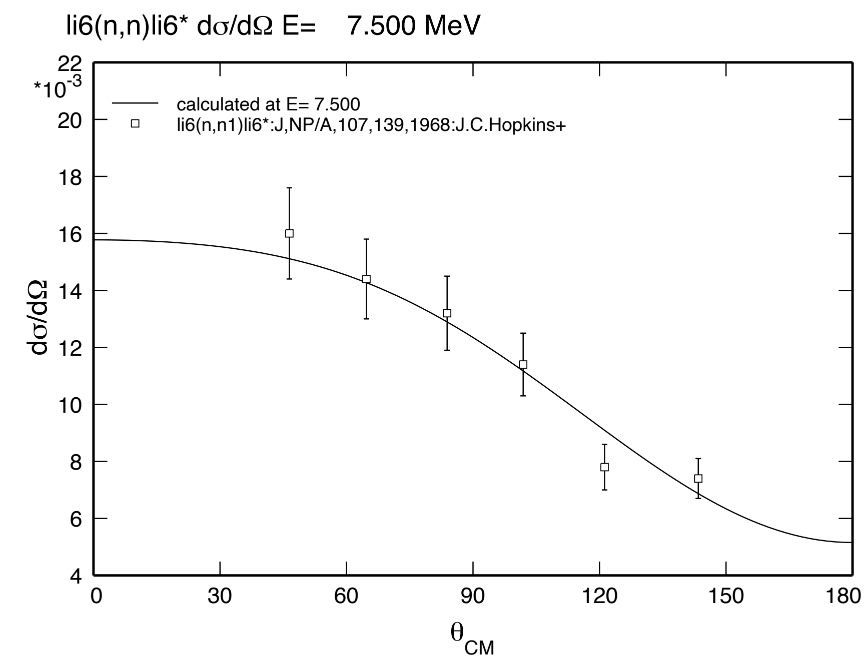

n+^{6}Li

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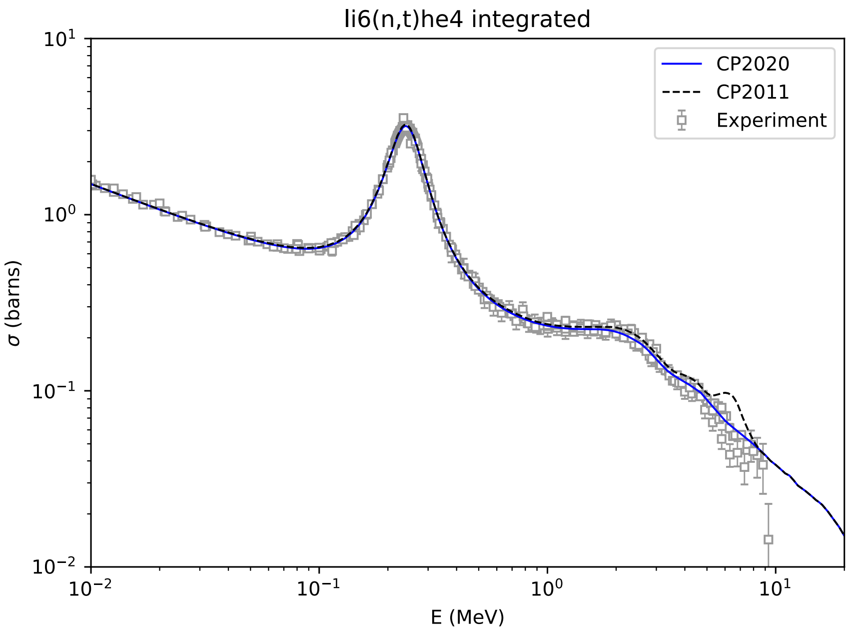

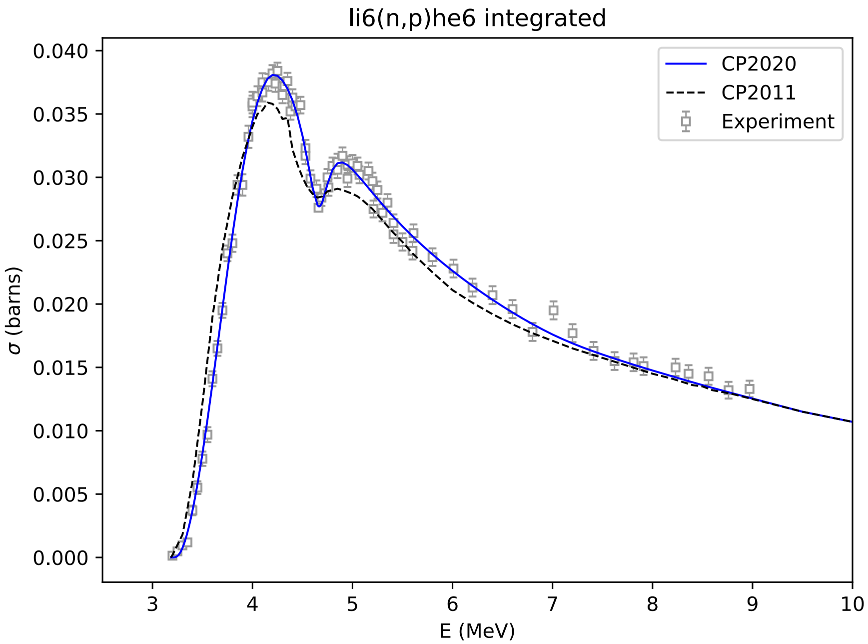

n+^{6}Li

R-matrix evaluation update/extension

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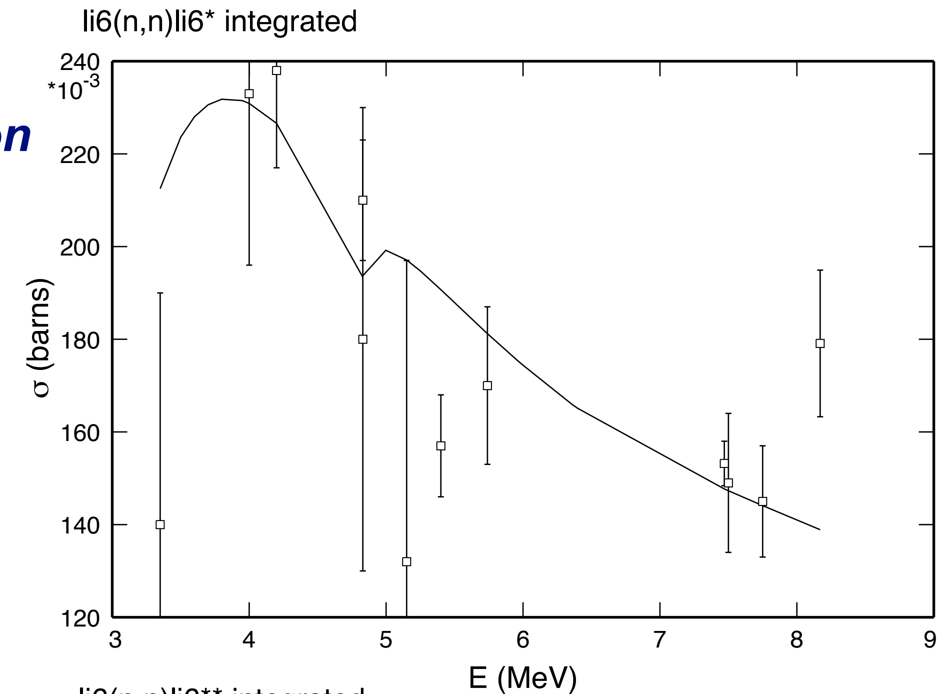
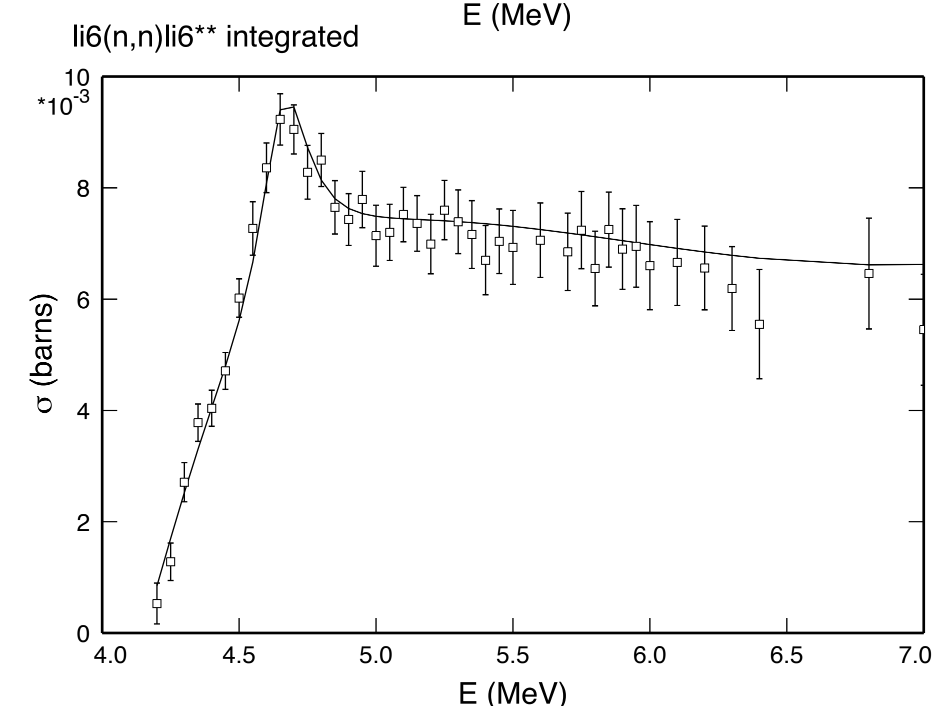
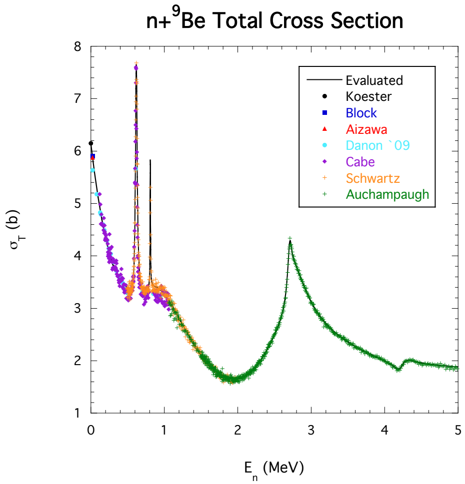
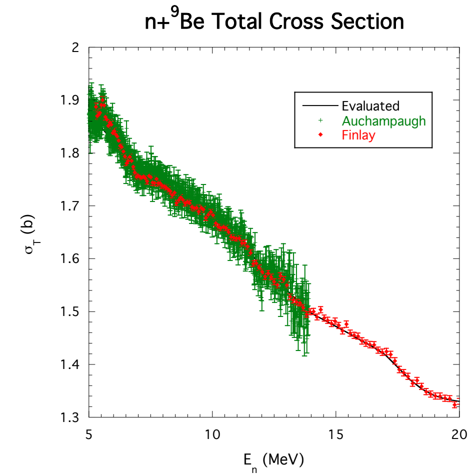


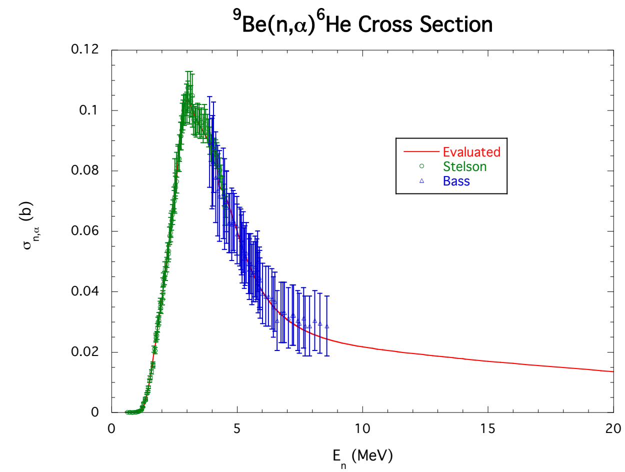


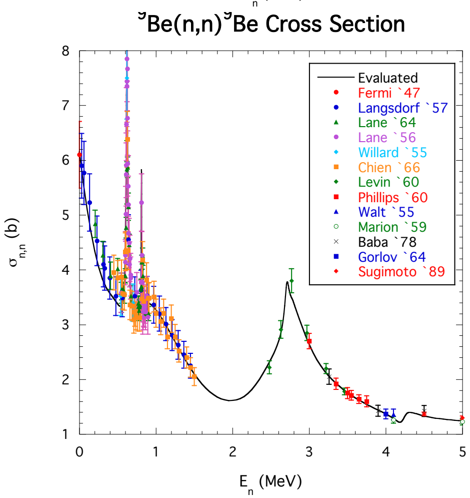
n+^{9}Be

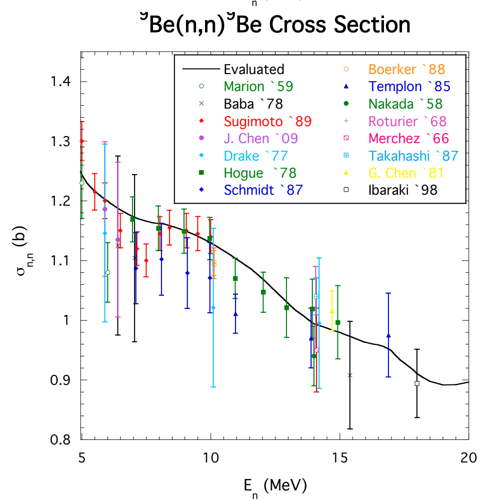
Integrated cross sections

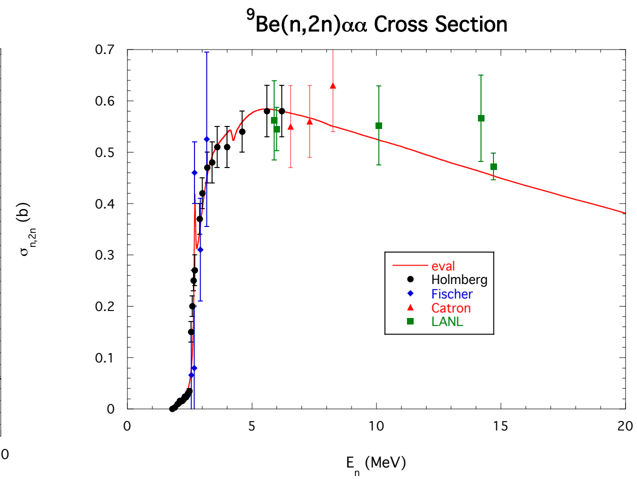






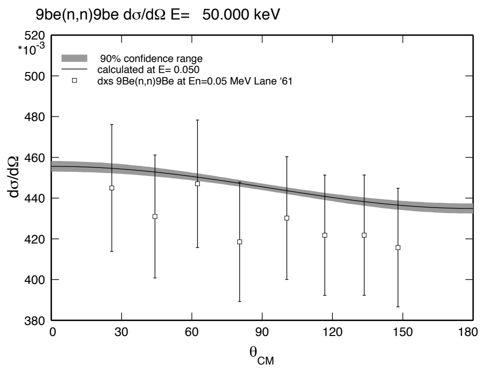


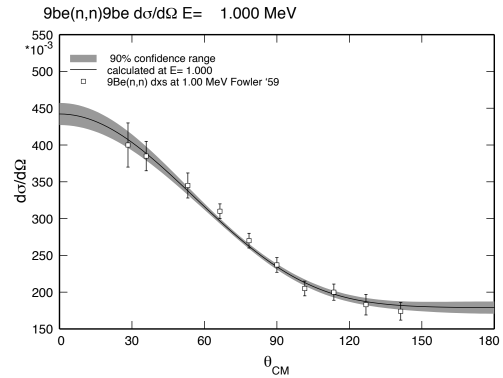


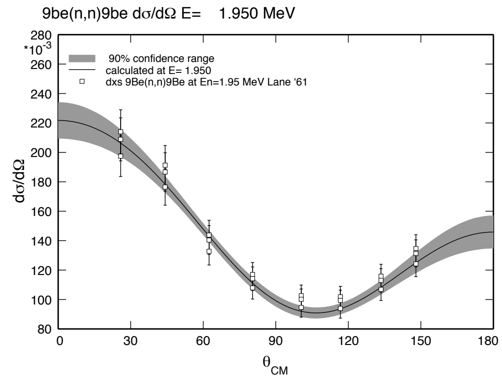


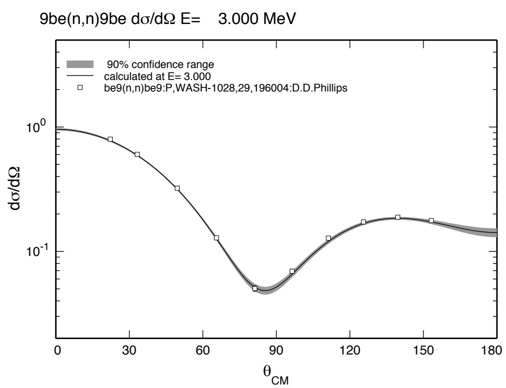
n+^{9}Be

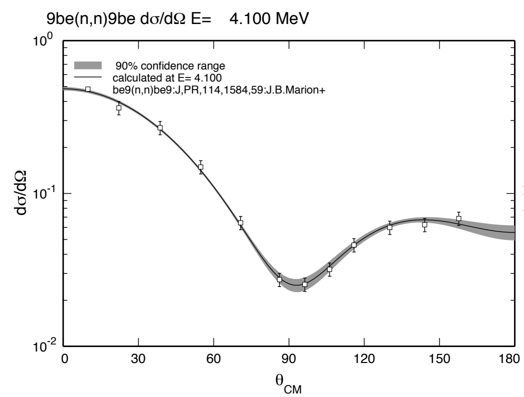
Differential cross sections $^9Be(n,n_0)^9Be$

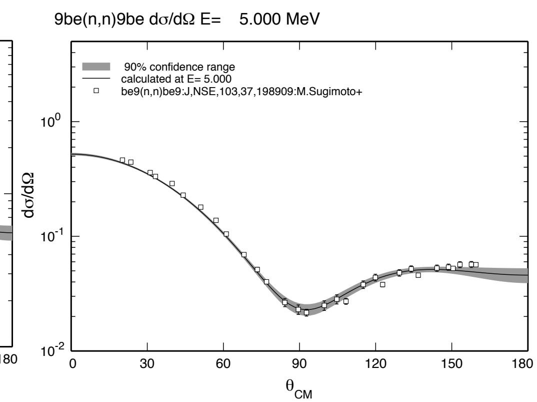






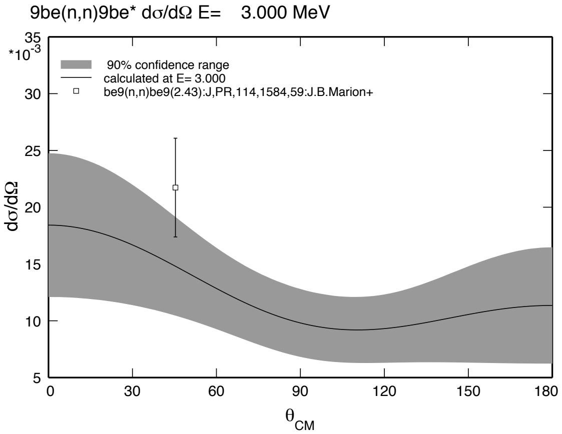


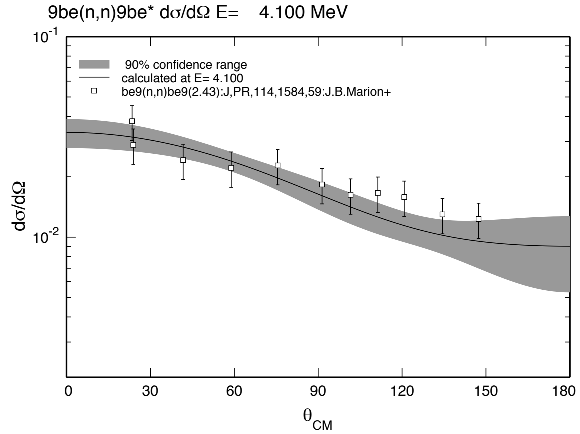


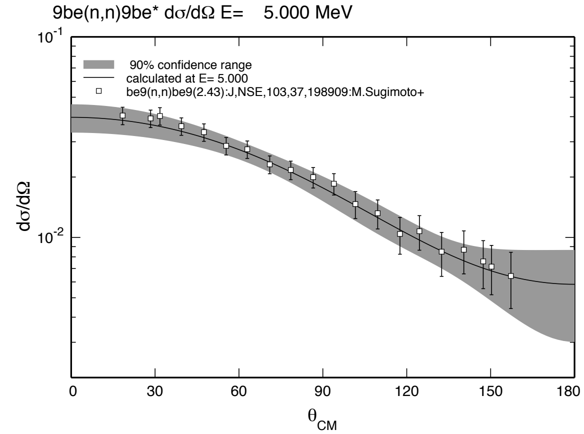


n+^{9}Be

Differential cross sections $^{9}Be(n,n_1)^{9}Be^*$







New Evaluation Summary:

- ^{10}Be analysis has produced a consistent set of cross sections and angular distributions that are in agreement with most of the experimental data at energies up to 5 MeV. Extensions above that energy were based on the experimental data alone.
- Level assignments for the overlapping resonances near E_n=2.7 MeV have the opposite parity ($4^-,3^+ \rightarrow 4^+,3^-$).
- Excited states of ^{9}Be make important contributions to the (n,2n) cross section (MT=16 → 24 in the new evaluation).
- Testing/benchmarking (on slides following n+^{16}O)