

# Light element evaluations for neutrons on ${}^6\text{Li}$ , ${}^9\text{Be}$ , and ${}^{16}\text{O}$

Nuclear Criticality Safety Program—Technical Program Review

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# Outline

- Overview of R-matrix evaluation procedure
- Evaluation & testing work
  - n+<sup>6</sup>Li
  - n+<sup>9</sup>Be
  - n+<sup>16</sup>O
- Conclusion

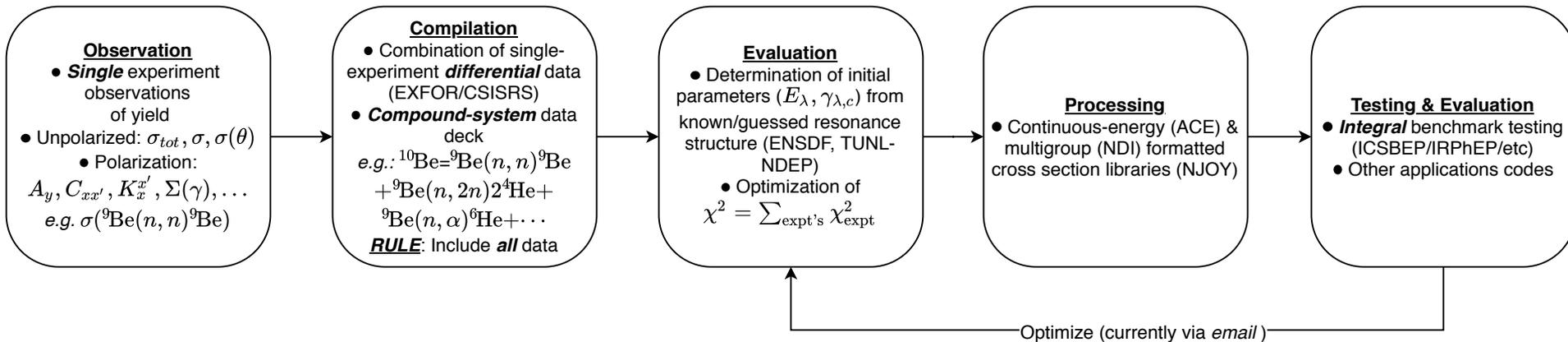


# Evaluation pipeline

## EDA R-matrix procedure

### Nuclear Data Pipeline

#### EDA cross section evaluation

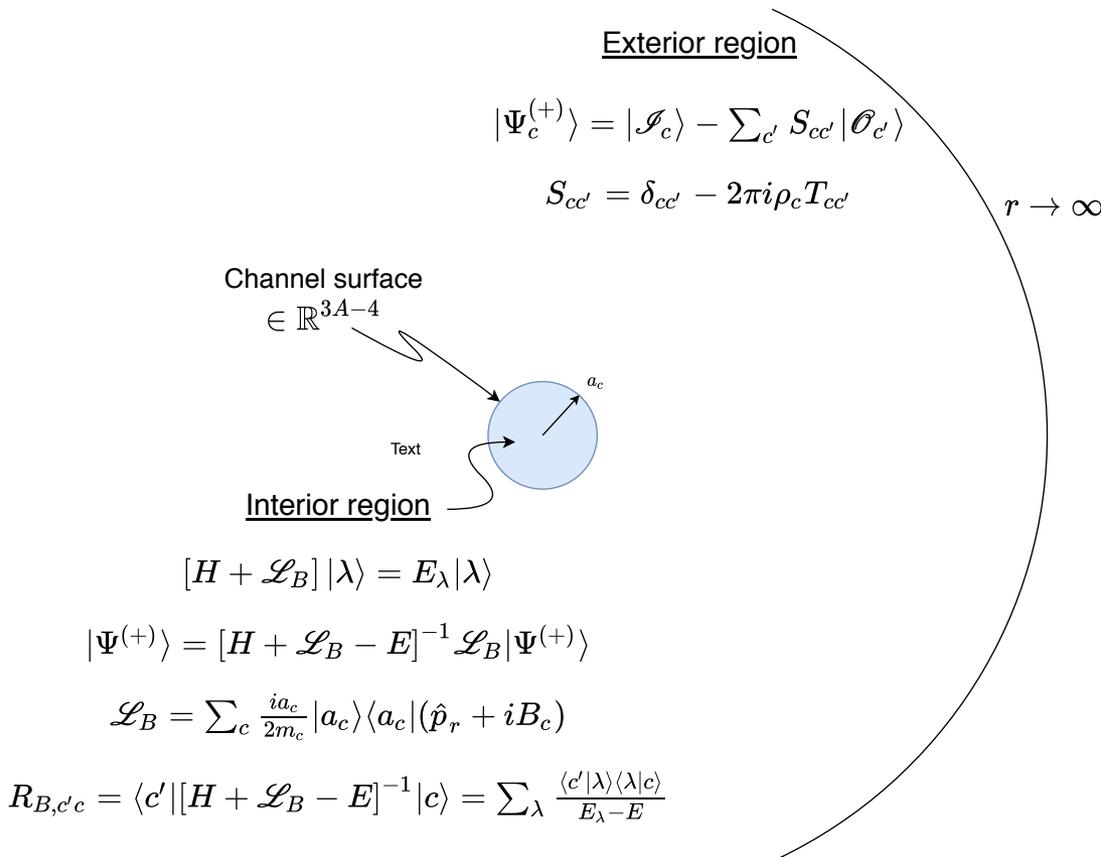


1. **EDAf90** code handles all types of data [*EXFOR/CSISRS; publications; priv. comm.*]
  - total, integrated, diff'l, polarized, unpolarized; neutron- and CP-induced: (n,X), (p,X), (d,X), (t,X),...
2. **EDAf90** handles all the compound system (here:  $^{10}\text{Be}$ ) data **simultaneously**
3. Optimization 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

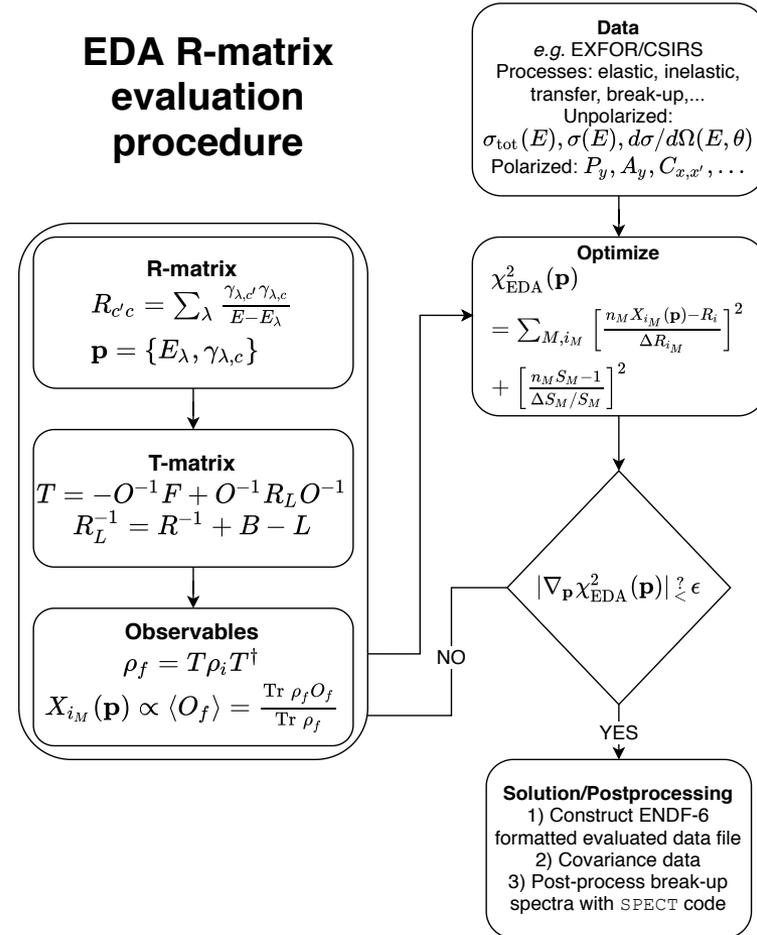


# R-matrix

## Overview of evaluation framework



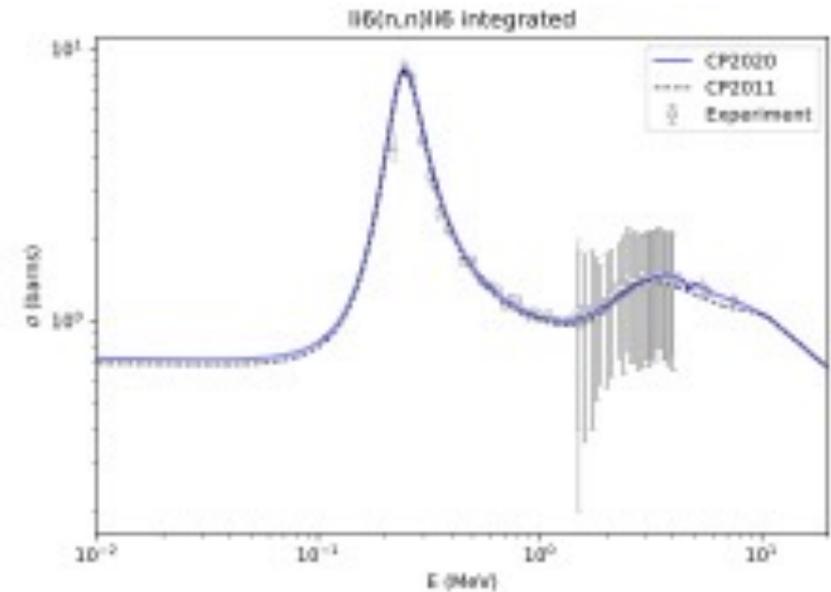
## EDA R-matrix evaluation procedure



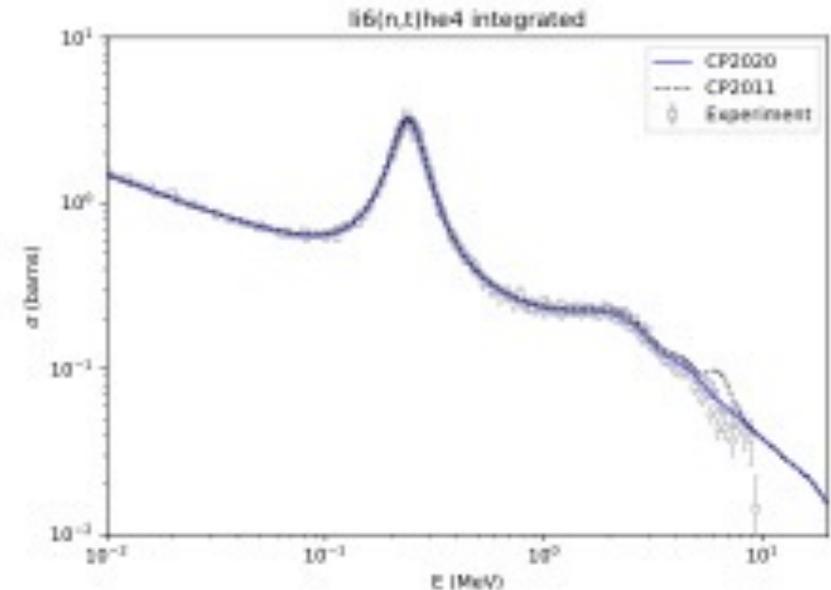
# $n+{}^6\text{Li}$

## *R-matrix evaluation update/extension*

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



(a)

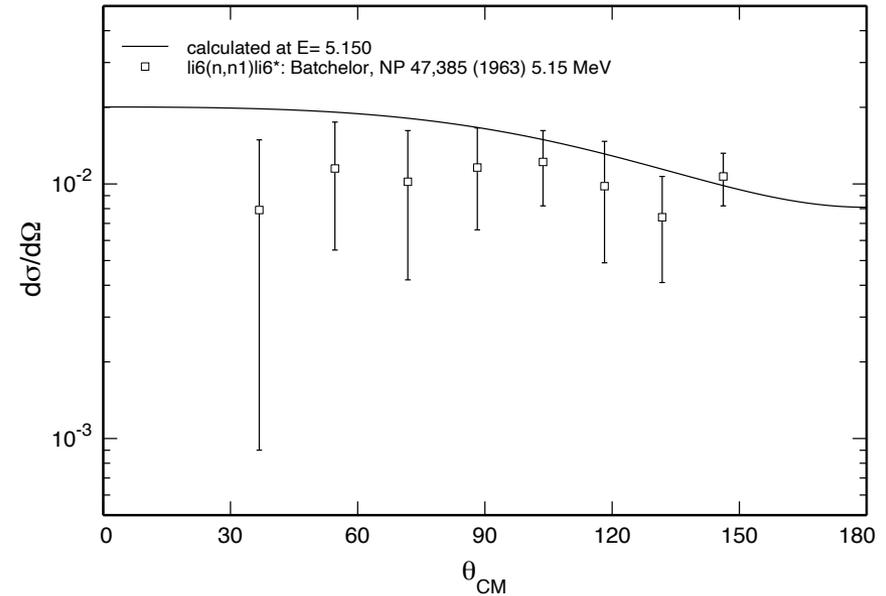


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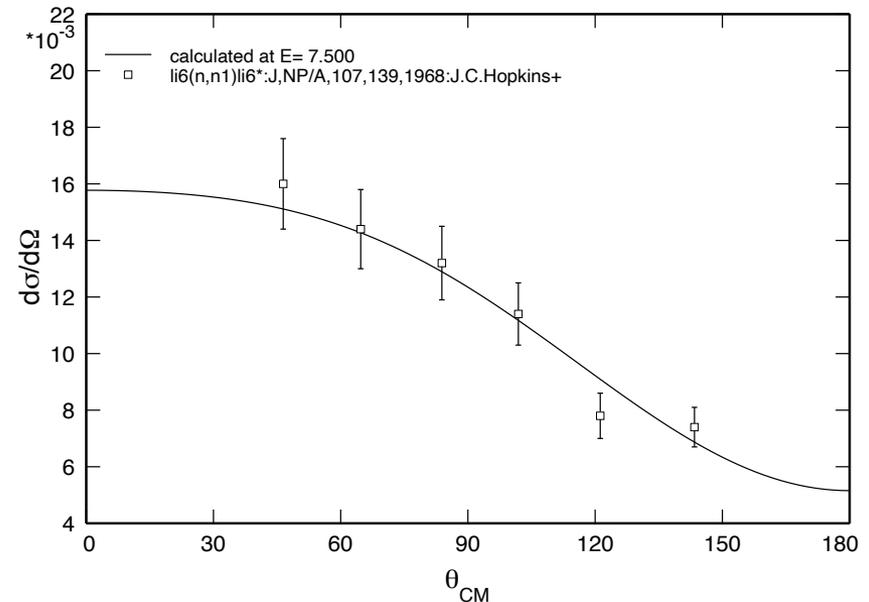
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${}^6\text{Li}(n,n){}^6\text{Li}^* \text{ d}\sigma/\text{d}\Omega \text{ E} = 5.150 \text{ MeV}$



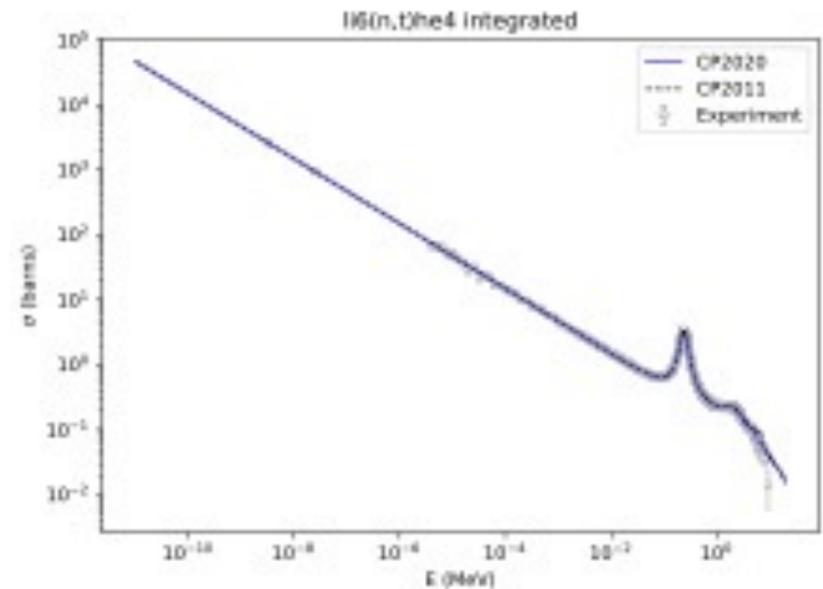
${}^6\text{Li}(n,n){}^6\text{Li}^* \text{ d}\sigma/\text{d}\Omega \text{ E} = 7.500 \text{ MeV}$



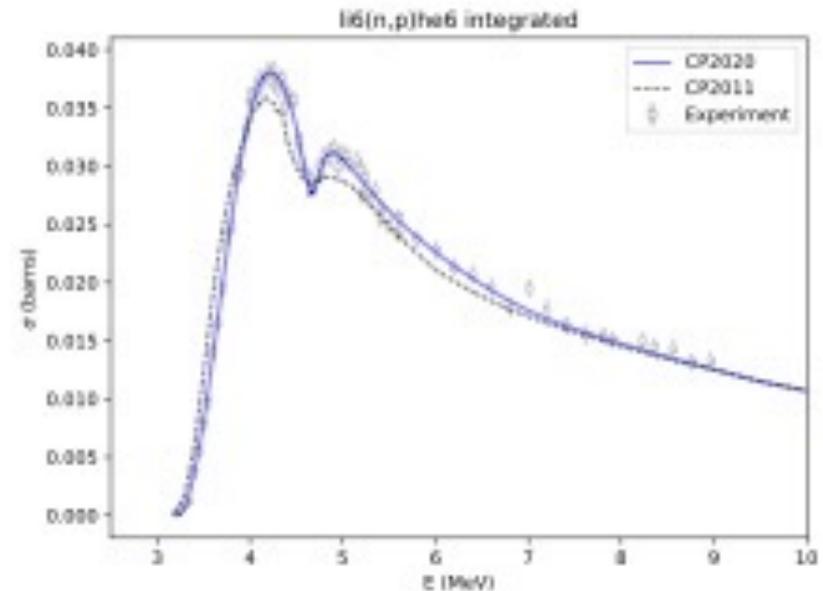
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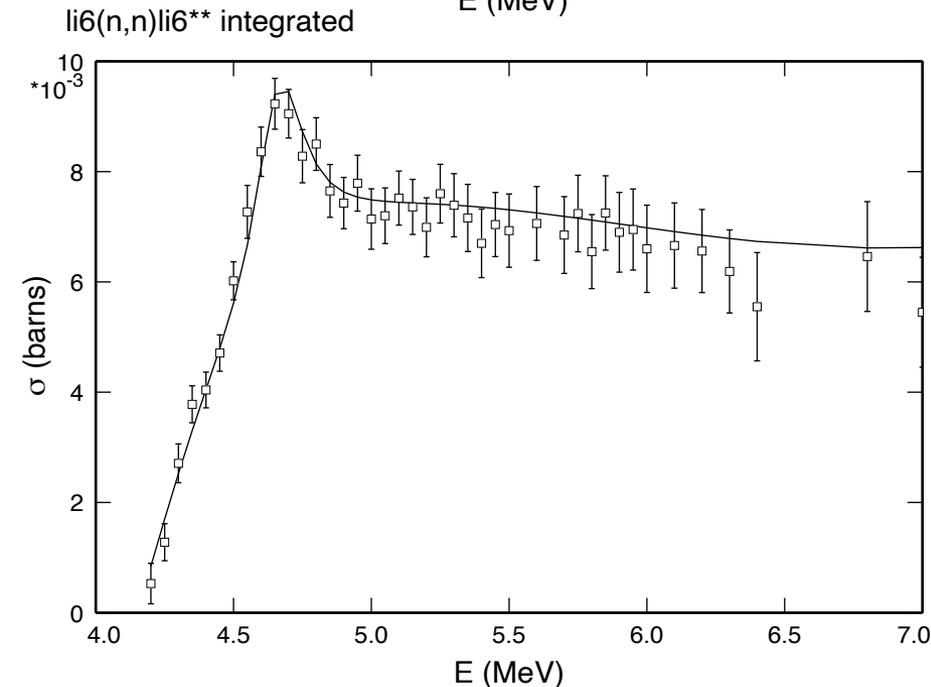
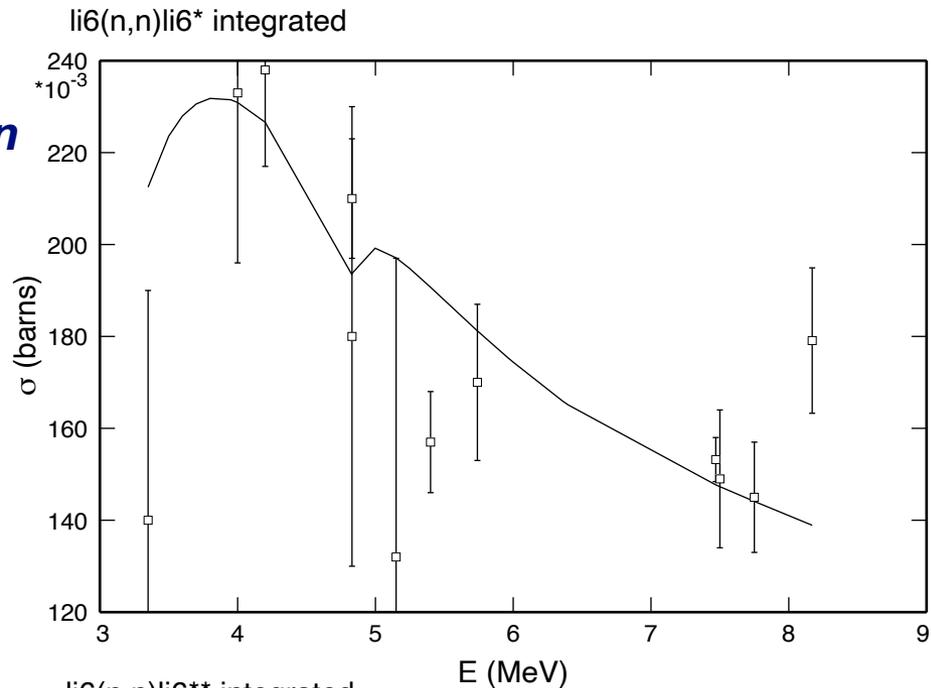
(b)



# $n+{}^6\text{Li}$

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# $n+{}^9\text{Be}$

## *R*-matrix configuration

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

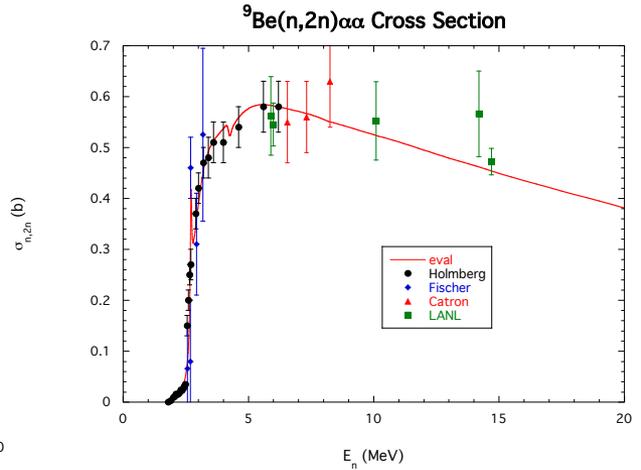
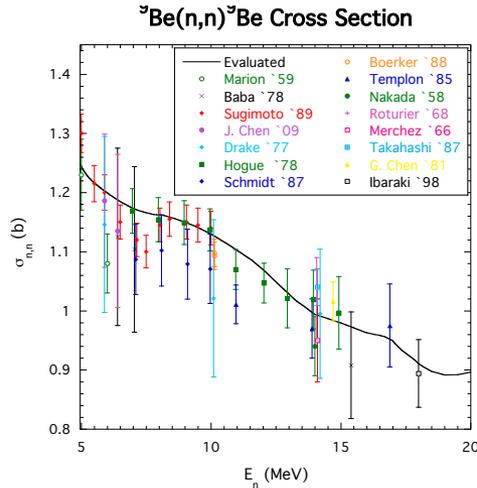
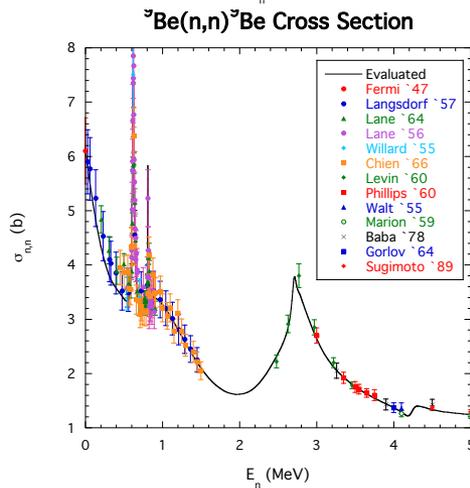
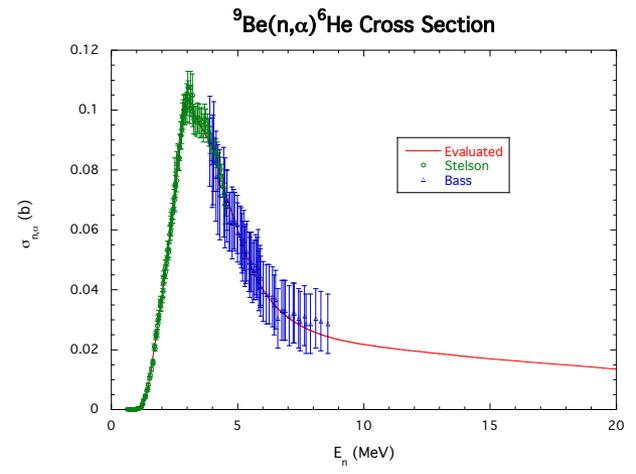
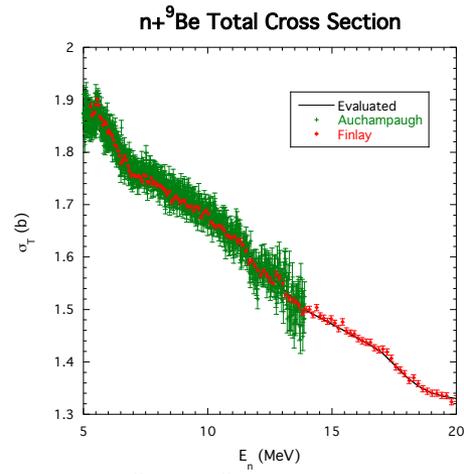
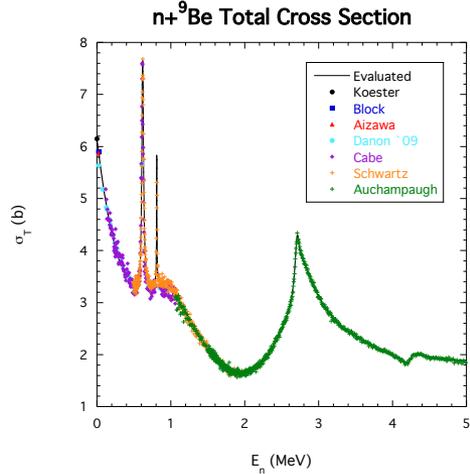
Process	$E_n$ range	Observables	$N_{\text{dat}}$	$\chi^2/N_{\text{dat}}$
${}^9\text{Be}(n, n_0){}^9\text{Be}$	(1.25 eV, 15.4 MeV)	$\sigma_{\text{tot}}, \sigma, \sigma(\theta), A_y(\theta)$	5782	1.65
${}^9\text{Be}(n, {}^4\text{He}){}^6\text{He}$	(0.63, 8.5) MeV	$\sigma, \sigma(\theta)$	178	1.40
${}^9\text{Be}(n,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

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



# $n+{}^9\text{Be}$

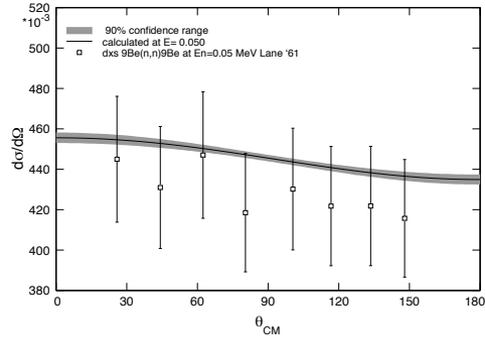
## Integrated cross sections



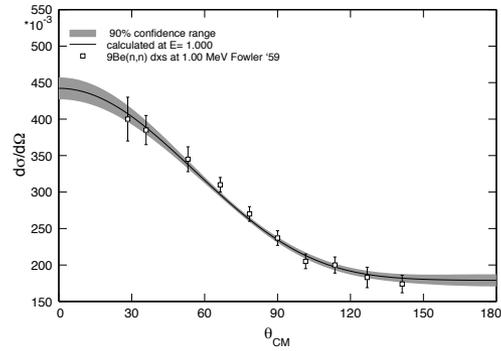
# $n+{}^9\text{Be}$

## Differential cross sections ${}^9\text{Be}(n,n_0){}^9\text{Be}$

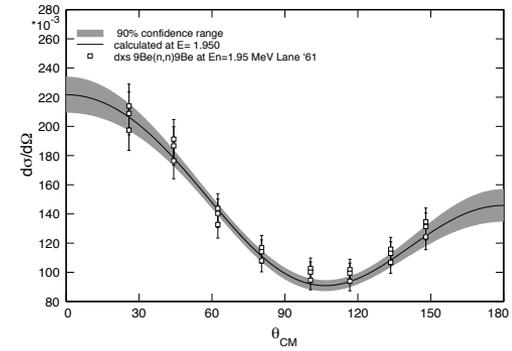
${}^9\text{Be}(n,n){}^9\text{Be}$   $d\sigma/d\Omega$   $E= 50.000$  keV



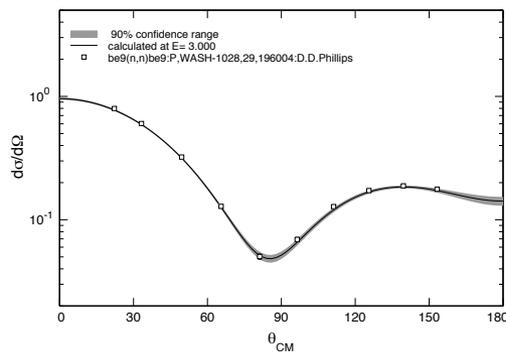
${}^9\text{Be}(n,n){}^9\text{Be}$   $d\sigma/d\Omega$   $E= 1.000$  MeV



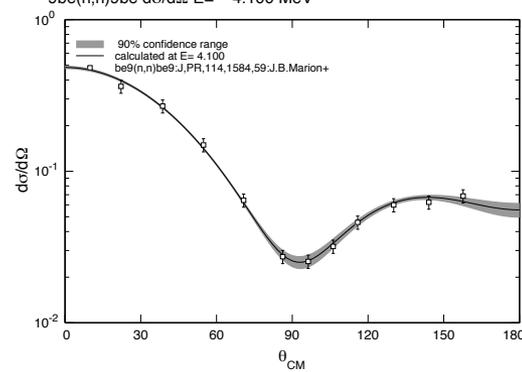
${}^9\text{Be}(n,n){}^9\text{Be}$   $d\sigma/d\Omega$   $E= 1.950$  MeV



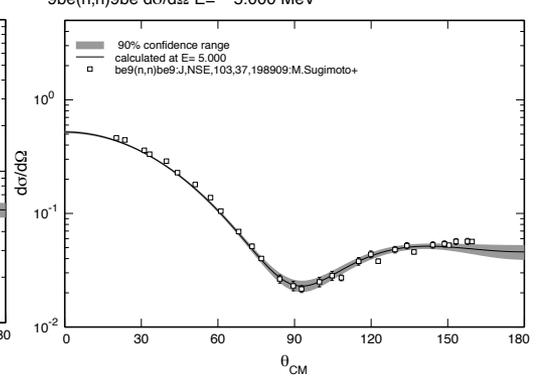
${}^9\text{Be}(n,n){}^9\text{Be}$   $d\sigma/d\Omega$   $E= 3.000$  MeV



${}^9\text{Be}(n,n){}^9\text{Be}$   $d\sigma/d\Omega$   $E= 4.100$  MeV

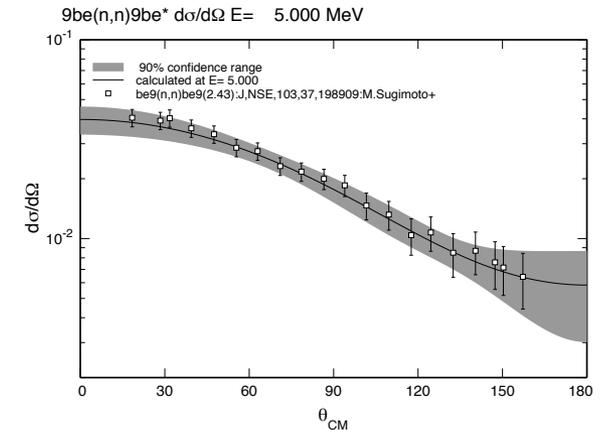
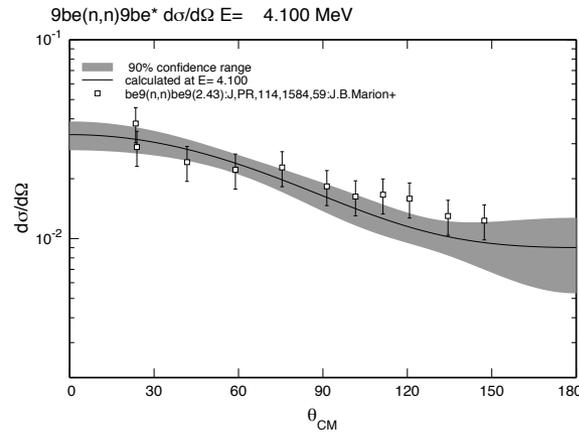
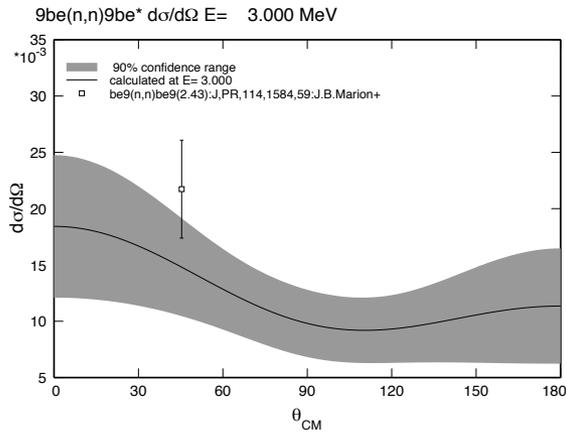


${}^9\text{Be}(n,n){}^9\text{Be}$   $d\sigma/d\Omega$   $E= 5.000$  MeV



# $n+{}^9\text{Be}$

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



### New Evaluation Summary:

- ${}^{10}\text{Be}$  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  ${}^9\text{Be}$  make important contributions to the  $(n,2n)$  cross section (MT=16  $\rightarrow$  24 in the new evaluation).
- Testing/benchmarking (on slides following  $n+{}^{16}\text{O}$ )

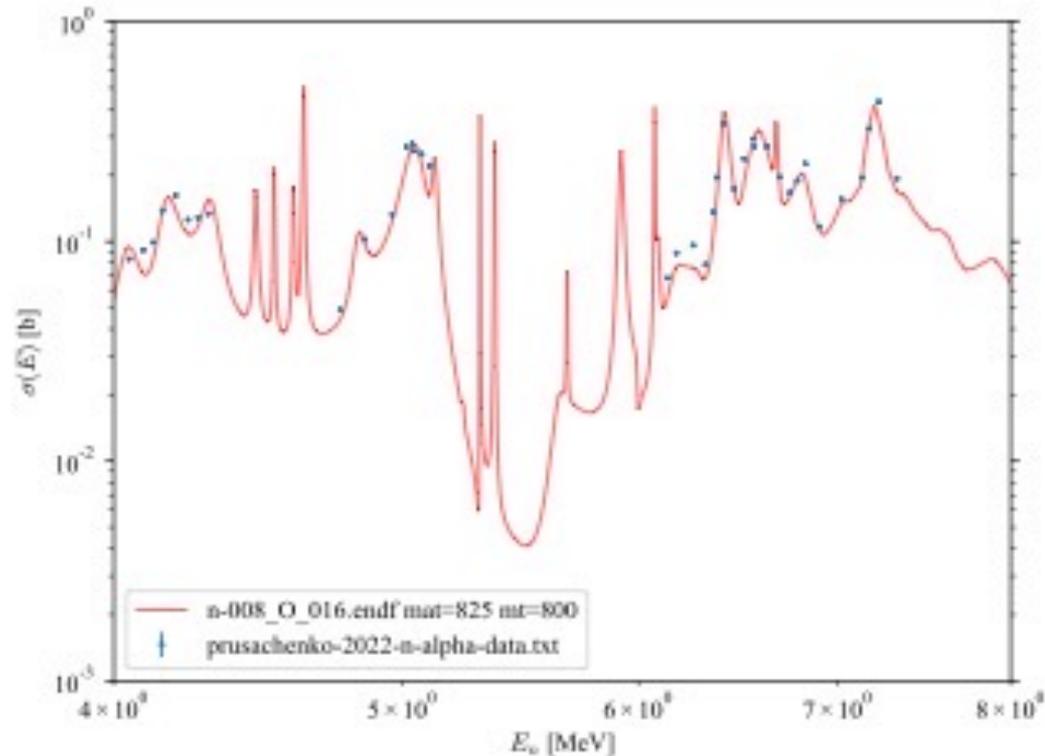


# $n+^{16}\text{O}$

## Evaluation adjustment for $^{16}\text{O}(n, \alpha_i)^{13}\text{C}^*$

- Abbreviated history
  - concern that  $^{16}\text{O}(n, \alpha)^{13}\text{C}$  absorption in ENDF/B-VIII.0 too large
  - LANL/EDA R-matrix fit considers  $E_n \leq 7.0$  MeV
  - Excited states  $E_n > 5.6$  MeV
- New data
  - supports ENDF/B-VIII.0 to 7.0 MeV
    - Prusachenko et al. IPPE 2022
    - H.-Y. Lee, S. Kuvin, et al. 2023
- Implement reduction in  $(n, \alpha_i)$ 
  - $i = 1, 2, 3 \leftrightarrow MT = 801, 802, 803$
  - reduced by factor of 2 to agree with Davis

$^A Z_i J^\pi$	$E_x(^{13}\text{C})$ (MeV)	$Q_{n\alpha_i}$ (MeV)	$E_n$ (MeV)
$^{13}\text{C}_0 \frac{1}{2}^-$	0.0	-2.215	2.355
$^{13}\text{C}_1 \frac{1}{2}^+$	3.08944	-5.304	5.639
$^{13}\text{C}_2 \frac{3}{2}^-$	3.68451	-5.899	6.271
$^{13}\text{C}_3 \frac{5}{2}^+$	3.85381	-6.068	6.451
$^{13}\text{C}_4 \frac{5}{2}^+$	6.864	-9.079	9.651



# $n+^{16}\text{O}$

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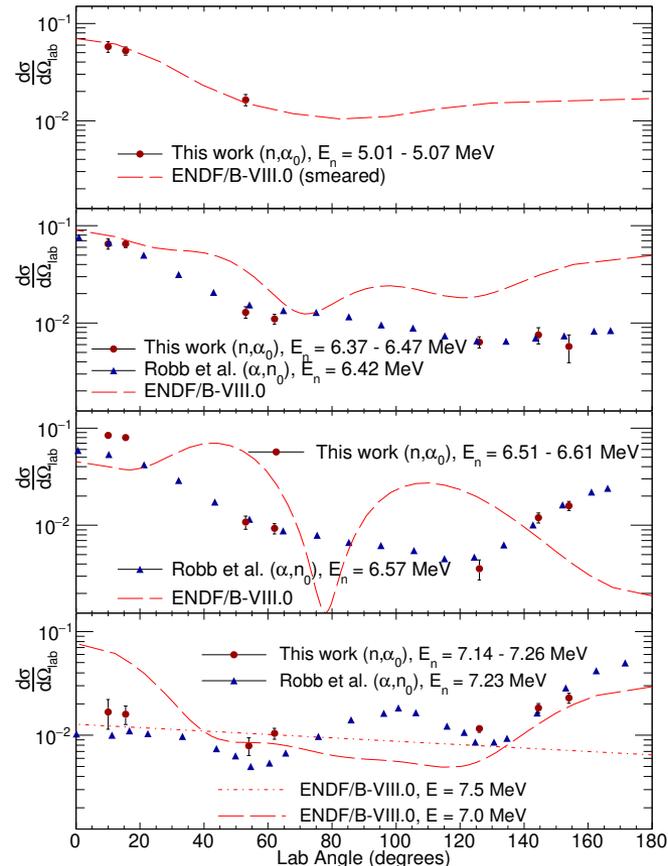
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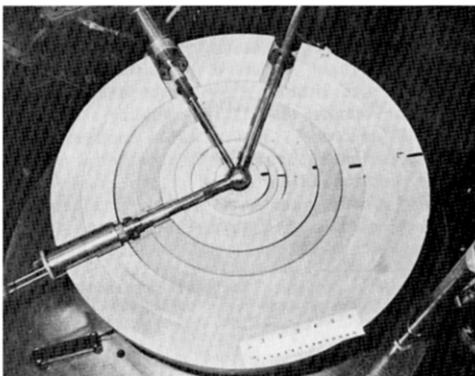
# n+<sup>6</sup>Li integral testing [preliminary]

*Kleedtke (LANL/XCP-5)*

Experiment	Measured $k_{\text{eff}}$	Calculated $k_{\text{eff}}$ (ENDF/B-VIII.0 XSDIR)		Calculated $k_{\text{eff}}$ (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  $k_{\text{eff}}$  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 spheres

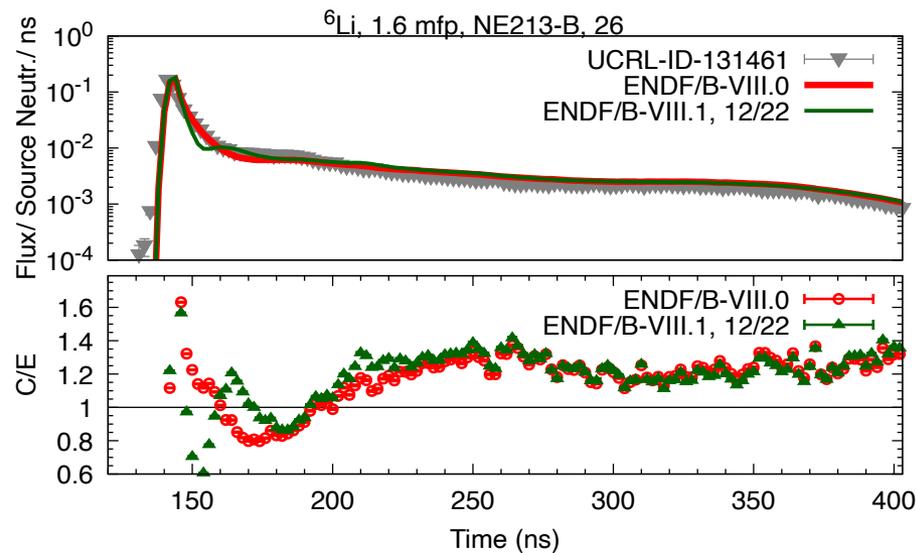
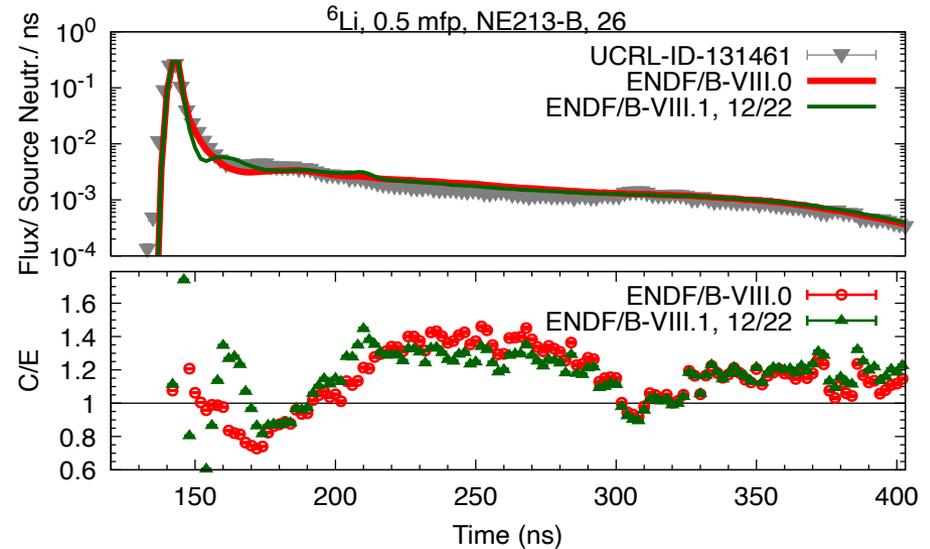
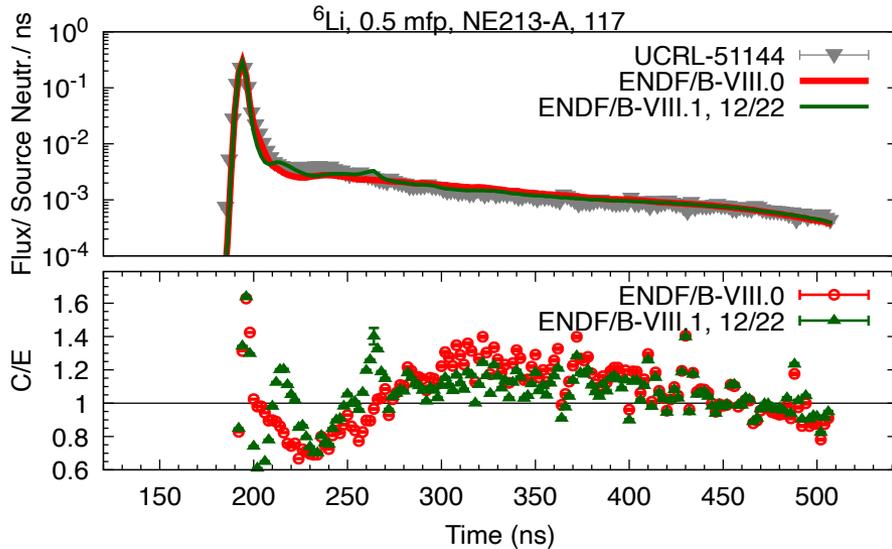
- Better for outer ampules
- Markedly worse (overshooting) for inner ampules
- **Puzzle: no change for 8.1b1 above 9 MeV**

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



# $n+{}^6\text{Li}$ integral testing [preliminary]

## LLNL pulsed spheres—Neudecker (LANL)



# $n+^9\text{Be}$ integral testing [preliminary]

*Kleedtke (LANL/XCP-5)*

Experiment	Measured $k_{\text{eff}}$	Calculated $k_{\text{eff}}$ (ENDF/B-VIII.0 XSDIR)		Calculated $k_{\text{eff}}$ (ENDF/B-VIII.1 XSDIR)	
		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)

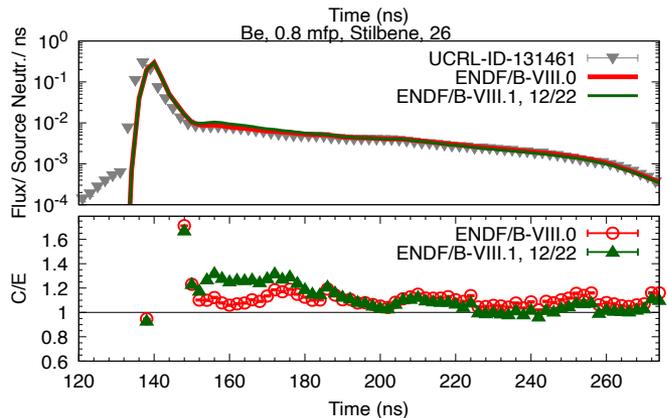
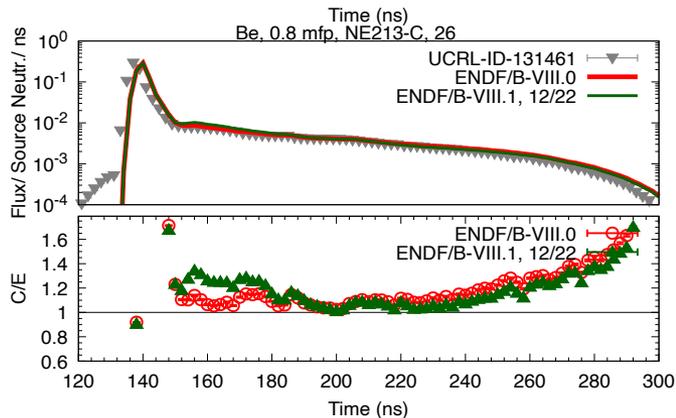
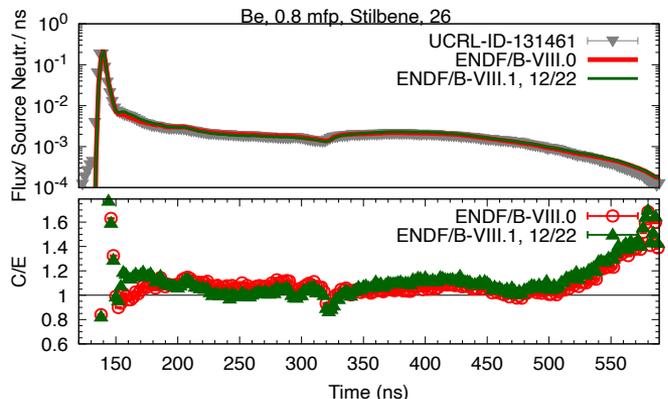
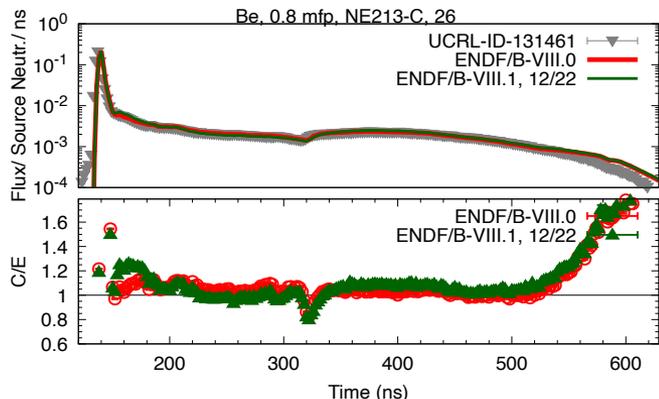
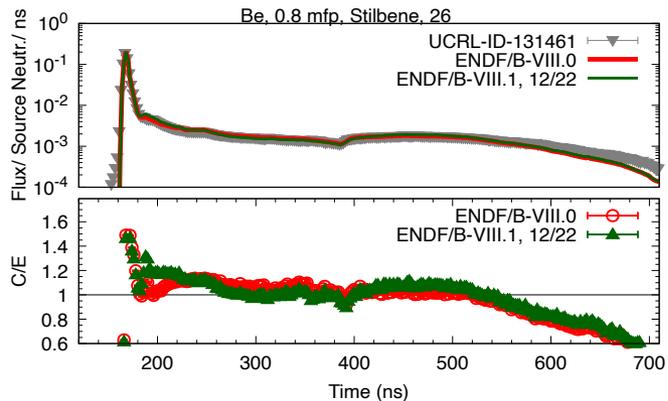
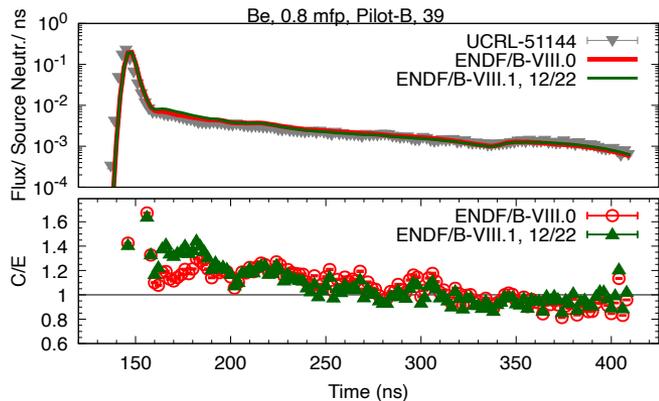
- Nominally worse on HMF/MMF

- HMF/MMF/PMF config: cyl. assys. of U5 or P9+HEU hemishells & P9 with  $^9\text{Be}$  reflectors
- Generally hotter by 100-200 pcm
- Need further testing with new  $^{16}\text{O}$



# n+<sup>9</sup>Be integral testing [preliminary]

## LLNL Pulsed spheres—Neudecker (LANL)



# $n+^{16}\text{O}$ integral testing [preliminary]

*Kleedtke (LANL/XCP-5)*

Experiment	Measured $k_{\text{eff}}$	Calculated $k_{\text{eff}}$ (ENDF/B-VIII.0 XSDIR)		Calculated $k_{\text{eff}}$ (ENDF/B-VIII.1 XSDIR)	
		ENDF/B-VIII.0	New	ENDF/B-VIII.0	New
LCT78, Case 1	0.9995(10)	0.99671(19)	0.99705(19)	0.99611(18)	0.99651(18)
LCT78, Case 11	0.9994(10)	0.99692(18)	0.99674(18)	0.99631(18)	0.99624(19)
LCT78, Case 15	0.9996(10)	0.99790(19)	0.99770(20)	0.99657(19)	0.99703(18)
LST1	0.9991(29)	1.01213(5)	1.01206(6)	1.00890(6)	1.00915(5)
PCF2, Case 1	0.9990(45)	1.02936(6)	1.02955(6)	1.02856(6)	1.02876(6)
PCF2, Case 2	0.9990(45)	1.02775(5)	1.02793(6)	1.02701(6)	1.02705(6)
PCF2, Case 3	0.9990(45)	1.02319(6)	1.02333(6)	1.02232(6)	1.02251(6)
PCF2, Case 4	0.9990(45)	1.01695(6)	1.01703(6)	1.01603(5)	1.01619(5)
PCF2, Case 5	0.9990(45)	1.01336(6)	1.01349(5)	1.01218(6)	1.01233(6)
PST28, Case 1	1.0000(12)	1.00362(12)	1.00366(12)	1.00326(12)	1.00356(12)
PST28, Case 7	1.0000(12)	1.00452(12)	1.00465(12)	1.00443(12)	1.00450(12)

- Nominally better on LCT/PCF/PST

- LCT:  $\text{H}_2\text{O}$  mod  $\text{UO}_2$  fuel lattice; LST unreflected  $\text{UO}_2\text{F}_2+\text{H}_2\text{O}$  cyl. assy.; PCF plexi-refl. polysty-mod  $\text{PuO}_2$ ; PST  $\text{H}_2\text{O}$  reflected annular cyl  $\text{PuNO}_3$
- No change/slight improvement



# Conclusion & Outlook

- $n+{}^6\text{Li}$ 
  - reasonably good description of differential data up to 8.0 MeV
  - well situated for FY24 target of  $E_n \leq 20$  MeV
  - integral benchmark testing puzzle: resolution of high-energy Bethe sphere ampules
- $n+{}^9\text{Be}$ 
  - improved description of differential data to 5.0 MeV
- $n+{}^{16}\text{O}$ 
  - reduced MT=801,802,803 by multiplicative factor of 0.5
- MF=2 resonance parameters
  - LRF=7 KRM=4 parameters are available
  - But NJOY doesn't process LRF=7, KRM=4
    - Goal: by end CY2023
  - Alternate, concurrent route
    - release EDA checking code, similar time frame
    - goes from MF=2 parameters to MF=3,6 (and 4,5)

Thanks.

