Los Alamos NATIONAL LABORATORY

$n+^{16}O$ & Charged-particle sublibrary evaluations in multi-channel unitary R-matrix approach

Cross section evaluation working group meeting
Brookhaven National Laboratory

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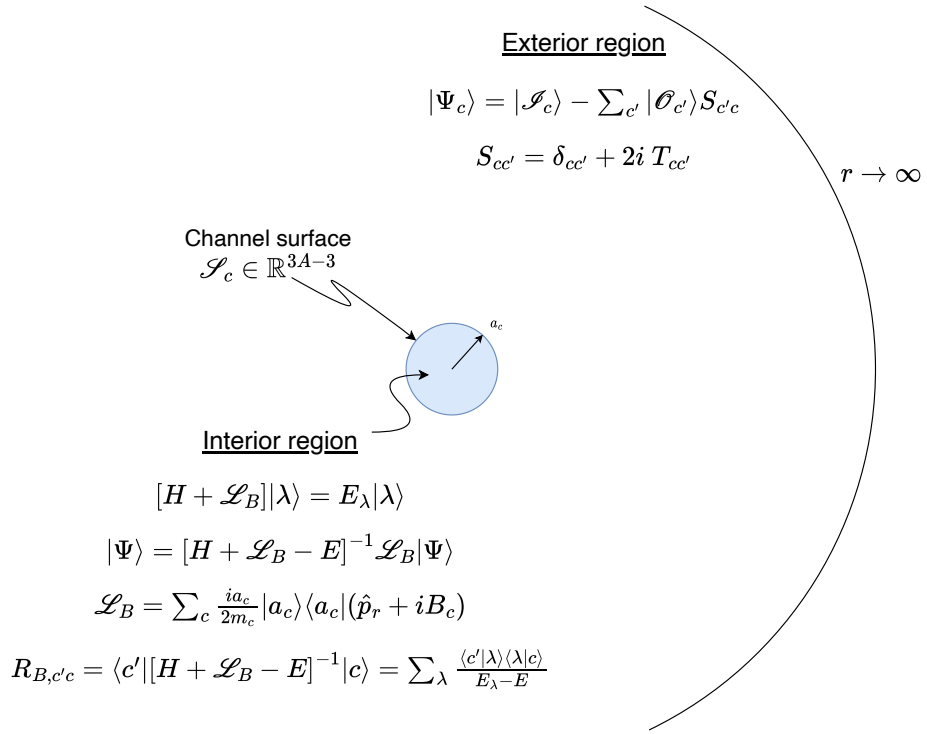
2022/11/01-04

LA-UR-22-31561

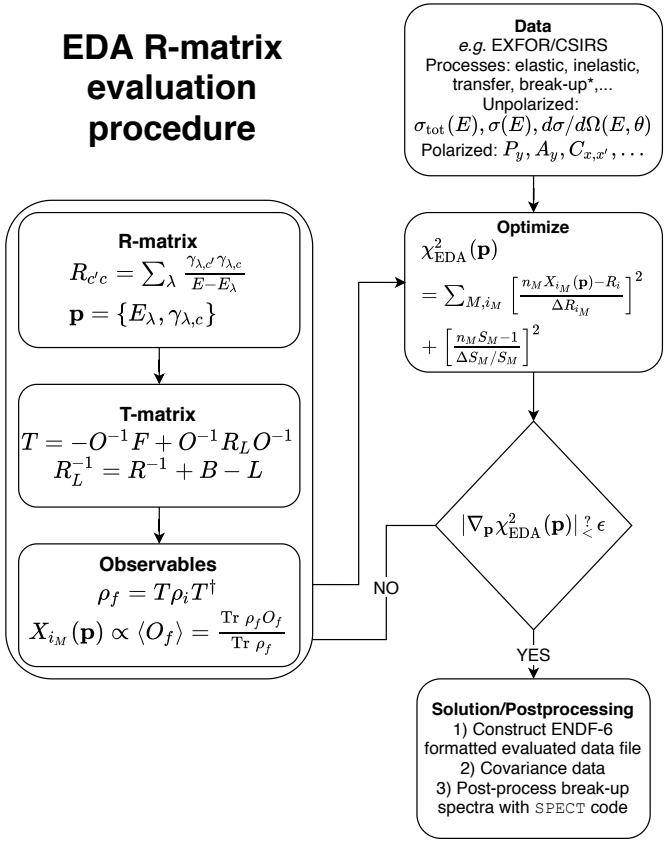
Outline

- R-matrix formalism
- Neutron sublibrary: ^{17}O system
  - n+^{16}O: focus on absorption by (n, α_{tot})

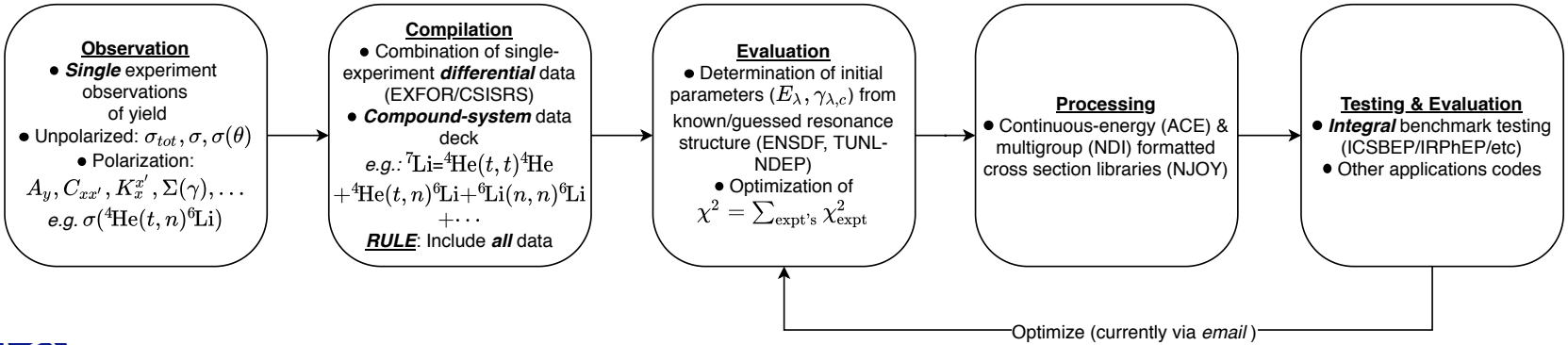
R-matrix formalism



EDA R-matrix evaluation procedure



Nuclear Data Pipeline
EDA cross section evaluation



LANL light-element program

- All compound systems A<20 (and a few above)
- Recent work in 2020:

Projectile\Target	^{1}H	^{2}H	^{3}H	^{3}He	^{4}He	^{6}Li	^{7}Li
n	2020	VIII.0	VIII.0	VIII.0	VIII.0	2020	VIII.0
p	2020	VIII.0	VIII.0	VIII.0	2020	VIII.0	VIII.0
d		VIII.0	VIII.0	2020	VIII.0[a]	VIII.0	VIII.0
t			VIII.0	VIII.0	2020	VIII.0	TENDL09
$h(^{3}\mathrm{He})$				VIII.0	VIII.0	VIII.0	TENDL09
α					VIII.0	TENDL09	TENDL09

^{11}B (α+^{7}Li, α+^{7}Li*, t+^{8}Be, n+^{10}B); ^{11}C (α+^{7}Be, p+^{10}B)
^{12}C (α+^{8}Be, p+^{11}B)
^{13}C (n+^{12}C, n+^{12}C*)
^{14}C (n+^{13}C)
^{15}N (p+^{14}C, n+^{14}N, α+^{11}B)
^{16}O (g+^{16}O, α+^{12}C)
^{17}O (n+^{16}O, α+^{13}C)
^{18}Ne (p+^{17}F, p+^{17}F*, α+^{14}O)

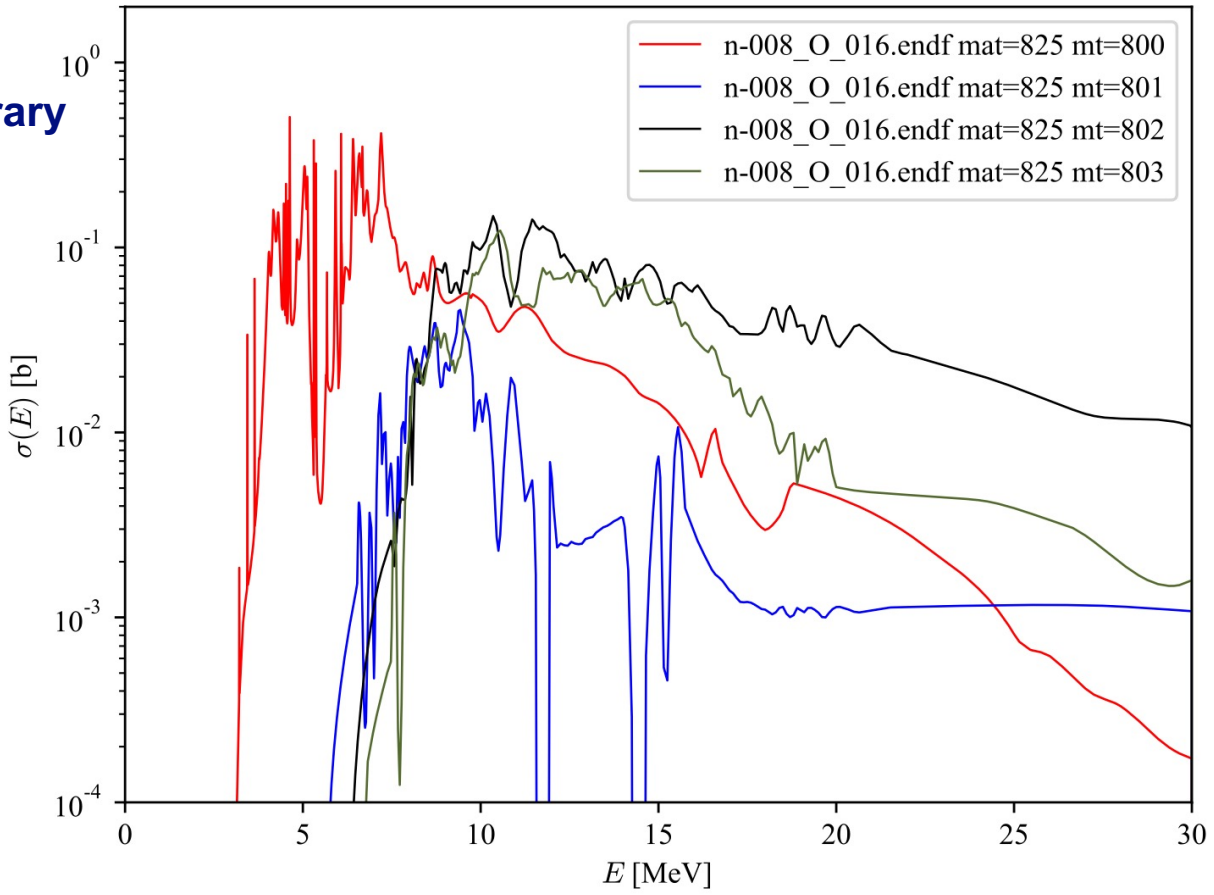
$$n + 160$$

Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

Neutron absorption

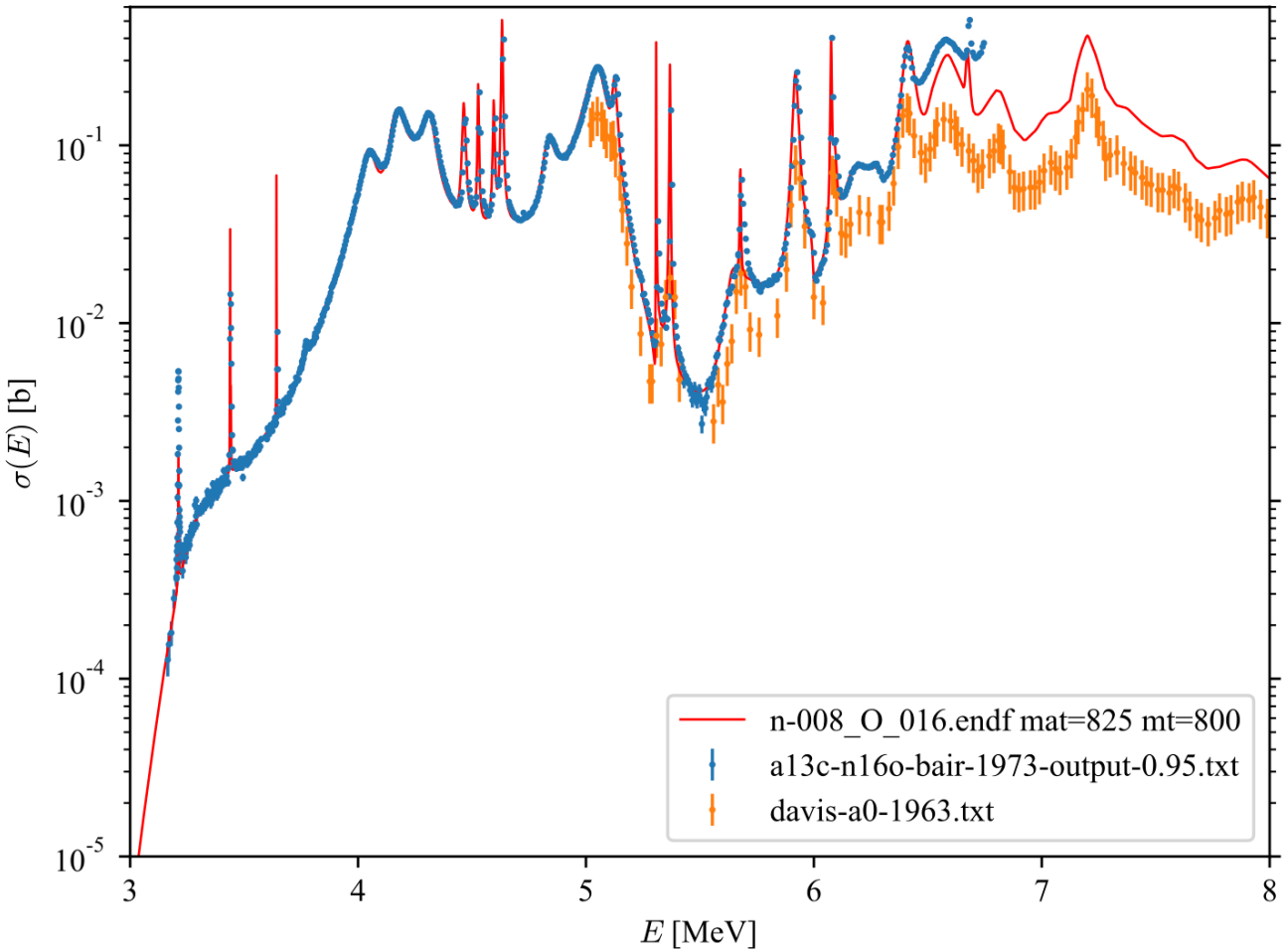
- mf3/mt800,…,803
- mt800 (n, α_0)
  - E_n~2.36 MeV
  - dominant until mt801
- mt801 (n, α_1)
  - E_n~5.64 MeV
  - exponential rise < 8 MeV
  - turn-over, dies
- mt802 (n, α_2)
  - E_n~6.27 MeV
  - Dominates > 8.5 MeV or so
- mt803 (n, α_3)
  - E_n~6.45 MeV
  - comparable to (n, α_2)10-15 MeV
  - dies > 15 MeV



${}^{A}Z_i\ J^\pi$	$E_x({}^{13}\mathrm{C})$ (MeV)	$Q_{n\alpha_i}$ (MeV)	E_n (MeV)	$E_x({}^{17}\mathrm{O})$ (MeV)
${}^{13}\mathrm{C}_0\ \frac{1}{2}^-$	0.0	−2.215	2.355	6.3587[1]
${}^{13}\mathrm{C}_1\ \frac{1}{2}^+$	3.08944	−5.304	5.639	9.447
${}^{13}\mathrm{C}_2\ \frac{3}{2}^-$	3.68451	−5.899	6.271	10.041
${}^{13}\mathrm{C}_3\ \frac{5}{2}^+$	3.85381	−6.068	6.451	10.211
${}^{13}\mathrm{C}_4\ \frac{5}{2}^+$	6.864	−9.079	9.651	13.219

Oxygen-16

ENDF/B-VIII.0 neutron sublibrary



(n, α_0)

- Bair & Haas '73
  - (α, n_0)
  - Time-reversal inv.

$$\left|T^J_{n_j \ell' s', \alpha_0 \ell s}\right|^2 = \left|T^J_{\alpha_0 \ell s, n_j \ell' s'}\right|^2$$

  - Applicable

$$1 \text{ MeV} < E_\alpha < 5.4 \text{ MeV},$$
$$\updownarrow$$
$$3.17 \text{ MeV} < E_n < 6.75 \text{ MeV}.$$

  - *cf.* Davis, Bonner, Worley & Bass 1963

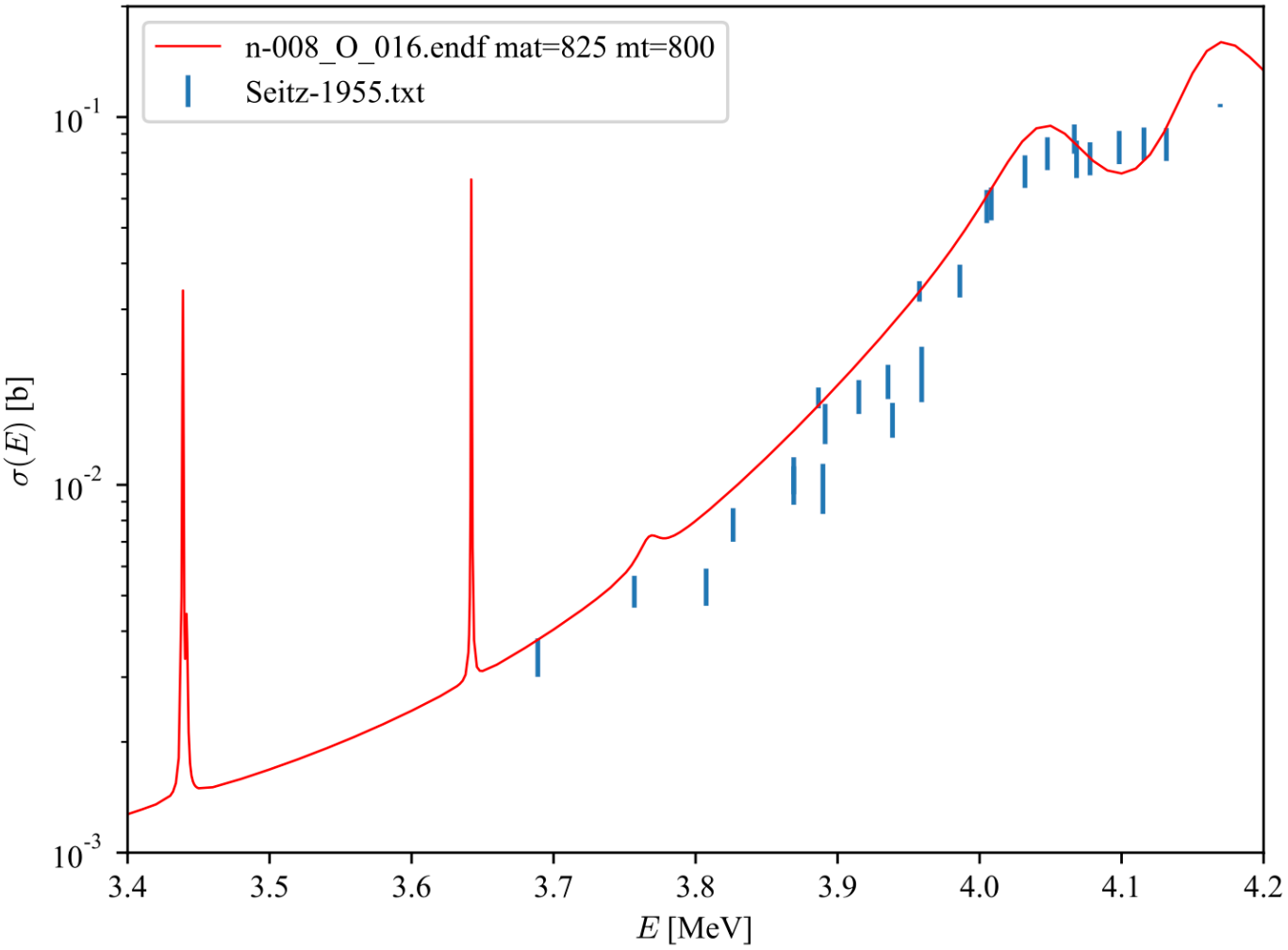
Figure 2: Comparison of $^{16}\mathrm{O}(n, \alpha_0)^{13}\mathrm{C}$ data by Davis[1] to that of Bair[2], converted from the Bair measurement of $^{13}\mathrm{C}(\alpha, n_0)^{16}\mathrm{O}$ to the inverse reaction $^{16}\mathrm{O}(n, \alpha_0)^{13}\mathrm{C}$ via Eq. (6) and compared to ENDF/B-VIII.0.

Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

(n, α_0)

− Seitz & Huber 1955



Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

(n, α_0)

– Ratio of Bair & Haas to Seitz & Huber

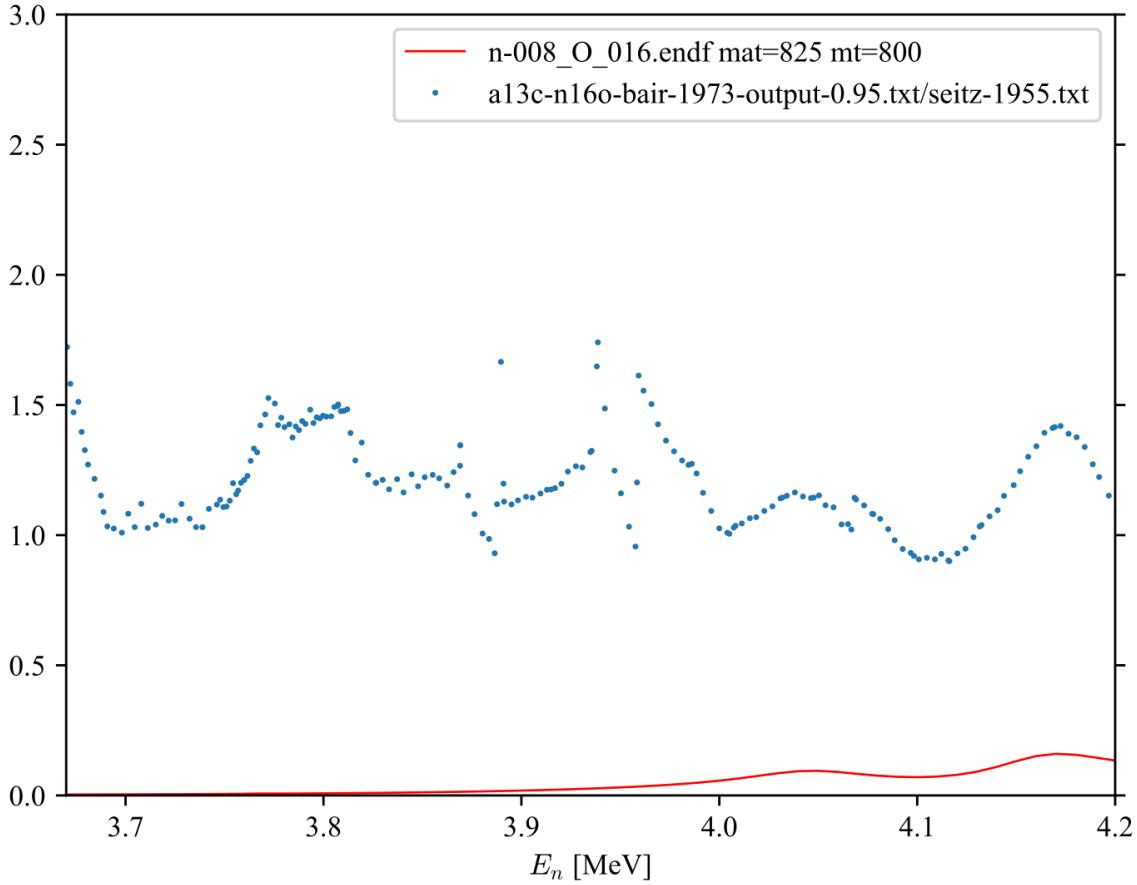


Figure 5: Ratio (dimensionless) of $^{16}\mathrm{O}(n, \alpha_0)^{13}\mathrm{C}$ data by Bair[2] to that of Seitz & Huber[3], converted from the Bair measurement of $^{13}\mathrm{C}(\alpha, n_0)^{16}\mathrm{O}$ to the inverse reaction $^{16}\mathrm{O}(n, \alpha_0)^{13}\mathrm{C}$ via Eq. (6) and compared, for purposes of resonance positions only, to the cross section in barns of ENDF/B-VIII.0. The ratio of these cross sections has been interpolated to energies corresponding to the unionized grid of both experiments in their region of overlap.

Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

(n, α_0)

- Ratio of Bair & Haas to Davis et al.

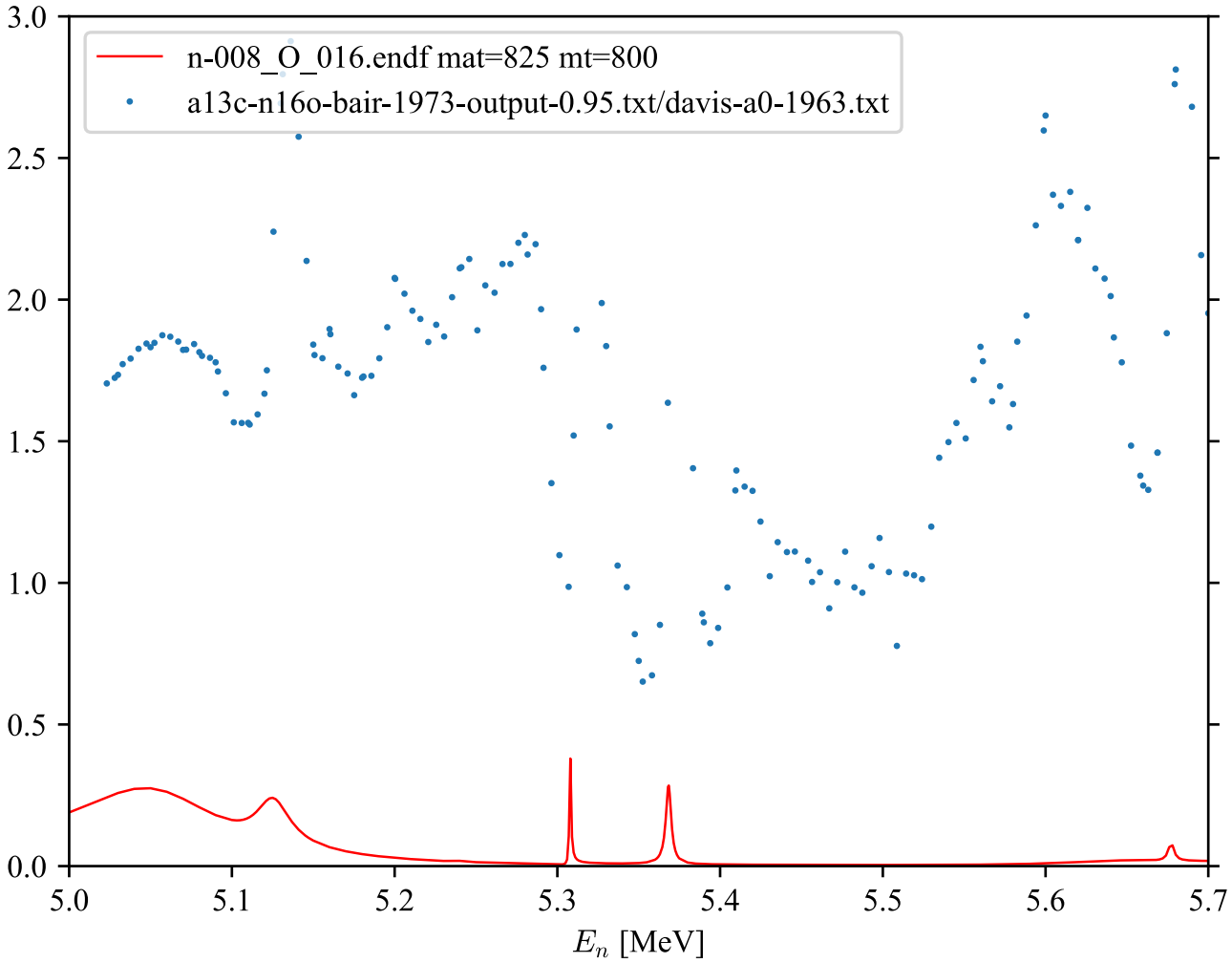


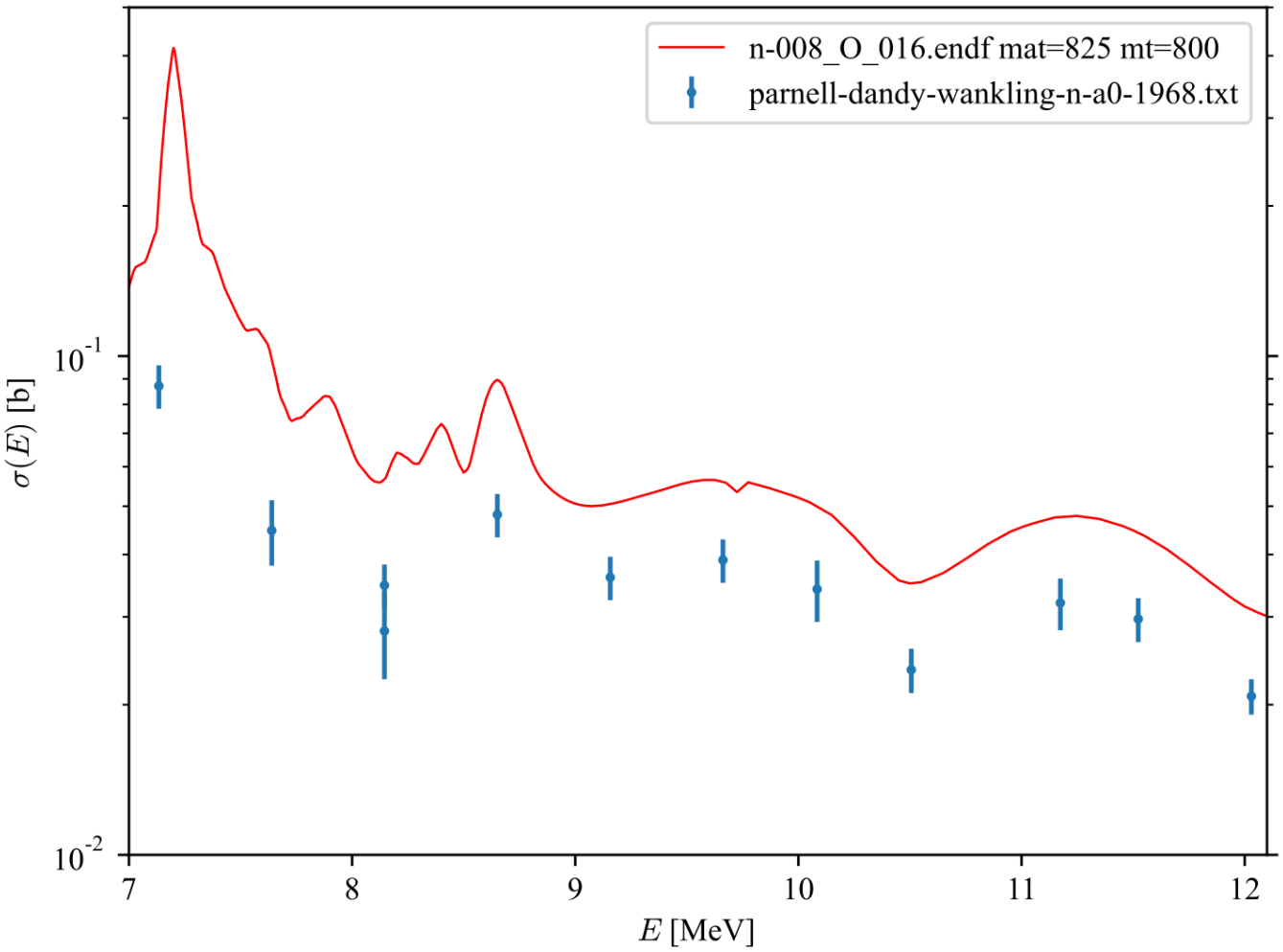
Figure 6: Ratio (dimensionless) of $^{16}\mathrm{O}(n, \alpha_0)^{13}\mathrm{C}$ data by Bair[2] to that of Davis *et al.*[1], converted from the Bair measurement of $^{13}\mathrm{C}(\alpha, n_0)^{16}\mathrm{O}$to the inverse reaction $^{16}\mathrm{O}(n, \alpha_0)^{13}\mathrm{C}$ via Eq. (6) and compared, for purposes of resonance positions only, to the cross section in barns of ENDF/B-VIII.0. The ratio of these cross sections has been interpolated to energies corresponding to the unionized grid of both experiments in their region of overlap.

Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

(n, α_0)

- Parnell, Dandy & Wankling 1968
  - 8.0 too large



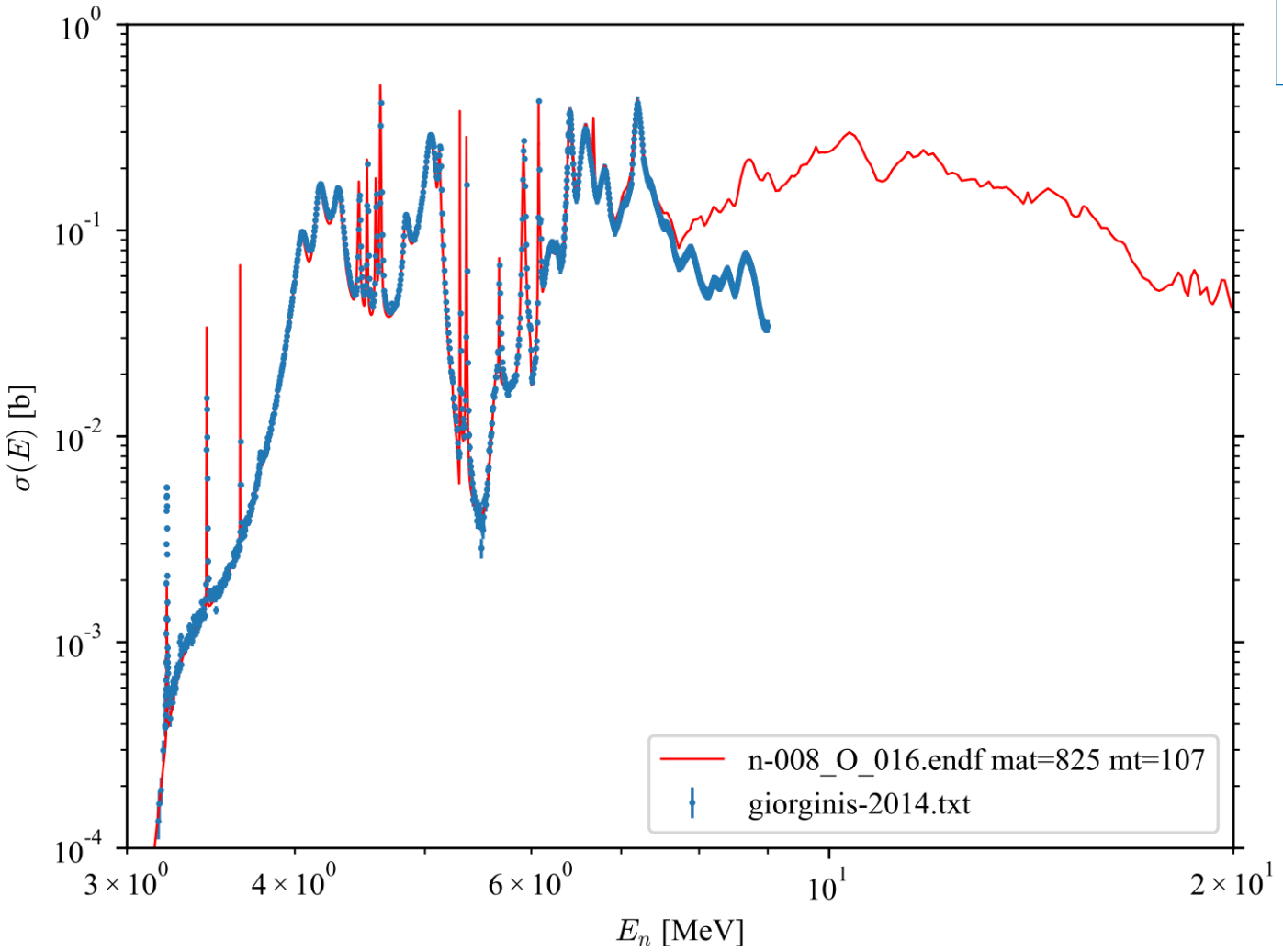
Comparison of $^{16}\mathrm{O}(n, \alpha_0)^{13}\mathrm{C}$ data by Parnell *et al.*[4] compared to ENDF/B-VIII.0.

Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

(n, α_0)

- Giorginis re-evaluation

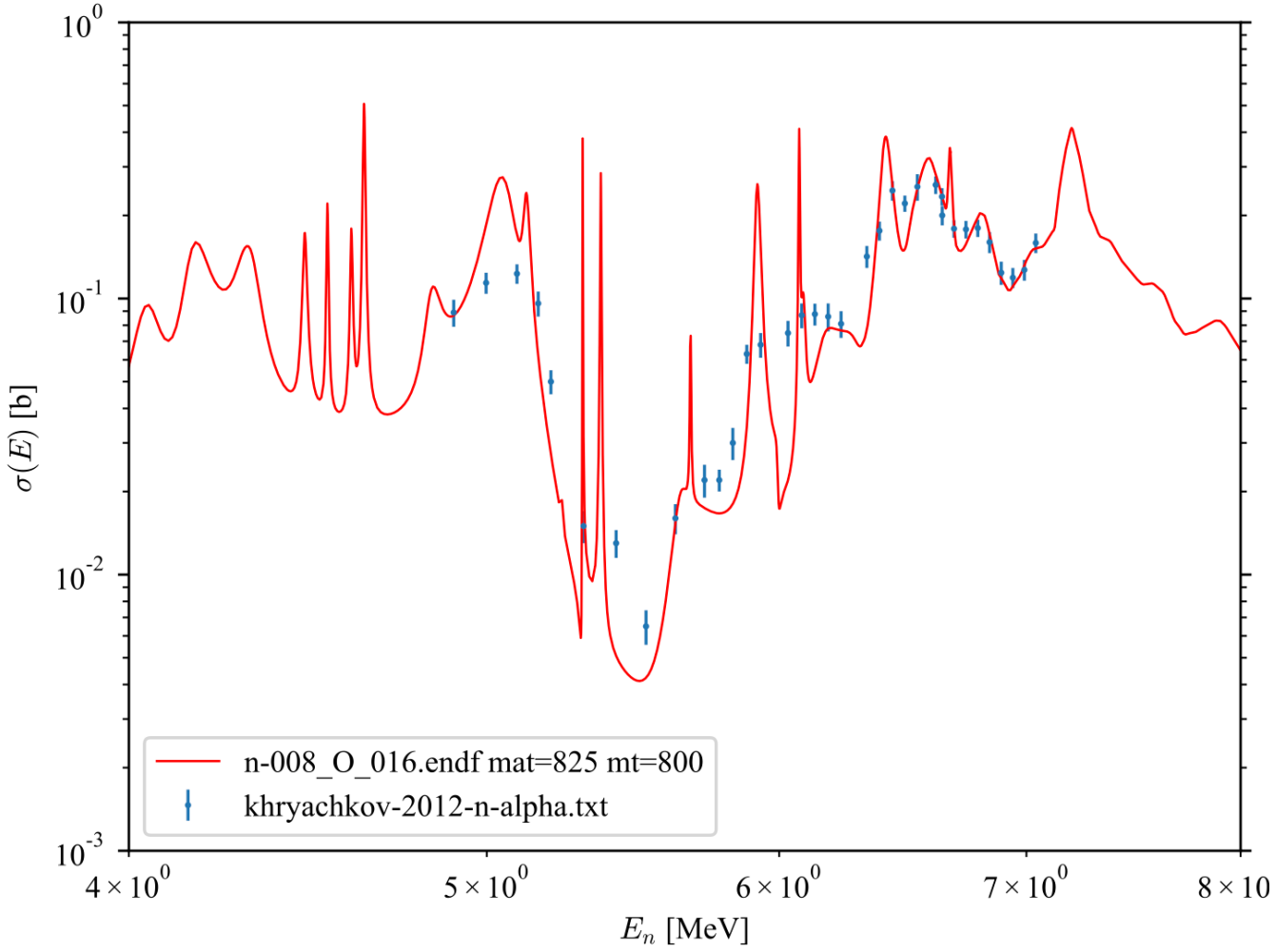


Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

(n, α_0)

– Khryachov updated



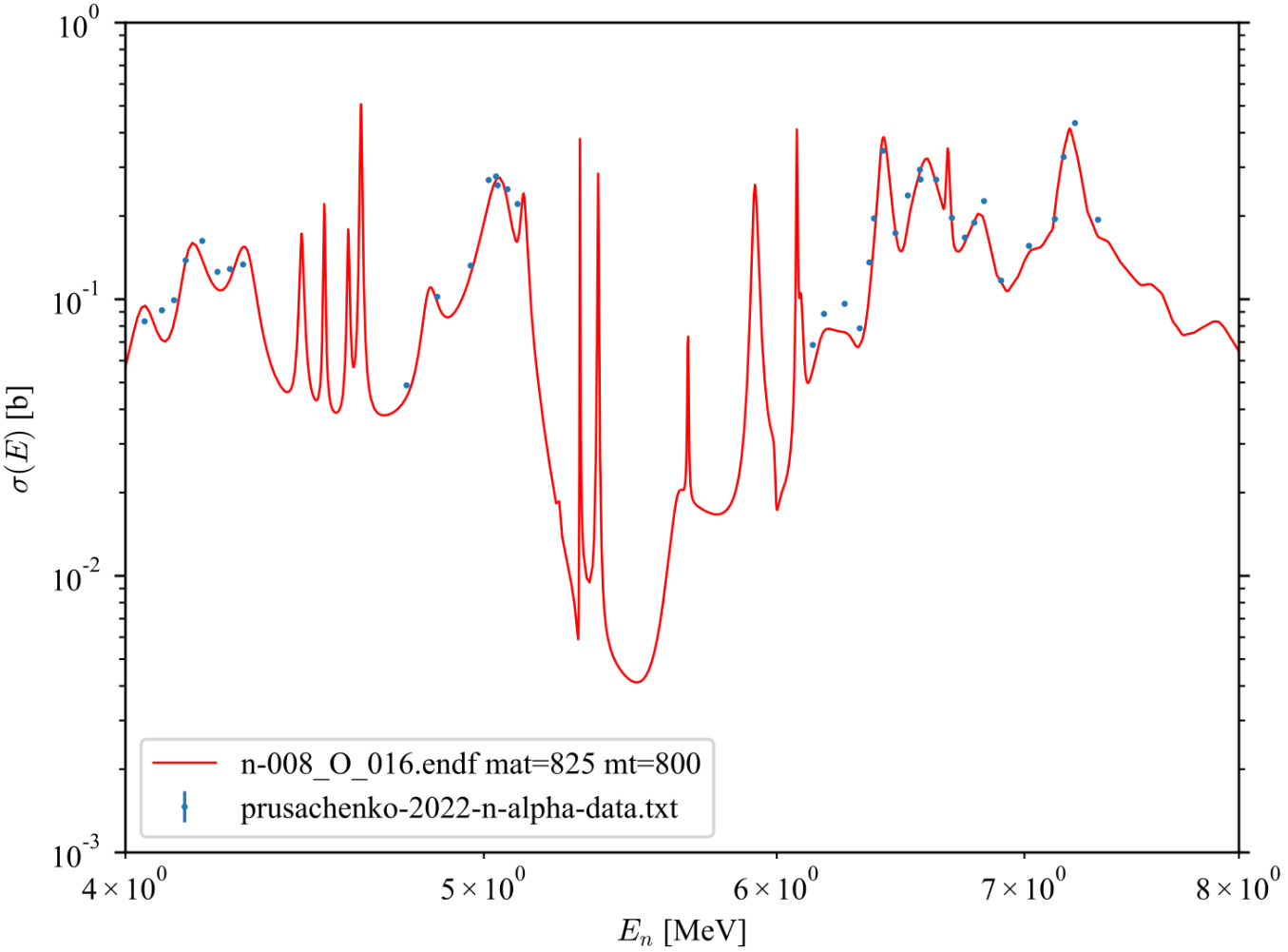
(20181001A) Subents 008,011 superseded
(20210401R) Data were received from T.Khromyleva and
(20210401A) added in Subents 005, 006, 007.

Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

(n, α_0)

- Prusachenko 2022 updated



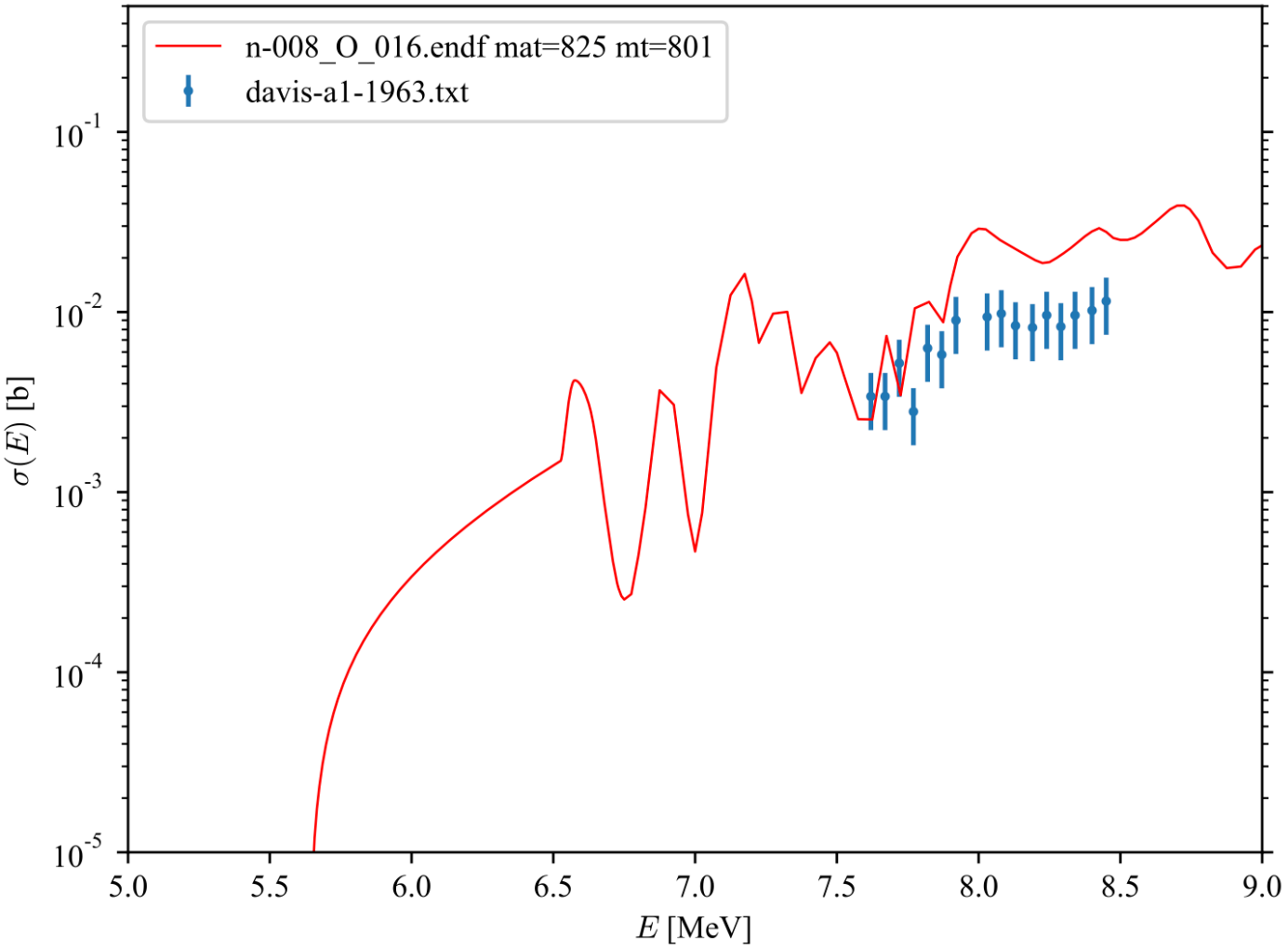
Comparison of $^{16}\mathrm{O}(n, \alpha_0)$ 2022 data by Prusachenko *et al.*[9] compared to ENDF/B-VIII.0.

Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

(n, α_1)

– Davis et al. 1963

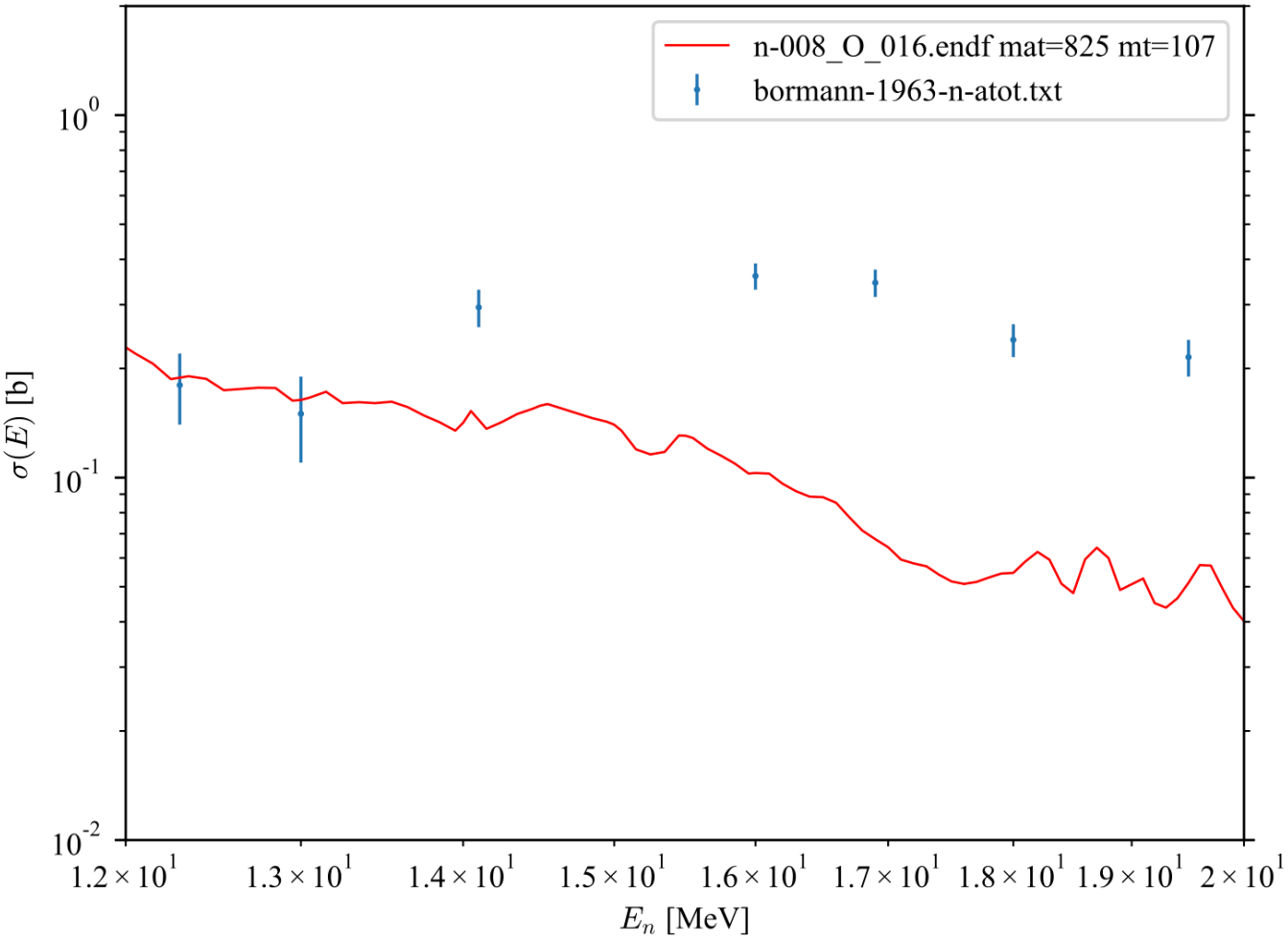


Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

(n, α_1)

– Borman et al. 1963



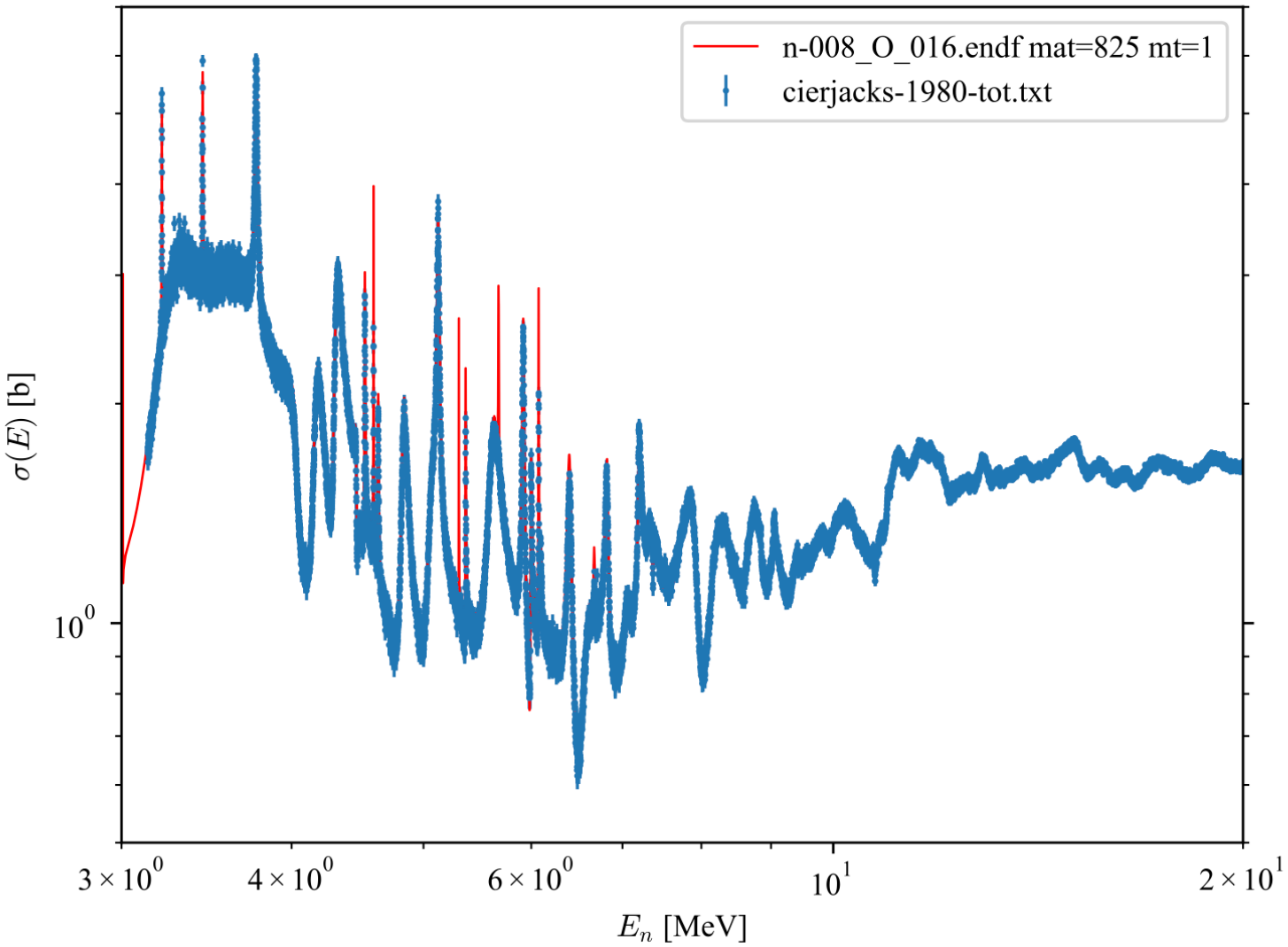
Comparison of $^{16}\mathrm{O}(n, \alpha_{tot})$ 1963 data by Borman[8] compared to ENDF/B-VIII.0.

Oxygen-16

ENDF/B-VIII.0 neutron sublibrary

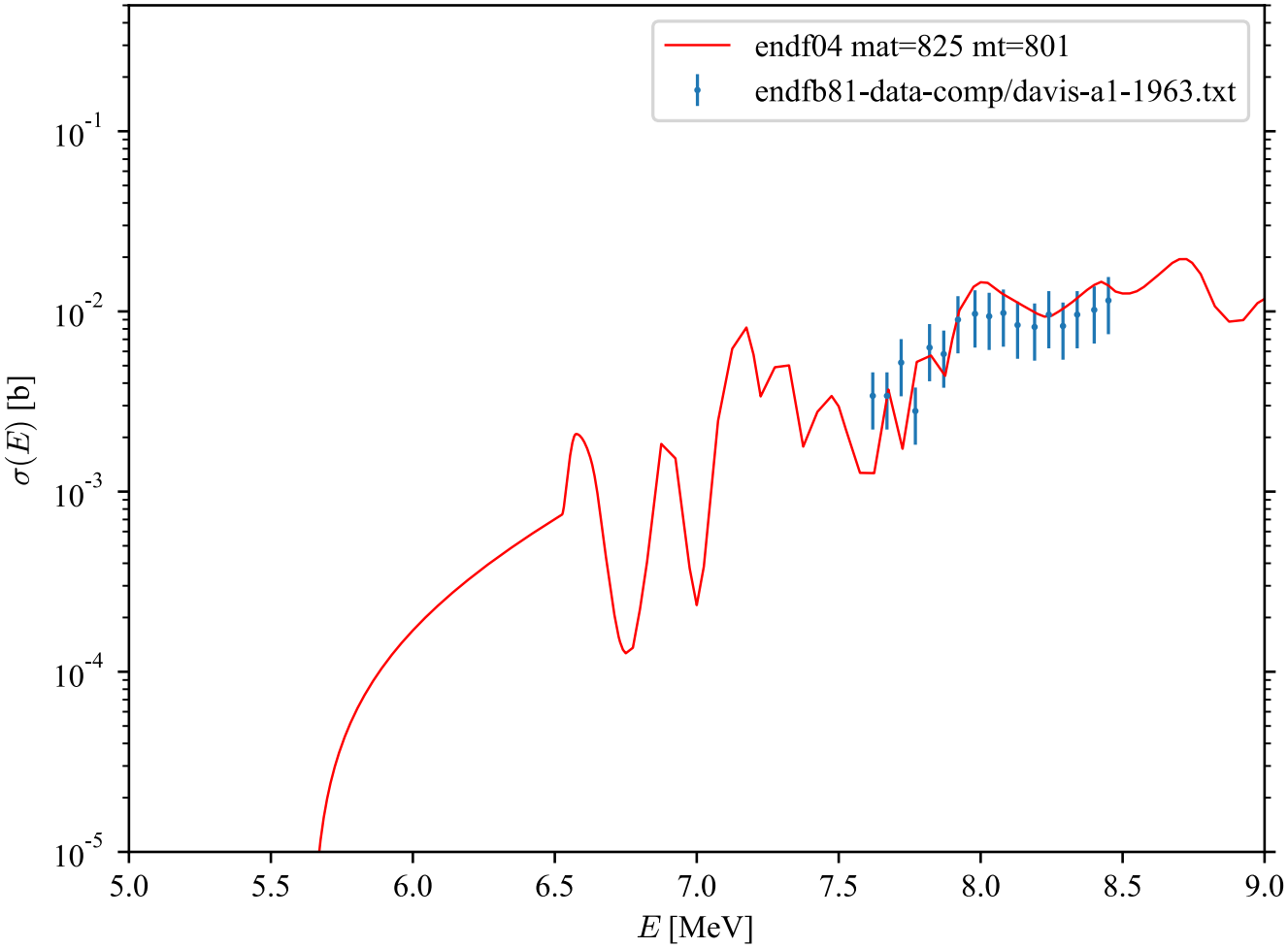
(n, n_{tot})

– Cierjacks 1980



Oxygen-16 Update for ENDF/B-VIII.1β0

- Bair & Haas / ENDF/B-VI.8 (pre-Harissopulos) scale is correct for (n, α_0)
- Scale mt=801,802,803 (n, α_x) $x = 1,2,3$ by factor 0.5



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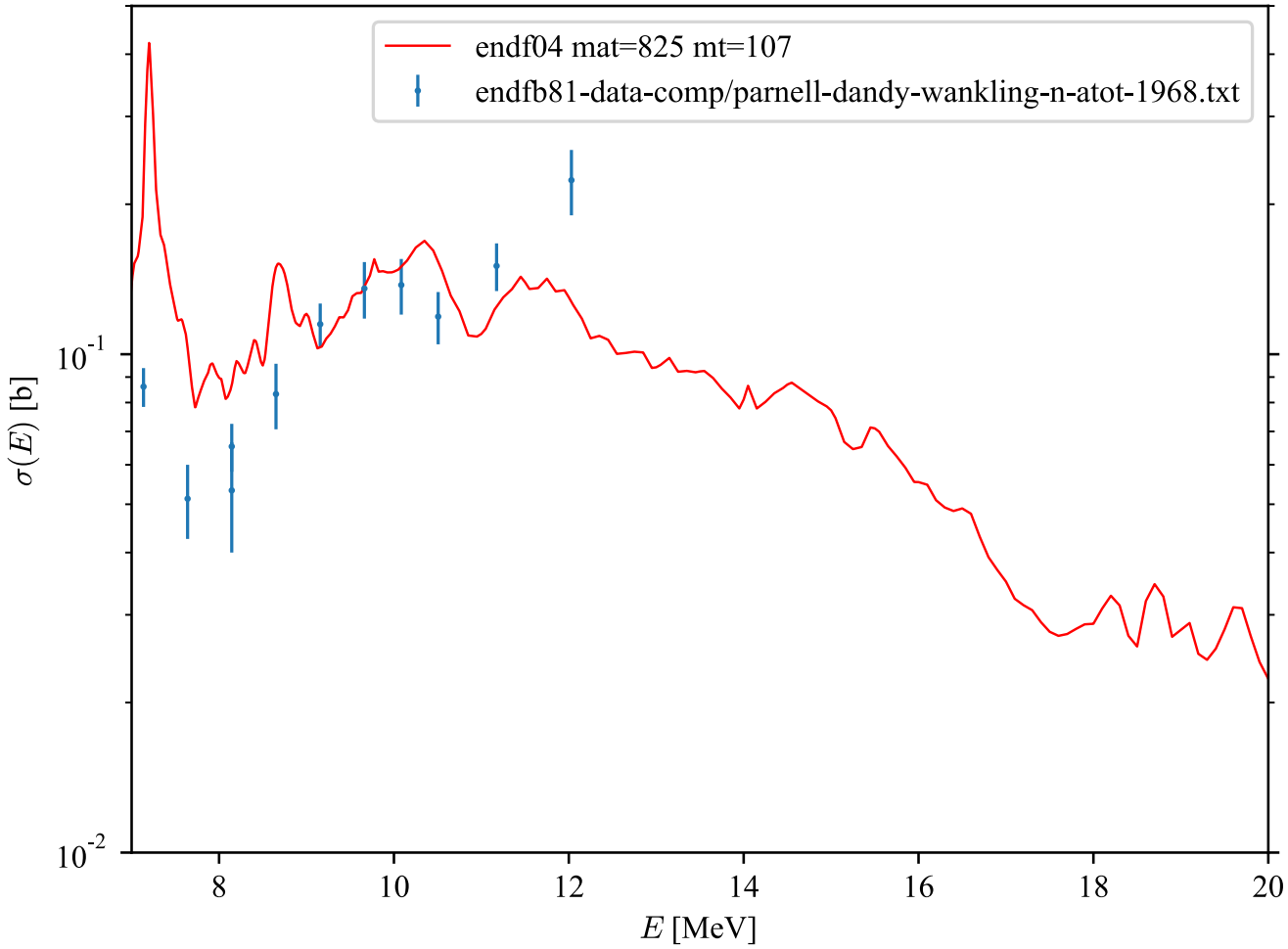

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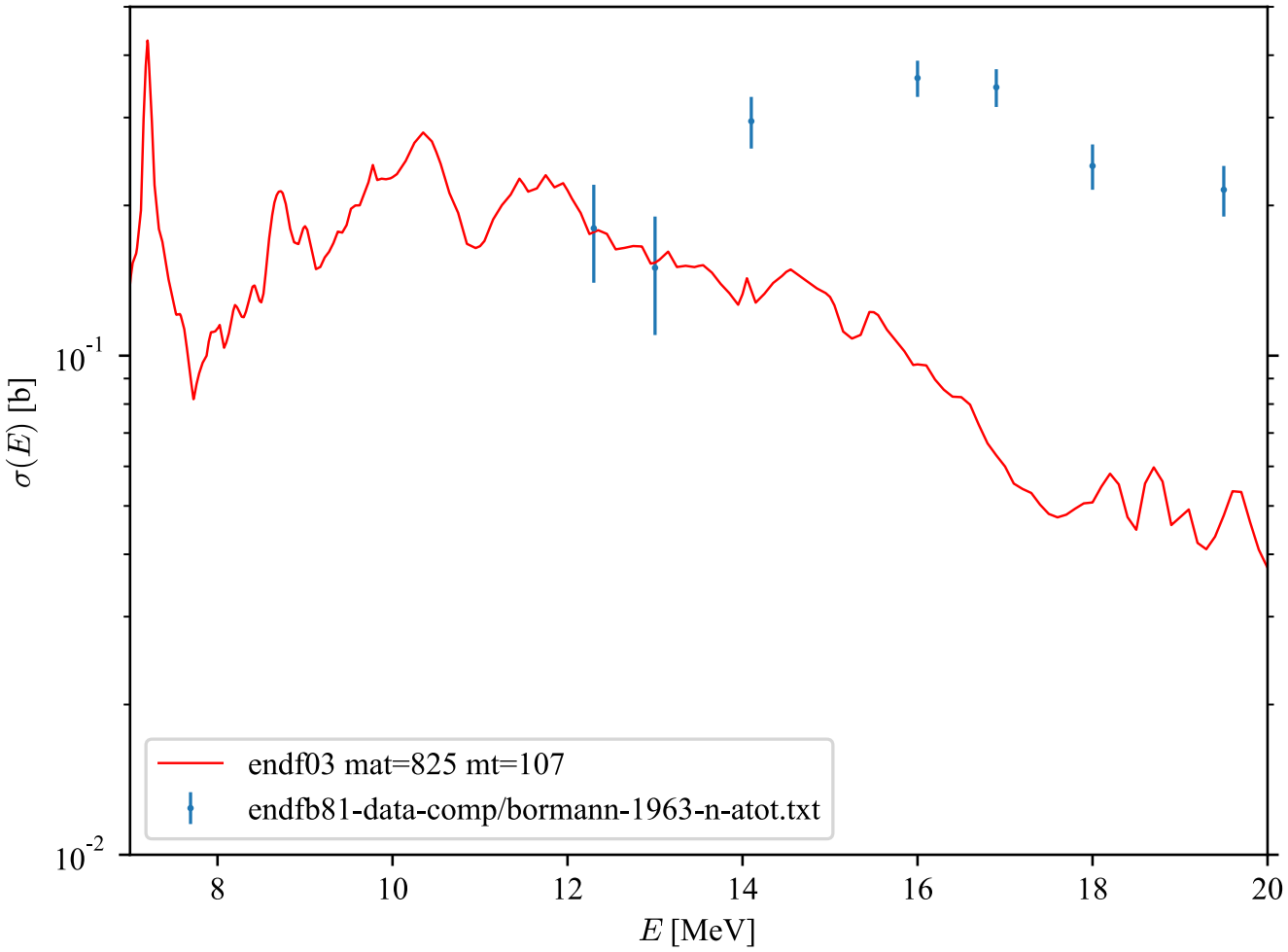
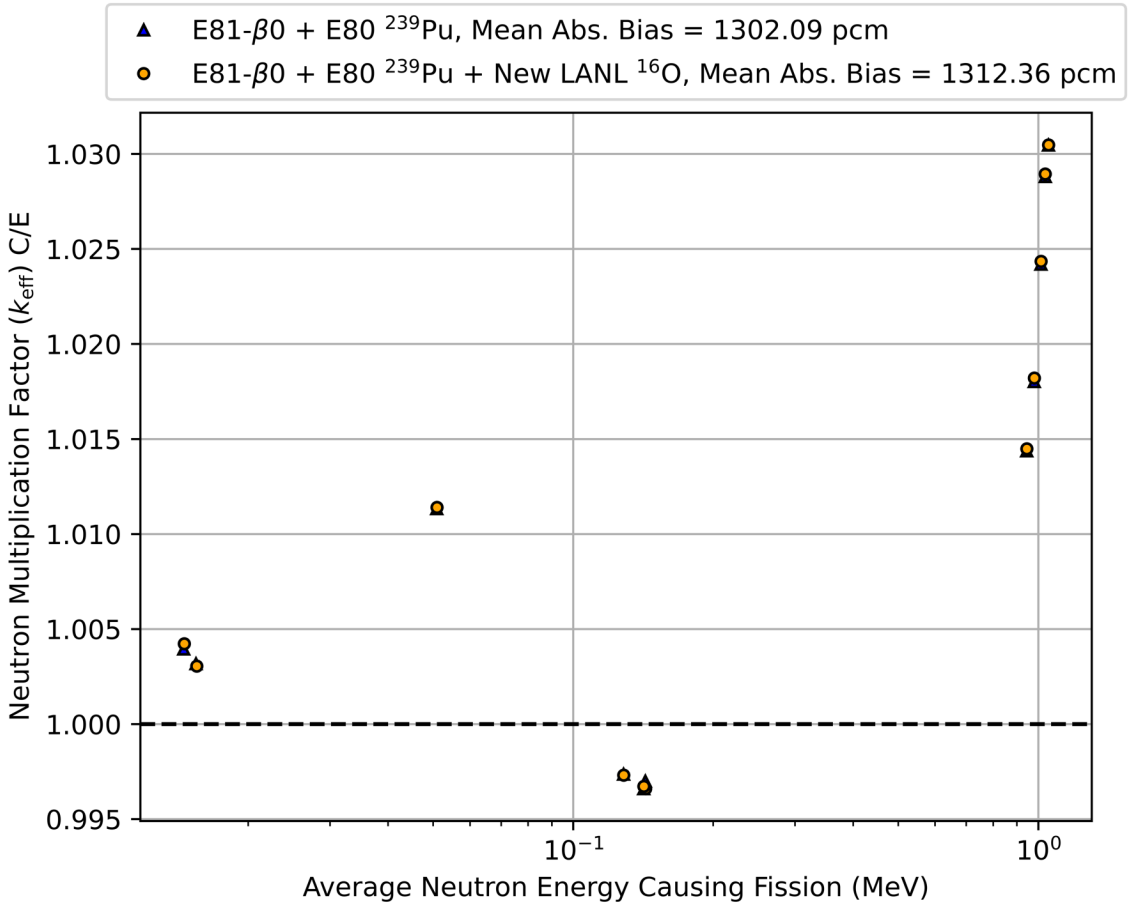


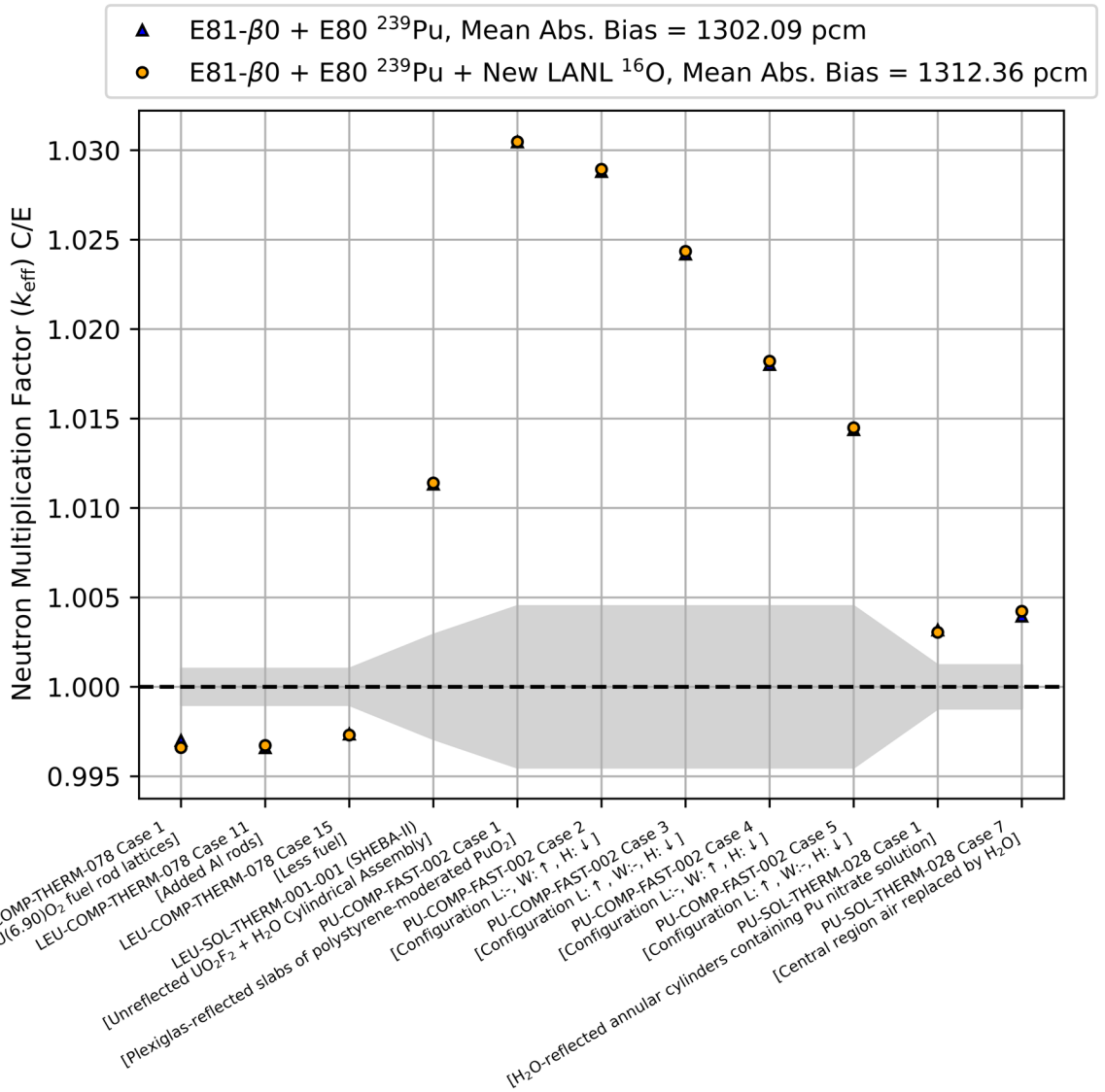
Preliminary n+16O testing

XCP-5 LANL



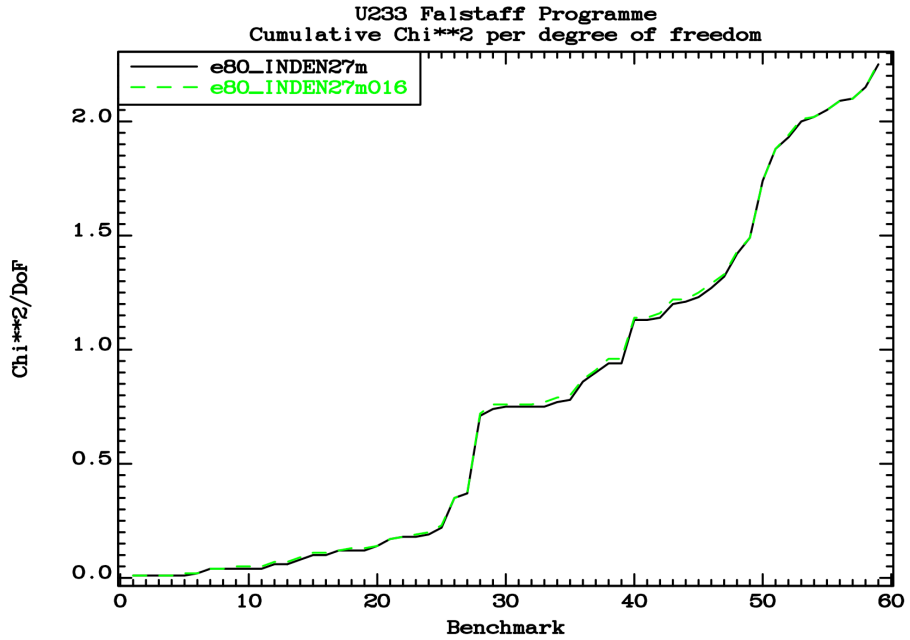
Preliminary n+16O testing

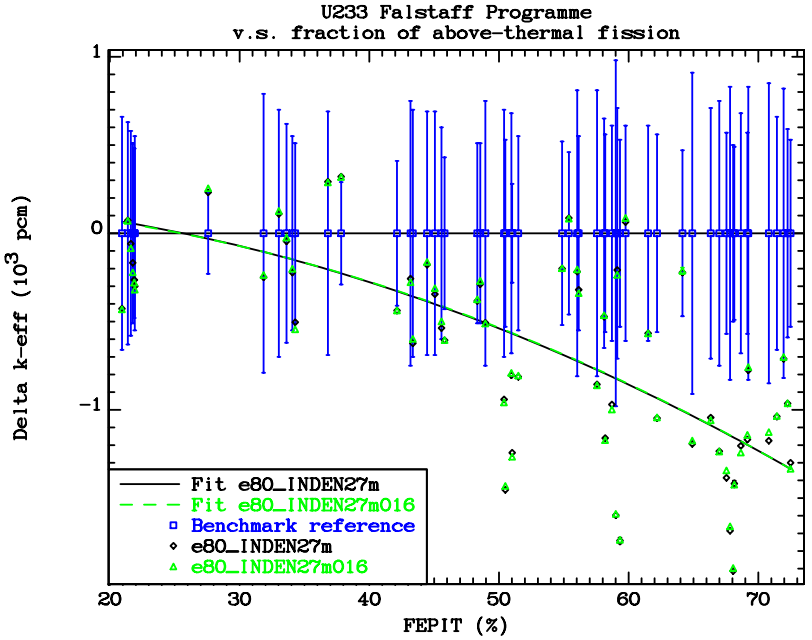
XCP-5 LANL

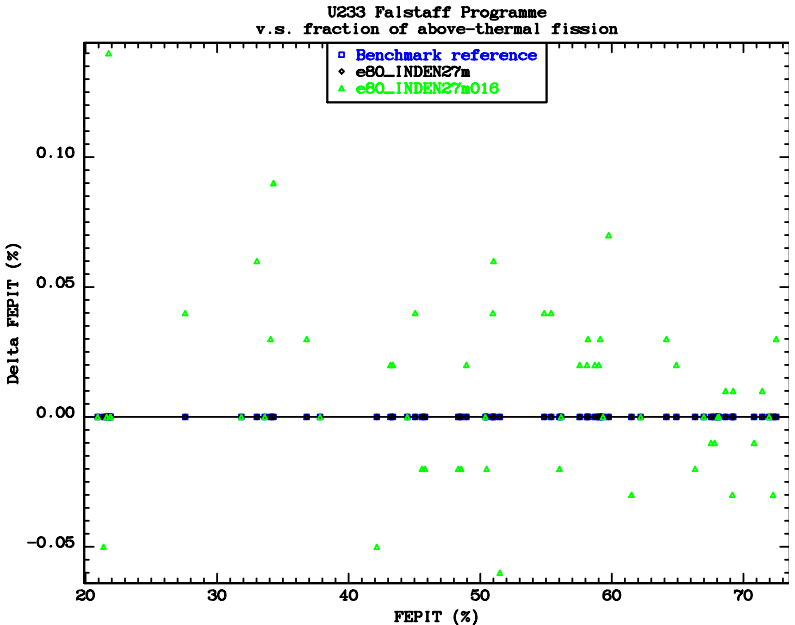


Preliminary n+16O testing

IAEA/NDS







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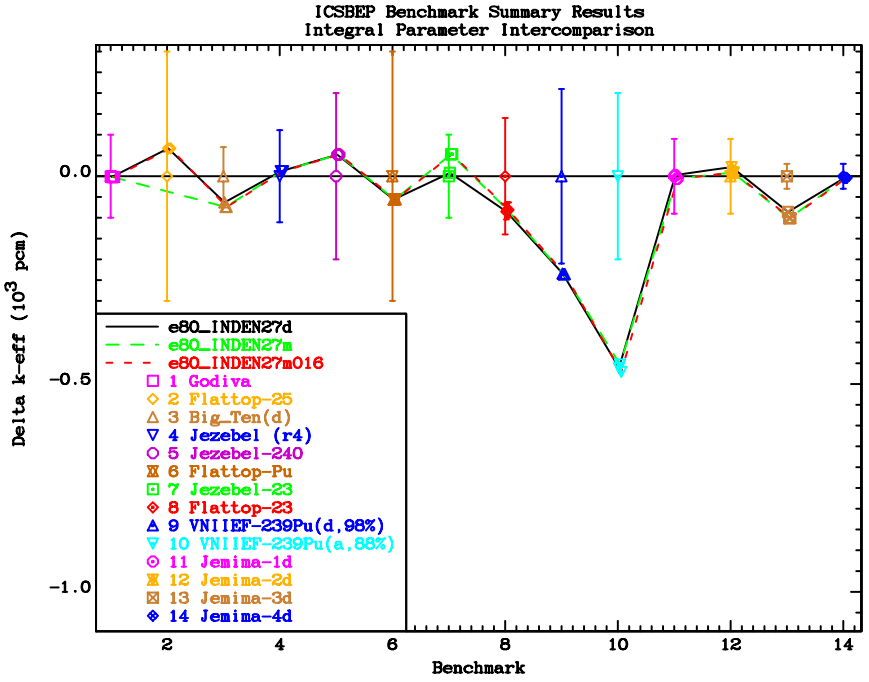
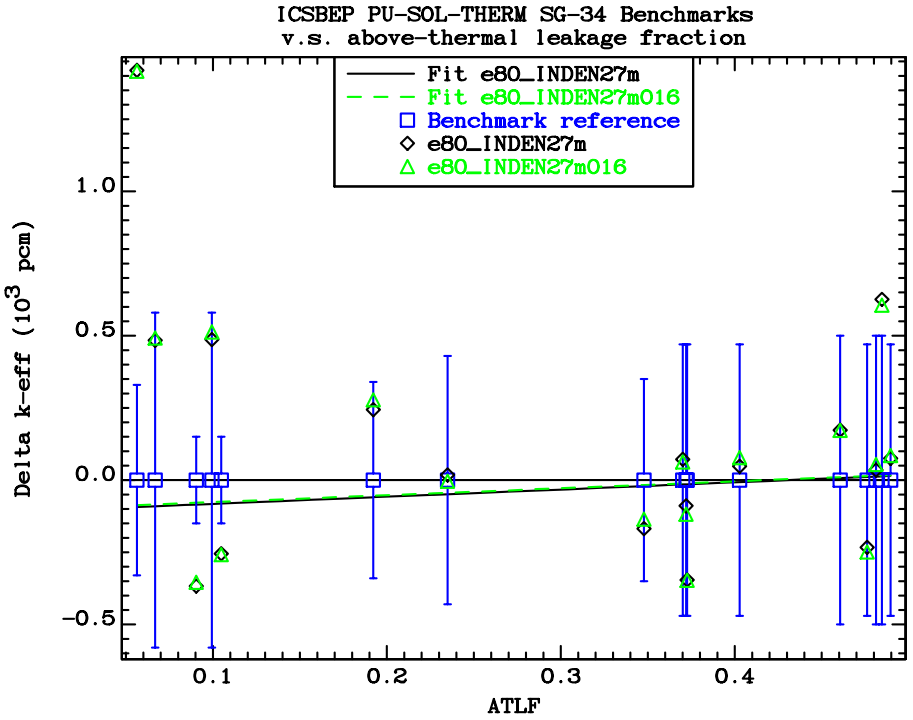


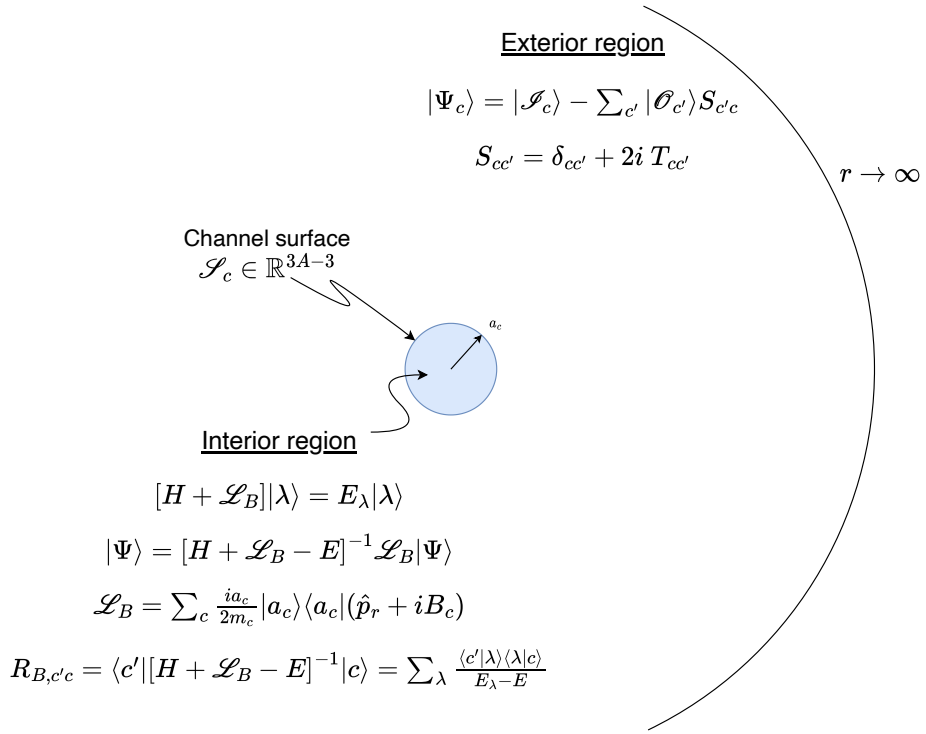


Charged-particle sublibraries

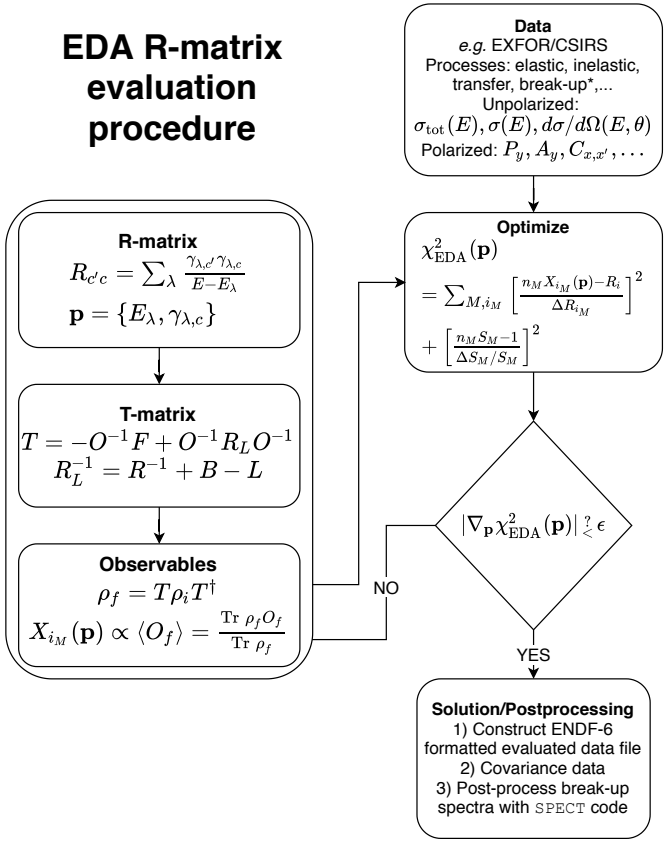
Outline

- R-matrix formalism
- Charged particle sublibrary
  - ^{5}Li system
- MF2 resonance parameters
  - ^{5}He test

R-matrix formalism



EDA R-matrix evaluation procedure



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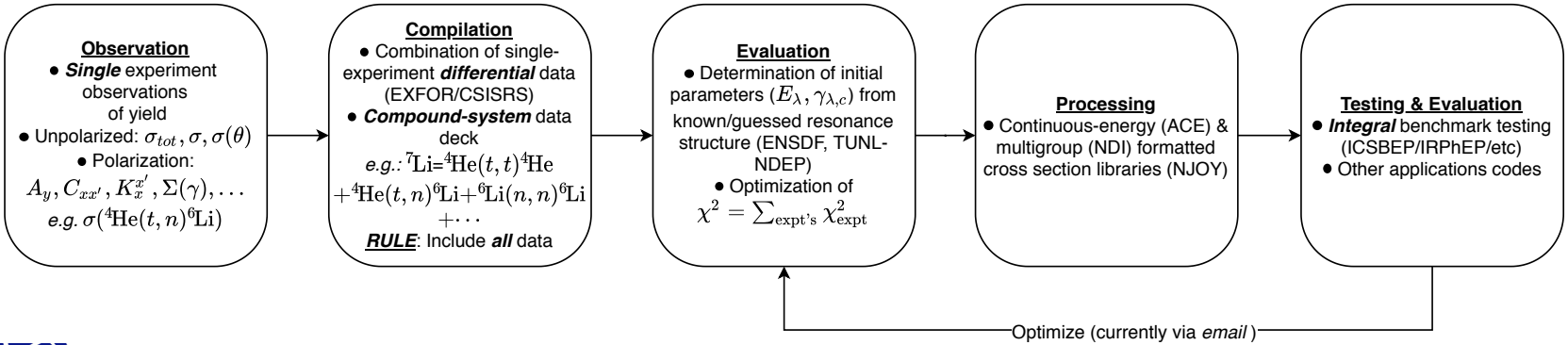
EDA cross section evaluation



LANL light-element program

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- Recent work in 2020:

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n	2020	VIII.0	VIII.0	VIII.0	VIII.0	2020	VIII.0
p	2020	VIII.0	VIII.0	VIII.0	2020	VIII.0	VIII.0
d		VIII.0	VIII.0	2020	VIII.0[a]	VIII.0	VIII.0
t			VIII.0	VIII.0	2020	VIII.0	TENDL09
$h(^{3}\mathrm{He})$				VIII.0	VIII.0	VIII.0	TENDL09
α					VIII.0	TENDL09	TENDL09

^{11}B (α+^{7}Li, α+^{7}Li*, t+^{8}Be, n+^{10}B); ^{11}C (α+^{7}Be, p+^{10}B)
^{12}C (α+^{8}Be, p+^{11}B)
^{13}C (n+^{12}C, n+^{12}C*)
^{14}C (n+^{13}C)
^{15}N (p+^{14}C, n+^{14}N, α+^{11}B)
^{16}O (g+^{16}O, α+^{12}C)
^{17}O (n+^{16}O, α+^{13}C)
^{18}Ne (p+^{17}F, p+^{17}F*, α+^{14}O)

Overview

Proposed additions/revisions to ENDF/B library

- **Tapes – all extended energy/better agreement with more data; Covariances planned**
  - `p-001_H_001.endf [EDA->ENDF]`
  - `p-002_He_004.endf [ready]`
  - `d-002_H_003.endf [EDA->ENDF]`
  - `d-002_He_003.endf` **`[submitted]`**
  - `d-003_Li_006.endf [ready]`
  - `n-003_Li_006.endf` **`[submitted]`**
  - `t-002_He_004.endf [ready]`
  - `a-006_C_013.endf [EDA->ENDF]`
- **Testing**
  - NJOY
  - IAEA/Dunford codes [checkr, stanef, fizcon, psyche, inter]
  - ENDF > ACE
    - checkace [LANL ACE format checking tool]
    - mcnp6.1 pencil beam (d+3He only)
- **Comparisons**
  - with ENDF/B-VII.1 (*aka*, “CP2011”), VIII.0
  - with LLNL *Evaluated Charged Particle Library (ECPL-2018)*

Changes
d-002_He_003.endf

MF	MT	Description	Energy range [MeV]
3		Reaction cross sections	
	2	(z,z0)	(0.01, 1.40)
	600	(z,p_0)	(0.00, 1.40)
6		Energy-angle distributions for emitted particles	
	2	(z,z0)	
	600	(z,p_0)	

Table 26: ENDF/B-VIII.0 library, file: d-002_He_003.endf

MF	MT	Description	Energy range [MeV]
3		Reaction cross sections	
	2	(z,z0)	(0.01, 20.00)
	600	(z,p_0)	(0.01, 20.00)
6		Energy-angle distributions for emitted particles	
	2	(z,z0)	
	600	(z,p_0)	

Table 27: CP2020 library new evaluation, file: d-002_He_003.endf

Changes

p-002_He_004.endf

MF	MT	Description	Energy range [MeV]
3		Reaction cross sections	
	2	(z,z0)	(0.11, 20.00)
6		Energy-angle distributions for emitted particles	
	2	(z,z0)	

Table 86: ENDF/B-VIII.0 library, file: p-002_He_004.endf

MF	MT	Description	Energy range [MeV]
3		Reaction cross sections	
	2	(z,z0)	(0.02, 34.30)
	650	(z,d_0)	(23.02, 34.30)
6		Energy-angle distributions for emitted particles	
	2	(z,z0)	
	650	(z,d_0)	

Table 87: CP2020 library new evaluation, file: p-002_He_004.endf

Changes

t-002_He_004.endf

MF	MT	Description	Energy range [MeV]
3		Reaction cross sections	
	2	(z,z0)	(0.14, 20.00)
6		Energy-angle distributions for emitted particles	
	2	(z,z0)	

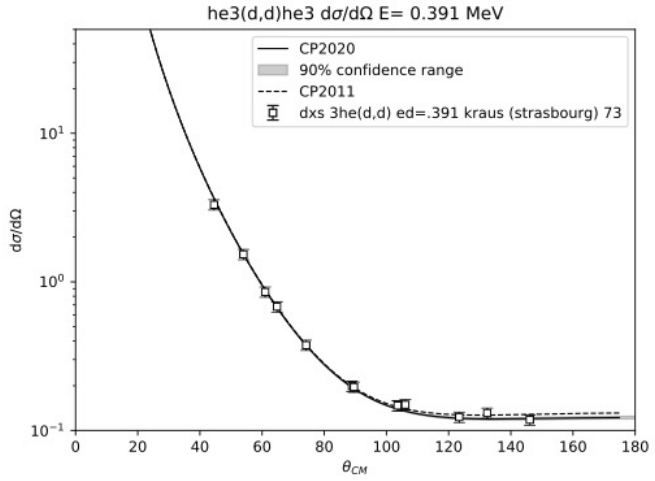
Table 120: ENDF/B-VIII.0 library, file: t-002_He_004.endf

MF	MT	Description	Energy range [MeV]
3		Reaction cross sections	
	2	(z,z0)	(0.10, 20.00)
	50	(z,n_0)	(8.39, 20.00)
	51	(z,n_1)	(12.28, 20.00)
	52	(z,n_2)	(14.65, 20.00)
	600	(z,p_0)	(13.18, 20.00)
	650	(z,d_0)	(10.98, 20.00)
6		Energy-angle distributions for emitted particles	
	2	(z,z0)	
	50	(z,n_0)	
	51	(z,n_1)	
	52	(z,n_2)	
	600	(z,p_0)	
	650	(z,d_0)	

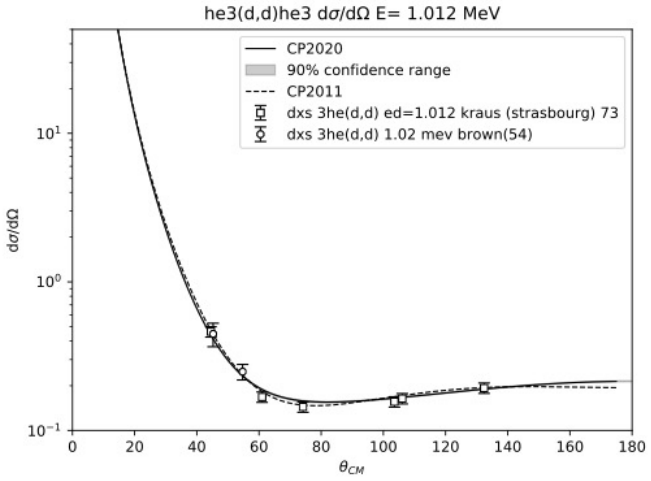
Table 121: CP2020 library new evaluation, file: t-002_He_004.endf

^{5}Li system evaluation

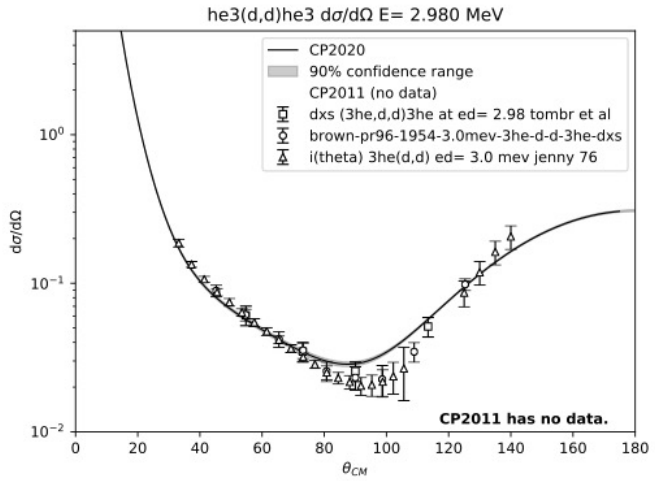
^{3}He(d,d)^{3}He



(a)



(b)



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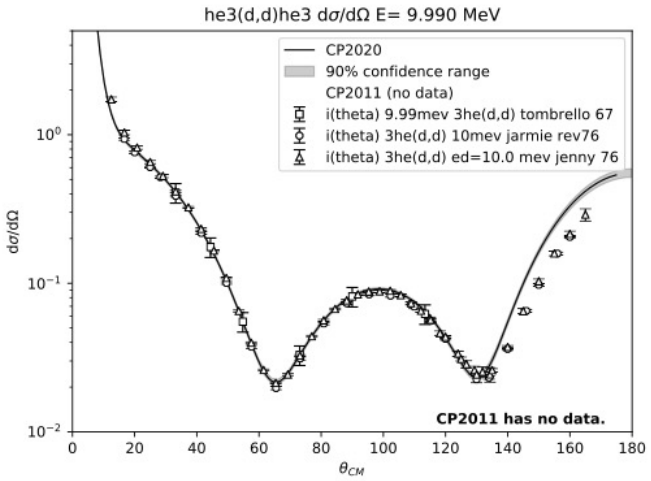
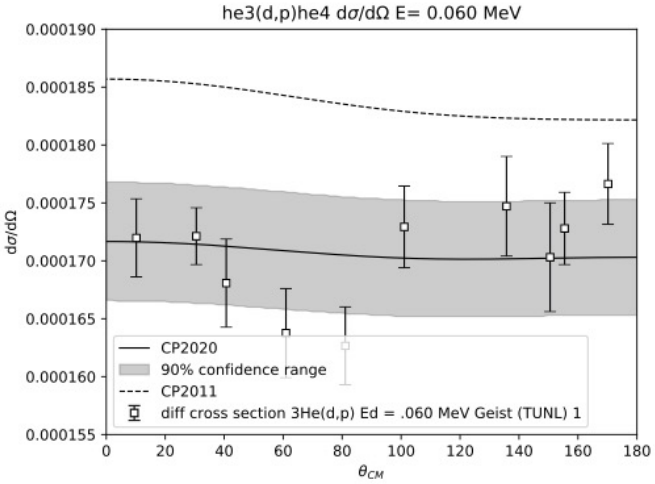


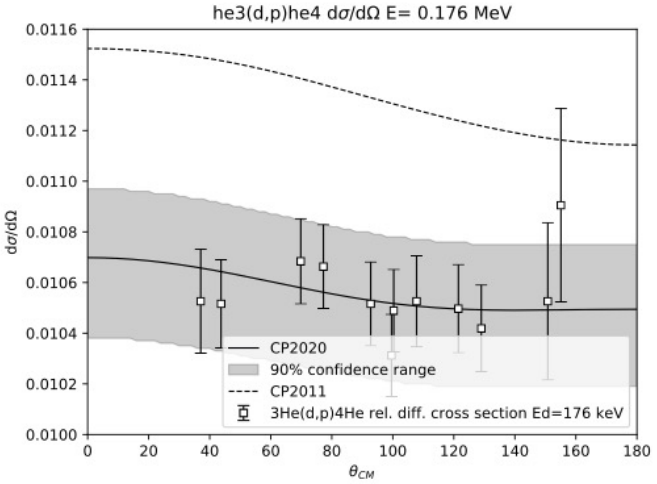
(d)

^{5}Li system evaluation

^{3}He(d,p)^{4}He



(a)



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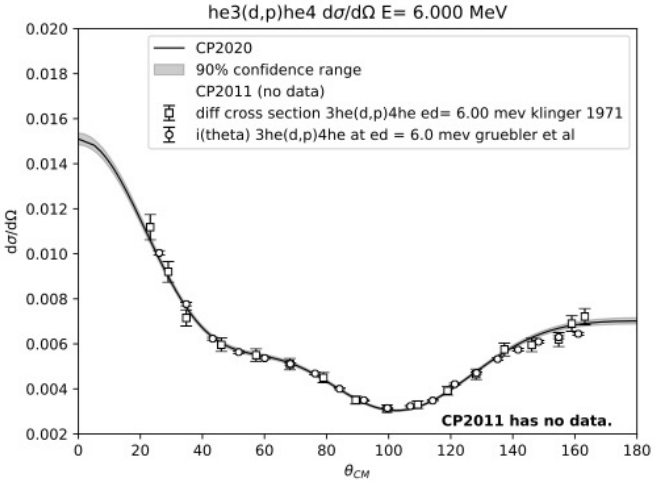

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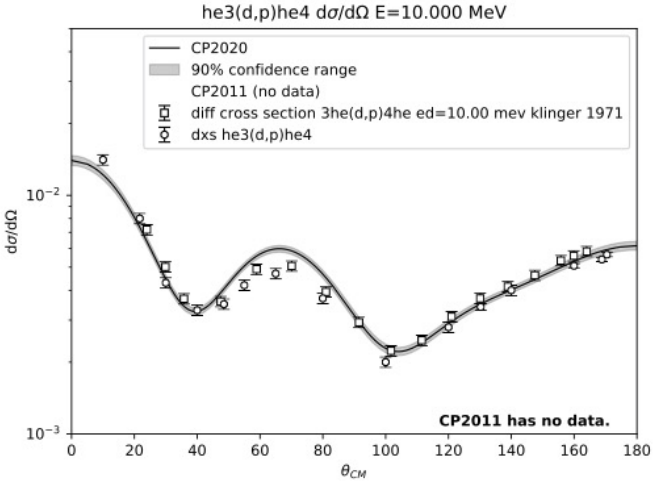
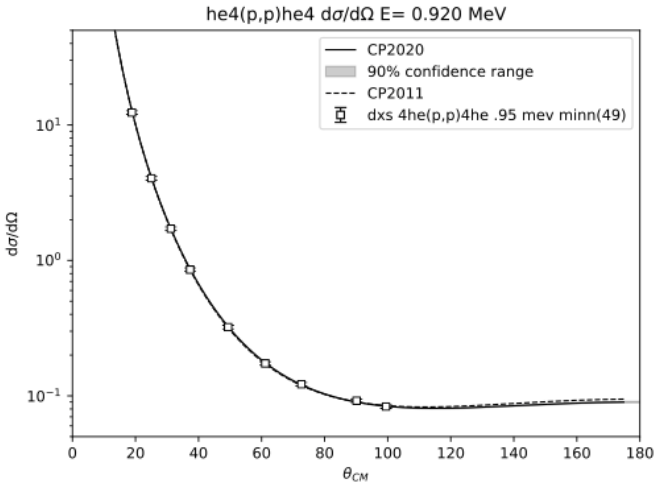


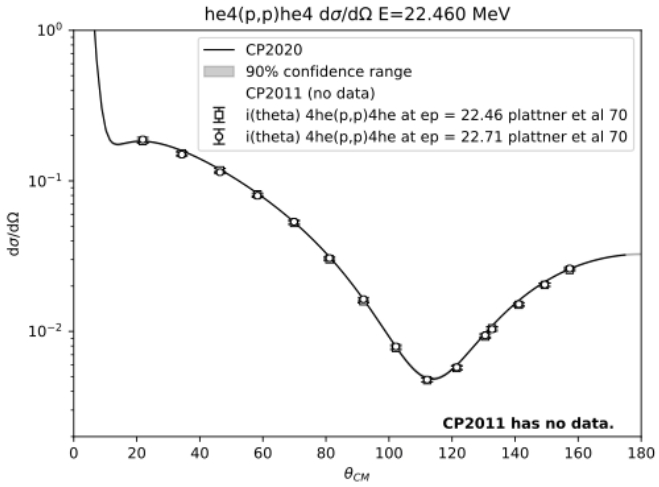
(d)

^{5}Li system evaluation

^{4}He(p,p)^{4}He



(a)



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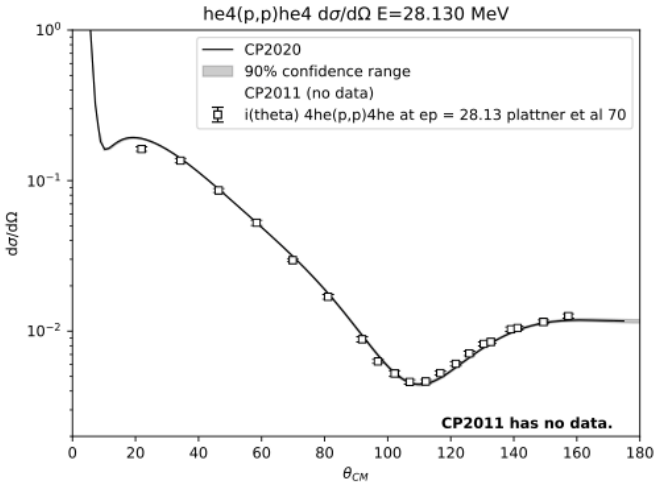

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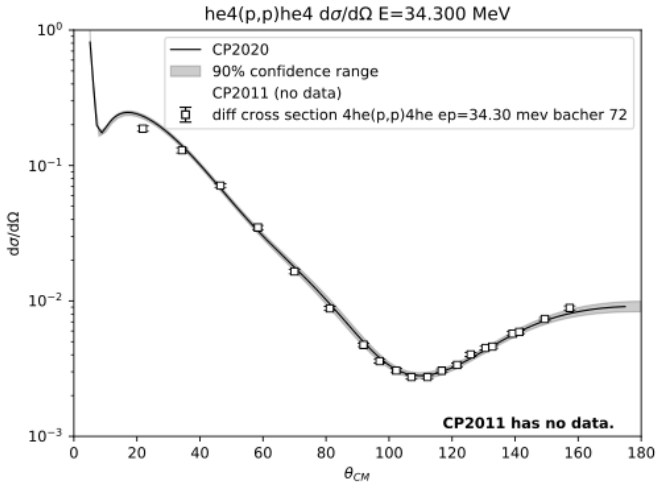
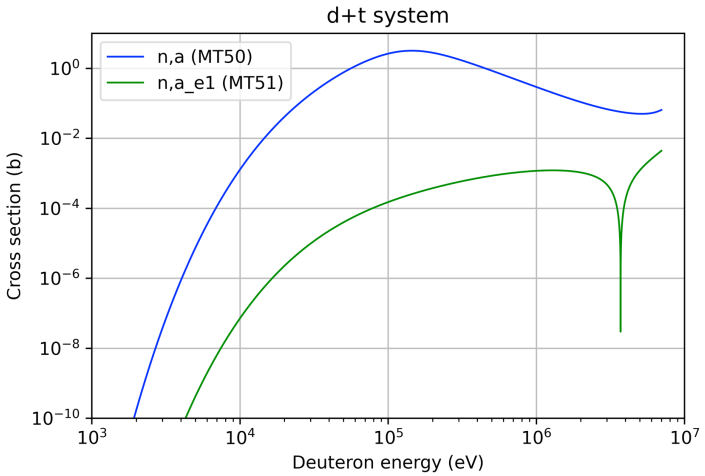


(d)

MF2 resonance parameters

- "Full" evaluation
- NJOY test buggy
  - We think we know why…
    - formatting

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 0.000000+0 0.000000+0          1          4         13          0 128 2151
 0.000000+0 0.000000+0          3          0         36          6 128 2151
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 0.000000+0 0.000000+0          0          4         24          4 128 2151
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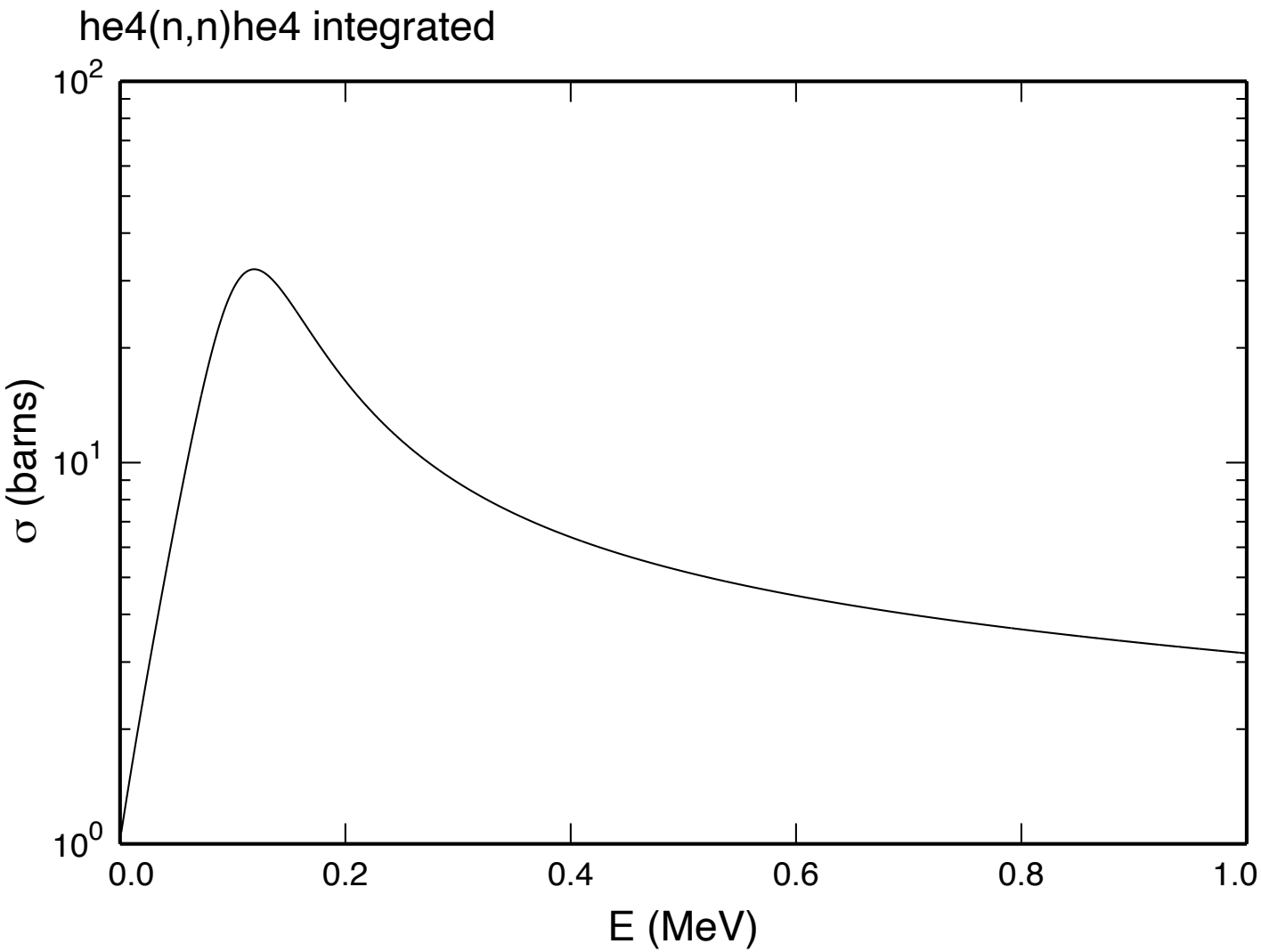
 0.000000+0 0.000000+0          0          4         24          4 128 2151
```

Manual update: beginning of revisions for resonance parameters sections

- https://git.nndc.bnl.gov/endf/format/endf6man.git
  - SHA: 56da8d2b

MF2 resonance parameters

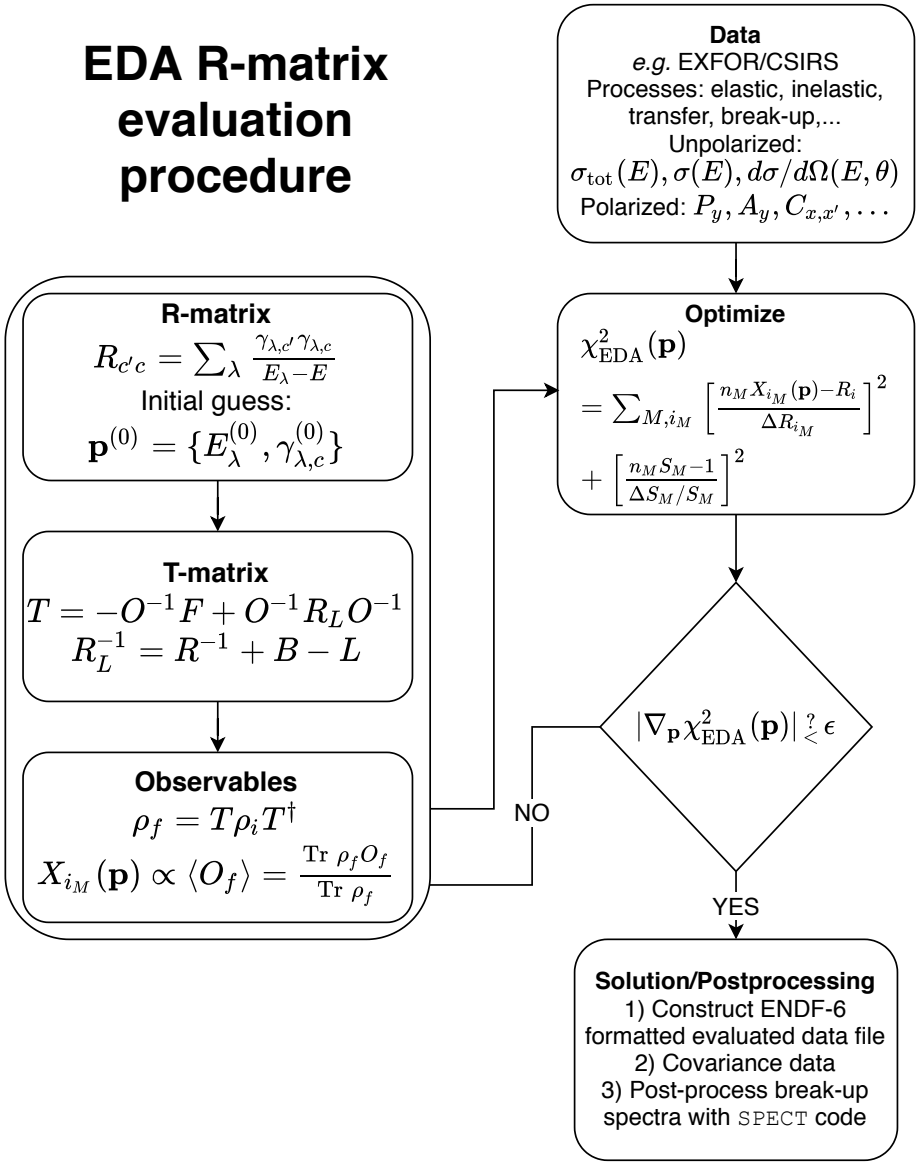
- "Test" evaluation
  - single channel, single resonance



Thank you!

^{17}O R-matrix evaluation [*NEW*]

EDA R-matrix evaluation procedure



Channel	a_c(fm)	$\ell_{\max}$
n+^{16}O(0^+;gs)	4.40	4
α+^{13}C($\frac{1}{2}^-$; gs)	5.40	5
n_1+^{16}O(0^+; 6.05 MeV)	5.00	3
n_2+^{16}O(3^-; 6.13 MeV)	5.00	2

Reaction	Range E_n, E_α (MeV)	$N_{\rm dat}$	Observables
^{16}O$(n,n)^{16}$O	(0.0, 7.0)	2,909	$\sigma_{\rm tot}, \sigma, \sigma(\theta), A_y(\theta)$
^{16}O$(n,n_2)^{16}$O(3^-; 6.13 MeV)	(6.6, 8.8)	45	$\sigma(\theta)$
^{13}C$(\alpha,\alpha)^{13}$C	(2.0, 5.7)	1,397	$\sigma(\theta)$
^{13}C$(\alpha,n)^{16}$O	(.23, 8.0)	1,054	σ_r
^{13}C$(\alpha,n_0)^{16}$O(0^+; gs)	(1.0, 6.5)	3,116	$\sigma, \sigma(\theta)$
^{13}C$(\alpha,n_1)^{16}$O(0^+; 6.05 MeV)	(5.1, 5.6)	113	$\sigma, \sigma(\theta)$
Total		8,634	5 types

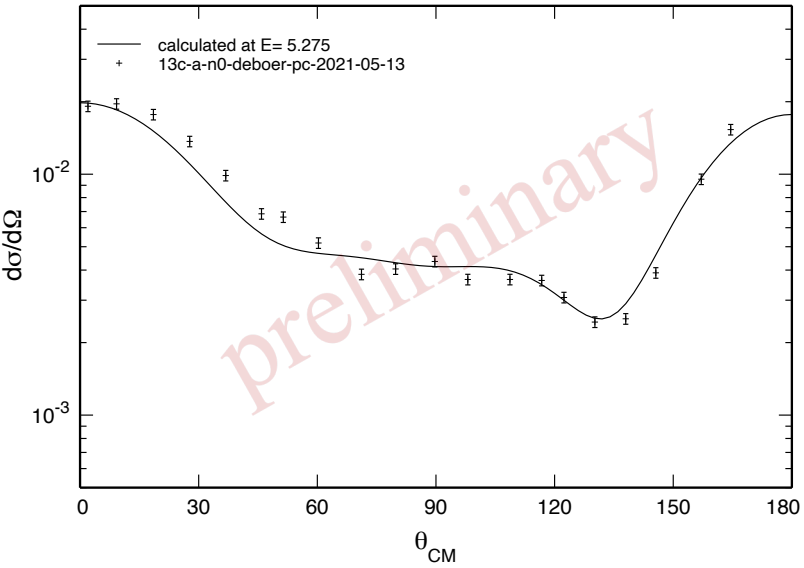
17O system channel/pars

- # channels: 45
  - J^{π}=1/2$^{\pm}$, ..., 11/2$^{\pm}$
- # parameters
  - E_λ: 81 level energies
  - $\gamma_{\lambda,c}$: 322 reduced widths
- # Normalizations
  - n_M: 95 norm scales
  - ΔE_M: 4 shift factors

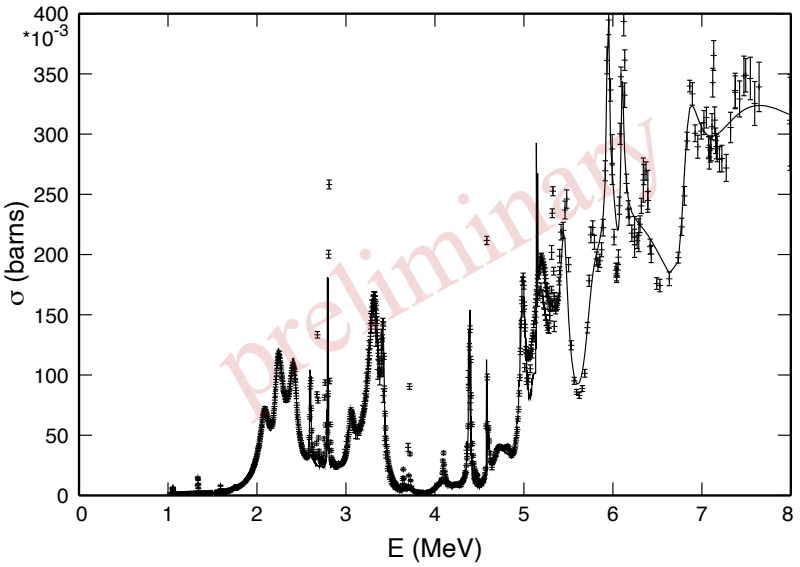
^{17}O Preliminary evaluation

Preliminary results: (α,n_0)

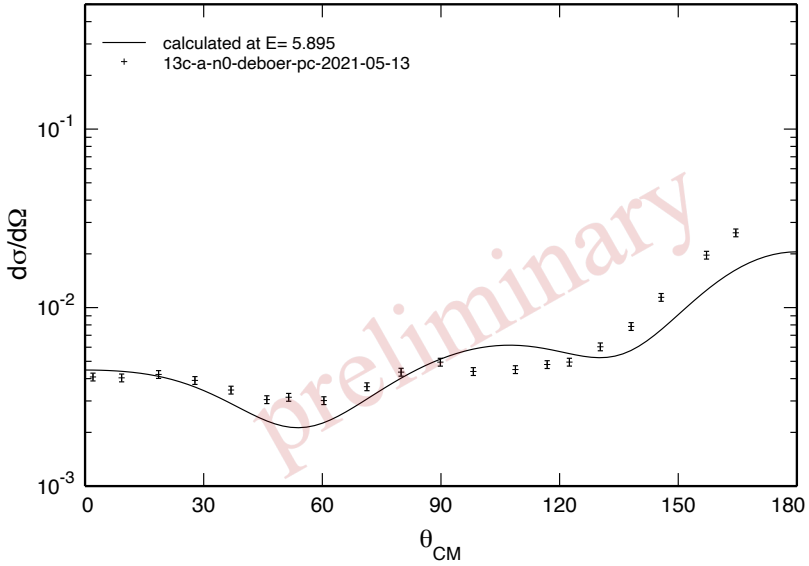
13c(4he,n)16o dσ/dΩ E= 5.275 MeV



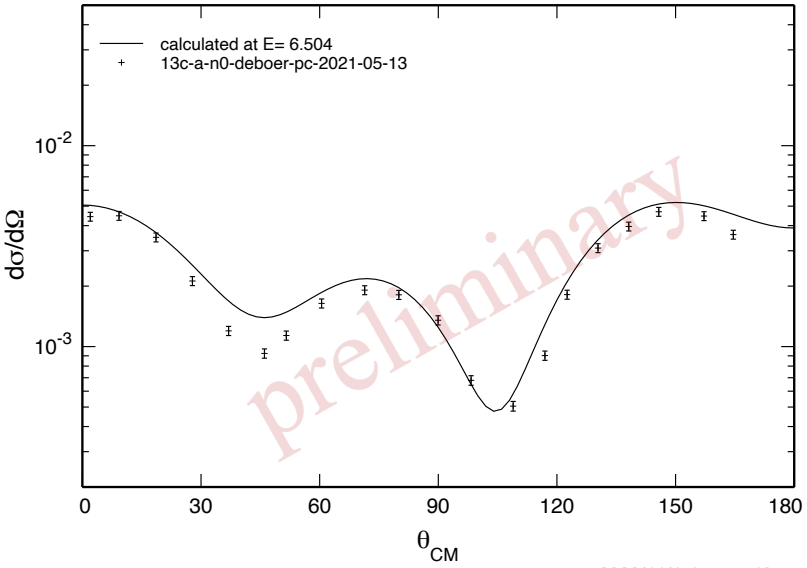
13c + 4he reaction



13c(4he,n)16o dσ/dΩ E= 5.895 MeV

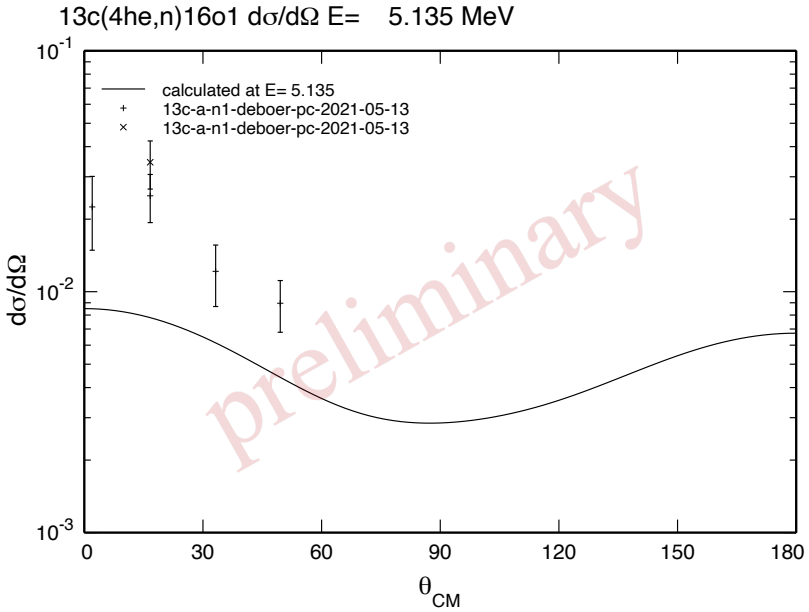


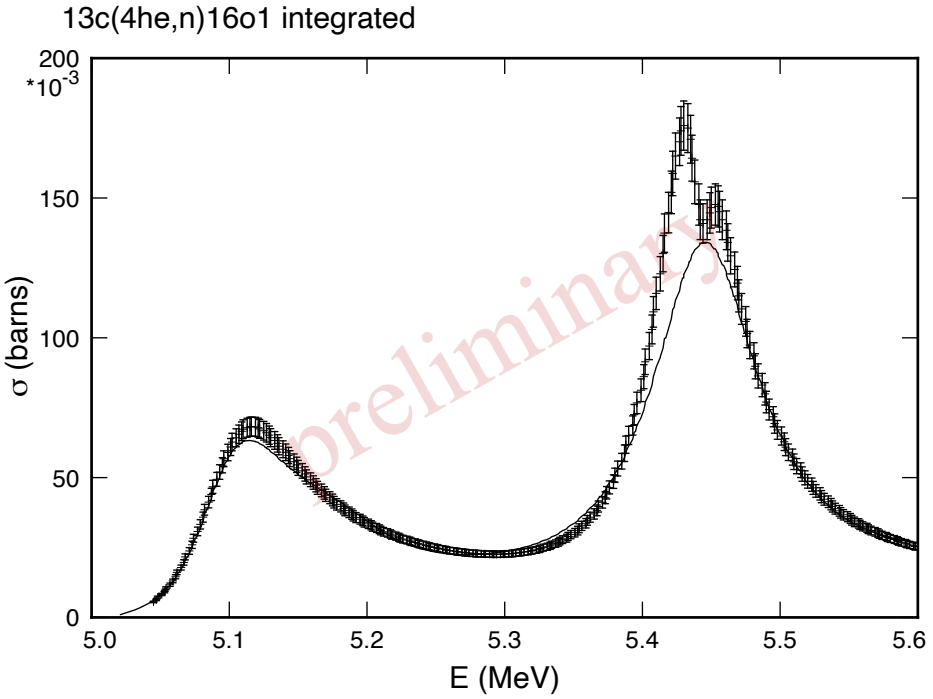
13c(4he,n)16o dσ/dΩ E= 6.504 MeV

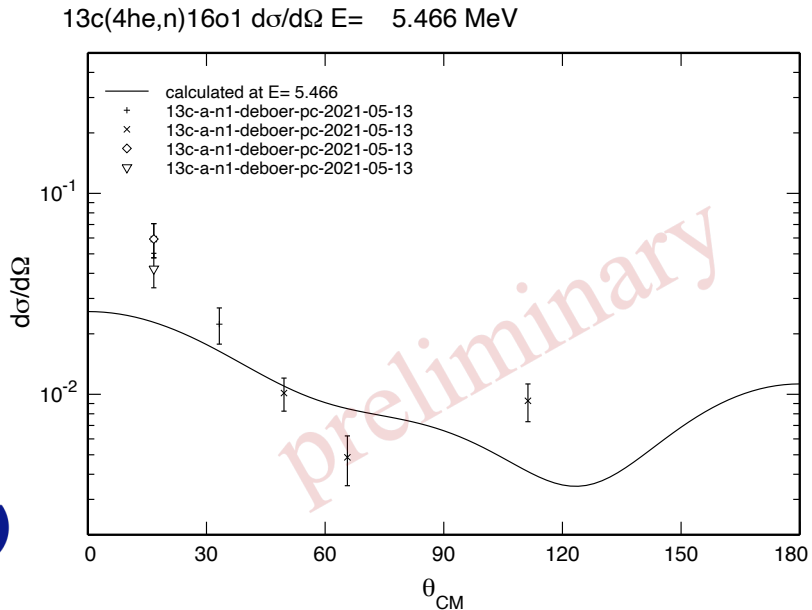


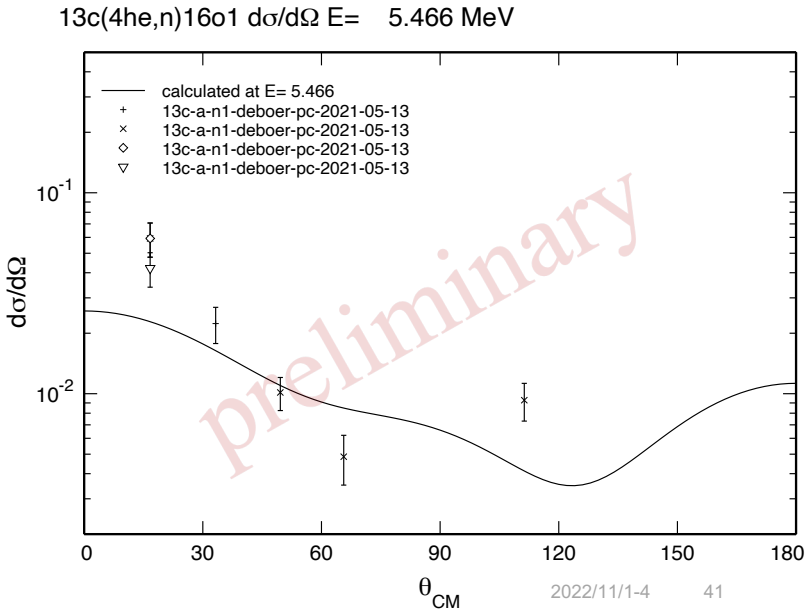
^{17}O Preliminary evaluation

Preliminary results: (α,n_1)



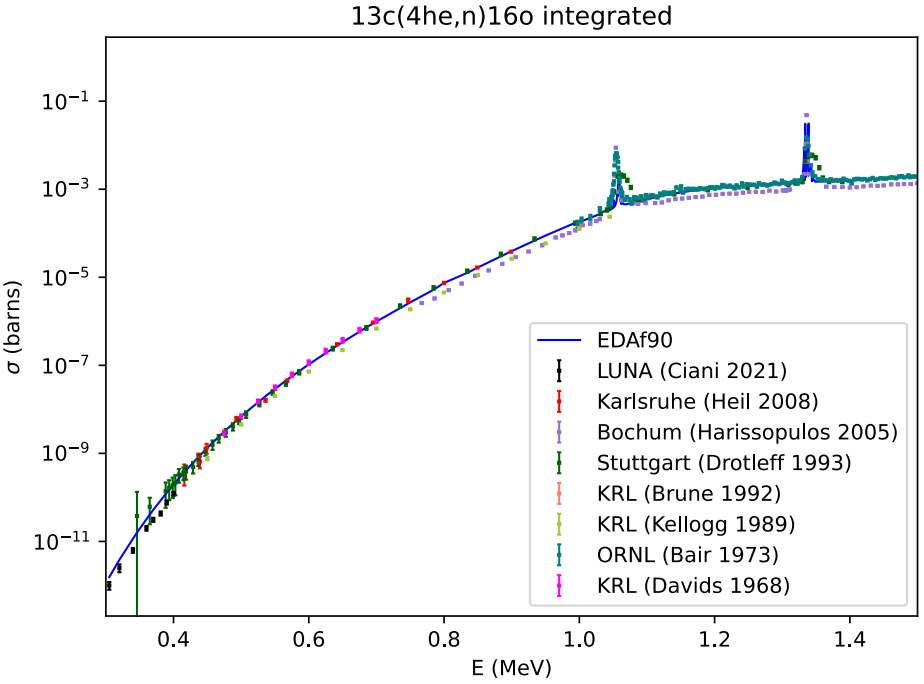


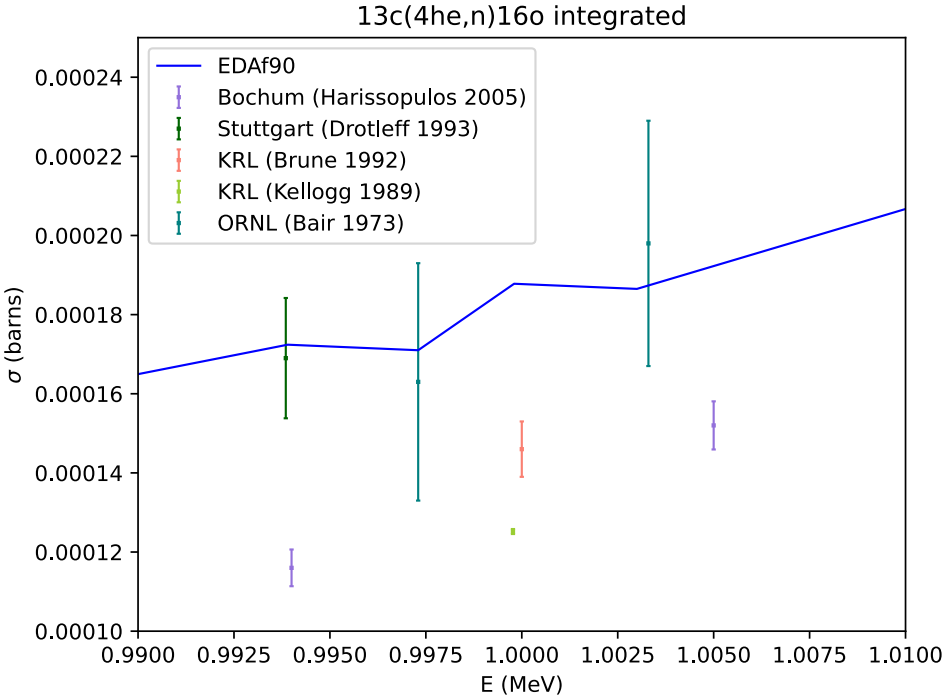




^{17}O Preliminary evaluation

Preliminary results: low energy



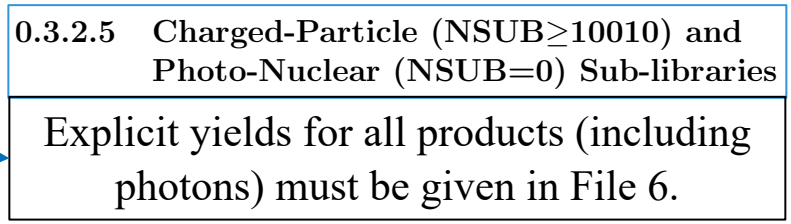


Experiment	E_α [MeV]	$\sigma_{(\alpha,n)}$ [μb]	1.000 MeV
KRL (Brune 1992)	1.0000	146(7)	146(7)
ORNL (Bair 1973)	1.0033	198(3)	179(4)
Stuttgart (Drotleff 1993)	0.9939	169(2)	187(3)
Bochum (Harissopulos 2005)	0.994	116(5)	136(7)
Bochum (Harissopulos 2005)	1.005	152(6)	–
KRL (Kellogg 1989)	0.9998	125(6)	126(8)

Measurements of $\sigma_{(\alpha,n)}(E_\alpha = 1.0$ MeV) for laboratory incident energies given in the first column, the value quoted in the second column, and the values linearly interpolated from the tabular data in the experiment's publication in the right-most column. No re-normalization factors have been applied to these values. In particular, the ORNL value of Bair & Haas[37]is quoted as originally presented without the 0.8 factor mentioned in their *Note added in proof.*

Charged-particle covariances
MF=30(!)

- Discussion at Monday's covariance session
  - MF=6 is *required* for CP induced tapes
  - there is no MF=36
- MF=30, however, admits covariance information for *any* MF>2
  - ENDF-6 format requirements
    - provide Cov_{ij} for any parameters
    - provide sensitivities for MF parameters
  - Advantages
    - Cov_{ij} can be diagonal (with eigenvector sensititivies)
    - MF=32 parameter covariances requires sensitivities (NJOY/ERRORR provides unc. for MF=3,4,5 only?)
  - Disadvantages
    - NJOY2016 doesn't process MF=30



Please correct me on any of this.