Summary of light-element charged-particle R-matrix evaluations for ENDF/B-VIII.1

Cross section evaluation working group
Evaluation Committee - Charged Particles
G. Hale & M. Paris (LANL/T-2)

2021-11-17

LA-UR-21-31260

Overview

Proposed additions/revisions to ENDF/B library

- **Tapes – all extended energy/better agreement with more data; Covariances planned**
  - `p-001_H_001.endf`
  - `p-002_He_004.endf`
  - `d-002_H_003.endf`
  - `d-002_He_003.endf`
  - `d-003_Li_006.endf`
  - `t-002_He_004.endf`
  - `a-006_C_013.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)	

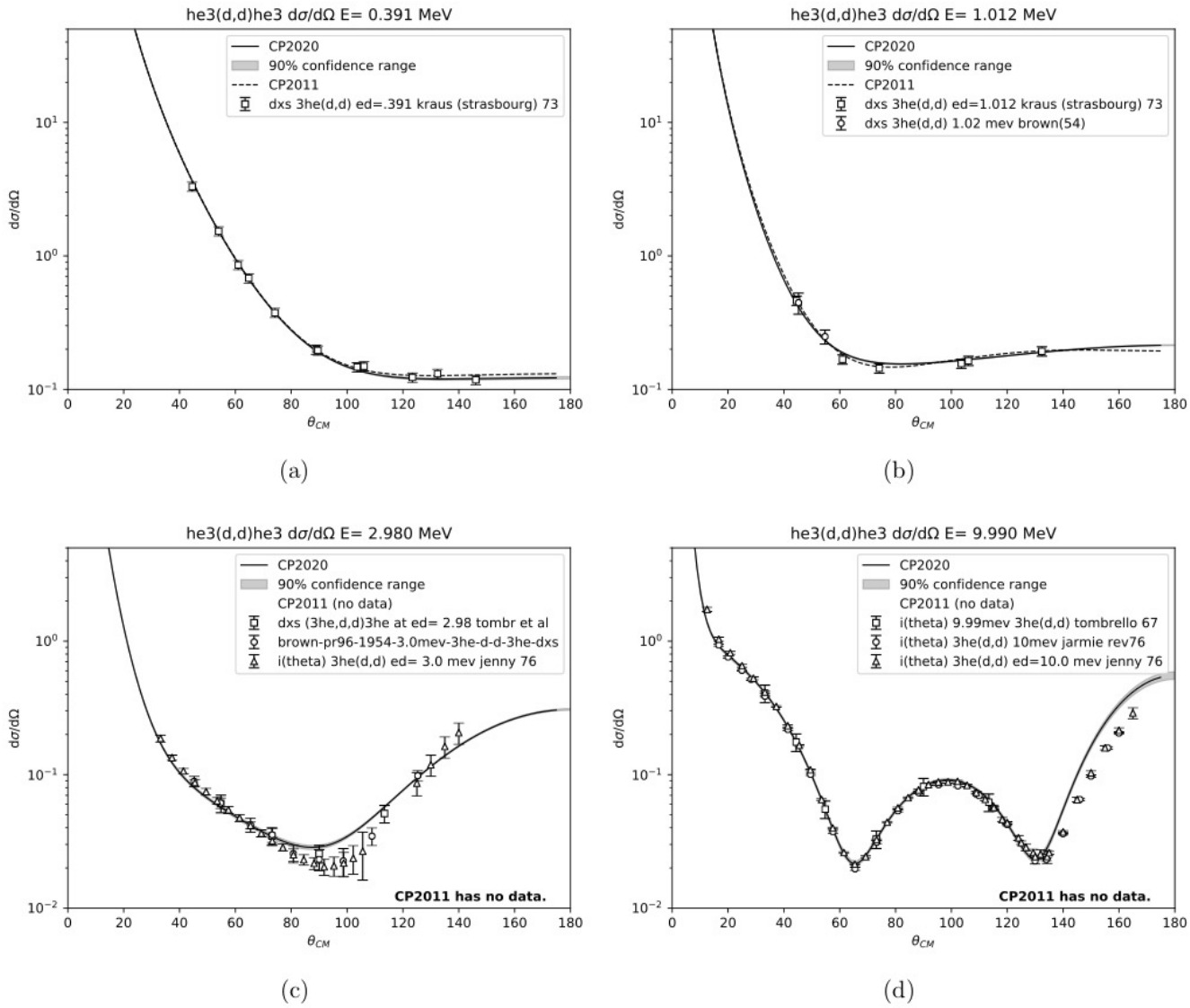
Table 120: ENDF/B-VIII.0 library, file: t-002_He_004.endf

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

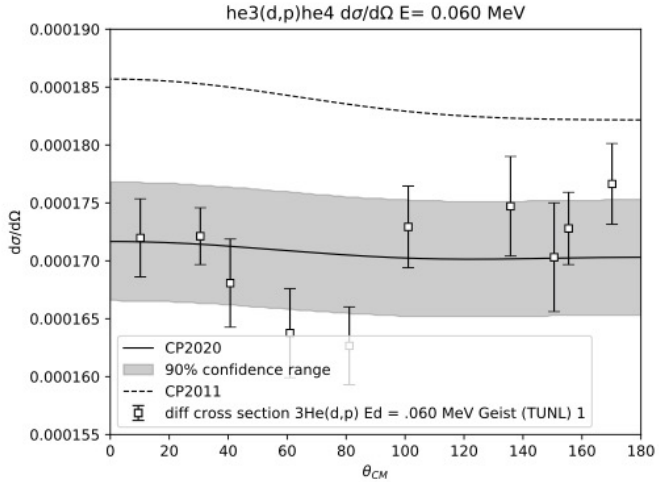
^{5}Li system evaluation

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

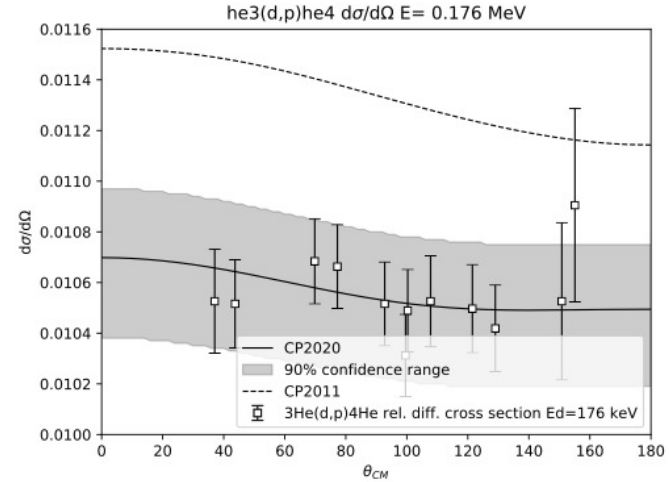


^{5}Li system evaluation

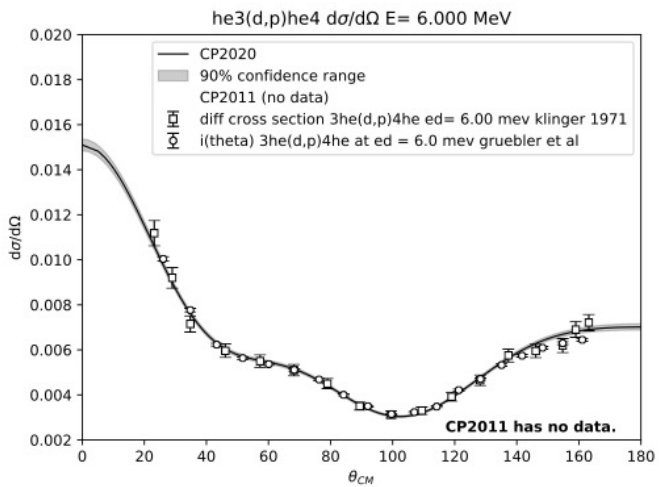
^{3}He(d,p)^{4}He



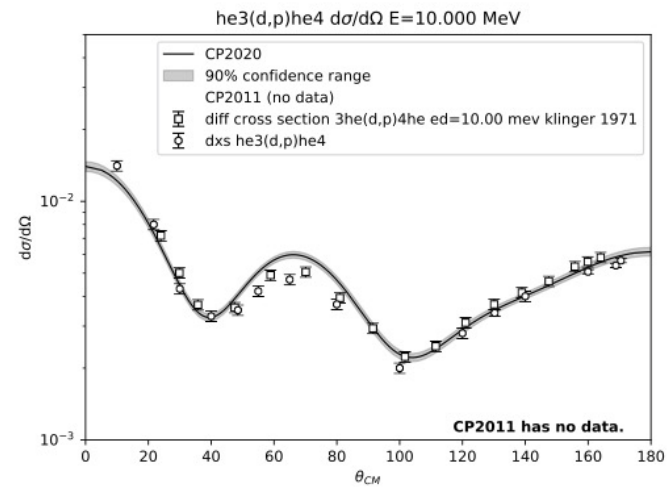
(a)



(b)



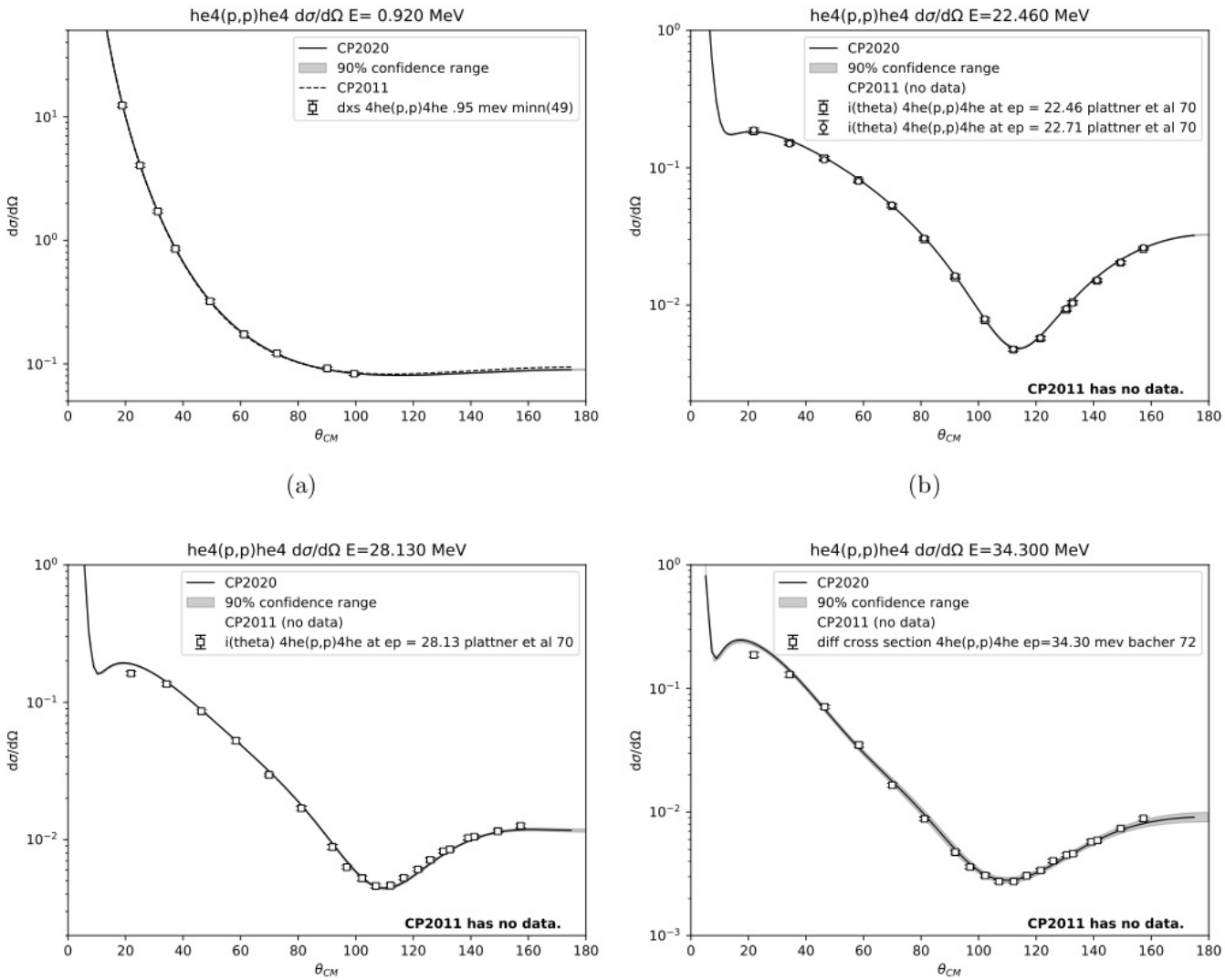
(c)



(d)

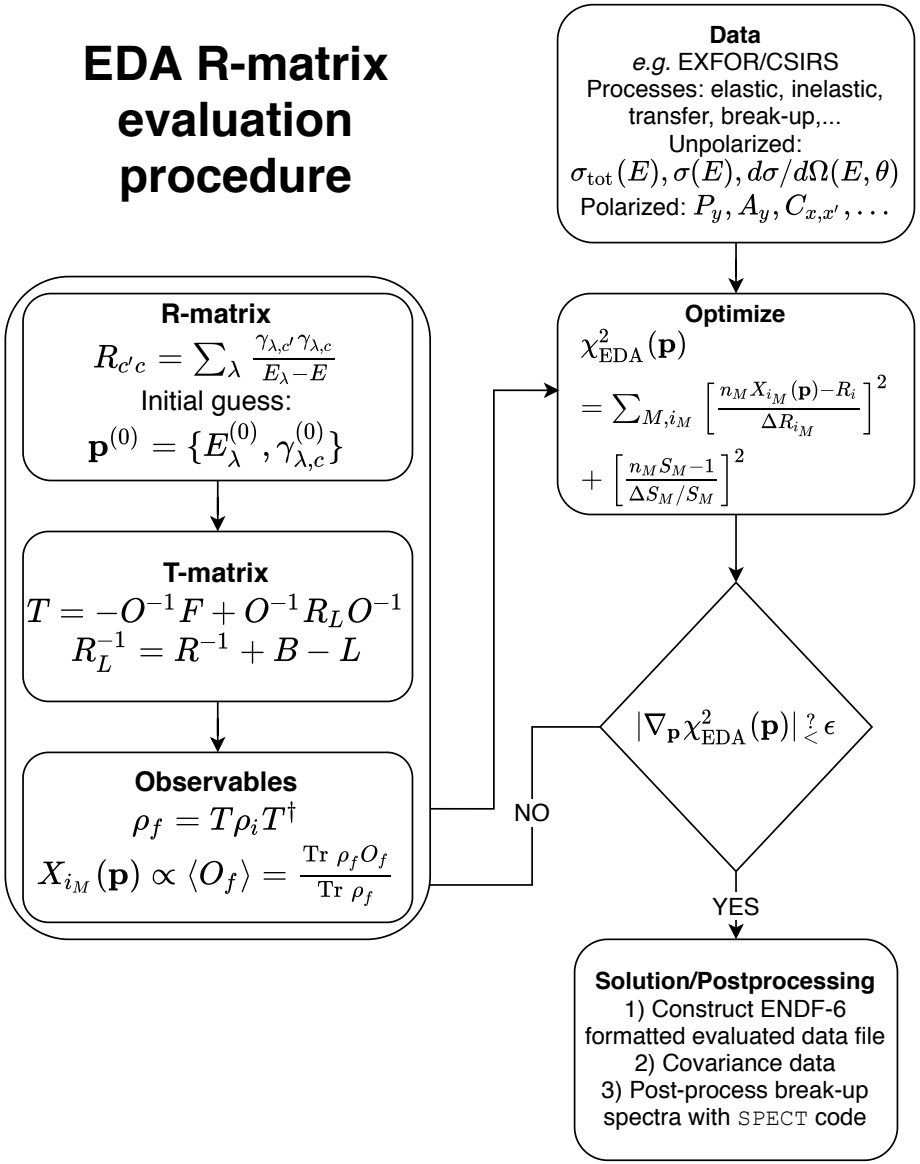
^{5}Li system evaluation

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



^{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

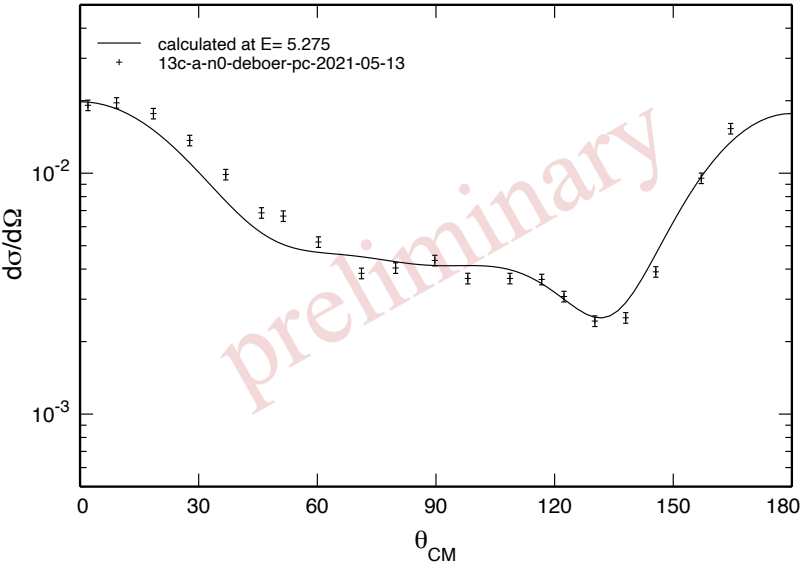
17O system channel/pars

- # 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

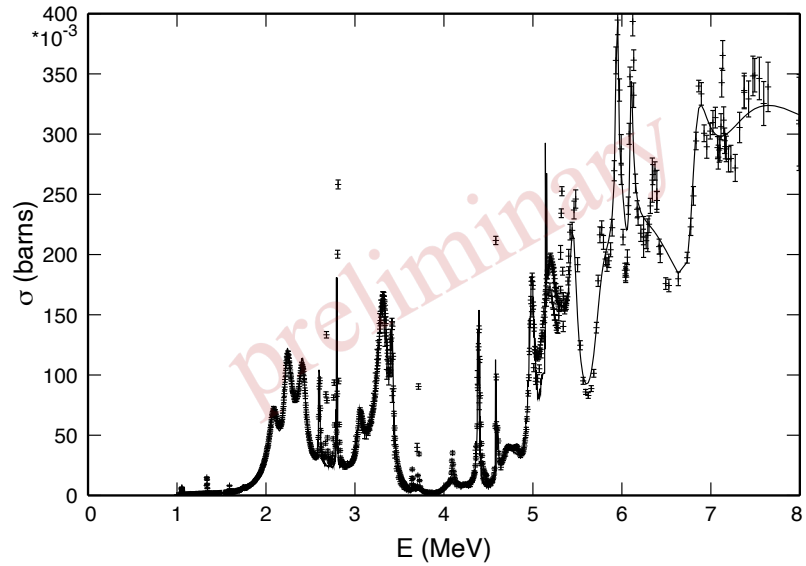
^{17}O Preliminary evaluation

Preliminary results: (α,n$_0$)

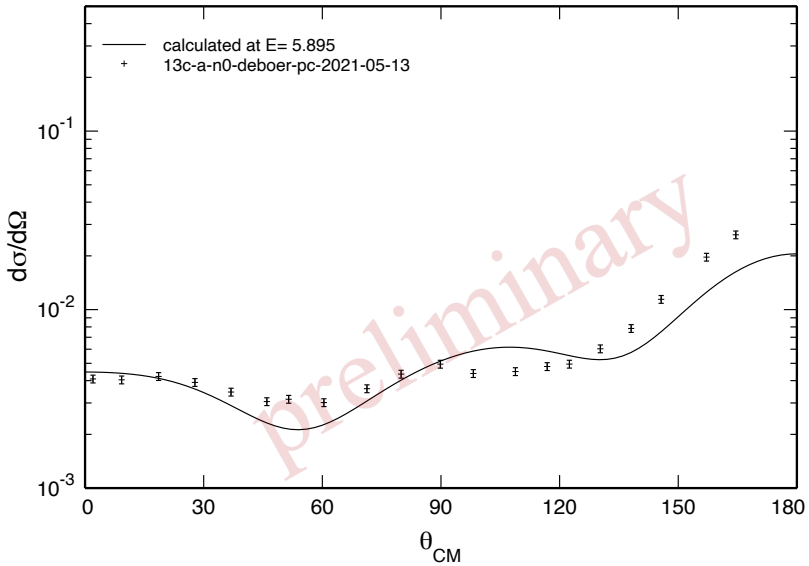
13c(4he,n)16o dσ/dΩ E= 5.275 MeV



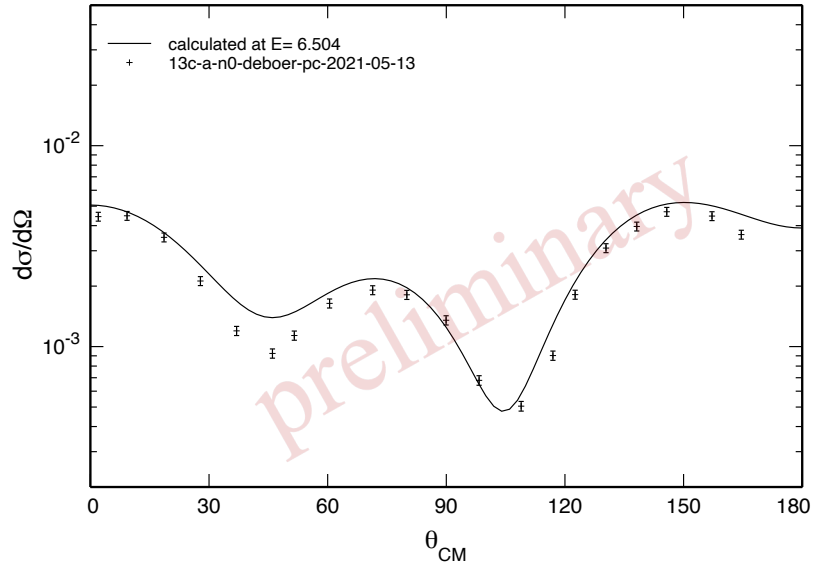
13c + 4he reaction



13c(4he,n)16o dσ/dΩ E= 5.895 MeV

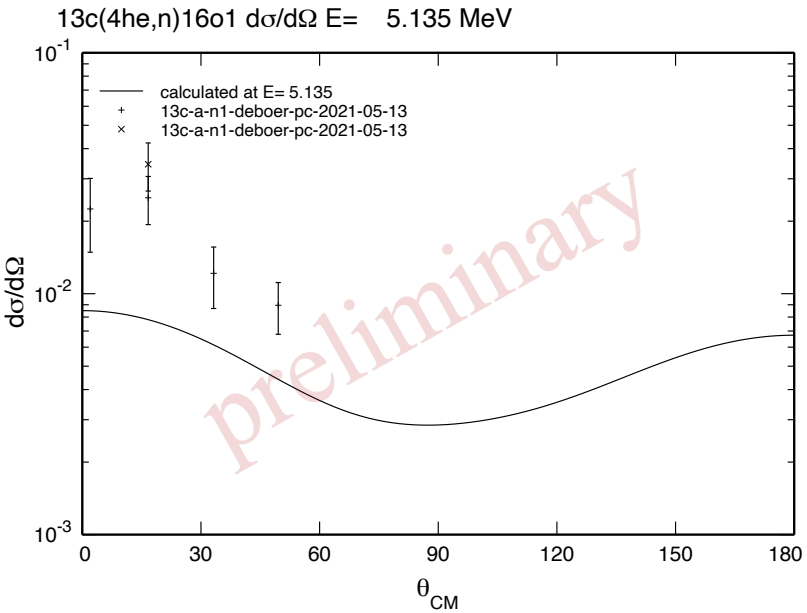


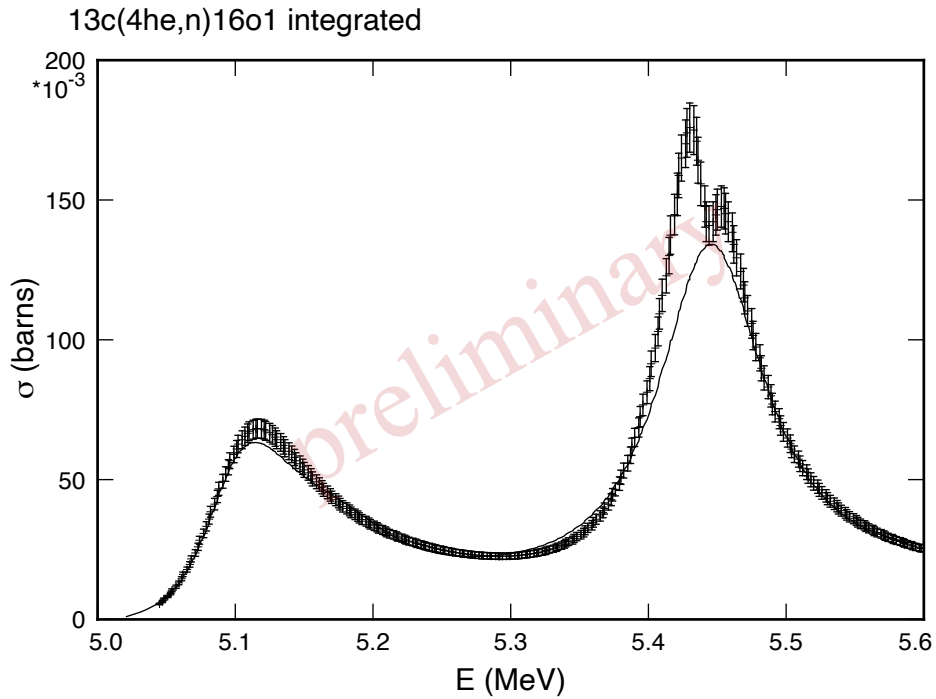
13c(4he,n)16o dσ/dΩ E= 6.504 MeV

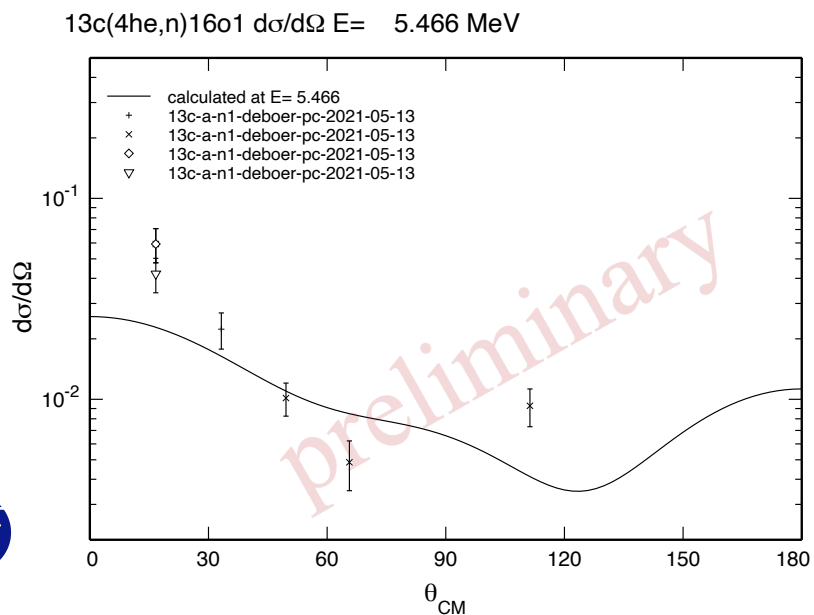


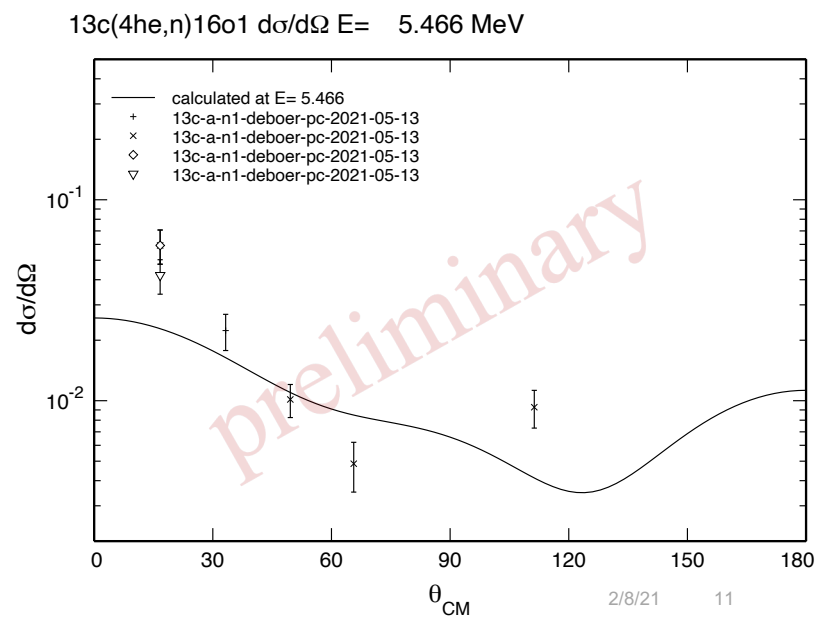
^{17}O Preliminary evaluation

Preliminary results: (α,n$_1$)



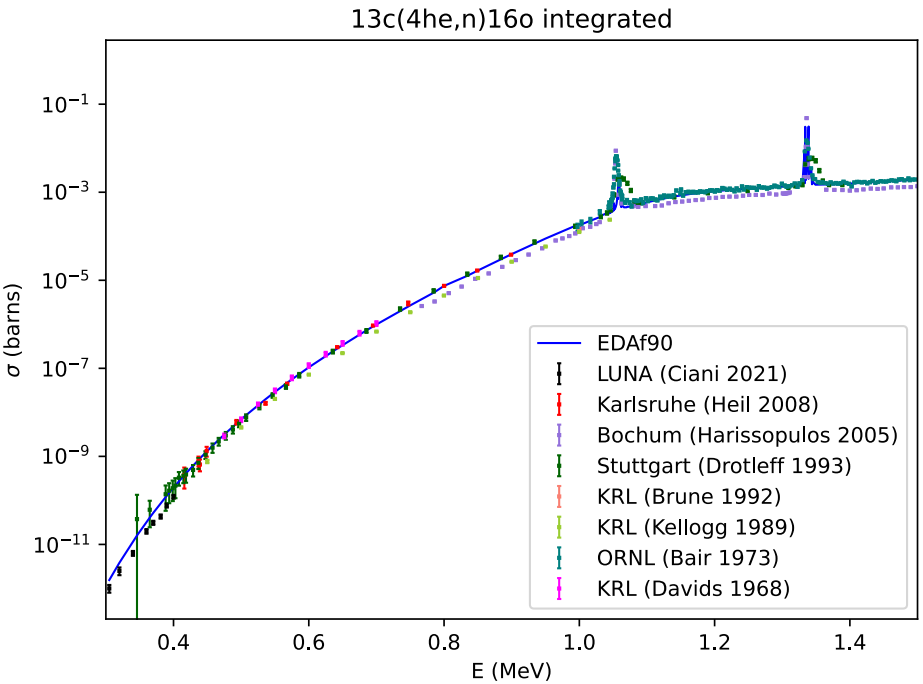


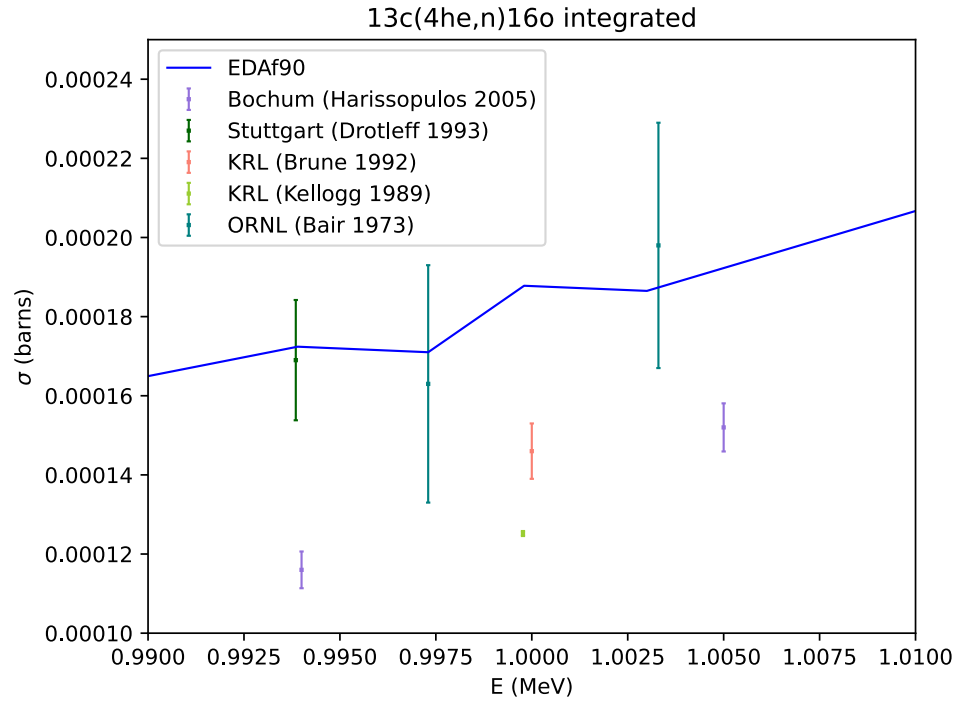




^{17}O Preliminary evaluation

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

0.3.2.5 Charged-Particle (NSUB≥10010) and Photo-Nuclear (NSUB=0) Sub-libraries

Explicit yields for all products (including photons) must be given in File 6.

Please correct me on any of this.

Conclusion

What is to be done

- `p-001_H_001.endf`
  - extension to 100 MeV of multichannel evaluation
  - punch `MF=2 LRF=7 (KRL=1)` sections
  - generate covariance sections
- `p-002_He_004.endf`
- `d-002_He_003.endf`
- `d-003_Li_006.endf`
  - ^{6}Li(d,n) now to 20 MeV
  - need to include angular distribution data
- `t-002_He_004.endf`
  - cross sections complete for all of the above
  - punch `MF=2 LRF=7 (KRL=1)` sections
  - covariance file generation needed
- `a-006_C_013.endf`
  - complete the ^{17}O system evaluation (~ 2 months)
  - punch ENDF files (`ENDFtk`)
    - `MF = 2,3,6,32,33`