Los Alamos NATIONAL LABORATORY

R-matrix evaluations of (α,n)

IAEA Technical Meeting on (alpha,n) nuclear data evaluation and data needs

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Outline

- Motivations
  - Nuclear security
  - Nonproliferation
  - Criticality safety
  - Energy
  - Basic science

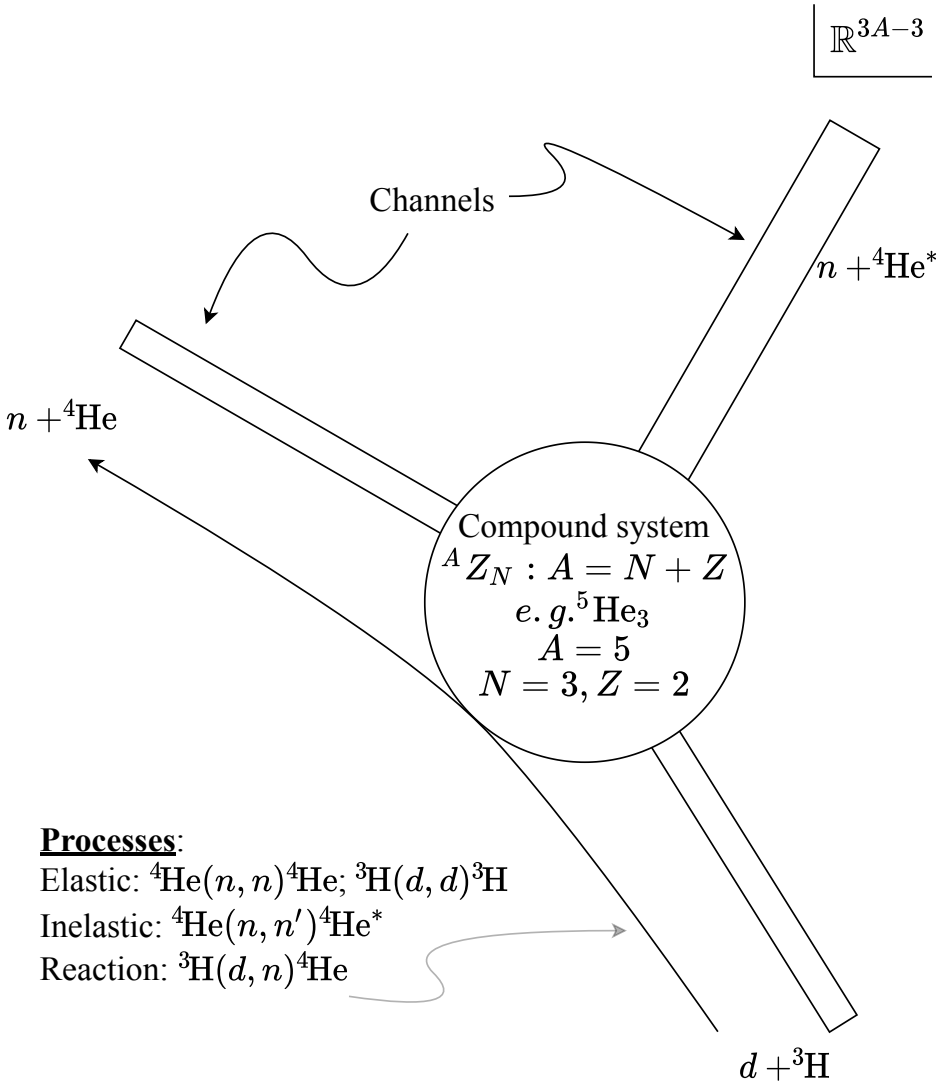
Myriad, high-impact; but we won't talk about these today

- R-matrix formalism & EDA_{f90} code
- Overview of ($\boldsymbol{\alpha}$, z) evaluations [z = *n, p, d, t, 3He,* $\boldsymbol{\alpha}$]
- ^{17}O system evaluation progress report:
  - $^{13}C(\boldsymbol{\alpha},n)$ evaluated data

Light-element R-matrix evaluation

Overview

- Main objective
  - Provide continuous (energy, energy-angle) representations of nuclear scattering and reaction cross section data
- Theoretical basis [Wigner&Eisenbud '47]
  - **Quantum theory:** unitary; causal; analytic
  - Unitarity: exp'l QA/UQ
  - Causal: ensures resonance parameter fidelity
  - Analyticity: threshold physics is right
  - Relativistic kinematics
- ***Why do "evaluation"?***
  - Correlate observables for processes coupled to particular compound system
    - ~10^5 data points (0, ~10) MeV < ~10^2 pars
  - Adjust for systematics in different experiments: *e.g.* resolution; norm; etc.
- High-fidelity data descriptions
  - ~30 compound systems
    - NN, ^{3}H, ^{3}He, ^{4}He, ^{5}He, ^{6}Li, ^{7}Li, ^{8}Li, ..., ^{17}O, ..., ^{29}Si



Light-element R-matrix evaluation

R-matrix formalism

Exterior region

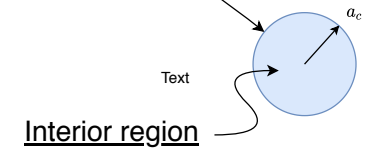
$$|\Psi_c^{(+)}\rangle = |\mathscr{I}_c\rangle - \sum_{c'} |\mathscr{O}_{c'}\rangle S_{c'c}$$

$$S_{cc'} = \delta_{cc'} + 2i\, T_{cc'}$$

$r \to \infty$

Channel surface

$\mathscr{S}_c \in \mathbb{R}^{3A-4}$



Interior region

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

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

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

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

EDA R-matrix evaluation procedure

R-matrix

$R_{c'c} = \sum_\lambda \frac{\gamma_{\lambda,c'}\gamma_{\lambda,c}}{E_\lambda - E}$

Initial guess:

$\mathbf{p}^{(0)} = \{E_\lambda^{(0)}, \gamma_{\lambda,c}^{(0)}\}$

T-matrix

$T = -O^{-1}F + O^{-1}R_L O^{-1}$

$R_L^{-1} = R^{-1} + B - L$

Observables

$\rho_f = T\rho_i T^\dagger$

$X_{i_M}(\mathbf{p}) \propto \langle O_f \rangle = \frac{\mathrm{Tr}\ \rho_f O_f}{\mathrm{Tr}\ \rho_f}$

Data

e.g. EXFOR/CSIRS

Processes: elastic, inelastic, transfer, break-up,...

Unpolarized:

$\sigma_{\mathrm{tot}}(E), \sigma(E), d\sigma/d\Omega(E,\theta)$

Polarized: $P_y, A_y, C_{x,x'}, \ldots$

Optimize

$\chi^2_{\mathrm{EDA}}(\mathbf{p})$

$= \sum_{M,i_M} \left[\frac{n_M X_{i_M}(\mathbf{p}) - R_i}{\Delta R_{i_M}}\right]^2$

$+ \left[\frac{n_M S_M - 1}{\Delta S_M / S_M}\right]^2$

$|\nabla_{\mathbf{p}} \chi^2_{\mathrm{EDA}}(\mathbf{p})| \lessgtr^{?} \epsilon$

NO

YES

Solution/Postprocessing

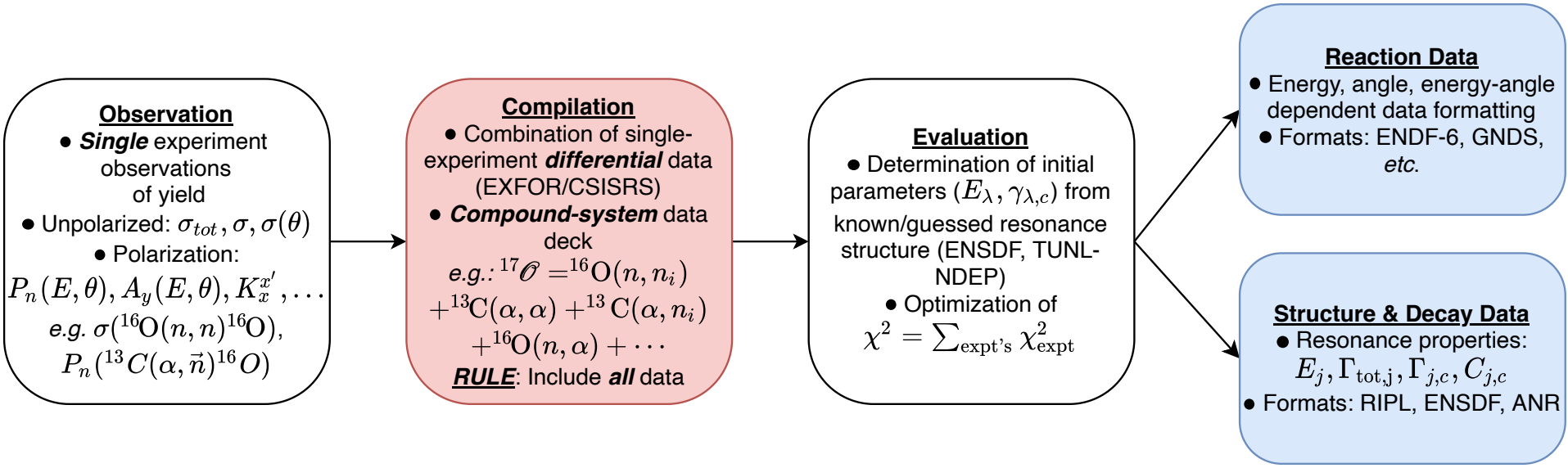
1) Construct ENDF-6 formatted evaluated data file

2) Covariance data

3) Post-process break-up spectra with `SPECT` code

Light-element R-matrix evaluation

Evaluation process



1. **EDAf90** code handles all types of data [*sources: EXFOR/CSISRS; publications; priv. comm.*]
   - total, integrated, diff'l, polarized, unpolarized; neutron- and CP-induced: (*n,z*), (*p,z*), (*d,z*), (*t,z*), (***α***,*z*), ...
2. **EDAf90** handles all the compound system (e.g.: $^{17}\mathbf{O}$) 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

Light-element evaluations

Overview

- All compound systems A<20 (and a few above)
- Recent work in 2020/2021 (*Charged-particle transport libraries* ***FY20 L2 Milestone***)

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	TENDL19
$h(^{3}\mathrm{He})$				VIII.0	VIII.0	VIII.0	TENDL19
α					VIII.0	TENDL19	TENDL19

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

^{17}O Preliminary evaluation

Preliminary results

- Configuration: channels, R-matrix parameters
- Observed data in `data` deck
  - Channels: (n,n_0), (n,n_2), (α,n_0), (α,n_1), (α,n)
  - Types: total, integrated, differential, *polarization* $[A_y, P_n]$

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

- New data
  - Ciani *et al.* (2021) (α,n_0)
  - Brandenburg & Meisel (2021) (α,n)
  - Febbraro, DeBoer *et al.* (2020) (α,n_0), (α,n_1)

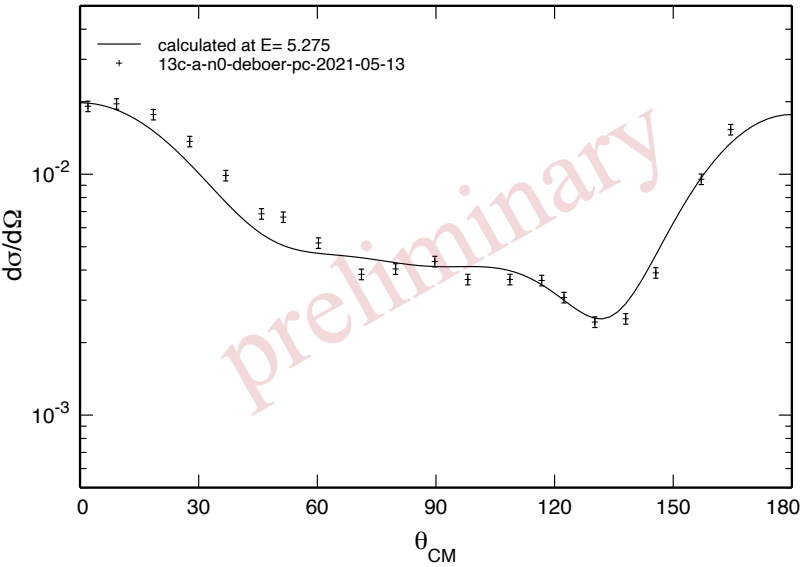
17O system channel/pars

- # 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

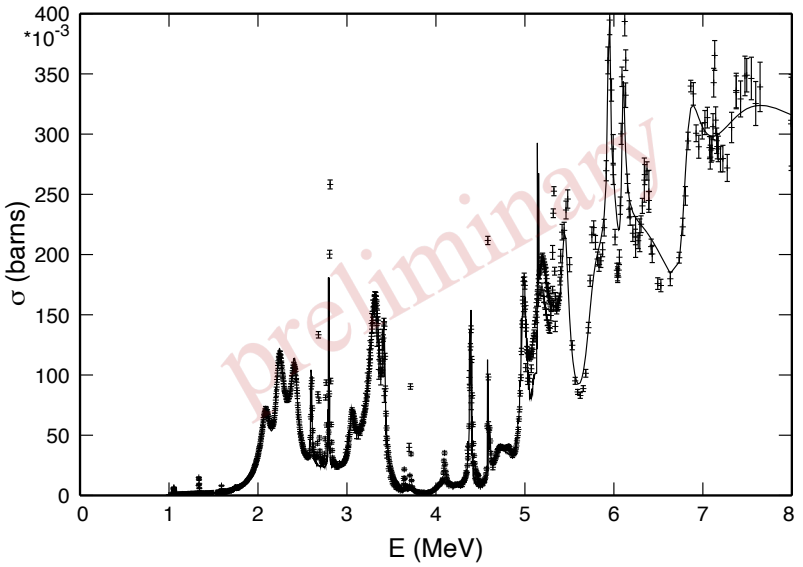
^{17}O Preliminary evaluation

Preliminary results: (α,n_0)

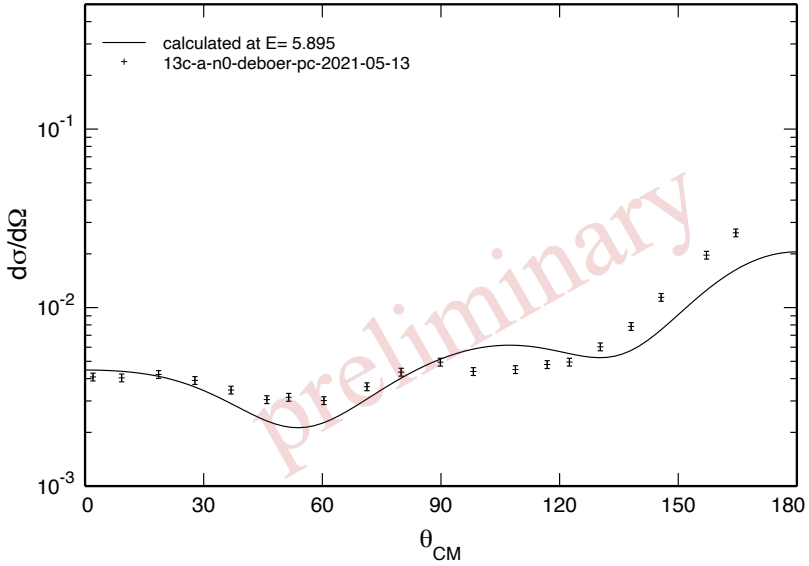
13c(4he,n)16o dσ/dΩ E= 5.275 MeV



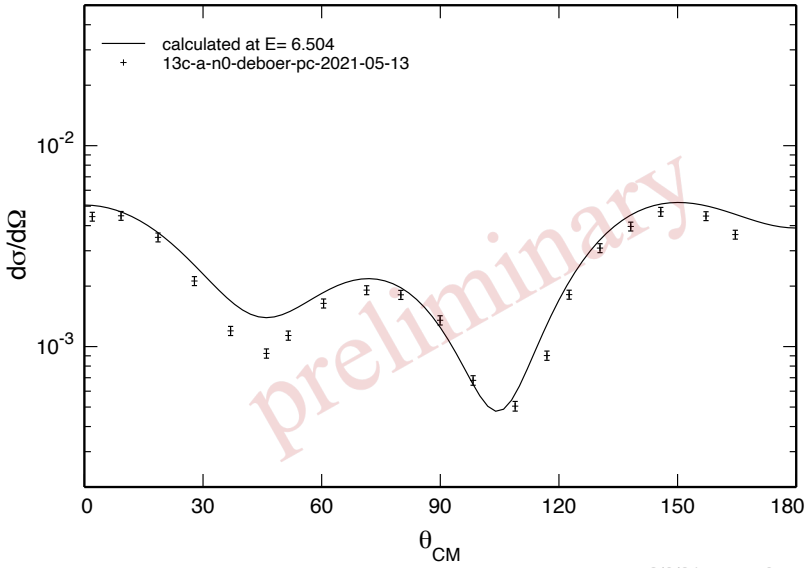
13c + 4he reaction



13c(4he,n)16o dσ/dΩ E= 5.895 MeV

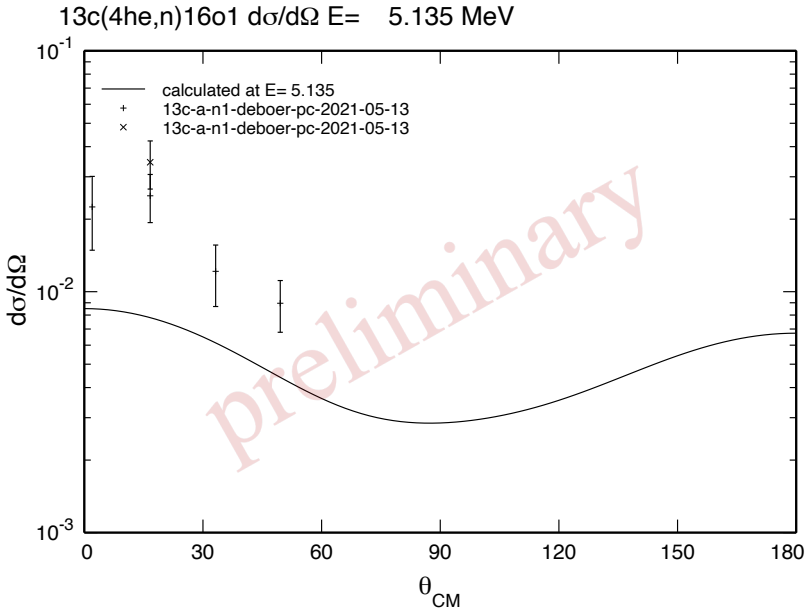


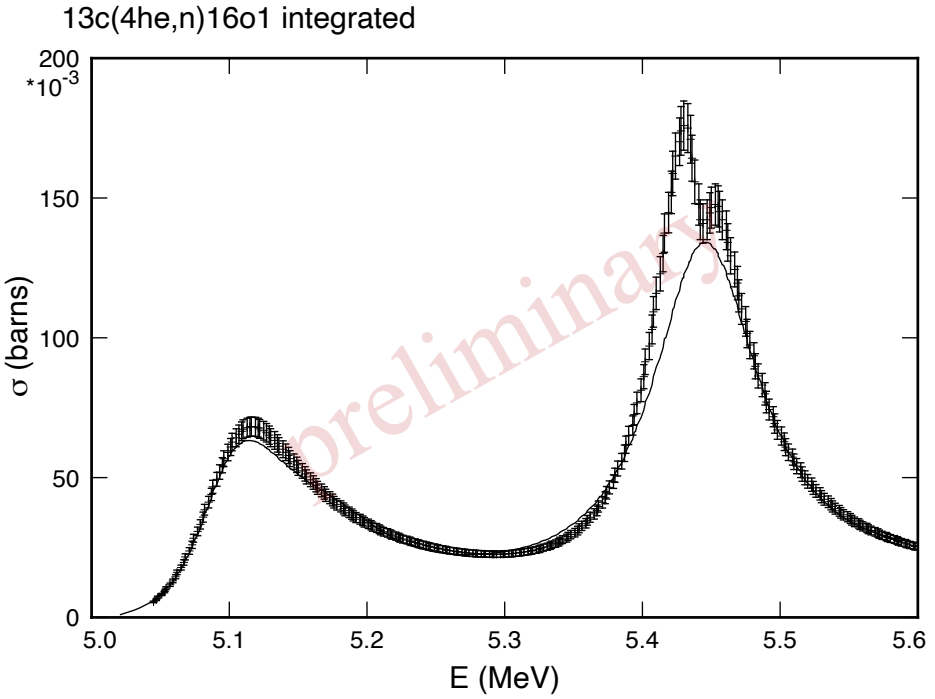
13c(4he,n)16o dσ/dΩ E= 6.504 MeV

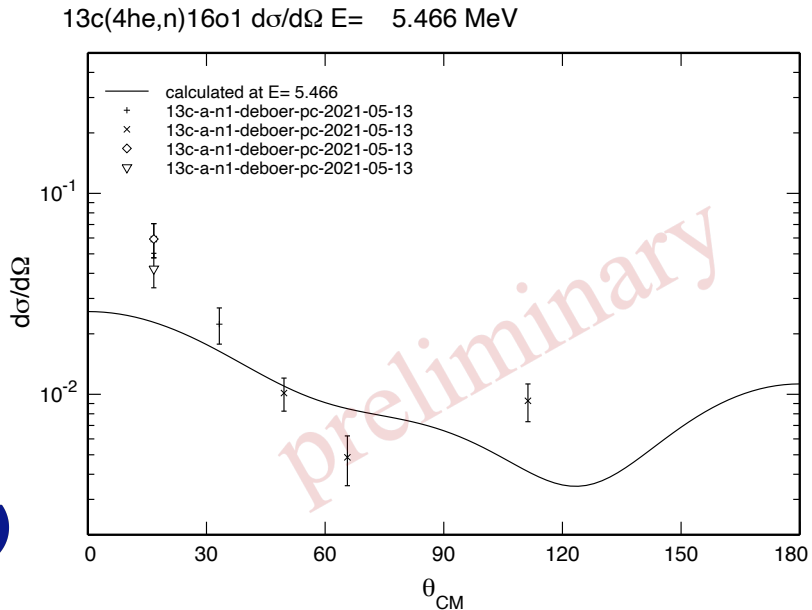


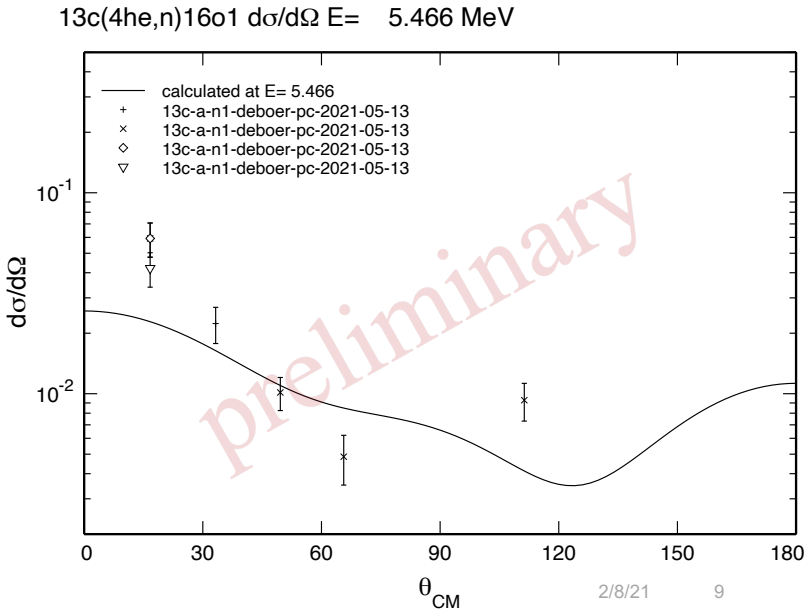
^{17}O Preliminary evaluation

Preliminary results: (α,n_1)



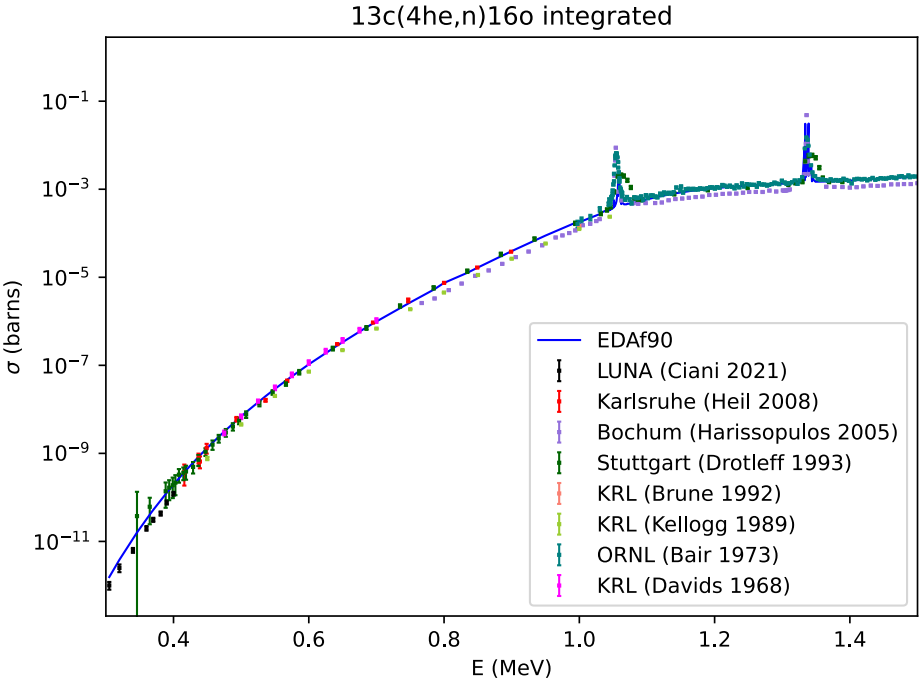


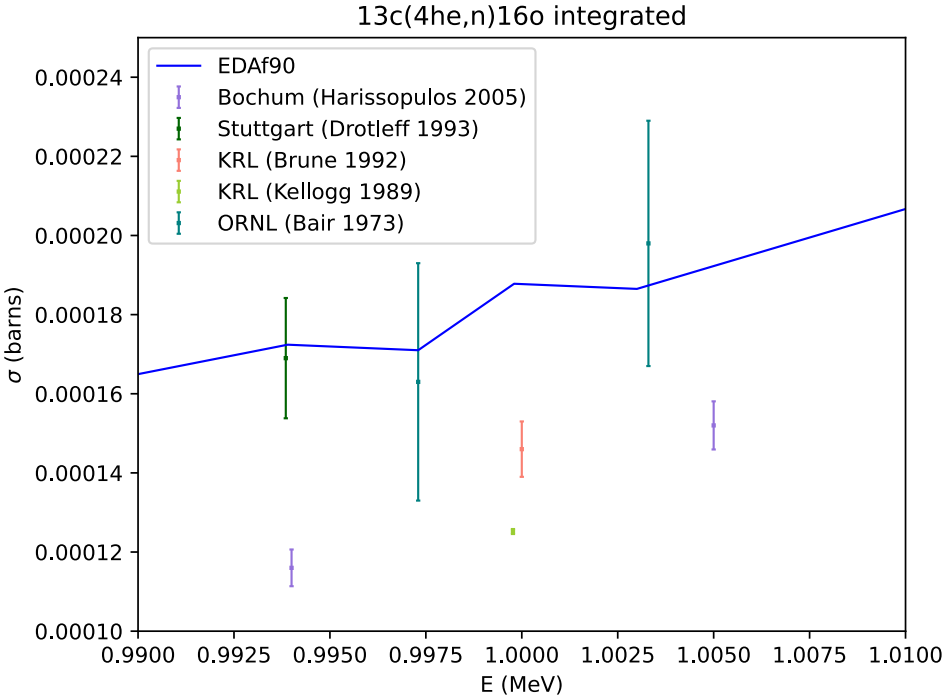




^{17}O Preliminary evaluation

Preliminary results: low energy



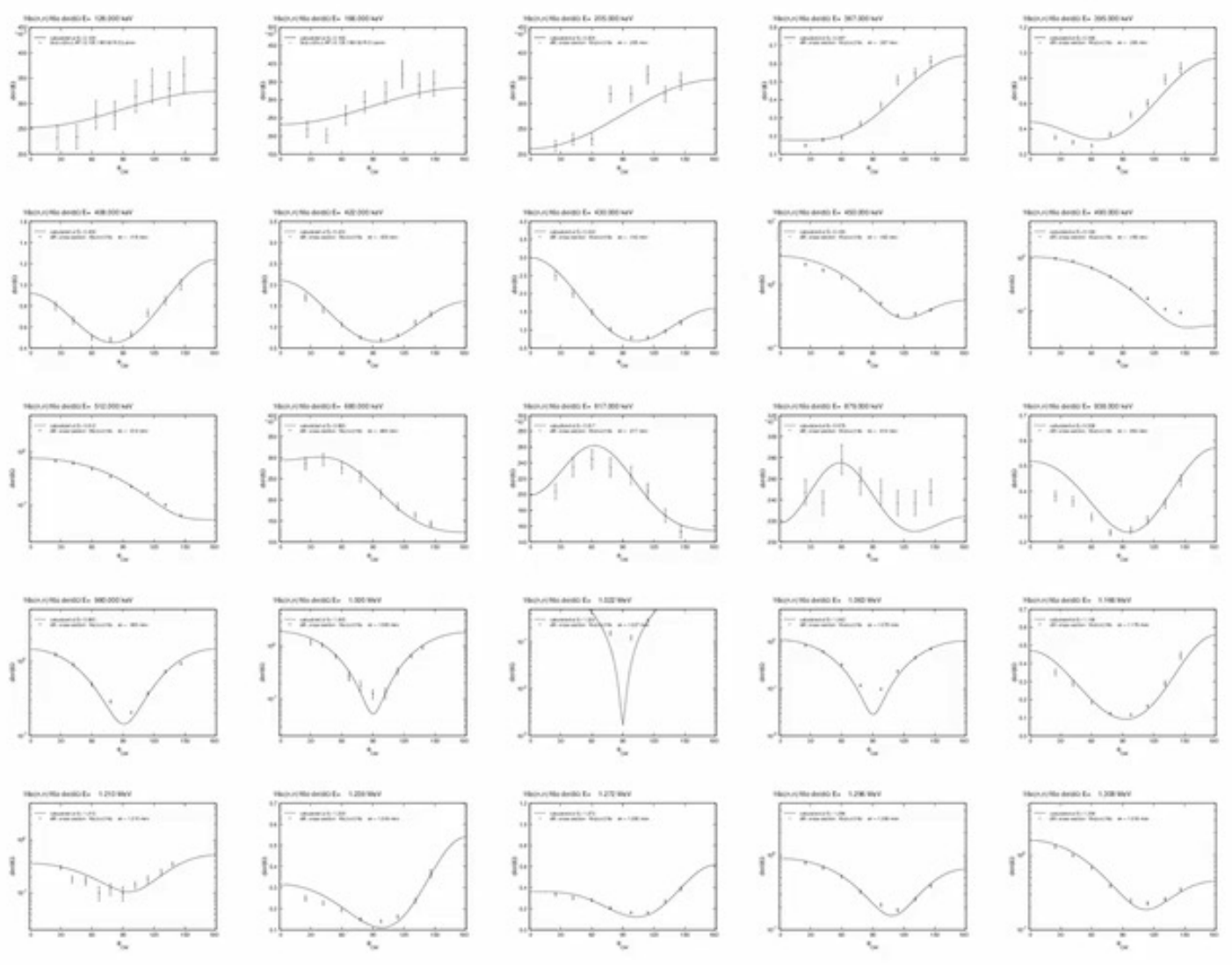


Experiment	E_α [MeV]	$\sigma_{(\alpha,n)}$ [μb]	1.000 MeV
KRL (Brune 1992)	1.0000	146(7)	146(7)
ORNL (Bair 1973)	1.0033	198(3)	179(4)
Stuttgart (Drotleff 1993)	0.9939	169(2)	187(3)
Bochum (Harissopulos 2005)	0.994	116(5)	136(7)
Bochum (Harissopulos 2005)	1.005	152(6)	–
KRL (Kellogg 1989)	0.9998	125(6)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

^{17}O Preliminary evaluation scope

Preliminary results



Conclusion

- Main task in CY2021
  - complete ^{17}O evaluation for $E_n \sim 10$ MeV
    - Check for additional low-energy (< 7 MeV) data
    - Incorporate (n,α) data
    - Check consistency of included data with normalization/energy-shift factors
    - Provide low-energy extrapolation for (α,n)
    - Publish R-matrix parameters (level energies, reduced widths, channel radii and BC)
- Ongoing work on (α,n) evaluations
  - 2→2 body reactions
    - $^{3}H(\alpha,n)^{6}Li$ [$E_\alpha \sim 11$ MeV]
    - $^{7}Li(\alpha,n)^{10}B$ [$E_\alpha \sim 4.5$ MeV]
    - $^{6}He^{*}(\alpha,n)^{9}Be$ [Q>0]
    - $^{8}Li^{*}(\alpha,n)^{11}B$ [Q>0] (no ^{12}B system evaluation yet)
    - $^{9}Be(\alpha,n)^{12}C$ [Q>0]
- Future capabilities
  - Larger A > 20 compound systems
    - $^{19}F(\alpha,n)^{22}Na$(2.3 MeV); $^{14}N(\alpha,n)^{17}F$(6 MeV); $^{15}N(\alpha,n)^{18}F$(8 MeV)
  - 2→3 body reactions
    - $^{13}C(\alpha,n\gamma)^{16}O$
    - $^{2}H(\alpha,np)^{4}He$ [$E_\alpha \sim 6$ MeV]
    - $^{9}Be(\alpha,n)3^{4}He$ [$E_\alpha \sim 2.2$ MeV]