Extending the Be7 evaluation to include Li6 exited states and also capture to Be7 excited state

Review for INDEN-LE

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R-matrix Framework

Contribution of He3+He4 to ENDF/B-VIII.1 :

1. The calculations should be made using $B_c = -L_c$
2. Background levels at 20 MeV (in this basis), 1 per spin group
3. Maximum orbital angular momentum $L_{ah}^{max} = 4$, $L_{pLi}^{max} = 1$, and all the spin groups up to $J^{\pi} = 9/2^{\pm}$.
4. R-matrix channel radii determined as a = 1.4 [fm] $(A_1^{1/3}+A_2^{1/3})$ and the same for all channels within a particle pair.
5. No capture channels yet
6. Most emphasis on h+α cross sections up to about 12 MeV: the data.

- Present Strategy:
  - Include Li6_e1 excited state (3+ resonance)
  - Include capture channels (either by Reich-Moore, or as primary channels)
  - Consider further data up to 20 MeV.
  - Consider for p+Li6 evaluation ?

Previous Experiment Data for the Be7 system

- Use *.dat files from de Boer to make 'Test3' calculation
- Still need to specify properties of these files:

projectile	ejectile	residual	file	sys-error	stat-error	norm	group	splitnorms	lab	abserr	scale	filedir	eshift	ecalib	splitshifts
h	h	0	Barnard_aa.dat	5	3	1	E	FALSE	TRUE	TRUE	b	Expt5/	0	0	FALSE
p	h	0	Elwyn_pa.dat	9	-1	1	A	FALSE	TRUE	TRUE	b	Expt5/	0	0	FALSE
p	p	0	Fasoli_pp.dat	-1	1.5	1	E	TRUE	TRUE	TRUE	b	Expt5/	0	0	FALSE
p	p	0	Harrison_pp0.dat	-1	2	2.2	A	FALSE	TRUE	TRUE	b	Expt5/	0	0	FALSE
p	p	1	Harrison_pp1.dat	-1	-1	0.2	A	FALSE	TRUE	TRUE	b	Expt5/	0	0	FALSE
p	h	0	Lin_pa.dat	10	-1	1	A	TRUE	TRUE	TRUE	b	Expt5/	0	0	FALSE
p	p	0	McCray_pp.dat	5	-1	1	E	TRUE	TRUE	TRUE	b	Expt5/	0	0	FALSE
h	h	0	Mohr_aa.dat	-1	5	1	A	TRUE	TRUE	TRUE	b	Expt5/	0	0	FALSE
h	h	0	Spiger-A1094004-lab_aa.dat	1.5	-1	1	E	TRUE	TRUE	TRUE	b	Expt5/	0	0.02	TRUE
h	p	0	Spiger-cm_ap0.dat	1.5	-1	1	A	TRUE	FALSE	TRUE	mb	Expt5/	0	0	FALSE
h	h	0	Tombrello_aa.dat	5	-1	1	E	FALSE	TRUE	TRUE	b	Expt5/	0	0.02	TRUE
a	h	15	LIMIT	4.001506	3.01550116										
p	Li6	2.79	LIMIT	1.008665	6.01347726										

Correct some data:

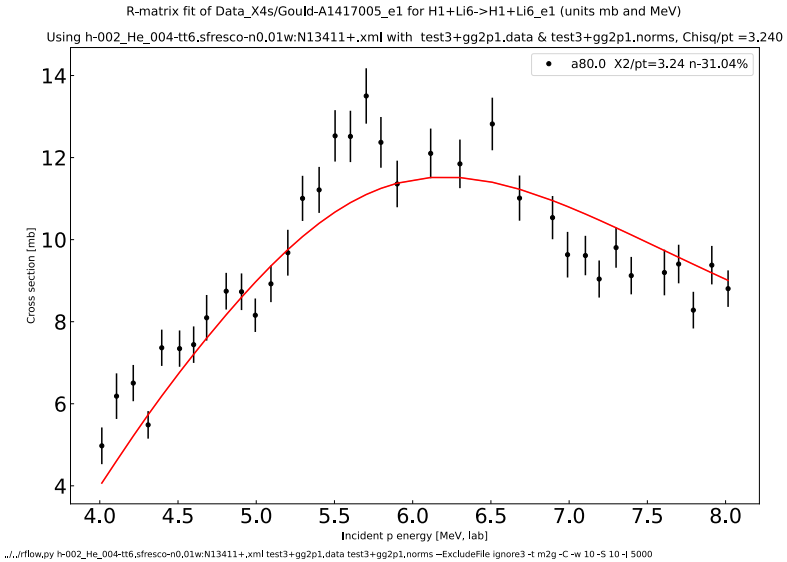
1. The 9.106 MeV point at 36.999 deg in the Spiger_aa data is not extracted from the plots properly.
2. The Tombrello_aa data (not A1039 but A1295) should have a constant discretization error of 0.5 mb/sr added in quadrature to the per-cent errors for the A1295002 data.
3. The points in Elwyn_pa at Ep = 2.277, 2.377, and 2.476 MeV were not plotted correctly, if checked by Legendre data.

Include also excited state Li6_e1 (3^+ resonance)

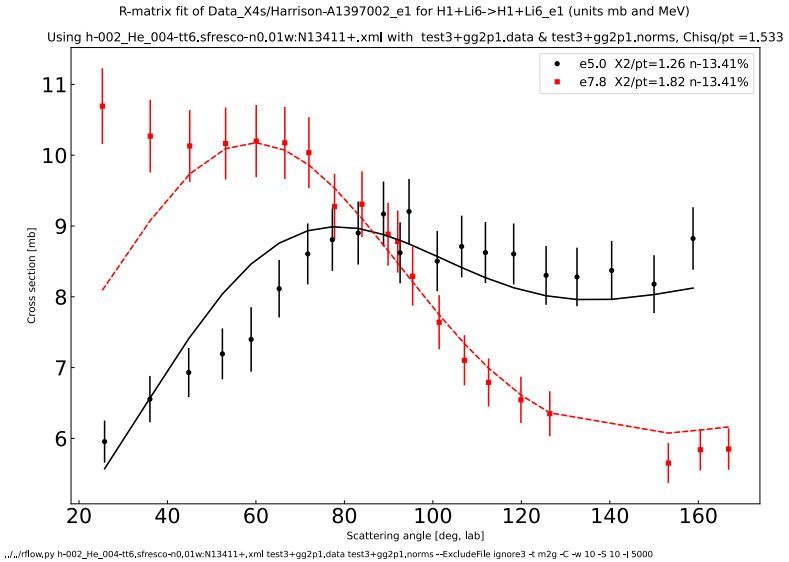
projectile	ejectile	residual	file	sys-error	stat-error	norm	splitnorms	lab	abserr	scale	Npoints	EXFOR
H1	H1	1	Gould-A1417005_e1.dat	5	5	1	FALSE	FALSE	TRUE	mb	35	A1417005
H1	H1	1	Harrison-A1397002_e1.dat	5	5	1	FALSE	FALSE	TRUE	mb	41	A1397002
H1	H1	1	Laurat-A1508006_e1.dat	5	5	1	FALSE	TRUE	TRUE	mb	18	A1508006
H1	H1	1	Laurat-A1508007_e1.dat	5	5	1	FALSE	FALSE	TRUE	mb	50	A1508007
H1	H1	1	Merchez-A1415002_e1.dat	5	5	1	FALSE	FALSE	TRUE	mb	54	A1415002
He3	H1	1	Spiger-A1094008_e1.dat	5	5	1	FALSE	TRUE	TRUE	mb	58	A1094008
He3	H1	1	Spiger-A1094009_e1.dat	5	5	1	FALSE	TRUE	TRUE	mb	44	A1094009
He3	H1	1	Spiger-A1094010_e1.dat	5	5	1	FALSE	TRUE	TRUE	mb	58	A1094010

- Combine with ‘test3’ data
- Refit
- Ferdinand: https://github.com/LLNL/ferdinand
- Rflow: https://github.com/LLNL/Rflow
  (uses tensorflow with cpus or gpus)

Fitting excited state Li6_e1 (slide 1)

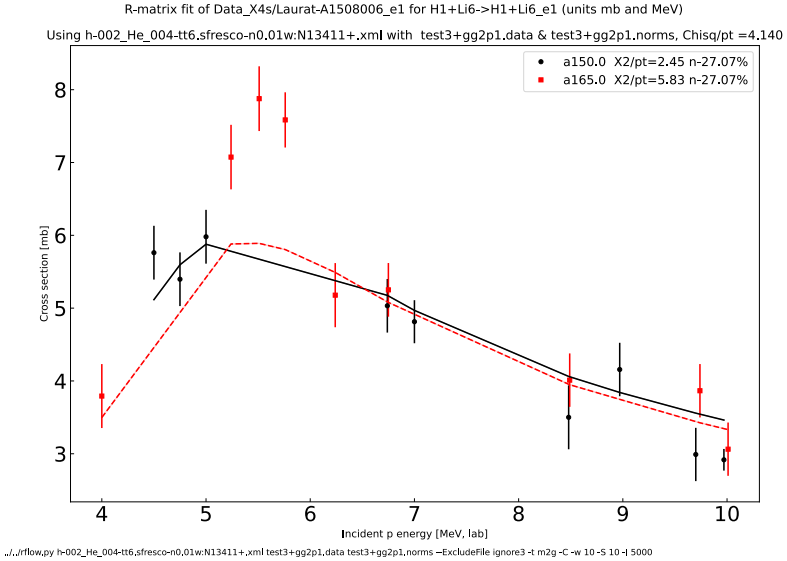


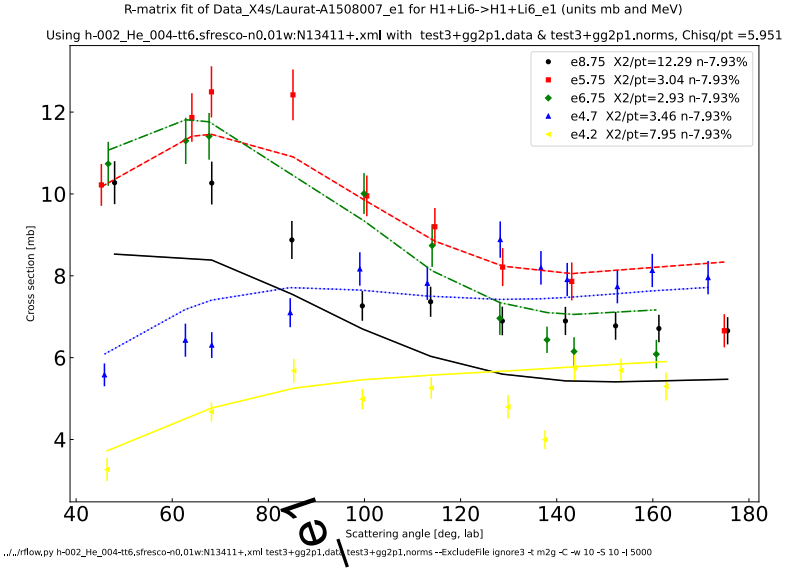
Gould-A1417005_e1



Harrison-A1397002_e1

Fitting excited state Li6_e1 (slide 2)

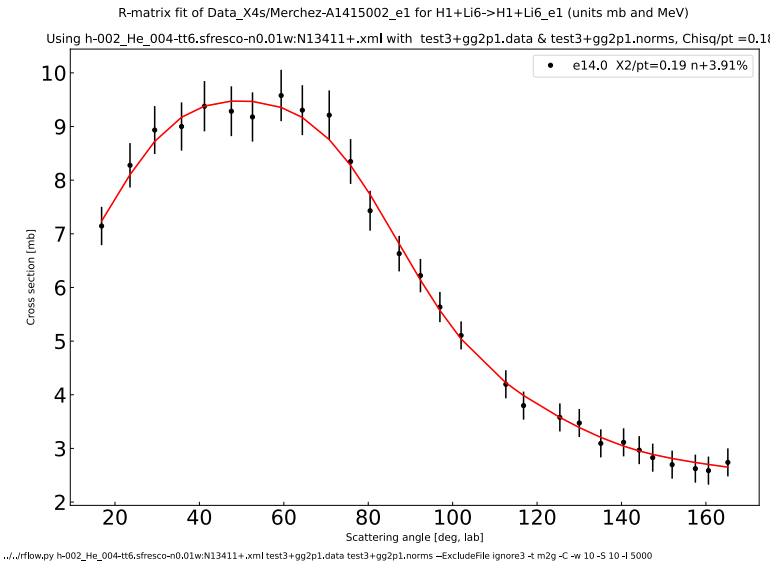


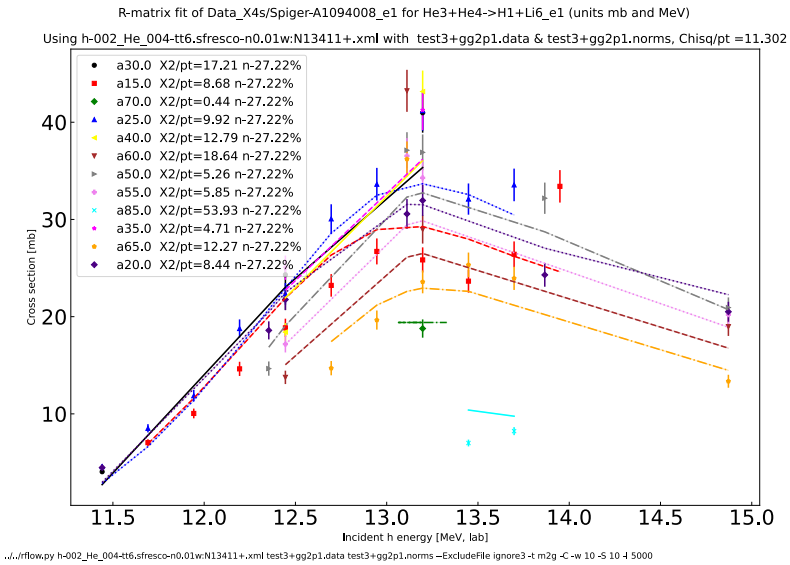


Laurat-A1508006_e1

Laurat-A1508007_e1

Fitting excited state Li6_e1 (slide 3)

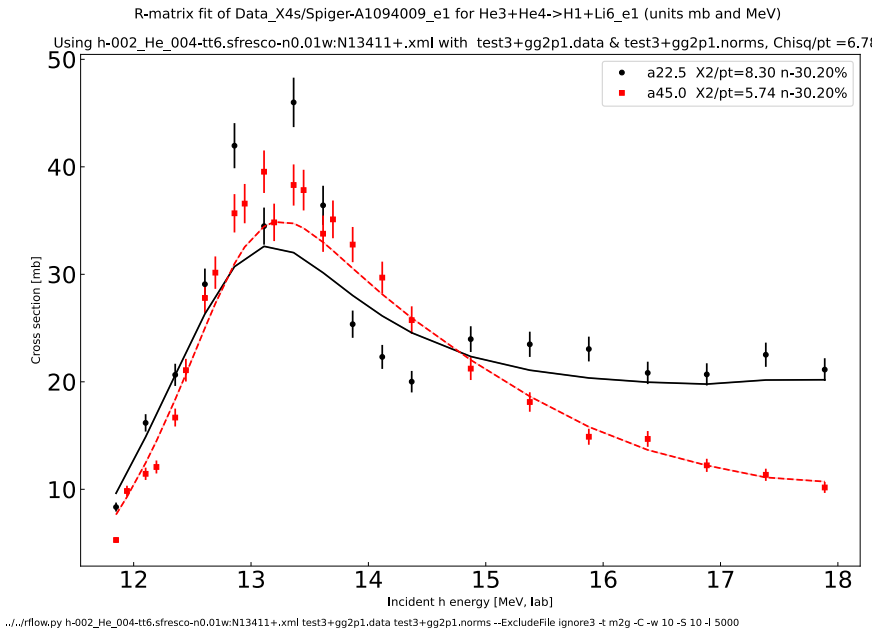




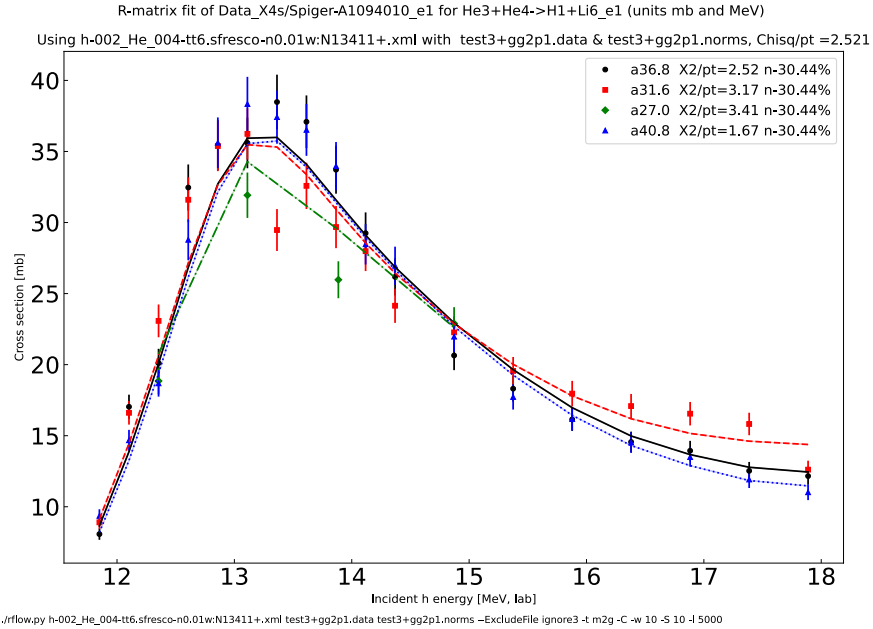
Merchez-A1415002_e1

Spiger-A1094008_e1

Fitting excited state Li6_e1 (slide 4)



Spiger-A1094009_e1



Spiger-A1094010_e1

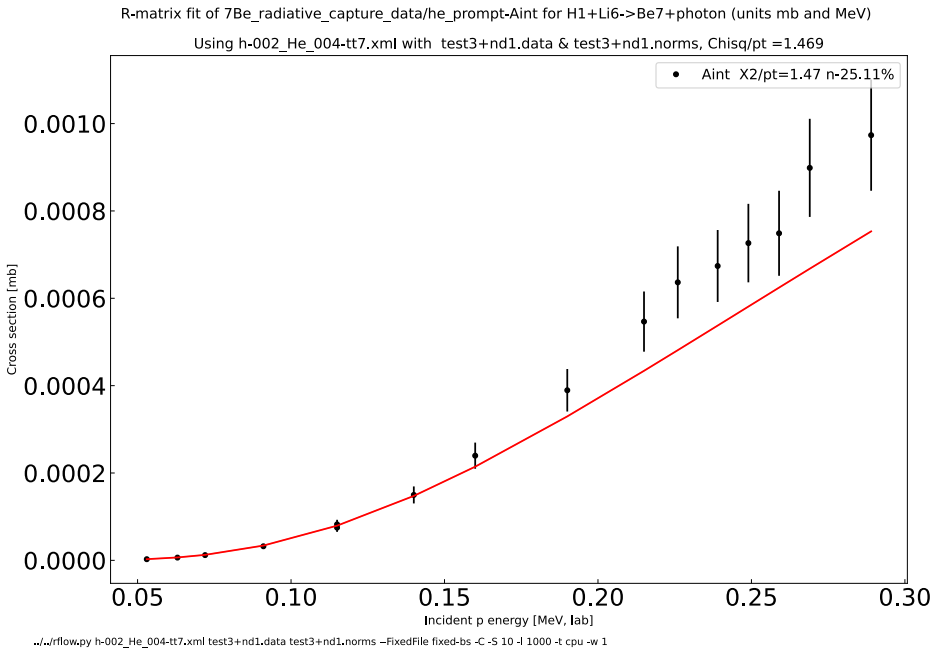
Discussion

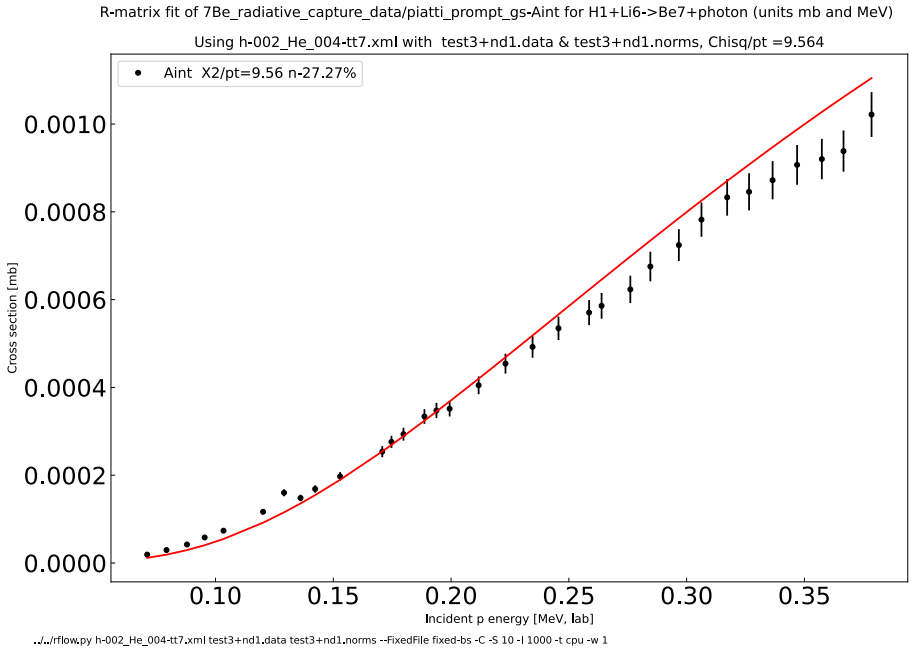
- Should be included
- Add to candidate for ENDF/B-VIII.1-beta3 ?

Include capture channels (a) primary gammas as two-body channels

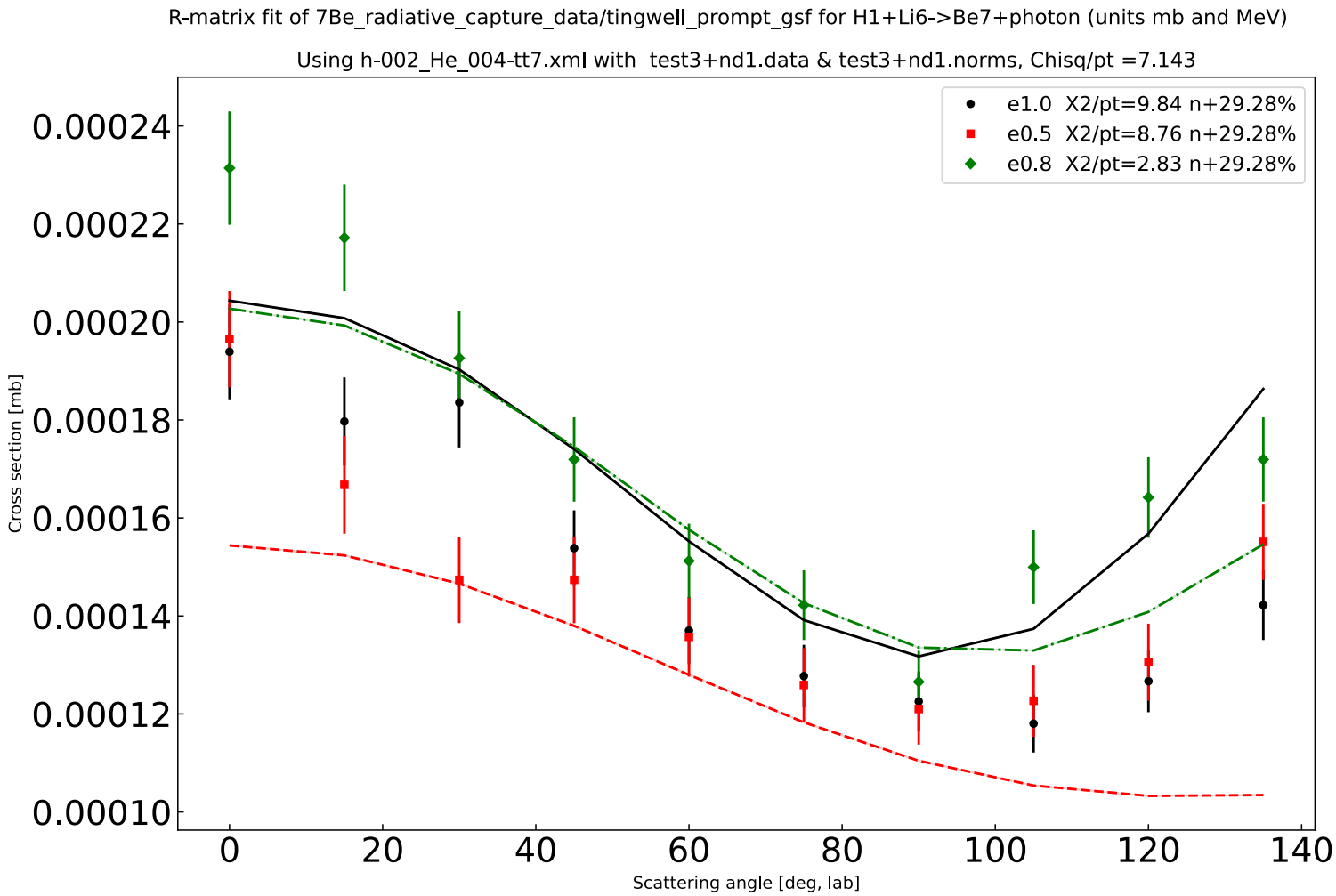
- Two channels:
  - Production of Be7 ground state
  - Production of Be7_e1 excited state
    - (Decay of excited state given by branching ratios. Here: 100% to gs)
- Easier in GNDS format:
  - <reaction label="Be7 + photon" >
  - <reaction label="Be7_e1 + photon" >
- Harder in ENDF:
  - need to use MT=900 and 901
  - I proposed this at Mini-CSEWG in April 2023.

Fitted primary gammas: (p,γ)Be7 (gs) Angle-integrated

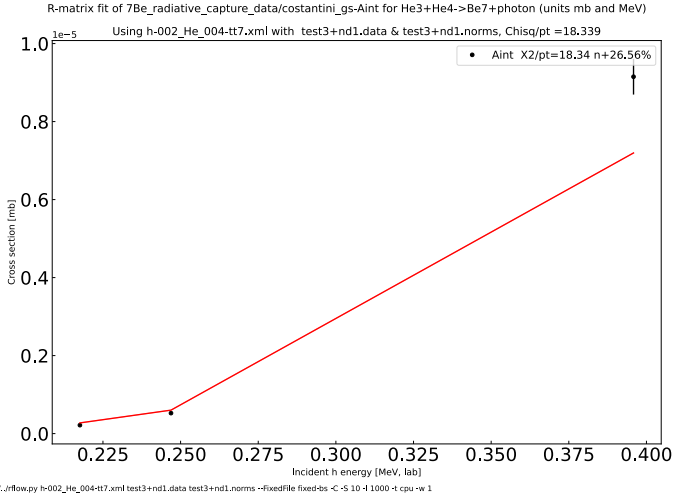


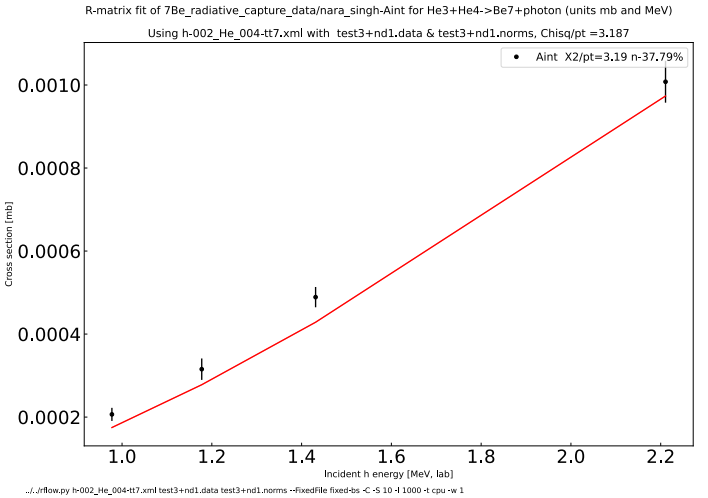


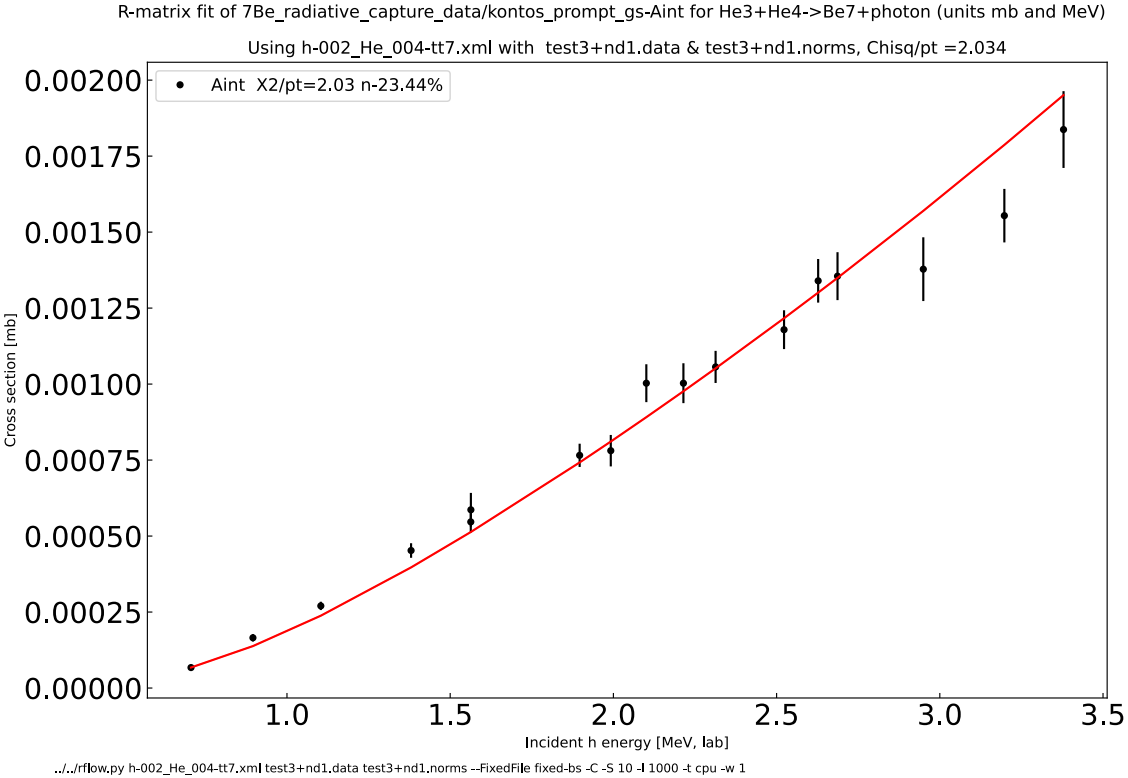
Fitted primary gammas: (p,γ)Be7 (gs) angular distributions



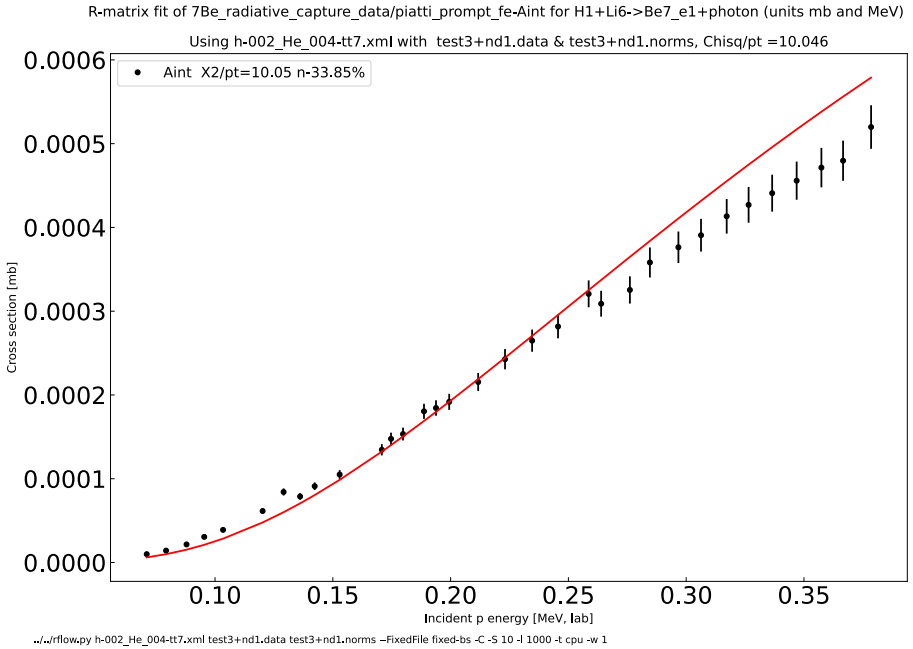
Fitted primary gammas: (h,γ)Be7 (gs)

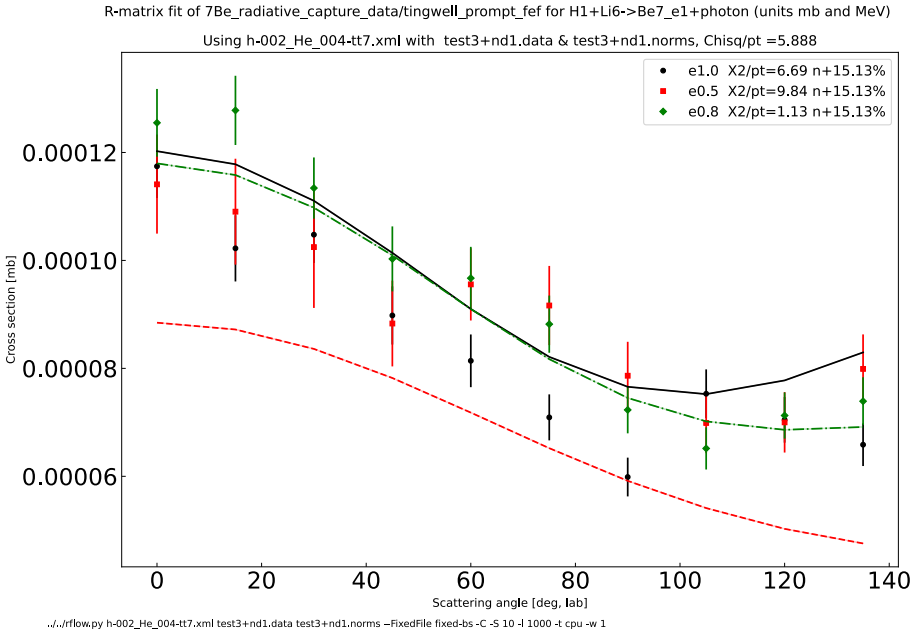






Fitted primary gammas: (p,γ)Be7_e1 (fe)

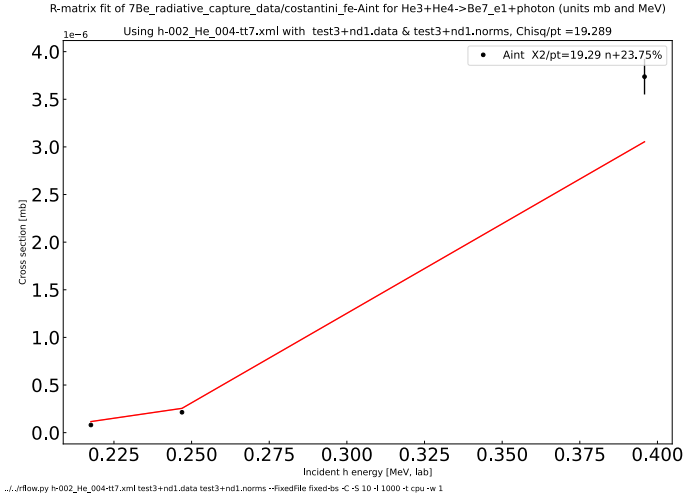


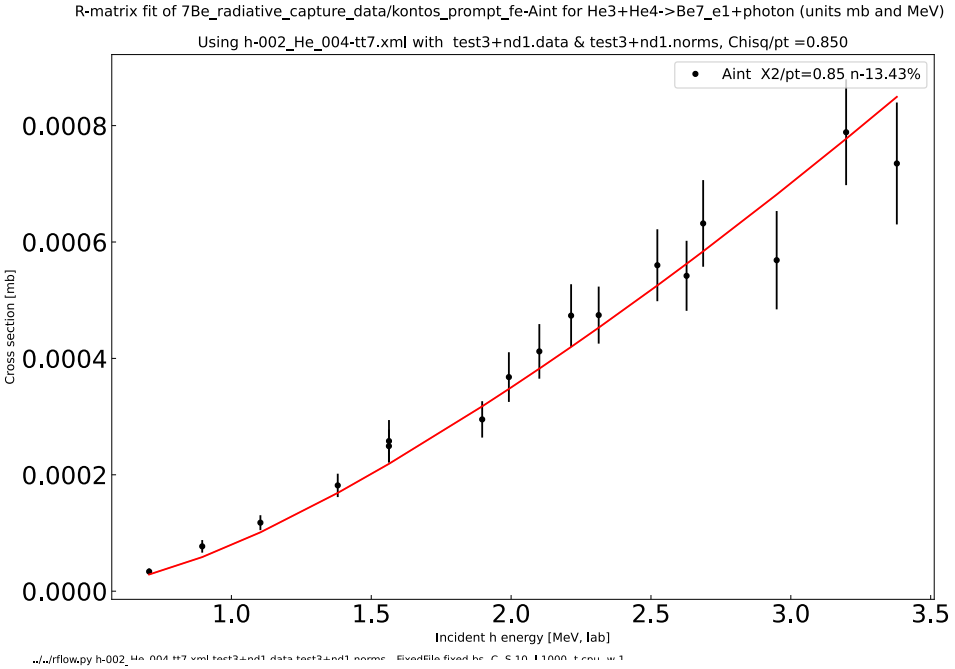


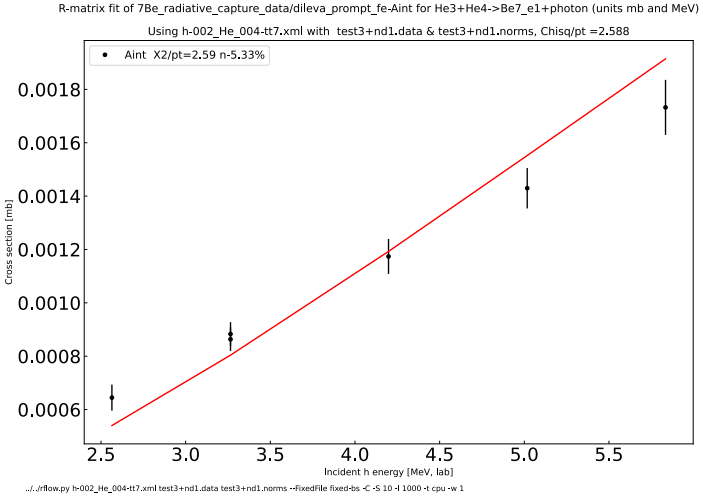
Piatti (angle-integrated)

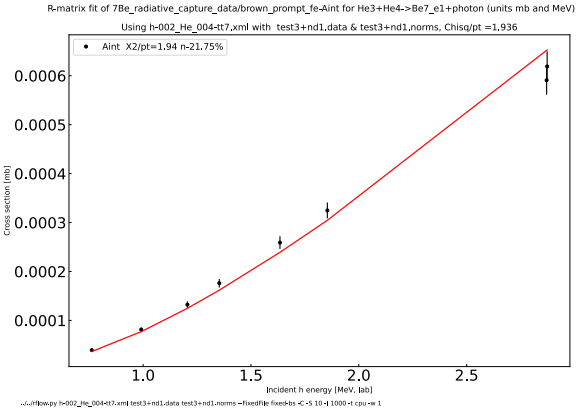
Tingwell (angular distributions)

Fitted primary gammas: (h,γ)Be7_e1 (fe)









Data renormalization factors from fit

- h-g/costantini_gs: +26.6 %
- h-g/kontos_prompt_gs -23.4 %
- h-g/nara_singh -37.8 %
- p-g/he_prompt -25.1 %
- p-g/piatti_prompt_gs -27.3 %
- p-g/tingwell_prompt_gs : +29.1 %

- h-g1/brown_prompt_fe -21.8 %
- h-g1/costantini_fe +23.8 %
- h-g1/dileva_prompt_fe -5.3 %
- h-g1/kontos_prompt_fe -13.4 %
- p-g1/piatti_prompt_fe -33.8 %
- p-g1/tingwell_prompt_fe +15.1 %

nd1

Data renormalization factors from fit Then with Rg = 50 fm, 100 fm

— h-g/costantini_gs:	+26.6 %	+14.4%	+25.2 %
— h-g/kontos_prompt_gs	-23.4 %	-5%	-23.6 %
— h-g/nara_singh	-37.8 %	-23.7%	-39.5 %
— p-g/he_prompt	-25.1 %	-19.4%	-21.9 %
— p-g/piatti_prompt_gs	-27.3 %	-18.9 %	-25.5 %
— p-g/tingwell_prompt_gs :	+29.1 %	+25.5%	+32.2 %
— h-g1/brown_prompt_fe	-21.8 %	-6.94 %	-9.4 %
— h-g1/costantini_fe	+23.8 %	+12.6 %	+18.4 %
— h-g1/dileva_prompt_fe	-5.3 %	-0.6 %	-0.62 %
— h-g1/kontos_prompt_fe	-13.4 %	+2.4 %	-1.71%
— p-g1/piatti_prompt_fe	-33.8 %	-24.4 %	-27.5%
— p-g1/tingwell_prompt_fe	+15.1 %	-10.7 %	+11.4 %

nd2

Data renormalization factors from fit (no He)
Then with Rg = 50 fm, 100 fm

— h-g/costantini_gs:	+26.6 %	+14.8%	+30.6 %
— h-g/kontos_prompt_gs	-23.4 %	-2.2%	-5.42 %
— h-g/nara_singh	-37.8 %	-21.6%	-23.3 %
— p-g/piatti_prompt_gs	-27.3 %	-23.8 %	-25.5 %
— p-g/tingwell_prompt_gs :	+29.1 %	+17.5%	+32.2 %
— h-g1/brown_prompt_fe	-21.8 %	-9.4 %	-9.4 %
— h-g1/costantini_fe	+23.8 %	+9.5 %	+18.4 %
— h-g1/dileva_prompt_fe	-5.3 %	-2.5 %	-0.62 %
— h-g1/kontos_prompt_fe	-13.4 %	+0.2 %	-1.71%
— p-g1/piatti_prompt_fe	-33.8 %	-23.2 %	-27.5%
— p-g1/tingwell_prompt_fe	+15.1 %	-13.5 %	+11.4 %

nd3 (but not Rg=100 fm

Data renormalization factors from fit (no He, Piatti, Tingwell). Then with Rg = 50 fm, 100 fm

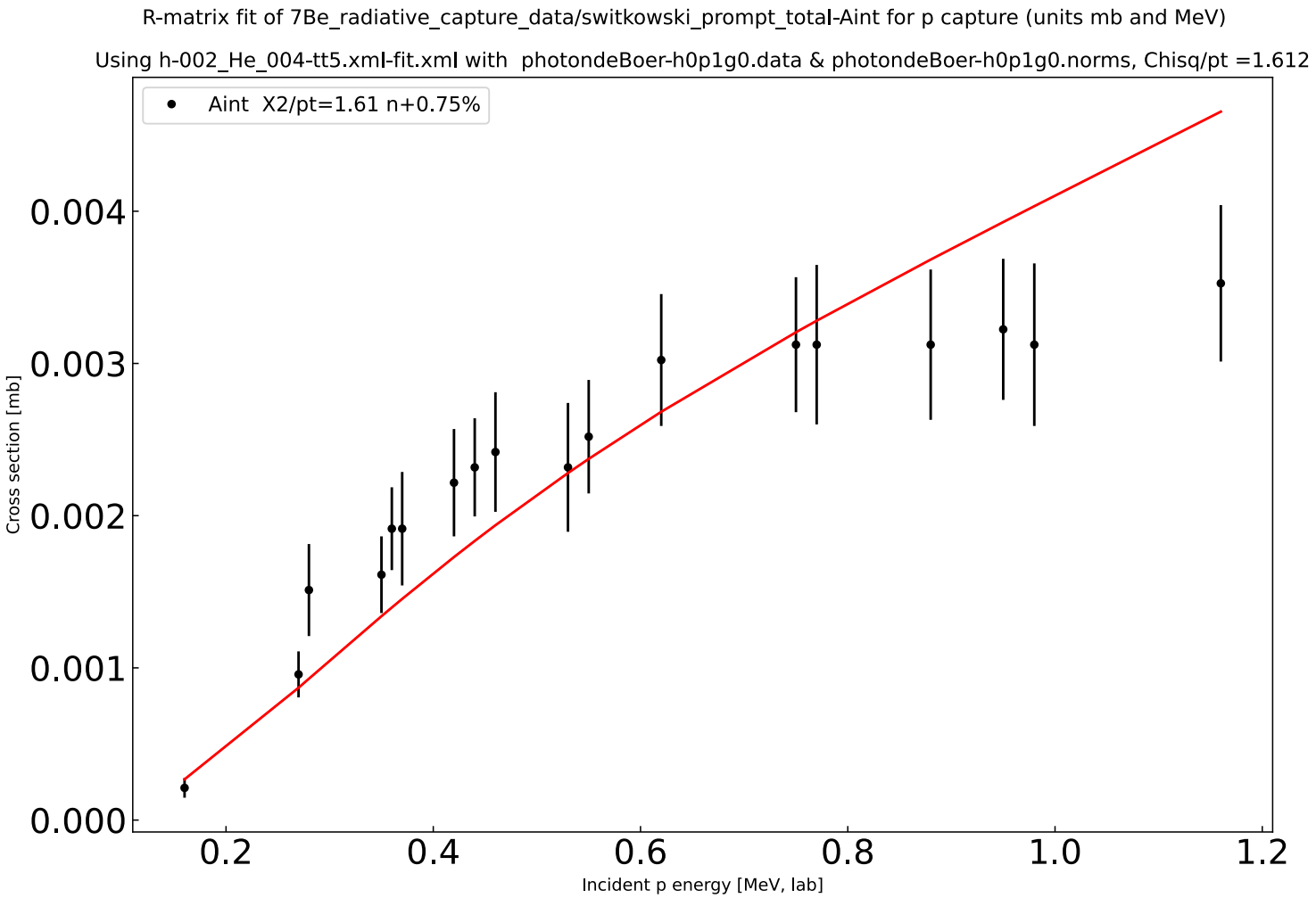
— h-g/costantini_gs:	+26.6 %	+18.2%	+30.6 %
— h-g/kontos_prompt_gs	-23.4 %	-9.03%	-5.42 %
— h-g/nara_singh	-37.8 %	-29.4%	-23.3 %
— p-g/piatti_prompt_gs	-27.3 %	-23.8 %	-25.5 %
— p-g/tingwell_prompt_gs :	+29.1 %	+17.5%	+32.2 %
— h-g1/brown_prompt_fe	-21.8 %	-12.2 %	-9.4 %
— h-g1/costantini_fe	+23.8 %	+12.8 %	+18.4 %
— h-g1/dileva_prompt_fe	-5.3 %	-8.1%	-0.62 %
— h-g1/kontos_prompt_fe	-13.4 %	+3.2 %	-1.71%
— p-g1/piatti_prompt_fe	-33.8 %	-23.2 %	-27.5%
— p-g1/tingwell_prompt_fe	+15.1 %	-13.5 %	+11.4 %

nd4 (but not Rg=100 fm)

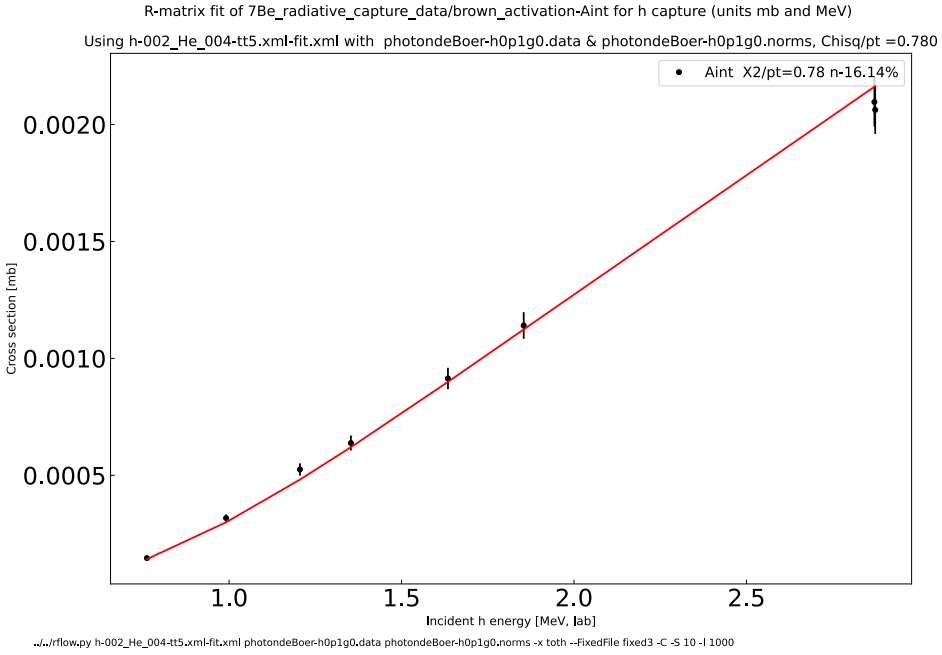
Include capture channels (b) inclusive gammas by Reich-Moore approx.

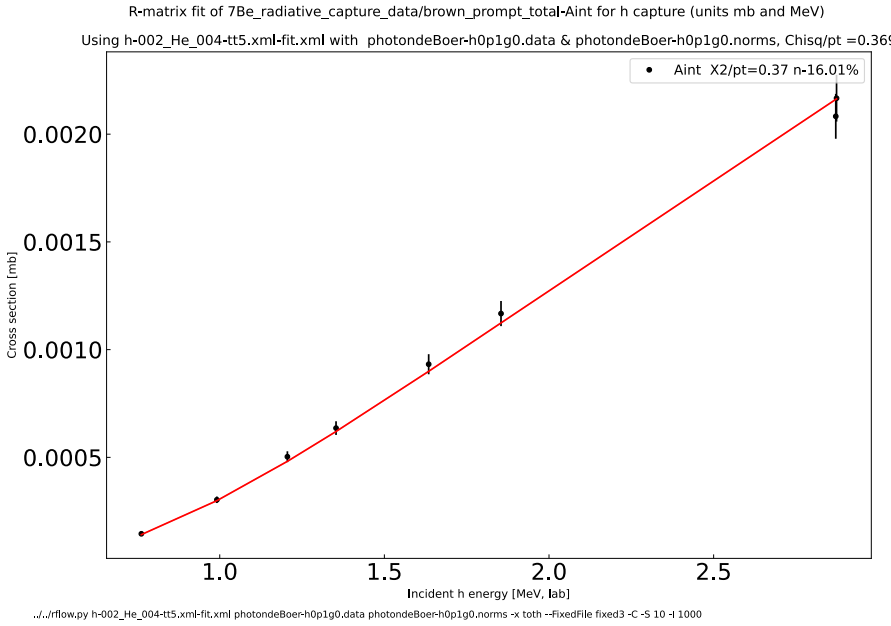
- Cannot distinguish these two channels in reaction model
  - Production of Be7 ground state and Be7_e1 excited state
  - Can split by hand afterwards
- Easy in GNDS format:
  - <reaction label="Be7 + photon [inclusive]" ENDF_MT="102" >
- Traditional in ENDF:
  - Use MT=102
- Fit damping width for each R-matrix pole above threshold

Reich-Moore gammas: (p,γ)Be7 (total=absorption) All angle-integrated

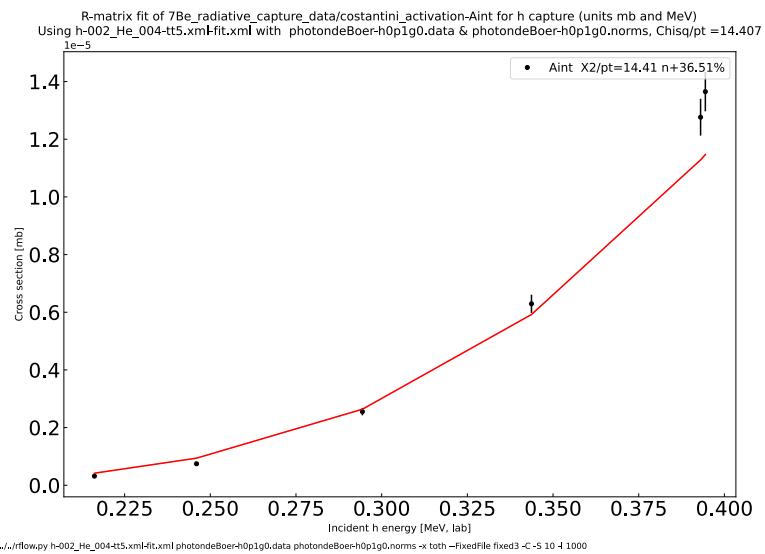


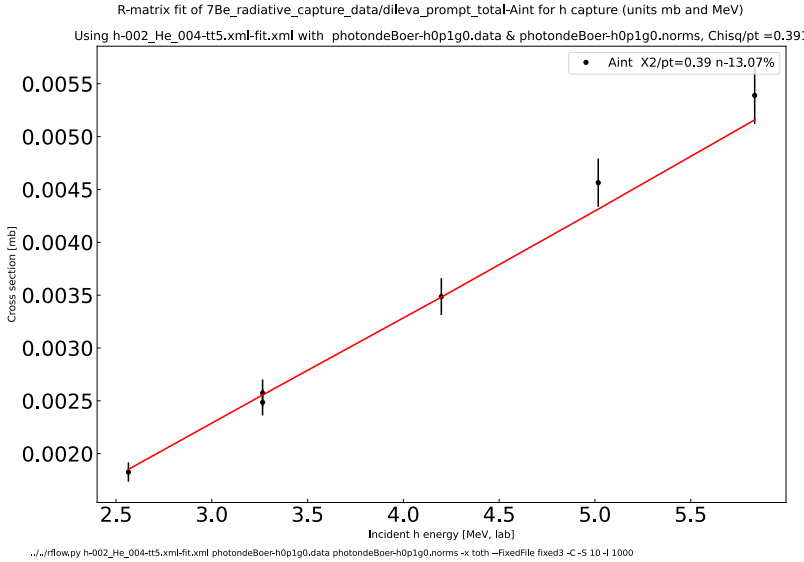
Reich-Moore gammas: (h,γ)Be7 (total=absorption) All angle-integrated

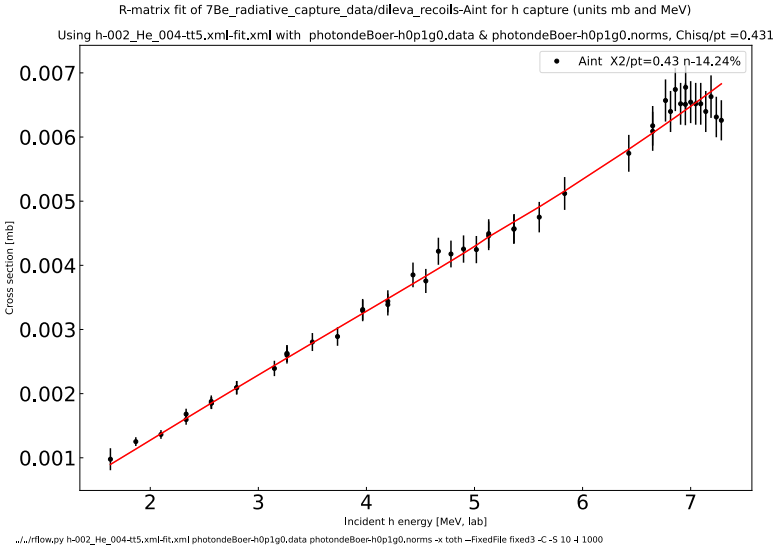


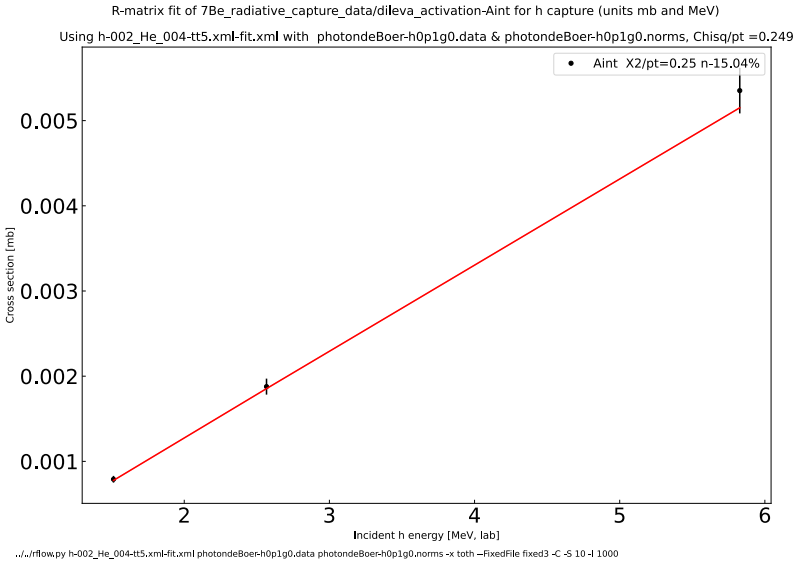


Reich-Moore gammas: (h,γ)Be7 (total=absorption) All angle-integrated









Data renormalization factors from fit

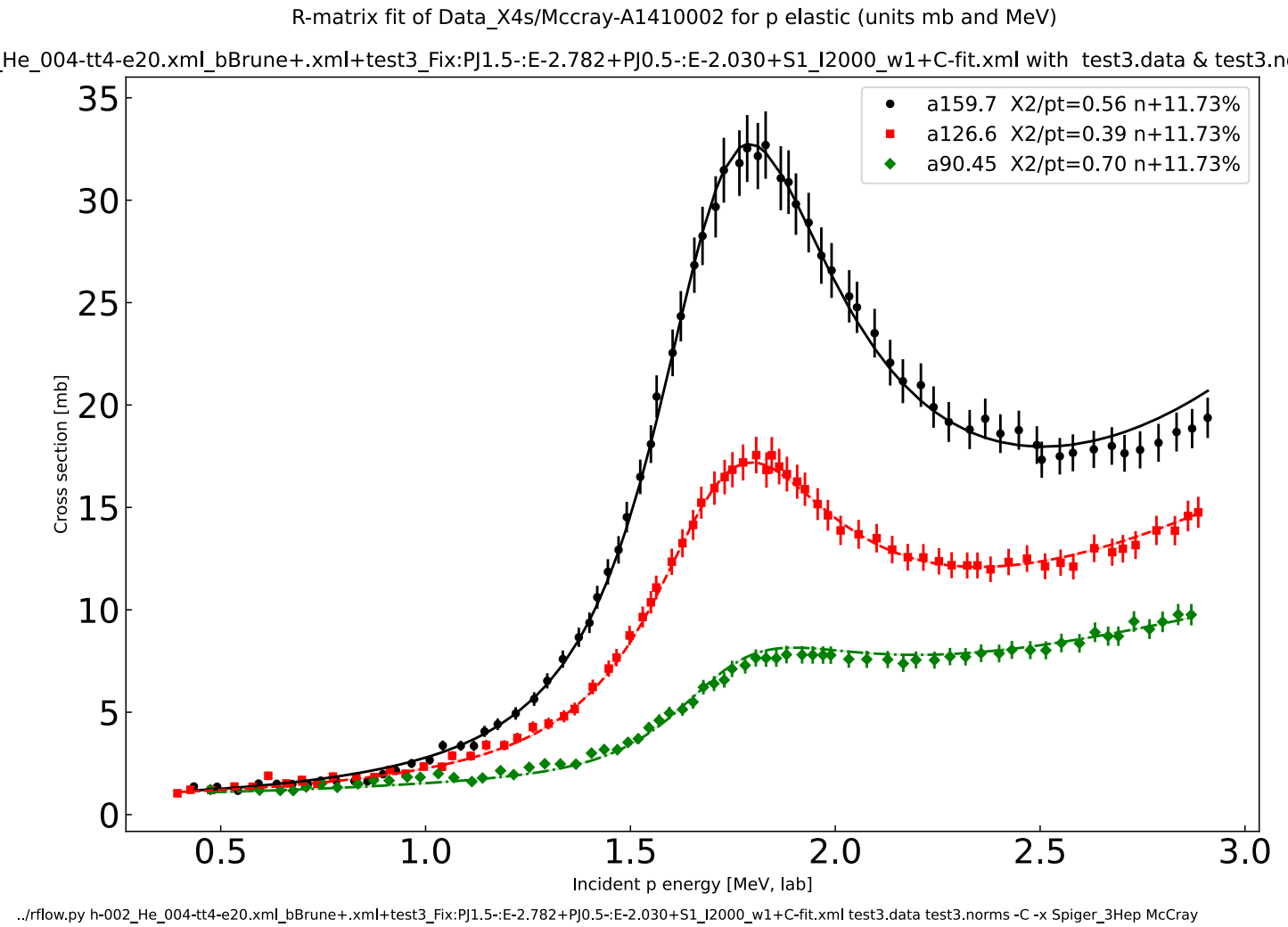
- h-g
  - brown_activation -16.2 %
  - brown_prompt_total -16.0 %
  - costantini_activation +36.5 %
  - dileva_activation -15.0 %s
  - dileva_prompt_total -13.0 %
  - dileva_recoils -14.3 %
  - parker_and_kavanagh_prompt -1.5 %
  - szucs_activation +2.6 %
- p-g
  - switkowski_prompt_total: +0.7 %

Discussion of gamma fits

- Which to choose: primary channels, or Reich-Moore ?
  - Which can be put in ENDF-6 format?
- Why large data renormalizations (up and down by 40%) ?

Further particle data up to 20 MeV: refit all data

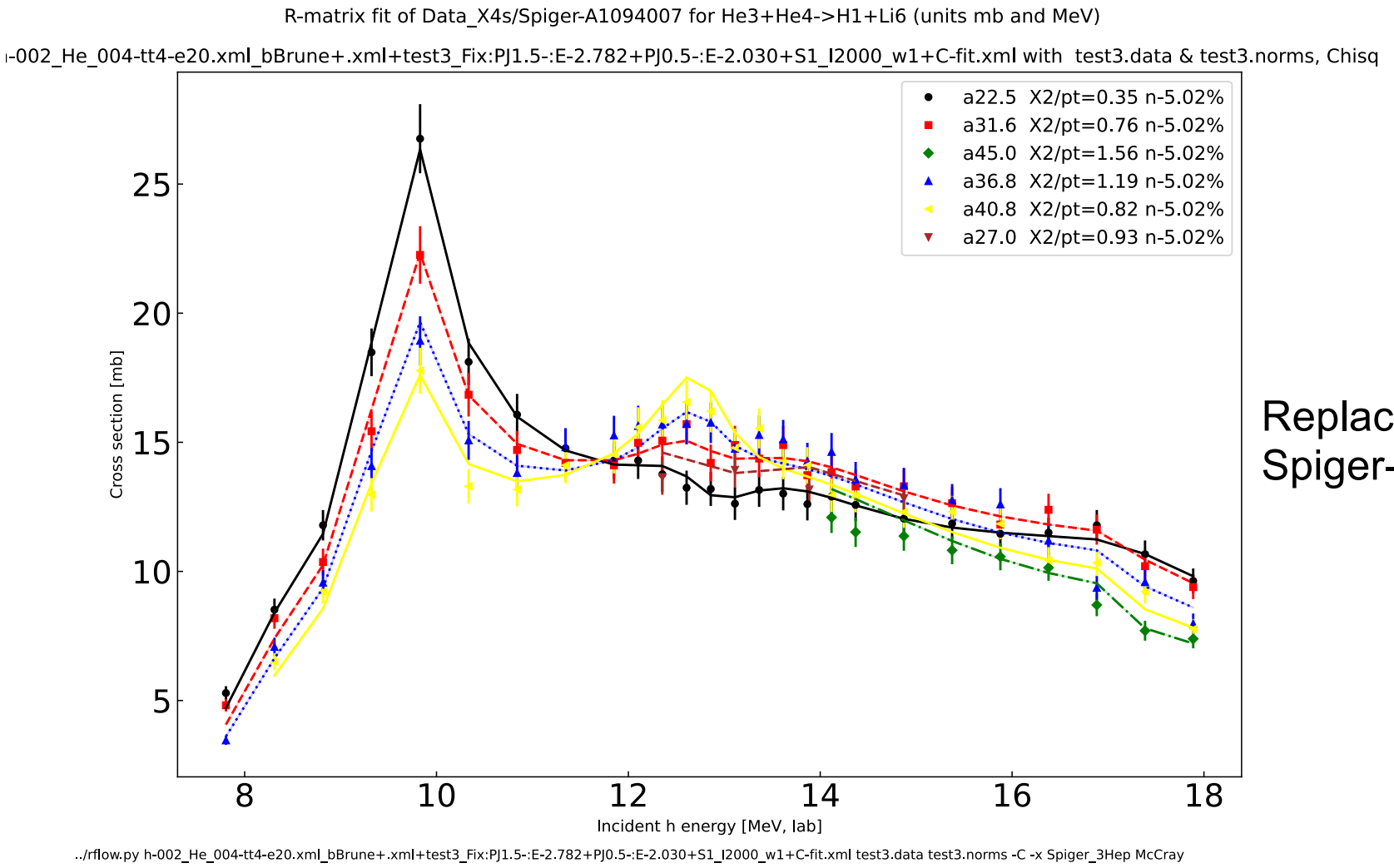
Now: **Mccray-A1410002 (p,p),** Spiger-A1094007 (h,p), Tombrello-A1295005 (h,p)



Replacing Mccray-pp.dat

Further proton data up to 20 MeV

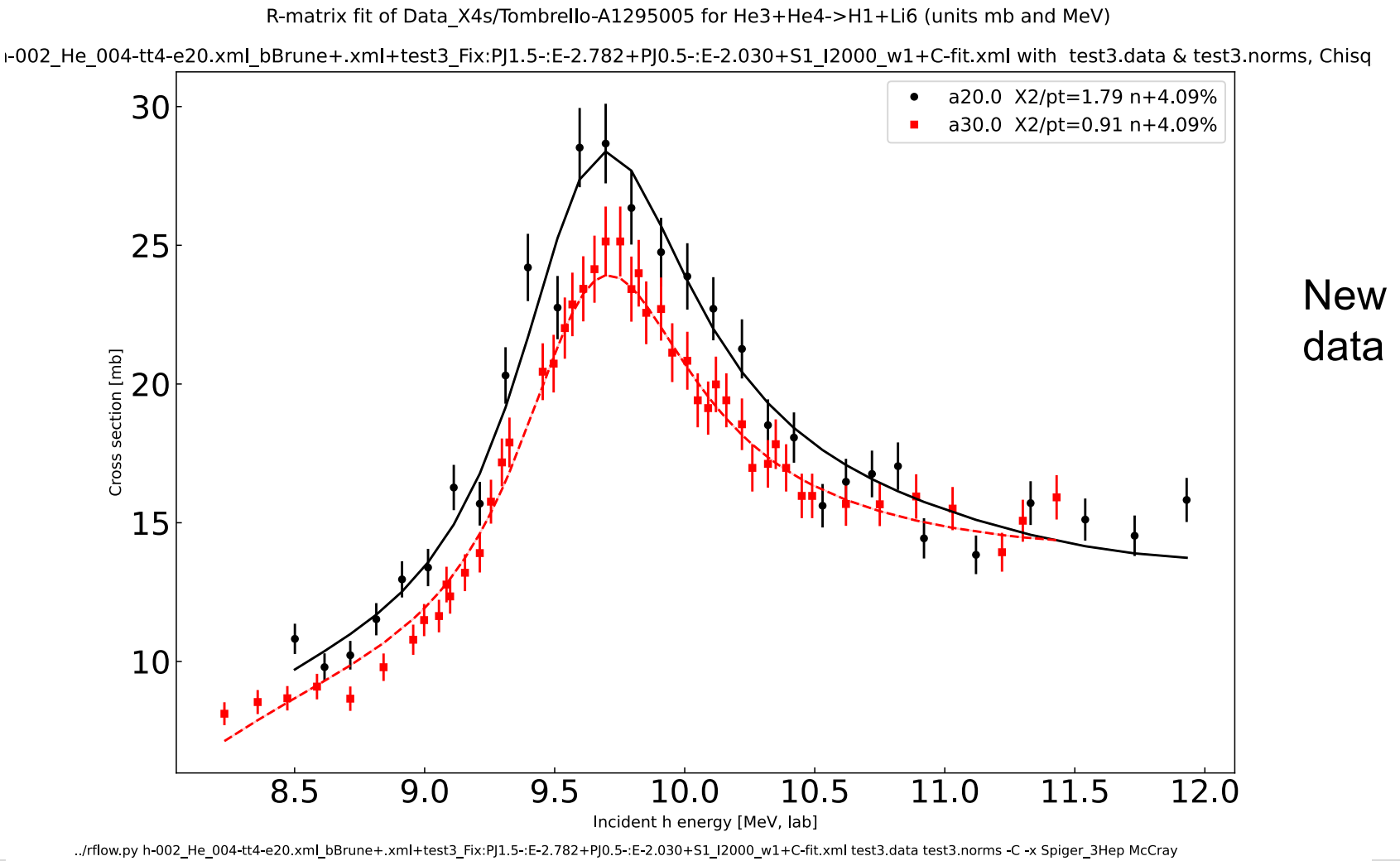
Now: Mccray-A1410002 (p,p), **Spiger-A1094007 (h,p)**, Tombrello-A1295005 (h,p)



Replacing
Spiger-cm_ap0.dat

Further particle data up to 20 MeV

Now: Mccray-A1410002 (p,p), Spiger-A1094007 (h,p), **Tombrello-A1295005 (h,p)**



New data

Discussion

- Are these improved enough to submit to ENDF/B-VIII.1 ?
- Submit a p+Li6 evaluation ?

Lawrence Livermore
National Laboratory