Candidate evaluation for He3 + He4 scattering from R-matrix theory

CSEWG 2022

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R-matrix Framework

- Strategy:
  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.

Specifying Experiment Data for the Be7 system

- Use *.dat files from de Boer, converted to ^{4}He on ^{3}He lab data.
- Still need to specify properties of these files:

> There are many errors in the EXFOR descriptions of these data sets.

projectile	ejectile	residual	file	sys-error	stat-error	norm	group	splitnorms	lab	abserr	scale	filedir	eshift	ecalib	splitshifts
a	a	0	Barnard_aa.dat	5	3	1	E	FALSE	TRUE	TRUE	b	Expt5/	0	0	FALSE
p	a	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	a	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
a	a	0	Mohr_aa.dat	-1	5	1	A	TRUE	TRUE	TRUE	b	Expt5/	0	0	FALSE
a	a	0	Spiger-A1094004-lab_aa.dat	1.5	-1	1	E	TRUE	TRUE	TRUE	b	Expt5/	0	0.02	TRUE
a	p	0	Spiger-cm_ap0.dat	1.5	-1	1	A	TRUE	FALSE	TRUE	mb	Expt5/	0	0	FALSE
a	a	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.

Search adventures

- The bound states should be at the observed Be7 energies, but that will not happen exactly since we are using the B=-L boundary conditions. So I ended up constraining the Brune-basis bound states at observed energy within 0.02 MeV.

- I ended up adding in some broad 3/2+ and 5/2+ poles lower than our 20 MeV background pole set.

- The amplitudes for the background poles were highly correlated in the final fit ($\rho > 0.995$). Since, strictly, these are not physical observables, I ended up fixing many of them, and only varying the norms and the middle-pole properties in order to obtain the final covariance matrix.

- I always plot the phase shifts, on a fine energy grid, from the final parameters: to make sure no unwanted poles have crept in.

- It is probable that the Spiger_aa elastic data is 0.1 MeV too high in its energy calibration. I fitted also the energy calibration of Spiger_aa and Tombrello_aa.

Results of fit

- I get $\chi^2/N = 2.884$ from the data,
  and $\chi^2/N = 3.037$ overall including contributions from norm factors differing from unity and shifts differing from zero.

Dataset	Chisq/pts	av norm	av shift
Barnard_aa.dat	0.967	0.990	
Elwyn_pa.dat	4.317	1.133	
Fasoli_pp.dat	3.895	0.996	
Harrison_pp0.dat	5.489	1.156	
Lin_pa.dat	3.885	1.305	
McCray_pp.dat	3.842	1.122	
Mohr_aa.dat	3.481	0.956	
Spiger-A1094004-lab_aa.dat	2.633	0.929	-0.048
Spiger-cm_ap0.dat	1.419	1.004	
Tombrello_aa.dat	3.559	1.080	-0.036

Fitted R-matrix parameters

TABLE III: R-matrix parameters in the $B = -L$ basis.
Pole energies in the centre-of-mass frame of the elastic channel.
Reduced width amplitudes γ_c in units of $\text{MeV}^{1/2}$ (cm).

$J^\pi = 1.5^-$

E (MeV)	He4+He3 LS: 1, 1/2	H1+Li6 LS: 1, 1/2	H1+Li6 LS: 1, 3/2	H1+Li6 LS: 3, 3/2
−5.444080	0.87557	−0.01150	−1.38640	1.06791
13.731600	0.16954	−1.39241	−2.26737	−1.02723
20.000 B	−1.62165	0.69621	0.18995	0.75548

$J^\pi = 0.5^-$

E (MeV)	He4+He3 LS: 1, 1/2	H1+Li6 LS: 1, 1/2	H1+Li6 LS: 1, 3/2
−16.412100	1.26282	3.16021	0.71913
20.000 B	−1.30080	0.02080	−1.29724

$J^\pi = 3.5^-$

E (MeV)	He4+He3 LS: 3, 1/2	H1+Li6 LS: 3, 1/2	H1+Li6 LS: 3, 3/2	H1+Li6 LS: 5, 3/2
−12.498600	−3.42797	−1.04027	−9.53490	3.45889
20.000 B	−2.82985	−0.86921	−3.70608	0.18067

$J^\pi = 2.5^-$

E (MeV)	He4+He3 LS: 3, 1/2	H1+Li6 LS: 1, 3/2	H1+Li6 LS: 3, 1/2	H1+Li6 LS: 3, 3/2
6.235800	−0.49320	0.88029	0.63581	−1.19863
7.058410	0.60011	1.10886	0.95826	−1.97907
20.000 B	2.29966	−0.05640	−2.71769	1.49483

$J^\pi = 0.5^+$

E (MeV)	He4+He3 LS: 0, 1/2	H1+Li6 LS: 0, 1/2	H1+Li6 LS: 2, 3/2
20.000 B	−3.04315	−2.93656	−1.35584

$J^\pi = 1.5^+$

E (MeV)	He4+He3 LS: 2, 1/2	H1+Li6 LS: 0, 3/2	H1+Li6 LS: 2, 1/2	H1+Li6 LS: 2, 3/2
12.737200	0.02992	2.00720	0.46536	2.69452
20.000 B	1.78531	−0.41199	1.60477	−0.87334

$J^\pi = 2.5^+$

E (MeV)	He4+He3 LS: 2, 1/2	H1+Li6 LS: 2, 1/2	H1+Li6 LS: 2, 3/2	H1+Li6 LS: 4, 3/2
15.502 B	−0.37654	1.29621	0.06419	−6.47263
20.000 B	−1.69761	−1.20948	0.10603	0.12602

$J^\pi = 3.5^+$ (zero for all L $\geq$ 0)

E (MeV)	

$J^\pi = 4.5^-$ (zero for all L $\geq$ 0)

E (MeV)	

$J^\pi = 4.5^+$ (zero for all L $\geq$ 0)

E (MeV)	

Brune Basis

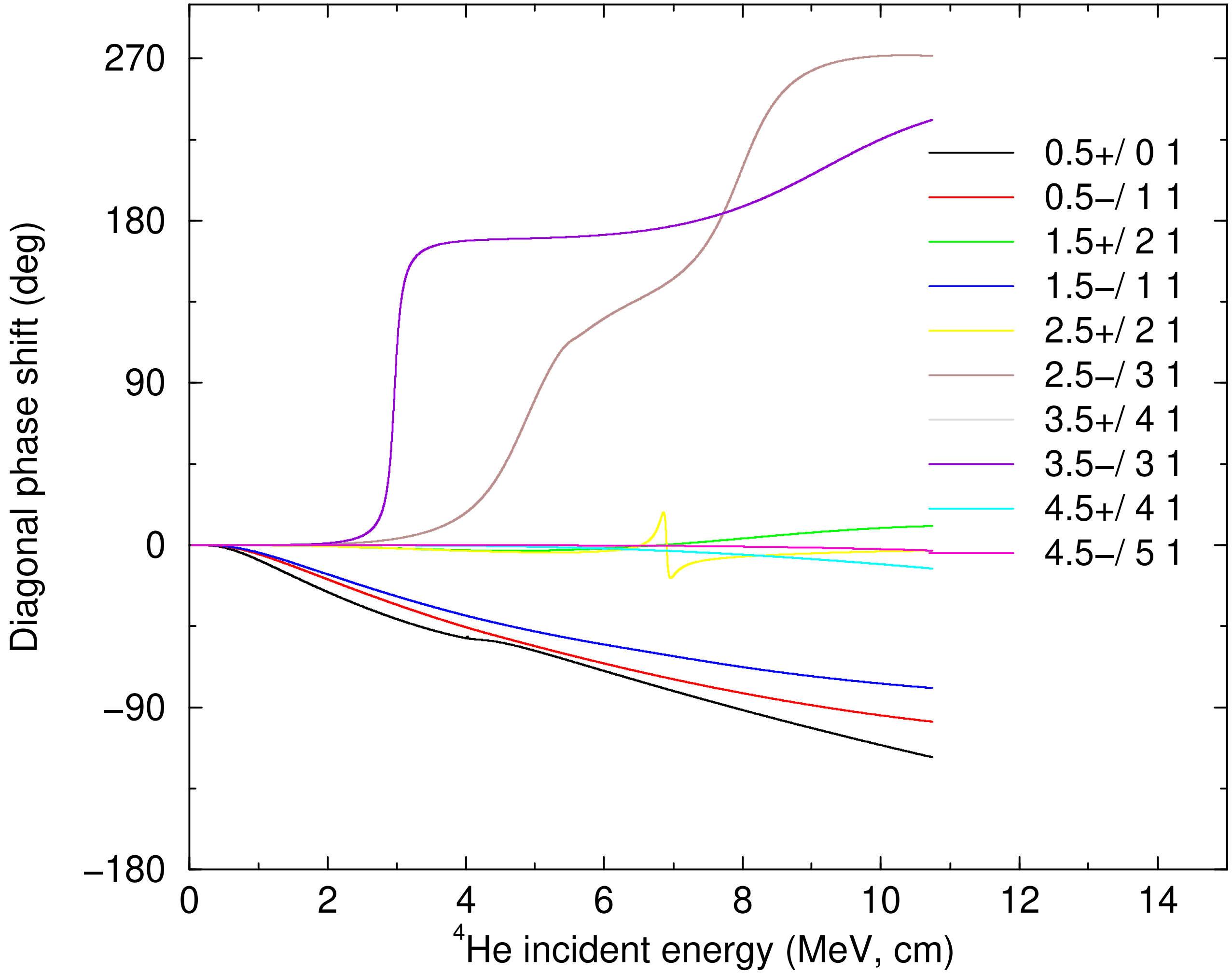
```
183 parameters and 226 fitted data sets
Spin-parity groups with no poles: [(3.5, 1), (4.5, -1), (4.5, 1)]

J,pi=1.5- from   -12.669 to    -3.682 took   31 iterations (cm:    -5.444 to    -1.582)
J,pi=1.5- from    31.955 to    19.747 took   60 iterations (cm:    13.732 to     8.486)
J,pi=1.5- from    46.542 to    39.136 took    6 iterations (cm:    20.000 to    16.817)
J,pi=0.5- from   -38.193 to    -2.641 took  278 iterations (cm:   -16.412 to    -1.135)
J,pi=0.5- from    46.542 to    39.743 took    6 iterations (cm:    20.000 to    17.078)
J,pi=3.5- from   -29.086 to     6.924 took  523 iterations (cm:   -12.499 to     2.975)
J,pi=3.5- from    46.542 to    24.676 took   18 iterations (cm:    20.000 to    10.604)
J,pi=2.5- from    14.511 to    11.713 took   48 iterations (cm:     6.236 to     5.033)
J,pi=2.5- from    16.426 to    13.016 took  262 iterations (cm:     7.058 to     5.593)
J,pi=2.5- from    46.542 to    19.809 took   38 iterations (cm:    20.000 to     8.512)
J,pi=0.5+ from    46.542 to    40.740 took    9 iterations (cm:    20.000 to    17.507)
J,pi=1.5+ from    29.641 to    18.132 took  268 iterations (cm:    12.737 to     7.792)
J,pi=1.5+ from    46.542 to    25.829 took   22 iterations (cm:    20.000 to    11.099)
J,pi=2.5+ from    36.075 to    15.979 took  358 iterations (cm:    15.502 to     6.866)
J,pi=2.5+ from    46.542 to    30.270 took   12 iterations (cm:    20.000 to    13.008)
```

constrained energies in red

Incident ^{4}He lab energies

CM energies in ^{4}He+^{3}He channel

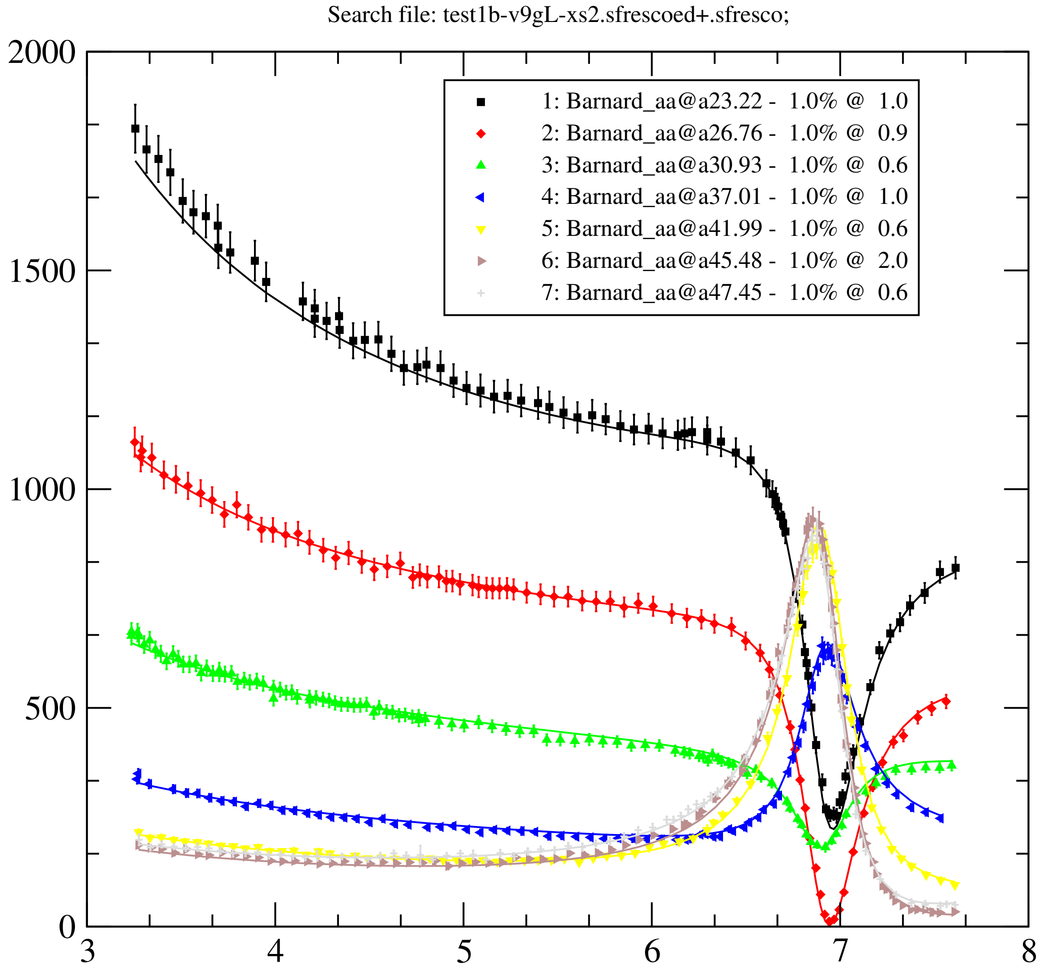
$^4He + ^3He$ diagonal phase shifts



Only 3 resonances in entrance channel:
1 in 7/2-
2 in 5/2-

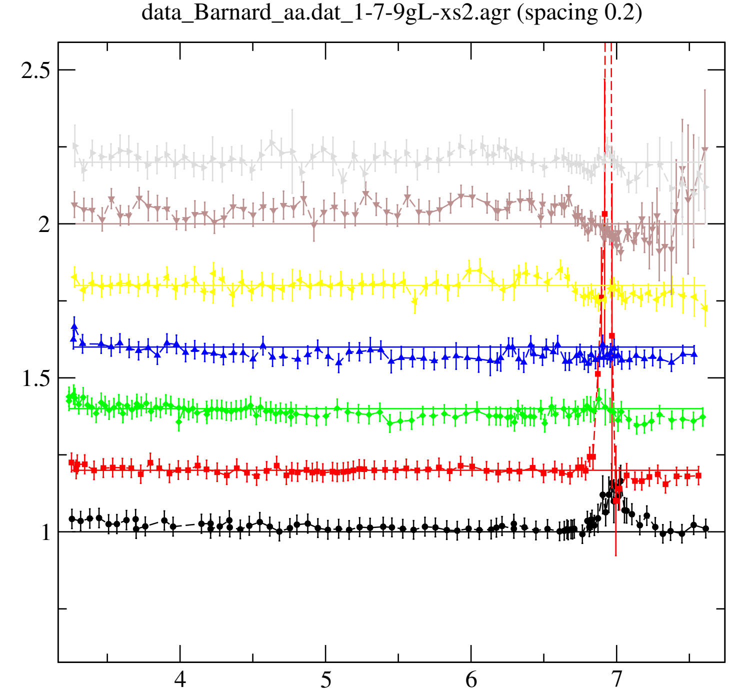
Hint of 5/2+ pole (no resonance)

Barnard_aa data



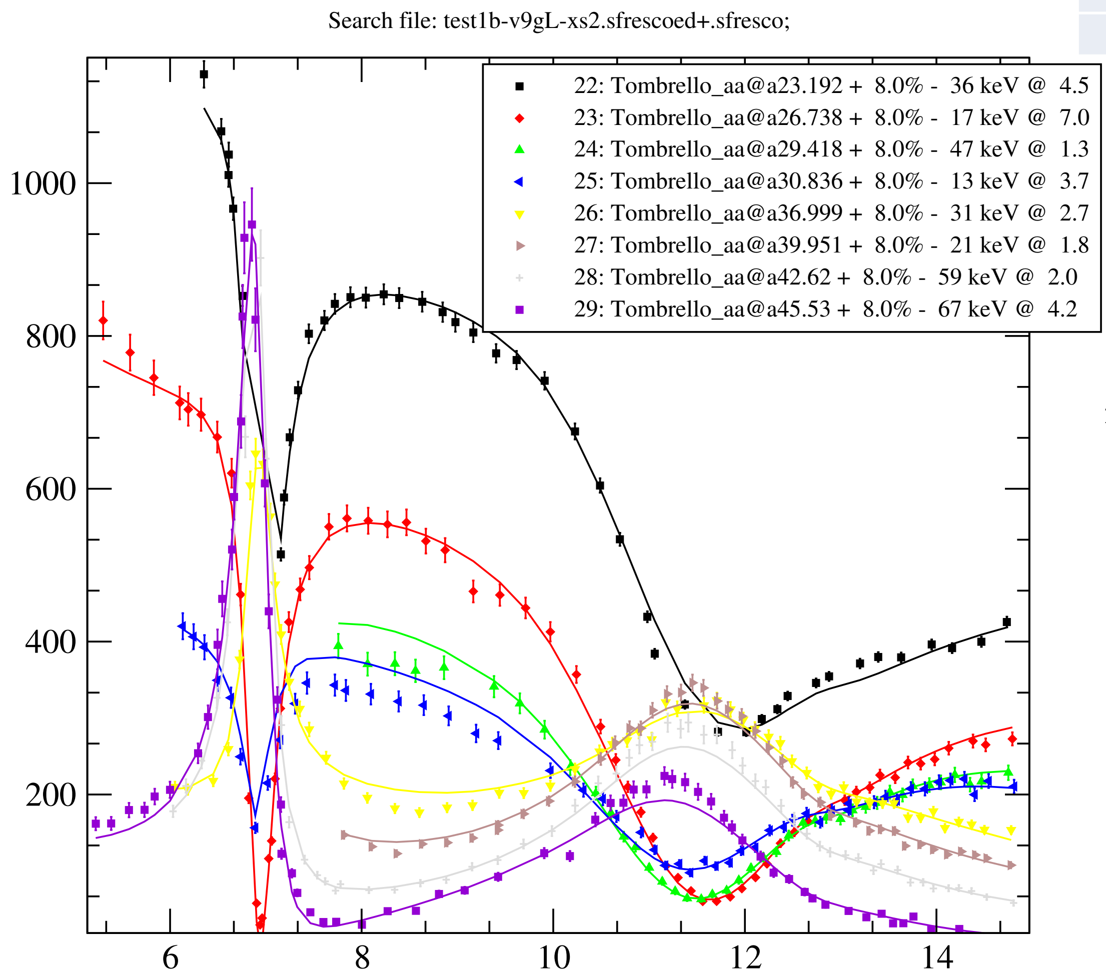
Dataset	Chisq/pts	av norm
Barnard_aa.dat	0.967	0.990

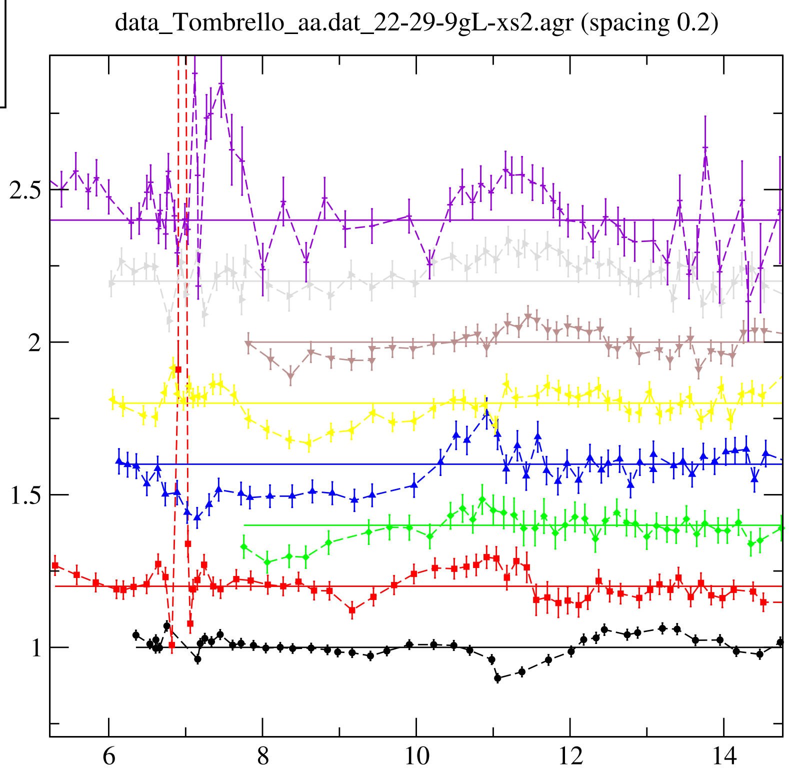
Experiment/R-matrix ratios



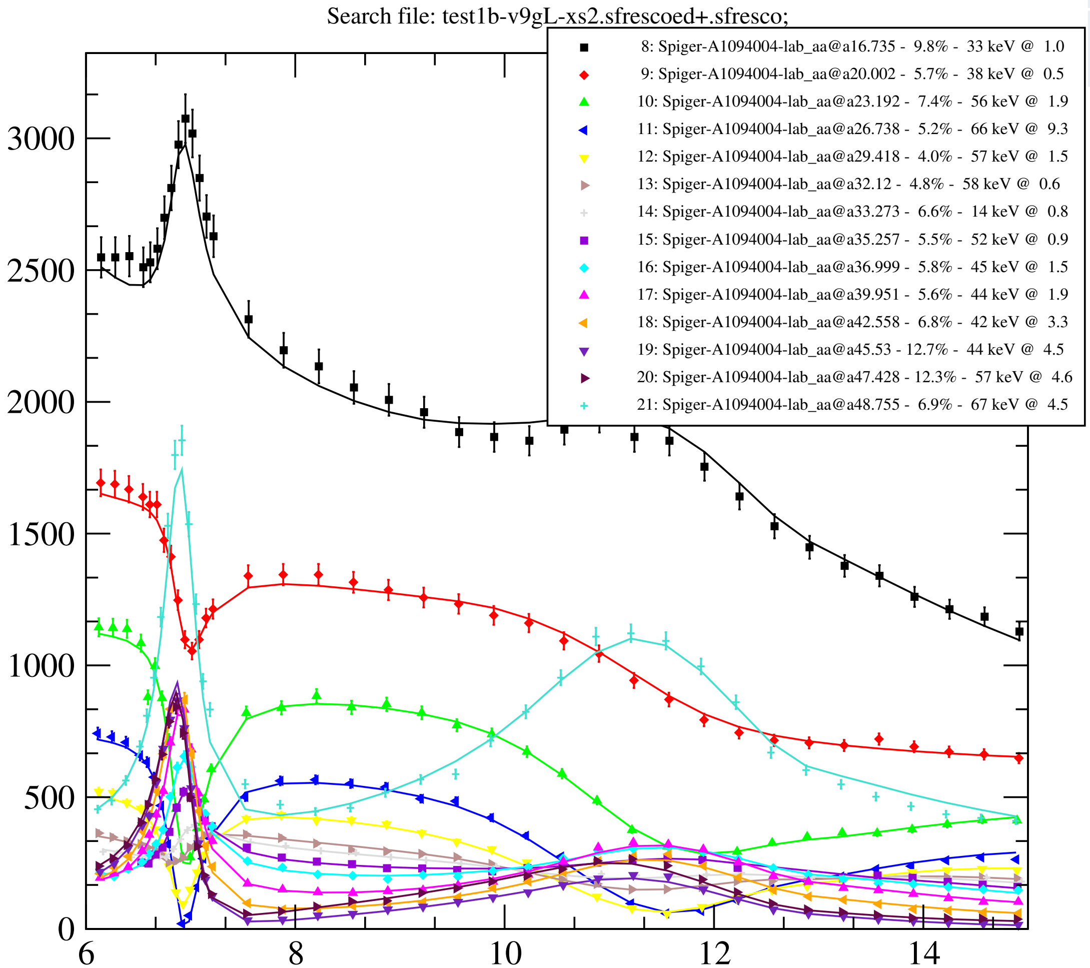
Tombrello_aa data

Dataset	Chisq/pts	av norm	av shift
Tombrello_aa.dat	3.559	1.080	-0.036

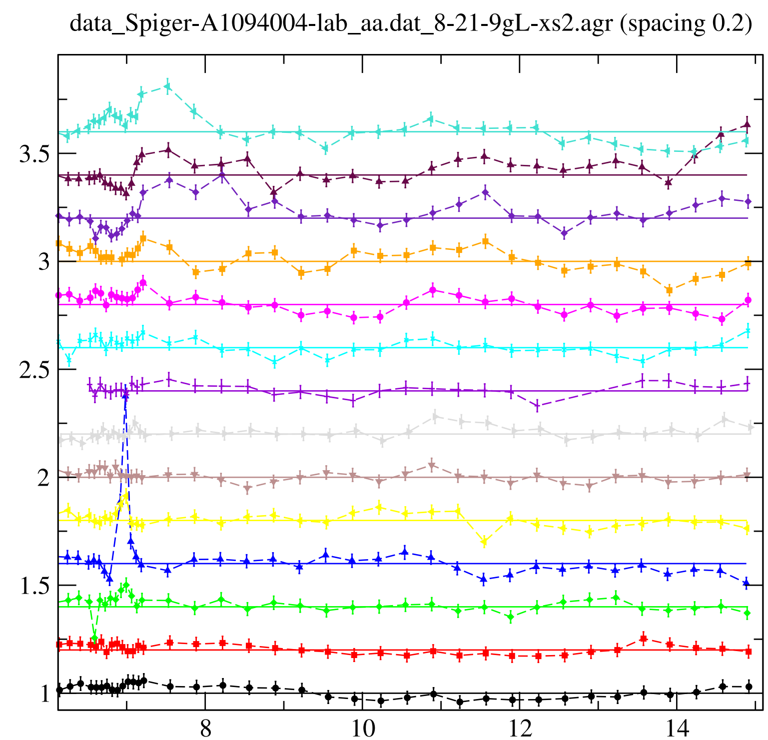




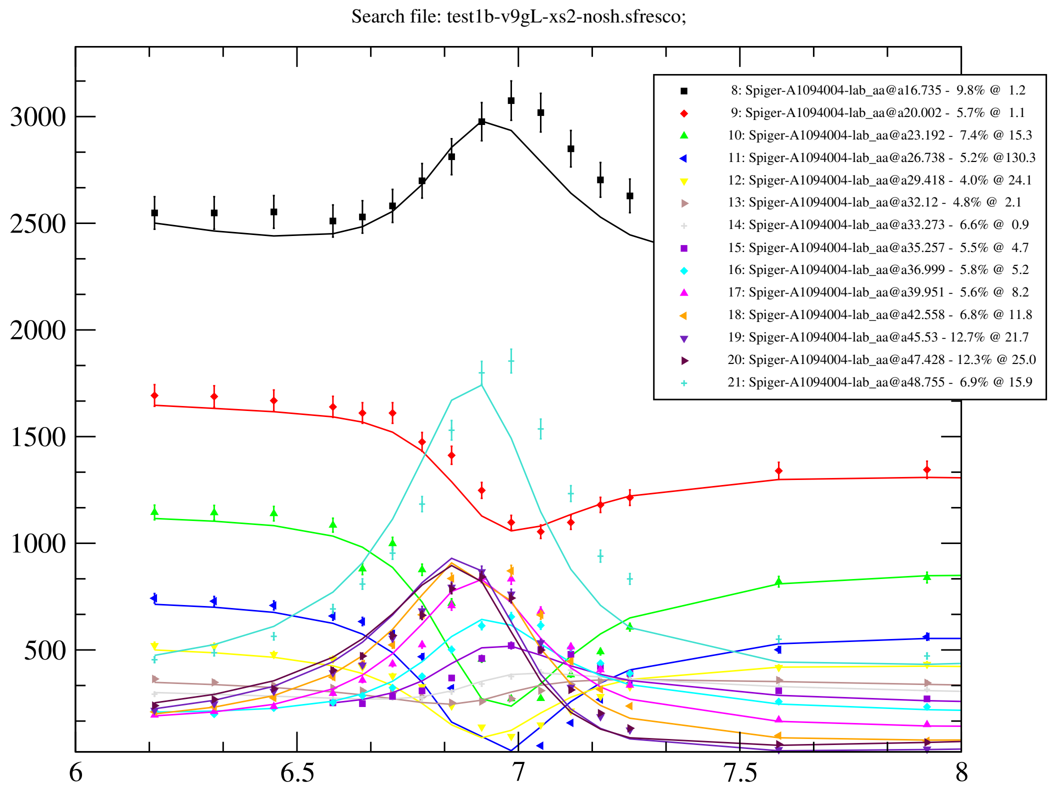
Spiger_aa data

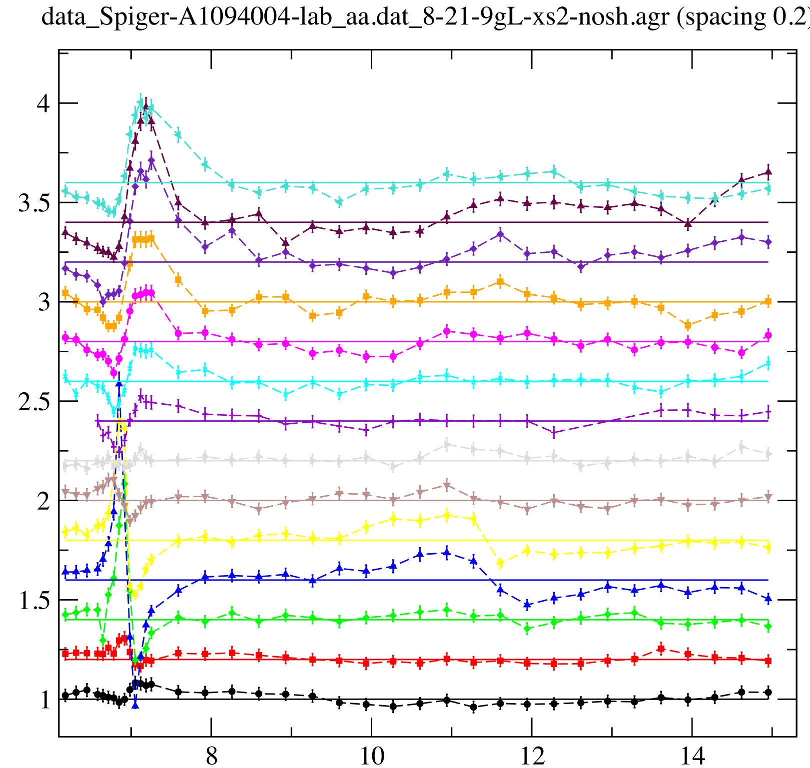


Dataset	Chisq/pts	av norm	av shift
Spiger-A1094004-lab_aa.dat	2.633	0.929	-0.048



Spiger_aa data (without energy shift adjusting)



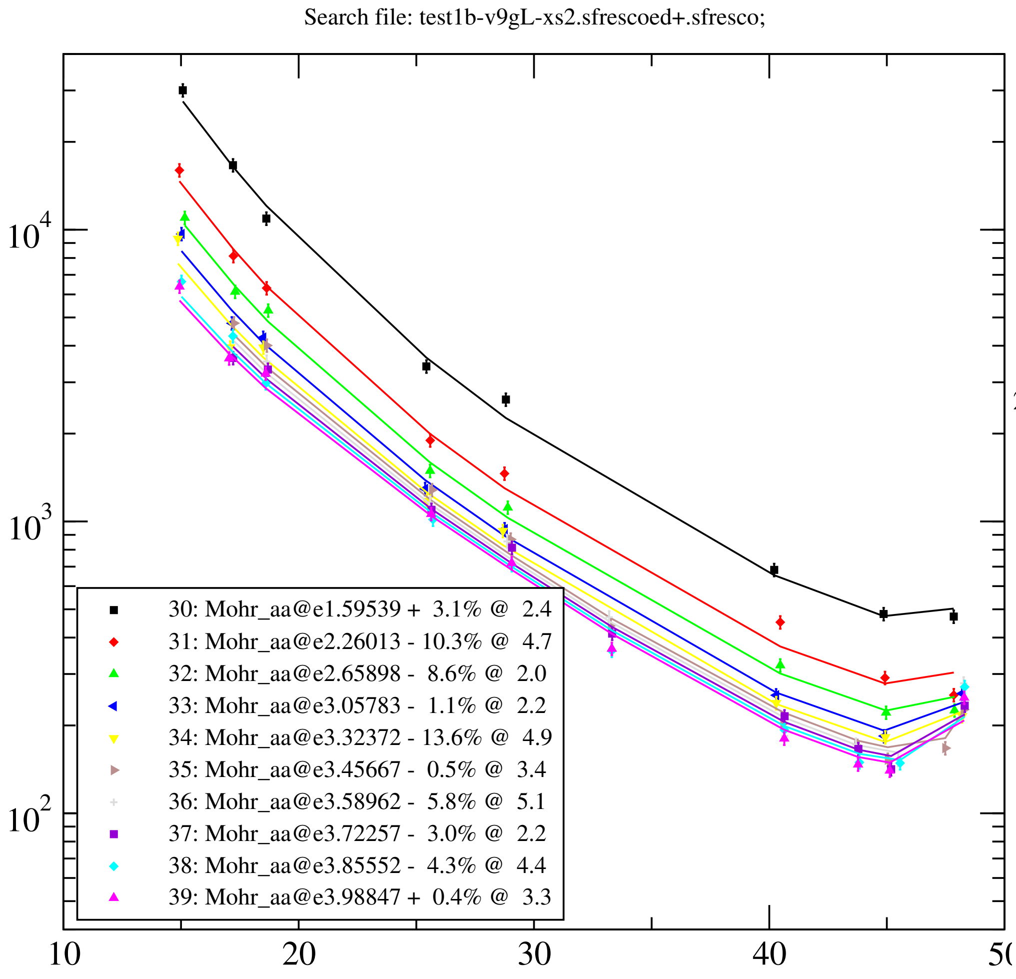


(normalizations **not** refitted)

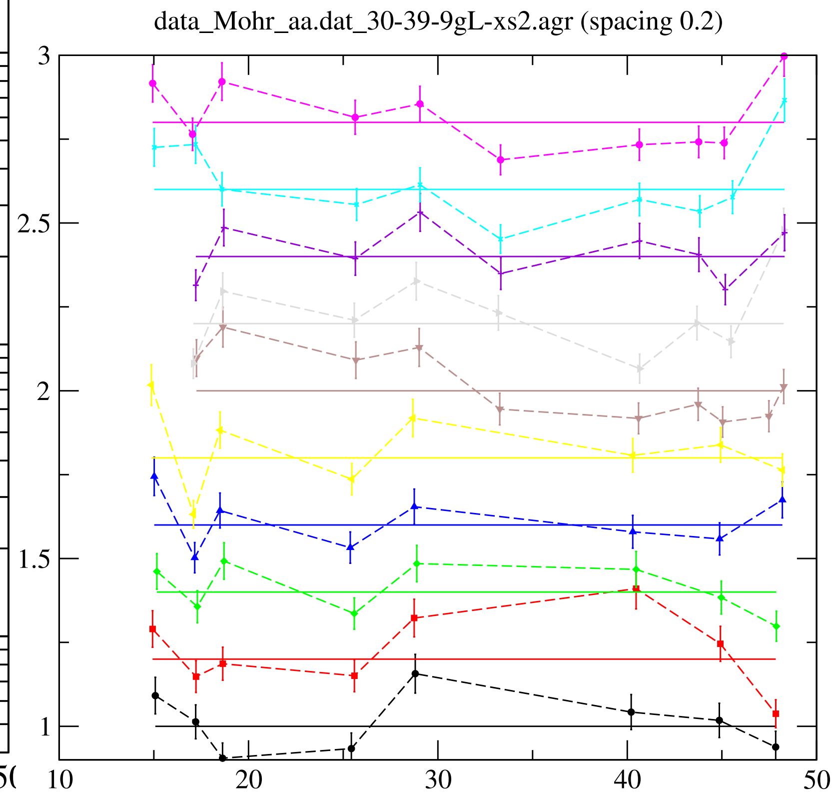
Dataset	Chisq/pts
Spiger-A1094004-lab_aa.dat	19.085

Barnard data not energy-shifted. Then discrepancies seen in other aa data sets near the 7 MeV pole.

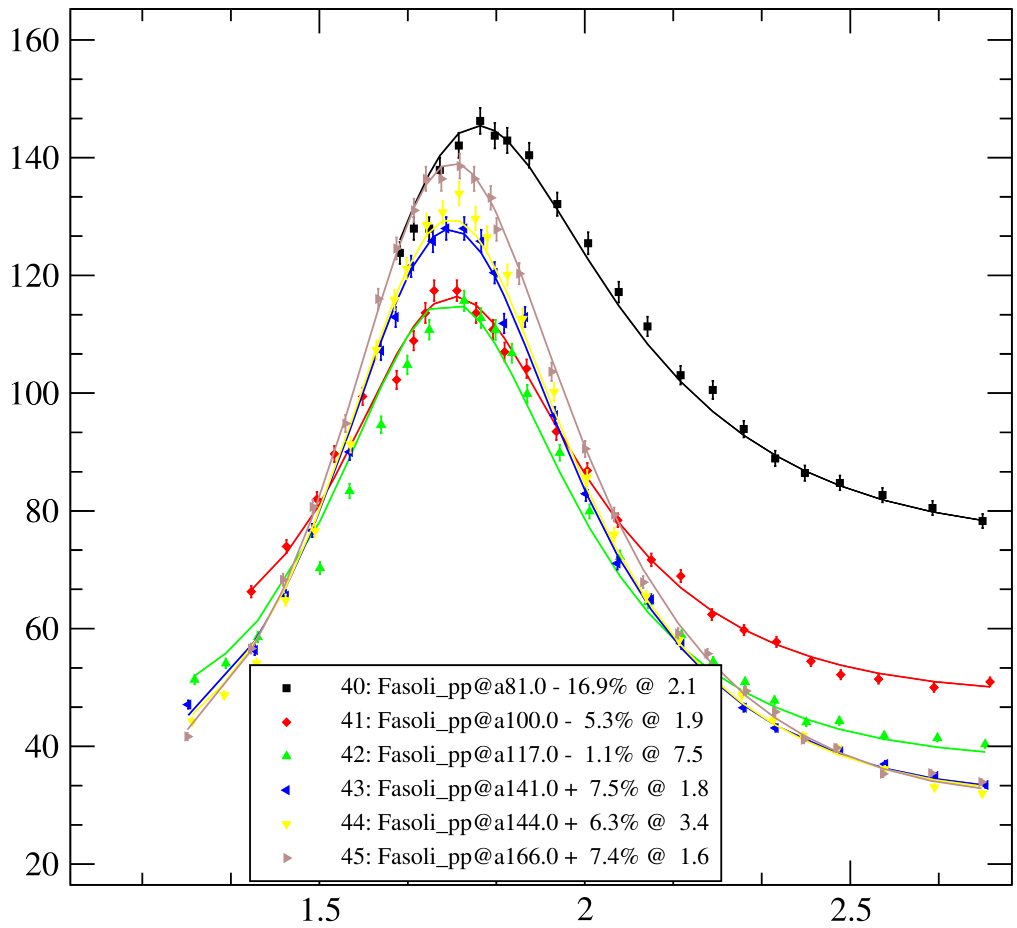
Mohr_aa data



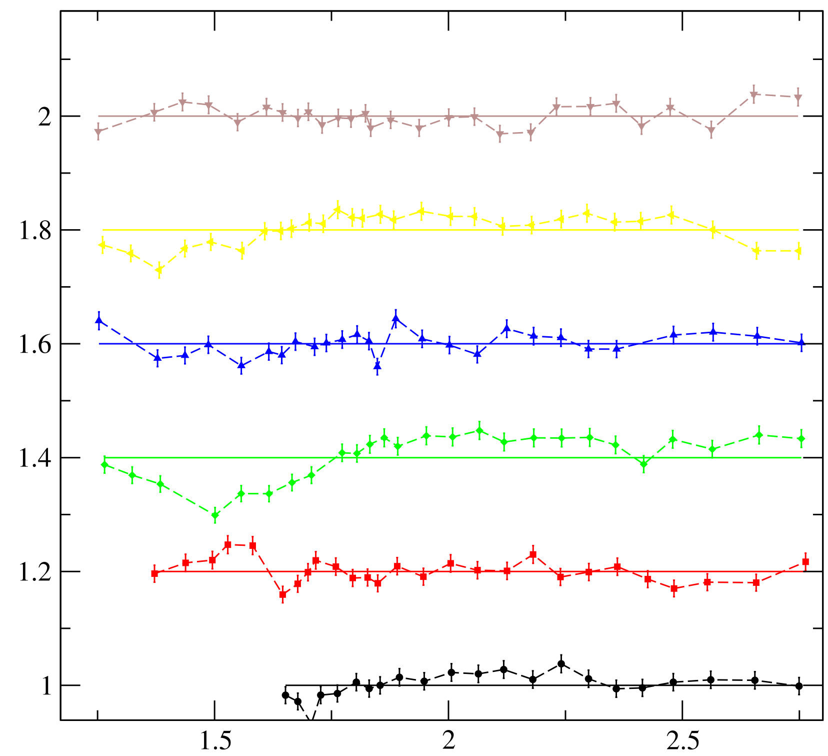
Dataset	Chisq/pts	av norm	av shift
Mohr_aa.dat	3.481	0.956	



Fasoli_pp data

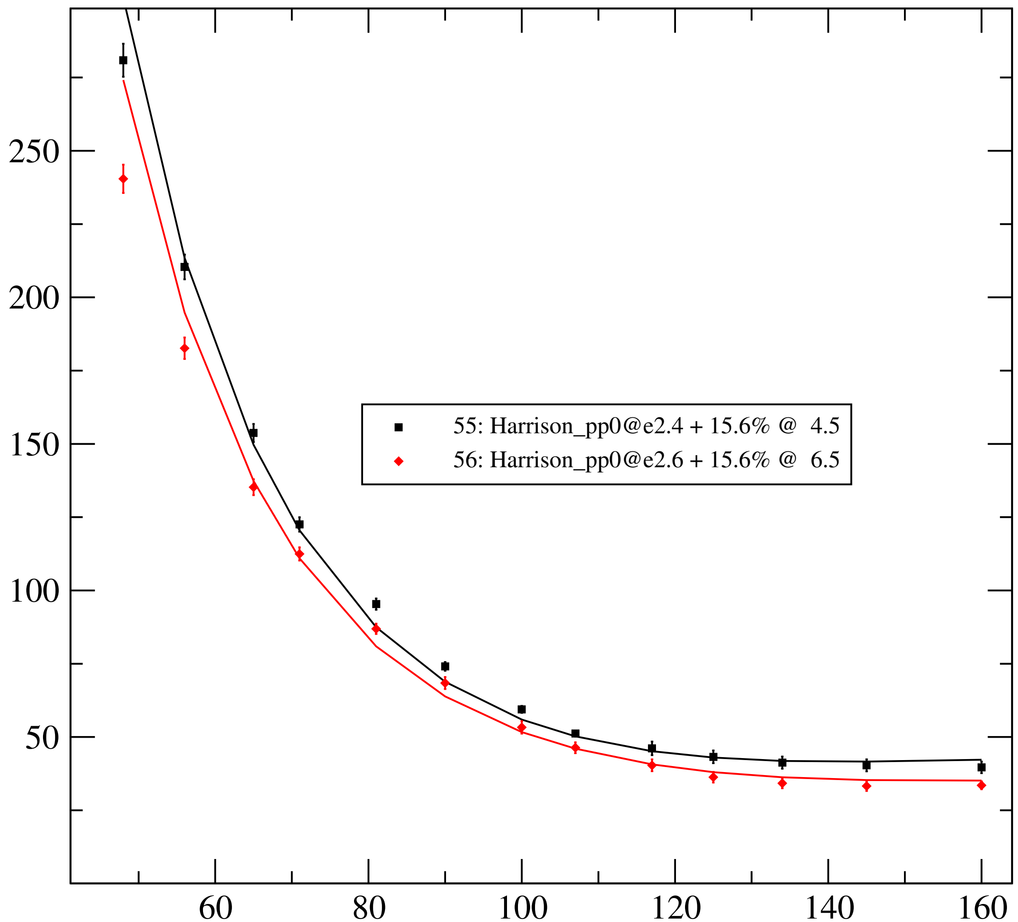


Dataset	Chisq/pts	av norm	av shift
Fasoli_pp.dat	3.895	0.996	



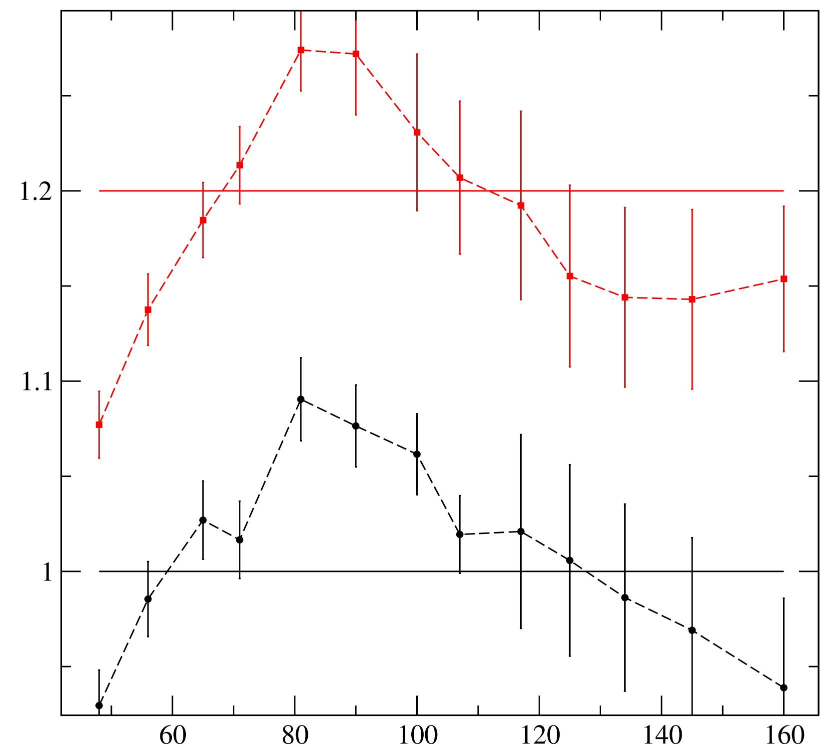
Harrison_pp0.data

Search file: test1b-v9gL-xs2.sfrescoed+.sfresco;

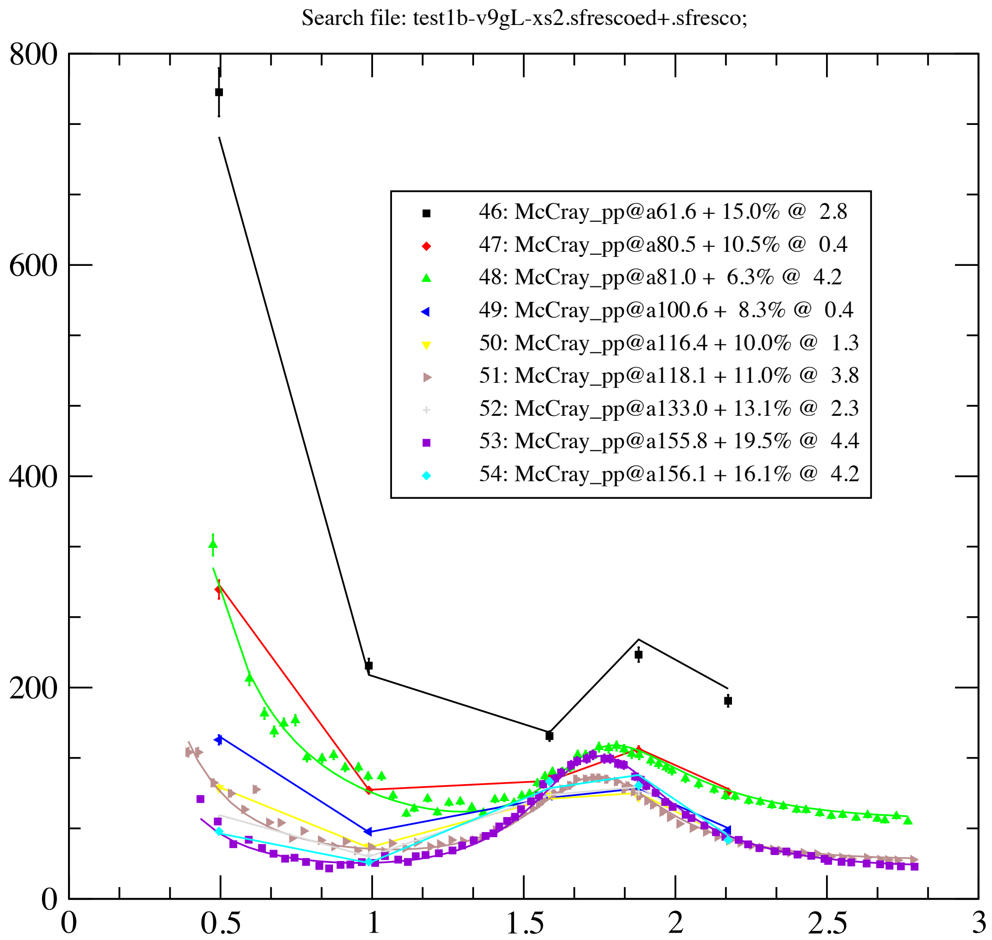


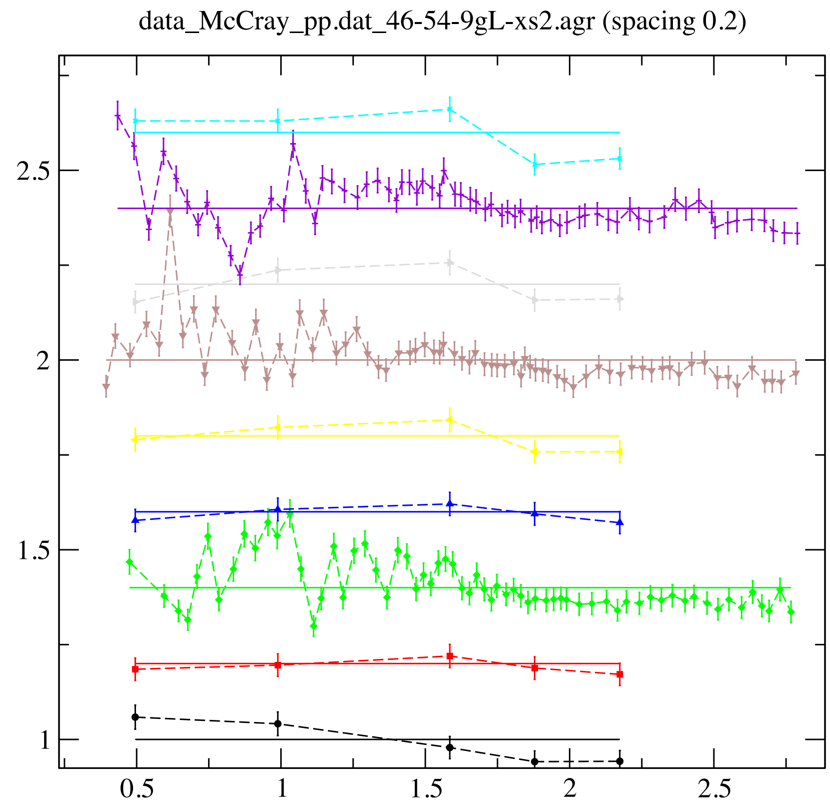
Dataset	Chisq/pts	av norm
Harrison_pp0.dat	5.489	1.156

data_Harrison_pp0.dat_55-56-9gL-xs2.agr (spacing 0.2)



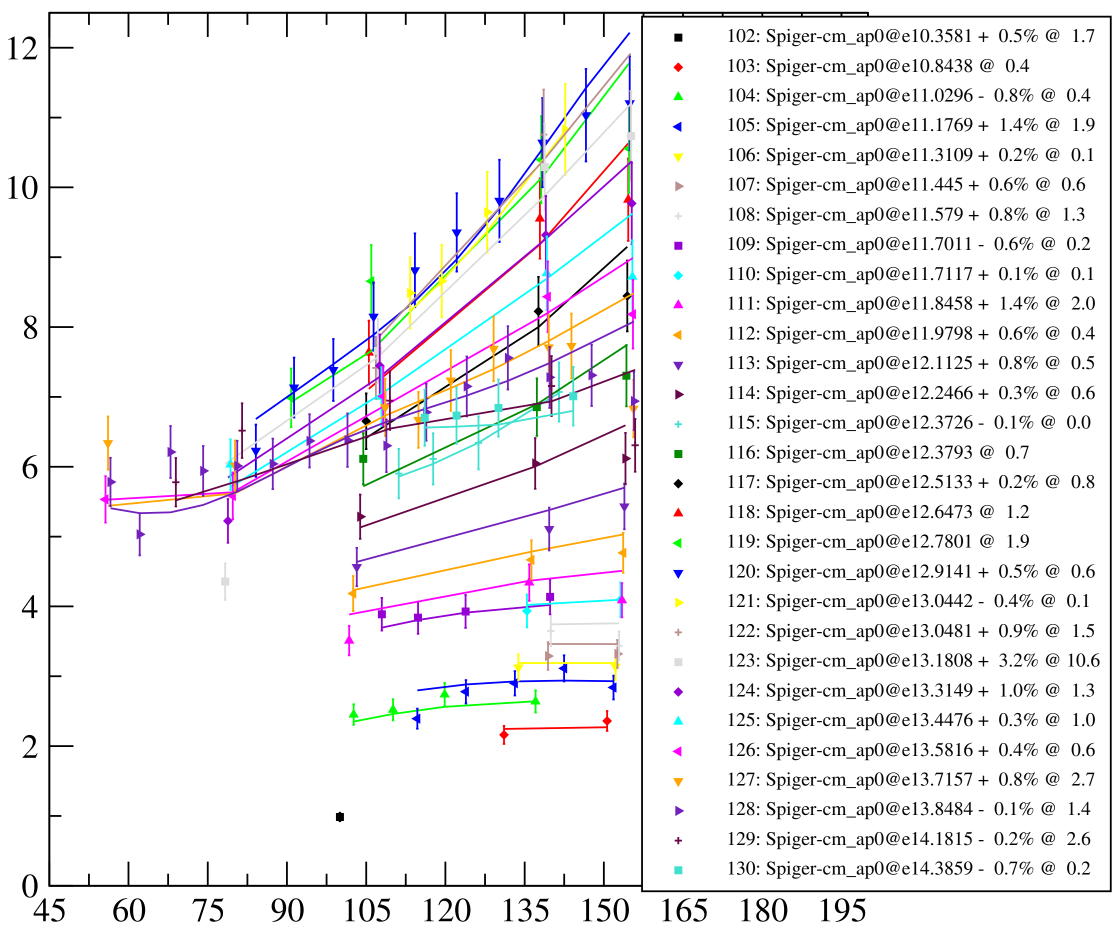
McCray_pp.data





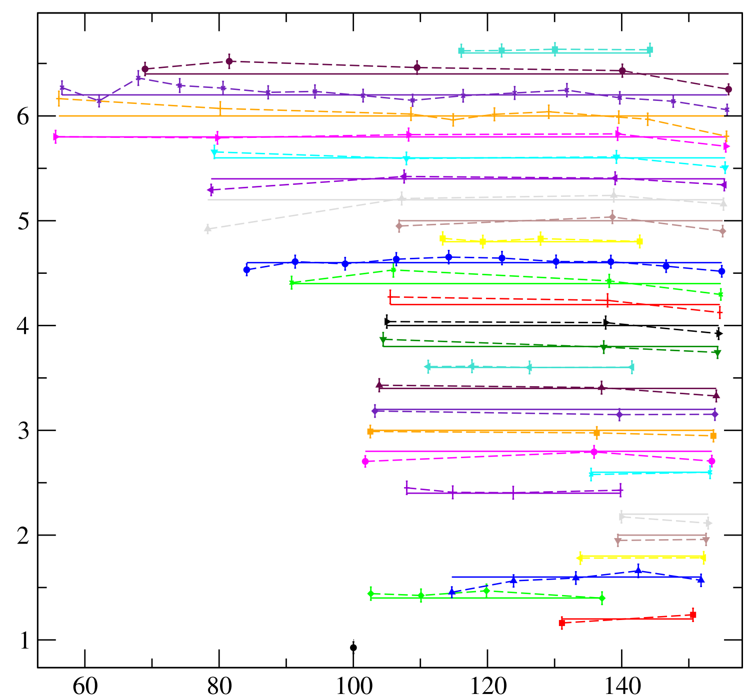
Spiger-cm_ap data

Search file: test1b-v9gL-xs2.sfrescoed+.sfresco;



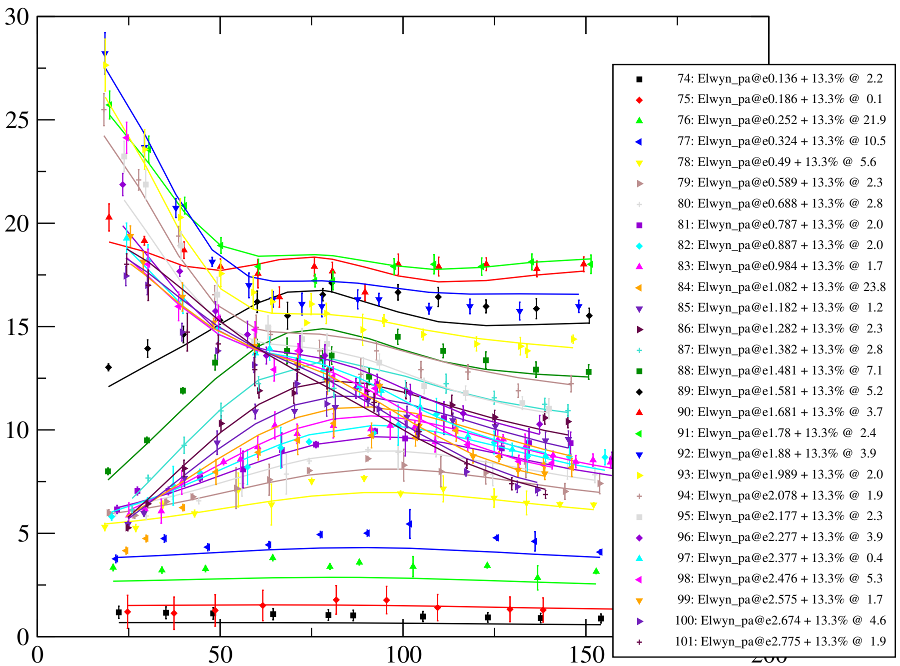
Dataset	Chisq/pts	av norm
Spiger-cm_ap0.dat	1.419	1.004

data_Spiger-cm_ap0.dat_102-130-9gL-xs2.agr (spacing 0.2)

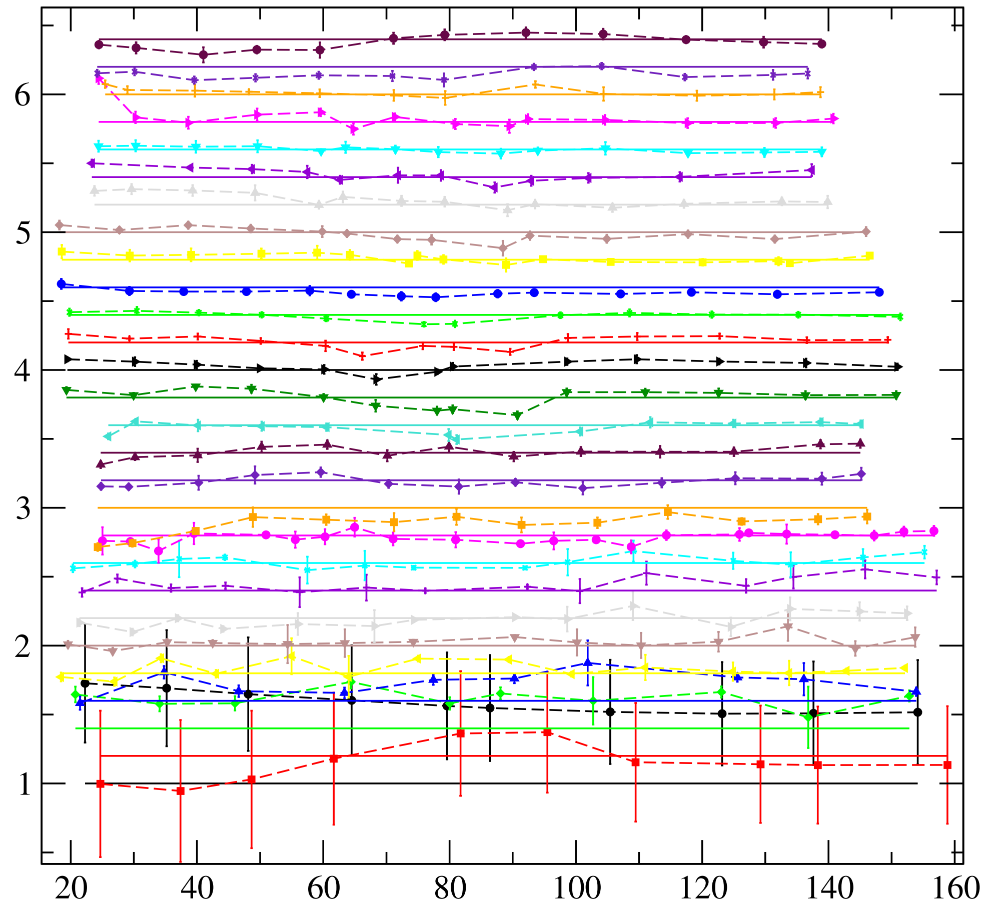


Elwyn_pa data

Dataset	Chisq/pts	av norm
Elwyn_pa.dat	4.317	1.133

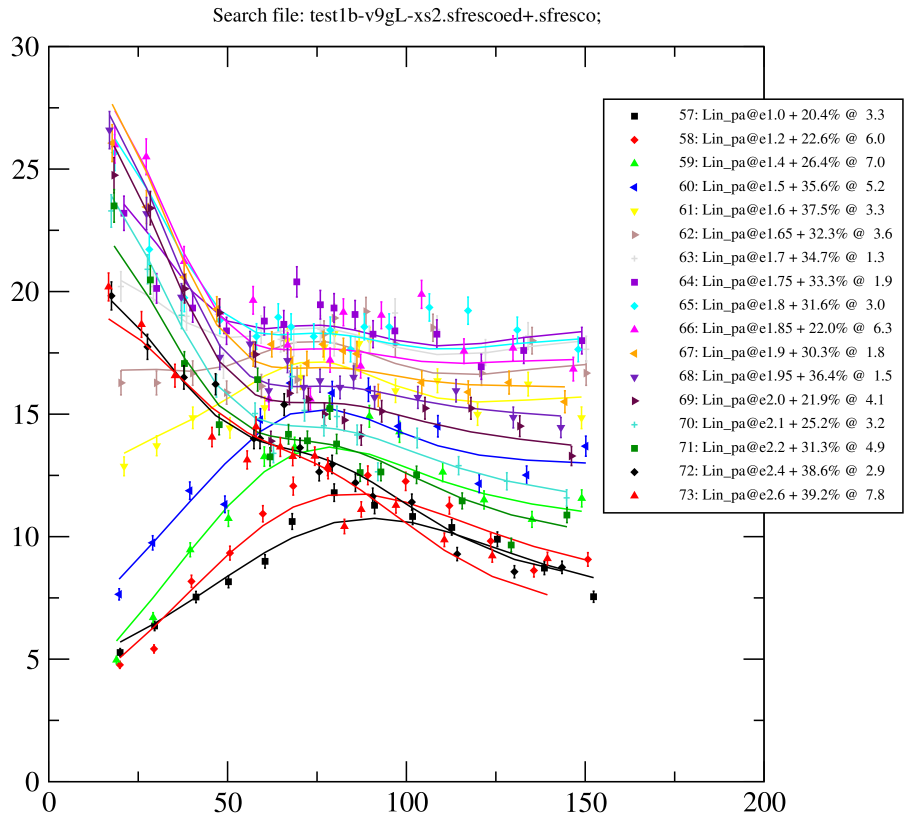


data_Elwyn_pa.dat_74-101-9gL-xs2.agr (spacing 0.2)

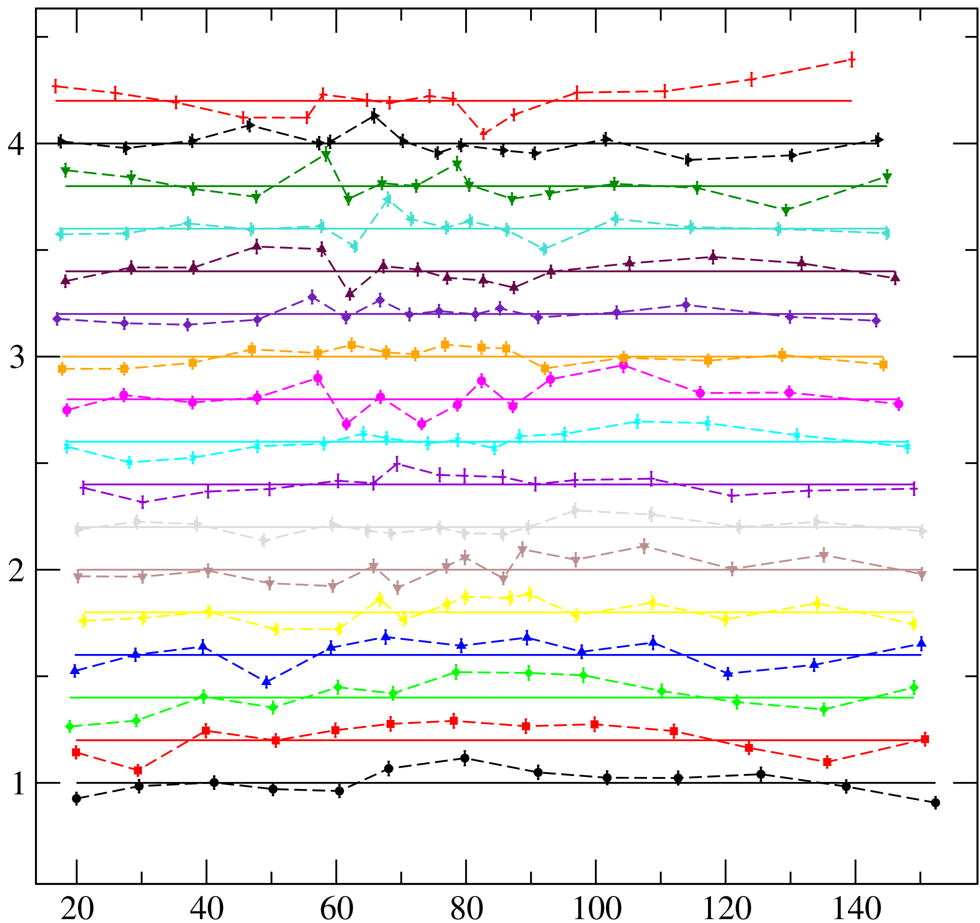


Lin_pa data

Dataset	Chisq/pts	av norm
Lin_pa.dat	3.885	1.305



data_Lin_pa.dat_57-73-9gL-xs2.agr (spacing 0.2)



On the Incompatibility of Lin and Elwyn data

Dataset	Chisq/pts	av norm	sys error %
Elwyn_pa.dat	4.317	1.133	9
Lin_pa.dat	3.885	1.305	10

My fitted norms are larger than the started systematic errors.
Elwyn: 13% > 9% !
Lin: 31% > 10% !

The figure shows these data sets are incompatible.

<u>Need some large scaling factors.</u>

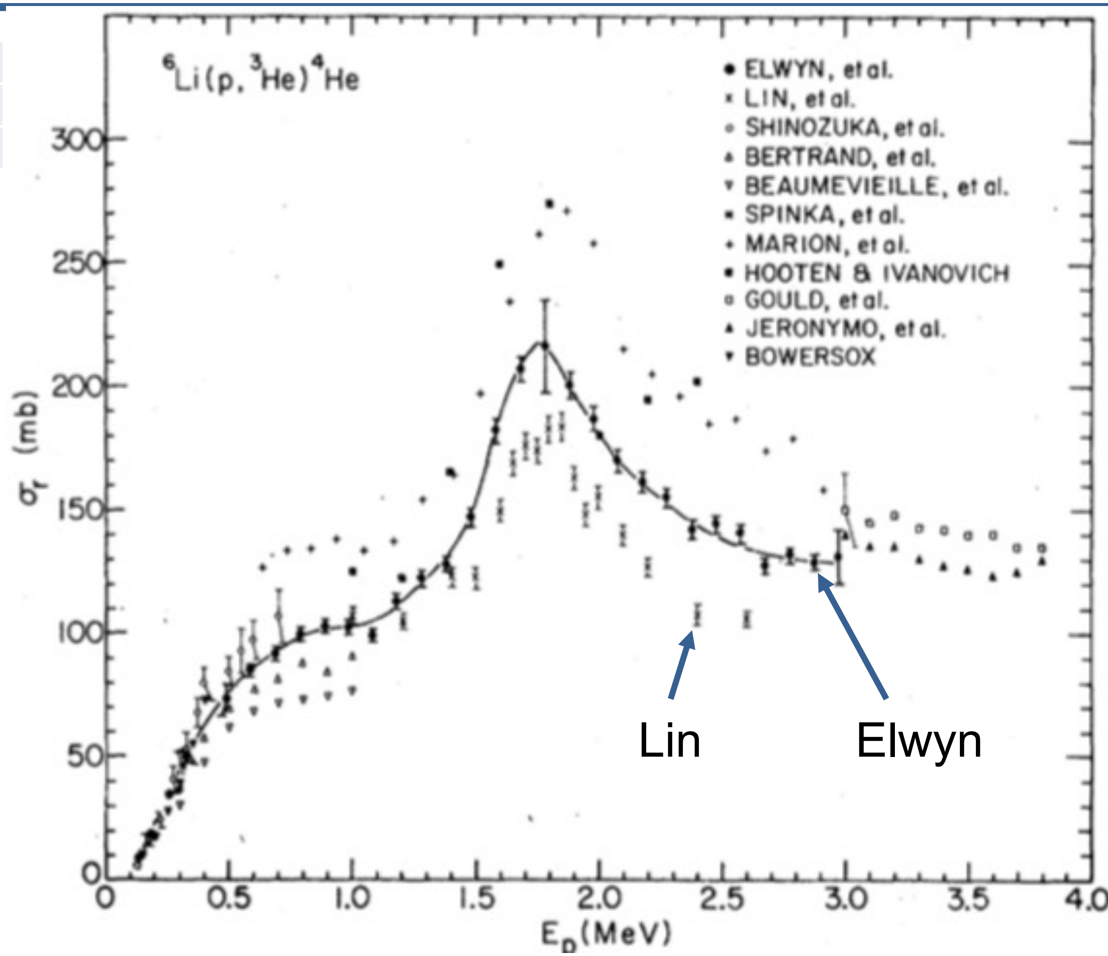


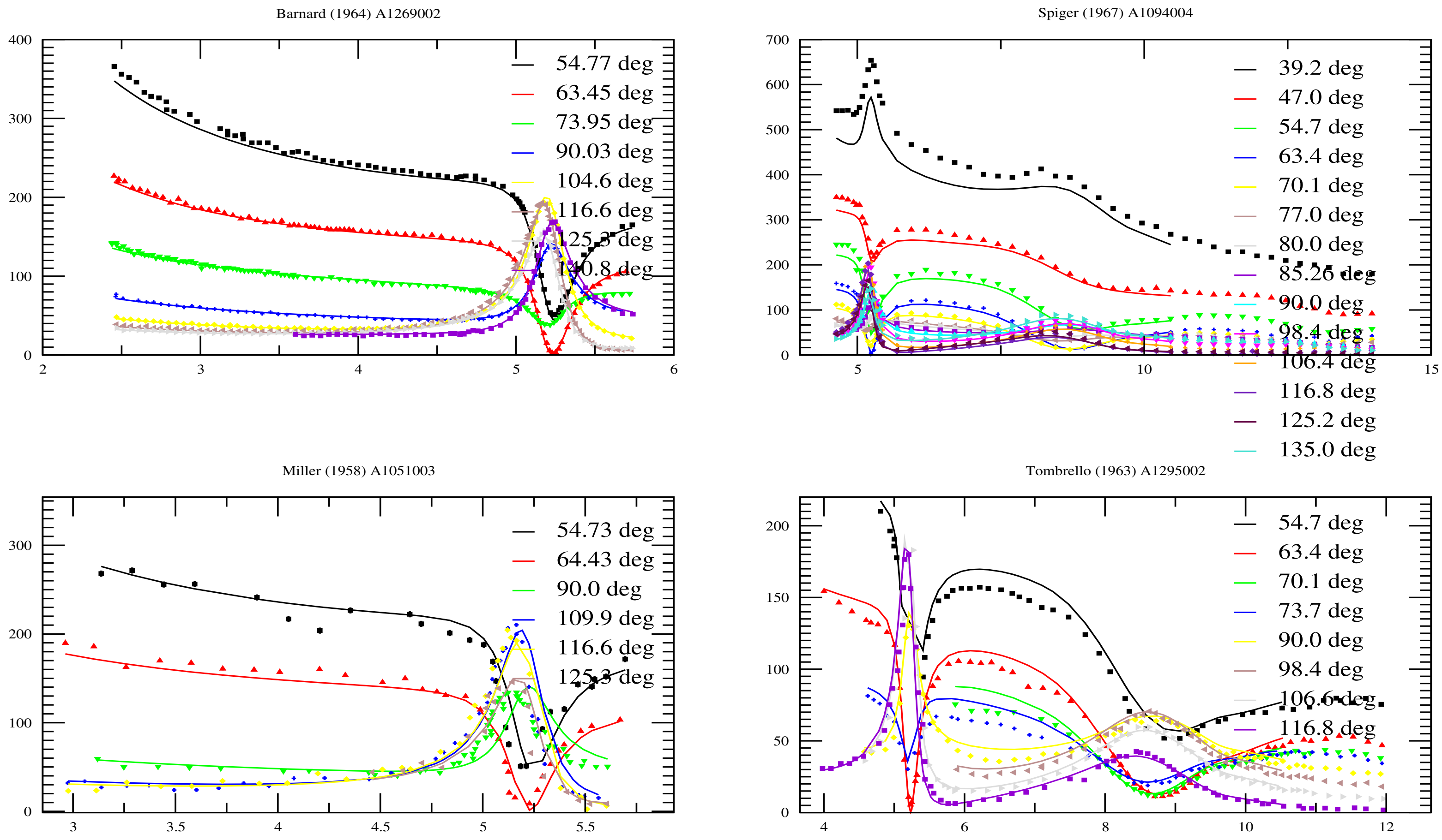
Fig 7 from Elwyn (1979) paper

Review of Fit

- Using ferdinand.py:
  - Make a GNDS or ENDF file of the R-matrix parameters
  - Pointwise reconstruction of elastic and non-elastic cross-sections and distributions, so Fudge .evaluate api works.
- Use validateWithX4plots.py:
  - Extract data from EXFOR independently
  - Compare with evaluate-d ENDF cross-sections
  - Make graphs, one for each EXFOR subentry.
- At least for ^{3}He incident on ^{4}He.
  - See next 6 slides to compare with compatible data from EXFOR
  - (but without normalization factors or energy shifts!)

Review ^{3}He + ^{4}He elastic scattering from EXFOR

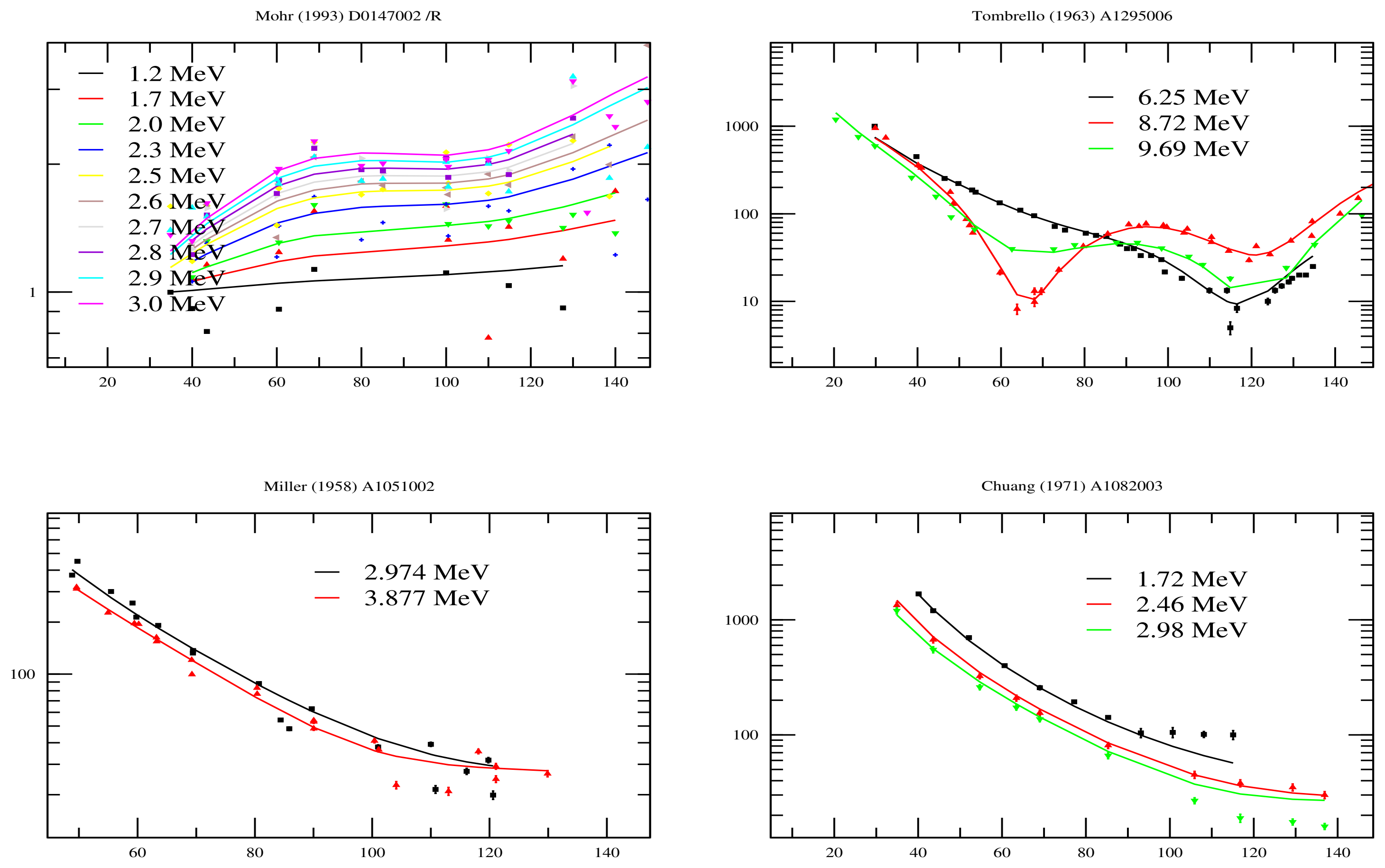
Excitation functions for He3 scattering on He4. Units: mb and MeV



validateWithX4plots.py test1b-v9gL-xs2.sfrescoed+.sfresco-P20,1pt4000eV+.xml -m all -o all -S 1.0 -g -f eps

Review ^{3}He + ^{4}He elastic scattering (2)

Excitation functions for He3 scattering on He4.   Units: mb and MeV

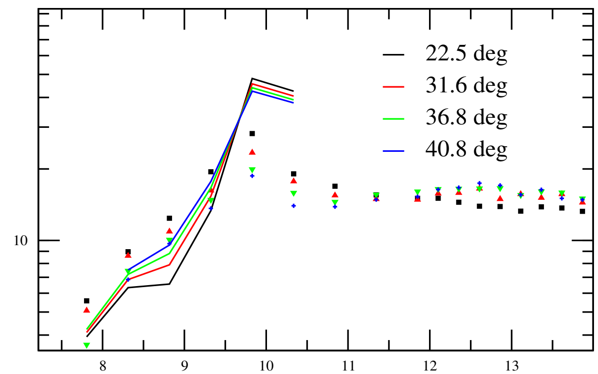


validateWithX4plots.py test1b-v9gL-xs2.sfrescoed+.sfresco-P20,1pt4000eV+.xml -m all -o all -S 1.0 -g -f eps

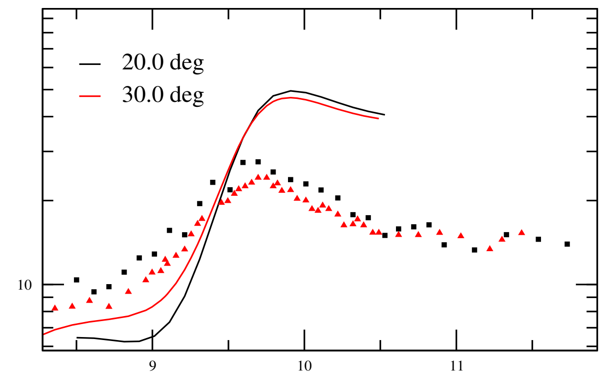
Review ^{3}He + ^{4}He → ^{1}H + ^{6}Li from EXFOR

Excitation functions for He3 scattering on He4. Units: mb and MeV, for H1 + Li6 outgoing channel. Page 2

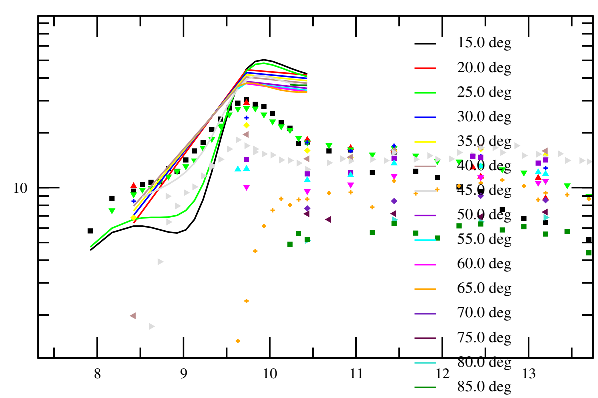
Spiger (1967) A1094007 E*=0.



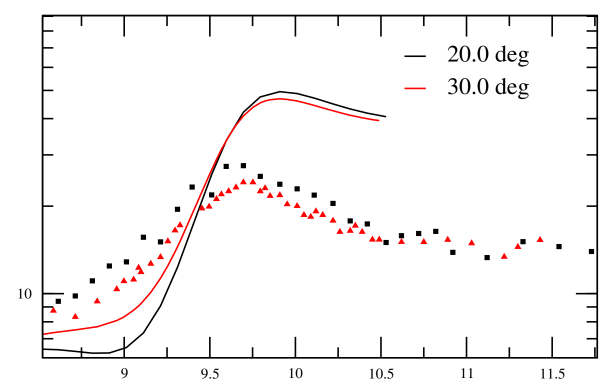
Tombrello (1963) A1295005 E*=0.



Spiger (1967) A1094006 E*=0.



Tombrello (1963) A1295004 E*=0.



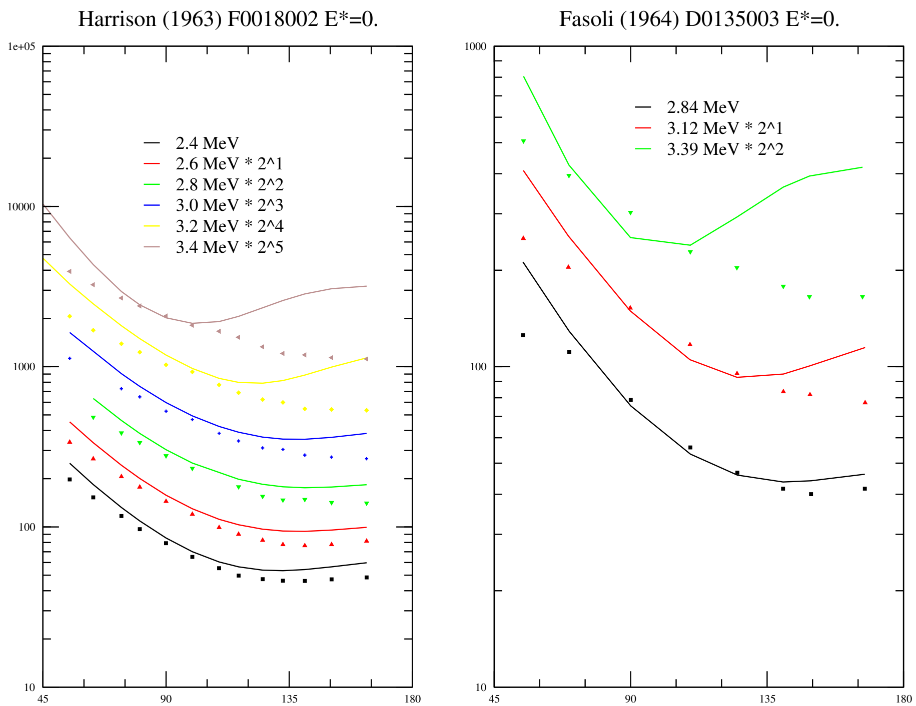
More work needed for higher H1 energies!

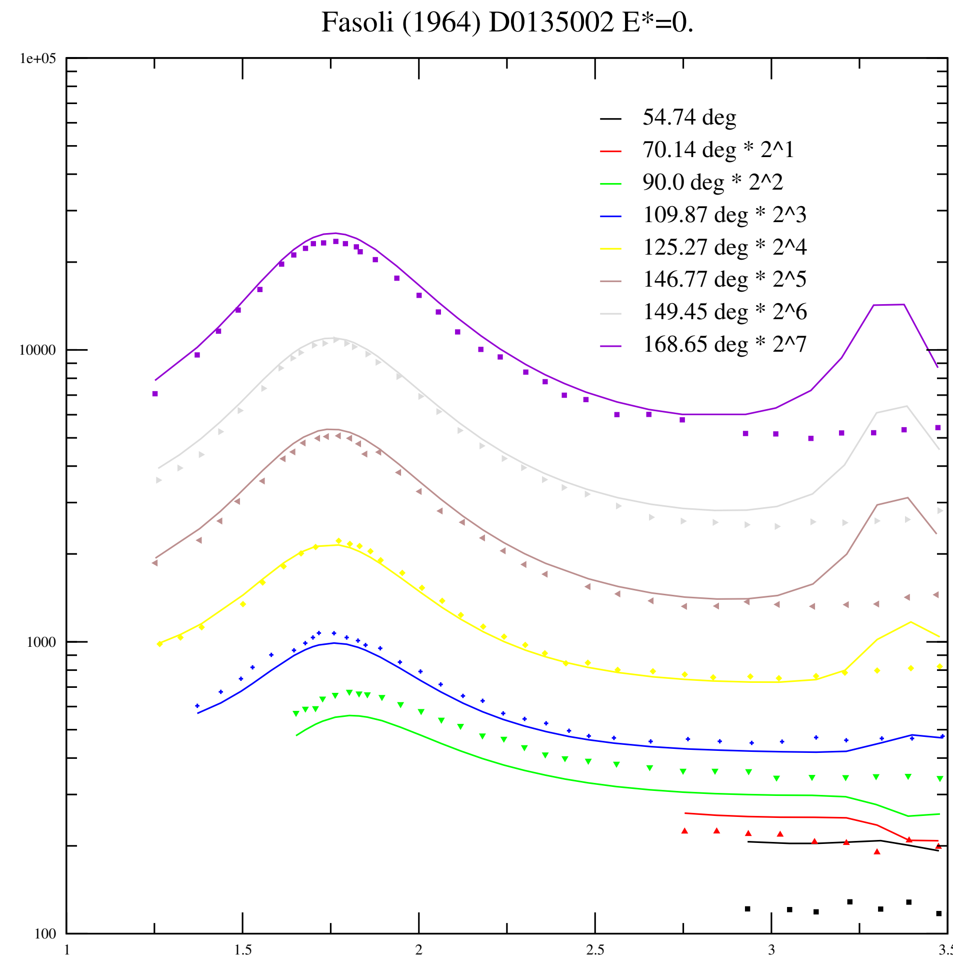
They are above original Test1b range.

validateWithX4plots.py test1b-v9gL-xs2.sfrescoed+.sfresco-P20,1pt4000eV+.xml -m all -o all -S 1.0 -g -f eps

Review $^{1}H + ^{6}Li$ elastic scattering (1)

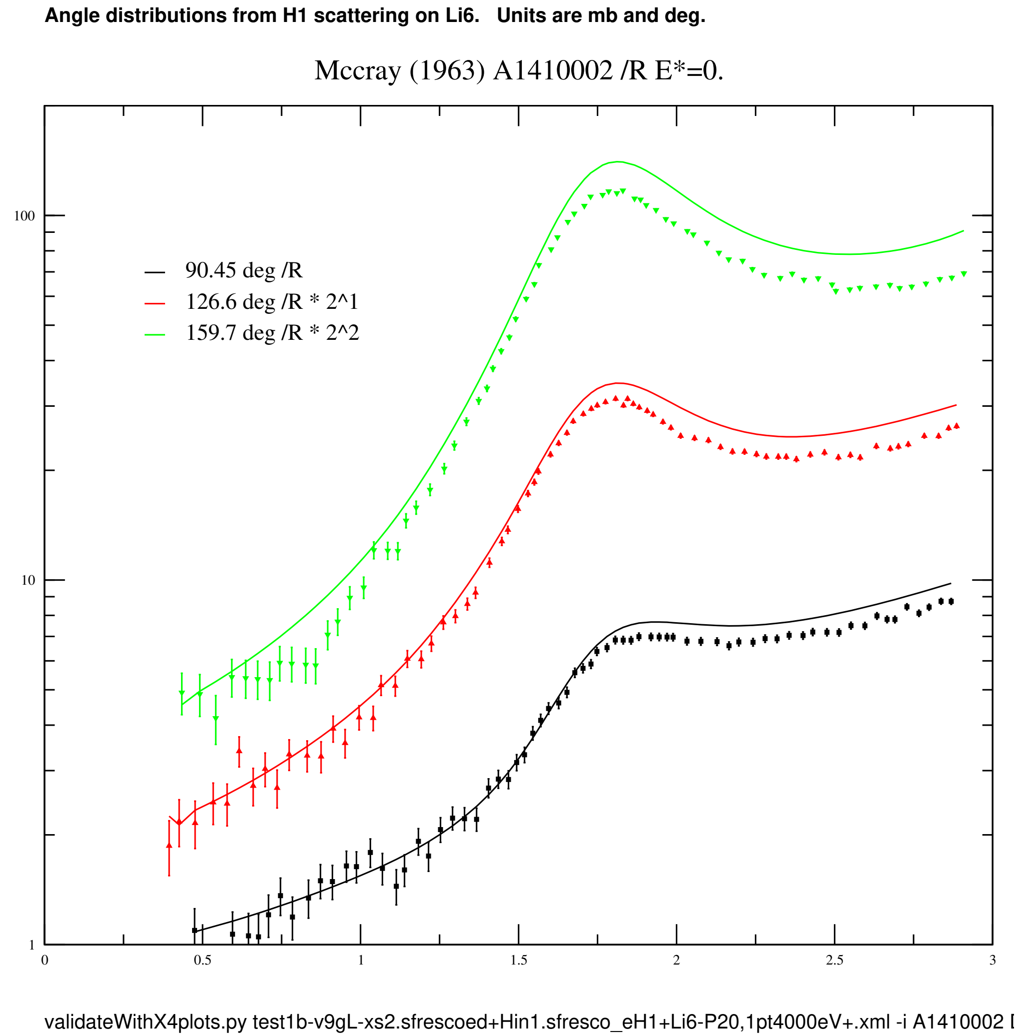
Angle distributions from H1 scattering on Li6. Units are mb and deg.



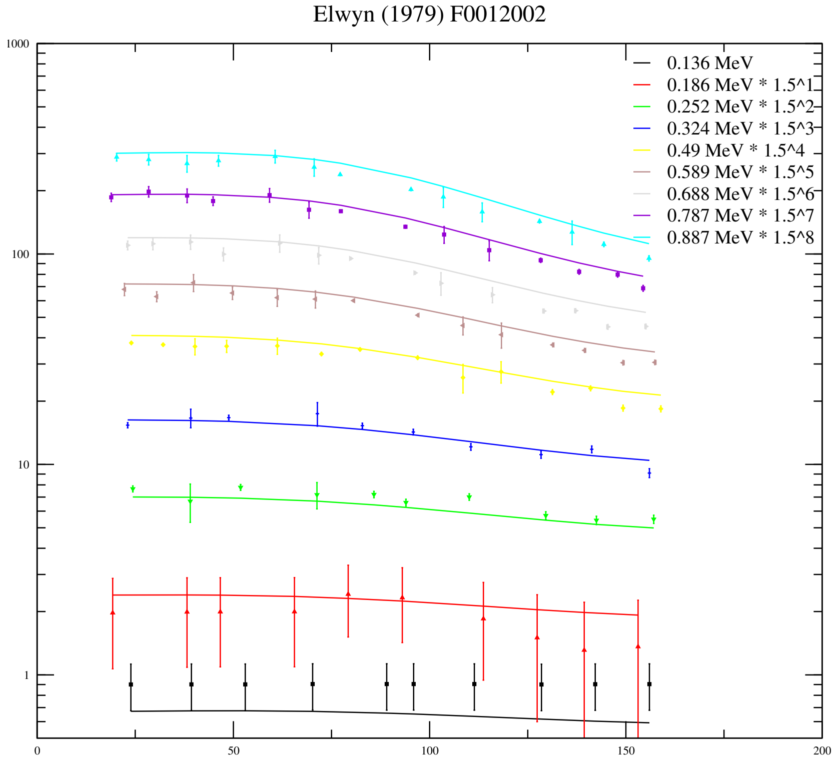


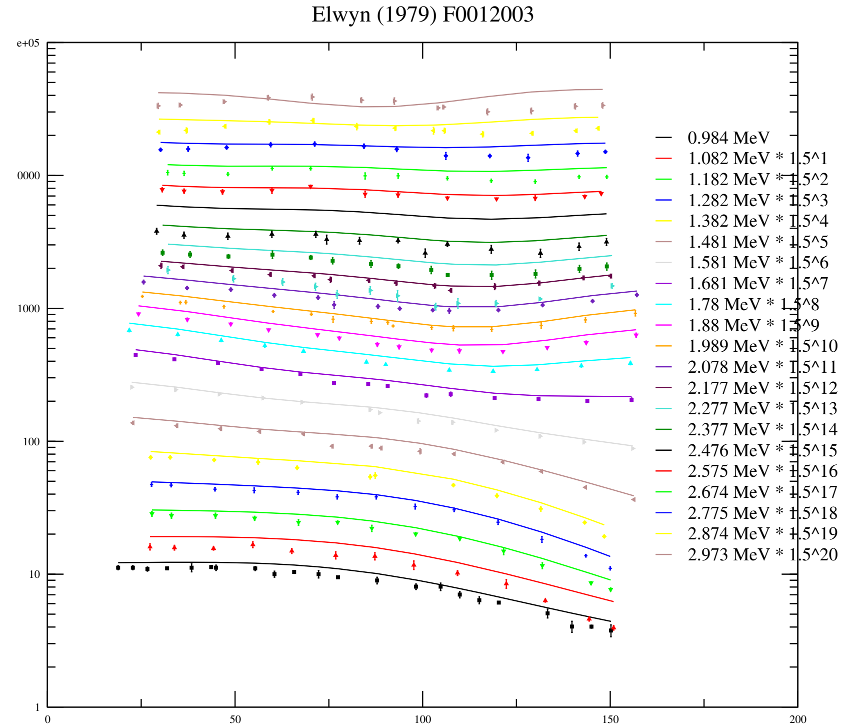
More work needed for higher H1 energies!

Review ^{1}H + ^{6}Li elastic scattering (2)



Review $^{1}H + ^{6}Li \rightarrow ^{4}He + ^{3}He$ from EXFOR





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