Charged Particle Libraries

Review of previous LLNL contributions to ENDF/B-VIII.0

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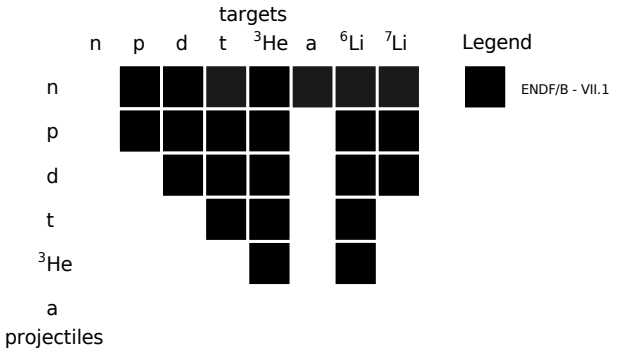
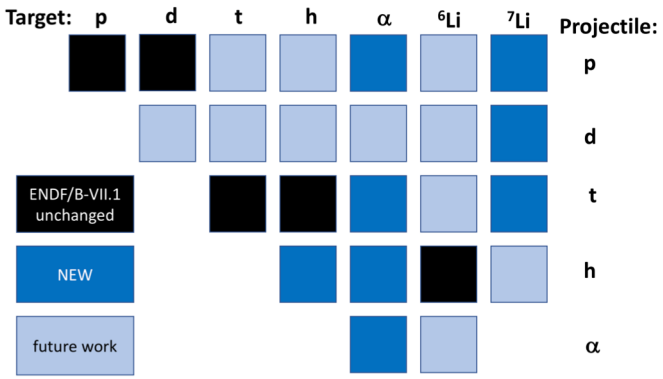
Past, Present and Future Evaluations
Today: talk on 8 Blue and 3 Green = 11 evals

ENDF/B-VII.1



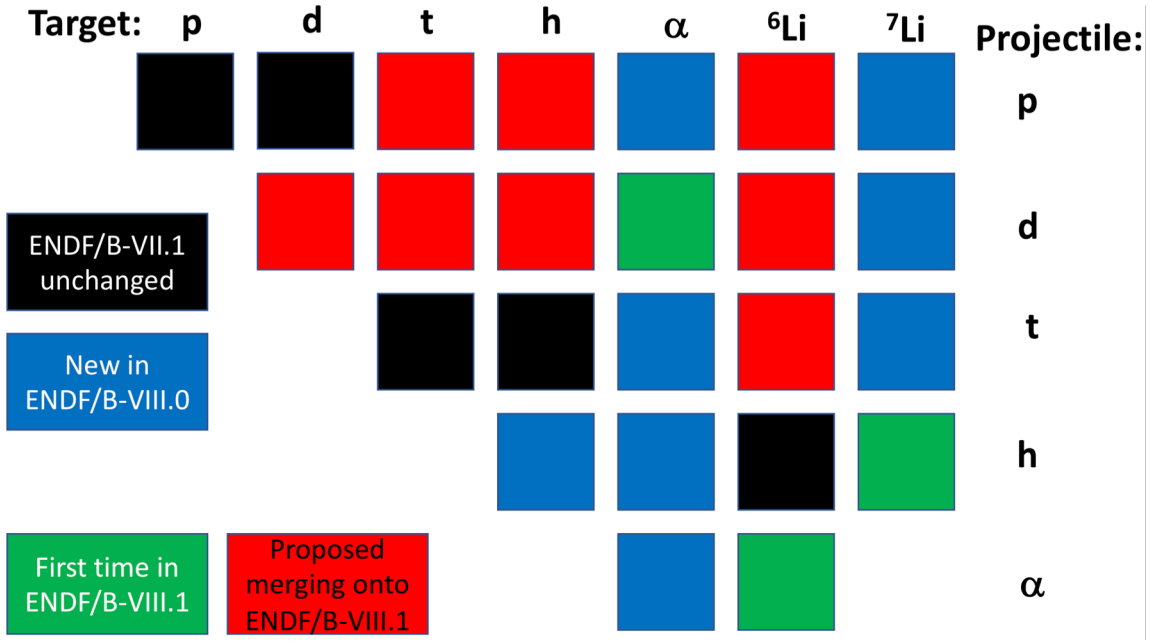
ENDF/B-VIII.0



The 8 submitted from LLNL in October 2016:

a+a, d+7Li, h+h, h+a, p+a, p+7Li, t+a, t+7Li

Proposals for adding and merging into ENDF/B-VIII. 1



Thermonuclear Reaction Library

- Legacy ECPL/ENDL99 evaluations
  - Incident charged particles (p,d,t,He3,He4), light targets Z<=3 (p,d,t,He3,He4,Li6,Li7)
  - R.M. White, D.A. Resler, S.I. Warshaw 'Evaluation of Charged-Particle Reactions for Fusion Applications,' Proc. from Nuclear Data for Sci. and Tech., Ed. S.M. Qaim, Juelich, Fed. Rep. Germany, 13-17 May (1991)
  - S.T. Perkins, D.E. Cullen, 'Elastic Nuclear plus Interference cross sections for light-charge particles' Nucl. Sci. Eng. 77, 20-39 (1981)

- 2010 evaluations at LLNL by Petr Navratil, David Brown & Chris Hagmann
  - Main sources for new evaluations
    - Descouvemont R-Matrix analysis
      - P. Descouvemont, A. Adahchour, C. Angulo, A. Coc, E. Vangioni-Flam, Atomic Data & Nucl. Data Tables 88, 203 (2004)
    - NACRE (Nuclear Astrophysics Compilation of REaction rate)
      - C. Angulo et al., Nucl. Phys. A656 (1999)3-187
    - Experimental data not in EXFOR

- Here: assess accuracy of evaluations contributed by LLNL.

- Most cross-sections were presented at CSEWG 2016 (supplemental slides below). So here we focus on the angular distributions of two-body channels vs. EXFOR.

  (Future methods will focus on breakup distributions)

Table of LLNL contributed evaluations

					ejectiles:								
ENDF/B-VIII version		n	2n	3n	p	2p	d	n+p	t	h	a		
0	p + a				elastic								p
0	p + Li7	50, 51			pt. Coul		650				800		p
1	d + a	50			600		elastic	28					p
0	d + Li7	22	16		103		elastic		700				p
0	t + a												p
0	t + Li7	50	24	17					pt. Coul				
0	h + h					111				elastic			
0	h + a									elastic			p
1	h + Li7				600		117	45	105	pt. Coul	800, 801		p
0	a + a										elastic		p
1	a + Li6				600		650, 651				pt. Coul		p

All distributions exist, but most are simple forms extrapolated from limited measurements.

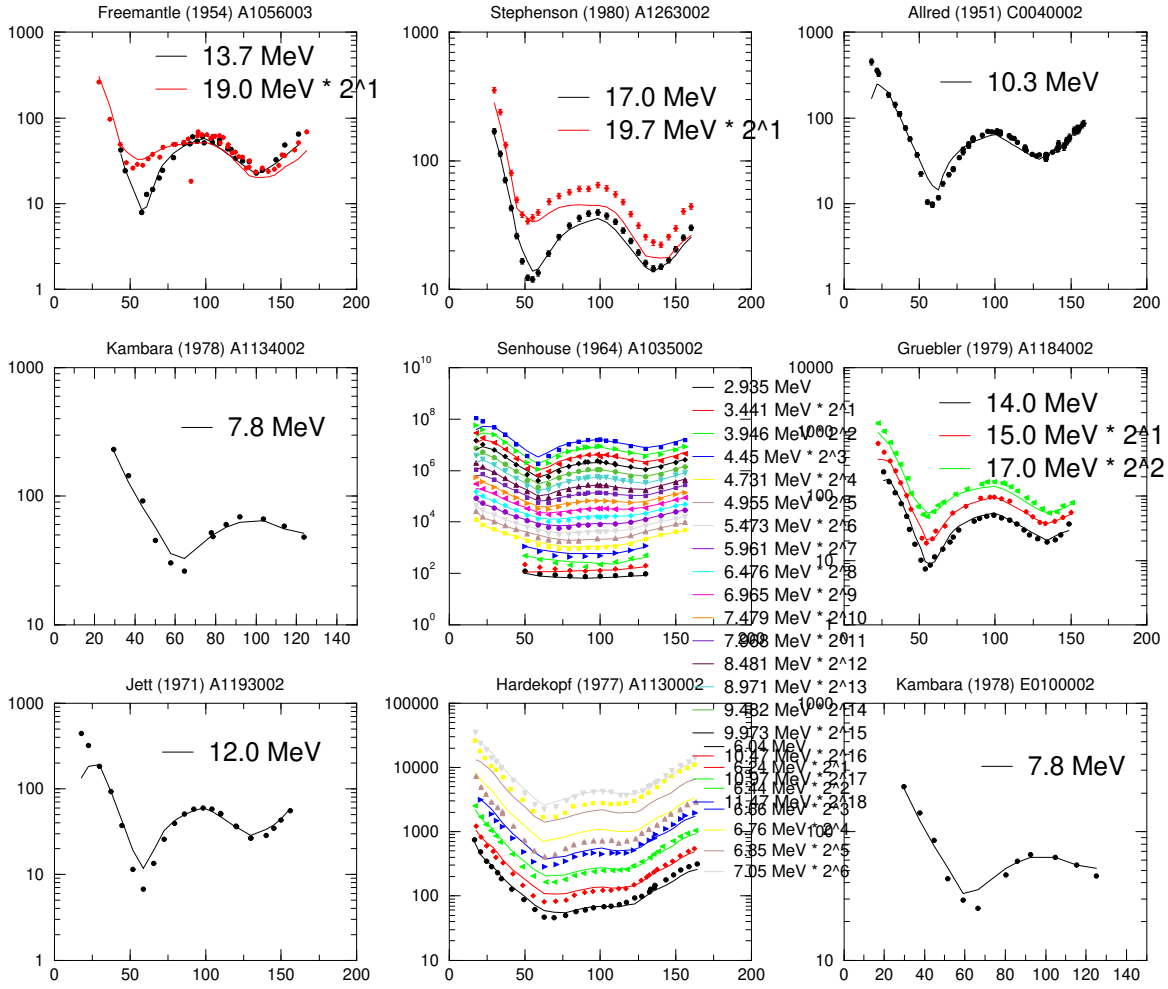
Many of these channels (2n, 3n, 2p, n+p) are too difficult for 2-body R-matrix models.

Evaluation Paths

- These from LLNL are temporary evaluations (2010 through 2020?)
  - Combination of cross sections and distributions from different sources
  - Trying to follow the experimental data evaluated as the best
- The future is to use full R-matrix evaluations!!
  - Where possible, publish R-matrix evaluations from LANL
  - Include all R-matrix parameters (even if relativistic kinematics)
  - Include all fitted data normalization factors
- Good way: convert from EDA, AZURE, FRESCO, SAMMY, HYRMA formats to GNDS and then ENDF
  - Using Ian's code Ferdinand.py
  - This is being developed with USNDP funding.
- Then can encourage, monitor and verify new R-matrix fits to data
  - Determine how to fit data above 3-body thresholds
  - Supplement with Hauser-Feschbach models above resonance region
- International effort through IAEA to verify and validate the above R-matrix codes.
  - Soon to be provided: h+α and p+6Li evaluations

d + α : Good elastic distributions vs. EXFOR data

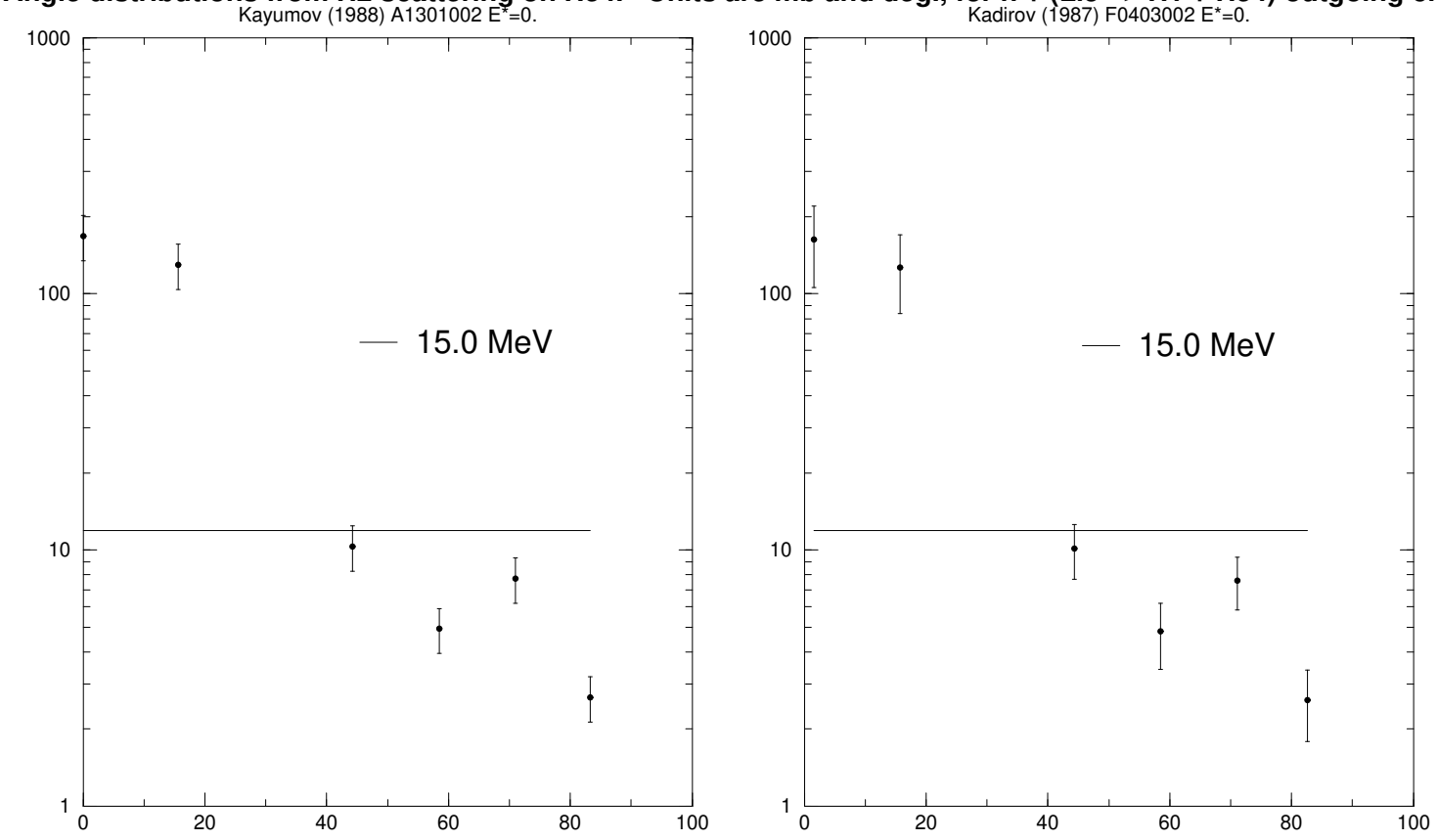
Angle distributions from H2 scattering on He4. Units are mb and deg.



validateWithX4plots.py d–002_He_004.xml –m all –o all –r 2 –l –f eps

d + α :
Poor fits to 2-step breakup channels

Angle distributions from H2 scattering on He4. Units are mb and deg., for n + (Li5 –> H1 + He4) outgoing channel. Page 3



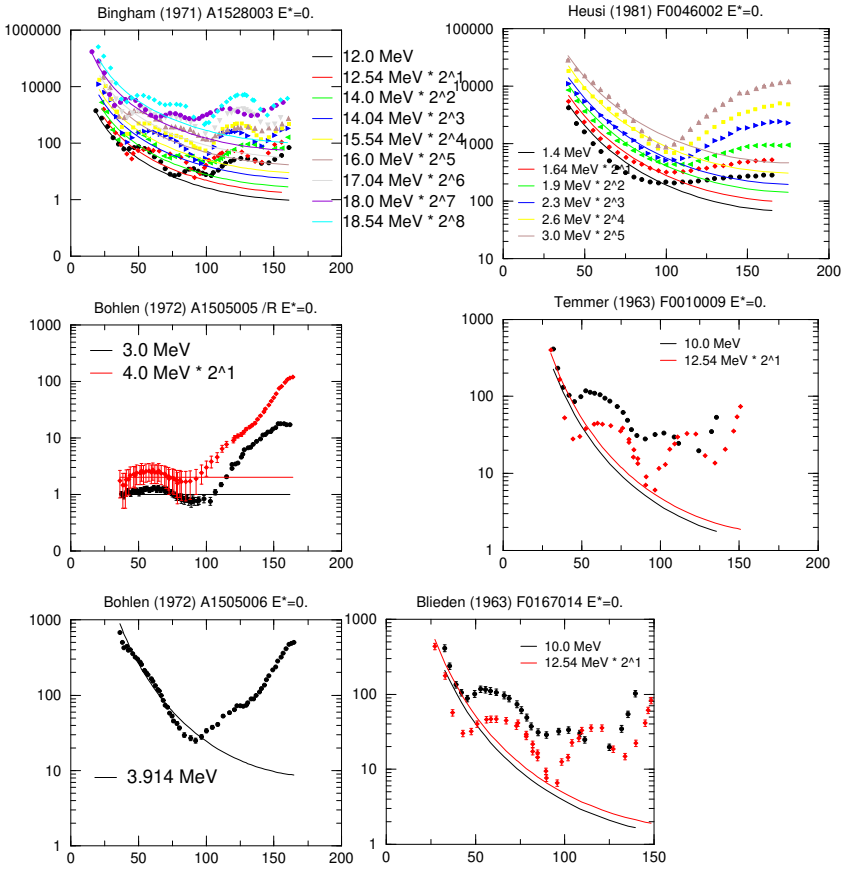
validateWithX4plots.py d–002_He_004.xml –m all –o all –r 2 –l –f eps

α + Li6

Elastic is only point Coulomb!

Starts ok at lowest energies & angles, but diverges.

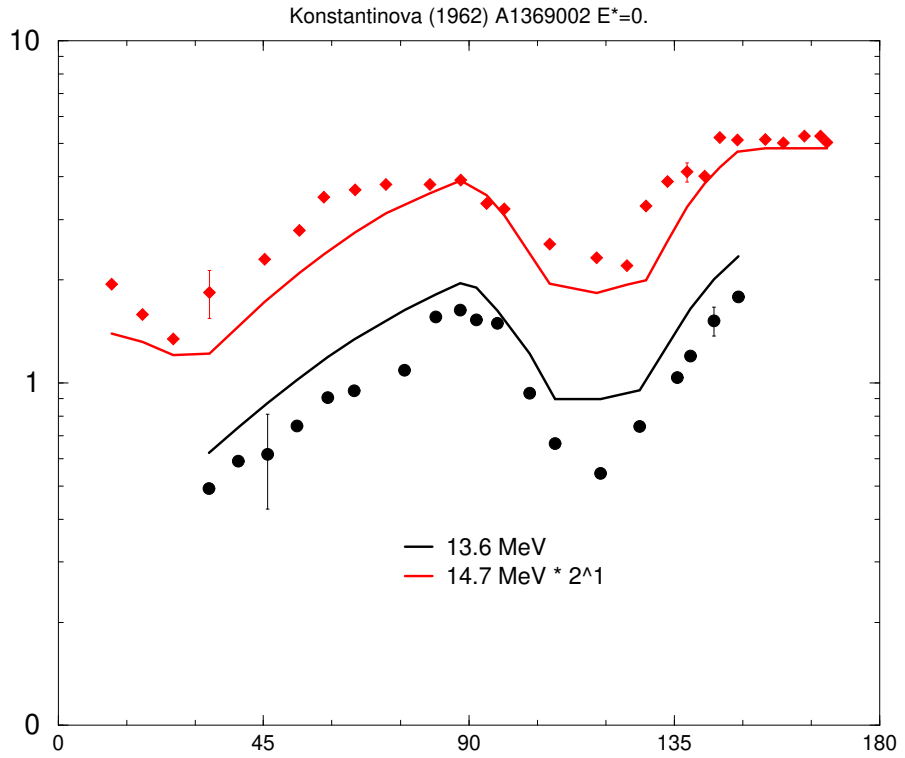
Angle distributions from He4 scattering on Li6. Units are mb and deg.



validateWithX4plots.py a–003_Li_006.xml –m all –o all –r 2 –l –f eps

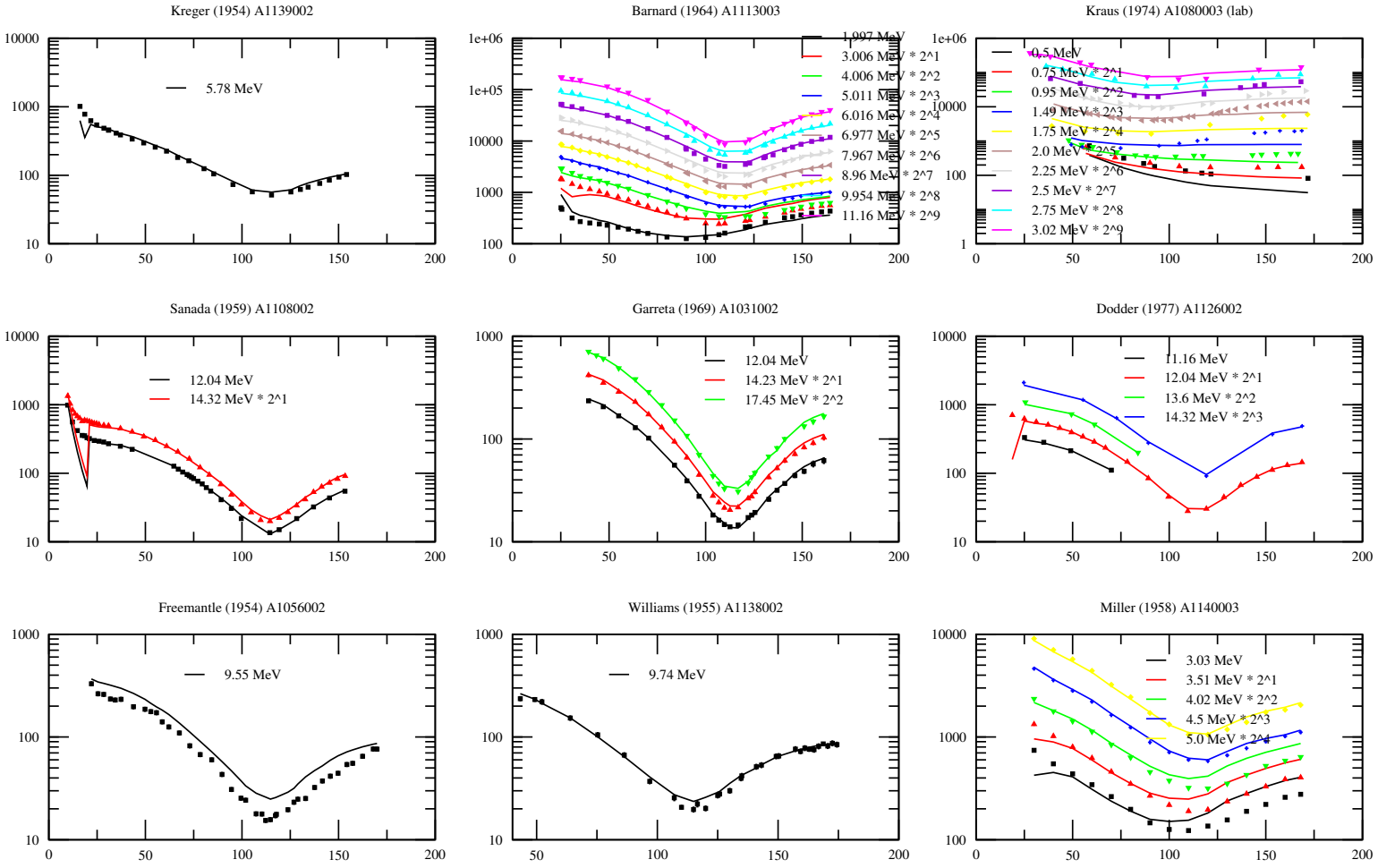
(a,p) and (a,d) distributions plausible

Angle distributions from He4 scattering on Li6. Units are mb and deg., for H1 + Be9 outgoing channel.



p + α:
good elastic distributions (the only channel!)

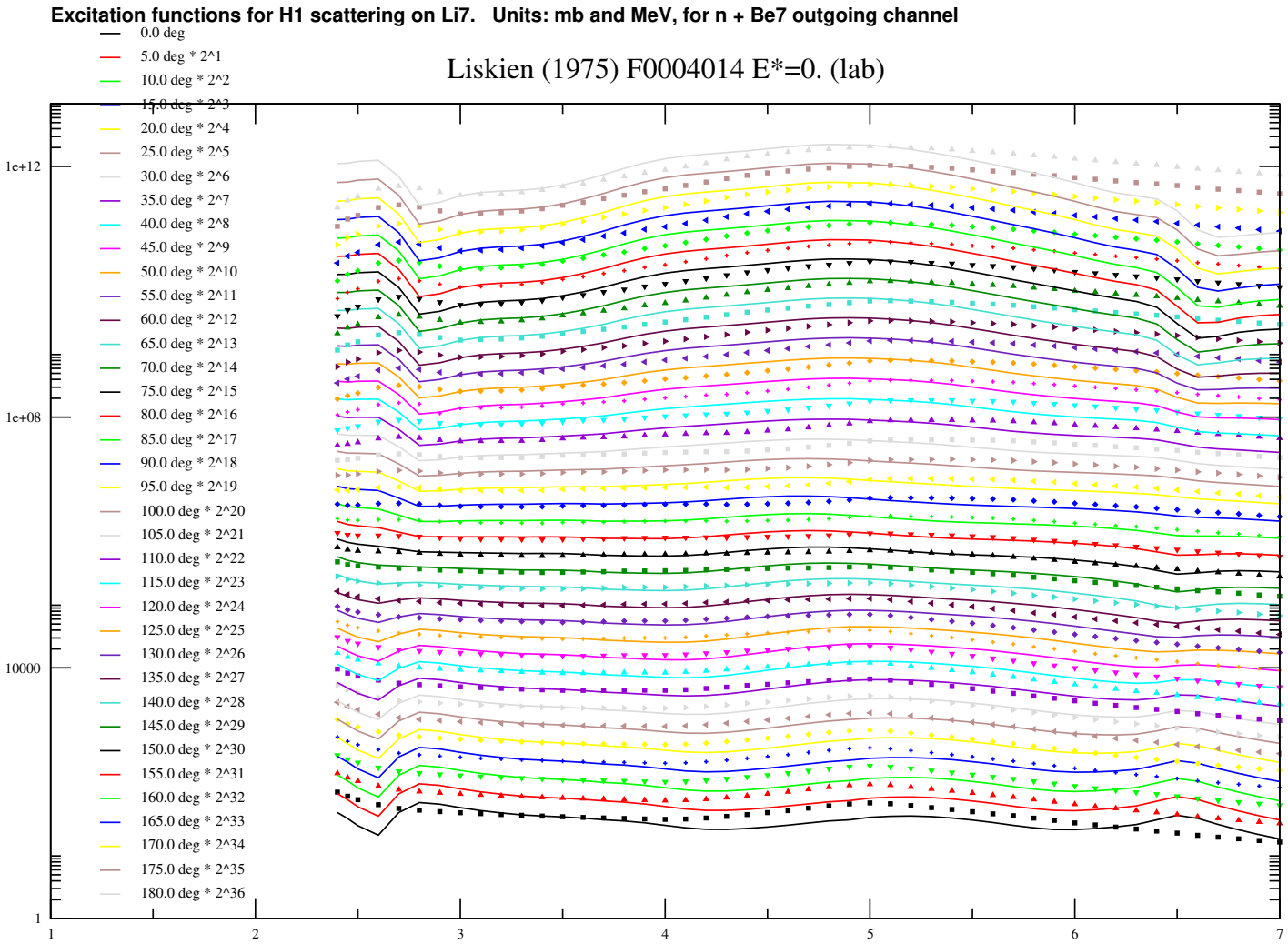
Angle distributions from H1 scattering on He4. Units are mb and deg.



Should reduce N+l cutoff below 20º!

validateWithX4plots.py p-002_He_004.xml -m all -o all -r 3 -g -l -f eps

p + Li7 -> n+Be7 :
From ENDF/B-VII.0 : mostly good!



validateWithX4plots.py p-003_Li_007.xml -i F0004014 -m all -o all -L 0.0 -e 2.4 -r 3 -g -l -f eps

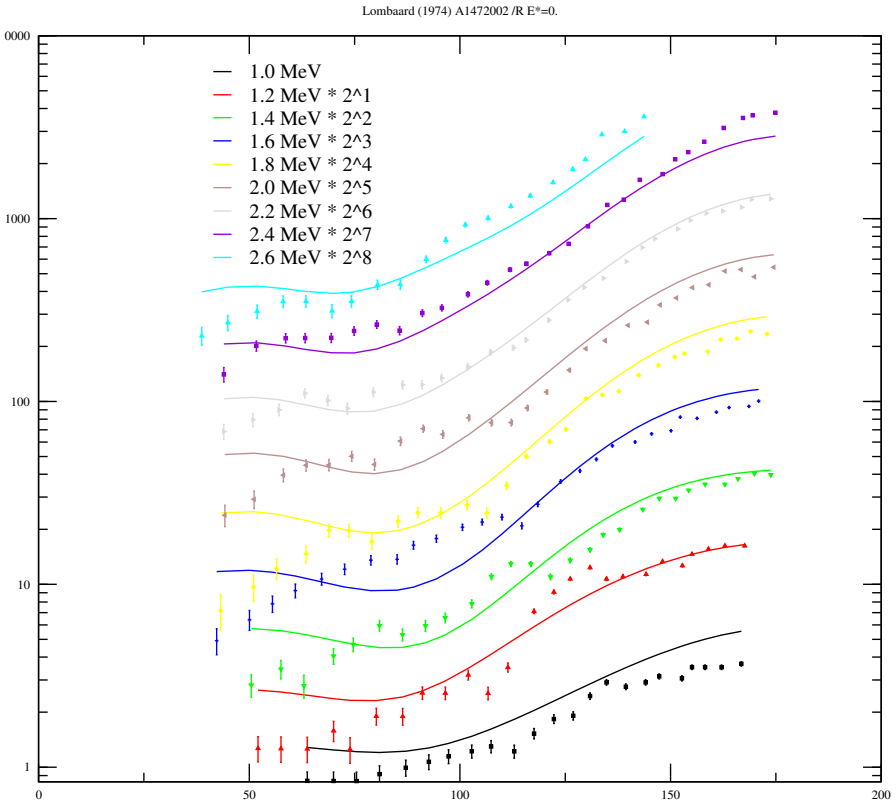
The p+Li7 elastic channel is Pure Coulomb.

Misses all resonances 0.4, 1, 2.1 MeV . . .

d + Li7:
elastic scattering

Elastic scattering ok at lowest energies

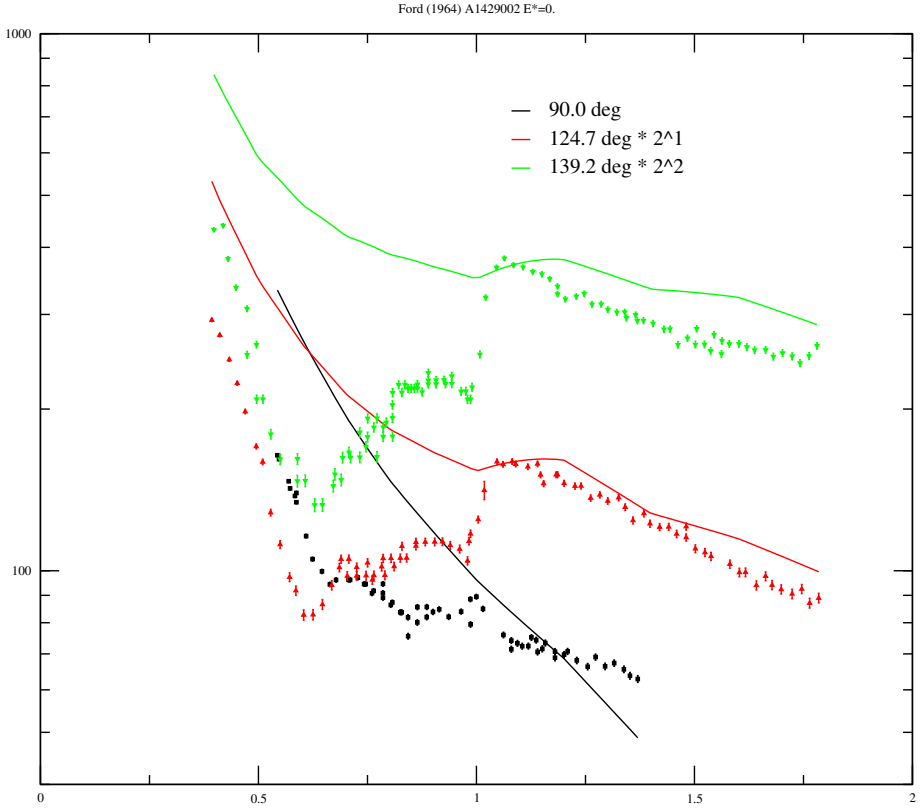
Angle distributions from H2 scattering on Li7. Units are mb and deg.



validateWithX4plots.py d-003_Li_007-rev.xml -i A1429002 A1472002 -m all -r 3 -g -l -f eps

But misses resonances if plotted as excitations:

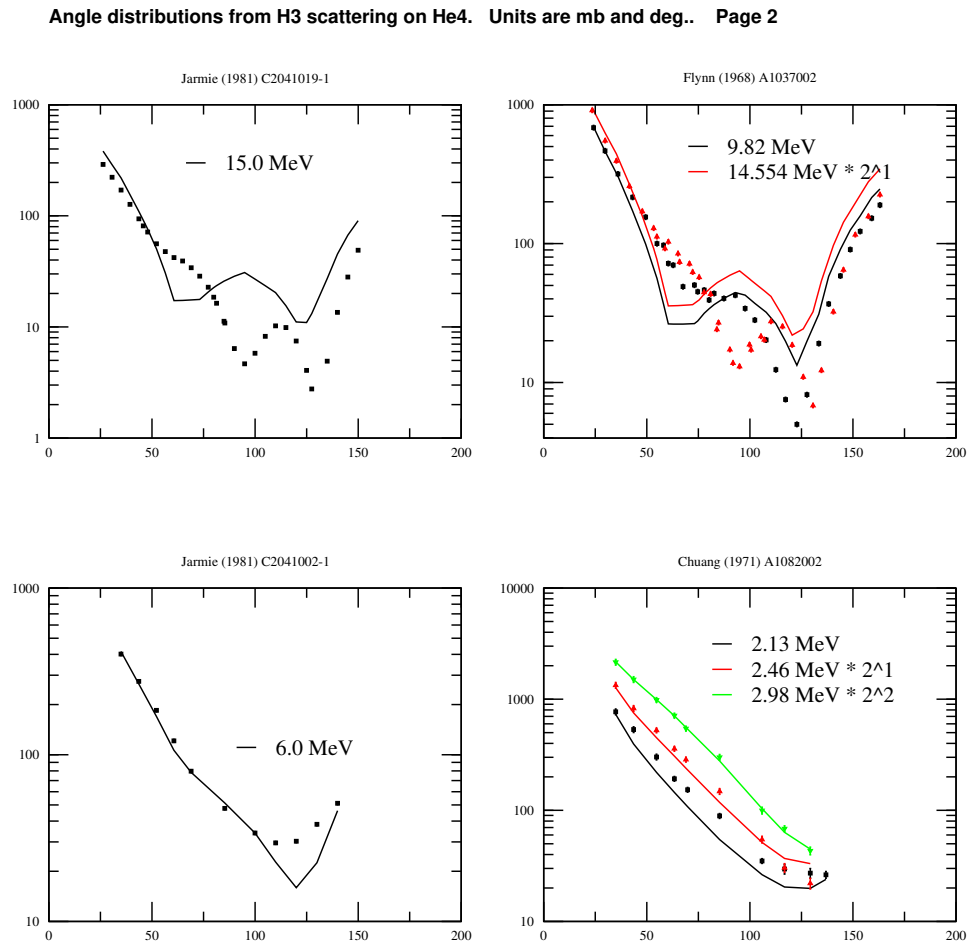
Angle distributions from H2 scattering on Li7. Units are mb and deg.



validateWithX4plots.py d-003_Li_007-rev.xml -i A1429002 A1472002 -m all -r 3 -g -l -f eps

t + α : elastic distributions (only channel) approximate

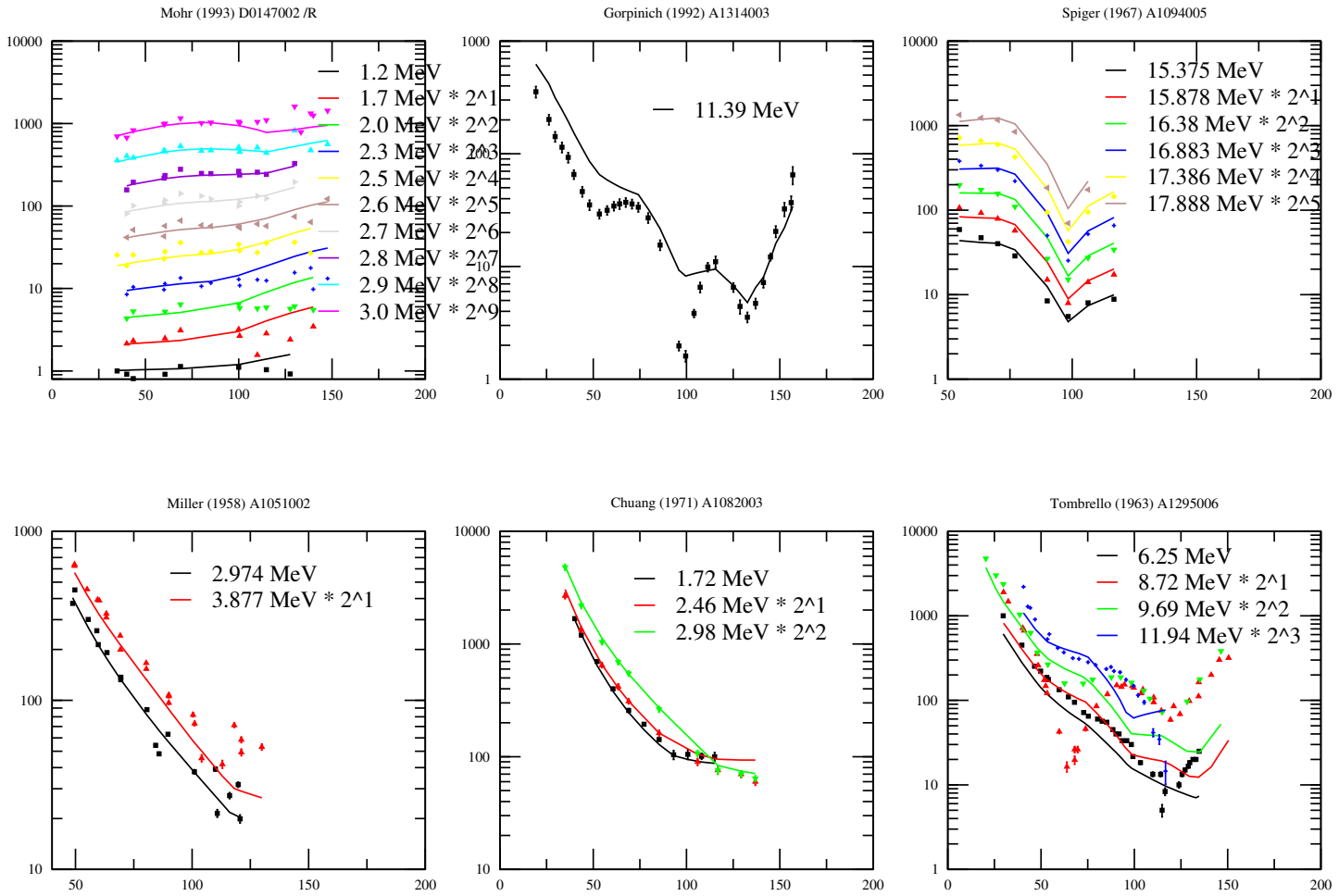
Elastic is approximate over many energies



validateWithX4plots.py t-002_He_004.xml -m all -o all -r 3 -g -l -f eps

h + α : elastic distributions (only channel) plausible

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



validateWithX4plots.py h-002_He_004.xml -m all -o all -r 3 -g -l -f eps

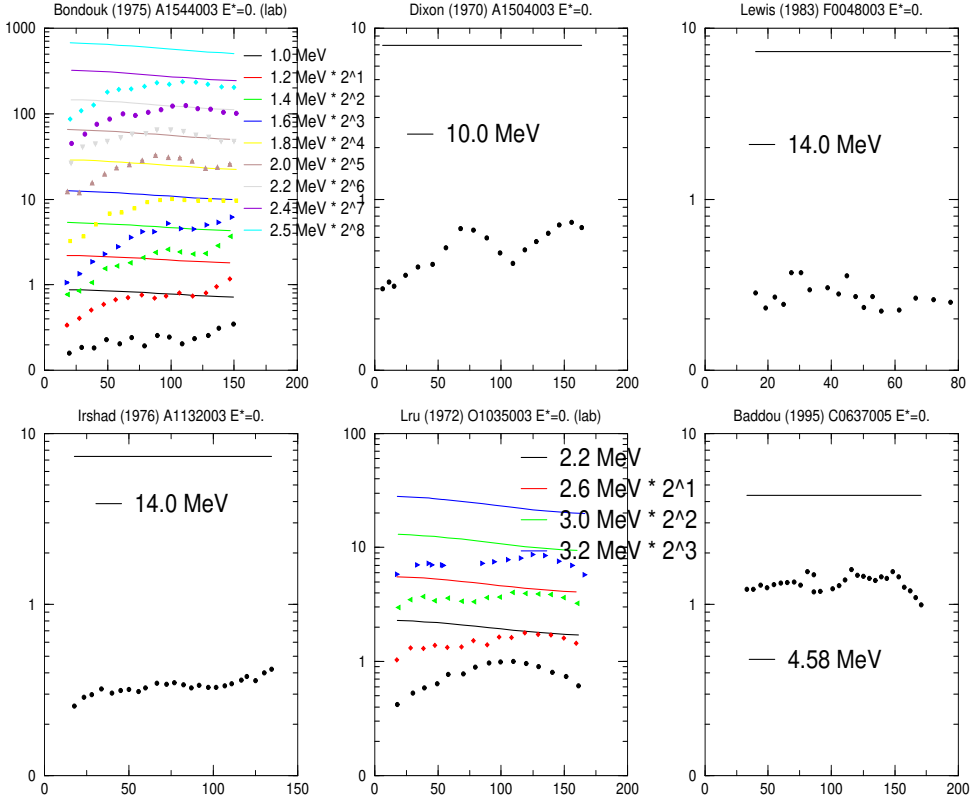
Maybe missing a resonance around 9 MeV?

h + Li7:
A primitive evaluation

Elastic is only point Coulomb!

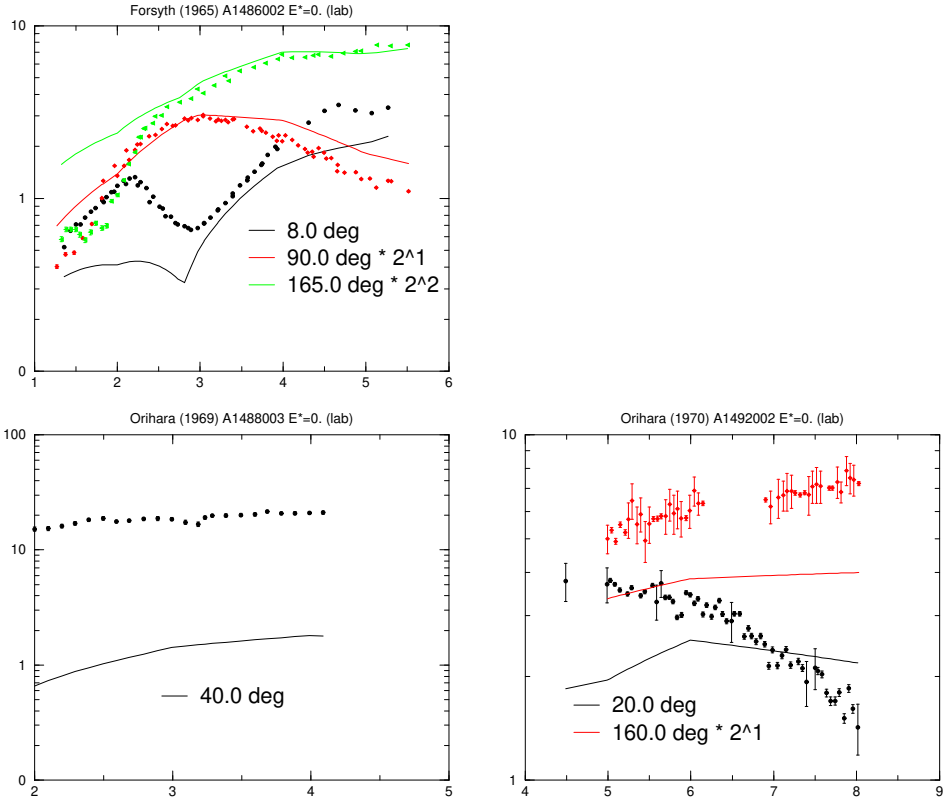
Li7(h,a)Li6 needs improvements!

Angle distributions from He3 scattering on Li7. Units are mb and deg., for H1 + Be9 outgoing channel



validateWithX4plots.py h–003_Li_007.xml –x C0139002 –m all –o all –r 2 –l –f eps

Angle distributions from He3 scattering on Li7. Units are mb and deg., for He4 + Li6 outgoing channel. Page



validateWithX4plots.py h–003_Li_007.xml –x C0139002 –m all –o all –r 2 –l –f eps

Summary

- Describing data with these ENDF contributions:
  - Elastic scattering is often well described for scattering on alpha particles.
  - Some principal two-body reaction channels are described
  - 3-body-channel fits not addressed here.
  - There are many channels that should be in ENDF/B evaluations.
  - Many of these channels are very sketchily described. For example by point-Coulomb elastic scattering.

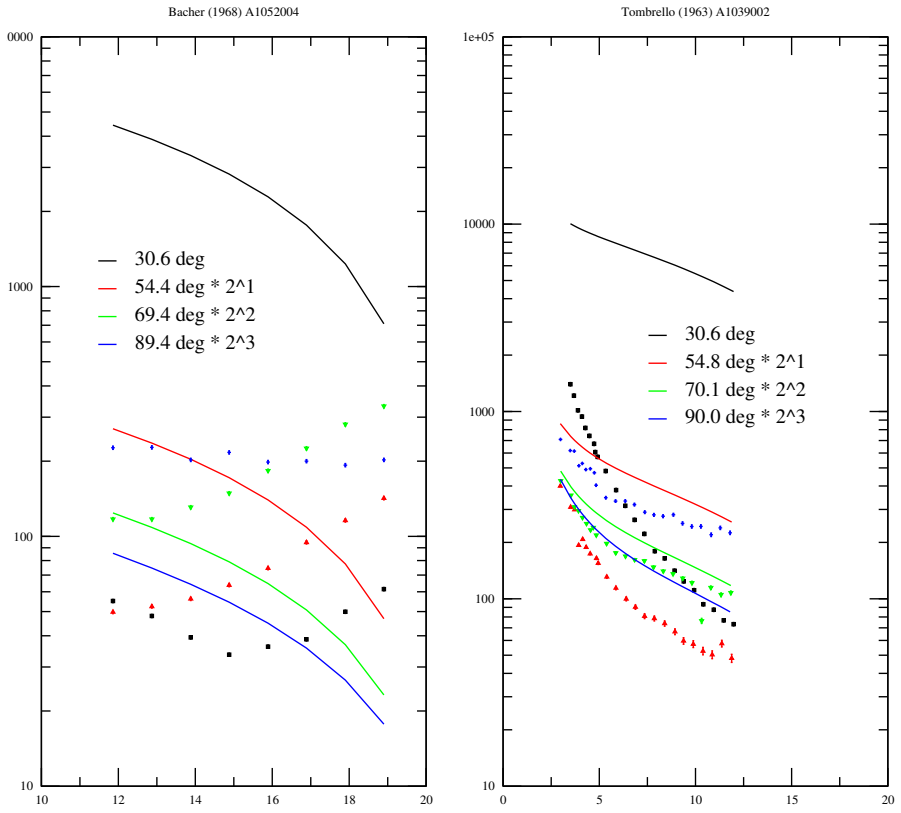
- Conclusions
  - These are definitely temporary evaluations needed because nothing there previously
    (e.g. no evaluations for charged-particle scattering on alphas,
    or missing channels in previous evaluations)
  - There are many resonance structures that are often missing in the evaluations
  - Used until replaced by something better

- We look forward to 2-body R-matrix models!
  - Assist LANL in making and checking MF=2 data sections in ENDF6 format libraries.

- Even more need for theory development of R-matrix for breakup channels!

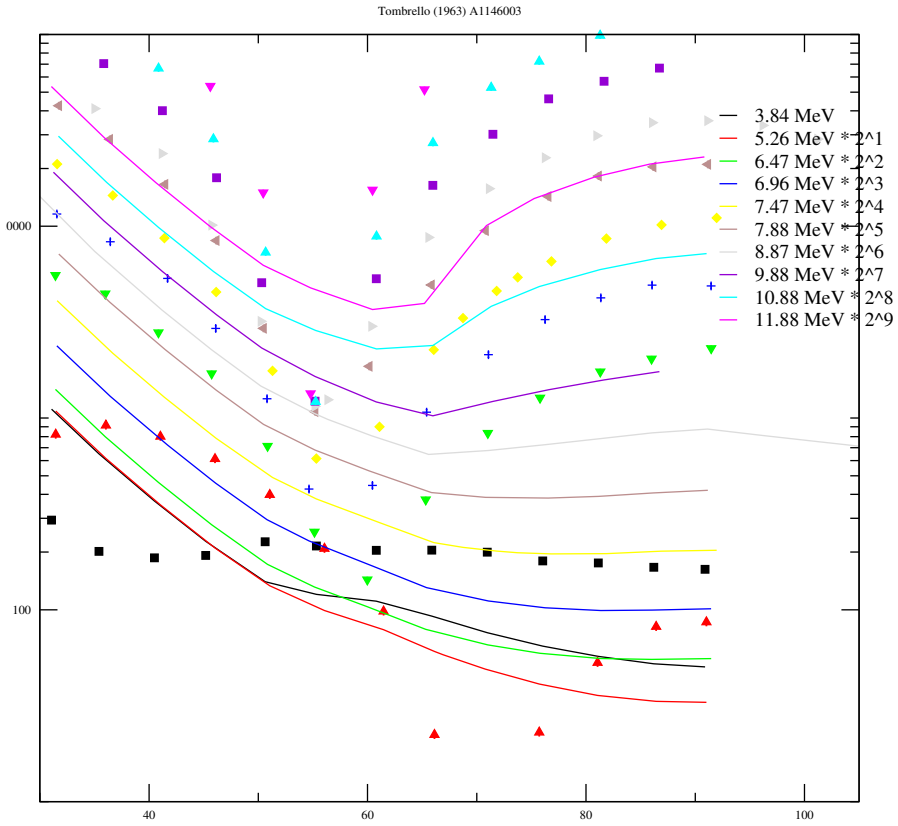
h + h and α + α : elastic distributions (only channel) not good!

Angle distributions from He3 scattering on He3. Units are mb and deg.



validateWithX4plots.py h-002_He_003.xml -m all -o all -r 3 -g -l -f eps

Angle distributions from He4 scattering on He4. Units are mb and deg.



validateWithX4plots.py a-002_He_004.xml -i A1146003 -m all -o all -r 3 -g -l -f eps

Have I made a mistake for identical particles?

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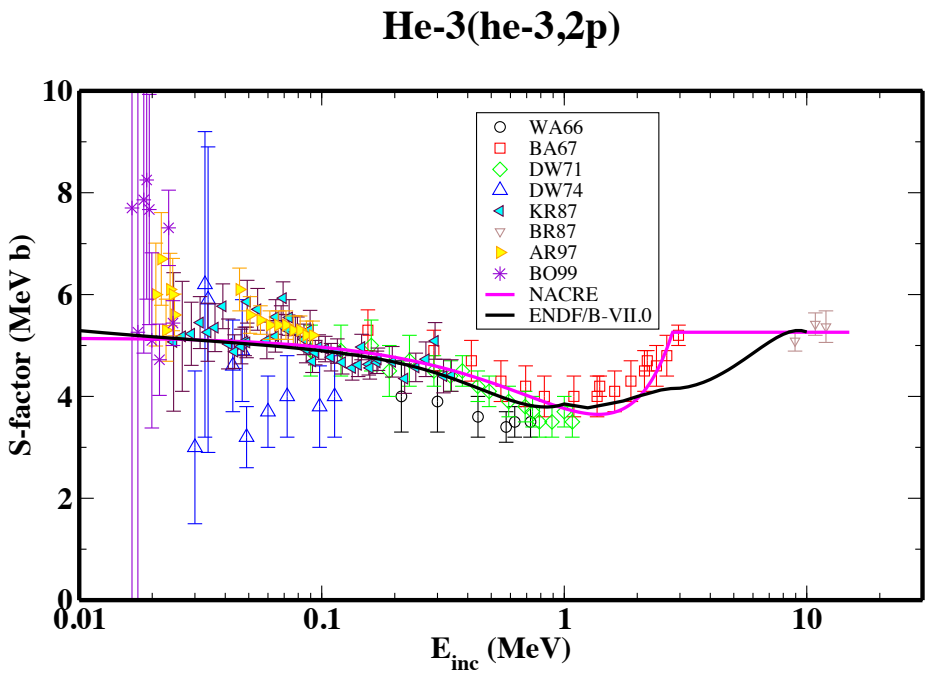
He3+He3 evaluation (from 2016 talk)

- ENDF/B-VII.0 (Hale 2001)
  - (He3,el), (He3,2p)
- ENDF/B-VIII.b3 (ENDL2011.0, Navratil 2010)
  - (He3,el) from ENDF
  - (He3,2p)
    - NACRE S-factor evaluation [4] that includes LUNA data [5]
    - Angle and energy distributions: from ENDF

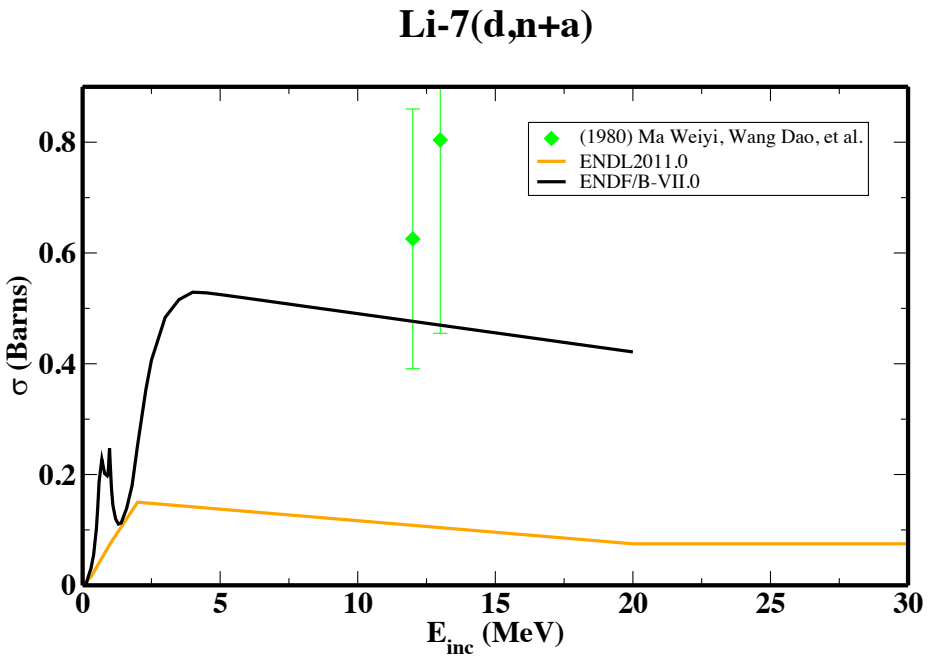


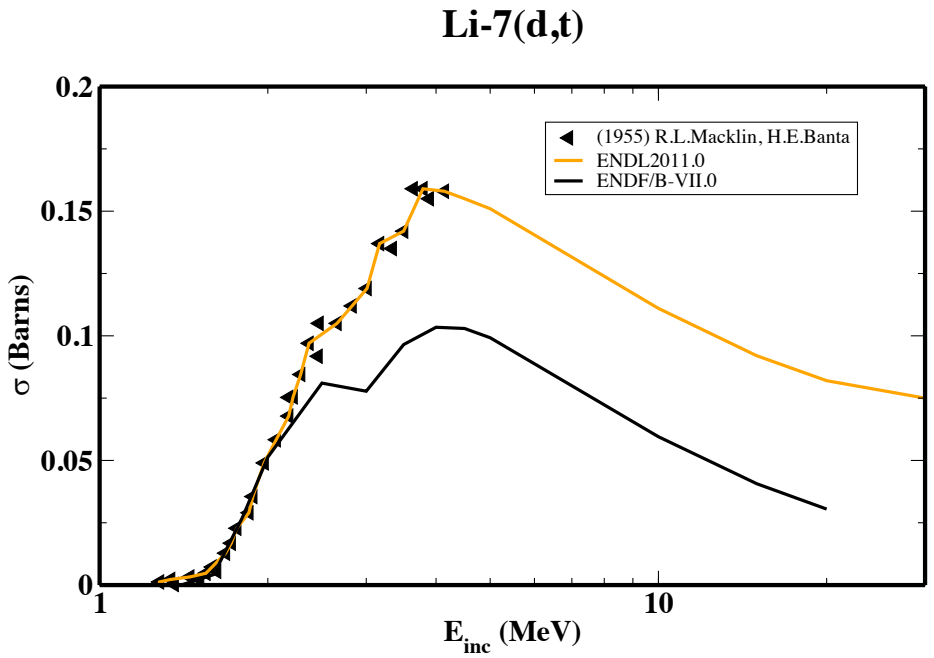
[4] C. Angulo et al. (NACRE Collaboration), Nucl. Phys. A656 (1999)3-187

[5] The LUNA Collaboration, M. Junker, et al., The cross section of 3He(3He,2p)4He measured at solar energies, Nuclear Physics B - Proceedings Supplements, Volume 70, Issues 1-3, Proceedings of the Fifth International Workshop on topics in Astroparticle and Underground Physics, January 1999, Pages 382-385, ISSN 0920-5632.

d+Li7 evaluation (from 2016 talk)

- ENDF/B-VII.0 (Hale 2003)
  - (d,el), (d,na), (d,t_0)
- ENDF/B-VIII.b3 (ENDL2011.0, Navratil 2010)
  - (d,el) from ENDF, extended up to 30 MeV
  - (d,na) from ECPL (but ENDF better fit to data)
  - (d,t) from R.L. Macklin [5] data up to 4 MeV; at higher energies scaled ENDF
    - Angular distributions: ENDF/B-VII.0

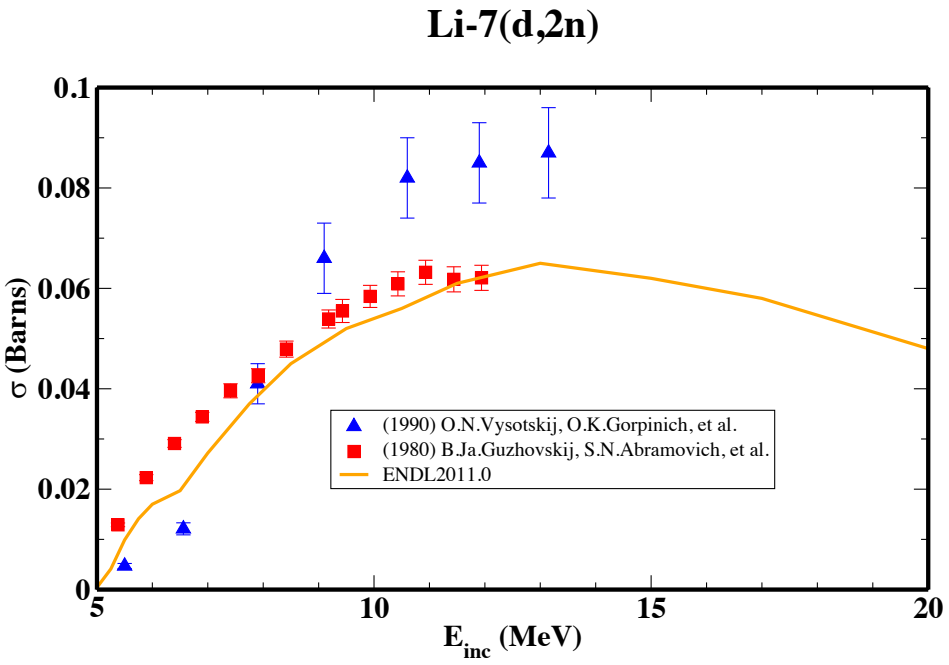


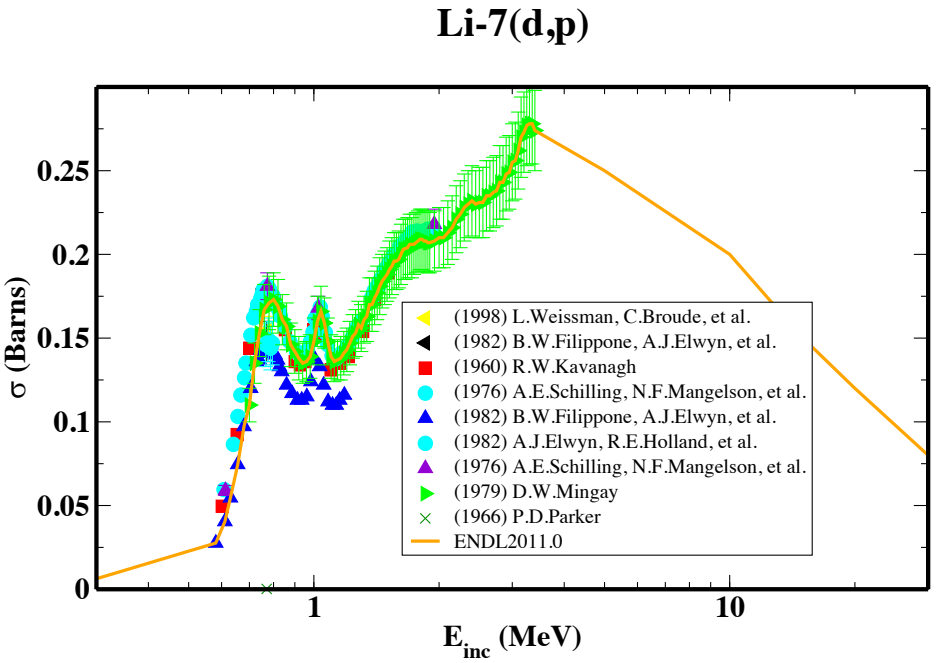


[5] R.L. Macklin, H.E. Banta, Phys. Rev., 97, 753 (1955)

d+Li7 evaluation (from 2016 talk)

- ENDF/B-VII.0 (Hale 2003)
  - (d,el), (d,na), (d,t_0)
- ENDL2011.0 (Navratil 2010)
  - (d,2n) from ECPL
  - (d,p)
    - < 0.7 MeV from Ref. [3]
    - 0.7 - 3.4 MeV from Ref. [4]
    - > 3.4 MeV educated guess
    - Angular distributions: from (d,na) neutron dist.



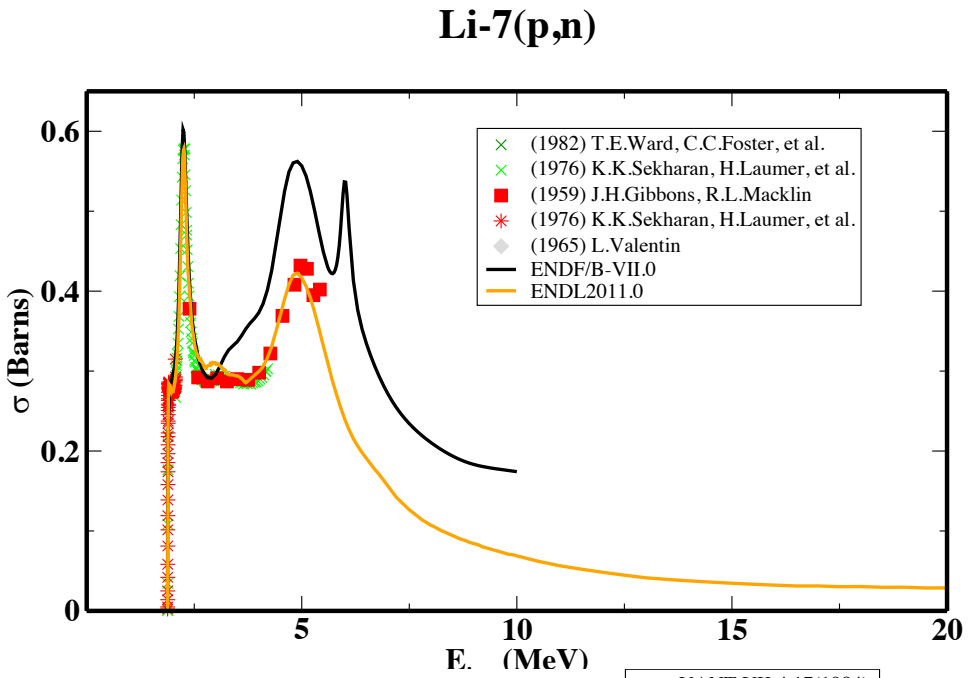


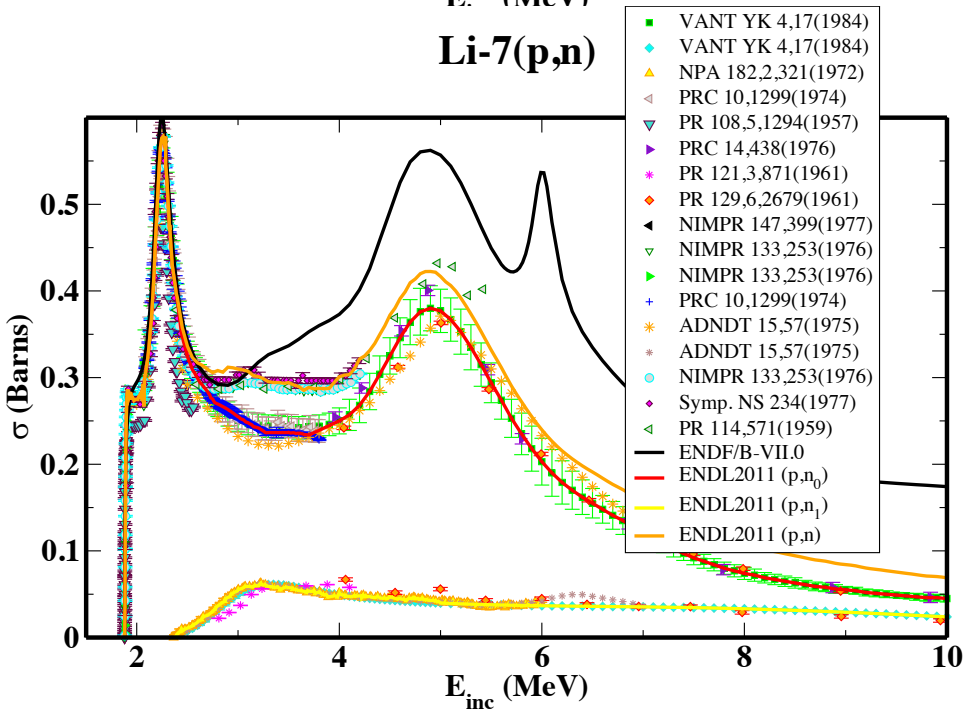
[3] B.W. Filippone, A.J. Elwyn, W. Ray Jr., D.D. Koetke, Phys. Rev. C, 25, 2174 (1982)

[4] D.W.Mingay, J, SAP, 2, (3), 107 (1979)

p+Li7 evaluation (from 2016 talk)

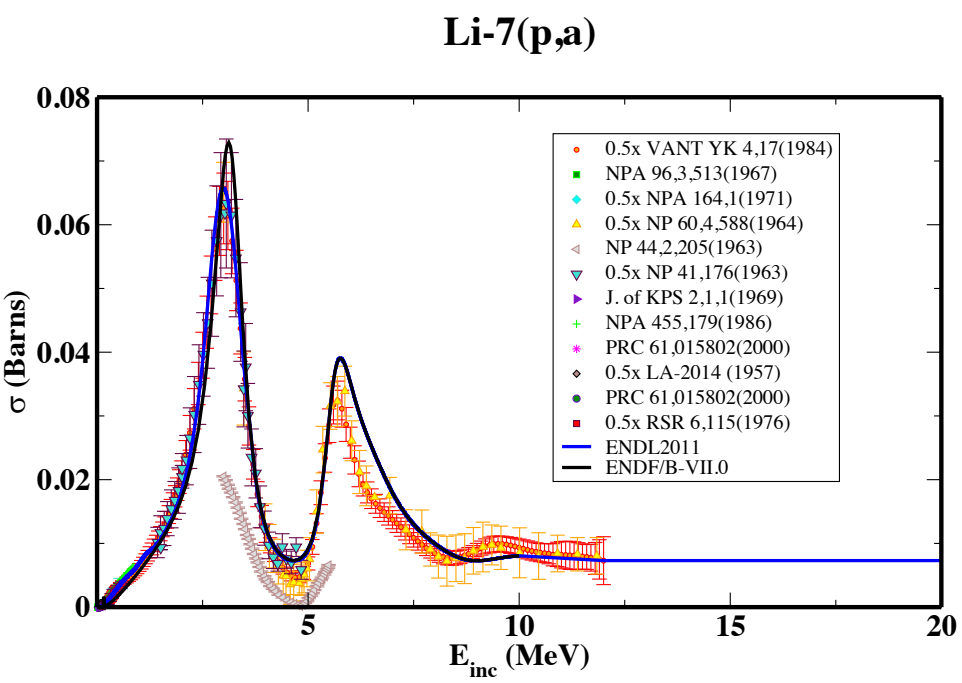
- ENDF/B-VII.1 (Page 2004)
  - (p,el), (p,n'$_0$), (p,d$_0$), (p,α$_0$)
- ENDF/B-VIII.b3 (ENDL2011, Navratil 2008)
  - 7Li(p,n)
  - Both ECPL and ENDF/B-VII.0 cross-sections were discarded. Evaluation is based purely on data
  - (p,n$_0$) [ground state]:
    - NIMPR 133, 253 (1976) for 0-2.35 MeV
    - PRC 10, 1299 (1974) for 2.4-3.6 MeV
    - VANT YK 4, 17 (1984) for 3.6-25 MeV
    - PRC 14, 438 (1976) for 25-26 MeV
    - Datasets matched with splines.
  - (p,n$_1$) [0.4291 MeV excited state):
    - NPA 182, 2, 321 (1972) for 2.3-5 MeV
    - VANT YK 4, 17 (1984) for 5-25 MeV
    - PRC 14, 438 (1976) for 25-26 MeV
    - Datasets matched with splines
  - Angular distributions
    - Taken from Page's ENDF/B-VII.0 evaluation
    - Distribution for excited state is same as ground state, but threshold is shifted.

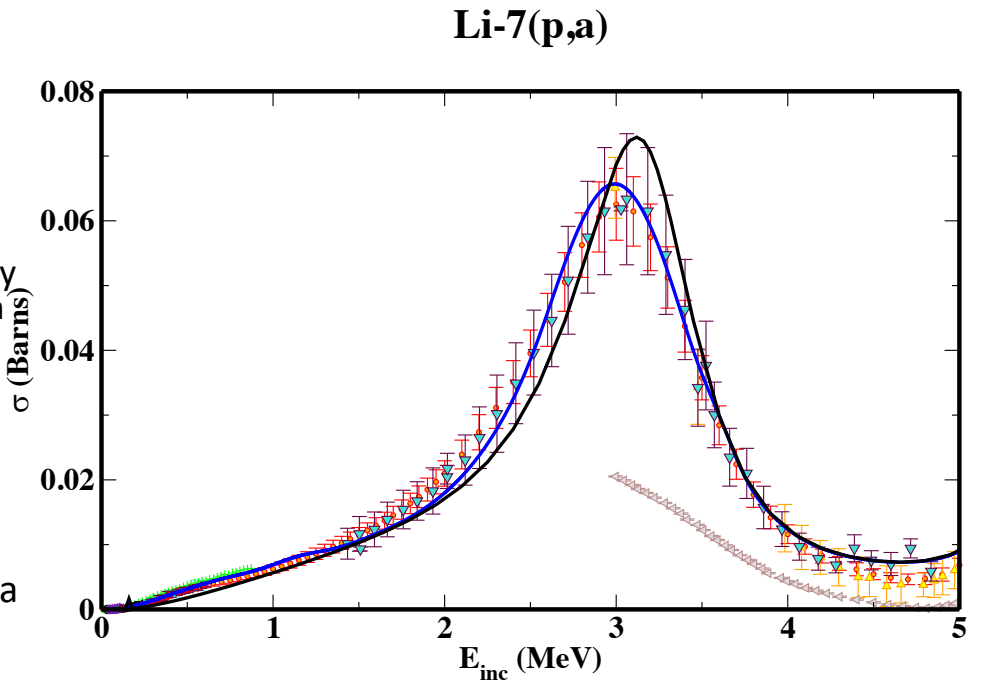




p+Li7 evaluation (from 2016 talk)

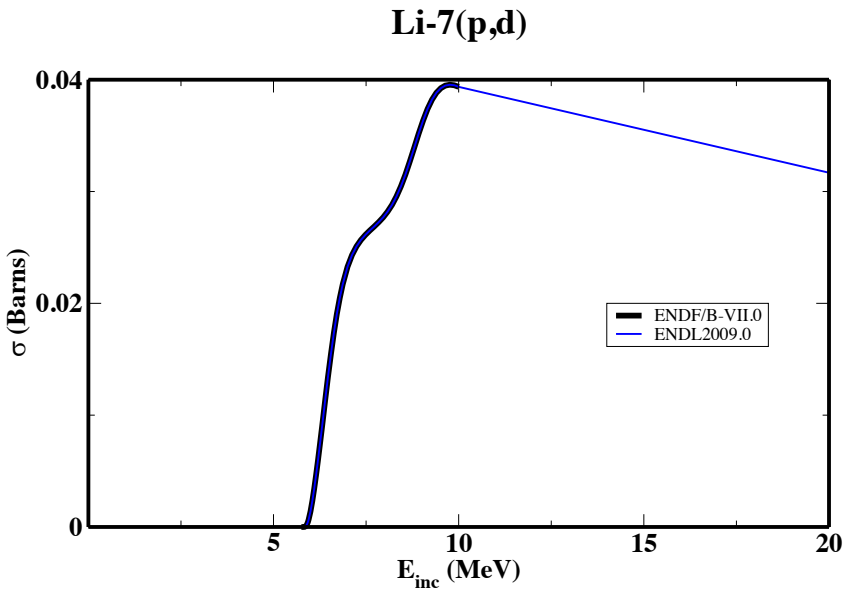
- ENDF/B-VII.1 (Page 2004)
  - (p,el), (p,n'$_0$), (p,d$_0$), (p,α$_0$)
- ENDF/B-VIII.b3 (ENDL2011, Navratil 2008)
  - (p,el) from ECPL
  - (p,a)
  - Cross-section
    - < 2.6 MeV : Descouvemont [3] S-factor
    - 2.6 - 3.15 MeV : three experimental points from the Rice measurement
    - > 3.15 MeV : Page evaluation
    - Note EXFOR file with the NP 33, 449 (1962) data is wrong as there was an erratum in NP 41, 176 (1963) (data needs to be multiplied by 10/7), divided by 2 as normalization based on 1958 measurement that counted alphas
  - Angular distributions from ENDF/B-VII.0
- Decouvemont 2004
  - [3] P. Descouvemont, A. Adahchour, C. Angulo, A. Coc, E. Vangioni-Flam, Atomic Data and Nuclear Data Tables 88, 203 (2004).





p+Li7 evaluation (from 2016 talk)

- ENDF/B-VII.1 (Page 2004)
  - (p,el), (p,n'$_0$), (p,d$_0$), (p,α$_0$)
- ENDF/B-VIII.b3 (ENDL2009, Navratil 2008)
  - 7Li(p,d)
  - Cross-section
    - < 10 MeV from ENDF/B-VII.0
    - To extrapolate to 30 MeV, integrated the cross section from Fig. 6 of PR 163,4,1066 (1967) and got 24 mb. Measurement was at 33.6 MeV proton energy. Recommend to use 24 mb at 30 MeV and make a linear interpolation to the 10 MeV point of Page
  - Angular distributions from ENDF/B-VII.0



New Evaluations at ENDF/B-VIII.1

- h + ^{7}Li evaluation
  - MT=2: elastic
  - MT=45: n + p + a + a
  - MT=600: p + Be9
  - MT=105: t + Be7
  - MT=800: a + Li6
  - MT=801: a + (Li6*(2.18 MeV)->Li6+γ) , with γ distribution in lab frame
  - MT=117: d + a + a

For these 3 evaluations, comprehensive reactions, but little documentation

- α + ^{6}Li evaluation
  - MT=2 elastic
  - MT=600: p + Be9
  - MT=650: Be8 -> 2a
  - MT=651: Be8_e1 -> 2a

- d + α evaluation, with 3-body breakup of deuteron via 3 routes:
  - MT=2 elastic
  - MT=600: p + (^{5}He -> α + n)
  - MT=50: n + (^{5}Li -> α + p)
  - MT=28: α + n + p (no resonances)