Data Evaluation and Extrapolation using *R*-matrix

James deBoer (for IAEA R-matrix consultant group)

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Nuclei in the Cosmos XV, LNGS Gran Sasso, Italy

UNIVERSITY OF NOTRE DAME

JINA-CEE

What is (phenomenological) *R*-matrix?

- Nuclear reaction framework (Compound Nucleus)
  - Reaction theory where nuclear part is parameterized in terms of individual levels
    - **reduced width amplitudes** (Partial widths) are treated as free parameters
    - **pole energies** (level energies) are also free parameters
  - Angular momentum, Coulomb potential in external region, unitarity, time reversal, resonance interferences
  - All decay channels must also be included

$$\sigma_{\alpha\alpha'} = \frac{\pi}{k_\alpha^2} \sum_{Jll'ss'} g_J |T_{cc'}|^2,$$

$$T_{cc'} = e^{2i\omega_c}\delta_{cc'} - U_{cc'},$$

$$U = \Omega\{1 + 2iP^{1/2}[I - R(L - B)]^{-1} R P^{1/2}\}\Omega,$$

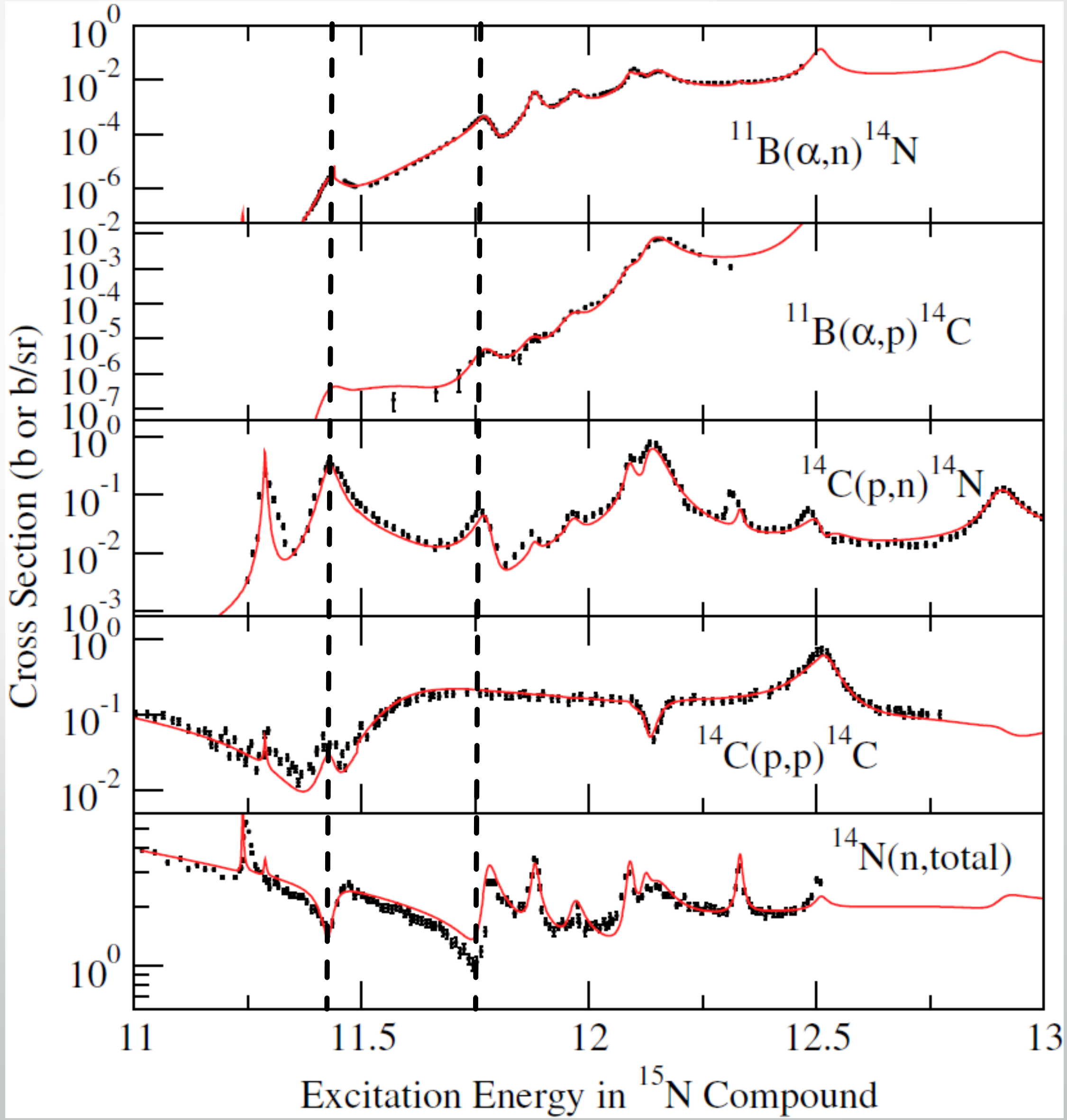
$$R_{c'c} = \sum_\lambda \frac{\gamma_{\lambda c'}\gamma_{\lambda c}}{E_\lambda - E}.$$

fit parameters to data

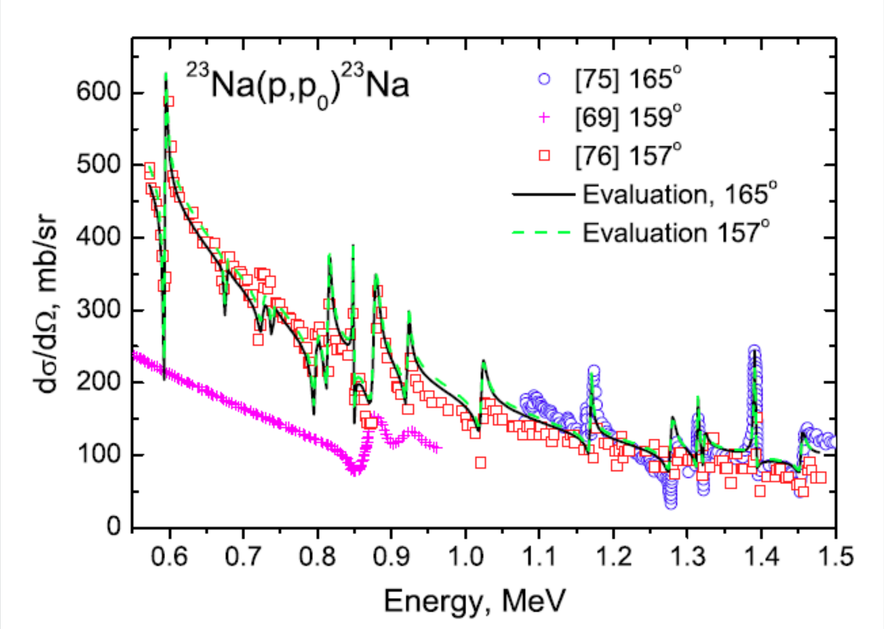
Main Use

- Reactions where resolved resonances are present (RRR)
  - Charged particle reactions on light nuclei
  - Low energy neutron induced reactions across the nuclear chart
- Cross Section data **evaluation**
  - Also across different reaction channels
  - Check of **systematic** uncertainties

Reactions populating the ^{15}N compound



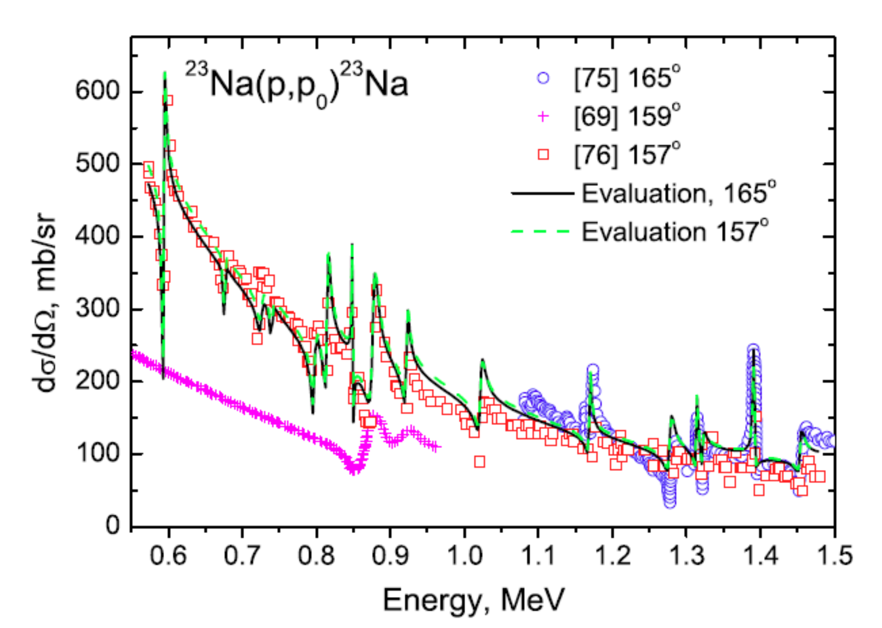
Many Applications



Ion Beam Analysis

Gurbich (2010)

Many Applications



Ion Beam Analysis

Gurbich (2010)

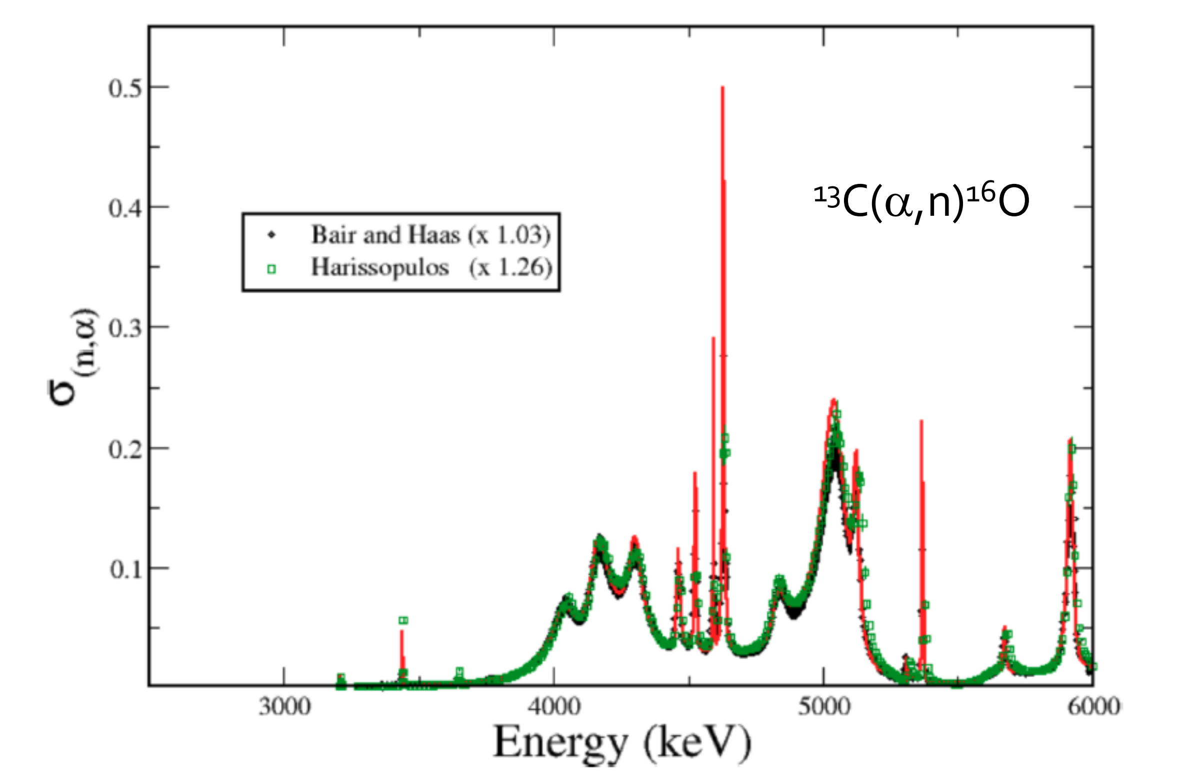
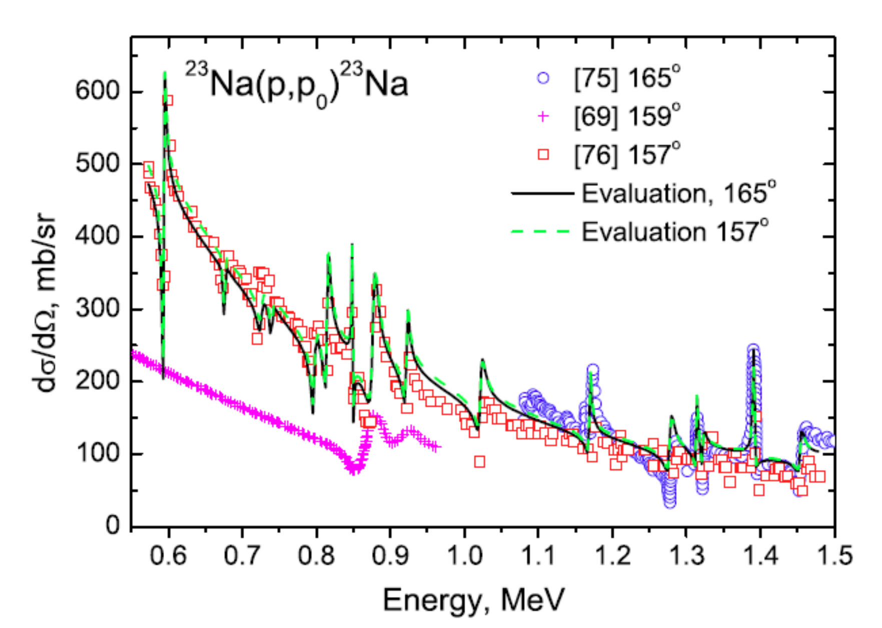


Fig. 5. SAMMY fits of the (n, α) cross sections of Bair and Haas and Harissopulos.

Nuclear Reactor and Safety

Leal et al. (2016)

Many Applications



Ion Beam Analysis

Gurbich (2010)

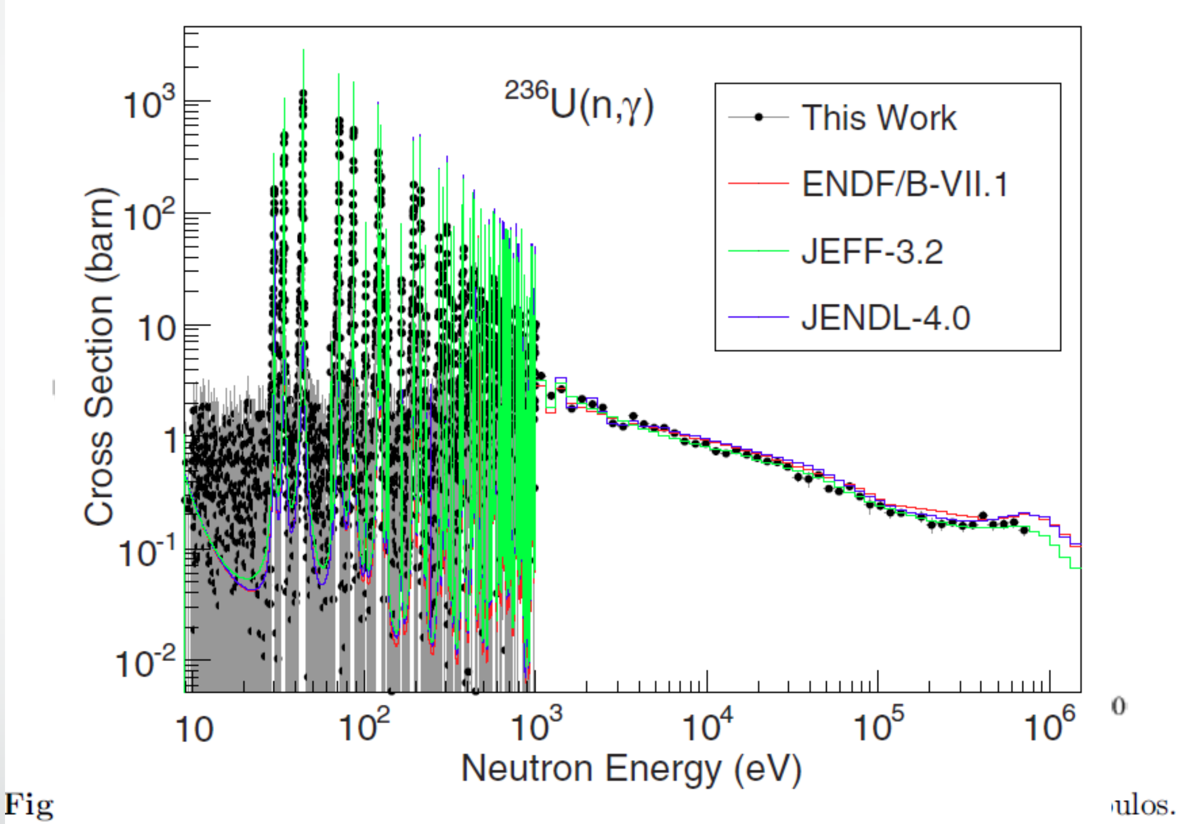
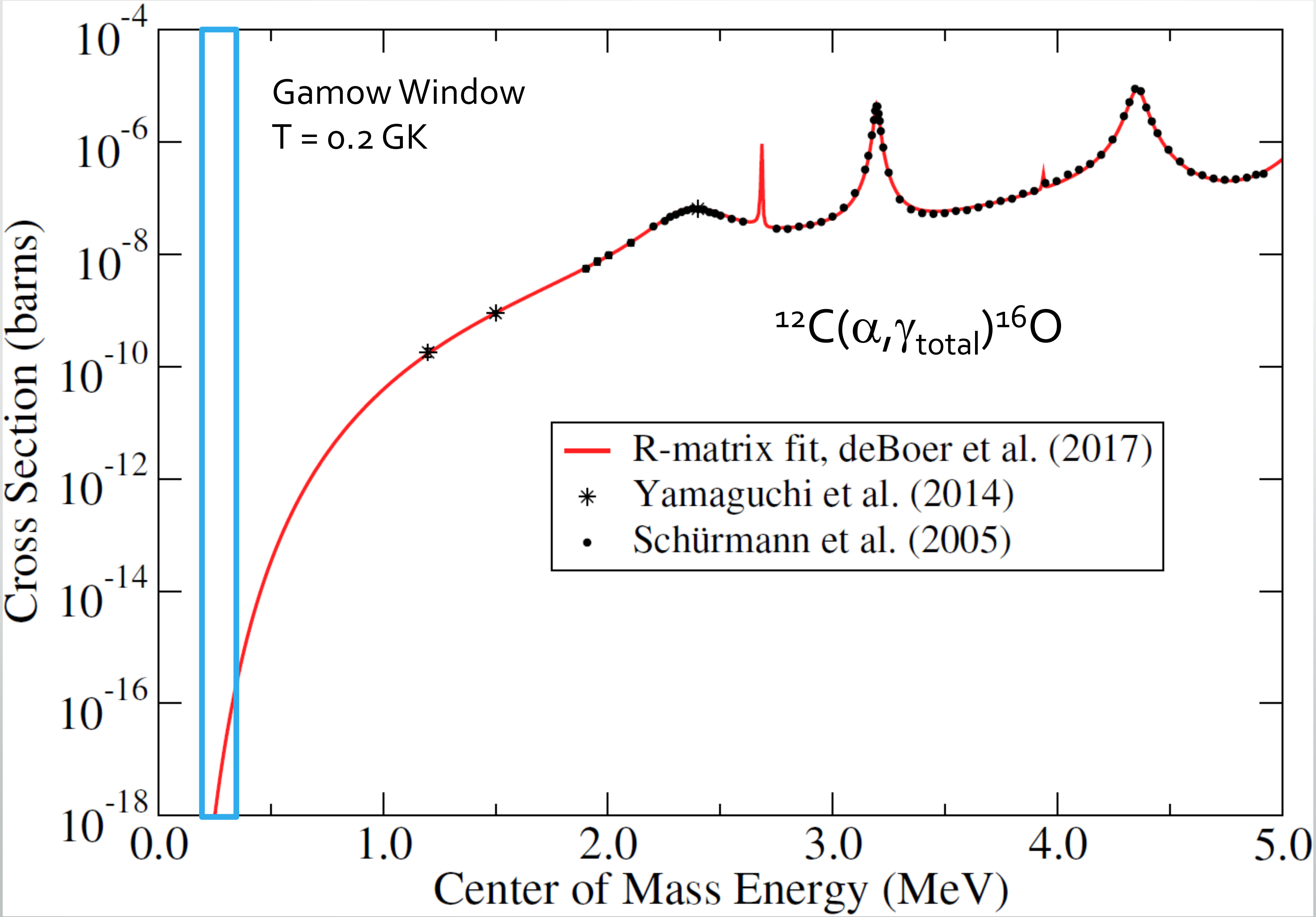


FIG. 7. ^{236}U neutron capture cross section.

Nuclear Reactor and Safety

Baramsai et al. (2017)

Cross Section **Extrapolation**

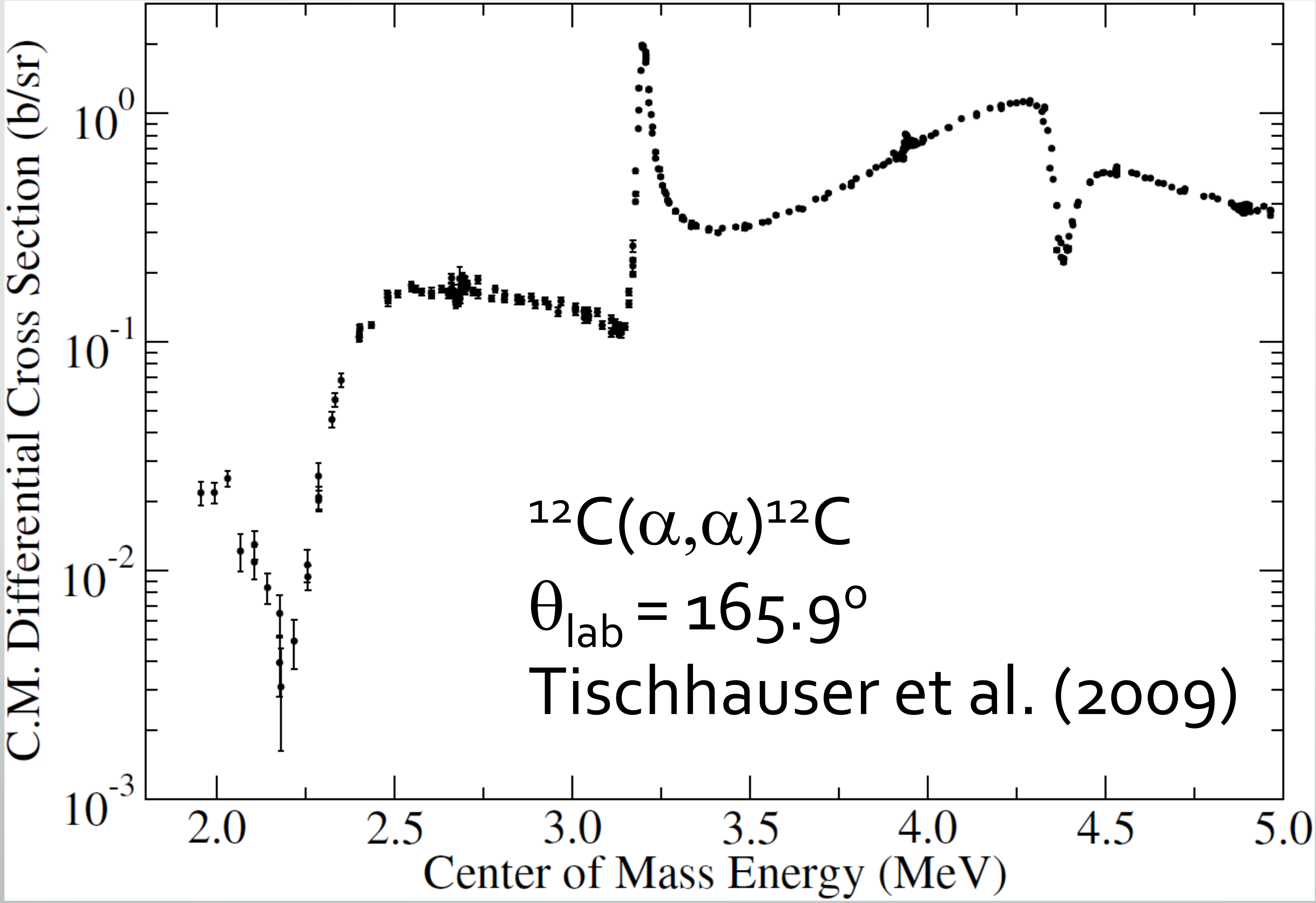


Just at this conference...

$d(p,\gamma)^{3}He$
$^{3}He(\alpha,\gamma)^{7}Be$
$^{4}He(d,\gamma)^{6}Li$
$^{6}Li(p,\gamma)^{7}Be$
$^{7}Be(p,\gamma)^{8}B$
$^{7}Be(n,p)^{7}Li$
$^{7}Be(\alpha,\gamma)^{11}C$

$^{12}C(\alpha,\gamma)^{16}O$
$^{13}C(\alpha,n)^{16}O$
$^{15}N(\alpha,\gamma)^{19}F$
$^{18}F(p,\alpha)^{15}O$
$^{19}F(p,\alpha)^{16}O$
$^{20}Ne(p,\gamma)^{21}Na$
$^{12}C+^{12}C$

Quick Example Calculation

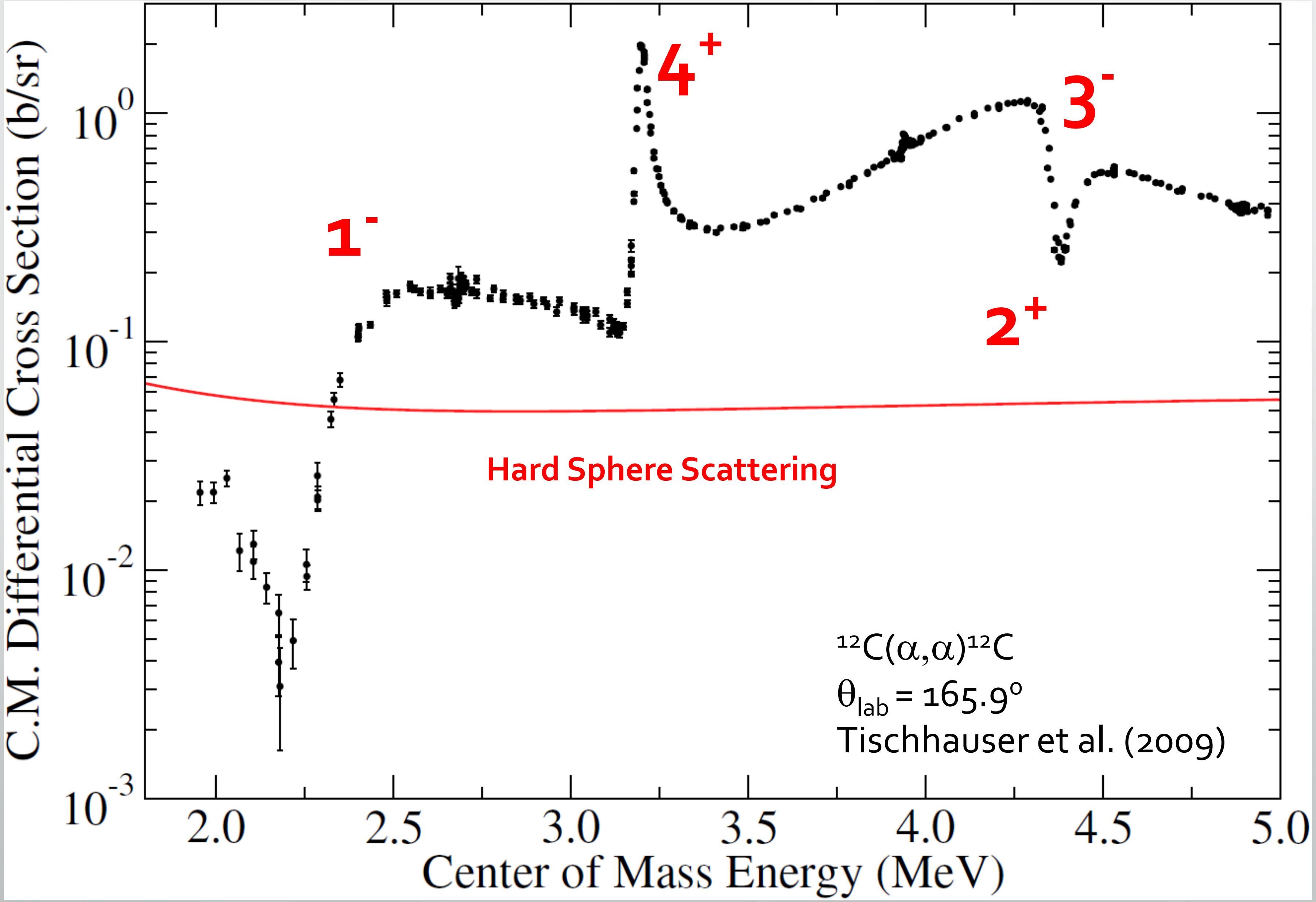


National Nuclear Data Center

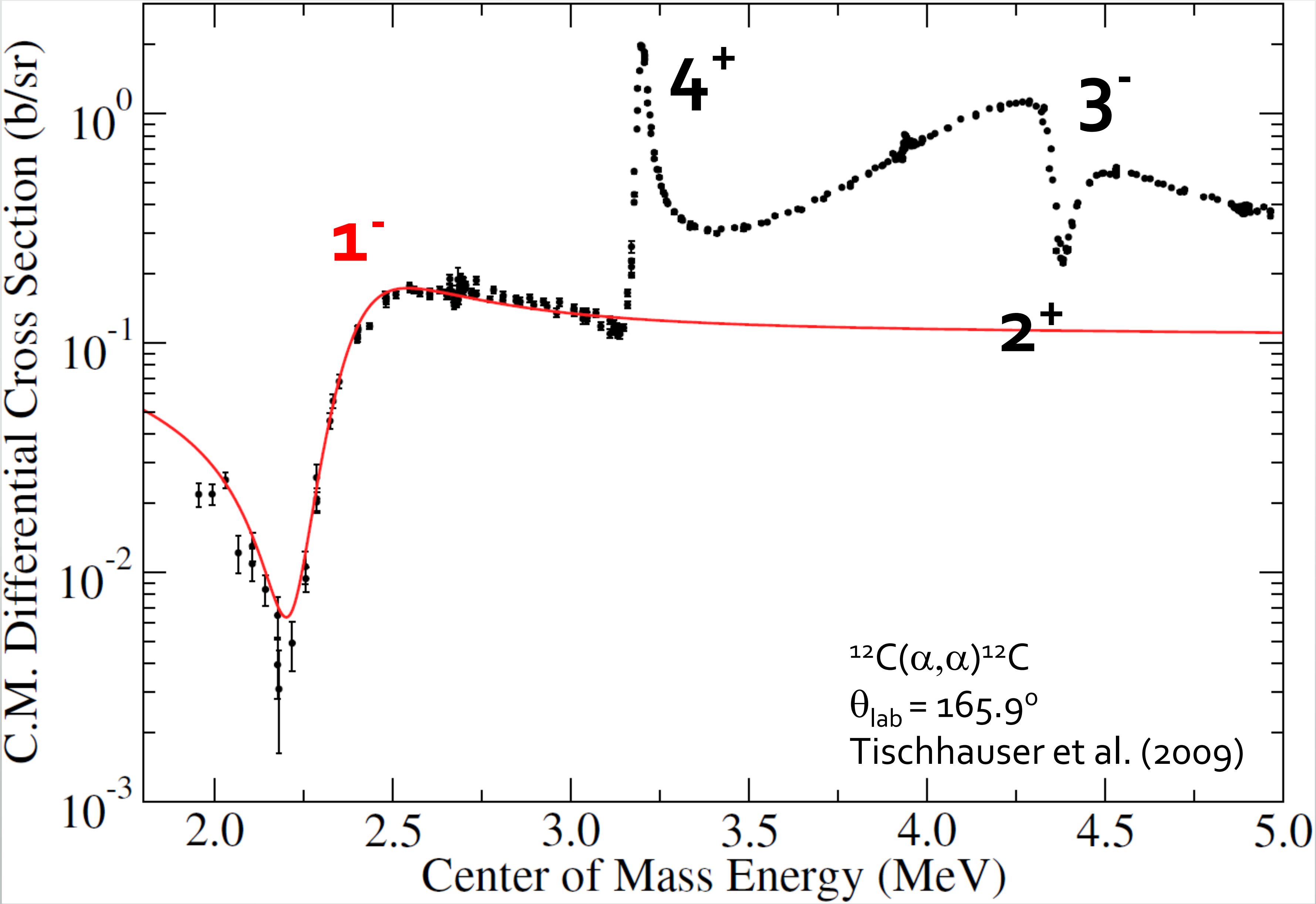
^{16}O

E_{level} (keV)	XREF	Jπ	$T_{1/2}$	E_{γ} (keV)	I_{γ}	γ mult.	Final level
0.0	ABCDEF HIJKLMNOPQ	0+	STABLE				
6049.4 *10*	ABC EF IJK M P	0+	67 ps *5*	6048.2 *10*		[E0]	0.0 0+
6129.89 *4*	ABC EF HIJKL NOPQ	3−	18.4 ps *5*	6128.63 *4*	100	[E3]	0.0 0+
6917.1 *6*	ABC EF HI KLMNOPQ	2+	4.70 fs *13*	787.2 *6* 867.7 *12* 6915.5 *6*	≤0.008 0.027 *3* 100	[E1] [E2] [E2]	6129.89 3− 6049.4 0+ 0.0 0+
7116.85 *14*	AB EF HIJKLM OPQ	1−	8.3 fs *5*	986.93 *15* 1067.5 *10* 7115.15 *14*	0.070 *14* <6E-4 100	[E2] [E1] [E1]	6129.89 3− 6049.4 0+ 0.0 0+
8871.9 *5*	A C E HIJKLMNOPQ	2−	125 fs *11*	1754.9 *6* 1954.7 *8* 2741.5 *5* 2822.2 *12* 8869.3 *5*	14.7 *7* 4.6 *7* 100 *21* 0.15 *5* 9.3 *10*	[M1+E2] [E1] [M1+E2] [M2] [M2]	7116.85 1− 6917.1 2+ 6129.89 3− 6049.4 0+ 0.0 0+
9585 *11*	A E IJ LMNO	1−	420 keV *20* % IT = 6.7E-6 *10* % α = 100	2688 *11* 9582 *11*	12 *4* 100 *16*	[E1] [E1]	6917.1 2+ 0.0 0+
9844.5 *5*	A C E HIJKLMNO Q	2+	0.62 keV *10* % IT = 0.0016 *3* % α = 100	2927.1 *8* 3794.6 *12* 9841.2 *5*	34 *7* 30 *7* 100 *7*	[M1] [E2] [E2]	6917.1 2+ 6049.4 0+ 0.0 0+
10356 *3*	A C E I KLMNO Q	4+	26 keV *3* % IT = 2.4E-4 *4* % α = 100	3439 *3* 4225 *3* 10352 *3*	100 *10* <1.6 9E-5 *3*	[E2] [E1] [E4]	6917.1 2+ 6129.89 3− 0.0 0+
10957 *1*	E HI LM Q	0−	5.5 fs *35*	3839.6 *10*	100	[M1]	7116.85 1−
11080 *3*	E HI Q	3+	< 12 keV				
11096.7 *16*	A C E KLMNO	4+	0.28 keV *5* % IT = 0.0020 *6* % α = 100	4179.0 *17* 4966.0 *16*	81 *20* 100 *42*	[E2] [E1]	6917.1 2+ 6129.89 3−
11260?	A I	(0+)	2500 keV % α = 100				
11520 *4*	A C E KLMNO	2+	71 keV *3* % IT = 9.4E-5 *3* % α = 100	4402 *4* 4602 *4* 5470 *5* 11516 *4*	≤0.9 4.4 *11* 4.6 *8* 100.0 *13*	[E1] [M1] [E2] [E2]	7116.85 1− 6917.1 2+ 6049.4 0+ 0.0 0+
11600 *20*	A	3−	800 keV *100* % α = 100				

Levels added individually: J^{π}'s?



Levels added individually

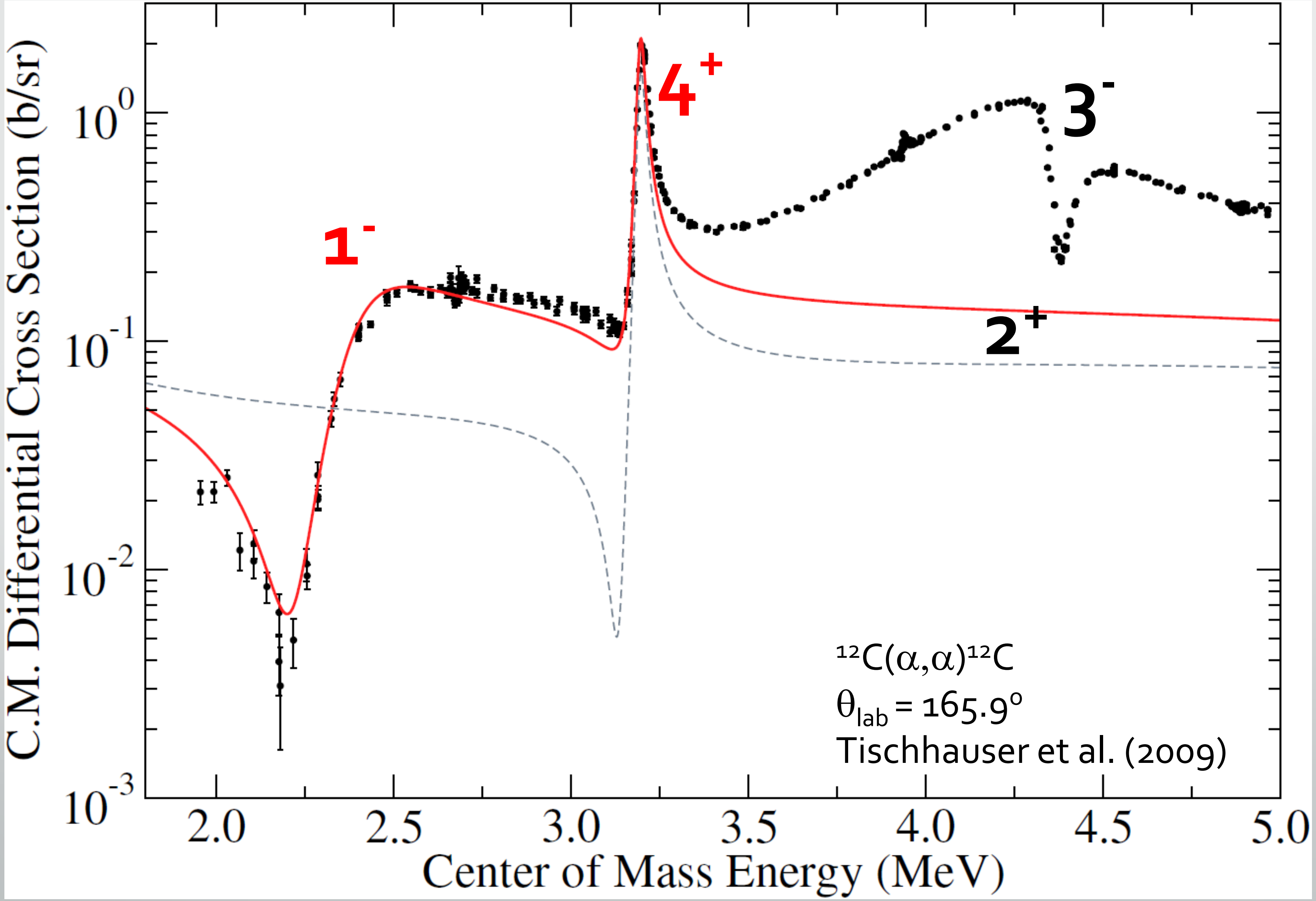


$^{12}C(\alpha,\alpha)^{12}C$

$\theta_{lab} = 165.9°$

Tischhauser et al. (2009)

Levels added individually



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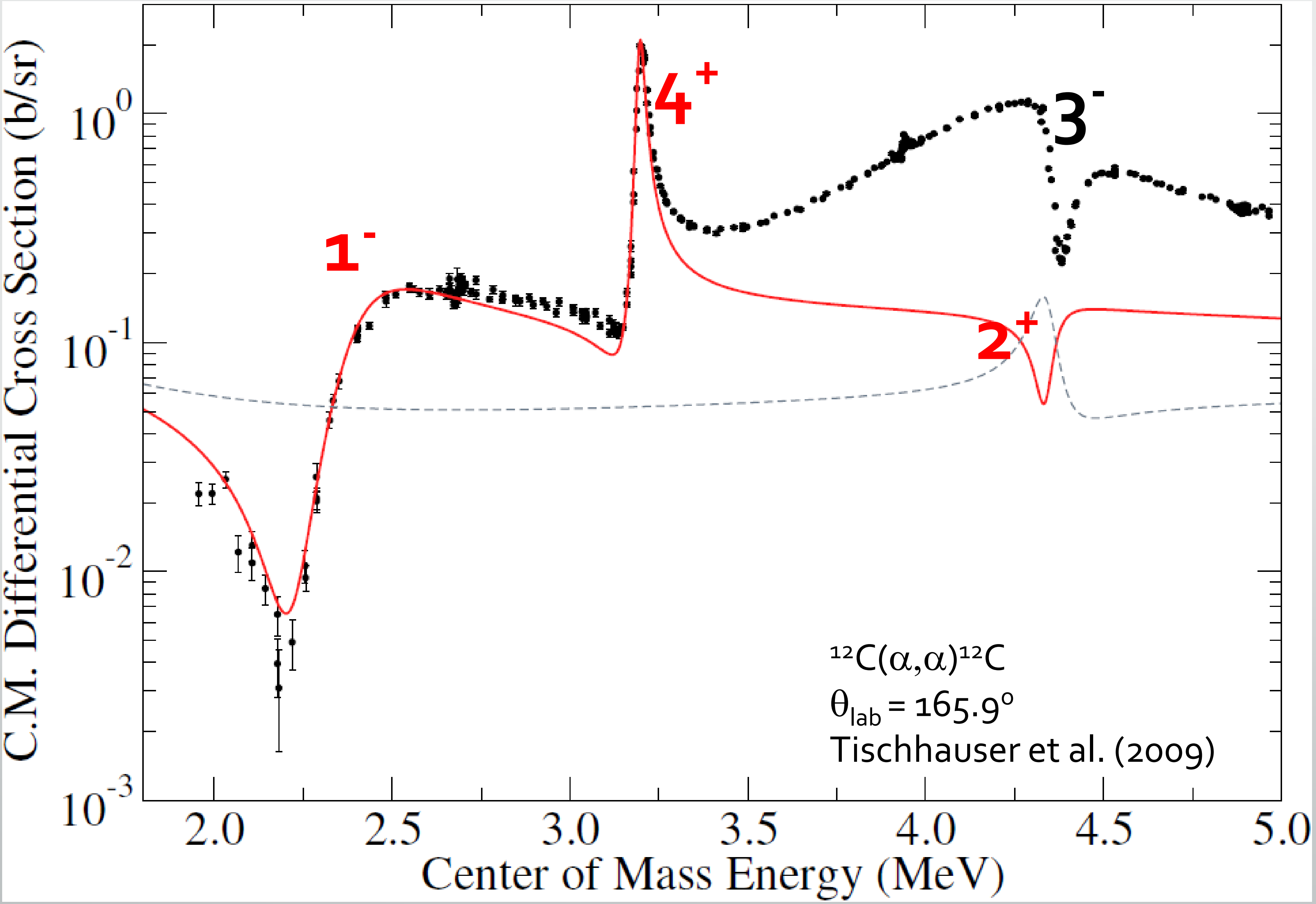

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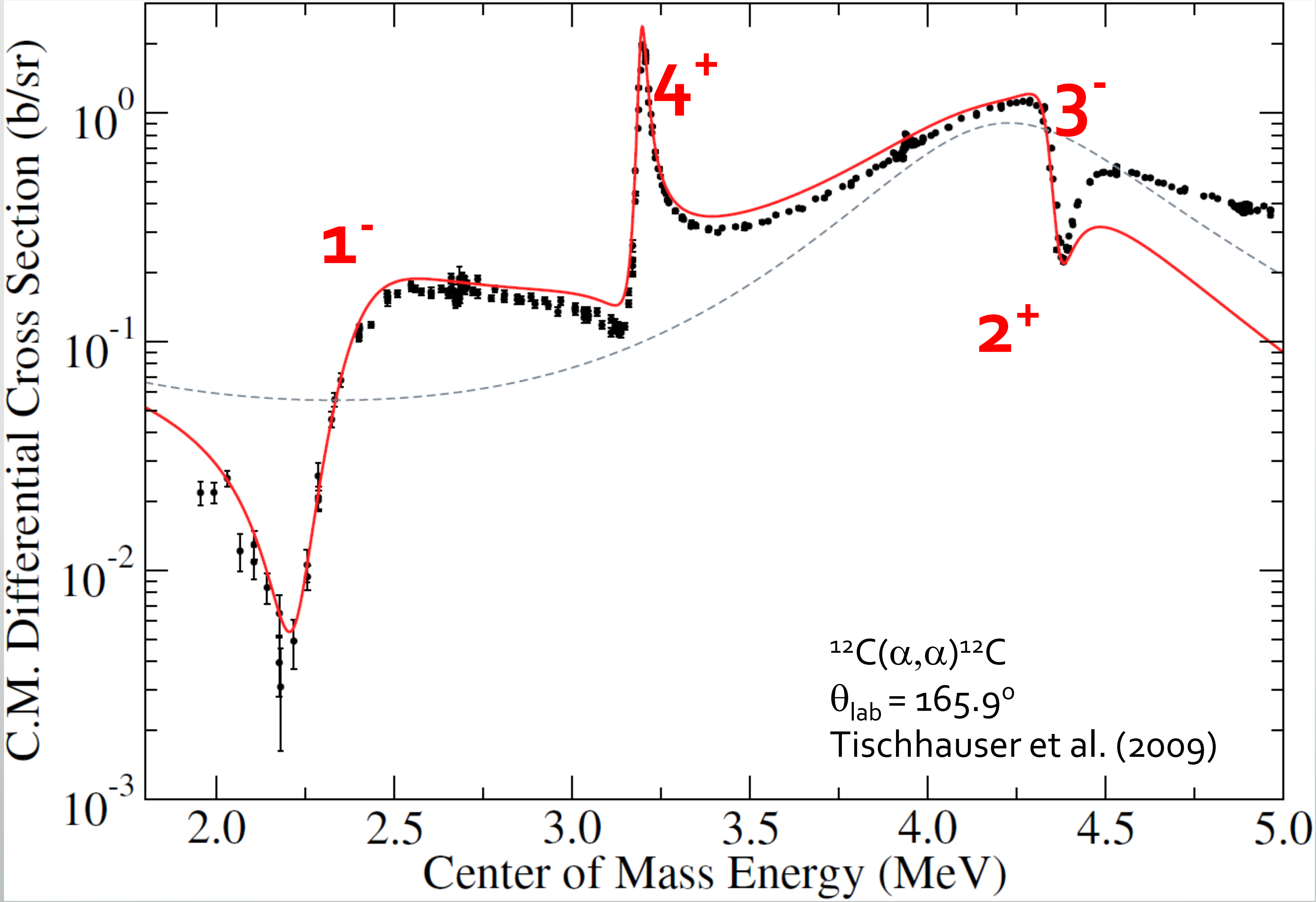
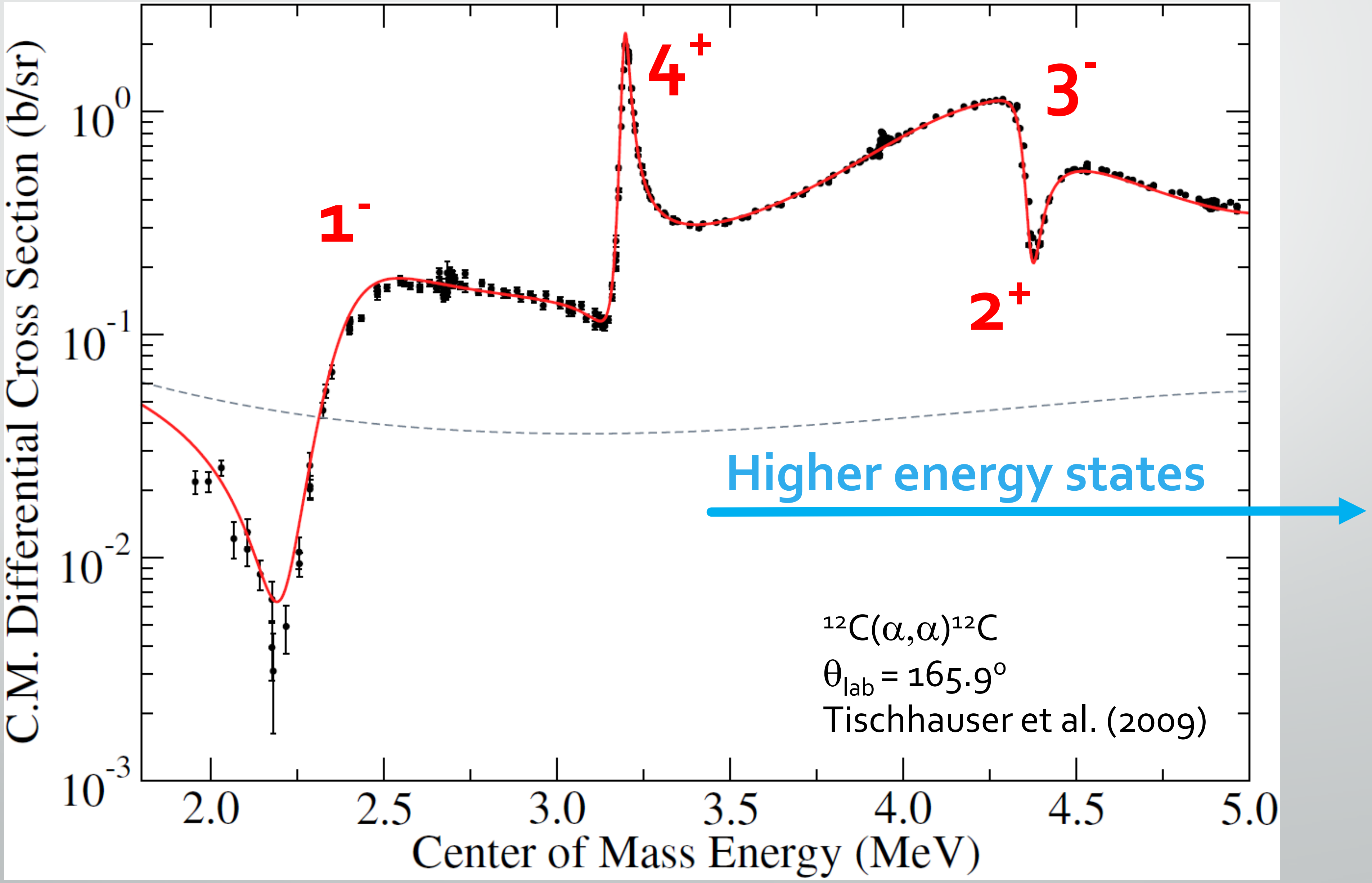
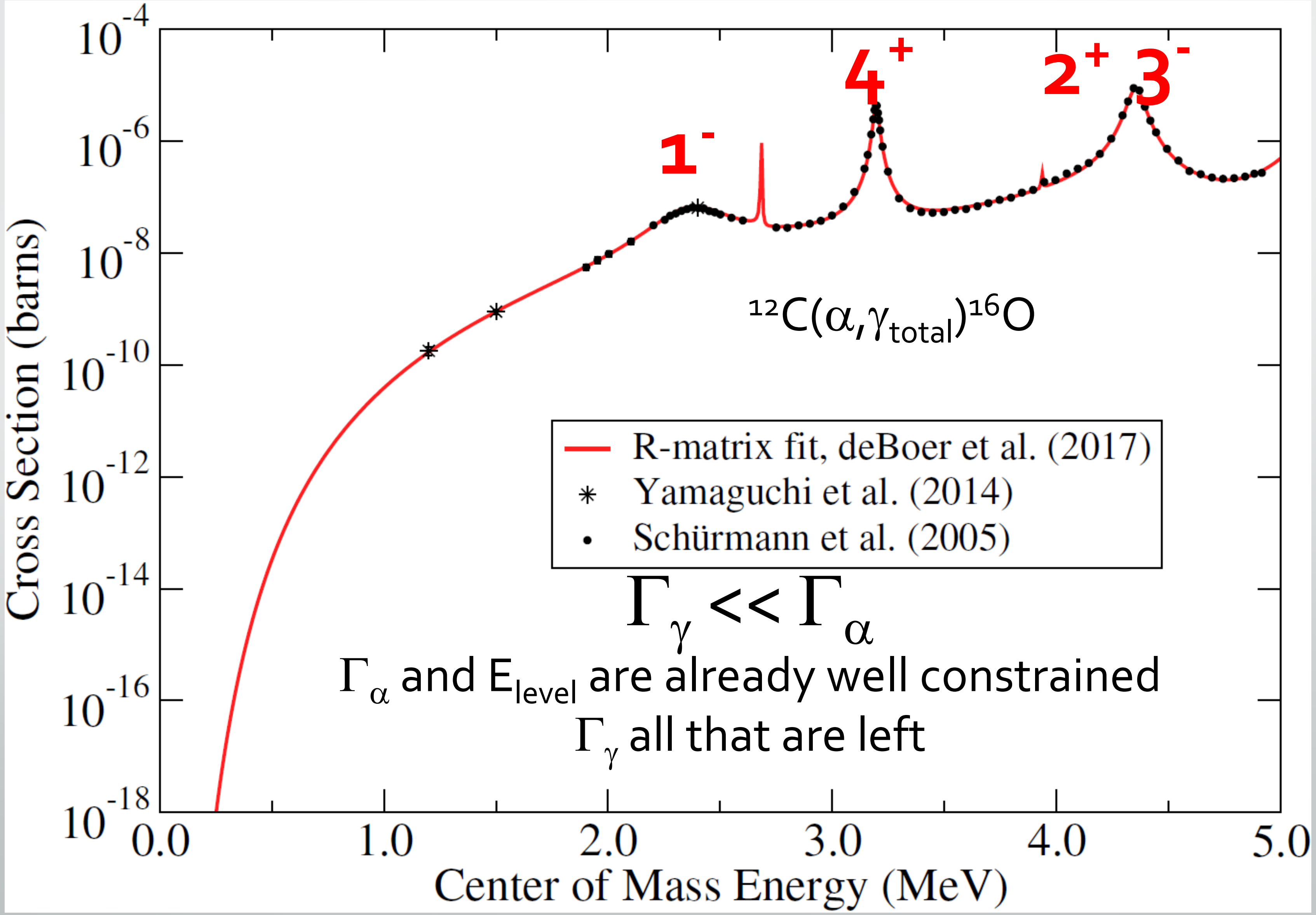


Higher Energy Levels



How does this scattering help for nuc astro?



That was easy!

Not really…

VOLUME 88, NUMBER 7 PHYSICAL REVIEW LETTERS 18 FEBRUARY 2002

Elastic $\alpha - {}^{12}C$ Scattering and the ${}^{12}C(\alpha,\gamma){}^{16}O$ $E2$ S Factor

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PHYSICAL REVIEW C **79**, 055803 (2009)

Measurement of elastic ${}^{12}C + \alpha$ scattering: Details of the experiment, analysis, and discussion of phase shifts

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(Received 23 September 2008; revised manuscript received 10 February 2009; published 12 May 2009)

Why does this take so long?

- Phenomenological model
  - Lots of flexibility
  - Unphysical solutions can be easily obtained
  - Closer attention to physical constraints, must be checked carefully

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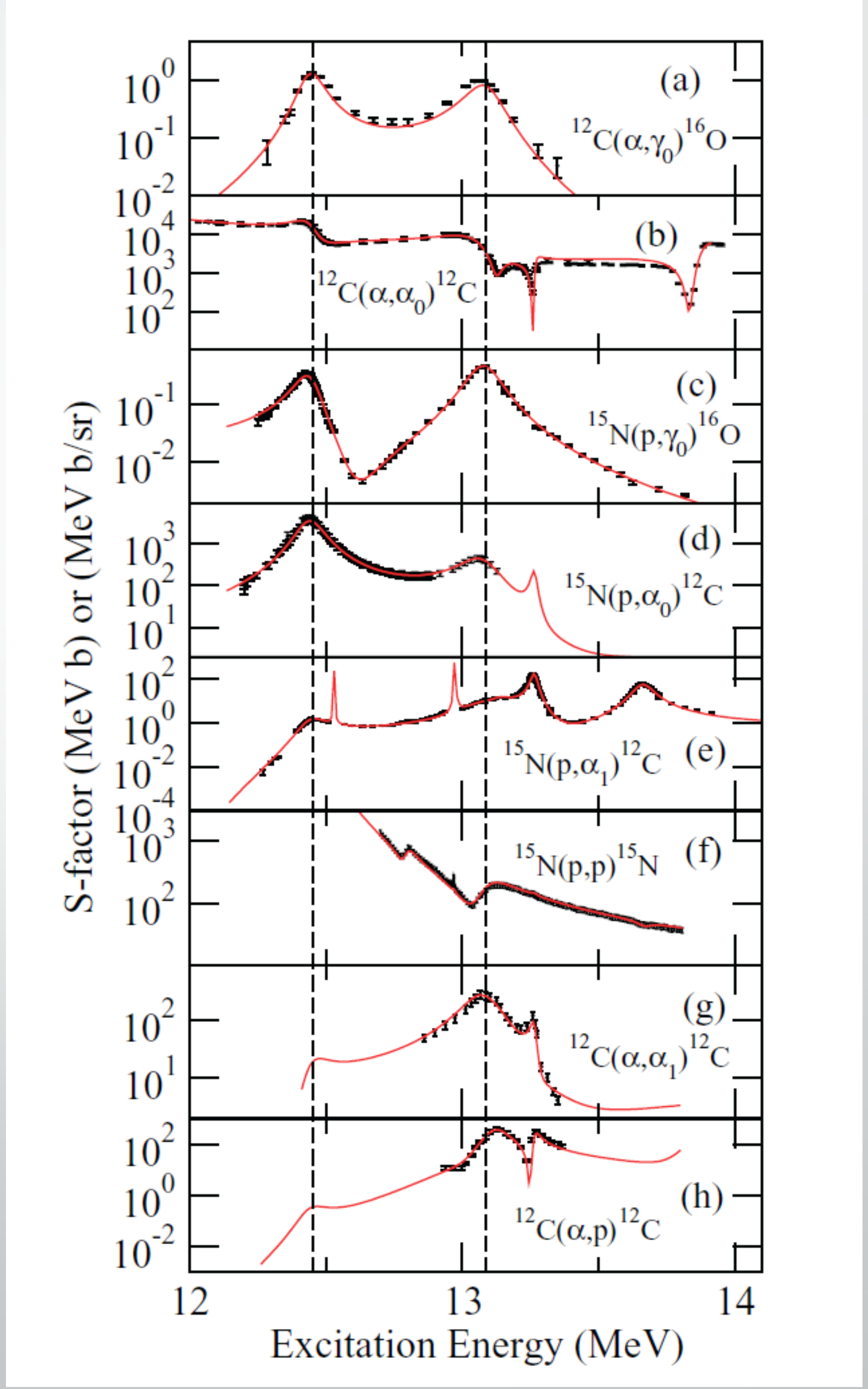

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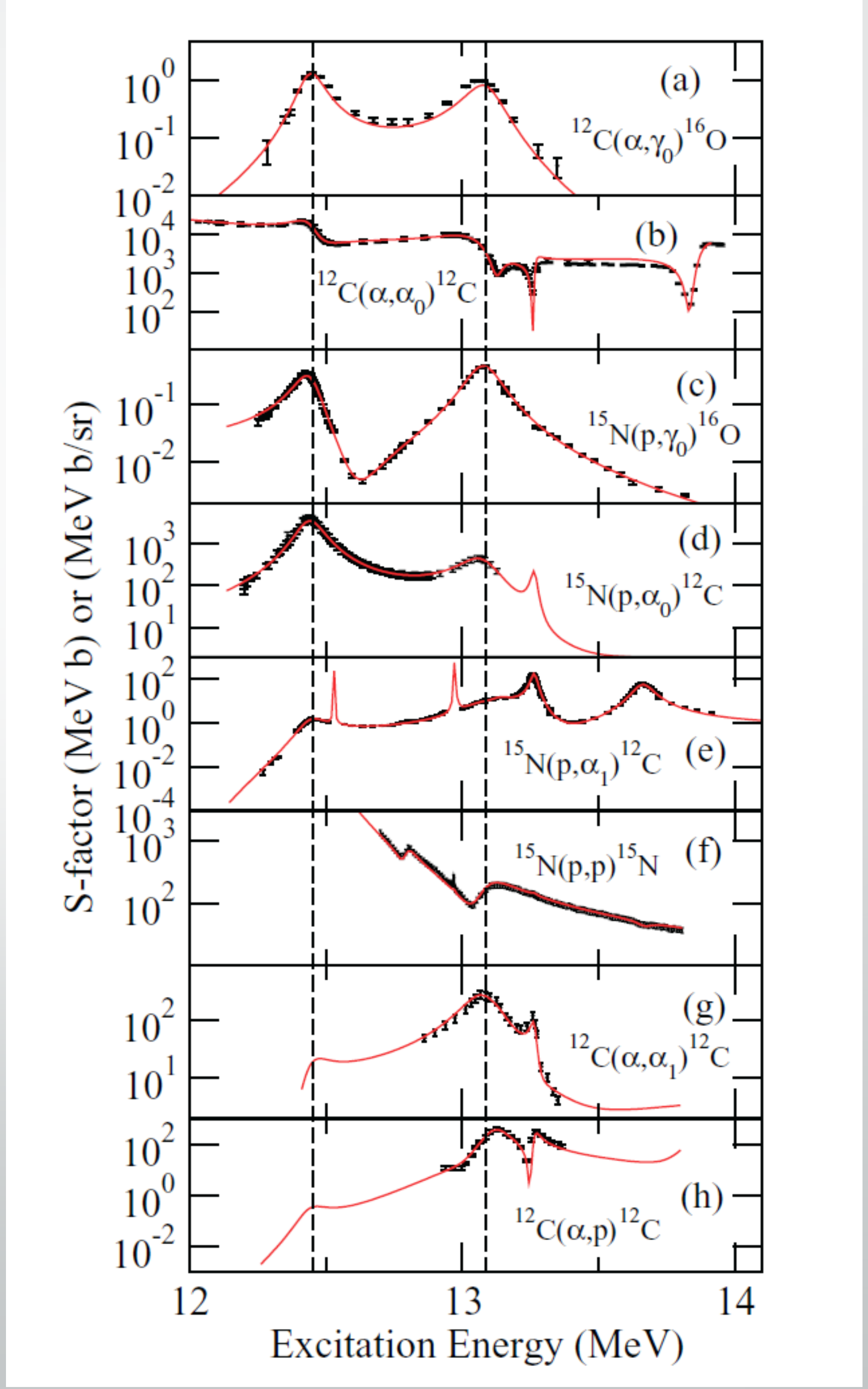
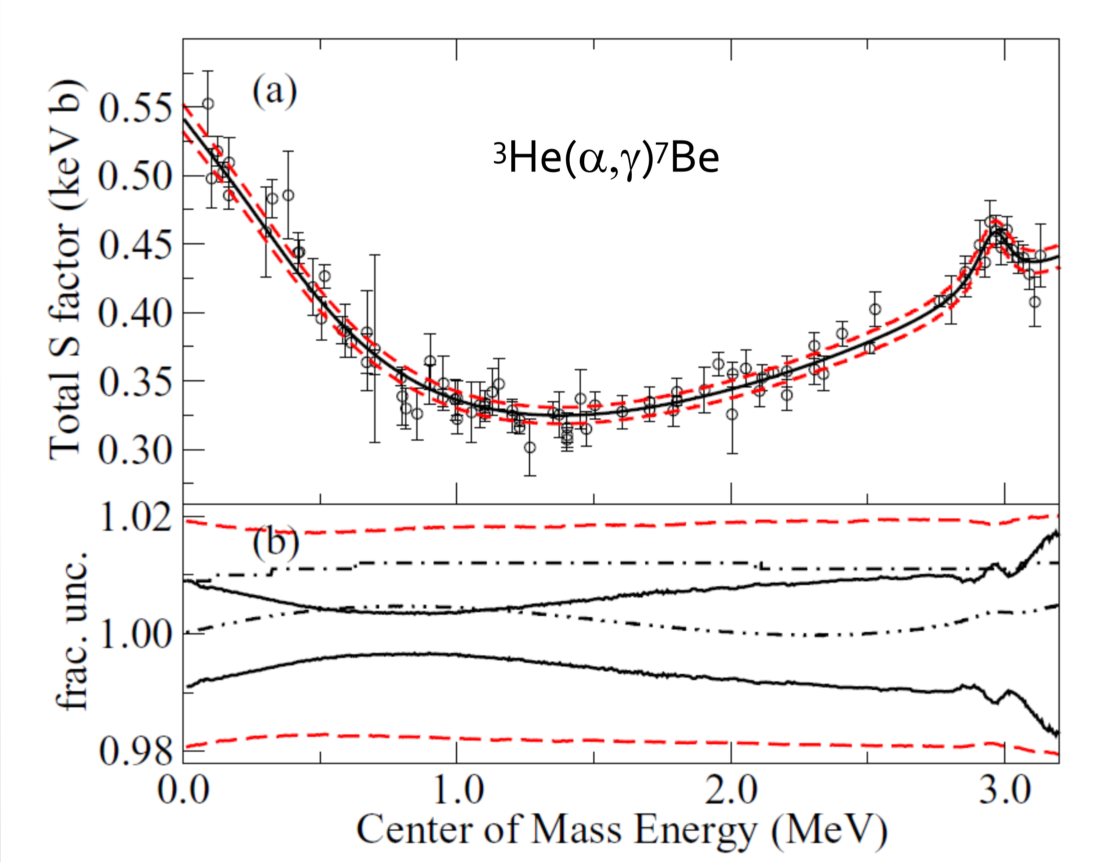
- The more global the fit, the **better** the results
- The more global the fit, the **harder** the results…

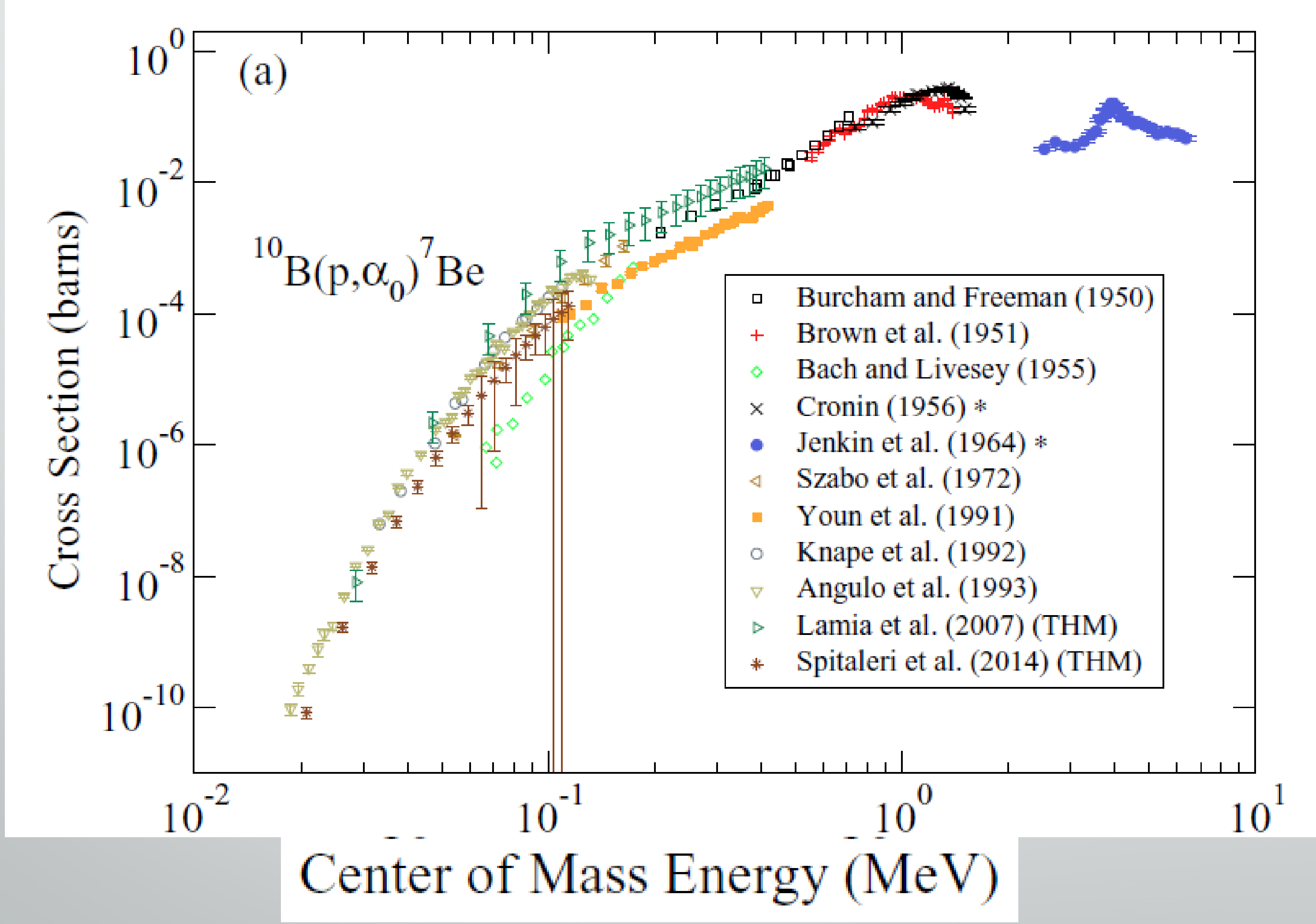


Global R-matrix analysis

- Desire for more accurate cross sections (reaction rates) drives the need for global analyses
- Data must exist
- Data must be consistent
- → Data Evaluation



Multiple data set fitting: systematic uncertainty



- Normalization differences
- Energy calibration differences
- Energy dependence differences

Shouldn't this be a standard calculation?

- Many different codes
- Many different R-matrix parameterizations
- Different fitting techniques
- Different uncertainty analysis techniques
- Many examples of calculation errors or analyses with where results cannot be reproduced

International Atomic Energy Agency: *R*-matrix Codes for Charged-Particle Reactions in the Resolved-Resonance Region

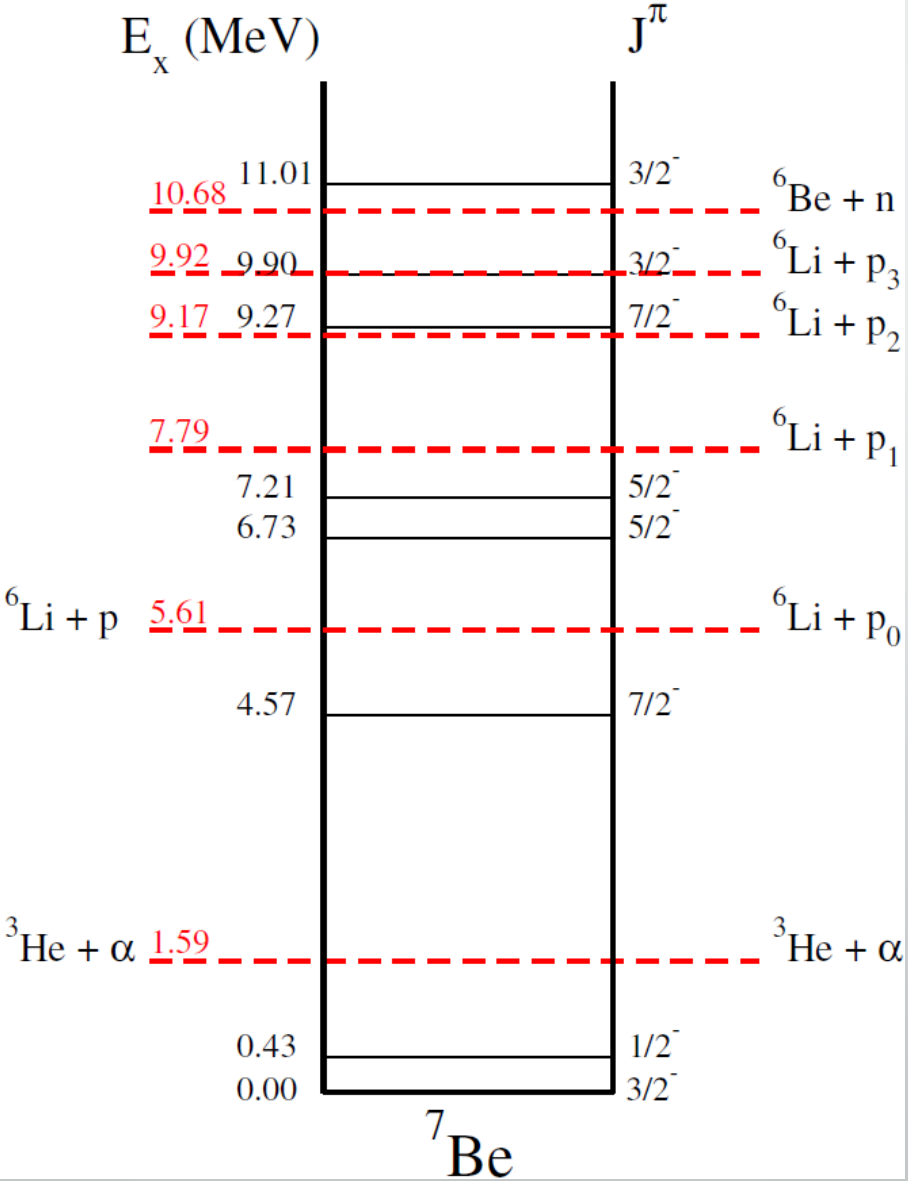
- Brings together people with *R*-matrix experience from a variety of backgrounds
  - Vivian Dimitriou (IAEA) – SAMMY
  - Ian Thompson (LLNL) – FRESCO
  - Sofia Quaglioni (LLNL) – personal code
  - Goran Arbanas (ORNL) – SAMMY
  - Marco Pigni (ORNL) – SAMMY
  - Mark Paris (LANL) – EDA
  - Satoshi Kunieda (JAEA) – AMUR
  - Zhenpeng Chen (Tsinghua University) – RAC
  - Helmut Leeb (TU Wien) – personal code
  - Thomas Srdinko (TU Wien/LANL) – personal code
  - James deBoer (University of Notre Dame and JINA) – AZURE2

Goals

- Develop standards for the evaluation of charged particle data in resolved resonance regions
- Obtain consistent set of codes that can be used for evolutions
- Produce evaluations for many different systems
- Store and make accessible evaluation results (ENDF)

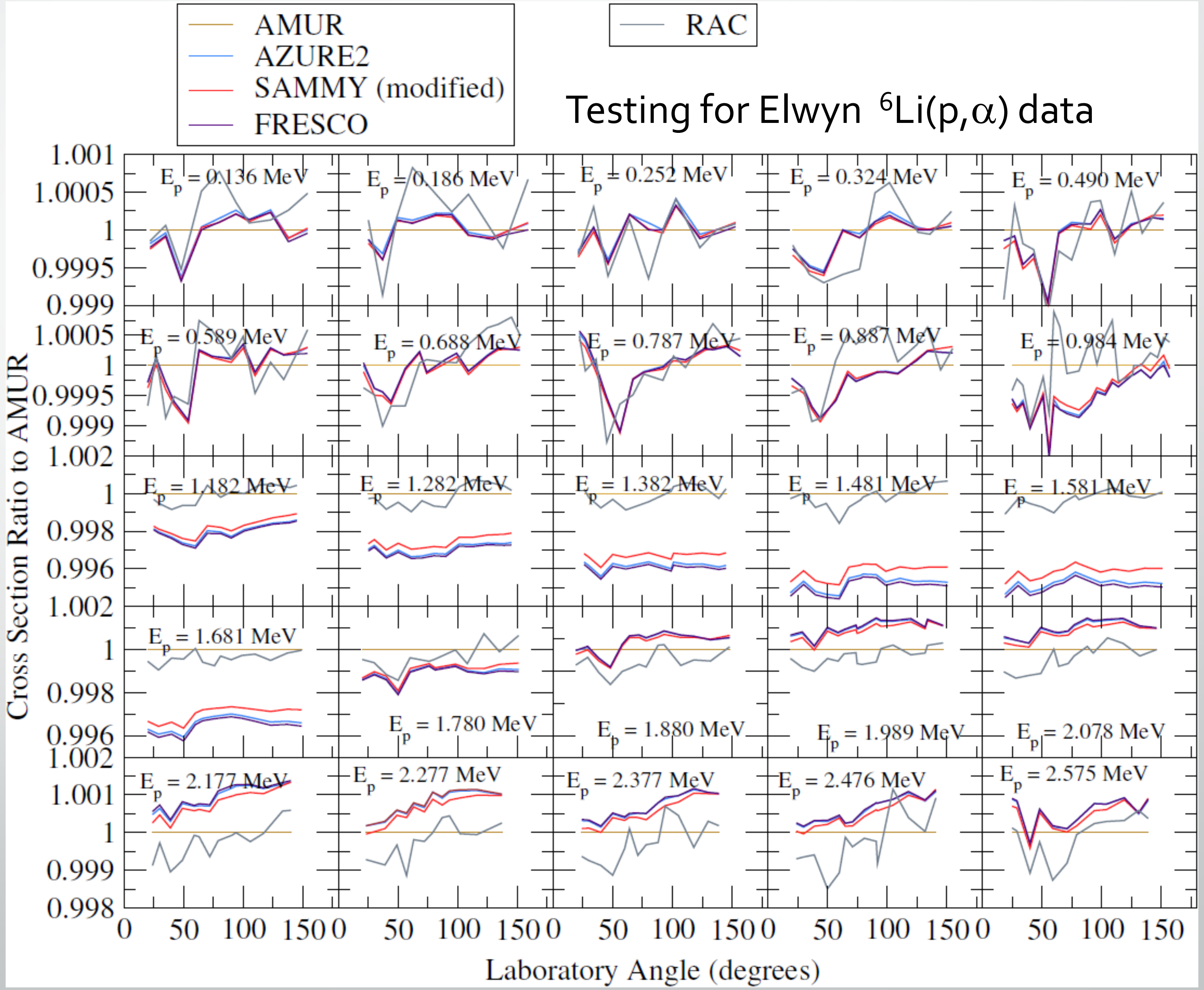
^{7}Be system for benchmarking

- ^{3}He(α,α)^{3}He, ^{6}Li(p,α)^{3}He, ^{6}Li(p,p)
- Not yet looking at γ-ray channels, but as we saw above this can be very helpful for ^{3}He(α,γ)^{7}Be and ^{6}Li(p,γ) analysis
- For those doing ^{6}Li(p,γ) analysis, can a low energy resonance be consistent with (p,p), (α,α) and (p,α) data?



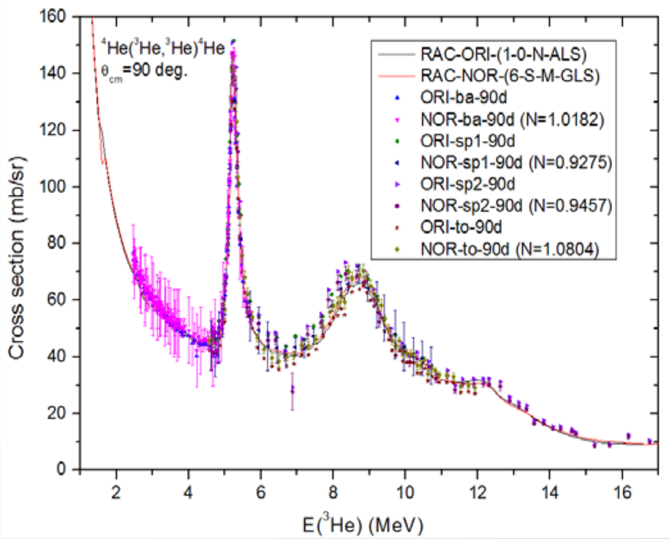
Lots of Benchmarking

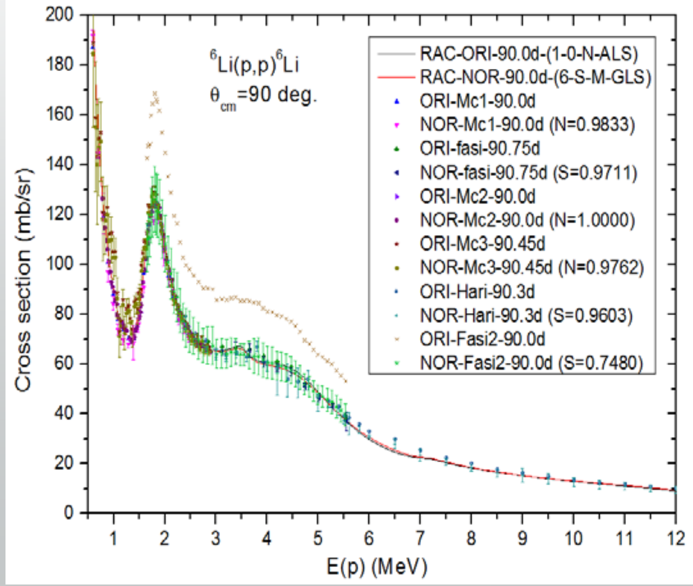
- Perform several test calculations to check consistency of codes
- Level of agreement is at about 1 / 10,000



Now actually fitting these data

- Do we get similar fits with similar parameters?
- Do different fitting techniques yield similar results (χ^2 vs. Bayesian approach)
- Treatment of systematic uncertainties





Preliminary fits by Zhenpeng Chen using RAC

Idea for evaluation procedure

- A member will perform an evolution of a system and then the group will check it over to verify
- Best fit parameters and covariance matrices will be stored in ENDF (evaluated nuclear data file) data base
- Input files for different R-matrix codes can be generated from the ENDF files with utility code Ferdinand (Ian Thompson)

Meeting websites

- https://www-nds.iaea.org/index-meeting-crp/CM-R-matrix/
- https://www-nds.iaea.org/index-meeting-crp/CM-R-matrix-2016/
- https://www-nds.iaea.org/index-meeting-crp/Rmatrix2017/

Application to Nuclear Astrophysics

- R-matrix **parameters** from evaluations can be used as a starting point for astrophysics analyses (extrapolation of data)
- More rigorous data evaluations will lead to better set of evaluated **starting data**
- More efficient analyses
  - Preliminary R-matrix fit already worked out
  - Preliminary evaluation of data sets
  - Can use a wide variety of codes and expect to get the same results

When can I use it?

- Some years down the road still
- Just finished code calculation comparisons (2 years)
- Just starting fitting comparisons
- Evaluation standards
- Actual evaluations

Summary

- R-matrix is a data analysis tool for interpreting resolved resonance region data
- The theory is best used when all decays to all significant channels are considered → this can complicate the analysis but leads to greater constraints on the phenomenological model
- The desire for increasingly accurate cross sections drives more global analyses
- This leads to a need for data evaluations to understand the level of agreement between the data
- An effort is underway at the IAEA to produce evaluations of charged particle data in the RRR. This will prove to be a valuable tool for the nuclear astrophysics community.

Acknowledgements

- IAEA working group on R-matrix analysis of charged particle reactions in the resolved resonance region
  - Vivian Dimitriou (IAEA)
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  - Sofia Quaglioni (LLNL)
  - Goran Arbanas (ORNL)
  - Marco Pigni (ORNL)
  - Mark Paris (LANL)
  - Satoshi Kunieda (JAEA
  - Zhenpeng Chen (Tsinghua University)
  - Helmut Leeb (TU Wien)
  - Thomas Srdinko (TU Wien/LANL)

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The $^{12}C(\alpha,\gamma)^{16}O$ reaction and its implications for stellar helium burning

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