European Commission

The status of data for ^{16}O and the program of work for CIELO

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Joint Research Centre

Contents

1. Program of work

2. Data for oxygen

Program of work
Goals, methods, timeline

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1) **Physics**
- Open points?
- Data to use?
- Available methods
  - R-matrix
  - Ext. Reich-Moore
  - Other?
- Handling of experimental effects

2) **Applications**
- Which applications are sensitive to ^{16}O?
- Which benchmarks to use?
- Interplay with other nuclides & physics
- Uncertainties & covar.

3) **Methods**
- Documentation for CIELO
  * Data
  * Codes
  * Decisions
  * Benchmarks
  * Improvements

4) **Timeline**
- Times
  * 2.5 year to tested file
  * 1.5 year to eval. File
  * 0.5 year to clarify data
- Times will be flexible except for the last year.
- Interconnection with other nuclides requires file to be ready on time.

Program of work
Tasks, assignments

1) What will we carry out?
2) Who will do what?
3) Parallel efforts?
   Allows comparing methods
4) How to merge?
   Decisions needed when E & C will not agree

Discussion end of the day & Friday

Data for oxygen

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Low energy data (<5keV)

Scattering & total: S. Kopecky

Capture: not touched upon (or ?)

High energy data (5 keV – 5.6/6.3 MeV)

Absorption

50% problem.

$^{16}O(n,a)^{13}C$: Khriatchkov (IPPE and IRMM data)

$^{13}C(\alpha,n)^{16}O$: Plompen (Harissopulos vs Bair&Haas)

Total cross section data (above 10 keV)

Brief summary of what is available (Plompen)

List of potential experimental effects to treat

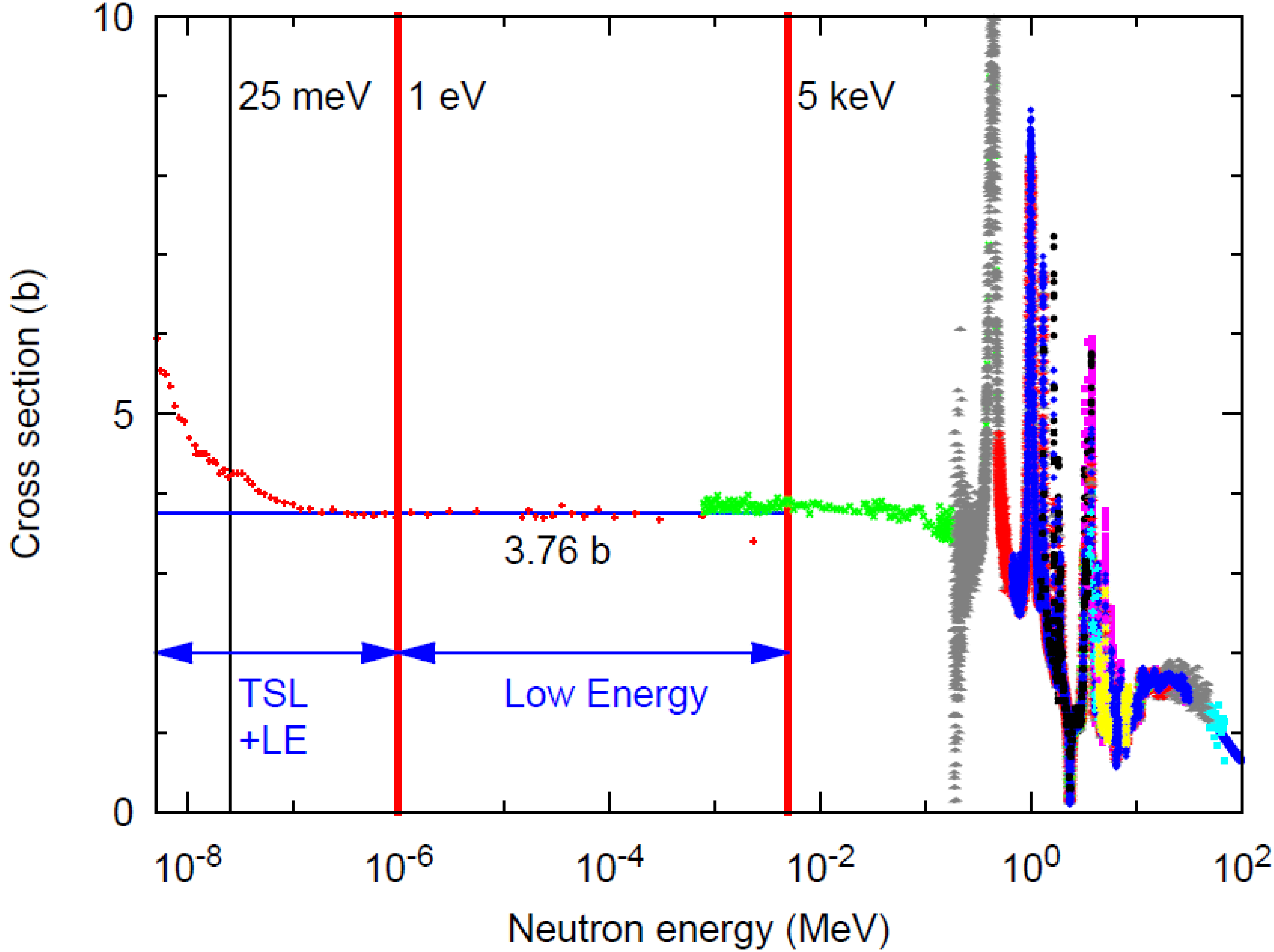
Analysis

Hale, Kunieda, Leal, Lubitz, Moxon

Implications for reactors:

Lubitz, Romano, Roubtsov, Kozier

Energy ranges

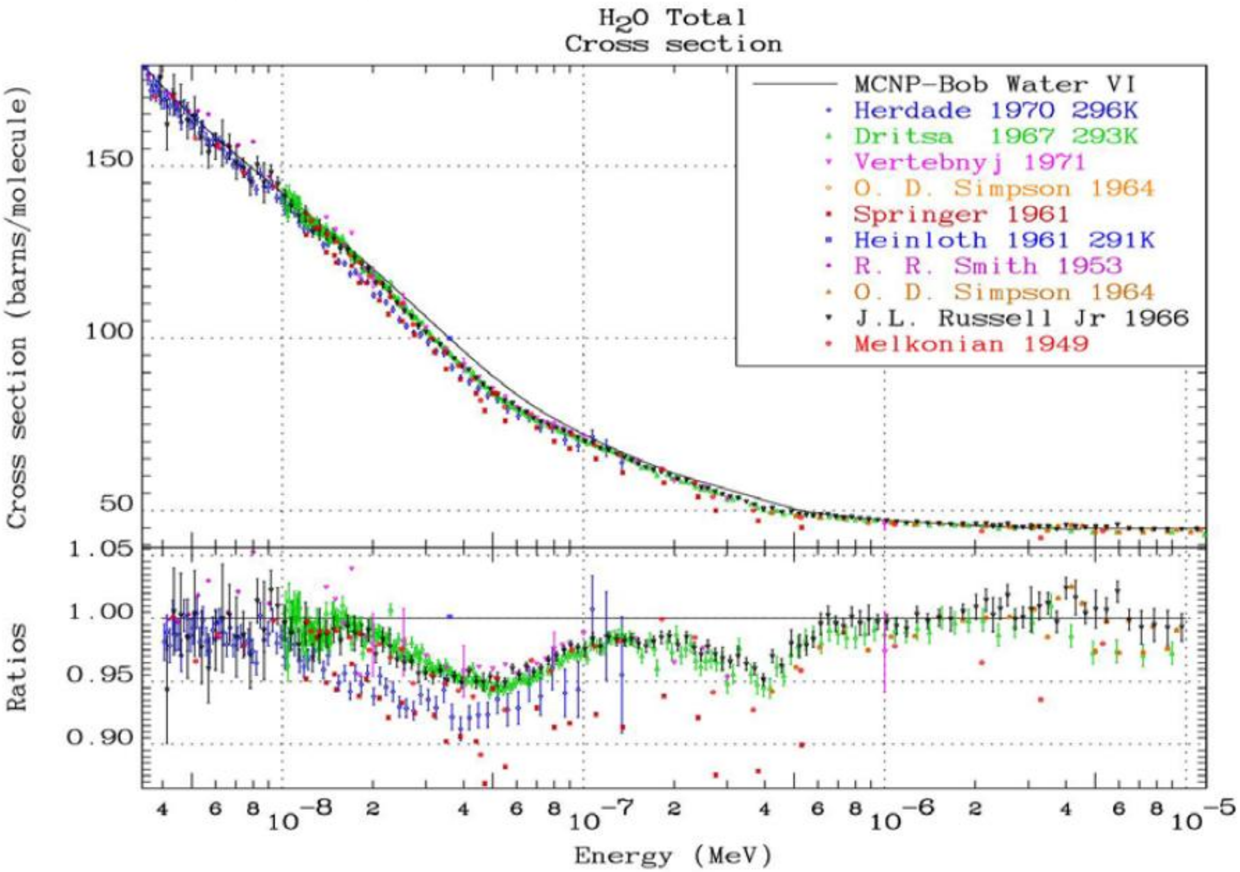


Thermal scattering

Contribution Sublet

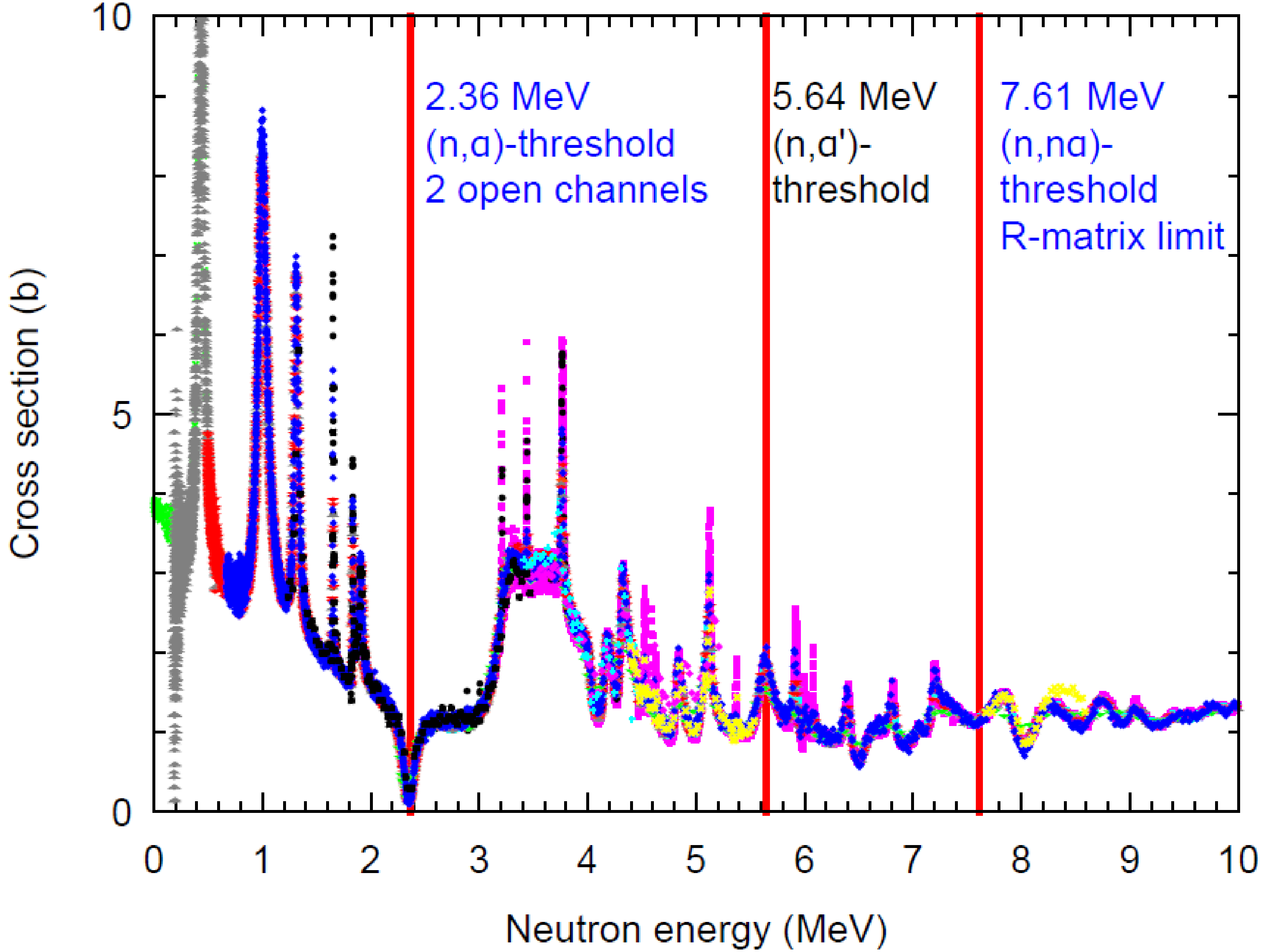
UCRL-TR-220605
"How Accurately Can We Calculate Neutrons Slowing Down In Water?"
Cullen et al. (2006)

Instances of E/C> 6%



"It is clear that the experimental data should be used if we are to be successful in calculating thermal critical assemblies.
Models are great when they can be verified by experimental data, but the experimental data should not be ignored and replaced by model calculations, particularly if the two do not agree."

Energy ranges



Absorption

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$^{16}O(n,\alpha)^{13}C$ and $^{13}C(\alpha,n)^{16}O$

$E_n > 2.36$ MeV
$^{16}O(n,\gamma)^{17}O$ is negligible

Microscopic reversibility

$$T_{a\to b} = T_{\bar{b}\to\bar{a}}$$

Principle of Detailed Balance

$$(2i_a+1)(2I_a+1)\,p_a^2\frac{d\sigma_{a\to b}}{d\Omega_b} =$$

$$(2i_b+1)(2I_b+1)\,p_b^2\frac{d\sigma_{\bar{b}\to\bar{a}}}{d\Omega_a}$$

(Reciprocity theorem)

a + A → B + b

n + ^{16}O → ^{13}C + α

n + ^{16}O ← ^{13}C + α

i_a	I_A	I_B	i_b
½	0	½	0

$$p_a^2\frac{d\sigma_{a\to b}}{d\Omega_b} = p_b^2\frac{d\sigma_{\bar{b}\to\bar{a}}}{d\Omega_a}$$

Up to threshold $^{16}O(n,\alpha')^{13}C^*$
2.36 MeV < E_n < 5.64 MeV
Up to threshold $^{13}C(a,n')^{16}O^*$
E_α < 5.01 MeV
6.36 MeV < $E_x(^{17}O)$ < 9.45 MeV

$^{13}C(a,n)^{16}O$

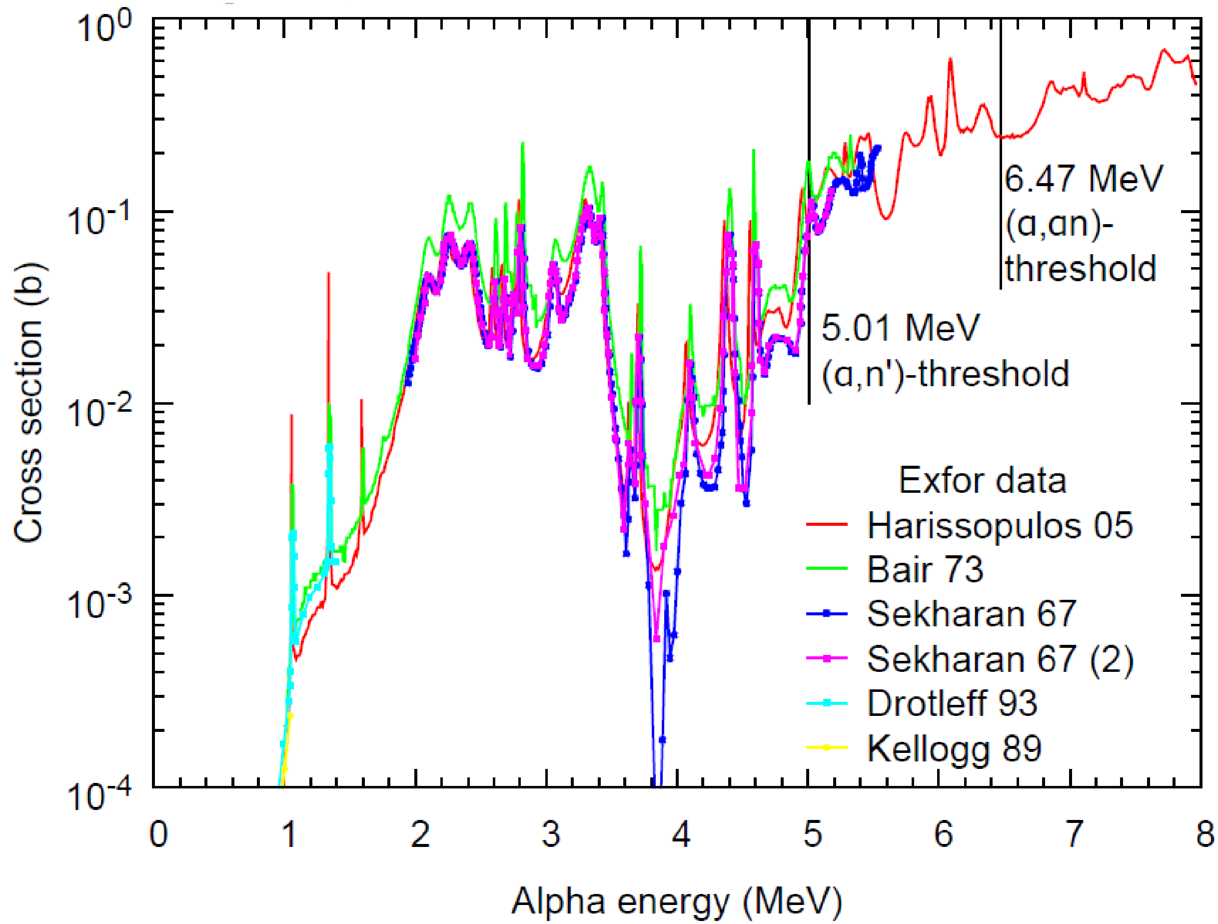
Considerable interest below E_{α}=1 MeV

Stellar neutron source reaction

Little concern to CIELO

Some data below 1.5 MeV are not shown (Heil, Brune, Ramström)

Data of interest to $^{16}O(n,\alpha)^{13}C$ are shown in the graph and discussed below



Issues

R-matrix puzzle (n,tot) vs (n,a)

Discrepancies & errors data

$^{13}C(a,n)^{16}O$

$$N_n = N_\alpha N_t \eta_n \sigma(E_{\rm eff})$$

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Harissopulos et al.

PRC72(2005)062801R

Expt. Ruhr U. Bochum

Dynamitron-tandem

Target

1) thin 22 μg/cm², 99% enr.

Thickness to 3% from resonance widths in (p,g) and (a,n) reactions and stopping powers.

ΔE_a=37(1)keV at Ea=1054 keV

ΔE_a=33(1)keV at Ea=1336 keV

2) thick natural to check enr.

Limited check, as nat.enr. 1.07(8)% ^{13}C has unc. 5%. Use of (p,g) react.

Nt = (10.2±0.3) $10^{17}/cm^2$ ^{13}C

Current

Biased Faraday cup 2% unc.

Neutron counter

1) PE cylinder 35 cm x 100 cm
2) 16 x 2.54 cm ø x 46 cm x 4 bar ^3He (2 rings of 8 at 16, 24 cm at rings at relative 22.5 degrees)
3) Outer shield Cd, PE, B-PE: 0.22 cps
4) Efficiency by MCNP: ^{252}Cf 31.6% (AP redo w.IAEA spectrum gives 32.7%: eff(<En>=2.3 MeV) vs. mean-eff.)
5) Efficiency ^{252}Cf 32.1(5)% (2.3 MeV)
6) Efficiency curve given (checks out)

$$\eta_n(E_n) = 0.7904 + 0.1607(E_n + 247.07)\exp(-0.114E_n)[\%]$$

Qualifications by authors

1. Overall uncertainty: 4%
2. Reproducibility: 2%
3. Energy steps/keV: 10

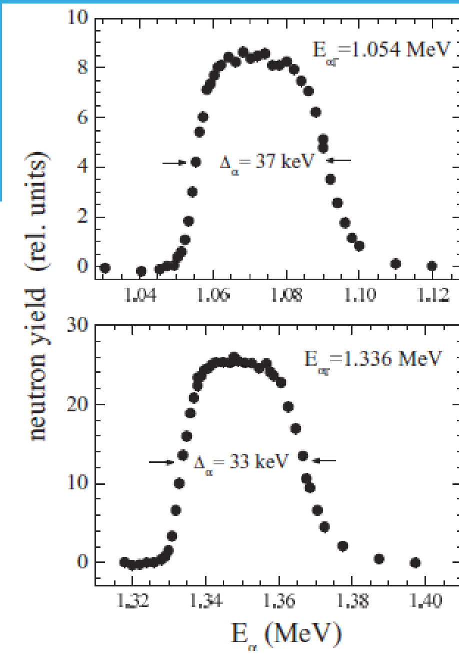
$^{13}C(a,n)^{16}O$

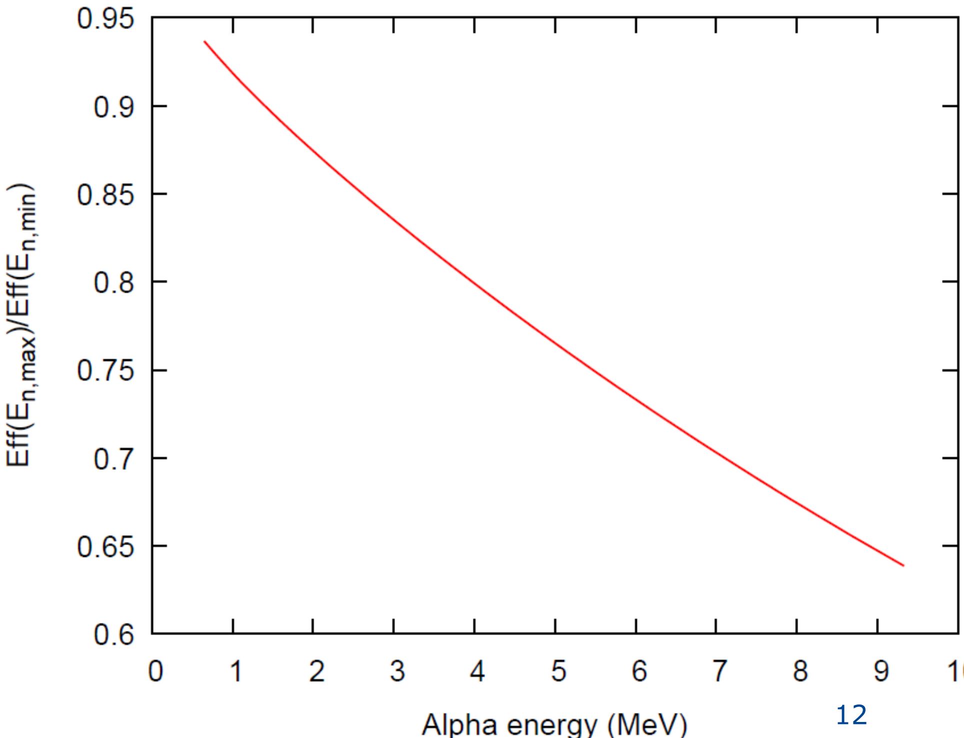
Discussion of Harissopulos et al.

1) Clerical error?
   Text has 157(7) μb at 1.000 MeV
   Table has 135 μb
   Correction factor table: 1.16
2) Efficiency calibration
   normalize to source data!

$\eta_n(^{252}Cf\text{-expt})$	32.1(5)%
$\eta_{n,calc}(<E_n(^{252}Cf)>)$	31.6%
$<\eta_{n,calc}>(^{252}Cf)$	32.7%

   Correction factor: 0.98 (32.1/32.7)
3) Impact angle dependence of neutrons on efficiency
   Use of $\eta_n(E_n(90^o))$ as efficiency
   Angle dependence ? worst case in graph, not included in following
4) Energy scale
   corrected to match transmission Cierjacks '80





$^{13}C(a,n)^{16}O$

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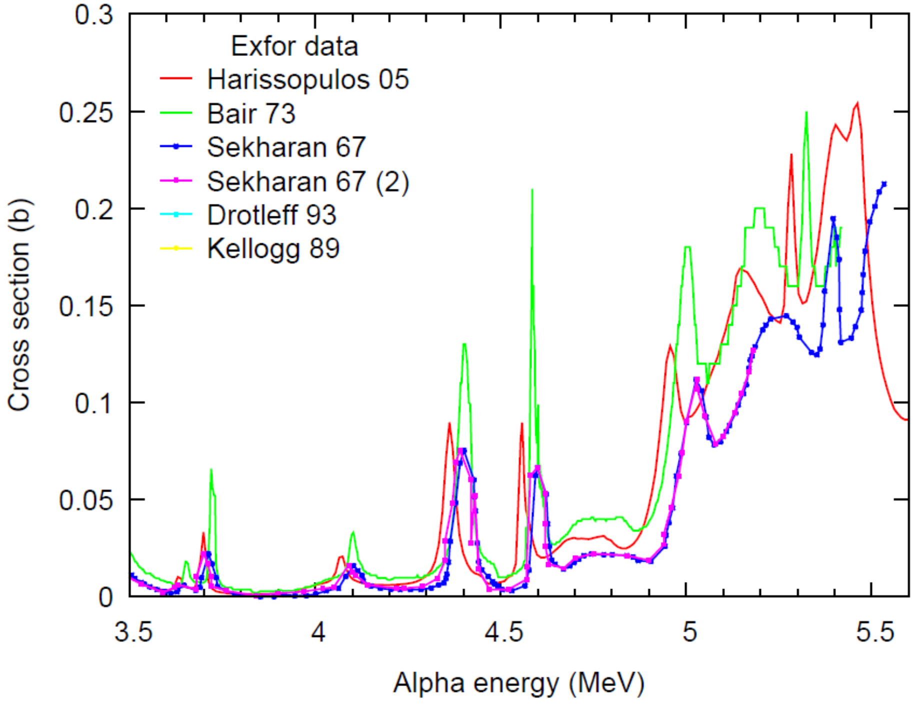
Discussion of Harissopulos et al.

I have had a lot to say about it but it is probably the best work for $^{13}C(a,n)^{16}O$ for our purpose.

1) Healthy measurement principle, good setup, good calibration

2) Good attention for detail for quantitative results

3) Sufficient detail to implement corrections, except resolution!
   a) Need neutron ang.dist.
   b) Some clarification authors

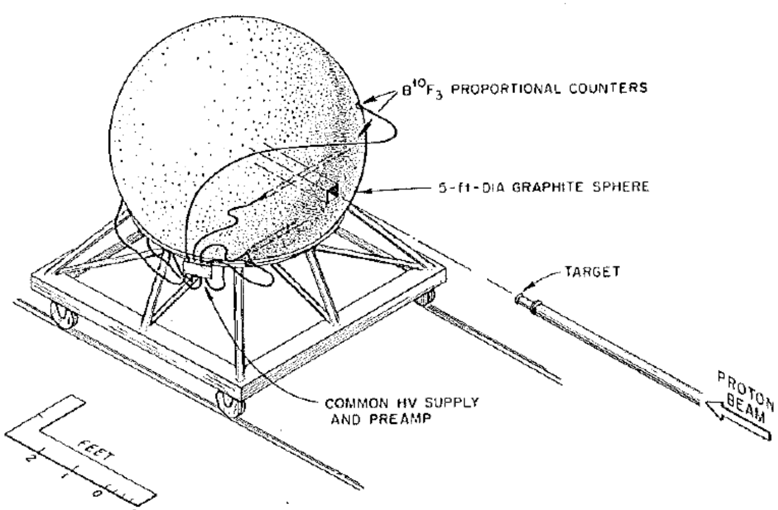


$^{13}C(a,n)^{16}O$

Bair and Haas

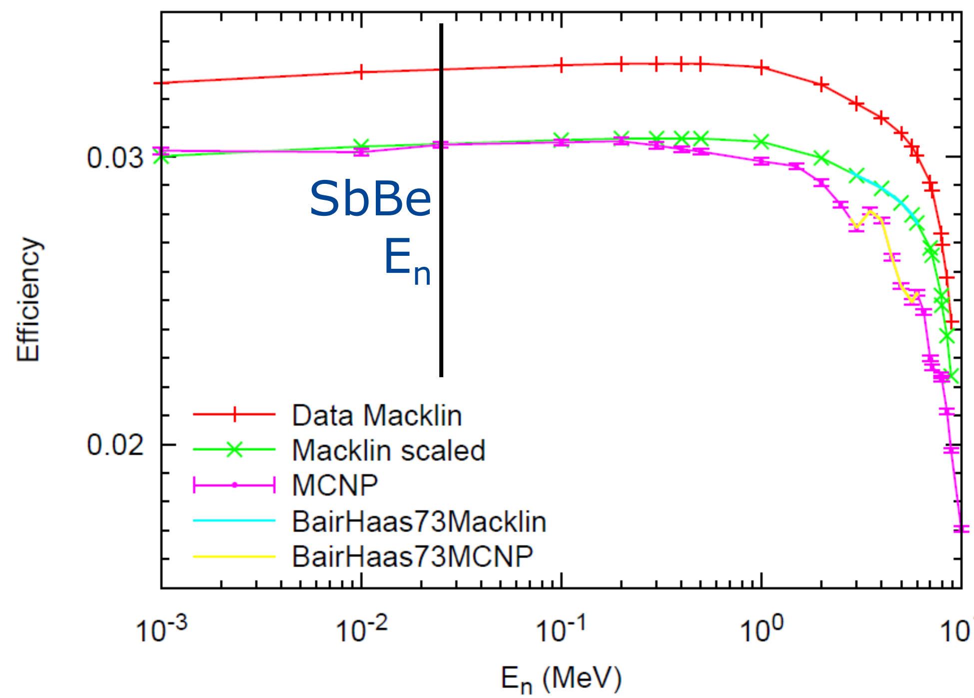
Bair and Haas PRC7(1973)1356
Bair NSE53(1973)83, TTY
Macklin and Gibbons
NSE31(1968)337, TTY
Macklin NIM1(1957)335, det.

Oak Ridge Van de Graaff
Oak Ridge Tandem (Bair TTY)



Graphite sphere moderator

1.5 m diameter
8 BF_3 counters
Sb-Be efficiency: 0.0306 (3%)
Eff(En): age theory
No shield.



$^{13}C(a,n)^{16}O$

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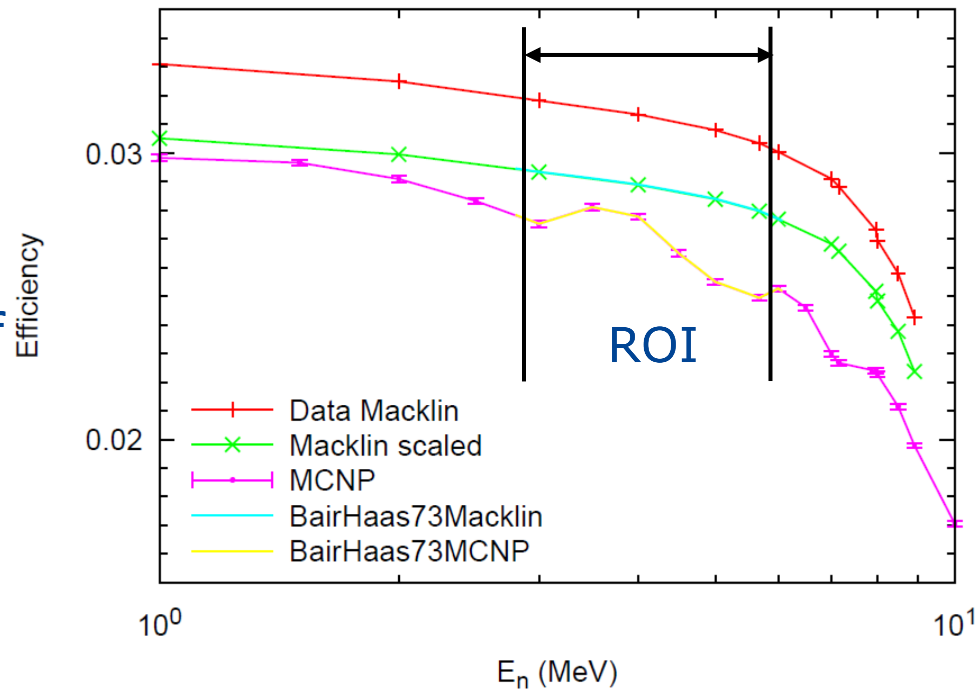
Bair and Haas

Macklin's SbBe and Age theory efficiencies disagree by 8.5%.
Rescaled to NBS source data

Energy dependence in range of interest (2-5 MeV) ?
MCNP vs. age theory or vs. a constant efficiency?



Other questions

1) No shield for room return
2) 80% of neutrons leak out !
3) Angular distribution: same problem as Harissopulos

$^{13}C(a,n)^{16}O$

Bair and Haas

Thick and thin target data

1) Thick ^{nat}C: resonance integrals
2) Thick ^{enr}C: weaker RI
3) Thin ^{enr}C: excitation curve

Thin target data: ^{13}C target

1) Excitation curve was obtained with "*cracked enriched acetylene on a Pt backing*".
2) ΔE_{α}= 5 keV at E_r=1054 keV
3) Enrichment unknown
4) Essentially unnormalized

Normalization

1) PRC paper
   RI thick ^{nat}C 1054 keV and
   RI thin ^{enr}C same resonance

2) PRC paper footnote:
   Reduce our data by 15-20%
   Reference: Bair NSE paper TTY

3) Note that data EXFOR show
   ΔE_{α}= 13 keV at E_r=1054 keV
   ΔE_{α}= 13 keV at E_r=1588 keV
   2.5 times claimed 5 keV!

$^{13}C(a,n)^{16}O$

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Bair and Haas

$$\mathrm{TTY}(E_\alpha) = \int_0^{E_\alpha} \frac{N(^{13}C)}{S(E'_\alpha)} \sigma_{\alpha,n}(E'_\alpha) dE'_\alpha$$

$N(^{13}C)$ number of ^{13}C atoms per atom

$S(E_\alpha)$ stopping cross section

$$\mathrm{TTY}^{\mathrm{exp}}(E_\alpha) = \frac{C_n^{\mathrm{net}}(E_\alpha)}{\langle \eta_n(E_\alpha) \rangle (Q_\alpha / q_\alpha)}$$

TTY for normalization?

- Same detector
- Data set Macklin and Gibbons
  - (w. 3 errors)
- Data set Bair
- Two NSE papers, data not in X4

Discussion

1) Very short papers
2) No comments about handling energy dependence of efficiency
3) Nevertheless each claims about 4-5 % uncertainty see below

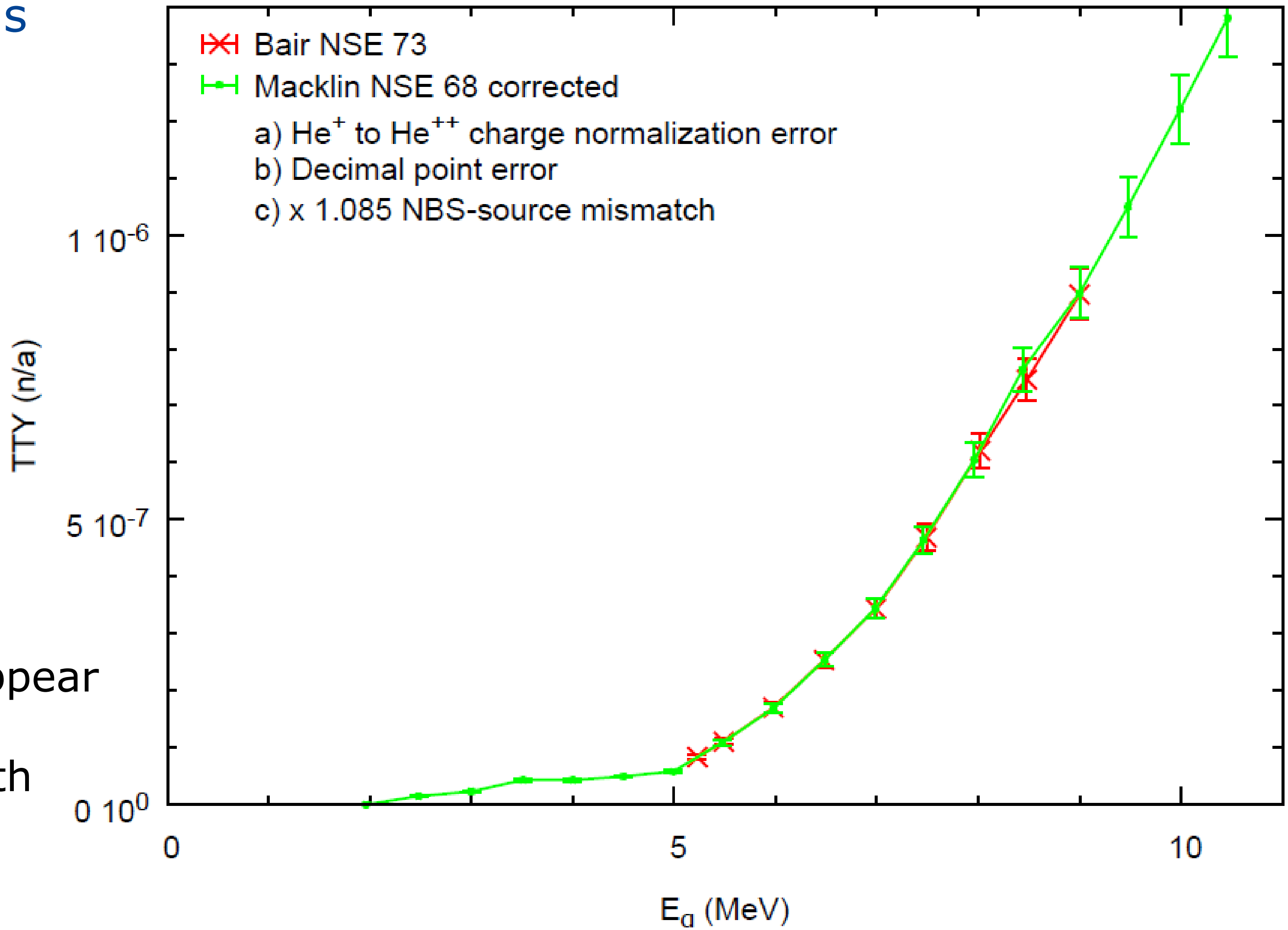
Corrections

1) Geometry from indicative numbers and drawing shown
2) Tube pressure 240 cm Hg instead of 120 cm in paper Macklin (NIM)
3) Effect of room cannot be modeled
4) Angular distribution

$^{13}C(a,n)^{16}O$

Bair and Haas

Discussion



TTY Macklin:

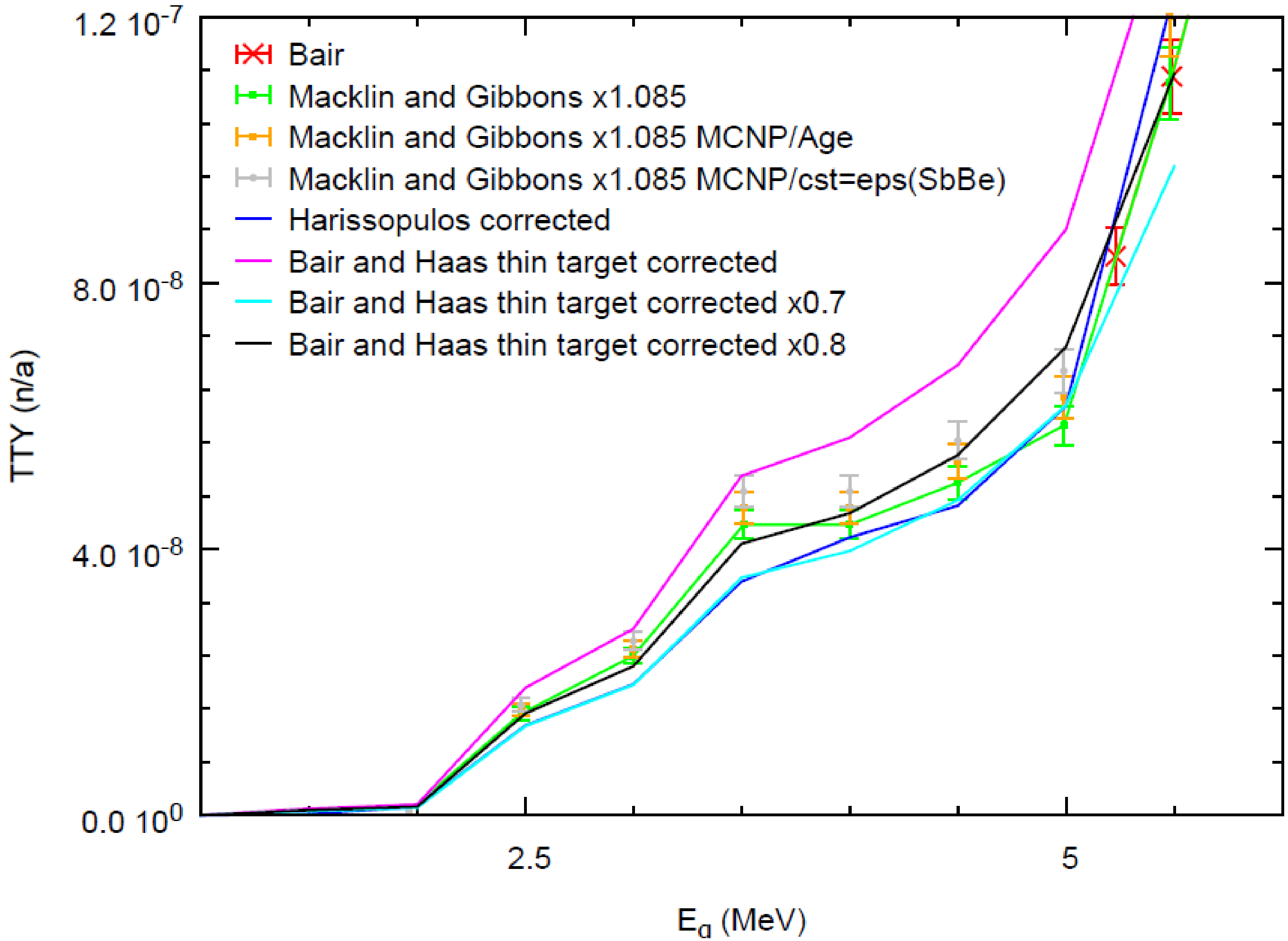
Corrections appear to give good agreement with Bair TTY

Bair and Haas Discussion TTY

Harissopulos agrees with Bair TTY
TTY eff.corr would improve agreement

Shape Harissopulos and Bair and Haas agrees up to 5 MeV, not above
Digitization error Bair data?

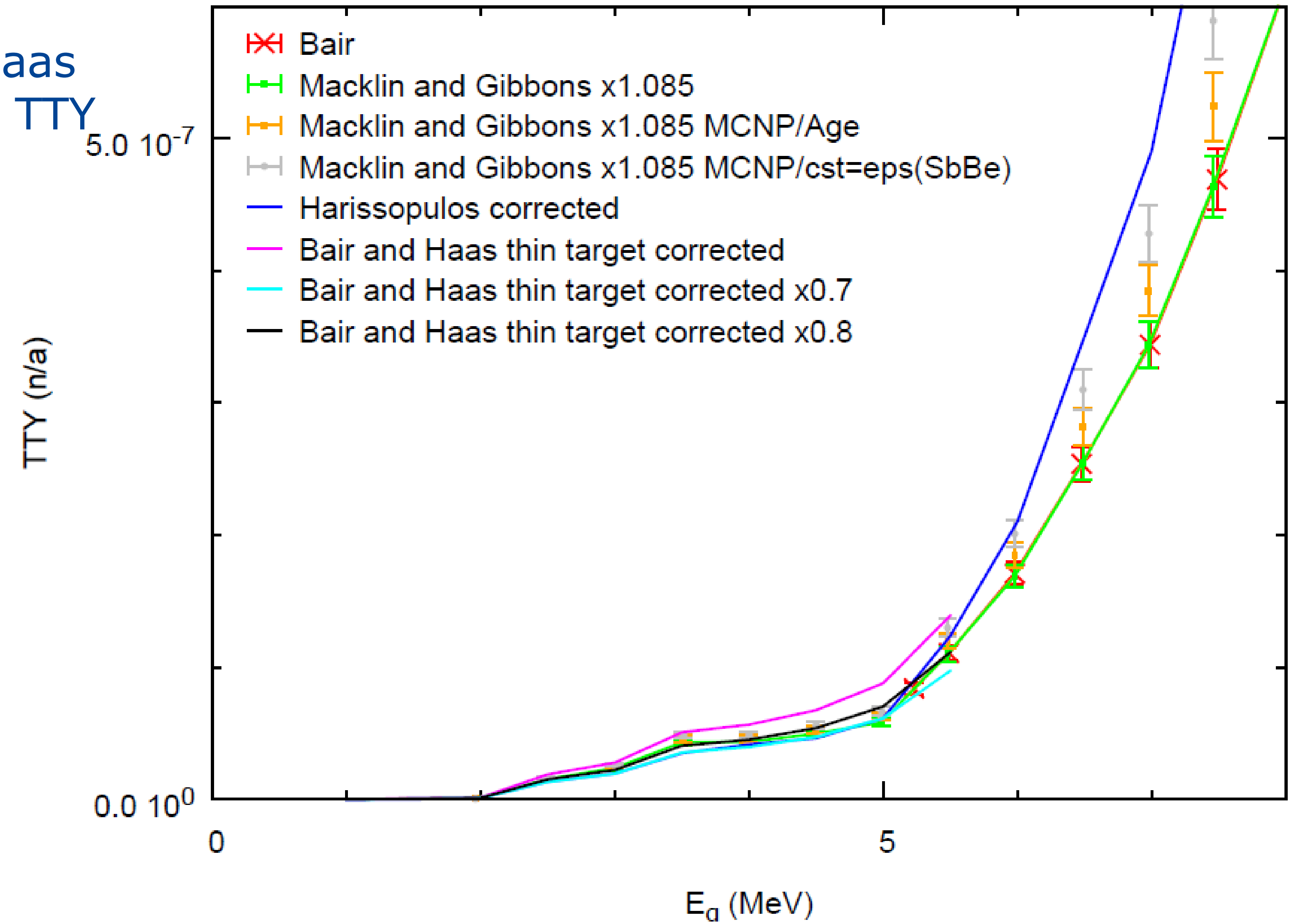
75-80% of efficiency corrected Bair and Haas agrees with Bair TTY



Present Harissopulos and Bair and Haas TTY calculations use SRIM2003 stopping powers

$^{13}C(a,n)^{16}O$

Bair and Haas Discussion TTY



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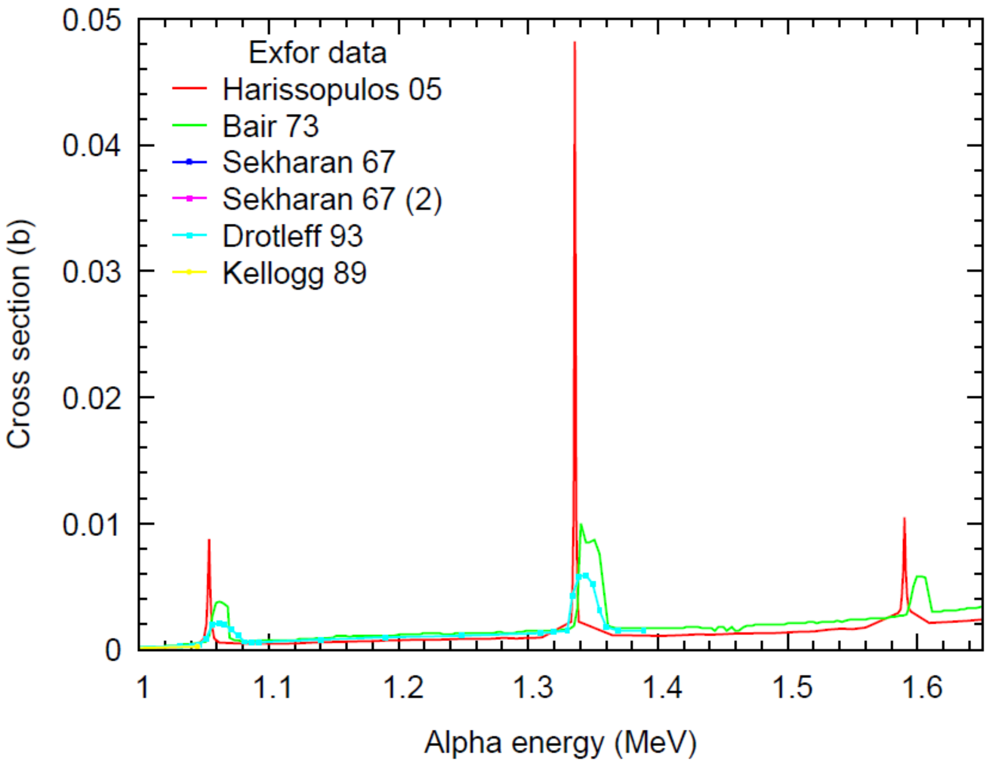
$^{13}C(a,n)^{16}O$

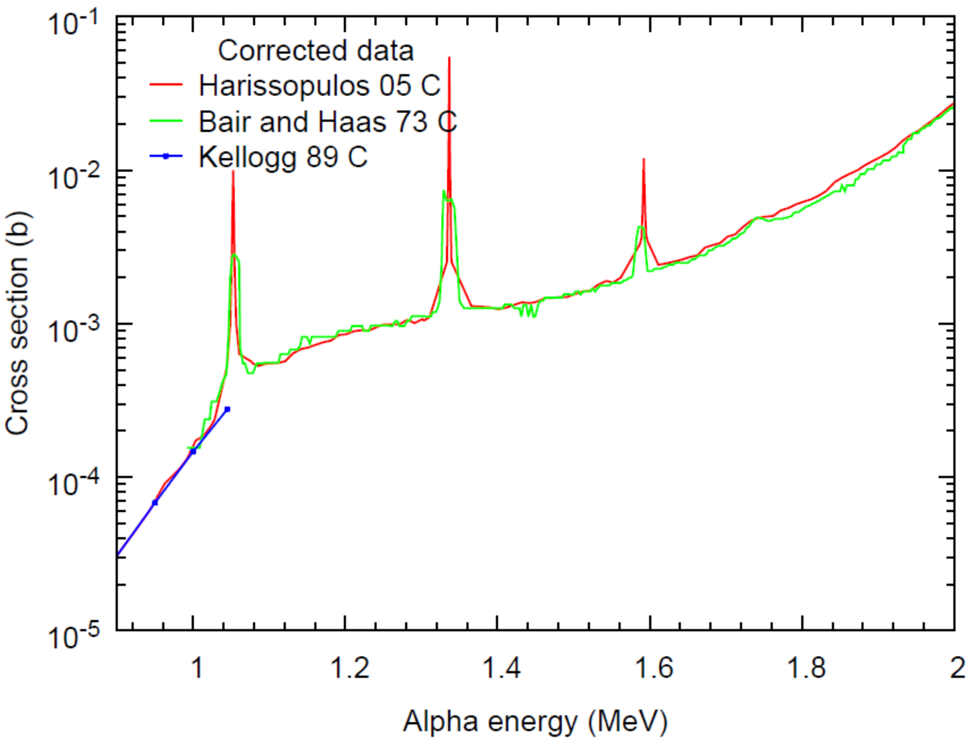
Resolution

Target thickness Harissopulos greater than that of Bair and Haas
For E_r = 1054 keV
Harissopulos: ΔE_a= 37(1) keV
Bair and Haas: ΔE_α= 13.1(2) keV

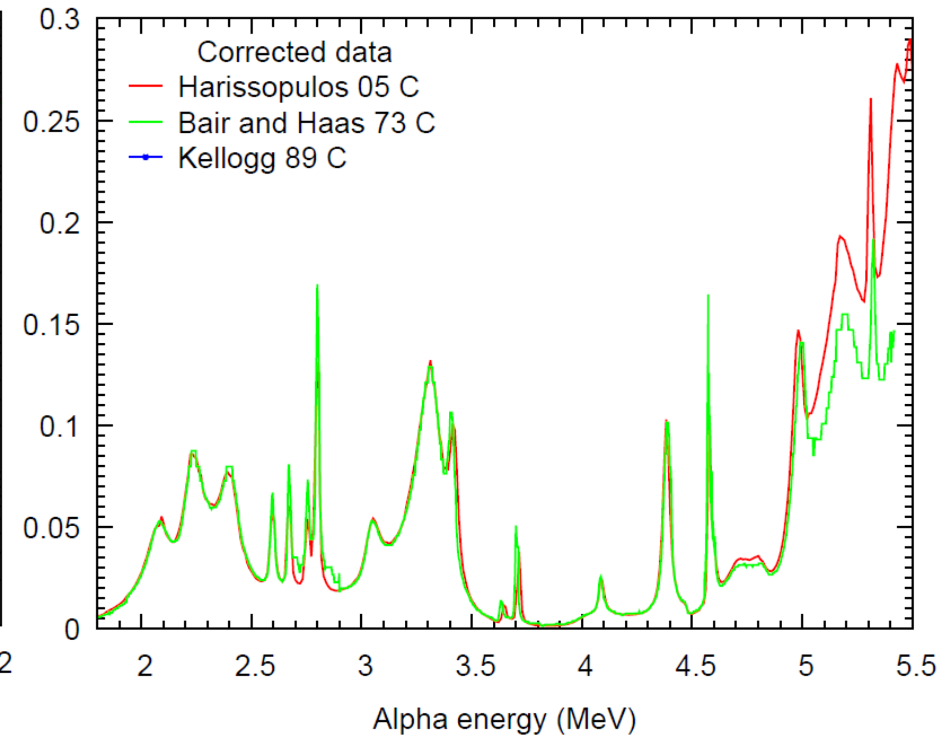
But Harissopulos corrected his data for energy loss.



$^{13}C(a,n)^{16}O$



Proposed corrected data



Bair and Haas reduced to 70%
(x age/MCNP x 70% ≈ 80%)
Kellogg to 0.156 mb at 1 MeV

Equivalent $^{16}O(n,a)^{13}C$

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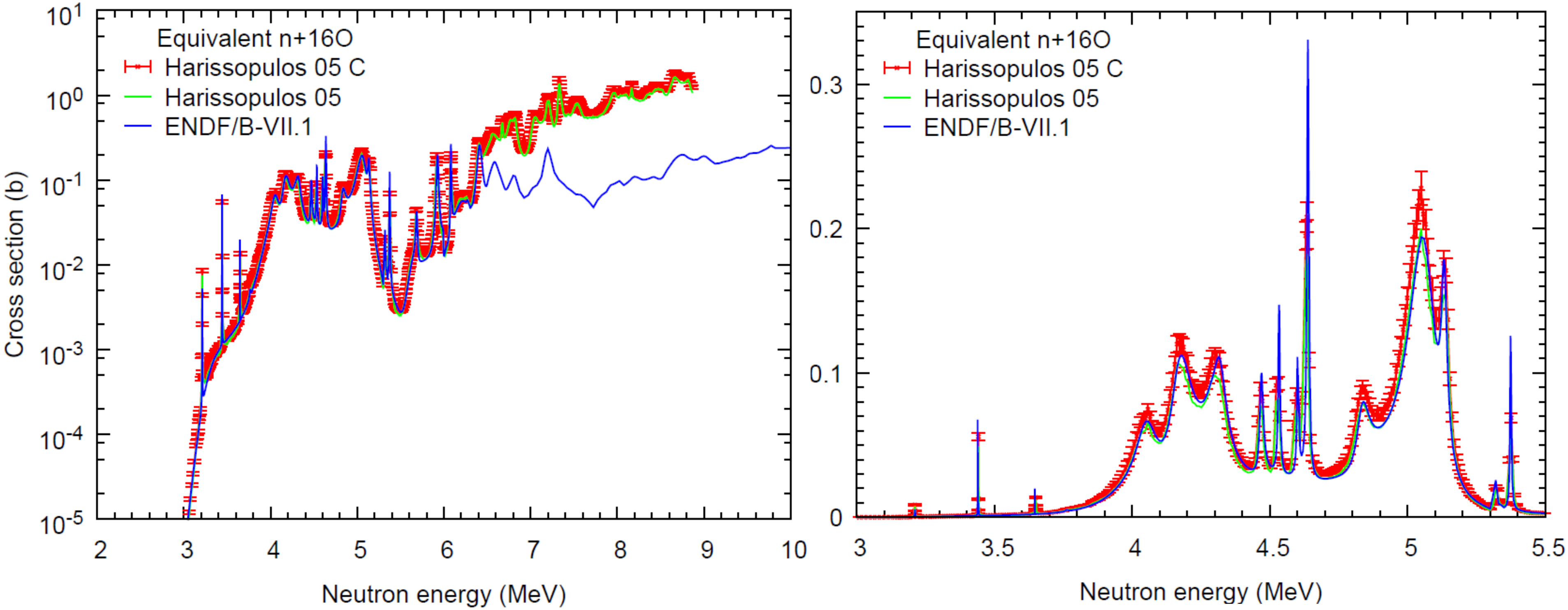


Note: 'Johnson data' n+^{16}O: Bair and Haas x 80% + changes !
So matches Harissopulos original data and ENDF/B-VII.1

Conclusion $^{13}C(\alpha,n)^{16}O$

No room for 50% up
For Harissopulos.

Bair&Haas should go down

Harissopulos data to do list

1. Raw data before target energy loss correction needed (from authors)
2. Clarify 14% issue (by authors)
3. Angular distribution data needed to correct energy dependence of efficiency.
4. Get their thick target data (if useful: perhaps only few resonances).

Bair and Haas normalization & E-dep.

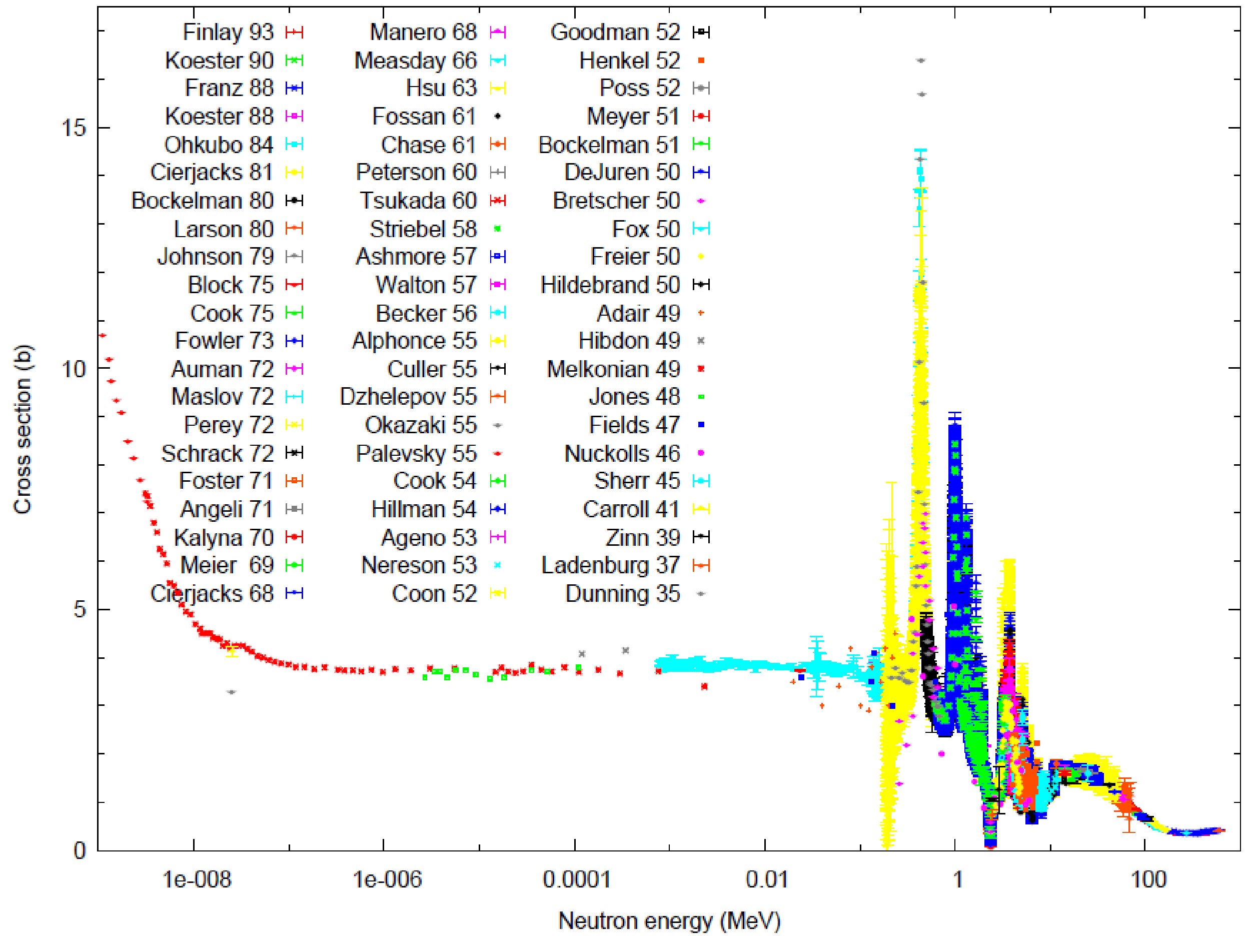
1. Every attempt at correction leads to lower cross sections, not higher.
2. Normalize by resonance integral? Needs Harissopulos resonance integrals and perhaps others (contact authors).

n+^{16}O total cross section

Widely studied above 100 keV

Above 100 keV:
Downselection needed
1) Large data sets
2) Good resolution
3) ‘Recent’

Below 100 keV:
Limited set of TOF data
Few very accurate results (Kopecky)



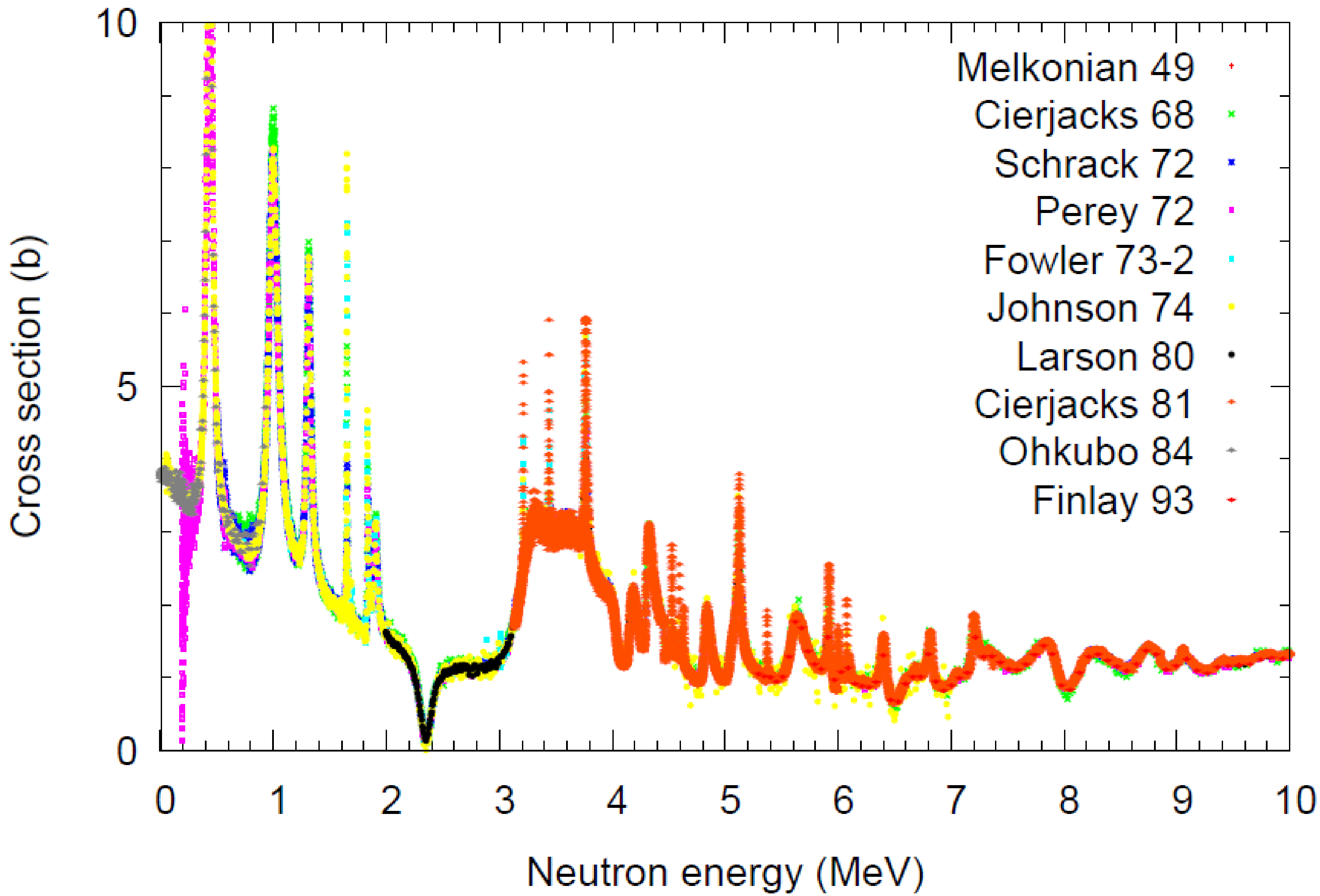
Selected Data Total $n+^{16}O$

First Author	Energy range MeV	Data # points	FPL m	Samples	Year	Lab
Finlay	5.3-600	474	38	BeO,Al_2O_3	1993	LANL/WNR
Ohkubo	0.0008-0.94	310	47	CeO,Ce	1984	JAERI e-linac
Larson	2-69	670	80	BeO,Be	1980	ORELA e+Ta,g+Be
Cierjacks	3.1-32	21058	189.25	LO_2	1980	KFK d+U 50 MeV, normalized to Cierjacks 1974
Johnson	0.04 – 7	2313	198.731		1974	ORELA
Fowler	0.6-4.3	538	0.47	BeO,Be	1973	ORNL VdG Li(p,n)
Schrack	0.5-20.5	3449	40	Quartz, Si	1972	NBS: e+W/Be
Perey	0.19-49	3688	47.35	SiO_2,Si	1972	ORELA
Cierjacks	0.67-32	4305	57.5	Al_2O_3	1968	KFK

Selected Data Total

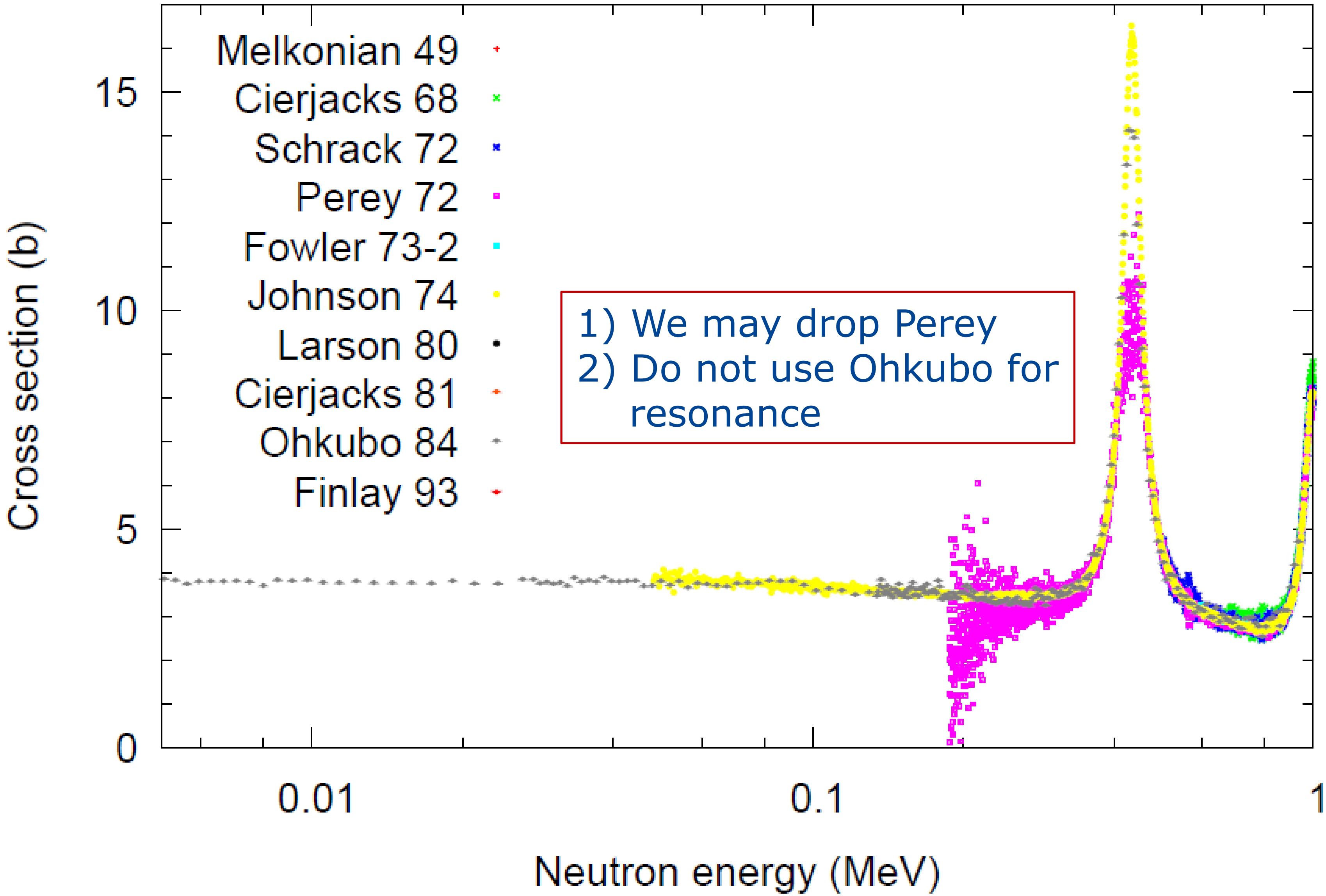
n+^{16}O

Large data sets, good resolution

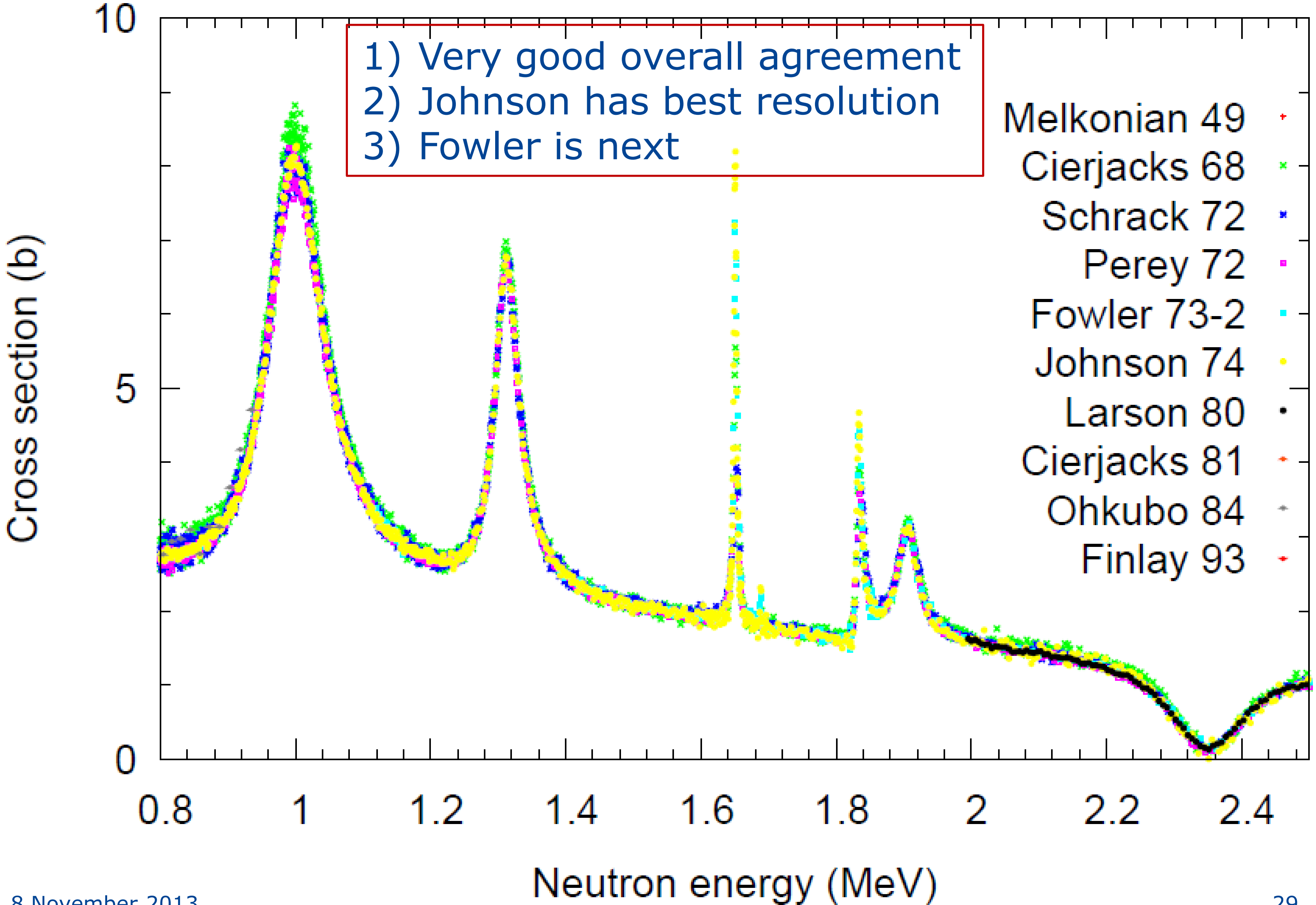


Selected Data Total

n+^{16}O



1) We may drop Perey
2) Do not use Ohkubo for resonance



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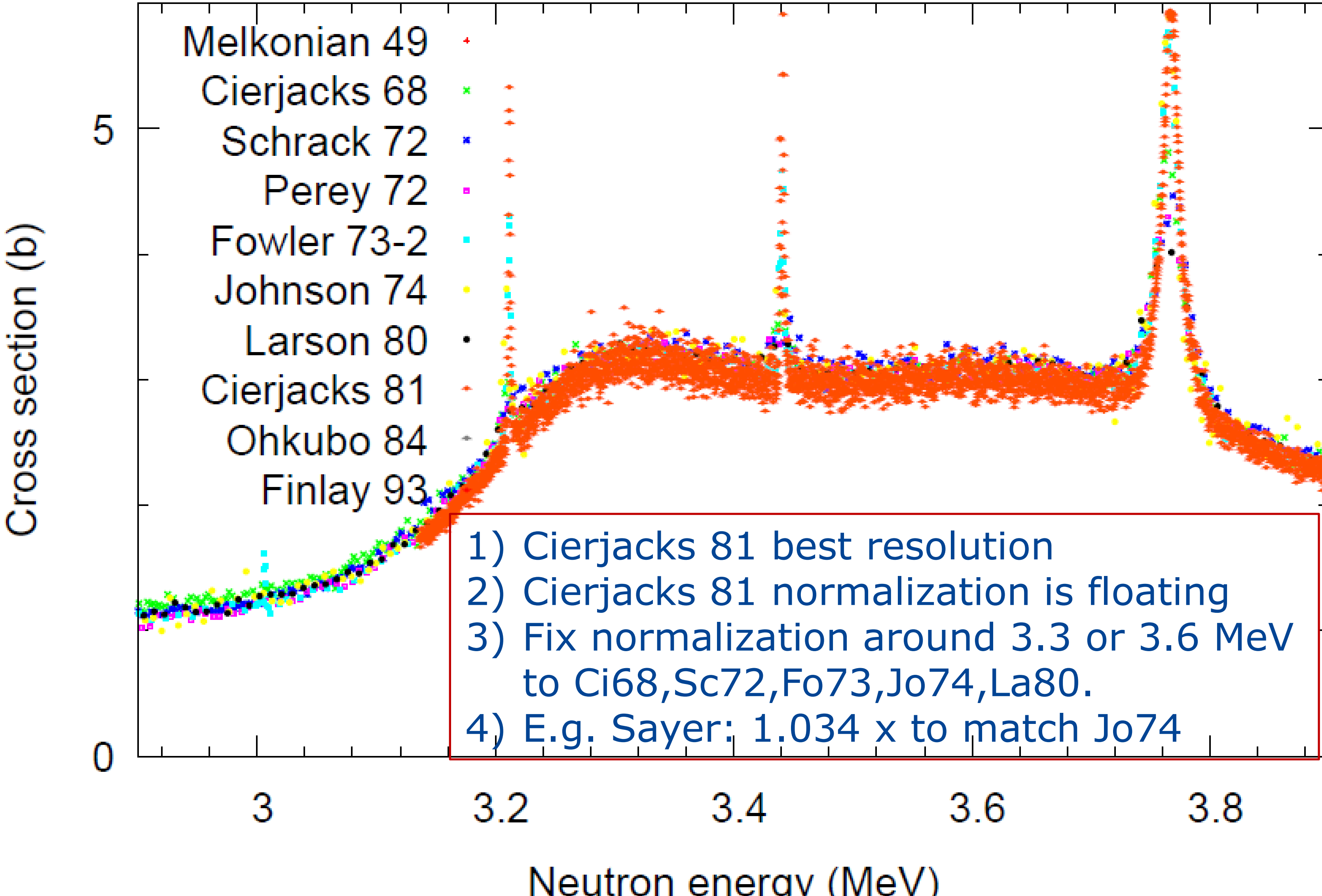
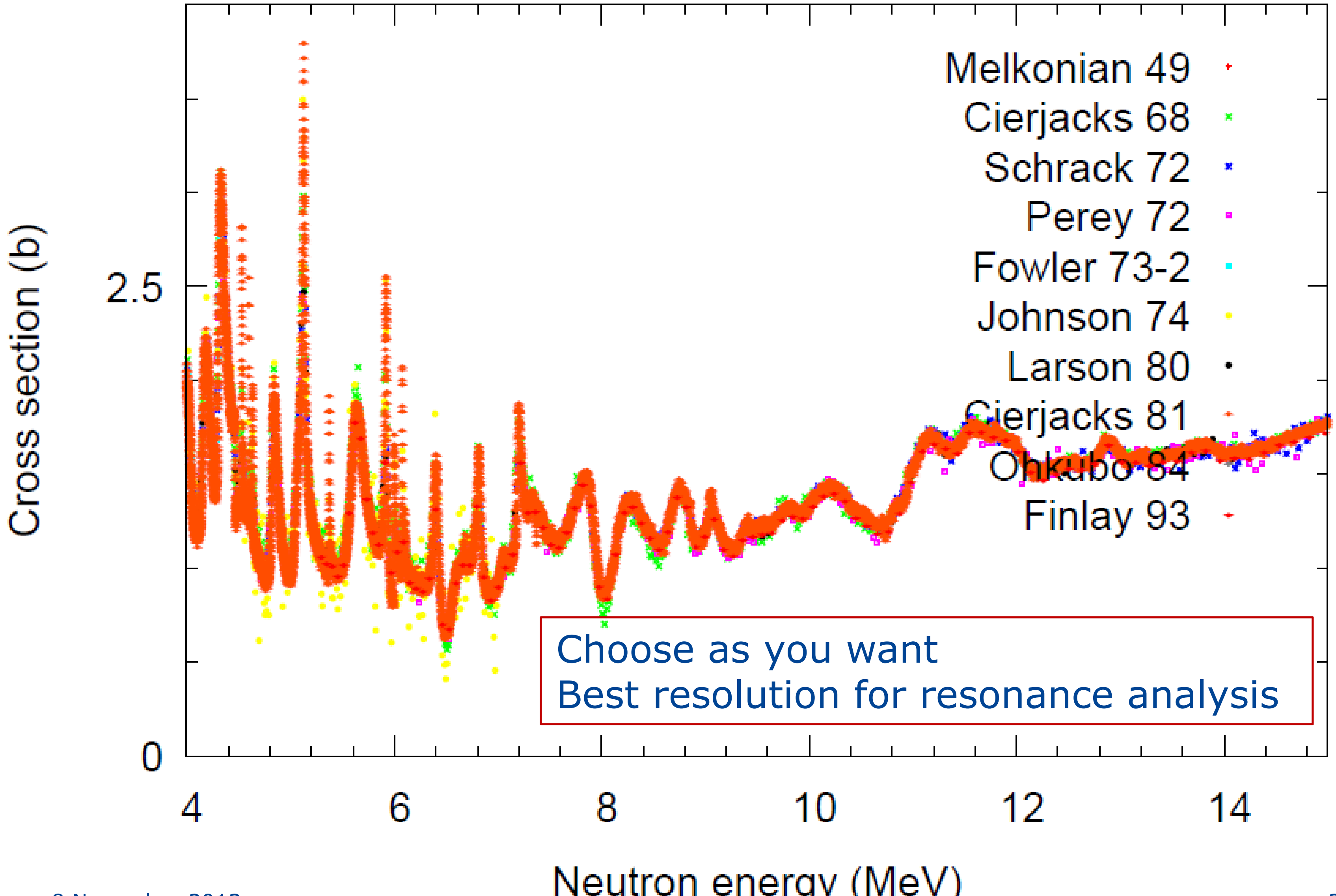
Selected Data Total n+^{16}O



1) Cierjacks 81 best resolution
2) Cierjacks 81 normalization is floating
3) Fix normalization around 3.3 or 3.6 MeV to Ci68,Sc72,Fo73,Jo74,La80.
4) E.g. Sayer: 1.034 x to match Jo74

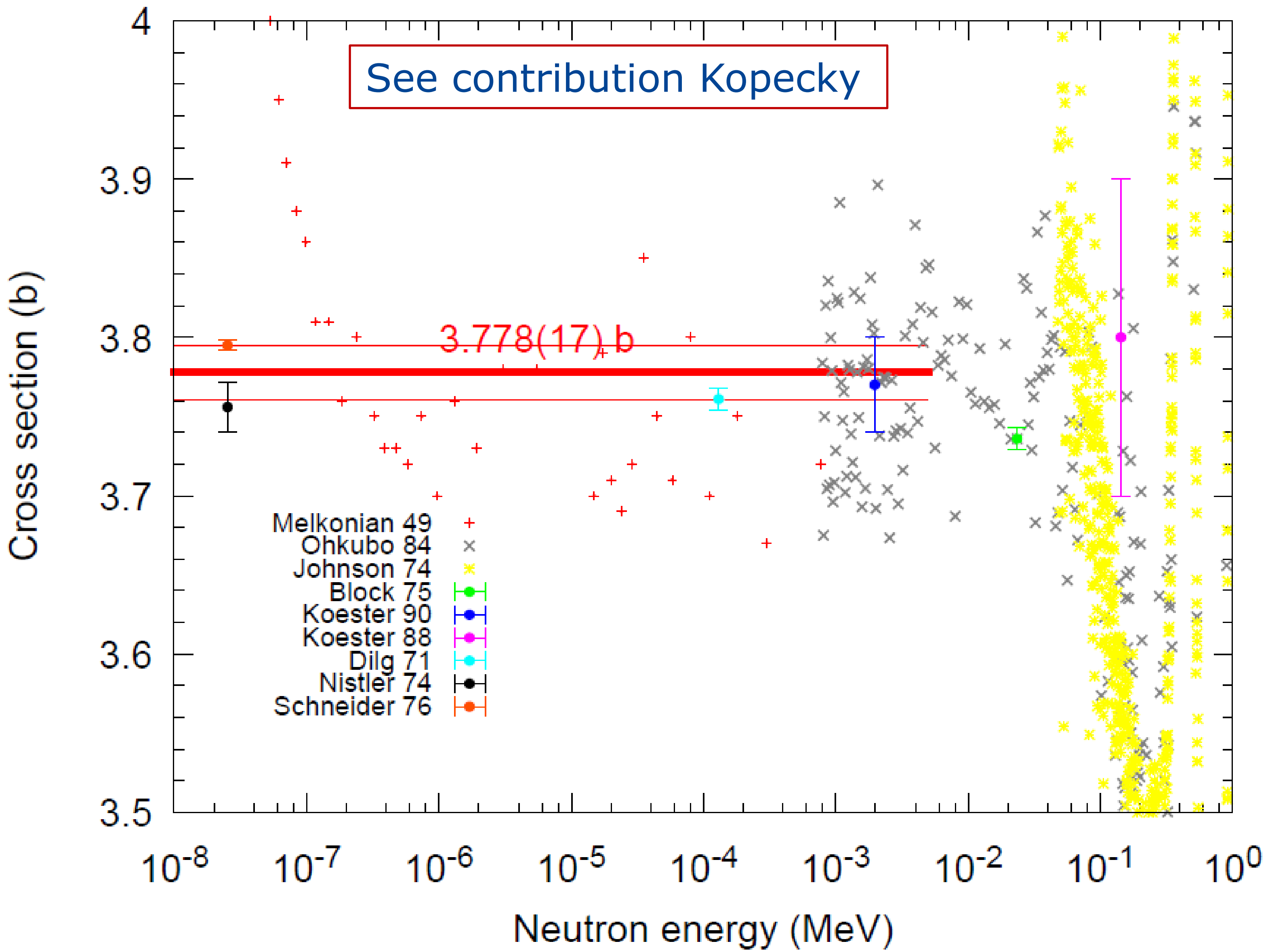
Selected Data Total

n+^{16}O



Selected Data Total

n+^{16}O

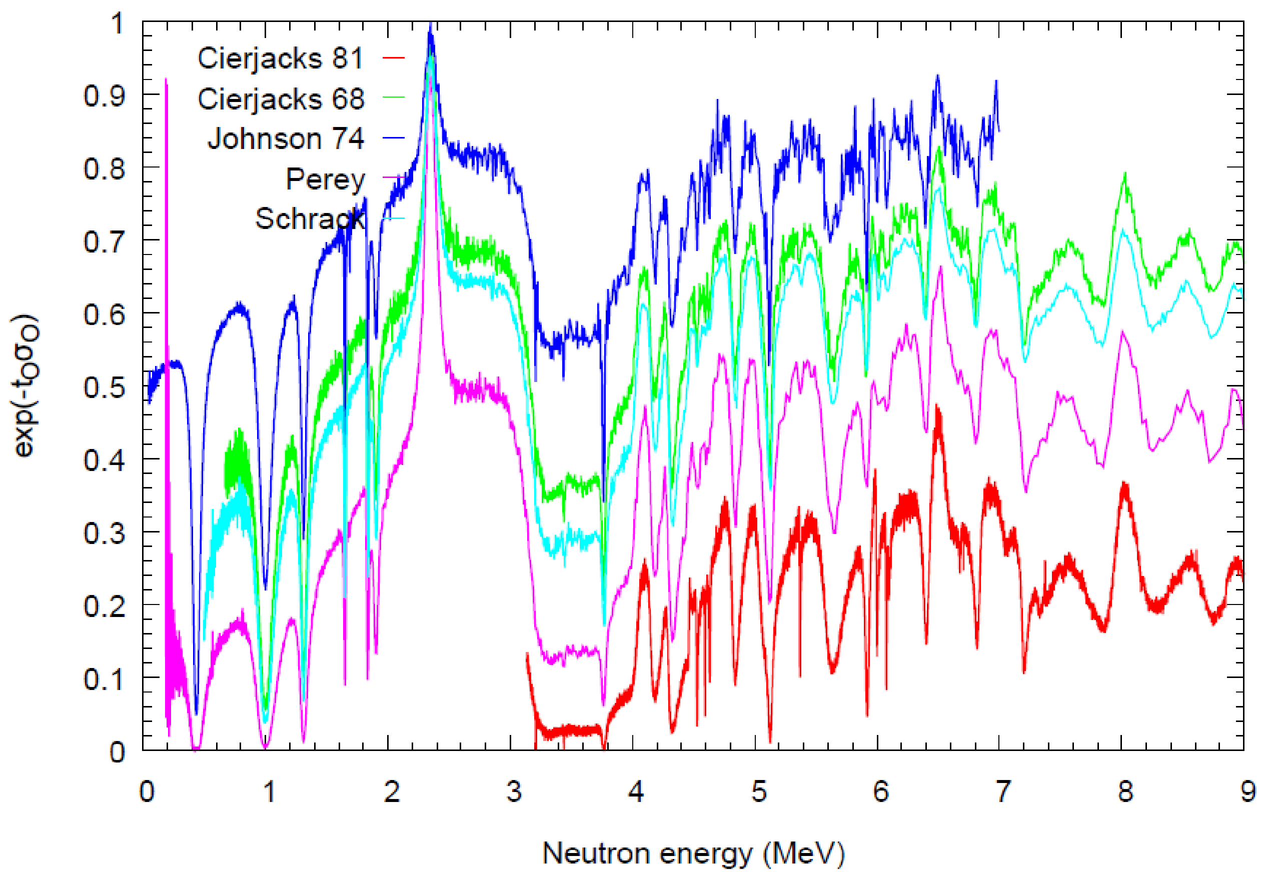


Conclusion $^{16}O(n,tot)$

1. Considerable number of good data sets above 100 keV

2. Accurate data available below 100 keV

3. One wide range transmission set from 25 meV – 200 keV is useful



4. Combination of thin and thick target data for best resonance parameters
5. Mind resolution effects before deducing $\Gamma\alpha$ from observed width and integral/height
6. Best to fit transmission data, with proper RF, sample thickness, but original data…
7. Good statistics, high resolution, thin and thick set for 0.1 – 20 MeV would be useful.

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Conclusion

^{16}O CIELO

Opportunity to make a clean start taking advantage of experience

Combine available data, expertise experiments, modeling, benchmarks

Establish

a) Target benchmarks sensitive to ^{16}O
b) Correlation other nuclides
c) Role of thermal scattering (LWR)

Agree on goals CIELO (Chadwick)

a) Best physics
b) Maintain performance benchmarks

Data to analyze

a) Total cross section (good shape, but room for improvement)
b) (n,a) confusing (expt/modeling)
c) a.d. (neutrons, alphas) spin assignments, impact transport
d) (n,g) so far ignored: take on