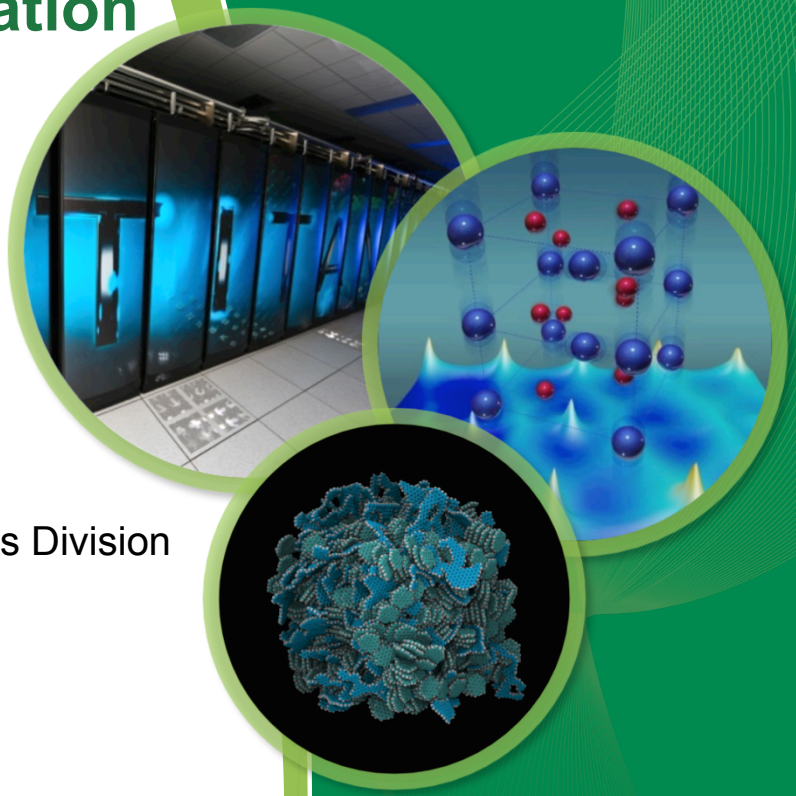
Reich-Moore R-matrix Parameters for n+^{16}O within CIELO Collaboration



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Outline

- Importance of n+^{16}O evaluation
- Status of n+^{16}O evaluation in ENDF/B-VII.1 library
- Evaluation procedure with the SAMMY code
  - Discussion on the boundary conditions
  - Treatment of the capture cross sections
- Experimental data overview
- Results and status on n+^{16}O evaluated cross sections
- Summary and conclusions
- Acknowledgments

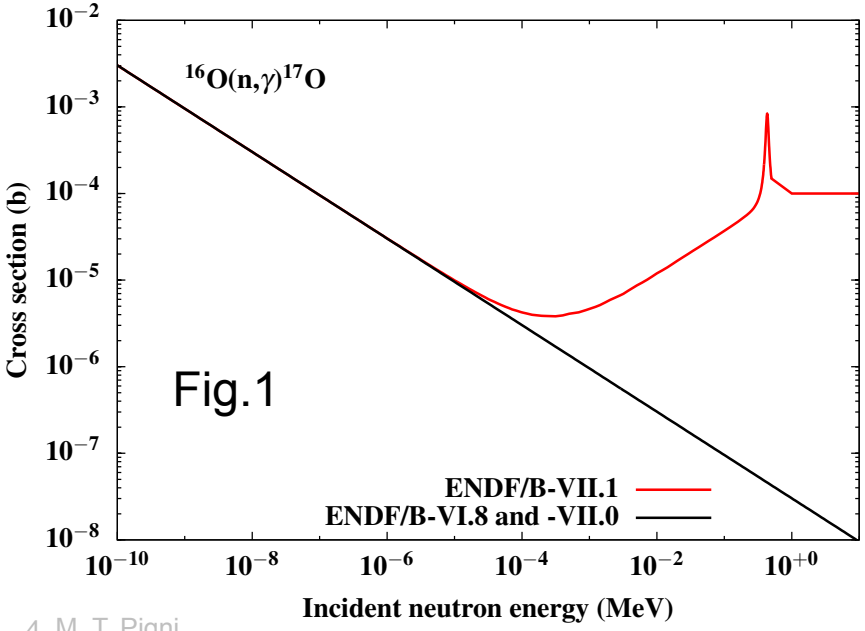
Motivation

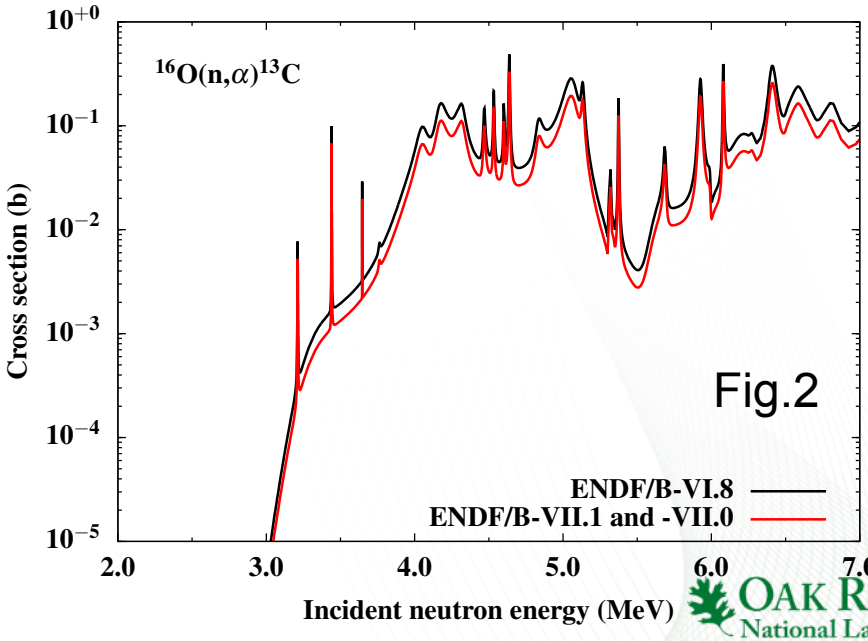
- Neutron scattering on oxygen is important in *criticality safety applications* where oxides are present in significant abundance
- Long standing issues in the evaluated cross sections deriving, e.g., from measured cross sections on $^{13}C(\alpha,n)^{16}O$
  - Discrepancies between Bair(1973) and Harissopulos(2005) data sets
  - This problem is recognized by the major nuclear data libraries and identified within the Collaborative International Evaluated Library Organization (CIELO) pilot project
- The aim of this work is to provide a set of resonance parameters able to describe $n+^{16}O$ cross sections within the recommendations of CIELO collaboration but, also, an alternative to the extant point-wise evaluation of oxygen in ENDF/B-VII.1 library

Status of ^{16}O Evaluation in ENDF/B-VII.1

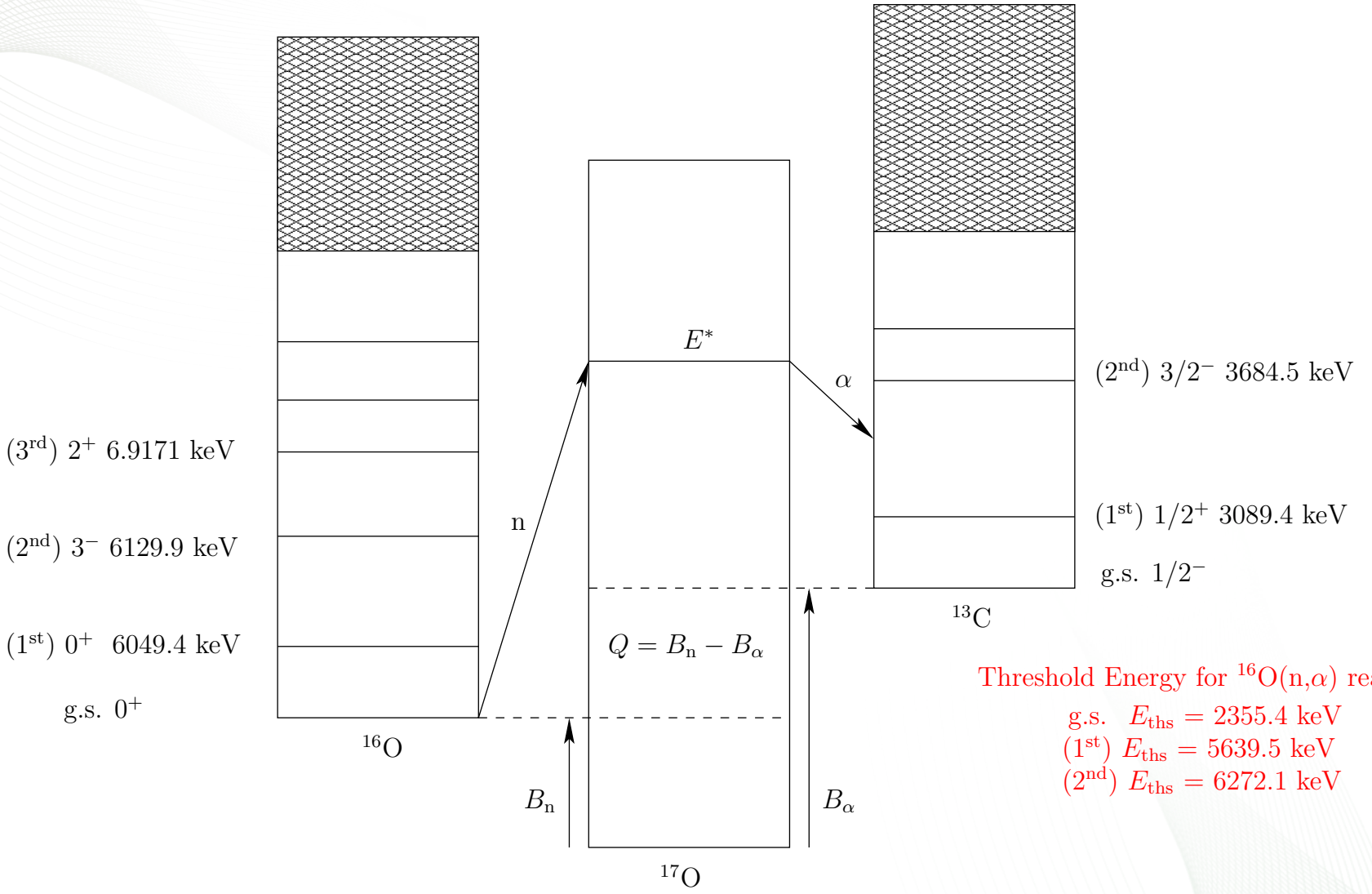
(in the resolved energy range up to about 7 MeV)

- The existing ENDF/B-VII.1 evaluation (2011) is expressed in terms of point-wise cross sections (at least since ENDF/B-VI.5 release)
  - As well as cross section covariance data
- In the resolved energy range ENDF/B-VII.1 and -VII.0 (2006) has no remarkable differences in the elastic and (n,α) cross sections. The capture cross sections were modified as shown in Fig.1
- From ENDF/B-VI.8 to –VII.0 and –VII.1 releases the (n,α) cross sections were normalized by more than -30% (Fig. 2)





Reaction Scheme of n+^{16}O Evaluation



Threshold Energy for ^{16}O(n,α) reactions

g.s. $E_{\rm ths}$ = 2355.4 keV
(1st) $E_{\rm ths}$ = 5639.5 keV
(2nd) $E_{\rm ths}$ = 6272.1 keV

Schematic of the ^{16}O(n,α)^{13}C nuclear reaction process

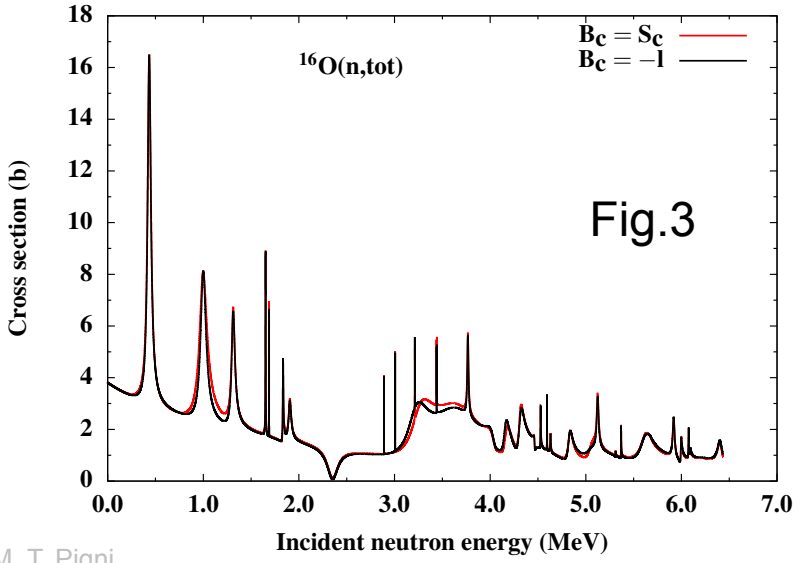
Evaluation Methodology

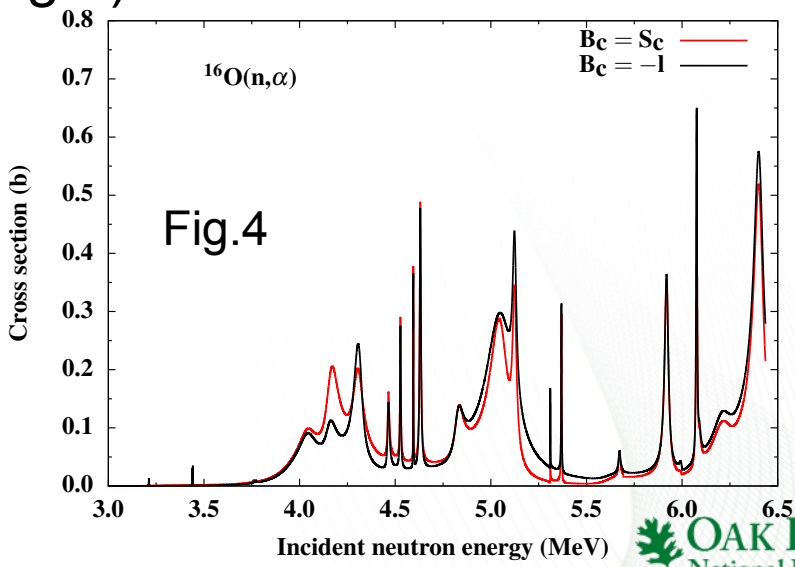
- The R-matrix SAMMY code was used to generate a set of resonance parameters for n+^{16}O reactions in the energy range of thermal up to E_{max}=6.43 MeV
  - E_{max} is the limit for which $^{13}C(\alpha_0,n_0)^{16}O$ (the target and residual nucleus are in the g.s.) : the $^{16}O(n,\alpha)$ cross sections are based on inverse kinematic of Bair's experimental data
- The evaluation work builds on a comprehensive resonance analysis performed by R.O. Sayer in 2000 (ORNL/TM-20000/212)
  - In Sayer's evaluation the Bair's (n,α) cross sections were normalized by -30%. In the present evaluation the normalization factor is -6%
- Two major features of the present evaluation
  - The first one is the use of the B_c=-l boundary condition commonly used in the formal R-matrix theory but never used in SAMMY evaluation work. Default option is the energy-dependent boundary condition B_c=S_c
  - The second one is the study of the capture channel treated as in the Reich Moore approximation or as particle channels whose penetrability factor are set to be unitary in SAMMY input file

Boundary Condition B_c=-l

(…starting from B_c=S_c boundary condition)

- **[First step]** Prior resonance parameters from Sayer's evaluation used in the Bayesian procedure to fit total cross sections, elastic angular distributions along with the newly normalized (n,α) cross sections
  - The Bayesian fitting procedure performed by using the default boundary condition in SAMMY, i.e., B_c=S_c
- **[Second step*]** Brune's transformation (Phys. Rev. C66 44611) was applied on the previous resonance parameters in order to obtain a set of resonance parameters satisfying the B_c=-l boundary condition (Fig.3 and Fig.4)



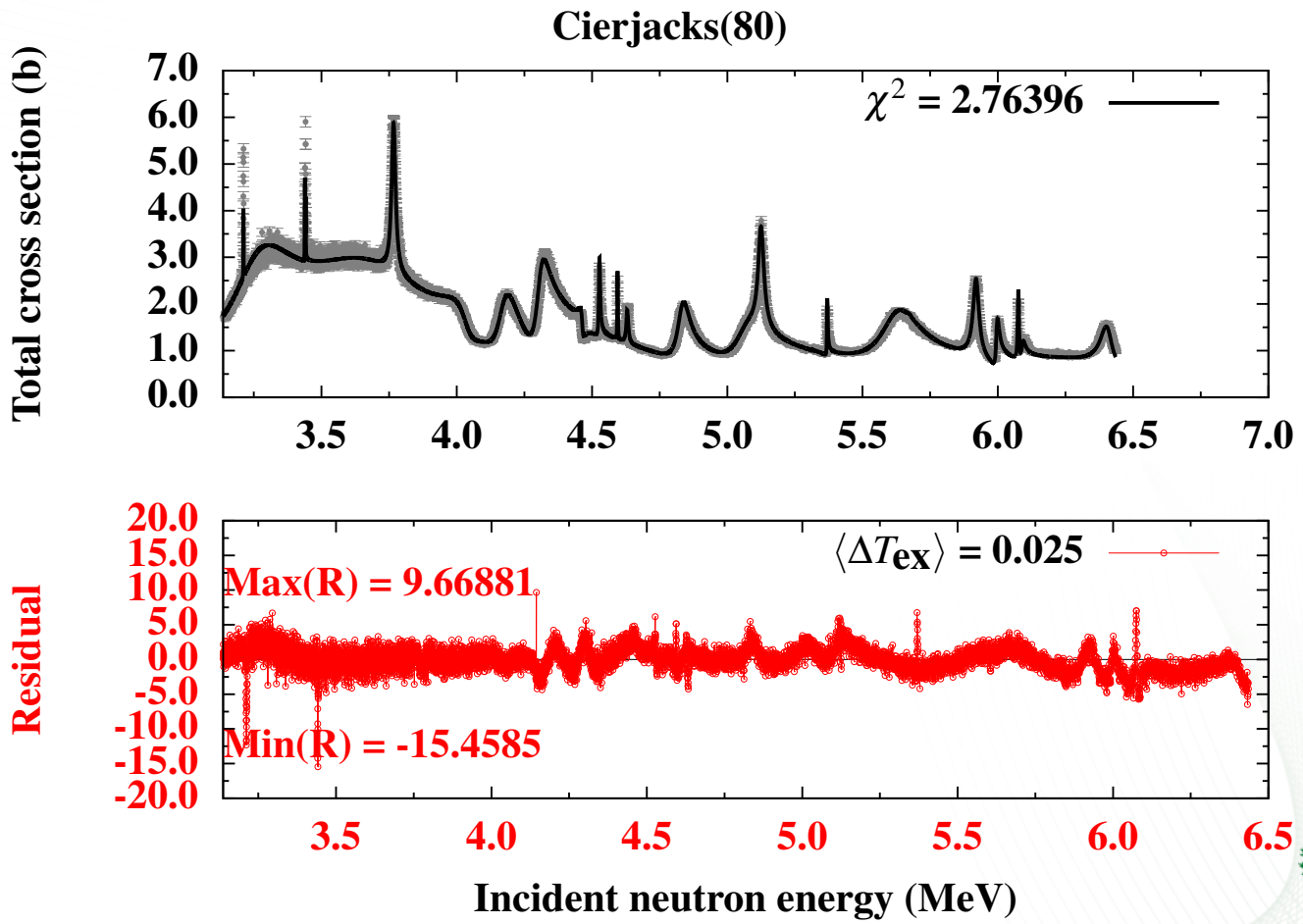


* A. Holcomb's code

Boundary Condition B_c=-l

(…starting from B_c=S_c boundary condition)

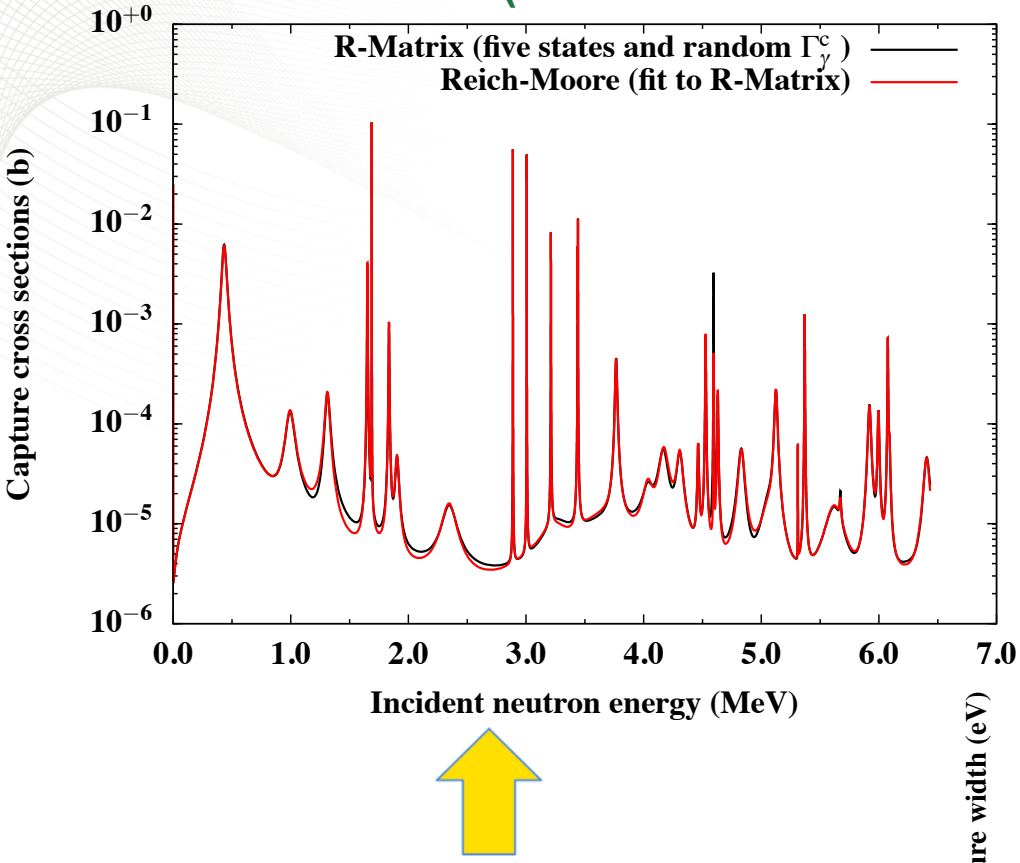
- **[Third step]** Converted resonance parameters from Brune's transformation used in the Bayesian procedure to fit experimental data
  - The Bayesian fitting procedure performed by using the boundary condition B_c=-l



Treatment of the Capture Channels

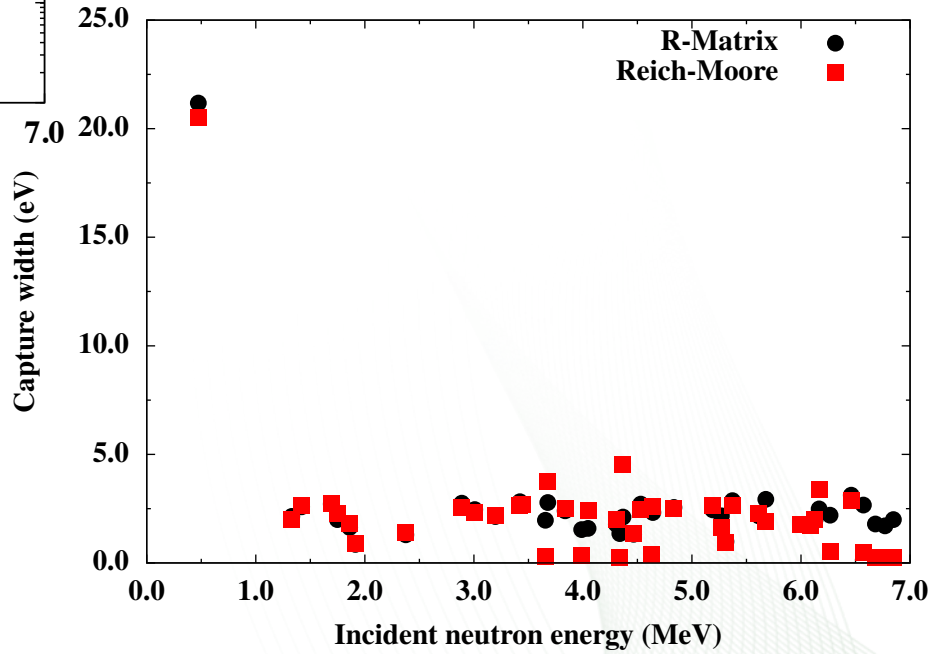
- The ^{16}O capture cross sections are small and a significant contribution is from the *direct* component
- The scarcity of experimental data makes it difficult to evaluate the resonant component of the capture cross sections
- Capture cross sections in the ENDF/B-VII.1 library need to be updated (Fig. 1)
- In view of this scenario SAMMY was used to study R-Matrix calculations without the Reich-Moore approximation by treating capture channels as particle channels whose penetrability factors were set to be unitary
  - The capture channels were defined on the basis of five states, i.e., $J^{\pi}=5/2^{+}$, $1/2^{+}$,$1/2^{-}$,$5/2^{-}$,$3/2^{-}$ (continuum) of the compound nucleus ^{17}O
  - For R-matrix calculations the capture widths (including sign +/-) were randomly sampled from a symmetric Porter-Thomas distribution
  - The aim is to study the accuracy of the Reich-Moore approximation compared to R-Matrix calculations specifically for n+^{16}O case

Treatment of the Capture Channels
(Reich-Moore vs R-Matrix calculations)



Good agreement between Reich-Moore and R-Matrix capture widths

$$\Gamma_{\mu\mu} = 2\sum_c \gamma_{\mu c}\gamma_{\mu c}$$



- R-matrix case (five states for ^{17}O) generated by randomly sampling capture widths (in black)
- The R-matrix capture cross sections were used to obtain capture widths in Reich-Moore approximation and related capture cross sections (in red)
- The fit of the capture cross sections did not impact other reaction channels

Summary and Conclusions

- We applied the R-matrix SAMMY method to determine a consistent set of neutron resonance parameters for ^{16}O including two major features
  - The use of boundary condition B_c=-l usually used in the formal R-matrix theory but never included in a formal evaluation work
  - Study on the accuracy of the Reich Moore approximation. Specifically for ^{16}O one can reasonably reproduce with Reich-Moore approximation the capture cross sections generated by R-Matrix calculations (5 states)
- In the analyzed energy range up to 6.4 MeV, this evaluation is intended to improve the current point-wise cross section evaluation in the US nuclear data library (ENDF/B-VII.1)
- 19 experimental data sets were used to ensure the calculated cross sections were in good agreement with multiple total, elastic angular distribution and also (n,α) data
  - Thermal capture cross sections based on Firestone et al. Phys. Rev. C93 44311 (2016)

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Thank you!