New perspectives in neutron reaction cross-section evaluation using consistent multichannel modeling methodology: Application to $^{17}O^*$

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Abstract. The traditional methodology of nuclear data evaluation is showing its limitations in reducing significantly the uncertainties in neutron cross sections below their current level. This suggests that a new approach should be considered. This work aims at establishing that a major qualitative improvement is possible by changing the reference framework historically used for evaluating nuclear model data. The central idea is to move from the restrictive framework of the incident neutron and target nucleus to the more general framework of the excited compound-system. Such a change, which implies the simultaneous modeling of all the reactions leading to the same compound-system, opens up the possibility of direct comparisons between nuclear model parameters, whether those are derived for reactor physics applications, astrophysics or basic nuclear spectroscopy studies. This would have the double advantage of bringing together evaluation activities performed separately, and of pooling experimental databases and basic theoretical nuclear parameter files. A consistent multichannel modeling methodology using the TORA module of the CONRAD code is demonstrated across the evaluation of differential and angle-integrated neutron cross sections of ^{16}O by fitting simultaneously incident-neutron direct kinematic reactions and incident-alpha inverse kinematic reactions without converting alpha data into the neutron laboratory system. The modeling is fulfilled within the Reich-Moore formalism and an unique set of fitted resonance parameters related to the $^{17}O^*$ compound-system.

1 Introduction

The ^{16}O isotope has been selected by the CIELO (*Collaborative International Evaluation Library Organisation*) project beside ^{235}U, ^{238}U, ^{239}Pu, ^{56}Fe and ^{1}H as having a significant impact on nuclear technology [1]. The main goal of the CIELO project was to solve discrepancies observed on one side between measurements and on the other side betwen evaluated data. Concerning the ^{17}O excited nucleus, both measured and evaluated data were discrepant of about 30 % according to the $^{16}O(n,\alpha)^{13}C$ cross section at the beginning of the project (2013) [2]. Discrepancies on the $^{16}O(n,n)$, $^{16}O(n,\gamma)$ thermal cross sections were also noticed. The $^{16}O(n,n)$ cross section impacts criticality calculations, especially for the D_2O-moderated reactors [3]. The $^{16}O(n,\alpha)^{13}C$ impacts criticality calculations in thermal and fast reactors, ^{4}He gaz production predictions in ractors [4, 5], and finally its inverse reaction is important for neutrons source calculations [4]. In the Resolved Resonance Region (RRR- the range of neutron kinetic energies between the neutron threshold S_n and S_n + 6 MeV), the status of the $^{16}O(n,\alpha)^{13}C$ evaluation that had arisen out of the CIELO project evolved towards two tendancies: the high and the low $^{16}O(n,\alpha)^{13}C$ cross section trend. The high $^{16}O(n,\alpha)^{13}C$ cross section was adopted for the ENDF/B-VIII.0 file release and the low $^{16}O(n,\alpha)^{13}C$ cross section was adopted for the JEFF-3.3 file distribution. Unbroadened values at thermal energy (E = 0.0253 eV) are as follows:

1. JEFF-3.3 recommendation
   - σ_{el} = 3.85181 b;
   - $\sigma_{\gamma} = 1.9 \times 10^{-4}$ b;
   - σ_{tot} = 3.852 b.
2. ENDF/B-VIII.0 recommendation
   - σ_{el} = 3.793904 b;
   - $\sigma_{\gamma} = 1.698355 \times 10^{-4}$ b;
   - σ_{tot} = 3.79407384 b.

Those two (n +^{16} O) files need definitive approval and the CIELO project has adviced further investigations to corroborate the choices made.

The work presented in this paper aims at proposing a new approach for the neutron cross section evaluation procedure using the multichannel unified framework. In the following sections, the physics features of a newly implemented module TORA (*Tool for Nuclear Reactions Analysis*) will be detailled. This tool has been designed with the objective of performing cross section evaluation using an unified technique relying on the center of mass of the compound-system framework, taking reference to the ground state energy of the excited compound-system. Present application is performed on the $^{17}O^*$ compound

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nucleus. TORA is an extra tool to the CONRAD (*COde for Nuclear Reaction Analysis and Data Assimilation*) code [6] developped in the Laboratory of Physics Studies at CEA-Cadarache.

2 The excited compound-system center of mass framework

Classical methods used in neutron cross section evaluation, in the field of reactors physics, are strongly attached to the laboratory system of the incident particle. Data from evaluations are historically constrained by neutron spectroscopy and evaluators usually rely on the method of the data inversion to treat reciprocal reactions. Even if a straight comparison of data [7] within the RRR validates the data inversion hypothesis, this method remains not recommended since it relies on the assumption of the formation of the same excited compound nucleus or accordingly, the total absence of the direct and semi-direct phenomena. The change of paradigm as proposed in this work, substitutes the laboratory system of the incident particle by a more unified one, the center of mass (CoM) of the excited compound-system. Within this new framework, the reference is not any more the separation energy of the projectile (or ejectile in the exit chanel) but the ground state energy of the excited compound-system. Thus, the energy of the resonance becomes the excitation energy of the corresponding excited compound-system state

$$\mathrm{E}_{\lambda}^{\mathrm{Lab}} \longrightarrow \mathrm{E}_{\mathrm{x},\lambda}^{\mathrm{CoM}} \tag{1}$$

Another concern is related to the adjusted resonance width. This common parameter is attached to the framework through its energy dependence carried by the penetration factor $\mathrm{P}(\mathrm{E}_{\lambda}^{\mathrm{Lab}})$ as follows

$$\Gamma(\mathrm{E}_{\lambda}^{\mathrm{Lab}}) = 2\mathrm{P}(\mathrm{E}_{\lambda}^{\mathrm{Lab}})\gamma^2 \tag{2}$$

The parameter γ is the reduced width decay amplitude, a nuclear structure energy-independent parameter. Given that the R-matrix formalism [8], a powerful theory applied to compute cross sections in the RRR, deals directly with γ, supplying the observed resonance width $\Gamma(\mathrm{E}_{\lambda}^{\mathrm{Lab}})$ is no longer needed. In this new framework, the reduced width amplitude γ is processed directly when computing R-matrix elements instead of recovering it from the resonance width $\Gamma(\mathrm{E}_{\lambda}^{\mathrm{Lab}})$ using the relation (2), as conventionally.

The benefit of redesigning cross sections evaluation in the framework of the center of mass system of the excited compound-system is that all the open reactions are observed and fitted simultanously. The consequence is that, these reactions are treated using an unique set of compound-system nuclear structure parameters.

3 Compound system CoM framework physics capabilities of the TORA module

The TORA module is designed to perform cross sections computation under R-Matrix theory in the RRR. The Reich-Moore [9] approximated R-matrix element from a channel c to another channel c′ is obtained as follows for a given J^{π} excited state

$$\mathrm{R}_{\mathrm{cc}'} = \sum_{\lambda} \frac{\gamma_{\mathrm{c},\lambda}^{\mathrm{CoM}} \gamma_{\mathrm{c}',\lambda}^{\mathrm{CoM}}}{\mathrm{E}_{\mathrm{x},\lambda}^{\mathrm{CoM}} - \mathrm{E}_{\mathrm{x}}^{\mathrm{CoM}} - \mathrm{i}\left(\gamma_{\gamma,\lambda}^{\mathrm{CoM}}\right)^2} \tag{3}$$

$\mathrm{E}_{\mathrm{x},\lambda}^{\mathrm{CoM}}$ and $\mathrm{E}_{\mathrm{x}}^{\mathrm{CoM}}$ are respectively the energy of the λ^{th} compound-system excited state belonging to the family of resonances that contribute to a same J^{π} (J and π describing respectively the total spin and parity) and the energy of the projectile (respectively ejectile) scaled with respect to the ground state energy of the excited compound-system and converted in the CoM system. The parameters $\gamma_{\mathrm{c},\lambda}^{\mathrm{CoM}}$, $\gamma_{\mathrm{c}',\lambda}^{\mathrm{CoM}}$ and $\gamma_{\gamma,\lambda}^{\mathrm{CoM}}$ are reduced width amplitudes attached to the λ^{th} compound-system excited state that belongs to the J^{π} family of resonances. They are converted in the CoM system as well. The subscripts c, c′ and γ appoint respectively the incident channel, the outgoing channel and the radiative gamma channel.

The wave number required to compute penetration factors, shift factors and hard sphere phase shifts, is calculated by rescaling the CoM projectile (resp. ejectile) energy with respect to the separation energy of the involved particle in order to treat correctly the opened and closed channels.

$$\mathrm{k}\left(\mathrm{E}_{\mathrm{x}}^{\mathrm{CoM}}\right) = \frac{1}{\hbar}\sqrt{\frac{2mM}{m+M}\left[E_{\mathrm{x}}^{CoM} - S_{\,part}\right]} \tag{4}$$

Where $\hbar$ is the reduced Planck constant, m the projectile (resp. ejectile) mass and M the target (resp. the residual) mass. $\mathrm{E}_{\mathrm{x}}^{\mathrm{CoM}}$ and $\mathrm{S}_{\mathrm{part}}$ are respectively the projectile (resp. ejectile) kinetic and separation energies scaled with respect to the the ground state energy of the excited compound-system. The subscript "part" appoints the particle which can be either projectile or ejectile.

The partial cross section of given reaction occuring through the formation of a compound-system from channels c obtained by a combination of a couple α (representing the target and the projectile) of particles with decay in a couple α' (representing the residual nucleus and the ejectile) of particles whose combination gives channels c′, is obtained as follows for a given J^{π}

$$\sigma_{\alpha\alpha'}^{\mathrm{J}^{\pi}}(\mathrm{E}_{\mathrm{x}}^{\mathrm{CoM}}) = \frac{\pi}{\mathrm{k}_{\alpha}^2\left(\mathrm{E}_{\mathrm{x}}^{\mathrm{CoM}}\right)} \mathrm{g}_{\alpha}^{\mathrm{J}} \sum_{\mathrm{c}} \sum_{\mathrm{c}'} |\delta_{\mathrm{cc}'} - \mathrm{U}_{\mathrm{cc}'}^{\mathrm{J}^{\pi}}|^2 \tag{5}$$

The factor $\mathrm{g}_{\alpha}^{\mathrm{J}}$ is the statistical spin factor related to the couple α (projectile and target) of particles interacting in the channels c. It is given by

$$\mathrm{g}_{\alpha}^{\mathrm{J}} = \frac{2\mathrm{J}+1}{(2\mathrm{i}+1)(2\mathrm{I}+1)} \tag{6}$$

I and i are respectively, the target and the projectile intrinsic spins. The two last components of the Eq. (5) are the kronecker symbol $\delta_{\mathrm{cc}'}$ (taking 1 if c = c′ and 0 otherwise) and the collision matrix element $\mathrm{U}_{\mathrm{cc}'}$.

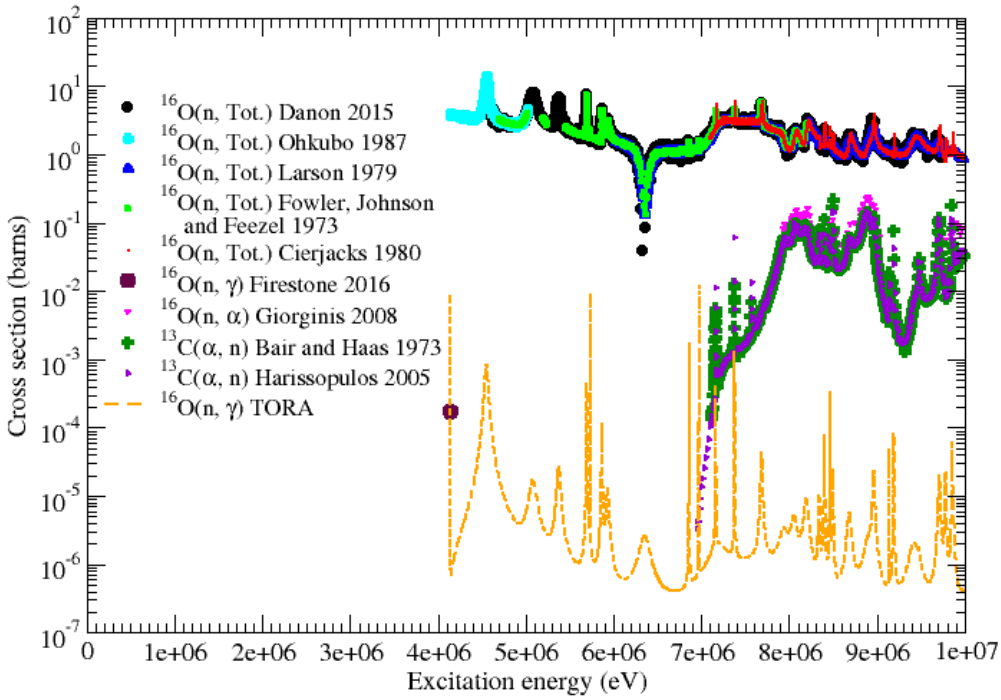

Figure 1. Partial and total cross sections of the $^{17}O^{*}$ system reconstructed within the unified framework from the JEFF33.T3 file parameters. The TORA results are compared to the experimental data presented in the references [16–24] . For better display, only the (n, γ) calculation by TORA is drawn on this picture.

Table 1. Comparison between bound states parameters from the Astrophysics and the reactors physics databases as extracted from the unified framework.

		Astrophysics database [13]		Reactors physics database [15]	
E_x(eV)	J^π	$\tau_{1/2}$	$\gamma_{\gamma,tot}\left(\sqrt{eV}\right)$	$\gamma_{\gamma,tot}\left(\sqrt{eV}\right)$	$\gamma_n\left(\sqrt{eV}\right)$
0.87e+06	1/2+	258.6 psec	7.97e-04	2.90e-01	1070.67
3.05e+06	1/2-	120 fsec	3.70e-02	3.65e-01	177.55
3.84e+06	5/2-	$\leqslant$ 25 fsec	$\geqslant$8.11e-02	3.97e-01	885.14

The total partial cross section of a reaction from α to α' is obtained by summing over all total spins and parities as follows

$$\sigma_{\alpha\alpha'}(E_x^{CoM}) = \sum_{J^\pi} \sigma^{J^\pi}_{\alpha\alpha'}(E_x^{CoM}) \quad (7)$$

Taking advantage of the unitary property of the collision matrix, the total cross section that includes all decaying possibilities is

$$\sigma_{tot}\left(E_x^{CoM}\right) = 2\frac{\pi}{k_\alpha^2\left(E_x^{CoM}\right)} \sum_{J^\pi} g^J_\alpha \sum_c \left[1 - Re\left(U_{cc}\right)\right] \quad (8)$$

The radiative channels being beforehand eliminated in the Reich-Moore approximation, the capture cross section must be computed from the total cross section by subtraction of the other partial cross sections as

$$\sigma^{J^\pi}_{c,\gamma} = \sigma^{J^\pi}_{c,tot} - \sum_{c'\neq\gamma} \sigma^{J^\pi}_{cc'} \quad (9)$$

The total capture cross section is obtained by summing over all total spins, parities and entrance channels

$$\sigma_{\gamma,tot} = \sum_{J^\pi,c} \sigma^{J^\pi}_{c,\gamma} \quad (10)$$

The TORA module is also able to generate angle differential cross sections of either charged or not charged particle channels, using Blatt and Biedenharn formalism [10].

4 Application to the compound-system: $^{17}O^{*}$

The application is made on the $^{17}O^{*}$ system from the (n +^{16} O) evaluated parameters of the JEFF33.T3 file [11]

that was released by L. C. Leal using R-Matrix Limited (RML) format (see ENDF manual [12]). This file contains both neutron and α channel parameters in addition to total gamma widths, making possible the testing of a simultaneous computation of the $^{16}O(n,\alpha)^{13}C$ reaction and its reciprocal $^{13}C(\alpha,n)^{16}O$ reaction under Reich-Moore hypothesis. For practical application, resonance widths tabulated in the file are first converted in their corresponding reduced width amplitudes using Eq. 2. Total gamma widths are processed by setting the penetration factor of Eq. 2 to unity. The JEFF33.T3 parameters being evaluated and tabulated within neutron laboratory framework, reduced width amplitudes and resonances energies supplied are converted and rescaled in the CoM. The conversion of the parameters is carried out as follows

$$E_{x,\lambda}^{CoM} = E_{\lambda}^{Lab}\frac{M_{^{16}O}}{M_n + M_{^{16}O}} + S_n\left(^{17}O^*\right) \tag{11}$$

$$\gamma_{c,\lambda}^{CoM} = \gamma_{c,\lambda}^{Lab}\sqrt{\frac{M_{^{16}O}}{M_n + M_{^{16}O}}} \tag{12}$$

The intermediate file generated is restrained to the parameters redesigned in the CoM system of the excited compound-system. That defines the backbone of the TORA module. Figure 1 shows the experimental data associated to $^{17}O^*$ and merged in the unique framework.

5 A challenge under investigation by means of the unified approach

The comparison of the Astrophysics (eg.[13, 14]) and Reactors Physics databases (eg.[15]) within the excited compound-system CoM framework reveals conceptual differencies for the three known bound states (see Table 1). On one hand, the neutron channel width does not show up in the Astrophysics database resulting logically in a total width assigned to the total gamma width (proportional to the half-life of the excited state). On the other hand, the Reactors Physics database is supplemented with a neutron width (of quite large magnitude) for reproducing correctly the thermal neutron energy partial cross sections. Indeed, the tail of bound states is observed at thermal energies, suggesting the assignment of neutron channel widths for bound states. Since the neutron penetration factor vanishes under S_n in the laboratory framework, the storage of reduced width amplitudes as suggested in the work by F. Fröhner and O. Bouland [25] is definitively more meaningful, and that especially for bound states.

6 Conclusion

A new approach for the evaluation of neutron cross sections using an unified consistent multichannel framework has been presented. This approach carries the advantage of using energy independent parameters, suppressing thus any inconsistency related to the choice of the working system. This enables simultaneous analyses of experimental data from reactions sharing the same excited compound-system. The use of a same set of parameters for all reactions, regardless the interacting couple of particles from the incident channel, ensures the consistency between all opened channels. This approach is as identical in its treatment of bound states as for unbound states.

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