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Testing Compound Nucleus Hypothesis Across the ^{17}O Nucleus Excitation

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Abstract. The excited compound nucleus ^{17}O* has been studied over (n,α) and (α,n) cross sections modelling, respectively for ^{16}O and ^{13}C targets in their ground states. The modelling is fulfilled within the Reich-Moore formalism. We were able to calculate the (α,n) cross section by two separate ways: the direct kinematic standard route and by inversion of the (n,α) cross section using the compound nucleus hypothesis. Resonance parameters of the resolved resonance range (0 to 6 MeV) were borrowed from the CIELO project. In a first stage, the modelling is carried out in the referential of the incident particle (either way neutron or α) requesting conversion of the CIELO neutron-type resonance parameters to the α-type. In a second stage, the implementation is uniquely designed in the center of mass system of the excited compound nucleus. The resonance parameters are thus converted in that unique reference framework. The present investigation shows the consistency of the kinetic transformation that relies on the compound nucleus hypothesis.

1 Introduction

The study of reactions that refer to the excited compound nucleus ^{17}O* is of strong concern for reactors physics nuclear data evaluators. ^{16}O is the most predominant isotope of oxygen in nature and contributes to ^{4}He gaz production observed in reactor through ^{16}O(n,α)^{13}C conversion. On this point of view, the ^{16}O constitutes an important safety issue in the operation of reactors. Furthermore, the oxygen is overriding in the oxide fuels and plays a role in neutron thermalization in water. One can also emphasize the interest of ^{17}O* excited compound nucleus as neutron source, especially meaningful in the *s*-process (astrophysics area), through the ^{13}C(α,n)^{16}O reaction. Taking into account nuclear structure aspect, the ^{17}O* compound nucleus is characterized by weak level density and subsequent wide resolved resonance range (RRR) that goes from 0 to 6 MeV. Two reaction types are fully open for this region: the neutron and α reactions. Due to its light nucleus structure feature, the ^{17}O* compound nucleus makes it a nice candidate for models testing in the RRR.

Existing nuclear data discrepancies between measured and evaluated data according to the ^{16}O(n,α)^{13}C and reciprocal ^{13}C(α,n)^{16}O reactions, have been the subject of strong

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discussions within CIELO [1, 2] project. In 2014, the CIELO team summarized the situation [1] pointing out 30% of discrepancies between lower (IRMM 2008 [3], Harrisopulos 2005 [4]) and higher (original Bair and Haas [5]) cross section trends. These discrepancies were also recorded between major evaluated data libraries. The old ENDF/B-VI evaluation was scaled on the higher cross section magnitude while the lower trend was adopted in the ENDF/VII.0 (unchanged in ENDF/B-VII.1) and JEFF-3.1 according the energy range below 6 MeV. Thereafter, that choice was completely re-examined in the last ENDF/B library. The CIELO team reported in 2018 [2] a raise up of about 40% to be applied to the ENDF/B-VII.1 (n,α) cross section. The modifications were included in the ENDF/B-VIII.0 file. However, the CIELO project recommended new experiments to corroborate these new changes.

Present work takes place in larger demarche that includes redesign of the technique of cross section evaluation meaning the determination of nuclear parameters using a unified framework approach. This paper presents the work on progress using a newly implemented computer branch [TOol for Reactions Analysis (TORA)] of the CONRAD code [6] whose purpose is to reach the above-cited objective. The TORA module has capability of achieving cross sections calculations not only in the laboratory framework attached to the incident particle (either charged or not) but also within the excited compound nucleus center of mass framework taking reference to the fermi energy of the latter. Based on this aspect, the TORA module acts as a complementary tool to the CONRAD code when analyzing data within the center of mass of the excited compound nucleus framework. The tool is tested across dedicated modelling of the $^{16}O(n,\alpha)^{13}C$ and $^{13}C(\alpha,n)^{16}O$ cross sections in both projectile laboratory respective frameworks and center of mass of the excited compound nucleus (defining the unified approach).

2 Theoretical background

This work is fulfilled in the Reich-Moore formalism [7]. The R matrix, in which the gamma channels are beforehand eliminated, is given by:

$$R_{cc'}^{J\pi} = \sum_{\lambda} \frac{\gamma_{\lambda c}^{J\pi}\gamma_{\lambda c'}^{J\pi}}{E_{\lambda}^{J\pi} - E - i\left(\gamma_{\lambda\gamma tot}^{J\pi}\right)^{2}} \tag{1}$$

The quantities $\gamma_{\lambda c}^{J\pi}$ and $\gamma_{\lambda c'}^{J\pi}$ are the reduced width amplitudes, $E_{\lambda}^{J\pi}$ is the resonance energy and the parameter $\gamma_{\lambda\gamma tot}^{J\pi}$ is the total gamma channel reduced width amplitude of the λth state in a group of states contributing to the same total spin J and parity π of the compound nucleus. E is the energy of the incident particle. Since these resonance parameters are expressed in the neutron laboratory system according to the ENDF format of the evaluated data libraries, a reference framework transformation is usually needed to calculate reciprocal cross sections (exchanging projectile-ejectile pair roles).

3 Direct kinematics calculations according to the $^{16}O(n,\alpha)^{13}C$ and $^{13}C(\alpha,n)^{16}O$ cross sections

The $^{16}O(n,\alpha)^{13}C$ and $^{13}C(\alpha,n)^{16}O$ cross sections calculations are fulfilled respectively in the neutron- and alpha-incident particle laboratory systems using TORA and validated by comparison to the calculations performed using SAMMY [8] and CONRAD [6] codes. The appropriate expressions are used to calculate neutrons and charged particles penetration

factors, shift factors and hard-sphere scattering phase shifts. The first step lies in the neutron to alpha laboratory system transformation of the CIELO resonance parameters to reconstruct the direct kinematics $^{13}C(\alpha,n)^{16}O$ cross section. The neutron laboratory frame is by definition scaled on the neutron separation energy (S_n= 4143890 eV) to be juxtaposed to corresponding alpha separation energy (S_α = 6359067 eV). The reaction Q-value is deduced accordingly. To achieve the framework transformation, formulas used are in the spirit of the SAMMY code [8] and have been implemented in the TORA module. The resonance energy $E_\lambda^{J\pi}$ and the reduced width amplitude $\gamma_\lambda^{J\pi}$ are transformed from the neutron laboratory framework to the alpha laboratory framework as below:

$$E_{\lambda(\alpha lab)}^{J\pi} = E_{\lambda(nlab)}^{J\pi} \frac{M_{16_O}}{M_{16_O}+M_n} \frac{M_{13_C}+M_\alpha}{M_{13_C}} - (S_\alpha - S_n) \frac{M_{13_C}+M_\alpha}{M_{13_C}} \tag{2}$$

$$\gamma_{\lambda(\alpha lab)}^{J\pi} = \gamma_{\lambda(nlab)}^{J\pi} \sqrt{\frac{M_{16_O}}{M_{16_O}+M_n}} \sqrt{\frac{M_{13_C}+M_\alpha}{M_{13_C}}} \tag{3}$$

$E_{\lambda(\alpha lab)}^{J\pi}$, $E_{\lambda(nlab)}^{J\pi}$, $\gamma_{\lambda(\alpha lab)}^{J\pi}$, $\gamma_{\lambda n}^{J\pi}$, M_{16_O}, M_{13_C}, M_n and M_{13_C} being respectively the resonance energy in the alpha laboratory framework, the resonance energy in the neutron laboratory framework, the reduced width amplitude in the alpha laboratory framework, the reduced width amplitude in the neutron laboratory framework, the mass of ^{16}O, the mass of ^{13}C, the neutron mass and the alpha particle mass. The subscripts αlab and $nlab$ indicate respectively for alpha laboratory framework and neutron laboratory framework.
The boundary limit (B) is assigned to the shift factor value (S) and channel radii are respectively chosen to a_c= 4.15 fm for the neutron channel and a_c = 6.68 fm for the alpha channel. Figure 1 shows corresponding simulations. The TORA calculations are compared to those fulfilled using the SAMMY code and to the experimental measurements. The (α,n) experimental cross section data are Bair and Haas 1973 [5] data and the forward (n,α) experimental data are Giorginis (IRMM 2008 [3]) data with their fixed EXFOR normalizations. The pseudo (n,α) Bair and Haas 1973 data are obtained by inversion of the forward (α,n) Bair and Haas 1973 data. The data inversion is based on the compound nucleus hypothesis presented in the subsection 4.2. The cross section of the reciprocal reaction is obtained as follow [9]:

$$\sigma_{(n,\alpha)}(E_n)\lambda\!\!\!^{-2}_\alpha = \sigma_{(\alpha,n)}(E_\alpha) \frac{(2i_\alpha+1)\left(2I_{13_C}+1\right)}{(2i_n+1)\left(2I_{16_O}+1\right)} \lambda\!\!\!^{-2}_n \tag{4}$$

E_α, i_α, I_{13_C} and $\lambda\!\!\!^{-}_\alpha$ are respectively the energy of the alpha projectile in the alpha laboratory framework, the spin of the projectile, the spin of the target and the reduced wavelength of the alpha projectile. E_n, i_n, I_{16_O} and $\lambda\!\!\!^{-}_n$ are reciprocal quantities in neutron laboratory framework. E_n is obtained by a transformation of E_α from the alpha laboratory framework to the neutron laboratory framework using equation (2).

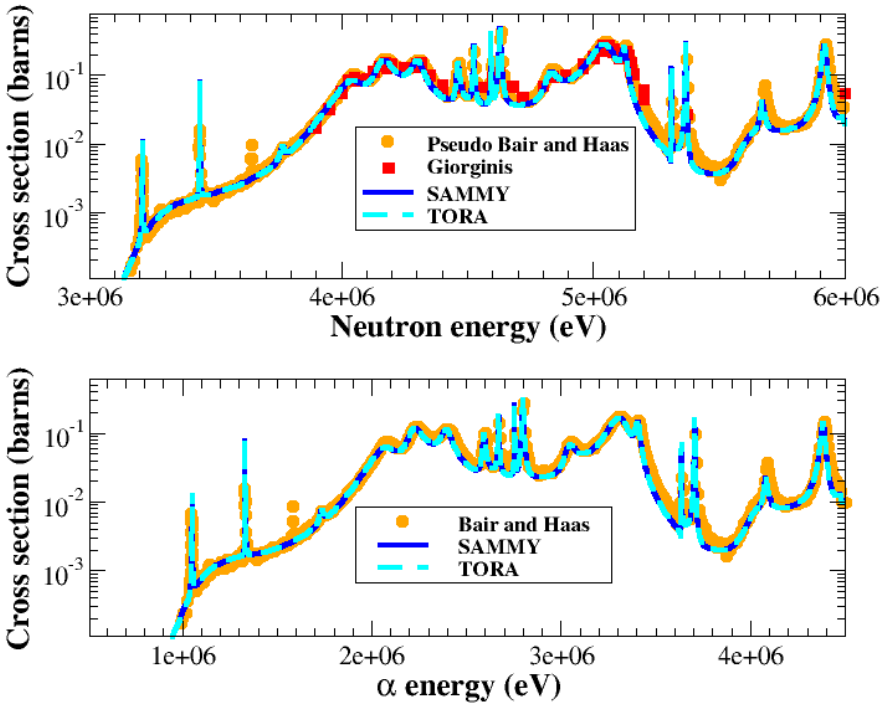

Fig.1. $^{16}O(n,\alpha)^{13}C$ (the top subfigure) and $^{13}C(\alpha,n)^{16}O$ (the bottom subfigure) unbroadened cross sections versus projectile energy. The long dash curves address the results from TORA. They are compared to reference calculations obtained using the SAMMY-8 (solid curve). On the top sub figure, the pseudo-experimental data are obtained by the inversion of the Bair and Haas 1973 (α,n) cross section which are plotted on the bottom subfigure (circular symbols). The forward (n,α) experimental data (square symbols) are Giorginis (IRMM 2008 [3]) data. The modeling is fulfilled using the Reich-Moore parameters kindly released by L.C. Leal [10].

4 Nuclear data computation involving compound nucleus CoM frame

4.1 Various calculated data for $^{17}O^*$ compound nucleus

Modelling of various neutron and α cross sections of reactions related to the $^{17}O^*$ compound nucleus has been fulfilled in the center of mass (CoM) system taking reference to the ground state energy of the $^{17}O^*$ nucleus. The main goal of this approach is to reduce the inconsistencies between data due to the frame reference dependence. All the parameters occurring in the equation (1) are now established in the CoM system. The reduced amplitudes being energy independent physical parameters (see equation 5 below taken from [11]), they become suitable for the purpose of present work suggesting to replace the total gamma width usually occurring in the denominator of the Reich-Moore R-Matrix formulation by its corresponding amplitude as shown in the equation (1).

$$\gamma_{\lambda c} = \left(\frac{\hbar}{2M_c a_c}\right)^{\frac{1}{2}} \int \varphi_c^* X_{JM}^{\lambda} dS \tag{5}$$

φ_c^* is the surface wave function for the channel c and X_{JM}^{λ} is the internal eigenfunction related to the energy E_{JM}^{λ}. The constants a_c and M_c are respectively the channel radius and the reduced mass. The integration is made over the totality of channel surfaces. The modelling of nuclear reactions in the CoM frame of the compound nucleus enables a consistent and simultaneous production of data for nuclear reactions involving the same compound nucleus. Figure 2 shows the results of a simulation of the four reactions: $^{16}O(n,n)^{16}O$, $^{16}O(n,\alpha)^{13}C$, $^{13}C(\alpha,n)^{16}O$ and $^{13}C(\alpha,\alpha)^{13}C$ in the same frame.

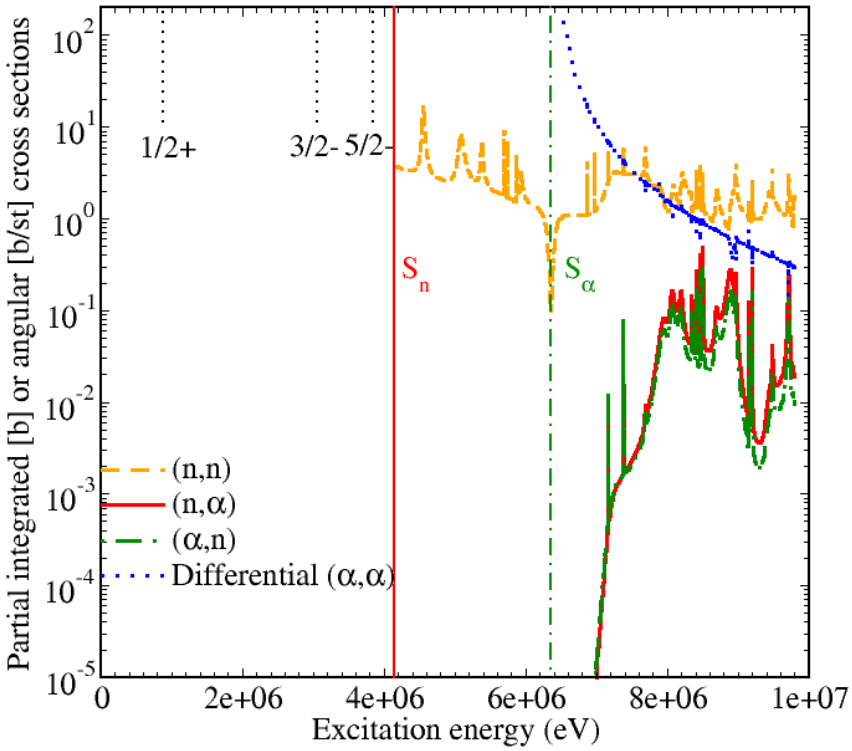

Fig.2. The $^{16}O(n,n)^{16}O$ (long dash curve), $^{16}O(n,\alpha)^{13}C$ (solid curve) ,$^{13}C(\alpha,n)^{16}O$ (long-short dash curve) and $^{13}C(\alpha,\alpha)^{13}C$ (dotted curve) cross sections. The targets are respectively ^{16}O and ^{13}C in their ground states. Vertical solid and dash lines indicate respectively the position of the separation energies of the neutron and α particle on the energy scale. The dotted vertical lines indicate the position of the three bound states of the $^{17}O^*$ nucleus below the separation energy of the neutron. Present differential cross section (α,α) is computed according Blatt and Biedenharn formalism [12] at the CoM angle of 54 degrees (the CoM angle of 54 degrees was chosen in concern of reproducing existing observable based on existing experimental data of Barnes [13] at 54.7 degrees).

In the CoM reference of $^{17}O^*$, the excited states must appear at the same excitation energy for all the simulated reactions since a unique energy scale is used. Furthermore, bound states energies are no longer expressed as a negative value of energy.

The use of the CoM frame gives also the tools to raise inconsistencies in the parameter files that support different energy scales. In the table 1 below, a straightforward comparison between resonance parameters from two separate databases (astrophysics [14] and reactors physics from CIELO project [10]) is done. Inconsistencies are highlighted. The three first total width values in the CIELO base are very large compared to those reported in the astrophysical base, suggesting very low life time assigned to these three levels. One unexpected J^{π} assignment (the second level in the Table 1) can also be noticed. On the

contrary, the level energies are in good agreement in spite of the highest level on which the energy is slight lower in the CIELO base.

Table 1. The comparison between resonances parameters for ten major levels from the Astrophysics and the CIELO project database using the unified framework. The bold numbers highlight most important differences between the two databases.

Astrophysics database (reference [14])			**CIELO Reich-Moore parameters (reference [10])**		
J^{π}	E_{λ} (eV)	Γ (meV)	J^{π}	E_{λ} (eV)	Γ (meV)
1/2+	8.70e+05	**1.27e-03**	1/2+	8.7267e+05	**3.6665e+09**
1/2-	3.05e+06	**2.74**	**3/2-**	3.0552e+06	**2.6721e+07**
5/2-	3.84e+06	**≤ 1.3e+01**	5/2-	3.8434e+06	**4.2045e+04**
3/2-	4.55e+06	4.0e+07	3/2-	4.5522e+06	4.1595e+07
7/2-	6.97e+06	< 1.0e+06	7/2-	6.9726e+06	7.9008e+04
5/2-	7.16e+06	1.38e+06	5/2-	7.1650e+06	1.6502e+06
3/2+	7.202e+06	2.80e+08	3/2+	7.2355e+06	3.0265e+08
5/2+	7.3792e+06	6.4e+05	5/2+	7.3784e+06	4.6646e+05
5/2-	7.3822e+06	9.6e+05	5/2-	7.3812e+06	1.4434e+06
3/2-	**7.559e+06**	5.00e+08	3/2-	**7.4224e+06**	6.7180e+08

4.2 Data reversibility

According to the assumption of Weisskopf and Ewing [15], the cross section of a reaction in which a projectile x collides with a target X to lead to a residual nucleus Y and an ejectile y, can be split as follows:

$$\sigma(x,y) = S_x(E) \times \xi_x(E) \times \eta_y(E_x) \tag{6}$$

Above hypothesis relies on the fact that given compound nucleus Y* is formed from the couple (x,X) and decays in the couple (y,Y). First product of right side term of Eq. (6) $S_x(E) \times \xi_x(E)$ represents the probability of the formation of compound nucleus. Among those two variables, $S_x(E)$ represents the cross section for reaching the surface of the target nucleus. The incident wave being partially reflected by the potential at the target nucleus surface, $\xi_x(E)$ is the probability denoting the fraction of the incident wave which interacts with the nucleons of the target nucleus. The last variable $\eta_y(E_x)$ quantifies the decaying probability of the compound nucleus giving the couple (y,Y). E is the energy of the projectile and E_x is the excited energy of a state of the compound nucleus created.

The interaction between a particle x and a target nucleus X does not always lead to the formation of a compound nucleus. Other interactions [16] may occur. A competition is possible between the reaction passing through the formation of the compound nucleus and other forms of reaction: surface and volume direct interactions, multiple collisions or even collective nucleon excitation (rotations and vibrations). The evaluation of the $^{16}O(n,\alpha)^{13}C$ cross section has been classically performed using the inverted $^{13}C(\alpha,n)^{16}O$ data from from Bair and Haas [5] and Harissopulos [4]. This inversion of data relies on the compound nucleus hypothesis suggesting that the entire energy brought by the incident wave is right away and equitably shared among all nucleons of the target. The process must last long enough so that the way of the formation of the compound nucleus is “forgotten” by the latter. Subsequent decay probability in given channel is thus independent from the formation channel but both must be connected to the same nuclear state of the compound nucleus. The compound nucleus hypothesis has been illustrated through the computation of

the $^{13}C(\alpha,n)^{16}O$ and $^{16}O(n,\alpha)^{13}C$ cross sections. Below are shown results of the comparison between the cross sections obtained by direct kinematics calculation on one side and those obtained by the data inversion on the other side. The inversion method used to obtain the inverse of a reaction cross section $\sigma_{cc'}(E_c^{CoM})$ for which a compound nucleus is formed from a channel c and decays into a channel c' relies on the expression [9]:

$$\sigma_{c'c}(E_{c'}^{CoM})\lambda\!\!\!^{-2}_{c} = \sigma_{cc'}(E_c^{CoM})\frac{(2i_c+1)(2I_c+1)}{(2i_{c'}+1)(2I_{c'}+1)}\lambda\!\!\!^{-2}_{c'} \quad (7)$$

E_c^{CoM}, i_c, I_c and $\lambda\!\!\!^{-}_{c}$ are respectively the energy of the projectile in the CoM framework, the spin of the projectile, the spin of the target and the reduced wavelength of the projectile in the channel c. $E_{c'}^{CoM}$, $i_{c'}$, $I_{c'}$ and $\lambda\!\!\!^{-}_{c'}$ are reciprocal quantities still in CoM system.

A quick eye on the Figure 3 shows that relative differences (down side plots) between the cross sections obtained from either the direct kinematics calculation or the pseudo cross sections obtained by inversion of data are very small. This trend is likely a confirmation of the predominance of a compound nucleus system at low excitation energy.

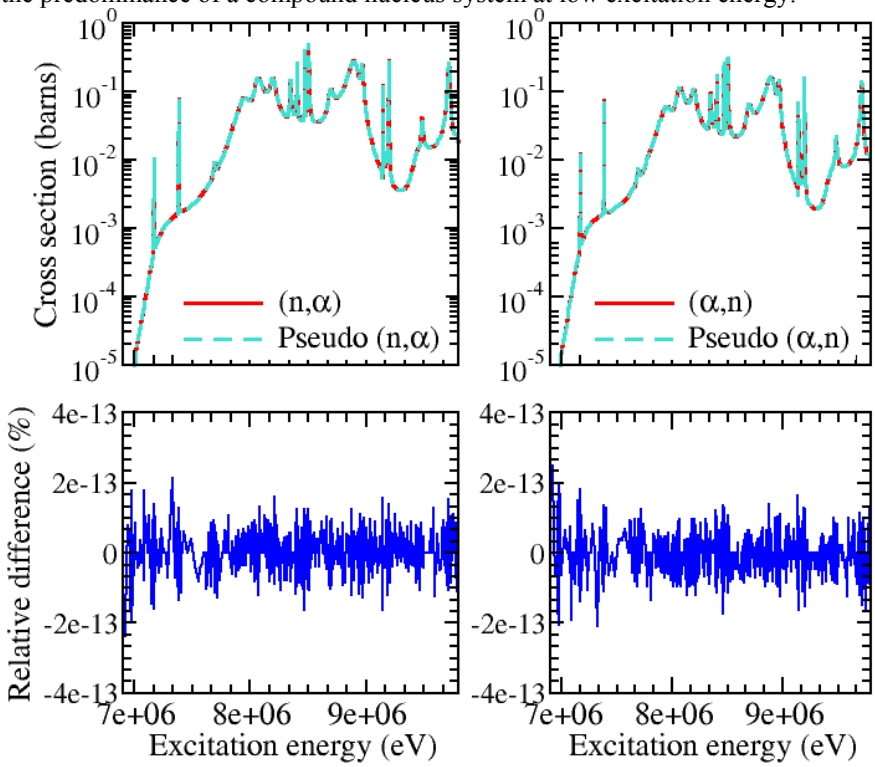

Fig.3. Comparison of the $^{16}O(n,\alpha)^{13}C$ and $^{13}C(\alpha,n)^{16}O$ cross sections obtained using direct kinematics calculation with the data obtained from the inversion of their reciprocal reaction cross sections labelled as pseudo data. The computation is performed using TORA. Relative differences in percentage are computed as the ratio [(Pseudo data – Direct kinematics calculated data)/Pseudo data].

5. Conclusion

A preliminary investigation of the $^{17}O^*$ compound nucleus has been made, using the CIELO Reich-Moore parameters, through a modelling of the $^{16}O(n,\alpha)^{13}C$ and $^{13}C(\alpha,n)^{16}O$ first in the incident particle laboratory frame and secondary in the CoM frame. Both two

cross sections have been benchmarked to the inversed cross sections retrieved from the reciprocal reactions. A comparison between nuclear parameters from the Astrophysics and Reactors physics databases highlighted notable differences. A solution to avoid the identified inconsistencies and reach a better accuracy is definitively the use of the CoM of the compound nucleus framework and energy-independent parameters in the nuclear reactions modelling. The approach has been set up by a simulation of the $^{16}O(n,n)^{16}O$, $^{16}O(n,\alpha)^{13}C$, $^{13}C(\alpha,n)^{16}O$ and $^{13}C(\alpha,\alpha)^{13}C$ reactions. A set of parameters obtained from a fit of experimental data within this unified framework, by the mean of a TORA full connexion to the CONRAD code, is foreseen.

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