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Impact of the ^{6}Li asymptotic normalization constant onto α-induced reactions of astrophysical interest

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Indirect methods have become the predominant approach in experimental nuclear astrophysics for studying several low-energy nuclear reactions occurring in stars, as direct measurements of many of these relevant reactions are rendered infeasible due to their low reaction probability. Such indirect methods, however, require theoretical input that in turn can have significant poorly-quantified uncertainties, which can then be propagated to the reaction rates and have a large effect on our quantitative understanding of stellar evolution and nucleosynthesis processes. We present two such examples involving α-induced reactions, ^{13}C$(\alpha,n)^{16}$O and ^{12}C$(\alpha,\gamma)^{16}$O, for which the low-energy cross sections have been constrained with (^{6}Li$,d$) transfer data. In this Letter, we discuss how a first-principle calculation of ^{6}Li leads to a 21% reduction of the ^{12}C$(\alpha,\gamma)^{16}$O cross sections with respect to a previous estimation. This calculation further resolves the discrepancy between recent measurements of the ^{13}C$(\alpha,n)^{16}$O reaction and points to the need for improved theoretical formulations of nuclear reactions.

Introduction: Nuclear fusion reactions involving the capture of a helium-4 nucleus (α-particle) from a light or medium-mass isotope to form a heavier nucleus and a neutron (n) or a high-energy photon (γ) are central to understanding the lifecycle of massive stars, from driving the nucleosynthetic processes that make them shine and evolve [1–3] to determining their remnants after their eventual death [4–7]. For example, the ^{13}C$(\alpha,n)^{16}$O and ^{22}Ne$(\alpha,n)^{25}$Mg reactions are the principal sources of neutrons fueling the slow neutron capture process (s-process) in asymptotic giant branch (AGB) stars, which is responsible for the formation of half of the elements heavier than iron [8]. Similarly, the ^{12}C$(\alpha,\gamma)^{16}$O reaction is not only a key process in the sequence of helium burning reactions that produces carbon and oxygen in red giant and supergiant stars [9] but also determines the ratio of the amount of ^{12}C to that of ^{16}O, which has profound repercussions on the later evolutionary phases and nucleosynthesis events of these stars, and their ultimate fate once they explode as supernovae [1]. Arriving at a quantitative and more fundamental understanding of the life and death of massive stars requires accurate and precise knowledge of α-induced reaction rates at stellar energies. In the case of ^{12}C$(\alpha,\gamma)^{16}$O, ideally the reaction rate would need to be known within $\approx 10\%$ uncertainty or less at center of mass energies of ≈ 300 keV [1, 10].

Typically, α-induced reactions are very difficult or impossible to measure in the range of (low) energies where they occur in stars because the Coulomb repulsion between the α particle and the nucleus suppresses the reaction probability (cross section) below the background of cosmic rays. Underground facilities, such as the Gran Sasso National Laboratories (LUNA) [11] or the China Jinping Underground Laboratory (JUNA) [12], help reduce this background and reach the low energies relevant for astrophysics. However, a direct measurement of, e.g., the ^{12}C$(\alpha,\gamma)^{16}$O reaction below ≈ 300 keV remains unfeasible and down extrapolations from higher-energy measurements rely on theory.

For the description of low-energy reactions involving systems made of more than A=12 nucleons, where accurate microscopic predictions based on validated models of the nuclear interactions [13, 14] are out of reach and few-body models using effective potentials between structureless reactants [15–17] do not provide the required predictive power, phenomenological R-matrix theory [18, 19] has been the tool of choice. In this technique, cross sections are reconstructed from a relatively small number of parameters that have a physical meaning and are adjusted to reproduce available experimental data. R-matrix analyses have been used extensively to evaluate S-factors[1] of astrophysical interest, including ^{13}C$(\alpha,n)^{16}$O [20, 21] and ^{12}C$(\alpha,\gamma)^{16}$O [1], and extrapolate them down to stellar energies. However, the fit of the parameters can result in sizeable uncertainties on the extrapolated S-factors, in particular when different data sets are inconsistent with each other. Moreover, the presence of loosely-bound states can further influence the extrapolation process [22]. To reduce uncertainties, parameters related to the asymptotic normalization of bound-state wave functions can be fixed using information gleaned from measurements of (^{6}Li$,d$) [or (^{7}Li$,t$)] α-transfer processes, in which an α-particle is transferred from a loosely-bound ^{6}Li (^{7}Li) to another nucleus A to form the A-α state of interest [23–26].

In this Letter, we discuss how a recent first-principle

[1] Astrophysical S-factors correspond to the cross sections rescaled to remove the effect of the Coulomb barrier.

prediction for the ^{6}Li nucleus [27] influences the low-energy properties extracted from $(^6\mathrm{Li}, d)$ transfer data and explains the discrepancy between two recent R-matrix evaluations of the $^{13}\mathrm{C}(\alpha, n)^{16}\mathrm{O}$ reaction by the LUNA [20] and JUNA collaborations [21]. We also estimate the significant impact of this ^{6}Li prediction on the R-matrix evaluation of the $^{12}\mathrm{C}(\alpha, \gamma)^{16}\mathrm{O}$ rate, and argue for future theoretical and experimental studies to improve the evaluation of additional α-induced reactions.

Peripheral reactions to extract ANCs: Non-resonant low-energy radiative α-capture reactions $A + \alpha \to B + \gamma$ dominated by electric transitions are peripheral, i.e., do not probe the interior of the A-α bound state (Fig. 1) and their cross sections scale with the square of its asymptotic normalization constant (ANC, denoted as $\mathcal{C}_{A\text{-}\alpha}$) [28]. The low-energy α-capture cross section can then be accurately approximated as [28, 29]

$$\sigma_{\alpha,\gamma} \simeq (\mathcal{C}_{A\text{-}\alpha})^2 \frac{\hat{\sigma}_{\alpha,\gamma}}{b^2_{A\text{-}\alpha}}, \tag{1}$$

where $\hat{\sigma}_{\alpha,\gamma}$ and $b_{A\text{-}\alpha}$ are the cross section and ANC obtained in a two-body model calculation that treats both the target nucleus (A) and the α as point particles ($b_{A\text{-}\alpha}$ is also referred as the single-particle ANC). More generally, the $(\mathcal{C}_{A\text{-}\alpha})$ ANC is connected with the α-partial width of the corresponding state in the $A + \alpha$ system [1, 28]. It is thus also an essential ingredient in the description and analysis of many low energy processes, such as the $^{13}\mathrm{C}(\alpha, n)^{16}\mathrm{O}$ reaction discussed in this work, but also in multiple other cases where α particles are involved in either the incoming or the outgoing channel [28, 30].

Transfer reactions at energies around the Coulomb barrier are also peripheral, and hence exhibit a similar proportionality with ANCs. For example, the cross section for A+^{6}Li$\to B(\equiv A + \alpha) + d$ at low energies can be accurately evaluated as

$$\sigma_{^6\mathrm{Li},d} \simeq (\mathcal{C}_{A\text{-}\alpha})^2 (\mathcal{C}_{\alpha\text{-}d})^2 \frac{\hat{\sigma}_{^6\mathrm{Li},d}}{b^2_{A\text{-}\alpha} b^2_{\alpha-d}}, \tag{2}$$

where, similar to before, $\hat{\sigma}_{^6\mathrm{Li},d}$ and $b_{\alpha\text{-}d}$ are the cross section and ANC obtained in simplified calculations that treat ^{6}Li, d and α as point particles. If the ANC of the ^{6}Li nucleus $\mathcal{C}_{\alpha\text{-}d}$ is well known, one can use Eq. (2) and experimental data on the transfer reaction to accurately extract $\mathcal{C}_{A\text{-}\alpha}$ by rescaling the theoretical cross sections $\hat{\sigma}_{^6\mathrm{Li},d}$, typically evaluated within the distorted-wave Born approximation (DWBA), to the data [28]. These calculations usually consider only the s-wave ANC of ^{6}Li and neglect the d-wave ANC, which is two order of magnitude smaller [27, 31].

A frequently adopted value of the s-wave α-d ANC in the analysis of peripheral $(^6\mathrm{Li}, d)$ transfer reactions [23, 24] has been $(\mathcal{C}_{\alpha\text{-}d})^2 = 5.3 \pm 0.5$ fm^{-1}. This value was determined by Blokhintsev *et al.* [32] using three different methods: 1) by analytic continuation of the α-d scattering phase shifts, 2) by computing the (two-body) α-d bound state using an interaction fitted to reproduce these phase shifts, and 3) by solving the Faddeev equations for the (three-body) α-n-p system using phenomenological α-nucleon interactions and neglecting the α-p Coulomb repulsion. Unfortunately, the uncertainties associated with the extrapolation procedure used in the first two methods and the ambiguity in the choice of the α-nucleon interactions combined with the omission of the Coulomb potential in the third method have not been quantified, raising the prospect for previously unrecognised systematic errors in the ANC determination. Other evaluations [31, 33] of $\mathcal{C}_{\alpha\text{-}d}$ relying on α-d phenomenological potentials are consistent with the values provided by Blokhintsev *et al.* but none of them have quantified the parametric uncertainties associated with the fit of the α-d interaction, which can be sizeable [15–17].

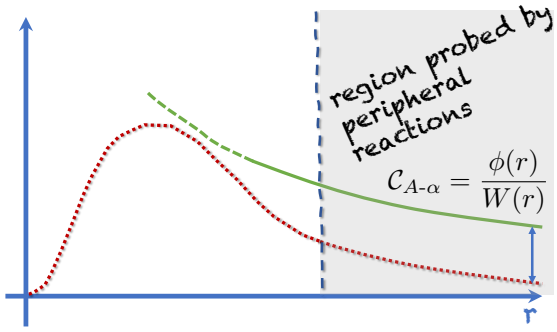


FIG. 1. Schematic representation of the radial part of the A-α wavefunction $\phi(r)$ (dotted red line) and the Whittaker function $W(r)$ (green continuous line). They differ by a constant factor, namely the asymptotic normalization constant $\mathcal{C}_{A\text{-}\alpha}$. Peripheral reactions are only sensitive to the asymptotic behavior of the A-α wavefunction (shaded area).

A new accurate determination of $\mathcal{C}_{\alpha\text{-}d}$ through (six-body) predictions of the ^{6}Li system starting from two- and three-nucleon forces derived within chiral effective field theory, recently became available [27]. These calculations, obtained within the framework of the *ab initio* no-core shell model with continuum (NCSMC) [34], treat the α-d scattering and bound ^{6}Li state on equal footing and accurately reproduce the low-energy properties of the system, including the $\alpha(d, \gamma)^6$Li capture rate and α-d elastic scattering at energies below 3 MeV. Contrary to the determination of Blokhintsev *et al.*, the uncertainties of these microscopic calculations stem from two clearly identified sources: the choice of chiral Hamiltonian and the convergence with respect to the size of the NCSMC model space (see Supplemental Material of Ref. [27]). Both uncertainties were significantly reduced by introducing a fine-tuning correction to exactly reproduce the experimental binding energy of the ^{6}Li

ground state. Compared to this first-principle prediction, $(\mathcal{C}_{\alpha\text{-}d})^2 = 6.864 \pm 0.210$ fm^{-1}, the ANC of Blokhintsev *et al.* [35] is 22% smaller and exhibits larger uncertainties.

Impact on s-process nucleosynthesis: Because of its key role in s-process nucleosynthesis, the ^{13}C$(\alpha, n)^{16}$O reaction has been measured in underground facilities in the last two years[2] at low energies relevant for astrophysics, i.e., at 0.23–0.3 MeV by the LUNA and at 0.24-1.9 MeV by the JUNA collaborations [20, 21]. Although the two data sets are consistent, the R-matrix analyses used to extrapolate the data to lower energies lead to different S-factors. The JUNA collaboration suggested that this discrepancy is explained by the use of a different α-ANC of the $1/2^+$ state in ^{17}O, located 3 keV below the α-threshold, which determines the overall normalization of the S-factor at the energies of astrophysics interest [20, 21, 28]. In the work of Ref. [21] this ANC is treated as a floating parameter in the R-matrix analysis of the data, while in the analysis of Ref. [20] it was fixed to the value inferred by Avila *et al.* from a sub-Coulomb (^{6}Li, d) transfer experiment [36] (Fig. 2). In turn, however, the work of Ref. [36] had adopted the s-wave α-d ANC of Blokhintsev *et al.* to extract the ANC of the $1/2^+$ state in ^{17}O following the relationship described in Eq. (2).

By reinterpreting the transfer data of Ref. [36] with the more accurate ANC obtained in Ref. [27], we extract[3] $(\tilde{\mathcal{C}}^{1/2^+}_{\alpha\text{-}^{13}\mathrm{C}})^2 = 2.8 \pm 0.5$ fm^{-1}, consistent with the value obtained by the JUNA collaboration, thus explaining the difference between the two R-matrix analyses. The new calculated value of $(\mathcal{C}_{\alpha\text{-}d})^2$ contributes by just 0.086 fm^{-1} to the quoted uncertainty. The rest is associated with the experimental and theoretical uncertainties arising from the (^{6}Li,d) experiment used to extract the α-^{13}C ANC, as described in [36]. This is in sharp contrast with the previous analysis of [36], where the Blokhintsev $(\mathcal{C}_{\alpha\text{-}d})^2$ value contributed to the total uncertainty by 0.34 fm^{-1}, a much more significant amount. The re-evaluated ANC from the (^{6}Li, d) transfer data also agrees with the values extracted from (^{11}B,^{7}Li) [37] and (^{7}Li, t) [38] transfer data (Fig. 2).

This work supports the JUNA analysis [21] of the thermonuclear reaction rate [40, 41], which is smaller than previous evaluations. This decrease in the flux of neutrons impacts the abundances of s-process branching point and heavier elements, in particular ^{60}Fe, ^{152}Gd and ^{205}Pb [20].

Interestingly, the rate of the other major neutron source in the s-process, ^{22}Ne$(\alpha, n)^{25}$Mg, has also been constrained using the α-partial width of resonances of ^{26}Mg extracted from (^{6}Li, d) data using the the s-wave α-d ANC of Blokhintsev *et al.* [30]. Based on the larger value of the α-d ANC of Ref. [27], we expect that this ^{22}Ne$(\alpha, n)^{25}$Mg rate is overestimated, and that the overall neutron flux in the s-process is even smaller than what is currently evaluated. Because the ^{22}Ne(^{6}Li, d)^{26}Mg transfer reaction populates unbound ^{26}Mg states, the DWBA analysis of the data should be revisited to account for model uncertainties associated with the approximation introduced by treating these states as bound and then extrapolating their properties up to energies in the continuum [42]. We reserve this study for future work, as some development in reaction theory is first needed to adequately describe transfer reactions to states in the energy continuum, e.g., through the generalization of the Green's function based formalisms [43–45] to α-transfer reactions.

Impact on ^{12}C$(\alpha, \gamma)^{16}$O*:* A recent R-matrix analysis of ^{16}O data (including ^{12}C$(\alpha, \gamma)^{16}$O capture, β-delayed α-emission, α-^{12}C elastic scattering measurements, and recent evaluations of bound- and resonant-state properties) found that the extrapolated ^{12}C$(\alpha, \gamma)^{16}$O S-factor at stellar energies of ≈ 300 keV depends strongly on the $\mathcal{C}_{\alpha\text{-}^{12}\mathrm{C}}$ ANC of the 1^- and 2^+ loosely-bound states in ^{16}O [1]. To arrive at their best R-matrix fit, the authors adopted (as fixed parameters) the ANCs of these and the other ^{16}O bound states determined from (^{6}Li, d)

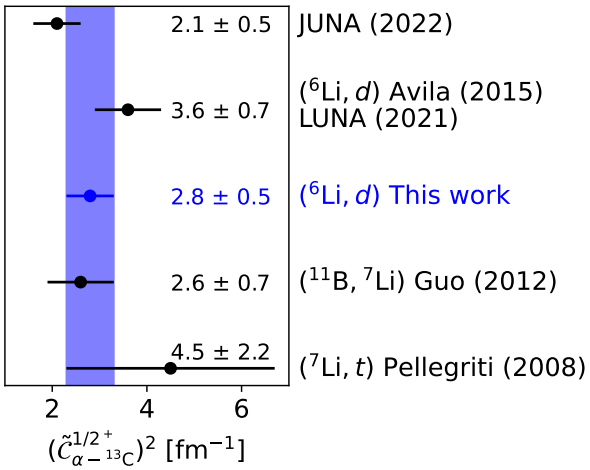


FIG. 2. Comparison of the square of the Coulomb-modified ANC of the $1/2^+$ threshold state in ^{17}O, $(\tilde{\mathcal{C}}^{1/2^+}_{\alpha\text{-}^{13}\mathrm{C}})^2$, deduced from: the R-matrix analysis of the JUNA collaboration [21], the values extracted from (^{6}Li, d) data [36] using the $(\mathcal{C}_{\alpha\text{-}d})^2$ of Ref. [35], our reinterpretation of the (^{6}Li, d) data [36] using a first-principle prediction of $(\mathcal{C}_{\alpha\text{-}d})^2$ [27], the values inferred from (^{11}B,^{7}Li) data [37, 39], (^{7}Li, t) data [38]. The numbers in the figure correspond to the values of the corresponding ANCs and their uncertainties.

[2] We cite here the year of the publications of the Phys. Rev. Lett. in which the data and analysis were published.

[3] The so-called Coulomb-modified ANC $\tilde{\mathcal{C}}$ is directly proportional to the usual ANC and given by $\tilde{\mathcal{C}} = \mathcal{C} \times \ell!/\Gamma(\ell + 1 + |\eta|)$, with ℓ being the relative angular momentum between the fragments and η the Sommerfeld parameter [28].

J^π	E_{ex}	Probe	$(\mathcal{C}^{J^\pi}_{\alpha\text{-}^{12}\mathrm{C}})^2$ Past Work	This Work	
0^+	6.05	$(^6\mathrm{Li}, d)$ [24]	2.43(30)	1.88(16)	$\times 10^6$
3^-	6.13	$(^6\mathrm{Li}, d)$ [24]	1.93(25)	1.49(14)	$\times 10^4$
2^+	6.92	$(^6\mathrm{Li}, d)$ [23]	1.24(24)	0.96(16)	$\times 10^{10}$
		$(^6\mathrm{Li}, d)$ [24]	1.48(16)	1.14(7)	
		$(^7\mathrm{Li}, t)$ [23]	1.33(29)		
		$(^7\mathrm{Li}, t)$ [46]	2.07(80)		
1^-	7.12	$(^6\mathrm{Li}, d)$ [23]	4.33(84)	3.34(58)	$\times 10^{28}$
		$(^6\mathrm{Li}, d)$ [24]	4.39(59)	3.39(34)	
		$(^7\mathrm{Li}, t)$ [46]	4.00(138)		

TABLE I. Square of ANCs (in units of fm^{-1}) for the 0^+, 3^-, 2^+ and 1^- bound states of ^{16}O extracted from $^{12}\mathrm{C}(^6\mathrm{Li}, d)^{16}\mathrm{O}$ [23, 24] and $^{12}\mathrm{C}(^7\mathrm{Li}, t)^{16}\mathrm{O}$ [23, 46] data. The first two columns indicate the excitation energy (in MeV), spin, and parity, of the corresponding state, and the third column specifies the reaction used for the extraction of the ANC. In the last two columns, we compare the original evaluation of the ANC using $(\mathcal{C}_{\alpha\text{-}d})^2$ of Ref. [32] with the analyses using a first-principle prediction of $(\mathcal{C}_{\alpha\text{-}d})^2$ [27].

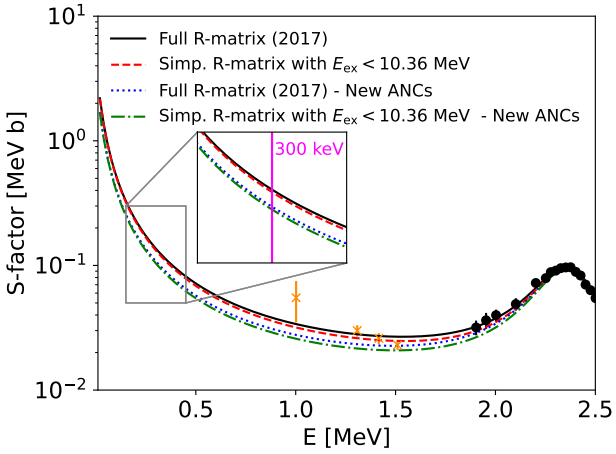


FIG. 3. Comparison of the $^{12}\mathrm{C}(\alpha,\gamma)^{16}\mathrm{O}$ S-factors as a function of the relative ^{12}C-α relative energy, obtained with the R-matrix analysis of deBoer *et al.* [1] (solid black line), a simplified version in which only the low-energy states and the α-channel are included (dashed red line), and predictions using our $(\mathcal{C}^{J^\pi}_{\alpha\text{-}^{12}\mathrm{C}})^2$ displayed in Table I (dotted blue and dash-dotted green lines). These S-factors have been obtained using the code AZURE2 [50, 51], and the input files are provided in Supplemental Material [52]. The total S-factor data from Refs. [49] (black circles) and [48] (orange crosses) are also shown for comparison. The inset show the S-factors around the stellar energies (in magenta).

reactions [23, 24] using the $\mathcal{C}_{\alpha-d}$ value of Blokhintsev *et al.* (fourth column of Table I). As in the previous case, the new accurate prediction of $\mathcal{C}_{\alpha-d}$ from Ref. [27] impacts the extracted ^{16}O $(\mathcal{C}^{J^\pi}_{\alpha\text{-}^{12}\mathrm{C}})^2$ values, yielding ANCs that are $\approx 22\%$ smaller and with reduced uncertainties (fifth column of Table I). These new evaluations are consistent with the $(\mathcal{C}^{1^-}_{\alpha\text{-}^{12}\mathrm{C}})^2$ and $(\mathcal{C}^{2^+}_{\alpha\text{-}^{12}\mathrm{C}})^2$ values extracted from $(^7\mathrm{Li}, t)$ transfer reactions in Ref. [46] and [23] respectively, but are in tension with the 2^+ ANC from Ref. [46] (Table I). The ^{7}Li ANC used in these DWBA analyses was determined using similar approaches as in Ref. [32] and model uncertainties are similarly not fully quantified [35, 47]. In this respect, a first-principle prediction of the ^{7}Li ANC $\mathcal{C}_{\alpha-t}$ would be desirable and may resolve the tension between the $\mathcal{C}_{\alpha\text{-}^{12}\mathrm{C}}$ values extracted from $(^6\mathrm{Li}, d)$ and $(^7\mathrm{Li}, t)$ transfer data.

To illustrate the impact of the $\mathcal{C}^{J^\pi}_{\alpha\text{-}^{12}\mathrm{C}}$ values determined in this work on the low-energy $^{12}\mathrm{C}(\alpha,\gamma)^{16}\mathrm{O}$ S-factor, we perform a reduced R-matrix calculation[4] starting from the best fit of Ref. [1], keeping only the ^{16}O states with excitation energies up to 10.36 MeV. At low energies, the S-factor from such reduced R-matrix calculation is close to the comprehensive fit of Ref. [1] (Fig. 3). We then rescale the ANCs of the bound states and perform an R-matrix calculation without refitting the rest of the parameters. As expected for a peripheral reaction, upon changing the α-^{12}C ANCs to the values determined in this work we obtain a reduced S-factor. At 300 keV, the S-factor is almost exactly proportional to $(\mathcal{C}^{J^\pi}_{\alpha\text{-}^{12}\mathrm{C}})^2$ and is reduced by 21% with respect to the original fit. It is worth noting that none of the S-factors are consistent with both data sets [48, 49]. Because of the need of renormalizing measurements, and the difficulties in extracting the overall normalization, R-matrix analyses lack predictive power for the determination of ANCs. It also indicates that these data alone do not sufficiently constrain the S-factor at stellar energies.

The 21% reduction of the S-factor at stellar energies will increase the ratio of the ^{12}C to ^{16}O abundances. Quantifying the impact of our new evaluations of the $\mathcal{C}_{\alpha\text{-}^{12}\mathrm{C}}$ ANCs on the other carbon burning scenarios at temperature 1-10 GK would require reevaluating the S-factor up to 6 MeV by means of a more complete R-matrix fit, similar to the one presented in Ref. [1], which included multiple reactions channels and data sets and used a robust statistical framework to quantify the uncertainties.

Conclusions and prospects: We have demonstrated how a recent first-principle prediction for $\mathcal{C}_{\alpha-d}$ impacts S-factors of astrophysical interest, for both the s-process and helium burning nucleosynthesis. Using this new $\mathcal{C}_{\alpha-d}$,

[4] We also included the cascade transitions, resulting from γ-ray de-excitations from the excited states to the ground state of ^{16}O.

the values for the ^{13}C-α ANC extracted from (^{6}Li, d) data now agree with values extracted from other α-transfer probes. Our analysis further provides an explanation for the discrepancy between the two recent LUNA and JUNA evaluations of the ^{13}C$(\alpha, n)^{16}$O S-factors and reaction rates, favoring the recent JUNA evaluation [21]. Since the other principal neutron source in the s-process, i.e., ^{22}Ne$(\alpha, n)^{25}$Mg, was also evaluated using (^{6}Li, d) data, our analysis suggests that the neutron flux in the s-process is smaller than what is currently evaluated.

The first-principle prediction of $\mathcal{C}_{\alpha\text{-}d}$ also impacts the ^{12}C$(\alpha, \gamma)^{16}$O reaction rate. We find that the S-factor at 300 keV is reduced by 21%, compared to Ref. [1]. This reduction, when propagated into a nucleosynthesis reaction network, will increase the abundance ratio of ^{12}C to ^{16}O and impact the abundances of heavier elements. This work advocates for a new R-matrix analysis, constrained with our new evaluation of the $\mathcal{C}_{^{12}\text{C-}\alpha}$, of the ^{12}C$(\alpha, \gamma)^{16}$O reaction rate over the all range of energies relevant for astrophysics.

Our approach will have a general impact on the accuracy and reliability of indirect measurements of reaction rates of astrophysical interest by significantly reducing the uncertainty associated with $\mathcal{C}_{\alpha\text{-}d}$. The uncertainties in the extraction of the relevant partial widths are now dominated by the experimental errors and the reaction model used to describe the process. Within this context, we have also pointed out some developments in reaction theory that should be conducted to improve our knowledge of any α-induced reaction rate of astrophysical interest. Because inaccuracies in the reaction model used to extract structure information from transfer data propagate to the astrophysical S-factor, it is crucial to push first-principle calculations, for which uncertainties are more straightforwardly quantifiable, to heavier systems [53]. In parallel, analysis of transfer data using few-body models could be improved to further constrain the S-factors: these methods should be generalized to the transfer to unbound states, without requiring any extrapolation techniques, and the treatment of the reaction dynamics formalism should be improved, i.e., by going beyond the one-step DWBA description. Finally, since uncertainties can be reduced by comparing the structure information extracted from various transfer probes, first-principle predictions of ^{7}Li and ^{11}B nuclei should be conducted and compared with experiments that provide stringent constraint on these ANCs, e.g., low-energy $d(^7\text{Li}, t)^6$Li measurements.

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