Suppression of Excited-State Contributions to Stellar Reaction Rates

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It has been shown in previous work [Phys. Rev. Lett. 101, 191101 (2008); Phys. Rev. C 80, 035801 (2009)] that a suppression of the stellar enhancement factor (SEF) occurs in some endothermic reactions at and far from stability. This effect is re-evaluated using the ground-state contributions to the stellar reaction rates, which were shown to be better suited to judge the importance of excited state contributions than the previously applied SEFs. An update of the tables shown in Phys. Rev. C 80, 035801 (2009) is given. The new evaluation finds 2350 cases (out of a full set of 57513 reactions) for which the ground-state contribution is larger in the reaction direction with negative reaction \(Q\) value than in the exothermic direction, thus providing exceptions to the commonly applied \(Q\) value rule. The results confirm the Coulomb suppression effect but lead to a larger number of exceptions than previously found. This is due to the fact that often a large variation in the g.s. contribution does not lead to a sizeable change in the SEF. On the other hand, several previously identified cases do not appear anymore because it is found that their g.s. contribution is smaller than inferred from the SEF.

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I. INTRODUCTION

Astrophysical reaction rates are central to any investigation in nucleosynthesis as they provide the quantitative description of temporal abundance changes in a hot plasma. They are related to reaction cross sections which, in turn, may be predicted in theoretical models or extracted from experiments. Compared to standard nuclear physics investigations of reactions on the ground state (g.s.) of nuclei, a treatment of reaction rates is complicated by the thermal population of excited states in the nuclei which are in thermal equilibrium with their hot environment. On the other hand, as long as thermal equilibrium is upheld, there is a mathematically rigorous reciprocity relation connecting the rates of forward and reverse reaction. This implies that only the stellar rate for one direction, say, \(A(a, b)B\) has to be determined by theoretical or experimental means. The stellar rate for its inverse reaction \(B(b, a)A\) automatically follows by applying the simple reciprocity relations.

Determining contributions of reactions proceeding on excited states of nuclei to the stellar rate remains an experimental challenge. Therefore it is interesting to theoretically investigate not only the magnitude of the contributions for each reaction but also which reaction direction is impacted less by such contributions. A determination of the rate in that direction would then be closer to the actually required stellar value. It is easy to show that fewer excited state transitions are involved in a stellar rate of a reaction with positive reaction \(Q\) value than in one with negative \(Q\) value. This is especially important for intermediate mass and heavy nuclei, whereas in light nuclei excited state contributions are often small in either reaction direction, anyway. The well-known “\(Q\) value rule” follows directly, stating that for astrophysical purposes it is preferable to use the direction of positive \(Q\) value. It has been shown recently, however, that an effect termed “Coulomb suppression of excited state contributions” can lead to a violation of this rule when the Coulomb barriers in entrance and exit channels are very different. Since the relevant contributions of reactions on excited states involve different relative interaction energies, depending on the excitation energies of the participating excited states and the reaction \(Q\) value, Coulomb barriers in entrance and exit channel act differently.

Ref. provided an in-depth investigation of this effect across the nuclear chart and also discussed the relevance in nucleosynthesis studies. It focused, however, on a comparison of the stellar enhancement factors (SEFs) in the forward and reverse reaction direction. Later it was shown that the SEF is not always a good measure of how reactions on excited states contribute to the stellar rate. In this work, a similar investigation of the suppression effect is performed but using the better suited g.s. and excited state contributions to the stellar rate to check whether the conclusions of the previous investigation still hold and to provide updated tables.

II. DEFINITIONS

The SEF \(f\) is defined as the ratio of the stellar rate \(r^*\) and reactivity \(R^*\) relative to the ground state (g.s.) rate

\[ f = \frac{r^*}{R^*} \]

\[ R^* = \sum_{\text{all reactions}} \frac{\text{d}R}{\text{d}E} \]

\[ \text{d}R = \text{d}N \times \sigma \]

where \(\text{d}R\) is the change in reactivity due to a reaction, \(\text{d}N\) is the number of nuclei participating in the reaction, and \(\sigma\) is the reaction cross section. The SEF can be used to estimate the contribution of excited state reactions to the stellar rate, and by comparing the SEF to the g.s. contribution, one can determine whether excited state reactions are important. The SEF is particularly useful for reactions that proceed through excited states, as it can provide insights into the relative importance of excited states versus ground states in determining the overall reaction rate.
formed similar to the one shown in \cite{5} but focusing by measurements.

shows what fraction of the stellar rate can be constrained the quantity of interest also to experimentalists because it naturally occurs in its long-lived isomer. Therefore, X is negligible and

Laboratory measurements only provide cross sections for r at excitation energy E. While Coulomb suppression certainly drives the SEF value towards unity, a value certainly differs by at least 30% between forward and reverse directions. Only plasma temperatures T \leq 4.5 GK were included to identify cases important in most nucleosynthesis environments and to eliminate those only occurring at very high temperature.

Using these restrictions, 2350 reactions (out of 57513) exhibiting a strong suppression effect of X forw remained, more than in the previous investigation. The reason for a larger number of cases being found is that a large variation in the g.s. contribution does not cause an equally big change in the SEF in many cases. On the other hand, some cases do not appear anymore because the g.s. contribution decreases although the SEF is remaining constant or becoming smaller. Figure 2 shows an example of this and also how the selection criteria work for the reaction 85Sr(n,p)85Rb and its reverse reaction. Although the SEF of 85Rb(p,n)85Sr (Q = –1.847 MeV) is close to unity for all temperatures, the actual g.s. contribution

\[ r^*(T) = \frac{r^*(T)}{r^*(T)} = \frac{R^*(T)}{R_0(T)} \]

at a plasma temperature T. While Coulomb suppression certainly drives the SEF value towards unity, a value close to 1.0 cannot be interpreted a priori as that excited state contributions are negligible. Later it has been shown that the more useful quantity to consider is the g.s. contribution to the stellar rate, \cite{4 8}

\[ X_0(T) = \frac{(2J_0 + 1)}{G(T)} \]

where J0 is the g.s. spin of the target nucleus and G is the temperature-dependent partition function, defined as

\[ G(T) = \sum_i (2J_i + 1)e^{-\frac{E_i}{kT}} \]

The sum runs over g.s. (i = 0) and excited states (i > 0) at excitation energy Ei.

The SEF can be close to unity even when excited state contributions are sizeable whereas X0 directly shows the impact of such contributions, being X0 \approx 1 when they are negligible and X0 \ll 1 when they dominate the rate \cite{3}. Laboratory measurements only provide cross sections for nuclei in their g.s., and thus r^*, except for 180mTa which naturally occurs in its long-lived isomer. Therefore, X0 is the quantity of interest also to experimentalists because it shows what fraction of the stellar rate can be constrained by measurements.

III. SUPPRESSION OF X0

Here, an investigation of the suppression effect is performed similar to the one shown in \cite{3} but focussing on X0, comparing the g.s. contribution of the forward rate X forw to that for its reverse rate X rev and identifying cases with X rev > X forw. The calculations were performed with the Hauser-Feshbach code SMARAGD \cite{4} using updated excited state information \cite{10 11} and masses \cite{12}. The code also uses an improved barrier penetration routine which is appropriate to treat low-energy α transmissions through high Coulomb barriers \cite{3}. As in the previous work, the forward reaction direction is defined as the one with positive reaction Q value, and reactions involving light projectiles (nucleons, α) are studied, with target nuclei ranging from Ne to Bi between the proton and neutron driplines. The selection criteria for the displayed cases had to be modified with respect to the ones used in \cite{5} because of the different properties of X0. To avoid trivial cases and find sizeable differences, only reactions with X rev/X forw > 1.3 and X rev > 0.8 were considered. This choice ensures that the stellar rate of the reaction with negative Q value is dominated by the g.s. contribution. It also implies that the g.s. contributions differ by at least 30% between forward and reverse direction. Only plasma temperatures T \leq 4.5 GK were included to identify cases important in most nucleosynthesis environments and to eliminate those only occurring at very high temperature.

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TABLE I. Targets for (α,γ) reactions with negative Q value but larger X₀ than their reverse reaction. Stable or long-lived targets are in italics. Underlined targets were also found in [2].

| Target | Lu | Gd | Tb | Ho | Er | Tm | Yb | Lu | Gd | Tb | Ho | Er | Tm | Yb |
|--------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|

...Table II. Same as Table I but for (p,γ).

...Table III. Same as Table I but for (γ,n).

...The present Tables I-III are in the same sequence as and formatted similarly to tables I-VIII in [2] and supersede those. Underlined target nuclei appeared already in the previous tables. Most nuclei are new entries, they are not underlined. Target nuclei which do not appear decreases with increasing temperature. Moreover, comparing the evolution of X₀ as function of temperature for forward and reverse reaction, it becomes apparent that X₀<sub>rev</sub> is larger than 1.3X₀<sub>forw</sub> only when both are smaller than 0.8. At lower T, both g.s. contributions are above the cutoff at 0.8 but there X₀<sub>forw</sub> > X₀<sub>rev</sub>. Therefore, the reaction <sup>85</sup>Rb(p,n)<sup>85</sup>Sr does not show up anymore in the tables given below.

Figure 2 can be directly compared to Fig. 2 of [2], illustrating the dependence of the suppression on the Coulomb barrier. Shown is the obtained range of Q val-
TABLE IV. Same as Table II but for (γ, p), (n, α), and (n, γ) reactions.

| (γ, p): | 40 Ca | 32 Si | 35 Cl | 36 Cl | 40 Ar | 42 Ar | 44 Mg | 54 Cr | 79 Cr | 98 Mo | 100 Mo |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 38 Ti | 46 Fe | 53 Co | 55 Zn | 64 Sr | 99 Sn | 137 Eu | 165 Ta | 90 Sr | 133 Xe | 159 Dy | 168 Ta |
| 44 Cr | 52 Co | 55 Zn | 75 Sr | 98 Sn | 137 Eu | 165 Ta |

TABLE V. Same as Table II but for (p, n).

| 32 Si | 36 Cl | 39 Ar | 40 Ar | 42 Ar | 44 Mg | 44 Mg | 45 Ca | 48 Ca | 48 Ca | 49 Ca | 49 Ca | 54 Cr | 55 Zn | 59 Co | 60 Co | 60 Co | 64 Ni | 64 Ni | 64 Ni | 66 Zn | 68 Zn | 68 Zn | 71 Ga | 72 Zn | 73 Zn | 73 Zn | 74 Zn |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 17 As | 36 Cl | 40 Ar | 55 Zn | 64 Sr | 99 Sn | 137 Eu | 90 Sr | 133 Xe | 159 Dy | 168 Ta | 165 Ta | 166 Dy | 168 Ta | 208 Hg | 208 Hg | 208 Hg | 208 Hg | 208 Hg | 208 Hg | 208 Hg | 208 Hg | 208 Hg | 208 Hg | 208 Hg | 208 Hg | 208 Hg |

far off stability – are purely based on theory, as neither spectroscopic information nor masses are available from experiment. In these cases, recommended mass values were taken [12, 13] or a theoretical mass model [14] was used to compute the separation energies. In the absence of knowledge about excited states, a theoretical nuclear level density was employed [15, 16]. Therefore new mass measurements could change the reaction Q values and also further experimental information on excited states may impact the results presented here, especially close to the driplines.

As already discussed in [3], to current knowledge most of the shown reactions are not of direct astrophysical importance. They are merely interesting cases to demonstrate the suppression effect and to study where the standard Q value rule can be applied and where this is not possible. Further developments in astrophysical models and experimental techniques should not be precluded, however, and therefore the full tables are given. For further details on the astrophysical relevance and on the limitations of the applied reaction model, see [3].

As has been pointed out previously, most remarkable in the current astrophysics context are the (α, γ) reactions on proton-rich targets listed in Table II especially the ones on stable targets with neutron number N ≥ 82. These are important to study (γ, α) rates and the optical α+nucleus potential required for predictions relevant to the synthesis of p nuclei [17]. Also important in the astrophysical γ- and in the νp process are (p, n) reactions with negative Q value (Table V) because (p, n) reactions on proton-rich isotopes play a role in these nucleosynthesis processes (see, e.g., [4, 5, 17–21]). Endothermic (α, p) reactions (Table VIII) on proton-rich nuclei are also of interest for νp process studies [22]. Further of interest are the (p, γ) reactions along the proton dripline shown in Table III because they appear in the rp-process [22]. Moreover, the large number of (α, γ) and (p, γ) reactions (and the comparatively small number of (γ, p) and (γ, α) in Table V) and given in the text above) found in this study underlines the fact that it is almost always preferable to measure in the capture direction, even for endothermic captures. This is consistent with the findings of [3, 24].

V. SUMMARY

A previous investigation was improved by studying the g.s. contributions in forward and reverse reaction directions instead of comparing the SEFs. Again, it was found that – contrary to common wisdom – some endothermic reactions exhibit smaller g.s. contributions to the stellar reaction rate than their exothermic counterparts and are thus preferable for experimental and theoretical studies, if one of the reaction directions is found to be important in a hot plasma. The main cause of suppression of the excited state contributions in an endothermic reaction is the Coulomb suppression of transitions with low relative
interaction energy [3]. The larger number of cases is due to the different temperature dependence of the g.s. contributions compared to the SEFs.

For experimental application, it is advisable to first search for a reaction with astrophysical importance and then to check in the above tables whether it belongs to the exceptions for which the experimentally accessible g.s. contribution to the stellar rate is larger in the endothermic direction. Otherwise, a determination of the cross sections of the exothermic reaction would be preferable for astrophysical application, if feasible.

Suppression of thermally excited state contributions is not limited to reactions treated in the Hauser-Feshbach model but also appears in resonant reactions and in direct reactions and similar considerations apply as those discussed above.

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TABLE VIII. Same as Table II but for (a,p).

| Element | Mass | Symbol | Element | Mass | Symbol | Element | Mass | Symbol | Element | Mass | Symbol |
|---------|------|--------|---------|------|--------|---------|------|--------|---------|------|--------|
| Ne      | 23   | 55Fe   | Zn      | 65   | 55Co   | Se      | 80   | 58Ni   | Cd      | 112  | 58Ni   |
| Na      | 28   | 56Fe   | Zn      | 65   | 55Co   | Se      | 80   | 58Ni   | Ca      | 44   | 59Co   |
| Mg      | 24   | 57Fe   | Zn      | 65   | 55Co   | Se      | 80   | 58Ni   | Ti      | 47   | 59Co   |
| Al      | 27   | 58Fe   | Zn      | 65   | 55Co   | Se      | 80   | 58Ni   | Ca      | 44   | 59Co   |
| Si      | 28   | 59Fe   | Zn      | 65   | 55Co   | Se      | 80   | 58Ni   | Ti      | 47   | 59Co   |
| P       | 31   | 60Fe   | Zn      | 65   | 55Co   | Se      | 80   | 58Ni   | Ca      | 44   | 59Co   |
| S       | 32   | 61Fe   | Zn      | 65   | 55Co   | Se      | 80   | 58Ni   | Ti      | 47   | 59Co   |
| Cl      | 35   | 62Fe   | Zn      | 65   | 55Co   | Se      | 80   | 58Ni   | Ca      | 44   | 59Co   |
| Ar      | 39   | 63Fe   | Zn      | 65   | 55Co   | Se      | 80   | 58Ni   | Ti      | 47   | 59Co   |
| Kr      | 85   | 87Se   | Br      | 81   | 87Se   | Br      | 81   | 87Se   | Br      | 81   | 87Se   |
| Xe      | 136  | 126Se  | Br      | 81   | 87Se   | Br      | 81   | 87Se   | Br      | 81   | 87Se   |
| Sr      | 88   | 164Br  | Br      | 81   | 164Br  | Br      | 81   | 164Br  | Br      | 81   | 164Br  |
| Ba      | 138  | 136La  | La      | 138  | 136La  | La      | 138  | 136La  | La      | 138  | 136La  |
| La      | 138  | 136La  | La      | 138  | 136La  | La      | 138  | 136La  | La      | 138  | 136La  |
| Ce      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Pr      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Sm      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Eu      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Gd      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Tb      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Dy      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Ho      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Er      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Tm      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Yb      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Hf      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Ta      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| W       | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Re      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Os      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Ir      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Pt      | 140  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  | Nd      | 142  | 140Nd  |
| Au      | 197  | 197Pt  | Pt      | 197  | 197Pt  | Pt      | 197  | 197Pt  | Pt      | 197  | 197Pt  |
| Hg      | 200  | 200Pt  | Pt      | 197  | 197Pt  | Pt      | 197  | 197Pt  | Pt      | 197  | 197Pt  |

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TABLE IX. Same as Table I but for (p,α).

| Atom | 48 Ar | 62 Ar | 70 Ca | 70 Se | 86 Zr | 92 Mo |
|------|-------|-------|-------|-------|-------|-------|
| 31 Si |       |       |       |       |       |       |
| 34 Si |       |       |       |       |       |       |
| 46 Si |       |       |       |       |       |       |
| 44 Ar |       |       |       |       |       |       |
| 47 Ar |       |       |       |       |       |       |

| Atom | 56 Ar | 63 Ar | 51 Ti | 116 Se | 87 Zr | 86 Tc |
|------|-------|-------|-------|---------|-------|-------|
| 31 Si |       |       |       |         |       |       |
| 34 Si |       |       |       |         |       |       |
| 46 Si |       |       |       |         |       |       |
| 44 Ar |       |       |       |         |       |       |
| 47 Ar |       |       |       |         |       |       |

| Atom | 43 Ca | 72 Ti | 70 Br | 80 Mo | 83 Ru | 88 Mo | 91 Ru | 89 Mo | 93 Ru | 95 Cd | 99 Cd |
|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 31 Si |       |       |       |       |       |       |       |       |       |       |       |
| 34 Si |       |       |       |       |       |       |       |       |       |       |       |
| 46 Si |       |       |       |       |       |       |       |       |       |       |       |
| 44 Ar |       |       |       |       |       |       |       |       |       |       |       |
| 47 Ar |       |       |       |       |       |       |       |       |       |       |       |