OPPORTUNITIES TO CONSTRAIN ASTROPHYSICAL REACTION RATES FOR THE s-PROCESS VIA DETERMINATION OF THE GROUND-STATE CROSS-SECTIONS

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Received 2011 May 5; accepted 2011 June 20; published 2011 August 19

ABSTRACT

Modern models of s-process nucleosynthesis in stars require stellar reaction rates of high precision. Most neutron-capture cross-sections in the s-process have been measured, and for an increasing number of reactions the required precision is achieved. This does not necessarily mean, however, that the stellar rates are constrained equally well, because only the capture of the ground state of a target is measured in the laboratory. Captures of excited states can contribute considerably to stellar rates that are already at typical s-process temperatures. We show that the ground-state contribution X to a stellar rate is the relevant measure to identify reactions that are or could be well constrained by experiments and apply it to (n,γ) reactions in the s-process. We further show that the maximum possible reduction in uncertainty of a rate via determination of the ground-state cross-section is given directly by X. An error analysis of X is presented, and it is found that X is a robust measure with mostly small uncertainties.

Several specific examples (neutron capture of 78Se, 90Zr, 121Sn, 187Os, and 193Pt) are discussed in detail. The ground-state contributions for a set of 412 neutron-capture reactions around the s-process path are presented in a table. This allows identification of reactions that may be better constrained by experiments and that cannot be constrained solely by measuring ground-state cross-sections (and thus require supplementary studies). General trends and implications are discussed.

Key words: nuclear reactions, nucleosynthesis, abundances

Online-only material: machine-readable table

1. INTRODUCTION

The astrophysical s-process is probably the best-understood nucleosynthesis process, contributing about half the natural nuclides beyond Fe (Käppeler & Mengoni 2006; Straniero et al. 2006; Käppeler et al. 2011). The main component of the s-process is produced in He-shell flashes of asymptotic giant branch (AGB) stars. A second, weak component comes from massive stars, additionally contributing to nuclei in the mass range A ≲ 90. The s-process proceeds by sequences of neutron-capture reactions to build neutron-richer isotopes within an isotopic chain. As soon as an unstable isotope is reached, β− decay moves the synthesis path to the next element with Z + 1. In some cases, neutron capture and β−-decay compete because of comparable reaction rates. This establishes branching points in the s-process path. The resulting abundances depend sensitively on the nuclear properties of these branching points. This fact may be used either to derive astrophysical parameters, such as temperature and neutron density, during the s-process or to test stellar s-process models that provide these parameters.

One prerequisite for the success of nucleosynthesis calculations regarding the s-process is the availability of excellent experimental neutron-capture data (see compilations by Bao et al. 2000; Dillmann et al. 2006, 2009). As the s-process path proceeds along the valley of stability, most nuclei (except unstable branching nuclei) can be used as stable targets. Typical s-process temperatures are on the order of kT ≈ 5–30 keV for the main component in the He-shell flashes of AGB stars, where the main neutron source 13C(a, n)16O operates at the lower end of the temperature range and the second neutron-producing reaction 22Ne(a, n)25Mg operates at the upper end (Käppeler & Mengoni 2006). The latter reaction also provides neutrons for the weak s-process component in massive stars, at slightly higher temperatures of up to about 80 keV (Rauscher et al. 2002). Experiments on stable targets are feasible at these energies, with typical cross-sections ranging from millibarns up to a few barns. However, many reactions in stable targets are still not measured in the full energy range important to the s-process. In the near future, cross-section measurements of unstable nuclei in the branchings will also become possible.

The central quantities in all s-process calculations are the astrophysical reaction rates. These must be determined by theoretical predictions in the absence of experimental data from the relevant energy range. Due to the impact of thermal excitation of nuclear states above the ground state in stellar plasma, however, a theoretical contribution may remain even when the ground-state cross-sections are measured. Although the s-process involves comparatively low plasma temperatures, transitions from low-lying excited states may contribute considerably to stellar rates.

We studied the contribution of ground-state transitions to stellar neutron-capture rates in the s-process to identify cases for which the astrophysical reaction rate is mainly given by the ground-state rate and thus can be constrained well by the measurement of ground-state cross-sections. These cases will allow us to pinpoint reactions for which an uncertainty in the astrophysical reaction rate will not be removed by the determination of ground-state cross-sections. This is also interesting for s-process modelers who want to estimate the uncertainties in the rates they are using. We also show a general
method to determine how the uncertainties in stellar rates are modified when better constraining one or more transitions from a ground state or an excited state, not limited to neutron captures in the s-process.

2. STELLAR RATES

2.1. Definition

Nuclear reactions occurring in astrophysical plasma are described by astrophysical reaction rates; e.g., for neutron capture, the rate is defined as (Fowler 1974; Rauscher 2011)

\[ r^* = n_n n_{\text{target}} \langle \sigma v \rangle^* = n_n n_{\text{target}} R^*, \]

where \( n_n \) and \( n_{\text{target}} \) are number densities of the neutrons and a species of target nuclei, respectively, and the stellar rate factor (also called reactivity) \( R^* = \langle \sigma v \rangle^* \). The relative velocities \( v \) between the neutrons and the target nuclei are given by the Maxwell–Boltzmann (MB) distribution \( \Phi_{\text{MB}}(v, T) \) at temperature \( T \). It can also be expressed as a function of the relative interaction energy \( \Phi(E, T) \).

In stellar plasma, nuclei are in thermal equilibrium with the plasma. This also implies that all excited states can be excited and the nuclei do not necessarily have to be in the ground state (g.s.), depending on the temperature. In most cases, the excited states within a nucleus are also in thermal equilibrium because the equilibration timescale is short (Gintautas et al. 2009). There are a few cases with isomeric or long-lived states that may not be thermalized at s-process temperatures, such as \(^{176}\text{Lu} \) (Heil et al. 2008; Mohr et al. 2009; Gintautas et al. 2009) or \(^{180}\text{Ta} \) (Belic et al. 1999; Mohr et al. 2007). Assuming thermal equilibrium, the total stellar reactivity \( R^* \) is (see, e.g., Ward & Fowler 1980)

\[ R^*(T) = w_0 R_0 + w_1 R_1 + w_2 R_2 + \cdots, \]

with the reactivities of the \( i \)th state in the target

\[ R_i(T) = \int_0^\infty \sigma_i(E_i) \Phi(E_i, T) dE_i. \]

The cross-section \( \sigma_i \) is the total neutron-capture cross-section of the \( i \)th state, i.e., summed over all final states \( j \) in the residual \((A + 1)\) nucleus: \( \sigma_i = \sum_j \sigma_i^{j \to i} \). The relative energy \( E_i \) between projectile and target is always measured in the system of the respective target state (i.e., the g.s. or excited state), and therefore the integration always starts at zero (Fowler 1974; Rauscher 2011). Thus, the full MB energy-distributed neutrons are also acting on nuclei that are in excited states, not only on nuclei in the g.s., and the reaction rate in Equation (1) has to be defined appropriately by the sum in Equation (2).

The normalized weights \( w_i \) of the excited-state contributions in Equation (2) are given by

\[ w_i = \frac{P_i}{\sum_i P_i} = \frac{P_i}{G}, \]

with the partition function \( G = \sum_i P_i \) or, normalized to the g.s., \( G_0 = G/(2J_0 + 1) \). The population factor \( P_i \) of the excited state \( i \) with excitation energy \( E_i \) and spin \( J_i \) is given by the usual Boltzmann factor:

\[ P_i = (2J_i + 1) \exp \left( -\frac{E_i}{kT} \right). \]

Normalized partition functions \( G_0(T) \) are usually given along with reaction rate predictions and can be found, e.g., in Holmes et al. (1976), Woosley et al. (1976), and Rauscher & Thielemann (2000).

Often, the integral in Equation (3) is divided by the mean thermal velocity \( v_i, T \), leading to the so-called Maxwellian-averaged cross-section (MACS). The MACS for the g.s. \((i = 0)\) can be derived from a measurement of the neutron-capture cross-sections over a properly chosen energy interval. The MACS for the g.s. and its uncertainty are provided in the compilations by Bao et al. (2000) and Dillmann et al. (2006, 2009).

Laboratory experiments are performed on nuclei in the g.s. (with the exception of \(^{180}\text{Ta} \), which is the only naturally occurring isomer and has a short-lived g.s.). Thus, experiments determine only the neutron-capture cross-section of the g.s., i.e., \( \sigma_0 \). Therefore, only the g.s. reactivity \( R_0 \) (or g.s. MACS) can be derived, instead of the desired astrophysical reactivity \( R^* \). To assess how much the g.s. rate differs from the astrophysical rate, the so-called stellar enhancement factor (SEF),

\[ f_{\text{SEF}} = \frac{R^*(T)}{R_0}, \]

is usually used. It is found that the SEF remains relatively close to unity, within about 20%–30%, for most nuclei in the s-process path up to temperatures of \( kT \approx 100 \text{ keV} \) (Bao et al. 2000; Dillmann et al. 2006, 2009). As shown below, however, this does not necessarily imply a small contribution of transitions from excited states or a small remaining uncertainty once \( R_0 \) has been well determined.

2.2. Excited-state Contributions

It can be shown that the weighted sum of integrals in Equation (2) can be transformed to an integral over a single MB distribution (Fowler 1974; Holmes et al. 1976; Rauscher 2011),

\[ R^* = \frac{1}{G_0(T)} \int_0^\infty \sigma^{\text{eff}}(E_0) \Phi(E_0, T) dE_0, \]

thereby avoiding the different energy scales found in Equation (2). Following Fowler (1974) and Holmes et al. (1976), \( \sigma^{\text{eff}} \) is the so-called effective cross-section, summing over all final states and initial excited states up to the interaction energy \( E \):

\[ \sigma^{\text{eff}}(E) = \sum_i \sum_j \frac{2J_i + 1}{2J_0 + 1} \frac{E - E_i}{E} \sigma^{i \to j}(E - E_i). \]

This transformation proves convenient in determining the actual weights with which transitions from excited states \( i \) are contributing to stellar rates. These are not the \( P_i \) as defined in Equation (5) because of the different MB distributions appearing in Equation (2). They are rather (Rauscher 2011)

\[ W_i = (2J_i + 1) \frac{E - E_i}{E} = (2J_i + 1) \left( 1 - \frac{E_i}{E} \right) \]

and are therefore linearly declining with increasing excitation energy \( E_i \). The energies \( E \) appearing in Equation (9) are given by the range of energies significantly contributing to the integral in Equation (7). Therefore, the maximum reference energy \( E \) that appears is the upper end of the relevant energy window.
(Gamow window). The relevant energy window for neutron captures is located close to the peak of the MB distribution, and its width is comparable to the width of the MB distribution (Iliadis 2007; Rauscher 2010). As can be seen in Iliadis (2007) and Rauscher (2010), the upper edge of the effective energy window for neutrons is located not far above the energy \( E = kT \), leading to \( \gamma_i \approx (2J_i + 1)(1 - E_i/(kT)) \).

The above discussion shows that for the \( s\)-process temperature of \( kT = 30 \text{ keV} \), excited states up to excitation energies of \( \approx 30-40 \text{ keV} \) can be important in the target nucleus due to the linearly decreasing weight; for a temperature of \( kT = 80 \text{ keV} \), excited states even up to \( \approx 80-100 \text{ keV} \) have to be considered. Obviously, \( \sigma^{-1}/f \) contains information on how strong the contribution from the excited state is. However, \( W \) allows us to estimate whether we have to bother with calculating \( \sigma^{-1}/f \).

Even though many nuclei in the \( s\)-process path show excited states below 100 keV, especially the heavier nuclides, the SEFs nevertheless remain close to unity in most cases. Clearly, this implies that the (predicted) stellar reactivity is close to that for the g.s., because either the \( w_i (\gamma_i) \) or the \( \sigma^{-1}/f \) is negligible for \( i > 0 \) or they conspire to yield a value close to that obtained for the g.s. transitions alone. The SEF does not allow us to distinguish those cases. For illustration, we examine a nucleus with only two levels characterized by excitation energies \( E_0 = 0 \) and \( E_1 \), spins \( J_0 \) and \( J_1 \), and thermal occupation weights \( w_0 \) and \( w_1 \). Let us consider two different cases in this simple model. For case A, we assume that 90% of the target nuclei are in the g.s. (\( w_0 = 0.9 \) and 10% are in the excited state (\( w_1 = 0.1 \)). Let us further assume that the cross-section of the excited state \( \sigma_1 \) is proportional to \( \sigma_0 \) but larger by a factor of two. This yields

\[
\frac{f^A_{\text{SEF}}}{R_0} = \frac{0.9R_0 + 0.1R_1}{R_0} = 0.9 + 0.1 \times 2 = 1.1. \tag{10}
\]

For case B, we assume that two-thirds of the target nuclei are in the first excited state and only one-third remain in the g.s. This can be easily achieved for a small excitation energy \( E_1 \ll kT \) and \( J_0 \ll J_1 \). Furthermore, we assume that the cross-section \( \sigma_1 \) is proportional to \( \sigma_0 \) but larger by 15%. This results in

\[
\frac{f^B_{\text{SEF}}}{R_0} = \frac{R_0/3 + 2R_1/3}{R_0} = 1/3 + 2/3 \times 1.15 = 1.1. \tag{11}
\]

Although the SEF is identical in both cases and close to unity, the essential difference is in the contribution of the excited state, which is small in case A but dominant in case B.

2.3. Ground-state Contribution

Instead of using the SEF, the importance of excited states in the stellar rate factor \( R^* \) can be better assessed by the g.s. contribution \( X \) to \( R^* \), which is given by

\[
X = \frac{w_0}{R^*} = \frac{w_0}{f_{\text{SEF}}} \tag{12}
\]

for the two simple examples above. The quantity \( X \) is positive and assumes its maximum value of unity when only the target g.s. is contributing to \( R^* \). It follows that in case A the g.s. contribution to the stellar rate factor is \( X = 0.9/1.1 \approx 0.82 \), i.e., the stellar rate factor is essentially defined by the dominating g.s. contribution. On the other hand, in case B, we find a g.s. contribution of only \( X = (1/3)/1.1 \approx 0.30 \), i.e., about 70% of the stellar rate stems from the excited state. This shows that the excited-state contribution may significantly exceed the g.s. contribution, even when \( f_{\text{SEF}} \approx 1 \).

The above result for the g.s. contribution can easily be generalized for many contributing thermally excited states. Equation (7) clearly shows that \( f_{\text{SEF}} \) is not a constant of order unity without the contribution of excited-state transitions; rather, \( f_{\text{SEF}} = 1/G_0 \) in this case (Rauscher 2011). Therefore, the g.s. contribution \( X \leq 1 \) in the general case is given by

\[
X(T) = \frac{1}{f_{\text{SEF}(T)}G_0(T)} = \frac{R_0}{R^*G_0}. \tag{13}
\]

The quantity \( X \) will be included in future versions of the KADoNiS (Karlsruhe Astrophysics Database of Nucleosynthesis in Stars) compilation (Dillmann et al. 2009). Even when it is not directly given in a compilation, however, it can be easily computed from \( G_0 \) and either \( f_{\text{SEF}} \) or \( R_0 \), as shown above.

The SEF itself is still interesting in the sense that it specifies whether the stellar rate, albeit incidentally, is similar to the g.s. rate.

2.4. Uncertainty in \( X \)

Note, however, that \( X \) itself is a theoretical quantity (like the SEF). The weighted uncertainties in the rates or cross-sections of the ground and excited states determine the total uncertainty in \( X \) and \( f_{\text{SEF}} \). Entering this total uncertainty, however, are the uncertainties in the ratios of the rates of excited states and the g.s., as well as the uncertainty in the ratios of the weights, i.e., of \( G_0 \). This can be seen easily when looking at the reciprocal of \( X \) (which must have the same relative uncertainty),

\[
\frac{1}{X} = 1 + \frac{w_1}{w_0} R_1 + \frac{w_2}{w_0} R_2 + \frac{w_3}{w_0} R_3 + \cdots. \tag{14}
\]

Similar considerations apply to the SEF. For example, using the simple two-level system from Section 2.2, we may assign some uncertainty, say a factor of two, to the term \( w_1 R_1/(w_0 R_0) \). This translates into uncertainties \( f^A_{\text{SEF}} = 1.1^{+0.30}_{-0.20} \times X^A = 0.85^{+0.08}_{-0.13} \) and \( f^B_{\text{SEF}} = 1.1^{+0.38}_{-0.20} \times X^B = 0.30^{+0.16}_{-0.12} \).

In the following, we study the influence of an uncertainty factor \( u \) on the calculations of the resulting g.s. contribution \( X \) and its inverse \( 1/X \). Only nuclei at or close to stability participate in the \( s\)-process. These nuclides generally have well-determined level schemes at low excitation energies, and therefore \( G_0 \) and the weights \( w_i \) are well determined. Thus, the uncertainties in \( X \) are limited to the uncertainties \( u_i \) arising from the predicted ratios \( R_i/R_0 \).

\[
u_{1/X} = 1 + \frac{w_1}{w_0} u_1 R_1 + \frac{w_2}{w_0} u_2 R_2 + \frac{w_3}{w_0} u_3 R_3 + \cdots. \tag{15}
\]

For the two-level system above, we assumed an uncertainty of a factor of two, i.e., \( u_1 = 2 \) and \( u_1 = 1/2 \), to arrive at the given total uncertainty in \( X \).

Another convenient property of \( X \) is that its uncertainty scales with \( X \) itself. This can be seen when assuming \( u = u_1 = u_2 = \cdots = 0 \). For realistic cases in the \( s\)-process, this is a good approximation of the actual errors in the ratios because only the first few terms in the sum will contribute to \( X \), and the weighted average of the uncertainties \( u \) will be close to the values of \( u_i \) and/or \( u_2 \). The applicability of the assumption can be checked.
averaged uncertainty factor through the normalized partition function. The closer \( G_0 \) is to unity, the better the above assumption holds.

Under the assumption above, we obtain

\[
\mu_{1/X} = 1 + \bar{\mu} \left\{ \frac{w_1 R_1}{w_0 R_0} + \frac{w_2 R_2}{w_0 R_0} + \frac{w_3 R_3}{w_0 R_0} + \cdots \right\} \\
= 1 + \bar{\mu} \left\{ \frac{1}{X} - 1 \right\}.
\]

Then, the factor \( X'/X \), by which \( X \) changes when assuming an averaged uncertainty factor \( \bar{\mu} \) in the rate ratios, is

\[
\mu_X = \frac{X'}{X} = \frac{1}{\bar{\mu} (1 - X) + X}.
\]

This is an important result because it shows that the uncertainties will be negligible for \( X \approx 1 \). Uncertainties will be larger for \( X \ll 1 \) but will still yield \( X' \ll 1 \) when they are included. In other words, large \( X \) values always remain large and very small \( X \) values remain small. Therefore, \( X \) is a robust measure of the g.s. contribution and can be used to determine the direct impact of measurements of g.s. cross-sections on the astrophysical reaction rate. This is another advantage of using \( X \) instead of the SEF. Figure 1 shows the connection between the uncertainty and \( X \).

The uncertainty factor will reach its maximum value, \( \max(\bar{\mu}, 1/\bar{\mu}) \), only for very small values of \( X \). Note that \( \bar{\mu} \) gives the uncertainty in the ratio \( R_i/R_0 \) and not in the rates or cross-sections. Global reaction rate predictions typically find average deviations from measurements of 30% for \((n,\gamma)\) MACS at 30 keV, with local deviations of up to factors of 2–3 (Rauscher et al. 1997; Hoffman et al. 1999; Bao et al. 2000). When using locally adjusted parameters, these uncertainties can be reduced further (at the expense of predictive power for unknown nuclides and their properties). It is commonly assumed, however, that the cross-section ratios \( \sigma_i/\sigma_0 \), and thus the reactivity ratios \( R_i/R_0 \), are predicted with much smaller uncertainty. This is especially true for the \( s \)-process. Unknown spins and parities of low-lying states would give rise to the largest part of the uncertainty in the prediction of \( \sigma_i/\sigma_0 \), but these are known for nuclei in \( s \)-process conditions. The remaining uncertainty is dominated by the uncertainty in the energy dependence of the \( \gamma \) widths (Rauscher 2010). However, note that neutron captures in the \( s \)-process generally have large reaction \( Q \) values, and therefore the relative change in energy for the contributing transitions \( (E - E_i + Q)/Q \) (Rauscher 2008, 2011), when varying \( E_i \), is small. This leads to an uncertainty much smaller than those in specific cross-sections, which are probably lower than 10%.

For a more conservative estimate, the uncertainties in \( X \) in Table 1 and Figures 2 and 3 are given for uncertainty factors \( \bar{\mu} = 1.3 \), i.e., 30%.

3. REDUCTION OF MODEL UNCERTAINTIES IN STELLAR RATES

3.1. Maximum Possible Reduction by Determining \( \sigma_0 \)

The g.s. contribution \( X \) to stellar rates, as derived in Section 2.3, is not just of theoretical interest. It gives directly the maximum reduction in a rate’s uncertainty that can possibly be achieved by completely determining the g.s. rate factor, e.g., by completely measuring the g.s. cross-sections \( \sigma_0 \) within the relevant energy window. Let us define an uncertainty factor \( \mathcal{U} \) of the stellar rate \( R^* \), implying that the “true” rate \( R^*_\text{true} \) is in the range \( R^*/\mathcal{U} \leq R^*_\text{true} \leq \mathcal{U} R^* \) for \( \mathcal{U} \geq 1 \). For instance, a 50% uncertainty in the rate is then expressed as \( \mathcal{U} = 1.5 \), and a rate known to be without uncertainty is characterized by \( \mathcal{U} = 1 \). This overall uncertainty factor \( \mathcal{U} \) of the rate can be split into a
contribution to the uncertainty stemming from the g.s. uncertainty $\mathcal{U}_{\text{gs}}$ and the combined uncertainty of the (usually only theoretically) predicted excited-state contributions $\mathcal{U}_{\text{exc}}$, leading to

$$\mathcal{U} = \mathcal{U}_{\text{gs}} X + \mathcal{U}_{\text{exc}} (1 - X).$$  \tag{18}$$

(It is important to note that the uncertainty factors $\mathcal{U}$, $\mathcal{U}_{\text{gs}}$, and $\mathcal{U}_{\text{exc}}$ defined here are different from, but related to, the factors $\mathcal{U} \equiv \mathcal{U}_{\text{exc}}/\mathcal{U}_{\text{gs}}$, $u_1$, $u_2$, ..., used in Section 2.4.)

The uncertainty $\mathcal{U}$ is determined by $\mathcal{U}_{\text{gs}}$ for $X \approx 1$ and by $\mathcal{U}_{\text{exc}}$ for $X \ll 1$. In both cases, it is safe to assume that the uncertainty of a theoretically predicted rate is $\mathcal{U} = \mathcal{U}_{\text{gs}} = \mathcal{U}_{\text{exc}}$ for simplicity. If the g.s. cross-section $\sigma_0$ can be experimentally determined without error, i.e., $\mathcal{U}_{\text{gs}}^{\exp} = 1$, within the full energy range required to compute the reaction rate integral, then the maximum possible percentage reduction of $\mathcal{U}$ will be simply 100%. It is immediately seen that the reduction is negligible for $X \ll 1$. On the other hand, if the experimentally determined g.s. rate $R_0$ has a non-negligible uncertainty $\mathcal{U}_{\text{gs}}^{\exp} > 1$, then the new, reduced uncertainty factor can be computed by replacing $\mathcal{U}_{\text{gs}}$ in Equation (18) with $\mathcal{U}_{\text{gs}}^{\exp}$. Again, this will only have appreciable impact on $\mathcal{U}$ when $X \approx 1$.

This maximum possible reduction in rate uncertainty is especially important for the $s$-process. Astrophysical modeling and cross-section measurements have entered a high-precision era, with $\sigma_0$ for many targets determined to a few percentage points of precision and with stellar models demanding very small uncertainties in stellar rates for a detailed understanding of the production of $s$ nuclei and for constraining the conditions within a star. It is important to realize, however, that the stellar rate is constrained by the experimental uncertainty only when $X = 1$. In the extreme case when $X \ll 1$, a measurement of g.s. cross-sections or MACS will not be able to constrain the rate in any way, even when performed with the highest precision. In this case, $R^*$ is essentially given by the theoretical prediction of the cross-sections of excited states, and further experiments are required to constrain theoretical predictions. For example, $(n, n')$ reactions populating excited target states (see, e.g., Mosconi et al. 2010b) or $(\gamma, n)$ reactions on the residual nucleus (e.g., Sonnabend et al. 2003a) have been suggested to study specific transitions to excited states in the target.

It should be noted that even when $X < 1$, the knowledge of $\sigma_0$ can be used to test and improve a model’s prediction of the reaction cross-section, even though the measurement will not directly constrain $R^*$. In many cases, deficiencies in the description of the cross-sections of the ground and excited states are correlated, and the prediction of a stellar rate may also be improved in such instances by a renormalization of the rate. Whether this is possible depends on reaction details and must be investigated separately for each target nucleus.

For completeness, it must be mentioned here that the uncertainties in the SEFs $f_{\text{SEF}}$ and g.s. contribution $X$ are not the only nuclear uncertainties playing a role in $s$-process nucleosynthesis calculations. In particular, for interesting branching nuclei, often only theoretical predictions of the capture cross-sections are available. The feasibility of a considerable reduction in theoretical uncertainties via measurements can be checked by inspecting $X$ for such nuclei. However, branching may be additionally affected by a temperature-dependent $\beta$-decay half-life (Takahashi & Yokoi 1987). Also, for decay rates (as for any other type of rate), the g.s. contribution can be determined by applying Equation (13). In this work, however, we focus on neutron captures that are close to stability.

### 3.2. General Results

We calculated SEFs $f_{\text{SEF}}$ and g.s. contributions $X$ for a set of nuclides important to $s$-process studies using the reaction rate code SMARAGD, version 0.8.1s (Rauscher 2011). This includes the excited states from the recent version of Evaluated Nuclear Structure Data File (ENSDF2010). Nuclides present in KADoNiS v0.3 (Dillmann et al. 2009) were supplemented with several additional nuclei under consideration for inclusion in future KADoNiS versions, yielding a set of 412 nuclei. Table 1 shows the nuclei considered with their $G_0$, $X$, and $f_{\text{SEF}}$ values at $kT = 30$ keV and $kT = 80$ keV (results for further temperatures will be included in future versions of KADoNiS). Also given is the relative uncertainty factor $\nu_x$, which defines the lower limit $X_{\text{lower}} = X/\nu_x$ and upper limit $X_{\text{upper}} = u_X X$ of $X$, as discussed in Section 2.4. The last column of Table 1 provides information on the current experimental status of the $(n, \gamma)$ reaction on the given target nucleus and identifies the nuclei marked in Figure 4 (marked by an asterisk in the comment column). When a reaction is measured (marked by “e”) and $X$ is close to unity, the uncertainty in stellar rate is directly connected to the experimental uncertainty. If $X$ is small, the theoretical

| $Z$ | $A$ | Nuclides | $G_0^{10}$ | $X^{10}$ | $u_X^{10}$ | $f_{\text{SEF}}^{10}$ | $G_0^{30}$ | $X^{30}$ | $u_X^{30}$ | $f_{\text{SEF}}^{30}$ | Comment $^a$ |
|-----|-----|----------|----------|---------|------------|--------------|----------|---------|------------|--------------|-----------|
| 10  | 20  | $^{20}\text{Ne}$ & 1.000 & 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| 10  | 21  | $^{21}\text{Ne}$ & 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| 10  | 22  | $^{22}\text{Ne}$ & 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| 11  | 23  | $^{23}\text{Na}$ & 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| 12  | 24  | $^{24}\text{Mg}$ & 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| 12  | 25  | $^{25}\text{Mg}$ & 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| 12  | 26  | $^{26}\text{Mg}$ & 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| 13  | 26  | $^{26}\text{Al}$ & 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| 14  | 26  | $^{26}\text{Si}$ & 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |

Notes.

$^a$ The marks appearing in the comments refer to KADoNiS v0.3 (Dillmann et al. 2009); n (not present), t (only theoretical estimate), 30 (only 30 keV MACS), e (measured in the relevant energy range), and * ($X_{\text{lower}} < 0.8$, appearing in Figure 4).

$^b$ $X$ and $f_{\text{SEF}}$ given for the g.s., not the isomeric state, and assuming thermal equilibration of the ground and excited states.

(This table is available in its entirety in a machine-readable form in the online journal. A portion is shown here for guidance regarding its form and content.)
uncertainty was not reduced, even when the rate was measured. For several reactions, only a 30 keV MACS was measured (marked by “30”), and the rates at other temperatures were determined by a renormalized rate prediction. Also listed are purely theoretical rates (marked by “t”) and rates not appearing in KADoNiS v0.3 (marked by “n”).

The table is useful for both astrophysicists and experimentalists and is meant to be interpreted as follows. The maximum possible reduction in theoretical uncertainty can be obtained by inserting the value of \( X \) into Equation (18) for a given reaction. When striving to better constrain reactions experimentally, those with values of \( X \) close to unity should be chosen. If reactions were measured previously, it is possible to better constrain them by measuring with higher precision across the full relevant energy range (see Rauscher 2010). An unmeasured rate will only be constrained by measuring \( \sigma_0 \) if \( X \approx 1 \). At the other extreme, some measured reactions show low \( X \) values (marked by the asterisk). It would be incorrect to assume for these cases that the uncertainty in stellar rates is similar to that of the measurements. Thus, this allows one to assess which reactions presently are well constrained in \( s \)-process calculations.

For a number of reactions, only \( kT = 30 \) keV MACS are directly obtained from experiments whereas the energy dependence is taken from theory. Obviously, this will only constrain stellar rates at 30 keV when \( X \approx 1 \). Although it is usually preferable to obtain a rate from a measurement within the full range of contributing energies, one has to realize that \( X \) may decrease with higher energy, even when it is close to unity at \( kT = 30 \) keV. In such a case, additional measurements above 30 keV may only partially reduce the uncertainty in the rates at higher temperatures. To see how \( X \) changes with energy, values for \( kT = 80 \) keV are also shown in Table 1.

For a better overview, further comparisons of g.s. contributions \( X \) to \((n,\gamma)\) rates at different temperatures are shown in Figures 2 and 3 for the nuclei included in Table 1. The error bars on the \( X \) values were computed as described in Section 2.4. We chose the reference temperature \( kT = 30 \) keV for the \( s \)-process and a high temperature of \( T = 2.5 \) GK, which is typical for explosive nucleosynthesis. As can be seen, the values of \( X \) are smallest in the region of deformed nuclei, where their deviation from the SEF is also the largest. This is because the level density in such nuclei is high, i.e., there are already many excited states at low excitation energies. At \( kT = 30 \) keV, we find \( X \approx 0.16–0.3 \) for several nuclei (with the lowest values of \( X \) = 0.04, 0.16, and 0.2 for \(^{166}\text{Ho}, \(^{193}\text{Pt}, \text{and} \(^{142}\text{Pt}\), respectively) and \( X \approx 0.5–0.8 \) for most nuclei in the mass range \( 150 \leq A \leq 190 \). Although experimental data with small uncertainties exist for most stable nuclei in this mass range (Bao et al. 2000; Dillmann et al. 2006, 2009), the stellar reactivity \( R^* \) is at least partially based on the calculated contribution of excited states. Consequently, the uncertainties in the stellar reactivities \( R^* \) may be much larger than the uncertainties in the g.s. MACS, which are provided in the compilations by Bao et al. (2000) and Dillmann et al. (2006, 2009).

At a glance, Figure 4 provides a guide to which targets are and are not well suited for experimentally constraining the theoretical uncertainties in stellar rates. The filled squares mark nuclei with \( X < 0.8 \) at 30 keV (using the lower limit of \( X \) from the errors discussed in Section 2.4). For neutron captures on these targets, even a complete experimental determination of g.s. rates will not be able to reduce the error from theory by more than 80%, and for even smaller \( X \) values it will not provide an improved rate. The open squares mark nuclei in our set that have \( X \geq 0.8 \) and therefore show cases for which the rate uncertainty mainly stems from experimental uncertainties. If not already measured, they may provide good opportunities for future experiments.

The limit of 80% error reduction was chosen because a significant reduction in the uncertainty from theory is required to achieve the precision desired for \( s \)-process nucleosynthesis. For example, assuming an 80% error reduction in an uncertainty of 30% in the rate predictions (Rauscher et al. 1997), the remaining error stemming from theory will then be on the order of 6%. On the other hand, an 80% reduction of the uncertainty factors of 2–3 in global reaction rate predictions would lead to a theoretical uncertainty in the stellar rate of about 40–60%, coming from uncertainties in the excited-state contributions. In addition, the experimental uncertainty for \( \sigma_0 \) also has to be included. This leads to uncertainties in stellar rates that already may be too large for high-precision \( s \)-process nucleosynthesis models.

Neutron captures and their inverse photodisintegration reactions at high temperatures are also important in the \( \gamma \)-process production of \( p \) nuclei (Woosley & Howard 1978; Rauscher 2006). For that reason, they are also included in KADoNiS (Dillmann et al. 2009). It is apparent from Figure 3 that \( X \) can assume very low values at high temperatures. This indicates that one must be very careful in extrapolating experimental rates from \( s \)-process temperatures (\( T = 0.384 \) GK is \( E = 30 \) keV), e.g., to a typical \( \gamma \)-process temperature of 2.5 GK. This implies an increasing theoretical contribution that is only constrained by experiments if, as pointed out above, the predictions of the ground- and excited-state cross-sections are correlated. Furthermore, although the partition function \( G_0 \) is well determined under \( s \)-process conditions by experimentally known level schemes, higher temperatures (and/or unstable nuclei) imply an increasing uncertainty in \( G_0 \).

### 3.3. Specific Examples

Finally, let us discuss some specific cases in more detail to further illustrate the difference between \( f_{\text{SEF}} \) and \( X \): neutron-capture reactions on \(^{79}\text{Se}, \(^{95}\text{Zr}, \(^{121}\text{Sn}, \(^{187}\text{Os}, \text{and} \(^{199}\text{Pt}\). We focus here on the stellar temperatures \( kT = 8 \) keV and \( kT = \)
30 keV. A temperature of $kT = 30$ keV is often taken as the reference temperature of the s-process (see, e.g., Dillmann et al. 2009). It is close to the typical burning temperature of the $^{22}$Ne(α, n)$^{25}$Mg reaction, which is one of the two neutron sources for the s-process in thermally pulsing AGB stars. The main neutron source in AGB stars is $^{13}$C(α, n)$^{16}$O, which operates at lower temperatures around $kT = 8$ keV. At these relatively low temperatures, the g.s. contribution to the stellar reaction rate factor $R^*$ is already far below unity in some cases. The weak s-process in massive stars operates at higher temperatures, and thus the g.s. contribution $X$ is even further reduced.

The reaction $^{79}$Se(n,γ)$^{80}$Se is an example of a case where $f_{\text{SEF}} < 1$ due to the weak influence of excited states. The nucleus $^{79}$Se has several low-lying levels ($J^\pi = 1/2^-, 95.8$ keV; $1/2^-, 128$ keV) above its $7/2^+$ g.s. (Singh 2002; ENSDF 2010). Because $J_0 = 7/2$ and $J_1 = 1/2$ in the first excited state, its population remains below about 1% up to $kT = 30$ keV, and a similar value is found for the large $J = 9/2$ state at 137.0 keV. This leads to $G_0 = 1.027$, $f_{\text{SEF}} = 0.99$, and $X = 0.98$ at $kT = 30$ keV. Moreover, $^{79}$Se is considered to be an important branching nucleus with a highly temperature-dependent half-life (Takahashi & Yokoi 1987) in the weak s-process. For $kT = 100$ keV, we find $f_{\text{SEF}} = 0.85$ and $X = 0.78$. This means that not only are the excited states more populated ($G_0 = 1.51$), but the captures in these states also impact the resulting stellar rates. Were this not the case, i.e., were the capture cross-sections of $^{79}$Se negligible in the excited states, then $X = 1$ and $f_{\text{SEF}} = 1/G_0 = 0.66$.

The reaction $^{95}$Zr(n,γ)$^{96}$Zr is an example of both $f_{\text{SEF}} < 1$ and $X = 1$ because the excited states are not populated. The first excited state of $^{95}$Zr is located at $E = 954$ keV, with $J^\pi = 1/2^+$. The g.s. has $J^\pi = 5/2^+$ (ENSDF 2010). The SEF and $X$ do not deviate from unity over the entire temperature range of the s-process because $G_0(T) = 1$. Note that there was an earlier claim for a low-lying, first excited state with $J^\pi = (3/2, 5/2)^+$ at 23 keV, but it was only observed in one particular experiment (Frota-Pessôa & Joffily 1986). The existence of such a level was excluded in a later high-resolution experiment (Sonnabend et al. 2003b). There is no evidence of another low-lying state “with quite different angular momentum,” as recently discussed by Huther et al. (2010). Consequently, the state at 23 keV was removed from the adopted levels of $^{95}$Zr (Basu et al. 2010; ENSDF 2010). An experimental determination of the $^{95}$Zr(n,γ)$^{96}$Zr capture cross-section would be extremely valuable because the experimental neutron-capture data completely define the stellar reaction rate. These data are a prerequisite for the understanding of isotopic patterns of zirconium and molybdenum isotopes in meteorites that may be of s-process origin.

The reaction $^{121}$Sn(n,γ)$^{122}$Sn is close to case B in Section 2.2. The g.s. of $^{121}$Sn has a low spin of $J^\pi = 3/2^+$. There is a very low-lying intruder state at $E = 6.3$ keV, with $J^\pi = 11/2^-$, and a further low-J state at $E = 60.3$ keV, with $J^\pi = 1/2^+$. Then, there is a gap in the level scheme up to the next state at $E = 663.6$ keV, which is too high to play a significant role in the s-process (Ohya 2010; ENSDF 2010). At $kT = 8$ keV, the population of the first excited state already exceeds the g.s., and we find a g.s. contribution to the stellar rate of $X = 0.36$. At the reference temperature of $kT = 30$ keV, the rate is further reduced to $X = 0.27$. The SEFs remain close to unity, with $f_{\text{SEF}} = 1.19$ and 1.07 at 8 keV and 30 keV. Because of the dominating contribution from the first excited state, experimental data for the $^{121}$Sn(n,γ)$^{122}$Sn reaction can only provide a minor one-third contribution to the stellar rate.

The reaction $^{187}$Os(n,γ)$^{188}$Os is important for the Re/Os cosmochronometer (Mosconi et al. 2010a, 2010b). The nucleus $^{187}$Os exhibits a very low-lying 3/2− state at 9.8 keV above the 1/2− g.s. The next levels appear at 74.4 keV, 75.0 keV, and 100.5 keV (3/2−, 5/2−, and 7/2−, respectively). Above the level at 117 keV and without spin assignment, the next levels are found at 187.4 keV and 190.6 keV, which are too high for the s-process (Busasia 2009; ENSDF 2010). At $kT = 8$ keV, the SEF is $f_{\text{SEF}} = 1.0$. The first excited state, however, is already populated, and we find a g.s. contribution of $X = 0.63$. At higher energies, the g.s. contribution reduces further to $X = 0.28$ for $kT = 30$ keV, although $f_{\text{SEF}} = 1.19$ remains close to unity. Because of the relevance of this reaction to the Re/Os cosmochronometer, neutron-capture experiments on $^{187}$Os have been performed (see, e.g., Mosconi et al. 2010a; Fujii et al. 2010, and references therein). The importance of the low-lying, first excited state was noticed in that work (Mosconi et al. 2010b; Fujii et al. 2010), and additional experiments on the inelastic neutron scattering of $^{187}$Os and the photodisintegration of $^{188}$Os have been performed (see, e.g., Shizuma et al. 2005; Mosconi et al. 2010b) to study transitions proceeding on this state.

Another example of the importance of including excited-state transitions is $^{193}$Pt(n,γ)$^{194}$Pt. An extremely low-lying 3/2− state at $E = 1.6$ keV is found above the 1/2− g.s. of $^{193}$Pt, and a further low-lying 5/2− state is located at $E = 14.3$ keV. Then, there is a small gap in the level scheme up to the next 3/2− state at $E = 114.2$ keV (Achterberg et al. 2006; ENSDF 2010). At $kT = 8$ keV, the first excited state already dominates the reaction rate factor $R^*$, and the g.s. contribution is only $X = 0.26$. At $kT = 30$ keV, the g.s. contribution drops to $X = 0.16$, and the reactivity $R^*$ is essentially determined by comparable contributions of the states at 1.6 keV and 14.3 keV. Again, as in the previous examples, the SEF remains relatively close to unity, with $f_{\text{SEF}} = 1.22$ at $kT = 8$ keV and $f_{\text{SEF}} = 1.31$ at $kT = 30$ keV. Thus, an experimental determination of the $^{193}$Pt(n,γ)$^{194}$Pt cross-section can be used only to restrict theoretical predictions of the g.s. cross-section. Similar to the above examples of $^{121}$Sn and $^{187}$Os, it is not possible to directly derive the stellar reaction rate from experimental neutron-capture data.

4. SUMMARY

In conclusion, SEFs close to unity should not be interpreted to mean that thermally excited states play only a minor role in stellar reaction rates. The g.s. contribution $X$ to a stellar reaction rate—given by $X = (f_{\text{SEF}} G_0)^{-1}$—may be significantly below 0.5 for target nuclei with low-lying excited states even when $f_{\text{SEF}} \approx 1$. Low values of $X$ indicate that it is impossible to determine the stellar reaction rate directly from experimental neutron-capture data. This should be taken into account in the planning of future neutron-capture experiments, in particular for the extremely difficult experiments on unstable branching nuclei in the s-process. Because of the importance of the g.s. contribution $X$, it will be included in future versions of the KADoNiS database (Dillmann et al. 2006, 2009).

Although $X$ is a theoretical quantity, it was shown that the uncertainties of $X$ remain relatively small for most nuclei in the s-process path, because the partition functions can be calculated from the well-known experimental level scheme for these nuclei. We showed that $X$ is a more useful quantity than the SEF. Experimentalists may still use both $X$ and SEF: the value of $X$
shows whether an experiment measuring g.s. cross-sections or rates contributes to the calculation of stellar rates; the SEF can be used to renormalize the g.s. rate to obtain a stellar rate. Such a renormalization, however, only makes sense when $X$ is close to unity. For modelers performing stellar network calculations, only $X$ provides valuable information. Usually, modelers assume that experimentally known rates are better constrained than theoretical ones or, at least, are constrained within the experimental error. However, this would only be the case for $X = 1$. A low value of $X$ for a reaction indicates that the modeler may allow for a larger uncertainty (e.g., in a rate variation study), using Equation (18) with appropriate experimental and theoretical uncertainties.

Obviously, these findings apply not only to neutron captures but also to any kind of reaction, and in other nucleosynthesis processes. Especially at the high temperatures found in explosive nucleosynthesis, reactions on nuclei in excited states often contribute significantly to stellar rates. Only the g.s. contribution $X$, which can be calculated in the same manner for all types of reactions, allows one to judge whether measurements of reactions on nuclei in the g.s. will be able to put direct constraints on stellar rates.

This work was supported by OTKA (NN83261). I.D. and R.P. are supported by the Helmholtz association in the Young Investigators projects VH-NG-627 and VH-NG-327. T.R. received support from the THEXO work package of the ENSAR project within the European Commission FP7.

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