Prediction of Astrophysical Reaction Rates: Methods, Data Needs, and Consequences for Nucleosynthesis Studies

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Abstract. The majority of nuclear reactions in astrophysics involve unstable nuclei which are not fully accessible by experiments yet. Therefore, there is high demand for reliable predictions of cross sections and reaction rates by theoretical means. The majority of reactions can be treated in the framework of the statistical model (Hauser-Feshbach). The global parametrizations of the nuclear properties needed for predictions far off stability probe our understanding of the strong force and take it to its limit.

The sensitivity of astrophysical scenarios to nuclear inputs is illustrated in the framework of a detailed nucleosynthesis study in type II supernovae. Abundances resulting from calculations in the same explosion model with two different sets of reaction rates are compared. Key reactions and required nuclear information are identified.

INTRODUCTION

Extensive reaction networks have to be employed in the investigation of nuclear energy generation and nucleosynthesis processes in astrophysics. Since stellar and explosive burning involves a considerable number of unstable isotopes which are currently unaccessible by experiments, the prediction of astrophysical reaction rates by means of nuclear reaction theory is unavoidable. There has been progress in the theoretical approaches, especially in the modelling and prediction of specific nuclear properties required for the determination of nuclear reaction rates. However, there is still need for experimental studies testing the predictions and providing more data to further improve theoretical models. After a discussion of statistical model inputs, this will be briefly addressed in the concluding section of the paper.

Considering the still remaining uncertainties in the prediction of nuclear reaction rates, it is of great interest to investigate the sensitivity of abundance yields to variations in the rates. This is also important if one wants to disentangle stellar
physics and nuclear effects in the comparison of models which differ in both aspects. A comparison of two sets of reaction rates by employing them in the same stellar model of [1] is presented in the second part of the paper.

**THE STATISTICAL MODEL**

In general, the cross section will be the sum of the cross sections resulting from compound reactions via an average over overlapping resonances (HF) and via single resonances (BW), direct reactions (DI) and interference terms:

\[
\sigma(E) = \sigma_{HF}(E) + \sigma_{BW}(E) + \sigma_{DC}(E) + \sigma_{int}(E) .
\]

Depending on the number of levels per energy interval in the system projectile+target, different reaction mechanisms will dominate [2]. Since different regimes of level densities are probed at the various projectile energies, the application of a specific description depends on the energy. In astrophysics, one is interested in energies in the range from a few tens of MeV down to keV or even thermal energies (depending on the charge of the projectile). It has been shown [2] that the majority of nuclear reactions in astrophysics can be described in the framework of the statistical model (HF) [3]. This description assumes that the reaction proceeds via a compound nucleus which finally decays into the reaction products. With a sufficiently high level density, average cross sections

\[
\sigma_{HF} = \sigma_{\text{form}} b_{\text{dec}} = \sigma_{\text{form}} \frac{\Gamma_{\text{final}}}{\Gamma_{\text{tot}}}.
\]

can be calculated which can be factorized into a cross section \(\sigma_{\text{form}}\) for the formation of the compound nucleus and a branching ratio \(b_{\text{dec}}\), describing the probability of the decay into the channel of interest compared with the total decay probability into all possible exit channels. The partial widths \(\Gamma\) as well as \(\sigma_{\text{form}}\) are related to (averaged) transmission coefficients, which comprise the central quantities in any HF calculation.

Many nuclear properties enter the computation of the transmission coefficients: mass differences (separation energies), optical potentials, GDR widths, level densities. The transmission coefficients can be modified due to pre-equilibrium effects which are included in width fluctuation corrections [4] (see also [2] and references therein) and by isospin effects. It is in the description of the nuclear properties where the various HF models differ. A choice of what is thought of being the currently best parametrizations is incorporated in the new HF code NON-SMOKER [5], which is based on the well-known code SMOKER [6].

**A REACTION RATE LIBRARY**

Utilizing the NON-SMOKER code, cross sections and reaction rates for reactions with nucleons, \(\alpha\) particles or \(\gamma\) rays in entrance and exit channels, respec-
tively, were calculated for all targets between proton and neutron drip line in the range \(9 < Z < 84\). Tabulated cross sections and rates can be found at http://quasar.physik.unibas.ch/~tommy/reaclib.html. Analytic fits to these rates, along with further information, can be obtained as an electronic file from the authors or on-line from Atomic Data and Nuclear Data Tables. A selection from these fits is published in [7].

In all applications, these rates should be supplemented or replaced with experimental rates as they become available. Such a combination of theoretical and experimental rates is provided, e.g., in the REACLIB compilation. Currently, a new version is being compiled, in which the theoretical rates presented here will be included. Latest information on REACLIB can be found on the WWW at http://ie.lbl.gov/astro.html. Further details on the NON-SMOKER code are presented at http://quasar.physik.unibas.ch/~tommy/reaclib.html.

**REACTION RATE SENSITIVITY OF NUCLEOSYNTHESIS IN TYPE II SUPERNOVAE**

When comparing results from different supernova models one faces the difficulty caused by the fact that it is hard to differentiate between influences of differing reaction rate sets and different stellar physics. We tried to segregate the abundance differences between the two models of [1] (WW95) and [8] (TNH) existing because of the dichotomy of stellar models from those reflecting purely the choice of nuclear physics. For that purpose, hybrid calculations were performed, using the same stellar evolution code as in [1] but with rates from both models. In addition to helping to understand why calculations of the two groups differ, the use of independent rate sets in identical stellar models helps determine the nuclear physics portion of the error bar one should assign to nucleosynthesis studies of this sort. The cause of the differences in the theoretical rates was further investigated, pointing to possibilities for future improvements of rate predictions. In the following, the findings are briefly summarized. A very detailed account of the work can be found in [9].

**The Rate Sets**

The reaction rates utilized in WW95 were those of [10] (WFHZ), TNH used [6] (TAT). As examples, Figs. 1 and 2 show a comparison of the two sets to each other and to experimental values for 30 keV neutron capture and proton capture at \(T_9 = 3\).

Typical differences at astrophysically interesting temperatures are less than a factor of two. There are individual cases, however, where the difference exceeds a factor of 10. Some of the larger differences occur for reactions where scarce experimental information is available and different assumptions were made regarding the photon transmission function, for example, \((\alpha,\gamma)\) reactions on \(Z = N\) nuclei.
Different assumptions were also made about the particle transmission functions, nuclear partition functions, and level densities. More modern and complete data used in the TAT rates makes them superior in cases where the partition function is important. WFHZ used an equivalent square well with empirical reflection factors; TAT used a more detailed optical model. Given the quite different values for, e.g., the neutron and proton transmission function, it is perhaps surprising that the rates differ so little. This is because the relevant temperatures for explosive burning are high. For incident particles in the Gamow window, the deviations in the particle transmission functions are typically smaller than a factor of two. In addition, higher partial waves contribute. A comparison of rates at a lower temperature would have revealed larger discrepancies.

Compared to experiment, both sets of theoretical rates give similar agreement, typically to a factor of two. The standard deviations between the two theoretical sets and cross section data are almost identical. In summary, the two rate sets have comparable merit when compared to experiment. All the authors of this paper agree that the new rate set, the “NON-SMOKER” set, will be preferable to both TAT and WFHZ and will be adopted by both groups (WW and TNH) for future work.
Results and Conclusions

The comparison of the yields obtained with the two reaction rate sets in the WW95 model is shown in Figs. 3 and 4 for a 15 and a 25 $M_\odot$ supernova, respectively.

When the two current rate sets are included in otherwise identical stellar models we find that the nucleosynthesis, with some interesting exceptions, is not greatly changed. For example, only about a dozen (out of 70) stable isotopes in the mass range 12 to 70 have nucleosynthesis that differ by over 20% in two supernovae of 15 $M_\odot$ that use the same rate for $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$. It can, however, be noticed that most of these isotopes - with one exception $^{44}\text{Ti}$ - are products of hydrostatic burning where individual reaction flows are governed by the cross sections involved. Nevertheless, none differ by more than a factor of 1.7. Given the significantly larger differences that exist in individual reaction rates, one may wonder at the robust nature of the final nucleosynthesis. We see three major causes.

First, as the star burns and becomes hotter, the nuclear flow follows the valley of $\beta$ stability making heavier nuclei as it goes. In doing so, it follows the path of least resistance – those reactions having the largest cross section for a nucleon or $\alpha$ particle reacting with a given nucleus. These large cross sections are reasonably well replicated by any calculation, normalized to experiment, that treats the Coulomb barrier and photon transmission function approximately correctly. Large differences...
FIGURE 3. Yield ratios for a 15 $M_\odot$ supernova.

may exist in rate factors for reactions that are in competition, especially a small channel in the presence of a large one, but these small channels are frequently negligible, at least for the major abundances while they can cause larger differences when one is interested in the abundances of trace isotopes, e.g. in isotopic anomalies of meteoritic inclusions.

If one is, however, interested in accurate abundance predictions resulting from these smaller flows in hydrostatic burning stages, these can in most cases only be obtained by improving the reliability of the cross sections (and reaction rates) that determine these weak flows on light and intermediate mass nuclei. As new experimental information becomes available, a continuous improvement is therefore highly warranted.

Second, beyond oxygen burning (nuclei heavier than calcium), nucleosynthesis increasingly occurs in a state of full or partial nuclear statistical equilibrium. There the abundances are given by binding energies and partition functions. As long as the “freeze-out” is sufficiently rapid, individual rates are not so important.

Third, the reaction rates varied here were only those theoretical values from Hauser-Feshbach calculations for intermediate mass nuclei, i.e., nuclei heavier than magnesium. The really critical reaction rates are, for the most part, those below magnesium. These reactions, like e.g., $^{12}$C($\alpha$, $\gamma$)$^{16}$O, govern the energy generation,
FIGURE 4. Yield ratios for a 25 \( M_\odot \) supernova.

major nucleosynthesis, and neutron exposure in the star. The rest are perturbations on these dominant flows.

This is not to say, however, that the nuclear and stellar details of heavy element synthesis are now well understood. Differences in the stellar model may account not just for 20\% variation, but orders of magnitude. That is, uncertainty in stellar physics – especially the treatment of convection and how it is coupled (or not coupled) to the nuclear network – accounts for most of the differences in current nucleosynthesis calculations – provided such calculations use the same nuclear reaction rates below magnesium.

Even in a perfect stellar model though, there will still be interesting nuclear physics issues. Stellar nucleosynthesis is becoming a mature field rich with diverse and highly detailed observational data. The “factor of two” accuracy that was adequate in the past may not do justice to the observations of the future. There are many individual cases where the nuclear physics uncertainty is still unacceptably large. We point out just a few examples for which experimental information would be of interest.
NUCLEAR DATA NEEDS

The suppression of radiative capture reactions into self-conjugate (isospin zero) nuclei is very uncertain. Past Hauser-Feshbach calculations have adopted empirical factors for this suppression. The new NON-SMOKER rates include a significantly improved treatment [11]. $\alpha$-capture reactions, like $^{24}\text{Mg}(\alpha, \gamma)^{28}\text{Si}$, $^{28}\text{Si}(\alpha, \gamma)^{32}\text{S}$, ..., $^{44}\text{Ti}(\alpha, \gamma)^{48}\text{Cr}$, are very important to nucleosynthesis in oxygen and silicon burning. The reaction $^{40}\text{Ca}(\alpha, \gamma)^{44}\text{Ti}$ also directly affects the synthesis of $^{44}\text{Ti}$. Modern accurate determinations of most of the reaction rates are missing (as well as $(p, \gamma)$ reactions into the same nuclei). Measurements here would be most welcome.

The Hauser-Feshbach rates are also only as good as the local experimental rates to which the necessary parameters of the calculation are calibrated. In that regard we would point out the near absence of charged particle reaction rate data for $A > 70$, even for stable nuclei. Charged particle reactions are important, especially on unstable nuclei, at significantly higher atomic weights in the $r$ process and in the $p$ process.

Extended systematics of other nuclear properties, such as level densities (especially around magic nucleon numbers), low energy behavior of the GDR, and optical potentials, would be highly appreciated for stable as well as unstable nuclei.

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