Astrophysical Reaction Rates From Statistical Model Calculations

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Abstract

Theoretical reaction rates in the temperature range $0.01 \times 10^9 \leq T(\mathrm{K}) \leq 10.0 \times 10^9$ are calculated in the statistical model (Hauser-Feshbach formalism) for targets with $10 \leq Z \leq 83$ (Ne to Bi) and for a mass range reaching the neutron and proton driplines. Reactions considered are (n,γ), (n,p), (n,α), (p,γ), (p,α), (α,γ), and their inverse reactions. Reaction rates as a function of temperature for thermally populated targets are given by analytic seven parameter fits. To facilitate comparison with experimental rates, the stellar enhancement factors are also tabulated. Two complete sets of rates have been calculated, one of which includes a phenomenological treatment of shell quenching for neutron-rich nuclei. These extensive datasets are provided on-line as electronic files, while a selected subset from one calculation is given as printed tables. A summary of the theoretical inputs and advice on the use of the provided tabulations is included.

Contents

1 Introduction

Nuclear reaction rates are an essential ingredient for all investigations of nucleosynthetic or energy generating processes in astrophysics. Highly unstable nuclei are produced in such processes which again can become targets for subsequent reactions. Cross sections and astrophysical reaction rates for a large number of nuclei are required to perform complete network calculations which take into account all possible reaction links and do not postulate a priori simplifications. Despite concerted experimental efforts, most of the involved nuclei are currently not accessible in the laboratory and therefore theoretical models have to be invoked in order to predict reaction rates.

In predictions of cross sections and reaction rates for astrophysical applications, slightly different points are emphasized than in pure nuclear physics investigations. Firstly, one is confined to the very low-energy region, from thermal energies up to a few MeV. Secondly, since most of the ingredients for the calculations are experimentally undetermined, one has to develop reliable phenomenological models to predict these properties with an acceptable accuracy across the nuclear chart. This task is made even harder by the lack of information on specific properties, such as optical potentials for α particles at the astrophysically relevant energies even for stable nuclei. Therefore, one has to be satisfied with a somewhat more limited accuracy, as compared to usual nuclear physics standards. The accuracy of the rates is estimated to be within a factor of $1.5-2$, with an even better average deviation, e.g. of 1.4 for neutron capture. Considering the substantially larger uncertainties in many astrophysical scenarios, this seems to be acceptable. Thus, the real challenge is not the application of well-established models, but rather to provide all the necessary ingredients in as reliable a way as possible, also for nuclei where no such information is available. Many efforts have been directed at addressing those problems and the current status of the investigations make it worthwhile to publish a full set of theoretical rates, intended to supersede early reaction rate tabulations [1, 2, 3, 4, 5, 6].

For the majority of nuclear reactions in astrophysics, the statistical model (Wolfenstein-Hauser-Feshbach approach) [7, 8] can be applied. This is appropriate provided the level density in the contributing energy window around the peak of the projectile energy distribution is sufficiently high to justify a statistical treatment. The critical level density is usually estimated between 5 and 10 MeV^{-1} [9]. Furthermore, the compound nucleus picture will only dominate when the energy of the incident particle is low enough ($<$ 20 MeV). While the latter point is practically always satisfied in astrophysical environments, the level density may fall below the critical value in certain nuclei lighter than Fe, at shell closures, and for very neutron-rich or proton-rich isotopes near the drip lines with correspondingly low separation energies. In these cases, single resonances or direct capture contributions will become significant and have to be treated individually. In this tabulation, we are not concerned with such effects but rather give a full set of rates calculated in the statistical model. However, the limits of its applicability will be discussed (Sec. 2.4).

In the following section, we concisely summarize the theoretical background for easy reference as well as the nuclear properties used as input in the calculations. This is followed by a section defining the reaction rates, explaining the fitting procedure and giving more details on the tabulated values. The paper is concluded by a summary and the rate tables.

2 The Statistical Model

2.1 Theory

The averaged transmission coefficients T comprise the central quantities in statistical model calculations. They do not reflect a resonance behavior, but rather describe absorption via an imaginary part in the (optical) nucleon-nucleus potential [10]. This leads to the well-known expression

$$\begin{aligned} \sigma^{\mu\nu}(E_{ij}) &= \frac{\pi\hbar^2/(2\mu_{ij}E_{ij})}{(2J_i^\mu+1)(2J_j+1)} \\ &\times \sum_{J,\pi}(2J+1)\frac{T_j^\mu(E,J,\pi,E_i^\mu,J_i^\mu,\pi_i^\mu)T_o^\nu(E,J,\pi,E_m^\nu,J_m^\nu,\pi_m^\nu)}{T_{\mathrm{tot}}(E,J,\pi)} \end{aligned} \tag{1}$$

for the cross section $\sigma^{\mu\nu}$ of the reaction $i^\mu(j,o)m^\nu$ from the target state i^μ to the excited state m^ν of the final nucleus, with a center of mass energy E_{ij} and reduced mass μ_{ij}. J denotes the spin, E the corresponding excitation energy, and π the parity of excited states. When these properties are used without subscripts they describe the compound nucleus; subscripts refer to states of the participating nuclei in the reaction $i^\mu(j,o)m^\nu$ and superscripts indicate the specific excited states. The total transmission coefficient $T_{\mathrm{tot}}=\sum_{\nu,o}T_o^\nu$ describes the transmission into all possible bound and unbound states ν in all energetically accessible exit channels o (including the entrance channel i). Experiments measure $\sigma^{\rm lab} = \sum_\nu \sigma^{0\nu}(E_{ij})$, summed over all excited states of the final nucleus, with the target in the ground state. Target states μ in an astrophysical plasma of temperature T^* are thermally populated and the astrophysical cross section σ^* is given by

$$\sigma^*(E_{ij}) = \frac{\sum_\mu (2J_i^\mu + 1)\exp(-E_i^\mu/kT^*) \sum_\nu \sigma^{\mu\nu}(E_{ij})}{\sum_\mu (2J_i^\mu + 1)\exp(-E_i^\mu/kT^*)} \quad , \tag{2}$$

k being the Boltzmann constant. The summation over ν replaces $T_o^\nu(E,J,\pi)$ in Eq. (1) by the total transmission coefficient

$$\begin{aligned} T_o(E,J,\pi) \quad &= \quad \sum_{\nu=0}^{\nu_m} T_o^\nu(E,J,\pi,E_m^\nu,J_m^\nu,\pi_m^\nu) \\ &+ \int_{E_m^{\nu_m}}^{E-S_{m,o}} \sum_{J_m,\pi_m} T_o(E,J,\pi,E_m,J_m,\pi_m)\rho(E_m,J_m,\pi_m)dE_m \quad . \end{aligned} \tag{3}$$

Here $S_{m,o}$ is the channel separation energy, and the summation over excited states above the highest experimentally known state ν_m is changed to an integration over the level density ρ. The summation over target states μ in Eq. (2) has to be generalized accordingly.

The important ingredients of statistical model calculations as indicated in Eqs. (1) through (3) are the particle and γ-transmission coefficients T and the level density of excited states ρ. Therefore, the reliability of such calculations is determined by the accuracy with which these components can be evaluated (often for unstable nuclei). It is in these quantities that various statistical model calculations differ. The reaction rates given in this paper are calculated with the code NON-SMOKER [11], derived from the well-known SMOKER code [5]. (The code MOST [12] is another code derived from SMOKER.) In the following we want to briefly outline the methods utilized in that code to estimate those nuclear properties. The challenge is in the goal to provide them in as reliable a way as possible, also for unstable nuclei for which no experimental information is available. Thus, global descriptions are employed which minimize the overall error and are trusted to be reliable also far from stability.

2.2 Transmission Coefficients

The transition from an excited state in the compound nucleus (E,J,π) to the state $(E_i^\mu,J_i^\mu,\pi_i^\mu)$ in nucleus i via the emission of a particle j is given by a summation over all quantum mechanically allowed partial waves

$$T_j^\mu(E,J,\pi,E_i^\mu,J_i^\mu,\pi_i^\mu) = \sum_{l=|J-s|}^{J+s} \sum_{s=|J_i^\mu-J_j|}^{J_i^\mu+J_j} T_{j_{l_s}}(E_{ij}^\mu). \tag{4}$$

Here the angular momentum $\vec{l}$ and the channel spin $\vec{s} = \vec{J}_j + \vec{J}_i^\mu$ couple to $\vec{J} = \vec{l} + \vec{s}$. The transition energy in channel j is $E_{ij}^\mu{=}E - S_j - E_i^\mu$, where S_j is the channel separation energy.

The total transmission coefficients for this tabulation are then calculated by applying Eq. (3) and utilizing up to 19 experimentally known excited states. The data are taken from [13], up to the first level for which the spin assignment was not known. Ground state spin and parities are known for many unstable nuclei. Far off stability, ground state spins and parities are taken from [14], if experimental values are not available.

2.2.1 Particle Transmission Coefficients

The individual particle transmission coefficients $T_{j_{l_s}}$ are calculated by solving the Schrödinger equation with an optical potential for the particle-nucleus interaction. We employ the optical potential for neutrons and protons given by [15], based on microscopic infinite nuclear matter calculations for a given density, applied with a local density approximation. It includes corrections of the imaginary part [16, 17].

The optical potential for α particles from [18] was shown to be quite accurate for a wide range of nuclei and is used in this work. However, it was realized [19, 20] that for heavily charged nuclei a more sophisticated potential had to be adopted at the comparatively low energies of astrophysical interest. Promising is the folding approach [21], with a parameterized mass- and energy-dependence of the real volume integral [22]. Microscopic and deformation information should be considered in the parametrization of the imaginary potential [23]. However, due to the scarcity of experimental data, the potential parameters can as yet only be extracted for a limited mass and energy range. The optical α+nucleus potential is likely to introduce the largest uncertainties in the charged particle rates presented here. Further experimental work is clearly necessary and most welcome.

Deformed nuclei are treated by using an effective spherical potential of equal volume, based on averaging the deformed potential over all possible angles between the incoming particle and the orientation of the deformed nucleus.

2.2.2 Radiative transmission coefficients

At least the dominant γ-transitions (E1 and M1) have to be included in the calculation of the total photon width. The smaller, and therefore less important, M1 transitions are treated, as usual, in the simple single particle approach ($T \propto E^3$ [24]), as also discussed in [2]. The E1 transitions are calculated on the basis of the Lorentzian representation of the Giant Dipole Resonance (GDR). Within this model, the E1 transmission coefficient for the transition emitting a photon of energy E_γ in a compound nucleus ${}^A_N Z$ is given by

$$T_{E1}(E_\gamma) = \frac{8}{3}\frac{NZ}{A}\frac{e^2}{\hbar c}\frac{1+\chi}{Mc^2}\sum_{i=1}^{2}\frac{i}{3}\frac{\Gamma_{G,i}E_\gamma^4}{(E_\gamma^2 - E_{G,i}^2)^2 + \Gamma_{G,i}^2 E_\gamma^2} \quad . \tag{5}$$

Here, M is the proton mass, $\chi(=0.2)$ accounts for the neutron-proton exchange contribution [25], and the summation over i includes two terms which correspond to the split of the GDR in statically deformed nuclei, with oscillations along ($i=1$) and perpendicular ($i=2$) to the axis of rotational symmetry. Many microscopic and macroscopic models have been devoted to the calculation of the GDR energies (E_G) and widths (Γ_G). Here, the (hydrodynamic) droplet model approach [26] is used for E_G, which gives an excellent fit to the GDR energies and can also predict the split of the resonance for deformed nuclei, when making use of the deformation, calculated within the droplet model. In that case, the two resonance energies are related to the mean value calculated by the relations [27] $E_{G,1}+2E_{G,2}=3E_G$, $E_{G,2}/E_{G,1}=0.911\eta+0.089$. η is the ratio of the diameter along the nuclear symmetry axis to the diameter perpendicular to it, and is obtained from the experimentally known deformation or mass model predictions. For the width Γ_G of the GDR the description of [28] is used, which applies to spherical and deformed nuclei and can be described as a superposition of a macroscopic width due to the viscosity of the nuclear fluid and a coupling to quadrupole surface vibrations of the nucleus (see also [6]).

Direct application of Eq. (5) would overestimate the radiation width by about 30% (see e.g. [29, 30]). This is due to the fact that, for low energy γ-transitions, the Lorentz curve is suppressed and the GDR width increases with excitation energy (e.g. [31, 32]). To account for these deficiencies, various treatments of an energy-dependent width have been suggested. We use the form [29]

$$\Gamma_G\left(E_\gamma\right)=\Gamma_G\sqrt{\frac{E_\gamma}{E_G}}\,. \tag{6}$$

Another effect has to be taken into account for certain α-capture reactions. Because of isospin selection rules, γ-transitions between levels with isospin $I=0$ are forbidden. This leads to a suppression of the cross section for (α,γ) reactions on self-conjugate ($N=Z$) targets, due to isospin conservation. A suppression could also be found for capture reactions leading into self-conjugate nuclei, although somewhat less pronounced because $I=1$ states can be populated according to the isospin coupling coefficients. The suppression is usually treated as a suppression of the γ-width. In previous rate tabulations it was either neglected [5] or accounted for in a phenomenological way by dividing the γ-width by quite arbitrary factors [2, 3]. In the code NON-SMOKER the appropriate γ-widths are obtained by explicitly accounting for isospin mixing and suppression of the appropriate γ-transitions [11]. A detailed account of the procedure can be found in [33].

2.2.3 Width fluctuation corrections

In addition to the ingredients required for Eq. (1), like the transmission coefficients for particles and photons, width fluctuation corrections $W(j,o,J,\pi)$ have to be employed. They define the correlation factors with which all partial channels for an incoming particle j and outgoing particle o, passing through the excited state (E,J,π), have to be multiplied. This takes into account that the decay of the state is not fully statistical, but some memory of the way of formation is retained and influences the available decay choices. The major effect is elastic scattering, the incoming particle can be immediately re-emitted before the nucleus equilibrates. Once the particle is absorbed and not re-emitted in the very first (pre-compound) step, the equilibration is very likely. This corresponds to enhancing the elastic channel by a factor W_j. In order to conserve the total cross section, the individual transmission coefficients in the outgoing channels have to be renormalized to T'_j. The total cross section is proportional to T_j and, when summing over the elastic channel ($W_j T'_j$) and all outgoing channels ($T'_{tot} - T'_j$), one obtains the condition $T_j = T'_j(W_j T'_j / T'_{tot}) + T'_j(T'_{tot} - T'_j)/T'_{tot}$ [34]. We can (almost) solve for T'_j

$$T'_j = \frac{T_j}{1 + T'_j(W_j - 1)/T'_{tot}} \quad . \tag{7}$$

This requires an iterative solution for T' (starting in the first iteration with T_j and T_{tot}), which converges rapidly. The enhancement factor W_j has to be known in order to apply Eq. (7). A general expression in closed form was derived [34], but is computationally expensive to use. A fit to results from Monte Carlo calculations gave [35]

$$W_j = 1 + \frac{2}{1 + T_j^{1/2}} \quad . \tag{8}$$

For a general discussion of approximation methods see [36, 37]. Eqs. (7) and (8) redefine the transmission coefficients of Eq. (1) in such a manner that the total width is redistributed by enhancing the elastic channel and weak channels over the dominant one. Cross sections near threshold energies of new channel openings, where very different channel strengths exist, can only be described correctly when taking width fluctuation corrections into account. The width fluctuation corrections of [35] are only an approximation to the correct treatment. However, it was shown that they are quite adequate [38].

2.3 Level Densities

Until recently, the nuclear level density has given rise to the largest uncertainties in the description of nuclear reactions in the statistical model [2, 5, 6]. Implemented in the NON-SMOKER code is a recently improved treatment [9]. It is based on a shifted Fermi-gas formalism [39] with an energy-dependent level density parameter a together with microscopic corrections from nuclear mass models. This leads to improved fits to known level densities in a wide range of masses [9]. More sophisticated Monte Carlo shell model calculations [40], as well as combinatorial approaches (see e.g. [41]), have shown excellent agreement with this phenomenological approach and justified the application of the Fermi-gas description at and above the neutron separation energy.

An in-depth description of the model and its application to astrophysical problems can be found in [9]. Here, we only want to briefly summarize the inputs used for calculating the rates presented in this tabulation. It should be noted that we applied our description throughout the nuclear chart, without relying on experimental level density parameters in specific cases as has been done before [2, 3, 12]. This may lead to locally slightly larger deviations from experiment but it improves the reliability when extrapolating to unknown isotopes.

The microscopic correction and the pairing corrections comprise crucial inputs for the level density formalism used here (see [9] for details). They can be extracted from mass models. There is a choice of several mass models in the NON-SMOKER code. The Finite Range Droplet Model (FRDM) [42] and an extended Thomas-Fermi approach with Strutinski Integral (ETFSI-Q) [43] have been chosen for the reaction rate calculations in this work. It has to be emphasized that experimental mass values [44] were included where possible. This is straightforward for the separation energies which were calculated from the mass differences; it was ensured that either only experimental or theoretical values were used in the differences, thus avoiding unphysical breaks at transition points from experiment to theory. The microscopic corrections were obtained by subtracting the well-defined spherical macroscopic (droplet) term of the FRDM from the total mass energy derived from experiment, from the FRDM or from ETFSI-Q, respectively (cf. Eq. (17) in [9]). The validity of the resulting rates is discussed in Sec. 3.3. Rates based on other mass models can be obtained from the authors on request or on-line (see Sec. 4).

The shifted Fermi-gas approach diverges for $U = E - \delta = 0$ (i.e. $E = \delta$, if δ is a positive backshift, with E being the excitation energy and δ being an energy shift due to pairing corrections). In order to obtain the correct behavior at very low excitation energies, the Fermi-gas description can be combined with the constant temperature formula ([39]; [36] and references therein)

$$\rho(U) \propto \frac{\exp(U/T_{\mathrm{nucl}})}{T_{\mathrm{nucl}}} \quad . \tag{9}$$

The two formulations are matched by a tangential fit determining the nuclear temperature T_{nucl}.

2.4 Applicability of the Statistical Model

The statistical model can be applied provided that the use of averaged transmission coefficients (Eq. (4)) is permitted. This will be the case for high level densities with completely overlapping resonances, typical for the compound nucleus reaction mechanism. For light nuclei, decreasing particle separation energies or at shell closures, level densities will eventually become too low for the application of the statistical model at astrophysical temperatures. In those cases, single resonances and contributions from the direct reaction mechanism have to be taken into account [45]. Based on the level density description outlined in Sec. 2.3, a quantitative criterion for the applicability was derived recently [9]. In the present work we give tables of all reaction rates regardless of applicability but specify the allowed temperature range in the tables. The estimate is quite conservative and thus the rates can still be accurate slightly below the given lower limits of the temperature.

3 Astrophysical Reaction Rates

3.1 Definition

The nuclear reaction rate per particle pair at a given stellar temperature T^* is determined by folding the reaction cross section $\sigma^*(E)$ from Eq. (2) with the Maxwell-Boltzmann velocity distribution of the projectiles [46]

$$\langle\sigma^* v\rangle = \langle\sigma v\rangle^* = \left(\frac{8}{\pi\mu}\right)^{1/2} \frac{1}{(kT^*)^{3/2}} \int_0^\infty \sigma^*(E) E \exp\left(-\frac{E}{kT^*}\right) dE \quad . \qquad (10)$$

It has to be emphasized that only the use of the stellar cross section σ^* (Eq. (2)) yields a reaction rate with the desired behavior that the inverse reaction can be calculated by using detailed balance. Therefore, laboratory rates – which only measure $\sigma^{\mathrm{lab}} = \sum_\nu \sigma^{0\nu}$, i.e. the cross section with the target being in the ground state – should always be measured in the direction that is least affected by excited target states. This is usually the reaction with positive Q-value (exoergic reaction). For astrophysical applications, such rates have to be corrected for the stellar enhancement effect due to the thermal excitation of the target [1]. The stellar enhancement factors (SEF) f^* are defined by

$$f^* = \frac{\sigma^*}{\sigma^{\mathrm{lab}}} \quad . \qquad (11)$$

The values of $f^*$for a range of temperatures for nuclei close to stability are given in the tables. Stellar enhancement factors for neutron capture reactions and a discussion of the involved uncertainties can also be found in a recent compilation of neutron cross sections for the s process [47].

3.2 Partition functions and reverse rates

The temperature-dependent partition function $G(T^*)$ normalized to the ground state target spin J_i^0 is defined as [48]

$$\begin{aligned}(2J_i^0+1)G(T^*) = \quad & \sum_{\mu=0}^{\mu_m}(2J_i^\mu+1)e^{-E_i^\mu/kT^*} \qquad (12) \\ & + \int_{E_i^{\mu_m}}^{E_i^{\mathrm{max}}} \sum_{J^\mu,\pi^\mu}(2J^\mu+1)e^{-\epsilon/kT^*}\rho(\epsilon,J^\mu,\pi^\mu)d\epsilon \quad ,\end{aligned}$$

with ρ being the level density and μ_m the last included experimentally known state. The included experimental levels were the same as for the calculation of the transmission coefficients (Eq. (3)). For the temperature range considered here, the maximum energy $E_i^{\max}$ above which there are no more significant contributions to the partition function is of the order of $20-30$ MeV. With that definition, the stellar reaction rate $\langle\sigma_i v\rangle^*$ for a reaction with particles in all channels is related to the rate of the reverse reaction $\langle\sigma_m v\rangle^*$ by

$$N_A \langle\sigma_m v\rangle^* = \left(\frac{A_i A_j}{A_o A_m}\right)^{3/2} \frac{(2J_i+1)(2J_j+1)}{(2J_o+1)(2J_m+1)} \frac{G_i(T^*)}{G_m(T^*)} e^{-Q/kT^*} N_A \langle\sigma_i v\rangle^* \quad , \tag{13}$$

where N_A is Avogadro's number, J and A are spins and masses A (in atomic mass units u) of the particles involved in the reaction $i(j,o)m$, Q is the reaction Q-value. To calculate photodisintegration rates from capture rates the appropriate relation is

$$\lambda_\gamma = \left(\frac{A_i A_j}{A_m}\right)^{3/2} \frac{(2J_i+1)(2J_j+1)}{(2J_m+1)} \frac{G_i(T^*)}{G_m(T^*)} (T^*)^{3/2} F e^{-Q/kT^*} N_A \langle\sigma_i v\rangle^* \quad . \tag{14}$$

For λ_γ in s^{-1} and using the usual practical units, i.e. temperatures $T_9 = T^*/10^9$ K and $N_A \langle\sigma v\rangle^*$ in cm^3 s^{-1} mole^{-1}, one obtains

$$(T^*)^{3/2} F = \left(\frac{ukT^*}{2\pi\hbar^2}\right)^{3/2} \frac{1}{N_A} = T_9^{3/2} 9.8685\times 10^9 \mathrm{mole\,cm}^{-3} \quad . \tag{15}$$

The numerical factor F as well as the spin and mass factors are already accounted for in the parameter a_0^{rev} which is tabulated. See Sec. 3.3.2 for further details.

In the tabulated rates, the thermal effects are already considered. Statistical model calculations not including full photon cascades may also be prone to some error arising from the decay of unbound particle states in reactions with negative Q-values (endoergic reactions). Furthermore, due to the exponential dependence of the inverse rate on the Q-value (Eqs. (13) and (14)), inaccuracies in the rate would be strongly enhanced when computing the exoergic rate from the endoergic one. In order to minimize the error, reactions are always calculated in the exoergic direction (with the exceptions of capture reactions, where photodisintegration is always treated as the reverse reaction regardless of Q-value) and detailed balance is applied to obtain the values for the endoergic reaction. This treatment has the additional advantage that it ensures consistent values for forward and reverse reactions, which is essential for application in astrophysical nuclear reaction networks. To calculate the actual (endoergic) reaction rate, those fits have to be multiplied by the ratio of the partition functions of the final nucleus and the target G_i/G_m at the appropriate temperature (see Sec. 3.3.2 and Sec. 3.3.6). For that purpose, partition functions are tabulated separately.

3.3 Analytic reaction rate fits

3.3.1 Parametrization

Reaction rates have been calculated for a temperature grid of 24 temperatures: T_9=0.1, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0. For easy application in astrophysical investigations, all reaction types ((n,γ), (n,p), (n,α), (p,γ), (p,n), (p,α), (α,γ), (α,n), (α,p), (γ,n), (γ,p), (γ,α)) are fitted with the same parametrization

$$\left.\begin{array}{c} N_A \langle \sigma v \rangle^* \\ \lambda_\gamma \end{array}\right\} = \exp\Big(a_0 + a_1 T_9^{-1} + a_2 T_9^{-1/3} + a_3 T_9^{1/3} + a_4 T_9 + a_5 T_9^{5/3} + a_6 \ln T_9\Big) \quad , \tag{16}$$

with the seven open parameters $a_0 - a_6$ and the stellar temperature T_9 given in 10^9 K. This parametrization proves to be flexible enough to accommodate the different temperature dependencies of the various reaction types across the fitted temperature range of $0.01 \leq T_9 \leq 10$. Parametrizations of the present rates in the form used in [2] and others can be obtained from the authors on request.

3.3.2 Parameters for the reverse rates

The parameters for the reverse rates are not given explicitly but can easily be computed from the information in the tables. To calculate the reverse rate of the reaction $i(j,o)m$, i.e. the reaction $m(o,j)i$, Eq. (16) is employed and the seven parameters $a_0^{\mathrm{rev}} - a_6^{\mathrm{rev}}$ for the reverse rate are determined as follows:

$$\begin{aligned} a_0^{\mathrm{rev}} &= a_0^{\mathrm{rev}}, \quad \text{as tabulated} \\ a_1^{\mathrm{rev}} &= a_1 - 11.6045Q \\ a_2^{\mathrm{rev}} &= a_2 \\ a_3^{\mathrm{rev}} &= a_3 \\ a_4^{\mathrm{rev}} &= a_4 \\ a_5^{\mathrm{rev}} &= a_5 \\ a_6^{\mathrm{rev}} &= \begin{cases} a_6 + 1.5 & \text{(i)} \\ a_6 & \text{(ii)} \end{cases} \end{aligned} \tag{17}$$

The above relations are derived from Eqs. (13) and (14), using Eq. (16) and taking the logarithms on both sides. For the coefficient a_6^{rev}, case (i) applies when calculating a photodisintegration rate from a capture rate, case (ii) for all other rates. Finally, for the reverse reaction case, *the value found by application of Eqs. (16) and (17) has to be multiplied by the ratio of the partition functions for residual and target nucleus G_i/G_m*. Examples are shown in Sec. 3.3.6.

3.3.3 Fit accuracy

The flexibility of the fitting function makes it prone to numerical problems outside the calculated range at low temperatures, where the rates should be close to zero. In some cases they tend to diverge strongly. This difficulty can be avoided by providing fit data at low temperatures additionally to the calculated values by appropriately extrapolating the rates to lower temperatures. This is achieved by either assuming s-wave capture for $T_9 < 0.1$ for exoergic neutron capture reactions (Maxwellian averaged capture cross sections in the energy range $5 \leq E \leq 100$ keV for targets along the line of stability can be found in another compilation [47]) or by considering proper Coulomb barrier penetration factors in the charged particle channels. Thus, both accuracy and flexibility can be ensured within a single parametrization. However, it has to be emphasized that *the given parameterization is only valid within the temperature range of* $0.01 \leq T_9 \leq 10.$, although many fits will show "proper" behavior down to lower temperature. Caution is advised when using derived (γ,p) and (γ,n) rates at the proton dripline (see below). For all cases, it is recommended to use the fits only down to the temperature $T_{\rm low}^{\rm fit}$ given in the table. The temperatures of the validity of the fits are given in the tables for each reaction, to emphasize the importance of the given fit ranges.

As a measure of the accuracy of a given fit, the quantity ζ is quoted in the tables. It is defined by

$$\zeta = \frac{1}{24}\sum_{i=1}^{24}\left(\frac{r_i - f_i}{f_i}\right)^2 \quad , \tag{18}$$

with r being the original rate value as calculated at each of the 24 temperatures $T_9 =$ 0.1, 0.15 ... 10.0, and f the rate calculated from the fit at these temperatures. Contributions with $r < 10^{-20}$ cm^3 s^{-1} mole^{-1} are neglected as lower accuracy at at low rates is inconsequential. Note that while a small value of ζ is indicative of an accurate fit over the entire temperature range, large ζ generally signify deviations of the calculated from the fitted rate at the lowest temperatures only.

The fit parameters are tabulated regardless of the validity of the statistical model of nuclear reactions in the given temperature range (see Sec. 2.4). The estimated lower temperature limit of the validity of the statistical model, $T_{\rm low}^{\rm HF}$ is given separately for each rate in the tables. Below that limit the calculation of the rate by means of the statistical model may not be justified, although the fit to the calculated rate will still be accurate. At temperatures below the applicability limit, rates may be over-estimated and should be compared to calculations considering single resonance and direct reaction contributions. Especially close to the driplines, fits of reactions with low Q-value cannot be applied at low temperatures. Although the fit may be valid, it should not be used at low temperature because the statistical model will not be applicable anymore.

3.3.4 Computed rate sets

Two different sets of rates have been calculated. They differ in the mass model used, which enters into the computation of the separation energies and Q-values as well as into the microscopic input to the level density calculation (see Sec. 2.3). One set was calculated employing the well-known FRDM mass model [42], which excellently reproduces masses and other ground state properties of nuclei close to stability. It is also the most comprehensive set across the nuclear chart.

Recently, it was suggested that so-called shell quenching effects may arise for neutron-rich nuclei far off stability [49, 50]. Fully microscopic calculations [51, 52] and experimental data [53, 54, 55, 56] indicate the weakening of nuclear shell gaps for neutron-rich nuclei. In the absence of microscopic calculations of the required nuclear properties for the whole nuclear chart, it is possible to phenomenologically include such quenching into existing mass formulae. This has been done in the ETFSI-Q model [43], based on the ETFSI-1 mass model [57, 58]. However, it does not cover the full range of isotopes. Therefore, we provide the alternative sets of reaction rates obtained with the two mass models, so that the rates based on the FRDM can be used for large-scale studies and close to stability, and the rates based on ETFSI-Q for investigations concerning neutron-rich unstable isotopes and the r process. It has to be noted that one should refrain from mixing rates from the two sets as this will lead to inconsistencies and artificial effects in the results.

3.3.5 Mass ranges of the tabulated fits

Due to the extensive number of nuclear reactions in the considered mass range, we have to limit the printed version of our reaction rate fits. Full rate libraries both for reactions calculated with the FRDM and with the ETFSI-Q (as well as ETFSI-1) mass model can be obtained on-line or from the authors on request (see Sec. 4). In the printed version, only the FRDM set is given and no capture rates for reactions with negative Q value are shown.

The full electronic versions of the tables available on-line include all reactions in the range $10 \leq Z \leq 83$ (FRDM) and $24 \leq Z \leq 83$ (ETFSI-Q). This amounts to 5369 (FRDM) and 4628 (ETFSI-Q) involved nuclei. The isotope ranges for which rate fits are available are given in Table A; for the FRDM, the mass range is also indicated by the heavy lines in Tables IA-IC. Rate fits are given for all n-, p-, and α-capture reactions and for those (n,p), (n,α), (p,n), (p,α), (α,n), and (α,p) reactions having positive Q-value. Reverse rates are not given explicitly but can be computed by a two-step procedure as described in Secs. 3.3.2 and 3.3.6. The stellar enhancement factors close to stability as well as the partition functions for all isotopes are given for a temperature grid of 24 temperatures: $T_9 = 0.1, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0$.

The printed Tables II−IV contain the following (calculated with the FRDM mass model):

- (n,γ) rate fits from stability to close to the neutron dripline in the range

$10 \leq Z \leq 49$, and to $N = Z + 59$ for $50 \leq Z \leq 83$ (Table II).

- (n,p) and (n,α) rate fits around stability in the range $10 \leq Z \leq 83$ (Table II).
- (p,γ), (p,n), (p,α), (α,γ), (α,n), and (α,p) rate fits from proton-rich nuclei to stability in the range $10 \leq Z \leq 50$ (Tables III and IV).
- Reverse (endoergic) rates are not given explicitly but can be computed with the help of partition functions from the information given in the tables (see Secs. 3.3.2, 3.3.6).
- Stellar enhancement factors f^* at selected 16 temperatures are only quoted close to the valley of stability (Tables II−IV).
- Partition functions for all involved isotopes are given at selected 20 temperatures in the range $0.1 \leq T_9 \leq 10$ (Table V).

An overview of the provided rates is given in Tables IA−IC, which show in detail for which n-, p-, and α-induced reactions rate fit parameters are available in Tables II−IV, respectively.

3.3.6 Examples of use of tables

This section is intended to help with interpreting the information given in the tables. We give two examples for calculating the reaction rate for a given reaction and its inverse reaction at a temperature of $T_9 = 2.0$.

The first example is the capture reaction ^{35}Ar(p,γ)^{36}K. From Table III one finds a Q-value of $Q = 1.666$ MeV and the parameters a_0 =128.39, $a_1 = -4.0033$, $a_2 = 137.67$, $a_3 = -276.87$, a_4 =17.691, $a_5 = -1.0728$, a_6 =123.68. With the help of Eq. (16) one calculates $N_A \langle\sigma v\rangle^* = 92.5$ cm^{3}s^{-1}mole^{-1} at $T_9 = 2.0$. Because both $T_{\rm low}^{\rm HF}$ and $T_{\rm low}^{\rm fit}$ are considerably smaller than our temperature T_9, it is safe to assume that the statistical model is applicable and the fit to the rate is valid. In order to obtain the value for the reverse rate, one first has to determine the parameter values in the given parametrization. The parameter $a_0^{\rm rev} = 151.83$ is given in the table. The remaining parameters are derived according to Eq. (17) for a photodisintegration rate. This yields $a_1^{\rm rev} = -23.3364$, $a_6^{\rm rev} = 125.18$; all other parameters assume the same value as for the forward reaction. Using those, Eq. (16) gives a value of $\lambda_\gamma{}' = 2.5\times10^8$ s^{-1}. This has to be multiplied by the ratio of the partition functions in order to obtain the valid rate factor for ^{36}K(γ,p)^{35}Ar:

$$\lambda_\gamma = \lambda'_\gamma \frac{G_{^{35}\rm Ar}}{G_{^{36}\rm K}} = \lambda'_\gamma \frac{1.001}{1.203} = 2.1 \times 10^8 \quad {\rm s}^{-1}.$$

The values of the partition functions at $T_9 = 2.0$ were taken from Table V. Note that for capture rates the procedure is always the same as described above regardless of whether it is an exoergic or an endoergic reaction.

The second example we consider is the reaction ^{34}S(α,n)^{37}Ar, again at $T_9 = 2.0$. It is not to be found in Table IV because of its negative Q-value. Therefore, one has to rely on Table II to calculate this reaction as the inverse reaction of ^{37}Ar(n,α)^{34}S. The parameters found in Table II are a_0 =20.072, $a_1 = -0.019613$, $a_2 = 1.8224$, $a_3 = -4.759$, a_4 =0.56437, $a_5 = -0.033893$, a_6 =1.7801, and $Q = 4.63$ MeV. Again, both $T_{\rm low}^{\rm HF}$ and $T_{\rm low}^{\rm fit}$ are lower than the temperature of interest. The rate $N_A \langle\sigma v\rangle^* = 5.2 \times 10^7$ cm^{3}s^{-1}mole^{-1} for ^{37}Ar(n,α)^{34}S results from the direct application of Eq. (16). In order to calculate the rate of ^{34}S(α,n)^{37}Ar, the parameters are determined by application of Eq. (17). This yields the value $a_1^{\rm rev} = -53.748448$. The value of $a_0^{\rm rev} = 20.199$ is taken from the table and all other parameters remain the same as for the forward reaction. With Eq. (16) one arrives at the rate value $r' = 1.272 \times 10^{-4}$ cm^{3}s^{-1}mole^{-1} at $T_9 = 2.0$. Multiplying this by the appropriate ratio of partition functions taken from Table V yields the final result

$$N_A \langle\sigma v\rangle^* = r' \frac{G_{^{37}\rm Ar}}{G_{^{34}S}} = r' \frac{1.0}{1.0} = 1.27 \times 10^{-4} \quad \rm cm^3 s^{-1} mole^{-1}.$$

4 Summary

Thermonuclear reaction rates for neutron-, proton- and α-induced reactions and their inverses have been calculated in the statistical model. All rates from the proton dripline to the neutron dripline for $10 \leq Z \leq 83$ (Ne to Bi) have been fitted to a unique function with seven free parameters. Tables of these parameters are provided on-line for two sets of rates, calculated with input from two different mass models. Furthermore, the stellar enhancement factors are given in order to facilitate comparison with experimental ground state rates. A printed subset of the on-line tables for the FRDM presented here shows fit parameters for (n,γ) and (p,γ) reactions from close to their respective driplines to stability, and for other n-, p-, and α-induced reactions with positive Q-values near stability. A prescription on deriving rates for inverse reactions with negative Q-values is given, as is a listing of the necessary partition functions.

It should further be noted that only purely theoretical rates are given here which do not use any direct experimental information (except for nuclear masses and excited state information where available). The methods to predict nuclear properties needed in the statistical model calculations are chosen to be as reliable as possible in order to retain predictive power. This is a compromise which may lead to locally enhanced inaccuracies but it emphasizes the importance of reliable predictions of rates far off stability.

In real 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. Latest information on the current version of REACLIB can be found on the WWW at *http://ie.lbl.gov/astro.html*. Further details on the NON-SMOKER code and the cross section and reaction rate calculations are presented at *http://quasar.physik.unibas.ch/~tommy/reaclib.html*. Rates including further mass models can also be obtained from the authors on request or directly at the latter URL.

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5 Explanation of Tables

Table IA: Neutron-Induced Reaction Rates Available in Table II

This is an overview of which neutron-induced reaction rates are available in the printed and the online versions. The full lines delimit the range of rates in the electronic version as given in Table A for the FRDM. The entries at a single neutron and proton number specify the reactions on the given target nucleus listed in the printed Table II. Only reactions with positive Q-value are shown. In addition to the marked rates, their reverse rates (with negative Q-value) can be inferred from the information in Table II as explained in Sec. 3.3.2. The reactions are denoted as follows:

G	(n,γ)
P	(n,p)
A	(n,α)

The box at the lower left corner gives the location in the Z, N plane of the final nucleus relative to the target nucleus for (n,γ), (n,p), and (n,α), thereby specifying also the inverse reaction fits derivable from Table II.

Table IB: Proton-Induced Reaction Rates Available in Table III

Same as Table IA but for proton-induced reactions. The marked reactions correspond to the entries in Table III. The reactions are denoted as follows:

G	(p,γ)
N	(p,n)
A	(p,α)

The box at the lower left corner gives the location in the Z, N plane of the final nucleus relative to the target nucleus for (p,γ), (p,n), and (p,α), thereby specifying also the inverse reaction fits derivable from Table III.

Table IC: Alpha Particle-Induced Reaction Rates Available in Table IV

Same as Table IA but for α-particle induced reactions. The marked reactions correspond to the entries in Table IV. The reactions are denoted as follows:

G	(α,γ)
N	(α,n)

P (α,p)

The box at the lower left corner gives the location in the Z, N plane of the final nucleus relative to the target nucleus for (α,γ), (α,n), and (α,n), thereby specifying also the inverse reaction fits derivable from Table IV.

Table II: Neutron-Induced Reaction Rates

Fits to stellar rates $N_A \langle\sigma v\rangle^*$ for (n,γ), (n,p), (n,α) reactions, calculated including masses from the FRDM. The rates in cm^3 mole^{-1} s^{-1} are computed by the use of Eq. (16), with the temperature given in units of 10^9 K. The fits are valid in the temperature range $T_{\rm low}^{\rm fit} < T_9 \leq 10$, with $T_{\rm low}^{\rm fit}$ given in the table. It should be noted that while the fit may still be formally valid and accurate, the application of the statistical model may not be justified at low temperatures. An estimate for the applicability of the statistical model is given by $T_{\rm low}^{\rm HF}$. The following information is provided:

Target — Reaction target

Reaction — Reaction type and final nucleus

Q — Reaction Q-value

$J_{\rm i}$ — Target ground state spin (same as in Table V)

$J_{\rm f}$ — Final nucleus ground state spin (same as in Table V)

$T_{\rm low}^{\rm HF}$ — Estimate of the lower temperature limit for the applicability of the (Hauser-Feshbach) statistical model; "n.c." indicates that the limit was not calculated for the given reaction.

$T_{\rm low}^{\rm fit}$ — Lower temperature limit for the fit; usually 0.01. Note that the fits give extrapolated rates below $T_9 = 0.1$, which may be less accurate, especially if they are very small.

Dev — Fit accuracy ζ (Eq. (18))

SEF — If the field is blank, the seven fit parameters below are followed by the stellar enhancement factors (SEF) f^* (Eq. (11)) at the 16 temperatures given in the head of the table.
A value of 1 indicates that all SEF are unity; no SEF are printed.
A value of 0 indicates that no SEF were calculated.

$a_0 \ldots a_6$ — Seven fit parameters for the forward rate

$a_0^{\rm rev}$ — First parameter for the reverse rate fit (see Sec. 3.3.2)

$T_9^{\rm SEF}$ — Temperatures at which the SEF were calculated

Table III: Proton-Induced Reaction Rates

Same as Table I for the reaction types (p,γ), (p,n), (p,α).

Table IV: Alpha Particle-Induced Reaction Rates

Same as Table I for the reaction types (α,γ), (α,n), (α,p).

Table V: Partition functions

Partition functions of isotopes for various temperatures calculated with a level density making use of FRDM input. Included are only those partition functions for nuclei involved in the reactions given in Tables II−IV.

Nuc — Isotope for which the partition functions are tabulated.

T_9 — Temperature (in 10^9 K) at which the partition functions have been calculated.

P — A value of 1 indicates that all partition function are unity; no partition functions are then printed explicitly.

Spin — Ground state spin of nucleus, either from experiment [44] or from theory [14].

Partition Functions: — Partition functions normalized to the ground state (Eq. (12)) for the 20 temperatures specified in the table header.

Table 1: This table lists the isotope range of the full rate tables which are available electronically. Given are the charge number Z of a target and the lower and upper limits $N_{\rm min}$ and $N_{\rm max}$ of the neutron number in the isotopic chain.

	FRDM		ETFSI-Q			FRDM		ETFSI-Q	
Z	$N_{\rm min}$	$N_{\rm max}$	$N_{\rm min}$	$N_{\rm max}$	Z	$N_{\rm min}$	$N_{\rm max}$	$N_{\rm min}$	$N_{\rm max}$
8	5	10			47	41	113	41	111
9	5	28			48	42	115	42	112
10	5	31			49	43	117	43	113
11	6	33			50	44	119	44	114
12	7	35			51	46	121	46	115
13	8	38			52	47	124	47	124
14	8	40			53	48	126	48	126
15	8	42			54	49	128	49	128
16	8	44			55	51	130	51	130
17	9	46			56	52	133	52	132
18	9	49			57	53	135	53	133
19	10	51			58	55	137	55	134
20	10	53			59	56	139	56	135
21	11	55			60	58	141	58	136
22	12	58			61	59	144	59	137
23	13	60			62	61	146	61	138
24	14	62	18	62	63	62	148	62	139
25	15	64	18	64	64	64	150	64	150
26	16	66	19	66	65	65	153	65	152
27	17	69	19	67	66	67	155	67	154
28	18	71	20	68	67	69	157	69	155
29	19	73	21	69	68	70	159	70	156
30	21	75	22	70	69	72	161	72	157
31	22	77	23	71	70	73	164	73	158
32	23	80	24	72	71	75	166	75	159
33	24	82	25	73	72	77	168	77	160
34	25	84	26	84	73	78	170	78	161
35	26	86	27	86	74	80	173	80	162
36	27	88	28	88	75	81	175	81	163
37	29	91	29	89	76	83	177	83	177
38	30	93	30	90	77	85	179	85	179
39	31	95	31	91	78	87	182	87	182
40	32	97	32	97	79	88	184	88	184
41	33	99	33	99	80	90	186	90	186
42	35	102	35	102	81	92	188	92	188
43	36	104	36	104	82	93	191	93	191
44	37	106	37	106	83	95	193	95	193
45	38	108	38	108	84	98	193	98	193
46	40	110	40	110	85	101	195	101	195