Radiative neutron capture reaction rates for nucleosynthesis:
The creation of the first r-process peak

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Abstract. In neutron star merger events, the occurrence of rapid neutron capture process (r-process) has been established. About half of the elements beyond iron are synthesised in stars by r-process. In stellar environments, very high neutron flux in a short time (\(\sim\) a few seconds) can be attained, leading to the creation of progressively neutron-rich nuclei until the waiting point is reached. At this point, further neutron capture reactions cannot happen and highly neutron-rich nuclei become stable via \(\beta^-\) decay. A detailed understanding of the r-process remains illusive. In the present work, the theoretical predictions of radiative neutron capture \((n, \gamma)\) cross-sections of astrophysical importance and the reaction rates using the Hauser–Feshbach statistical model formalism have been investigated for Fe, Co, Ni, Cu, Zn, Ga, Ge, As and Se isotopes (around the first r-process peak near mass \(= 80\)). These calculations have been compared with the JINA REACLIB reaction rates. The inherent uncertainties remain large in neutron-rich nuclei. When there is low-energy enhancement, a significant increase in the reaction rate occurs for neutron capture.

Keywords. Binding energies and masses; r-process; \((n, \gamma)\) cross-sections; level density; nucleosynthesis.

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1. Introduction

The nucleosynthesis via rapid neutron capture process (r-process) occurring in astrophysical environment is regarded as carrying the load of producing nearly half of the heavy elements present in nature. This broad-spectrum problem poses a great challenge for physics. The properties of nuclei like masses, neutron capture and \(\beta^-\)-decay rates along with \(\beta^-\)-delayed neutron emission probabilities are crucial physical quantities which are required for calculating r-process nucleosynthesis. While nuclear properties in the neighbourhood of stability are well known, much remains to be explored in the domain of neutron-rich nuclei far away from the stability line which may aid the r-process. The studies of sensitivity ascertain the response of a change in nuclear physics input(s). It facilitates the fixing of critical nuclear properties that decide the observed final elemental abundances in nature.

The recognition of locations responsible for the synthesis of heavy elements [1,2] is a matter of great interest in astrophysics. It is well known for decades that the nuclear abundances in our solar system of elements which are heavier than iron can be divided into two major processes that synthesise them. In the slow neutron capture process (s-process), substantial time elapses for the \(\beta^-\)-decay to follow before capturing another neutron. This process produces nuclei around the line of stability. On the contrary, rapid neutron capture process (r-process) is rather fast in time-scale, producing nuclei on the neutron-rich side of the valley of stability. There also exists another process called the proton capture process (p-process) that primarily produces elements with low abundances on the proton-rich side [3,4]. While the basic physics [5] of the s-process [6] and heavy p-process [7,8] is better understood and astrophysical locations well identified, the same is not true in the case of the r-process [9–11].

In principle, by subtracting the p- and s-process contributions [12,13] from the solar system abundances, the r-process pattern can be extracted which consists of three predominant peaks in the abundances at mass numbers \(\sim 80, 130\) and 195, linked with the neutron magic numbers 50, 82 and 126. In order to produce the heaviest r-process elements, of the order of 100 neutrons per seed nucleus are necessary. Additional constraints arise from observations of r-process elements in old stars in the galactic halo [14,15] and meteoritic
data [16]. These data point towards specific origins for the r-process nuclei of light mass number $<120$ and heavy mass number $>120$. The distribution of main r-process elemental abundances is much the same among r-process-enhanced halo stars and is similar to the residuals of the solar system. This is indicative of the fact that since early galactic times [17–20], identical process that operates in a consistent manner created these elements. Though the time-scale argument is obeyed by the core-collapse supernovae, the promise of early studies [21,22] is yet to be achieved by the simulations [23–26] of recent times. The neutron star mergers cause low-temperature outflows which are highly neutron-rich [27–31] and due to fission recycling [32,33] have consistent abundance pattern. But mergers suffer from time delay [34] uncertainty. Other major astrophysical sites explored comprise hot accretion disk outflows from the mergers of neutron stars or neutron star-black hole [30,31,35,36], supernova neutron-rich jets [37–39], γ-ray burst collapsar outflows [40–42], shocked surface layers of O–Ne–Mg cores [43,44] and neutrino-induced nucleosynthesis in the helium shell of exploding massive stars [45].

The aforementioned astrophysical objects are governed by definitive environments such as initial composition, temporal distribution of density and temperature and neutron-richness which lead to elemental abundances that are unique and bear the signatures of these conditions. In principle, about $10^{24}$ free neutrons per cm$^3$ are required at temperatures in the range of $10^9$ K ($T_0$) prevalent in these environments, to match the waiting points, at which no more neutrons can be captured, with the mass numbers of the abundance peaks for r-process nuclei. The preciseness and near-universality [46] of the pattern should have led to the main astrophysical sites for the r-process. But the uncertainties of the nuclear rates used in the network calculations for predicting the r-process estimates would cause large-scale correlations to be unreliable. Moreover, the complications involved in simulating astrophysical environments and characteristics of the properties of a large number of neutron-rich nuclei participating in the r-process lead to additional uncertainties. In the present work, the radiative neutron-capture (n,γ) cross-sections and reaction rates around the r-process peak near mass number = 80 have been calculated and inherent uncertainties in the case of neutron-rich nuclei have been investigated.

2. Analytical framework for the statistical model

The thermonuclear reaction rates can be obtained by convoluting fusion cross-sections with Maxwell–Boltzmann distribution of energies. These cross-sections can vary by several orders of magnitude across the required energy range. The low-energy fusion cross-sections $\sigma$, some of which are not sufficiently well known, can be obtained from laboratory experiments. However, there are cases, in particular involving the weak interaction such as the basic p+ p fusion to deuterium in the solar p–p chain, where no experimental data are available and one completely relies on theoretical calculations [47]. The theoretical estimates of the thermonuclear reaction rates depend on the various approximations used. Several factors influence the measured values of cross-sections. We need to account for the Maxwellian-averaged thermonuclear reaction rates in the network calculations used in primordial and stellar nucleosynthesis.

The reaction rates used in the big-bang nucleosynthesis (BBN) reaction network are temperature-dependent except $^6$Li(n,γ)$^7$Li, $^{10}$B(n,γ)$^{11}$B, $^{12}$C(n,γ)$^{13}$C and $^{14}$N(n,γ)$^{15}$N which are constant with respect to temperature. The computer code TALYS [48] allows comprehensive astrophysical reaction rate calculations apart from other nuclear physics calculations. To a good approximation, in the interior of the stars the assumption of a thermodynamic equilibrium holds and nuclei exist both in the ground and excited states. This assumption, along with cross-sections calculated from the compound nucleus model for various excited states, facilitates Maxwellian-averaged reaction rates. For stellar evolution models, this is quite an important input. The nuclear reaction rates are generally evaluated using the statistical model [49,50] and astrophysical calculations mostly use these reaction rates. Stellar reaction rate calculations have been routinely done in the past [51,52]. However, TALYS has extended these Hauser–Feshbach (HF) statistical model [53] calculations by adding some new and important features. Apart from coherent inclusion of fission channel, it also includes reaction mechanism that occurs before equilibrium is reached, multiparticle emission, competition among all open channels, width fluctuation corrections in detail, coupled channel description in deformed nuclei and level densities that are parity-dependent. Different approaches are also used while normalising nuclear models on available experimental data, such as level densities on s-wave spacings or E1 resonance strength on photoabsorption data.

2.1 Mathematical expressions for the (n,γ) reaction cross-sections

In the low-energy domain, a compound nucleus is formed by the fusion of the projectile and the target nuclei. While the total energy $E_{\text{tot}}$ is fixed from energy conservation, the total spin $J$ and parity $\Pi$ can have a
range of values. The reaction obeys the following conservation laws:

\[ E_a + S_a = E_{a'} + E_x + S_{a'} = E_{\text{tot}}, \]

energy conservation,
\[ s + I + l = s' + l' + l' = J, \]
arbitrary momentum conservation,
\[ \pi_0 \Pi_0 (-1)^l = \pi_f \Pi_f (-1)^l' = \Pi, \]
parity conservation.

The formula for binary cross-section, assuming the compound nucleus model, is given as follows:

\[
\sigma_{\alpha\alpha'}^{\text{comp}} = D_{\alpha\alpha'}^{\text{comp}} \pi \frac{l_{\text{max}} + l + s}{k^2} \sum_{J=\text{mod}(l+s,1)} \sum_{l'-s'} \frac{\sum_{l''} \sum_{l'''} \delta_{\Pi}^{(\alpha)}(\delta_{\Pi}^{(\alpha')} W_{a''a'j''j'''}(E_{a''}))}{\sum_{a''a'''j''j'''}} \sum_{a''a'''j''j'''}
\]

where \( E_a \) is the energy of the projectile, \( I \) is the orbital angular momentum of the projectile, \( s \) is the spin of the projectile, \( J \) is the total angular momentum of the projectile, \( \pi_0 \) the parity of the projectile,

\[ \delta_{\Pi}^{(\alpha)} = \begin{cases} 1 & \text{if } (-1)^l \pi_0 \Pi_0 = \Pi, \\ 0 & \text{otherwise}, \end{cases} \]
\[ \delta_{\Pi}^{(\alpha')} = \begin{cases} 1 & \text{if } (-1)^l' \pi_f \Pi_f = \Pi, \\ 0 & \text{otherwise}, \end{cases} \]

\( \alpha \) is the designation of the channel for the initial projectile–target system: \( \alpha = \{ a, s, E_a, E_{a'}, I, \Pi_0 \} \), where \( a \) and \( E_{a'} \) are the types of the projectile and the excitation energy (which is zero usually) of the target nucleus, respectively, \( l_{\text{max}} \) is the maximum \( l \)-value of the projectile, \( S_a \) is the separation energy, \( E_{a'} \) is the energy of the ejectile, \( l' \) is the orbital angular momentum of the ejectile, \( s' \) is the spin of the ejectile, \( J' \) is the total angular momentum of the ejectile, \( \pi_f \) is the parity of the ejectile,

\[ G(T) = \sum_{\mu} (2I_{\mu} + 1)/(2I^0 + 1) \exp(-E_{\chi_{\mu}}/kT) \]
is the temperature-dependent normalised partition function. By using the reciprocity theorem [54], the reverse reaction cross-sections or rates can also be estimated.

3. Astrophysical implications of rapid neutron capture process

In nuclear astrophysics, the \( r \)-process is a series of nuclear reactions which is responsible for the synthesis of approximately half of the heavy nuclei resulting in the origin of elements beyond iron. The neutron star mergers, Type-II supernovae and low-mass supernovae [55] are thought to be the three probable \( r \)-process
candidate sites where appropriate conditions necessary for nucleosynthesis are expected to exist.

In a Type-II supernova, shortly after the extreme compression of electrons, $\beta^-$ decay is forbidden. This happens due to the high electron density which occupies all the states available to free electrons up to a Fermi energy that is larger than the $\beta^-$ decay energy. However, these free electrons capture by the nuclei do occur causing increasing neutronisation of the nuclear matter. This causes high temperatures and extremely high density ($\sim 10^{24}$) of free neutrons per cm$^3$ [3] that cannot decay. At this stage, it bloats and the expansion cools it and neutron capture by heavy nuclei present in the environment advances more rapidly than the $\beta^-$ decay. Consequently, the r-process progresses along the path of the neutron drip line and neutron-rich unstable nuclei are synthesised.

The dampening process of photodisintegration, the rapid decrease in the neutron-capture cross-section as it approaches closed neutron shells and the magnitude of nuclear stability in the domain of heavy isotopes are the three major processes which influence the ascent of neutron drip line. Thus, the neutron-rich, weakly bound nuclei are formed with neutron separation energies as low as $2$ MeV [3,56] due to neutron captures during r-process nucleosynthesis. At this stage, the neutron capture is temporarily paused as it reaches the neutron shell closures at $N = 50, 82$ and 126. These pauses or the so-called waiting points are characterised by the increased binding energy compared to heavier isotopes, resulting in low neutron capture cross-sections and a growth of semi-magic nuclei which are more stable towards $\beta$ decay. Additionally, nuclei beyond the shell closures, owing to their proximity to the drip line, are inclined to $\beta$ decay quickly. The $\beta$ decay happens before further neutron capture [57] for these nuclei. The waiting point nuclei then prefer $\beta$ decay to move towards stability ahead of any more neutron capture [3], causing deceleration or freeze-out of the reaction.

The decrease in the stability of nuclei puts an end to the r-process when its heaviest nuclei develop instability towards spontaneous fission. At this point, the total number of nucleons reaches 270 but before that, sufficiently low fission barrier might induce fission at neutron capture and continuation towards neutron drip line [58] terminates. After the decrease in neutron flux, these radioactive nuclei which are highly unstable undergo successive $\beta$ decays rapidly until they approach neutron-rich nuclei which are more stable [59]. In neutron-rich predecessor nuclei, the r-process produces an abundance pattern of radioactive nuclei $\sim 10$ amu below the peaks of slow neutron-capture process after they decay back to stability whereas the slow neutron capture process produces an abundance of closed neutron shell stable nuclei.

4. Results and discussions

4.1 Theoretical calculations of the $(n,\gamma)$ cross-sections

We have theoretically calculated the radiative neutron capture $(n,\gamma)$ cross-sections of astrophysical importance for Fe, Co, Ni, Cu, Zn, Ga, Ge, As and Se isotopes using the Hauser–Feshbach statistical model reaction calculations. The calculations have been performed using the most recent level density based on temperature-dependent Hartree–Fock–Bogolyubov calculations using the Gogny force and for the $\gamma$-ray strength function Brink–Axel Lorentzian has been used [48]. In figures 1–6, the plots of these estimates for the radiative neutron capture cross-sections as functions of incident neutron energy for the aforementioned elements and their different isotopes are given. These excitation functions highlight the variations of $(n,\gamma)$ cross-sections with energy and show a different dependence from $1/E_n^{1/2}$ behaviour valid at very low energies in the thermal domain. The energy variation of radiative capture cross-section is more expeditious in the astrophysical realm of energy range of 10 keV to 1.2 MeV than in the thermal domain.

4.2 Computations of the $(n,\gamma)$ reaction rates

In a stellar plasma, the kinetic energy available to nuclei is that of their thermal motion. Hence, reactions initiated by this motion are called thermonuclear
reactions. The nuclei in a stellar plasma move non-relativistically and are non-degenerate at temperatures in the range of $10^9$ K ($T_9$) ubiquitous in these environments. In stellar interiors, nuclides not only exist in their ground states but also in different thermally excited states and a thermodynamic equilibrium holds locally to a very good approximation. Therefore, velocities of nuclei can be described by a Maxwell–Boltzmann distribution. The cross-sections for nuclear reaction and their convolution with Maxwell–Boltzmann distribution of energies are important for explaining various processes occurring under extreme conditions [3,60,61].

In the main-sequence stars and compact stars which are in their ultimate stages of evolution, such environments of very high density and temperature prevail. The exothermic fusion reactions cause nuclear explosions in the surface layers of the accreting white dwarfs (nova events), in the cores of massive accreting white dwarfs (Type-Ia supernovae) [62,63] and in the surface layers of accreting neutron stars (Type-I X-ray bursts and superbursts [64–67]). Precise knowledge of the rates of thermonuclear reactions obtained by folding Maxwell–Boltzmann distribution of energies
with energy-dependent cross-sections becomes necessary for describing these astrophysical phenomena. The Maxwellian-averaged thermonuclear reaction rate per particle pair $\langle \sigma v \rangle$ at temperature $T$, can be represented by the integral [47,68,69] described as follows:

$$\langle \sigma v \rangle = \left[ \frac{8}{\pi m (kT)^3} \right]^{1/2} \int \sigma(E) E \exp(-E/kT) dE,$$

where $v$ is the relative velocity, $E$ is the energy in the centre-of-mass system, $k$ and $m$ are the Boltzmann constant and the reduced mass of the reacting nuclei, respectively. Thus, the reaction rate between two nuclei can be written as

$$r_{12} = \frac{n_1 n_2}{1 + \delta_{12}} \langle \sigma v \rangle,$$

where $n_1$ and $n_2$ are the number densities of nuclei of Types 1 and 2. The Kronecker delta $\delta_{12}$ prevents double counting in the case of identical particles.

Some key reactions [70] which may have particularly large impact on the final abundances in the $A \sim 80$ region have been investigated. Several works [71–75] regarding reaction rates have been done in the past. Except a few neutron-induced reactions, all other reaction rates have temperature dependencies. The neutron capture cross-sections show $\approx 1/v$ behaviour at very low energies in the thermal domain. Therefore, in eq. (3), using $\sigma(E) \propto E^{-1/2}$ one finds immediately that at thermal energies the reaction rates are more or less constant with respect to temperature. However, only for very low-energy neutrons ($\sim 0.025$ eV) this fact is true where energies are about an eV or less. On the other hand, at energies in the region of astrophysical interest, the capture cross-sections for the neutron-induced reactions can be best described by $\sigma(E) = R(E)/v$ [76], where $R(E)$ varies gently as a function of energy [77]. It is, therefore, similar to the astrophysical S-factor and one expects $\langle \sigma v \rangle$ to be temperature-dependent. Due to this reason, since Bao–Käppeler fit [78] to experimental data has been independent of temperature, we have excluded it and retained I Dillman et al ($ka$, $kd$) [79] and KADoNiS ($ks$) [80] for comparison with experimental results. The comparisons of the present $(n,\gamma)$ reaction rate calculations with the JINA REACLIB reaction rates [79,80] are presented in figures 7–15 as functions of $T_9$ for Fe, Co, Ni, Cu, Zn, Ga, Ge, As and Se. Although the JINA REACLIB reaction rates $kd$ and $ks$ follow the trends of the Hauser–Feshbach statistical model estimates, $ka$ behaves in a different manner beyond temperatures in the range of a giga Kelvin or more because of the limitation in the temperature dependence of the polynomial used for $ka$ in the higher temperature range. The results of the present calculations matches quite well with $kd$ and $ks$ reaction rates for $^{65}$Cu($n,\gamma$), $^{66}$Zn($n,\gamma$), $^{69}$Ga($n,\gamma$), $^{74}$Ge($n,\gamma$), $^{75}$As($n,\gamma$) and $^{78}$Se($n,\gamma$) reactions as evident from figures 10–15. This trend implies that the estimates of the present calculations are better for higher mass nuclei. The observations mentioned above can be summarised as: a few of the estimated rates are quite similar while others are somewhat different when compared with those from REACLIB and even JINA REACLIB reaction rates, $ka$, $kd$ and $ks$, among themselves are markedly different for quite a few cases. The possible reason for these is that REACLIB data exist only for a very limited range of neutron energies and $ka$,
Figure 8. Comparison of the predictions of $^{59}$Co(n,γ) reaction rates (HF) with the data from JINA REACLIB [79,80].

Figure 9. Comparison of the predictions of $^{62}$Ni(n,γ) reaction rates (HF) with the data from JINA REACLIB [79,80].

Figure 10. Comparison of the predictions of $^{65}$Cu(n,γ) reaction rates (HF) with the data from JINA REACLIB [79,80].

Figure 11. Comparison of the predictions of $^{66}$Zn(n,γ) reaction rates (HF) with the data from JINA REACLIB [79,80].

$kd$ and $ks$ rates themselves were fitted to different forms of polynomial functions of the temperature $T_9$ with different fitting parameters. Moreover, the errors associated with measured data were also not always small.

The microscopic nuclear inputs used for the radiative neutron capture reaction cross-section and reaction rate calculations are given in table 1. The flag ‘asys n’ opted here is for using all level density parameters from systematics and for neglecting the connection between the level density parameter $a$ and the s-wave resonance spacing $D_0$, even if an experimental value is available for the latter. The normalisation factor for γ-ray transmission coefficient ‘gnorm’ is an adjustable parameter that can be used to scale the (n, γ) cross-sections. To enforce automatic normalisation, ‘gnorm’ has been chosen as $−1$. As the flag ‘localomp’ has not been used, whenever enough experimental scattering data of a certain nucleus are available, a local optical model potential (OMP) can be constructed. The local OMP parameters are automatically obtained by TALYS from the database containing nuclear structure and model parameters. In case the database does not have a local OMP representation, the existing global OMPs are utilised. Furthermore, as there is no usage of the ‘massmodel’ or ‘expmass’ flags, theoretical mass models are employed only if there is no access to an experimental mass.
5. Summary and conclusion

To summarise, in the present work the theoretical predictions of radiative neutron capture \((n,\gamma)\) cross-sections of astrophysical importance and the reaction rates for Fe, Co, Ni, Cu, Zn, Ga, Ge, As and Se isotopes using the Hauser–Feshbach statistical model reaction calculations have been investigated. It is observed that the experimental results are uncertain by a few orders of magnitude for nuclei even in the vicinity of the valley of stability. Some key reactions [70] which may have significantly large impact on the final abundances in the region of mass number around 80 have been explored. The calculations of the \((n,\gamma)\) reaction rates have been compared with the JINA REACLIB reaction rates. Since in several cases large deviations among fits to experimental data of \(ka, kd\) and \(ks\) do exist, estimates of the present calculations can be termed as good. In addition, it is recognised that the uncertainties due to factors, such as level densities and mass models may have substantial effects on the rates while the low-energy upbend in the \(\gamma\)-strength function has a little (though non-negligible) effect on the rates.

To conclude, the present calculations have important bearings on the relative abundance of the elements involved in the r-process nucleosynthesis. The full reaction network calculations with varying neutron densities...
should be performed for a more detailed determination of the resulting abundances and isotopic ratios to study the consequence of incorporating present results. It is envisaged that to constrain the \((n,\gamma)\) reaction rates near the mass region \(=\) eighty, there is an acute need of more data. In order to exclude or establish certain model inputs, new experimental techniques, namely, the surrogate method for neutron-rich nuclei \[81]\ and the beta-Óslo method \[82]\ may contribute some crucial information.

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