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Astrophysical S-Factor Calculations under the Effects of Gamma-Ray Strength Functions for Some Alpha Capture Reactions

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Abstract—The reaction cross section and the energy, at which this value is obtained, are extremely important parameters in the calculation of astrophysical S-factor. Astrophysical S-factor values can be shown as one of the most notable values not only for nuclear reactions occurring at low energies but also for deeper understanding of astrophysical processes too. Considering the importance of this variable, it has been made possible to calculate it with theoretical methods when it cannot be measured experimentally. Theoretical calculations require the energy and the reaction cross section values. While the reaction cross section value, which can be explained as the probability of occurrence of a reaction, is obtained by theoretical calculations, the result can be affected by many parameters. In this study, it is aimed to investigate the effects of gamma-ray strength functions on the calculations of the astrophysical S-factor values of ^{96}Ru(α, γ)^{100}Pd, ^{106}Cd(α, γ)^{110}Sn, ^{112}Sn(α, γ)^{116}Te, ^{113}In(α, γ)^{117}Sb, and ^{144}Sm(α, γ)^{148}Gd reactions by using the cross section values obtained via utilizing different gamma-ray strength functions, which is one of the parameters known to have an effect on the cross section calculations. All calculation results were obtained using a well-known computation code TALYS, and the data obtained were analysed both graphically and statistically against available experimental data from the Experimental Nuclear Reaction Data (EXFOR) Library.

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1. INTRODUCTION

Some situations do not allow experimental studies to be carried out completely or partially. As a result of these kind of situations, the importance of theoretical studies has been understood and they have become more valuable. Although theoretical models provide many conveniences, they contain complex and long mathematical operations. Overcoming this difficulty has been achieved by the development of computer-aided calculation codes. Some examples of the abilities of these kind of codes could be given as obtaining the reaction cross section calculations, studying the dependencies of different level density models, understanding the influences of the γSF models on the calculations, effects of various optical model potentials and etc. There exist many studies in the literature which could be pointed within this scope in addition to the others that address the importance of the alpha particle induced reactions and γSF studies [1–6].

Among many parameters and outcomes of a nuclear reaction one particular quantity could be pointed as more interesting and remarkable, which is known as reaction cross section. This quantity accounts for the probability of a reaction occurrence and could provide very important information to the researchers. For some cases and energy ranges, it may possible to measure a reaction's cross section value. However, due to the decrease of charged particle cross sections because of the reduction of the tunnelling effect, it may not possible to have that value experimentally in some cases, especially in lower energies. A solution for such situations has been proposed by extrapolating the possibly observable high energy cross section data to the low energies by using estimations and mathematical approaches. On the other hand, a quantity named as astrophysical S-factor, which is able to be used in low energies and has better outcomes rather than employing such previously mentioned methods, is also available [7].

One of the aims of this study is to obtain the astrophysical S-factor values of ^{96}Ru(α, γ)^{100}Pd,

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^{106}Cd$(\alpha,\gamma)^{110}$Sn, ^{112}Sn$(\alpha,\gamma)^{116}$Te, ^{113}In$(\alpha,\gamma)^{117}$Sb and ^{144}Sm$(\alpha,\gamma)^{148}$Gd reactions. All of these investigated reactions are alpha capture reactions and each of the selected target nuclei of these reactions has importance in the astrophysical processes. The origin of these investigated elements in the solar system are dying low-mass stars and merging neutron stars. A visual for the distribution of these events at variable rates for each element is given by Johnson [8]. On the other hand, selected energy ranges for each reaction examined in this study are chosen to be the same as the values in the experimental data of the related reactions. It is thought that the relationship between the calculation results obtained with the theoretical models and the experimental data will be analysed more accurately by choosing the same energy intervals with the experimental data.

All calculations performed in accordance with the purpose of the study are made with TALYS [9] and its 1.8 versions, which is a widely used and known calculation code in the literature. In these calculations, firstly the cross section values are obtained by using different γSF models available in the TALYS code. Later on, S-factor values are calculated by using these cross section values and by doing so, the effects of different γSF models on the calculations of astrophysical S-factor values are aimed to be investigated. To validate the calculation results, available literature data for each of the investigated reaction are taken from the EXFOR [10] library. These data are used to provide a graphical comparison in addition to a numerical analyses in where mean weighted deviation [11] method is used.

2. CALCULATION METHODS

It is possible to show various parameters and models that may slightly or deeply effect the cross section calculation results. One thing which needs more attention is to select the appropriate model during the theoretical investigations which provides a better realization on the nature of the reaction and also contribute to both the development and improvement of the selected model. In this manner, by considering the investigated reactions within this study, the effects of various γSF models are utilized in the calculations. These models, which are Kopecky—Uhl generalised Lorentzian [12], Brink—Axel Lorentzian [13], Goriely's hybrid [14], Hartree—Fock BCS tables [15] and Hartree—Fock—Bogolyubov tables [15], are available in the TALYS code and utilized one by one on the cross section calculations of each investigated reaction. The main reason of selecting the TALYS code for this study could be given as its success and high preference in the literature. It is possible to list some other codes that are capable to perform various nuclear reaction calculations like TALYS yet it could be given as one of the most cited and utilized code among them due to some of its superior abilities such as the ease of target and incident particle definition, wide energy range in the calculations, user defined input generation, the ability of modification the theoretical model parameters and etc. However, TALYS v1.8 is not capable to directly perform the S-factor calculations. Due to that, TALYS based S-factor values are obtained by using Eq. (1) with the cross section values from the γSF model utilized TALYS calculations.

$$\sigma\left(E\right)=E^{-1}\exp\left(-2\pi\eta\right)S\left(E\right) \qquad (1)$$

In Eq. (1), the astrophysical S-factor value, which is denoted by $S\left(E\right)$, has a dependency to the center of mass energy of the reactants'. It is possible to say that, this dependency varies more slowly with respect to the energy rather than the other two parameters which are $\exp\left(-2\pi\eta\right)$ and $\sigma\left(E\right)$. η is known as the Sommerfeld parameter which is equal to $\left(Z_1Z_2\mathrm{e}^2\right)/\hbar\nu$ where Z_1 and Z_2 are the charges of projectile and the target, respectively. $\hbar$ and e are known constants while ν represents the magnitude of the incident particle's relative velocity. The term $\sigma\left(E\right)$, represents the total reaction cross section and considering the Coulomb repulsion between the charged particles, as they can be projectile and target, the astrophysical S-factor could be given with a rescaled value of $\sigma\left(E\right)$ which shows the importance of the connection between those two quantities [4, 5].

On the other hand, in addition to the importance of astrophysical S-factor, it is also aimed to investigate the effects of various γSF models on the S-factor calculations in this study. Among the above mentioned γSF models employed within this study, TALYS 1.8 utilizes Brink—Axel Lorentzian Model for all types of transitions rather than $E1$ where a generalized Lorentzian model of Kopecky'Uhl has been adopted as the default model for $E1$ radiation. In addition to these models, there are two microscopic model options for $E1$ radiation within TALYS code which are generated according to the Hartree-Fock BCS model and indicated in this study as Hartree—Fock BCS tables while the other one is derived from the Hartree—Fock—Bogolyubov model which is given as Hartree—Fock—Bogolyubov tables in the rest of the study. Certain differences and the details of all used models can be found from the Koning et al. [9].

Statistical analyses are performed to examine the consistency of the calculation results with the experimental data in addition to the determination of the least bad model for each investigated reaction with respect to the literature data. The mean weighted

Table 1. Statistical analyses of γSF models

Target	Kopecky–Uhl generalised Lorentzian	Brink–Axel Lorentzian	Goriely's hybrid	Hartree–Fock BCS tables	Hartree–Fock–Bogolyubov tables
^{96}Ru	4.52	4.87	3.69	3.85	3.80
^{106}Cd	8.53	8.57	8.15	8.17	8.18
^{112}Sn	6.05	6.25	6.13	6.10	6.12
^{113}In	10.53	4.36	7.87	8.68	8.61
^{144}Sm	14.93	16.24	15.68	15.50	15.62

deviation method is used for statistical investigations and the calculations are performed by using Eq. (2),

$$F = \left\{ \frac{1}{N} \sum_{i=1}^{N} \left[\left(\sigma_i^{calc} - \sigma_i^{exp} \right) / \Delta\sigma_i^{exp} \right]^2 \right\}^{1/2} \qquad (2)$$

where the results denoted with F tend to be the lowest one among others for better agreement between the literature data and calculation results. In this equation, σ_i^{calc} represents the theoretical calculations where the experimental cross section values and their uncertainties are represented via σ_i^{exp} and $\Delta\sigma_i^{exp}$, respectively for N number of experimental data points [11].

3. RESULTS AND DISCUSSION

Comparisons of astrophysical S-factor values of calculations and literature data for ^{96}Ru(α, γ)^{100}Pd, ^{106}Cd(α, γ)^{110}Sn, ^{112}Sn(α, γ)^{116}Te, ^{113}In(α, γ)^{117}Sb and ^{144}Sm(α, γ)^{148}Gd reactions are given in Figs. 1–5. Also, the mean weighted deviation analysis calculations are listed in Table 1.

In Fig. 1, comparisons of the S-factor calculations for alpha capture reaction of ^{96}Ru with the literature data of Rapp et al. [16] are given. All model results are in an acceptable compliance with the EXFOR data after neutron separation energy and Goriely's hybrid model could be pointed as the least bad γSF model option for this reaction with 3.69 mean weighted deviation value.

^{106}Cd(α, γ)^{110}Sn reaction's S-factor calculations are compared in Fig. 2 with the available literature data of Gyürky et al. [17]. All models are succeed to produce similar S-factor values with respect to each other. However, it seems that they are mismatched the EXFOR data up to 9 MeV alpha incident energy. After this energy, calculation results are in an acceptable compliance with the literature data. As can be seen from the statistical analysis results given in Table 1, Goriely's hybrid model could be pointed as the least bad γSF model for this reaction.

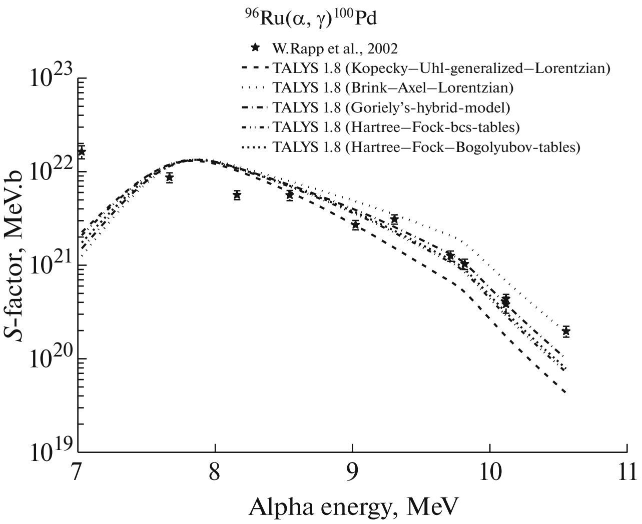

Fig. 1. Graphical comparisons of the calculated S-factor values for ^{96}Ru(α, γ)^{100}Pd reaction.

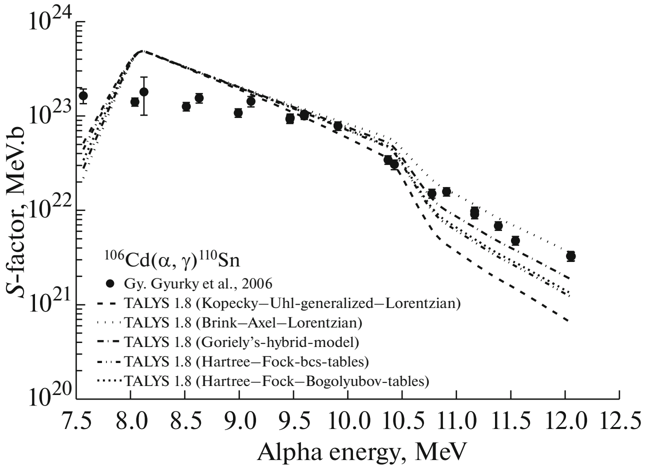

Fig. 2. Graphical comparisons of the calculated S-factor values for ^{106}Cd(α, γ)^{110}Sn reaction.

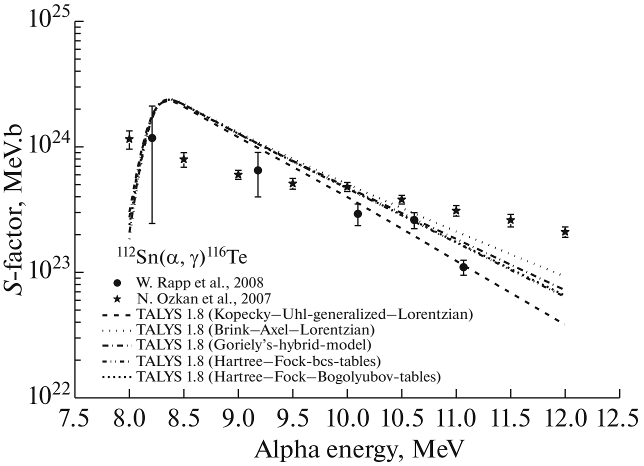

Fig. 3. Graphical comparisons of the calculated S-factor values for ^{112}Sn$(\alpha, \gamma)^{116}$Te reaction.

Calculation results obtained by using the Eq. (1) for ^{112}Sn$(\alpha, \gamma)^{116}$Te reaction are presented with the literature data of Rapp et al. [18] and Özkan et al. [19] in Fig. 3. All γSF models are able to produce similar geometrical shapes with the literature data. According to the mean weighted deviation analysis results, Kopecky–Uhl generalised Lorentzian model could be given as the γSF model that generated the least bad calculations with respect to the literature data.

Comparisons of S-factor calculations and the literature data taken from the studies of Yalɜın et al. [20] for the alpha capture reaction of ^{113}In are given in Fig. 4. All calculation results are generate similar geometries with the EXFOR data. Maximum S-factor values are observed at 9 MeV for this reaction. Brink–Axel Lorentzian model is the least bad γSF model option with 4.36 mean weighted deviation result for this reaction. As it can be seen from the Fig. 4, for the whole investigated energy range of this reaction Kopecky–Uhl generalised Lorentzian model generate lower S-factor values with respect to the literature data.

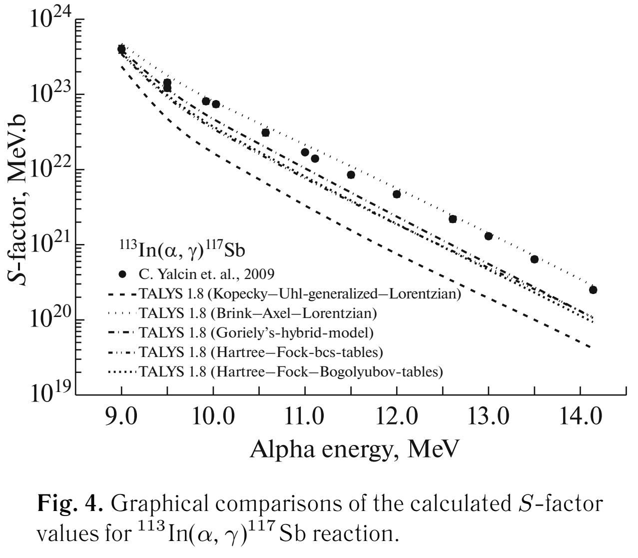

Fig. 4. Graphical comparisons of the calculated S-factor values for ^{113}In$(\alpha, \gamma)^{117}$Sb reaction.

^{144}Sm$(\alpha, \gamma)^{148}$Gd reaction S-factor calculations are compared with the literature data of Somorjai et al. [21] are shown in Fig. 5. All calculation results are obtained as following the literature data from above up to 13 MeV. The mean weighted deviation analysis results from Table 1 show that Kopecky-Uhl generalised Lorentzian model could be pointed as the least bad γSF model among all used models.

4. SUMMARY AND CONCLUSIONS

In this study, the astrophysical S-factor calculations for alpha capture reactions of ^{96}Ru, ^{106}Cd, ^{112}Sn,^{113}In and ^{144}Sm isotopes are obtained via Eq. (1). The cross section values used in Eq. (1) are obtained by utilizing different γSF models of TALYS code. Hereby, obtained results can be summarized as follows:

1. γSF models have an undeniable importance and impact on the S-factor calculations of alpha capture reactions.
2. Similar studies to this one may provide good theoretical contribution to the literature in where the γSF models, S-factor values and their relations are investigated. In accordance to that, this particular study and furthermore studies should be considered.

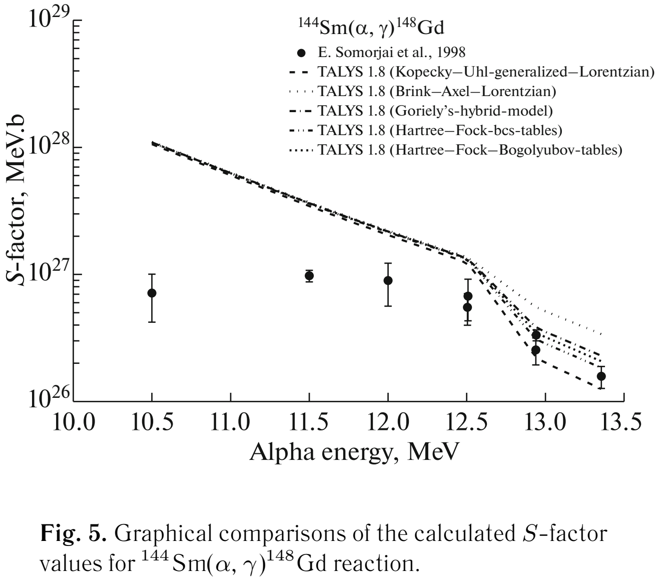

Fig. 5. Graphical comparisons of the calculated S-factor values for ^{144}Sm$(\alpha, \gamma)^{148}$Gd reaction.

3. Generally, all γSF models are in an acceptable compliance with the literature data. In the TALYS calculations performed in this study, only γSF models are varied and all other parameters are kept as default of the TALYS code. The TALYS code uses Hauser–Feshbach model up to the energy of the last discrete level of the target nucleus. It is thought that, the Hauser–Feshbach model could be the reason of the mismatch for the mentioned reaction.

4. Goriely's hybrid model results are generated harmonic calculation results with respect to the available literature data.

5. Hartree–Fock tables should be improved for ^{96}Ru, ^{106}Cd, ^{112}Sn,^{113}In and ^{144}Sm isotopes.

6. Generally, the astrophysical S-factor calculations obtained by using the cross section results from the utilization of Kopecky–Uhl generalised Lorentzian γSF model are generated the least bad outcomes with the available experimental data.

7. Brink–Axel Lorentzian model could be pointed as the least bad γSF model for the alpha capture reaction of the ^{113}In isotope. This model was developed based on the level density parameters. By considering this, the level density parameter effects should also be investigated for ^{100}Pd, ^{110}Sn, ^{116}Te, ^{117}Sb and ^{148}Gd isotopes.

8. As one of the main results of the whole study, it can be said that some models in the TALYS code should be improved.

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