ЯДЕРНА ФІЗИКА
NUCLEAR PHYSICS

УДК 539.17.02+539.172 https://doi.org/10.15407/jnpae2018.04.350

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CROSS-SECTION CALCULATIONS OF (n, 2n) and (n, p) REACTIONS FOR ^{69,71}Ga and ^{75}As TARGET NUCLEI UP TO 20 MeV

In the present research, neutron induced reaction cross sections of ^{69,71}Ga(n, 2n), ^{69,71}Ga(n, p), ^{75}As(n, 2n) and ^{75}As(n, p) were investigated up to 20 MeV. Three theoretical calculation codes (EMPIRE 3.2, TALYS 1.6 and ALICE/ASH) were used for model calculations based on the Weisskopf - Ewing and Hauser - Feshbach theories. The results of theoretical calculations were compared with some empirical formulas developed by different researches, with evaluated nuclear data sets (JENDL-4.0u2 (2012), TENDL-2015, JEFF-3.2 (2014), and ENDF/B-VIII.0 (2018)) and also with the available experimental data found in literature.

Keywords: nuclear reactions, ^{69,71}Ga, ^{75}As, TALYS 1.6, EMPIRE 3.2, ALICE/ASH, cross section.

1. Introduction

Due to lack of experimental data in literature, several reaction models have been developed by many researchers to estimate the reaction cross sections in recent years [1 - 4]. The neutron and proton induced nuclear reaction cross section calculations are very important for many technical applications in nuclear physics. In the present study, reaction cross section calculations of gallium and arsenic nuclei were investigated. Gallium (Ga) with atomic number 31 is a rare Earth element and does not occur as a free element in nature. There are five isotopes of gallium (^{66,68,69,70,71}Ga) and only two of them are stable and occur naturally: ^{69}Ga (~60 %) and ^{71}Ga (~40 %). All the other isotopes are radioactive. Gallium is widely used in nuclear reactors in the semiconductor industries and in the medical field [5, 6]. Arsenic (As) is a chemical element with atomic number 33 occurring in many minerals. Arsenic is known as a fission product and is also important for nuclear energy applications material science [7].

2. Theoretical Model Calculations

In this study, the cross sections of the ^{69,71}Ga(n, 2n), ^{69,71}Ga(n, p), ^{75}As(n, 2n) and ^{75}As(n, p) reactions were calculated for incident neutron energies ranging from 5.5 to 20 MeV. The calculations were performed with the EMPIRE-3.2 [8], TALYS-1.6 [9], and ALICE/ASH [10] codes, which are extensively used for nuclear data evaluation. The details on the input files used in each code are given in the following subsections.

2.1. The EMPIRE 3.2 calculations

EMPIRE [8] is a modular system of nuclear reaction codes, comprising various nuclear models, and it is designed for calculations over a broad range of energies (from keV to several hundred MeV) and incident particles.

In the present work, cross section theoretical calculations were performed in the framework of the Hauser - Feshbach theory [11], while width fluctuation corrections were taken into account according to the HRTW model. The default option was chosen for the description of the nuclear level densities, which is referred to as “EMPIRE-specific level densities”. The optical model parameters for the outgoing particles (=1 neutrons, =2 protons) were selected from Reference Input Parameter Library (RIPL) catalog. More specifically, the parameters given by Koning and Delaroche (2003) were adopted for outgoing neutrons and protons (input keyword OMPOT = -2408). Concerning pre-equilibrium reactions, the classical exciton model was implemented by means of the PCROSS module (default value 1.5). Moreover, the Feshbach - Kerman - Koonin (FKK) [12] fully quantum mechanical theory was used for multiple pre-equilibrium emissions, while the multi-step compound (MSC), multi-step direct (MSD) and hybrid Monte Carlo pre-equilibrium (HMS) calculations were not enabled in the present calculations. In addition, cluster emission was calculated in terms of the Iwamoto - Harada model [15].

2.2. The TALYS-1.6 calculations

TALYS-1.6 code [9] is also a nuclear reaction program which provides complete and accurate cross section calculations for reactions that involve neutrons, protons, γ-rays, deuterons, tritons, ^{3}He and α-particles in the 1 keV - 200 MeV energy range and for target nuclides of mass 5 and heavier. It takes into account the three basic nuclear reaction mechanisms, such as direct, compound nucleus and pre-equilibrium processes by using the appropriate parameterization (optical model, nuclear level densities, gamma-ray strength functions etc.) [10]. The TALYS-1.6 code can calculate elastic and total reaction cross sections, non-elastic cross sections per discrete state, elastic and non-elastic angular distributions, discrete and continuum gamma-ray production cross sections, isomeric and ground state cross sections, single and double-differential particle spectra, fission cross sections and fission yields, astrophysical reaction rates etc. [17].

In the present work, the compound nucleus reaction cross sections were calculated in the framework of the Hauser - Feshbach theory, while width fluctuation corrections were activated by implementing the HRTW model for incident neutron energies up to 9.3 MeV. Regarding the nuclear level densities, the option "ldmodel 1" was used, which corresponds to the combination of the constant temperature model (CTM) [14], as introduced by Gilbert and Cameron and the Fermi gas model, as given by Dilg et al. [18]. The phenomenological optical model parameters given by Koning and Delaroche (2003) [16] were used and furthermore the option to use a local, nucleus-specific optical model, when available, was enabled (localomp y). Furthermore, pre-equilibrium reactions were taken into account by means of the exciton model (preeqmode 1).

2.3. The ALICE/ASH calculations

The ALICE/ASH code [10], which is a modified version of the ALICE code developed by Blann, is used for the calculation of excitation functions, energy and angular distribution of secondary particles emitted in nuclear reactions, residual nuclear yields, and total nonelastic cross sections for nuclear reactions induced by nucleons and nuclei with energies up to 300 MeV [17]. Moreover, the geometry dependent hybrid (GDH) model is used successfully for description of the pre-equilibrium (pre-compound) particle emission from nuclei [20, 21].

In the theoretical calculations using the ALICE code, the standard Weisskopf-Ewing model was used for equilibrium reactions. The nuclear level densities were described according to the Fermi gas model, while the "ldopt = 0" parameter was determined by the expression a = A/9, where A is the mass number of gallium and arsenic isotopes. Concerning pre-equilibrium reactions, the geometry dependent hybrid (GDH) model was implemented, while in order to take into account the ratio of elementary (p-n) and (p-p) cross sections, the initial neutron and proton exciton numbers were multiplied by a factor of 2.73. Moreover, the separation energy of the projectile was calculated by using the MSL (Myres, Swiatecki and Lysekikl) mass formula [21] and the nucleon mean free path was multiplied by a factor of 2. Regarding the optical model parameters for the outgoing particles, the ones by Wilmore and Hodgson [23] were adopted for neutrons and the ones by Bechetti and Greenless [24] were used for protons. In addition, total pre-single alpha cross section was calculated according to the Iwamoto - Harada model [15]. Pairing option (MP) was selected to be 1 for pairing term in masses, while level density ground state shifts (LDGS) were calculated from MSL formula and applied back-shifted. IFIS = 0 was used for the rotating finite range barriers due to A. J. Sierk [21].

3. Semi-empirical formulae

Accurate cross sections for neutron induced reactions around 14 - 15 MeV are essential for testing nuclear models and nuclear reaction theories, as well as for practical applications such as designing of fusion reactors and neutron dosimetry [25 - 28]. Many experimental data have been published in literature concerning (n, charged particle) and (n, 2n) reaction cross sections induced by 14 - 15 MeV neutrons. Thus, many semi-empirical cross section formulae have been developed and proposed by different authors [25 - 36] for cross-section calculations around 14 - 15 MeV incident neutron energies for the (n, α), (n, 2n), (n, p), (n, t), and (n, ^{3}He) reactions [25 - 36].

In the present work, in order to compare with the theoretical calculations results, five semi-empirical cross section formulae have been used (Table 1) and their results are presented in Tables 2 and 3. The semi-empirical formulae have been developed by Tel et al. (2003, 2008) [32, 33], Lu and Fink (1971) [29], Konno et al. (1993) [34], Kasuage et al. (1996) [35], Broeders and Konobeyev (2006) [36]. In the first three rows of Table 1, the semi-empirical cross section formulas for the (n, p) reactions are presented, while in the rest rows the formulae for the (n, 2n) reactions are shown. As clearly seen from Table 1, all the semi-empirical cross section formulae present an exponential dependence from the mass number A, the neutron number N and the proton number Z of the target nucleus.

Table 1. **Semi empirical formulae for (n, 2n) and (n, p) reactions at 14 - 15 MeV neutron energies**

Author	Cross section formulae, mb	Energy, MeV
Lu and Fink (1971) [29]	$\sigma(n,2n) = 47.011(A^{1/3}+1)^2[1-3.9808\exp(-24.127(N-Z)/A)]$	14.8
Tel et al. (2008) [33]	$\sigma(n,2n) = \exp[7.65(1-1.59\exp(-23.06(N-Z)/A))]$	14.7
Konno et al. (1993) [34]	$\sigma(n,2n) = \exp[7.434(1-1.484\exp(-27.37(N-Z)/A))]$	14.5
Tel et al. (2003) [32]	$\sigma(n,p) = 7.31(A^{1/3}+1)^2\exp\left[-20.21(N-Z)/A\right]$	14.7
Kasugai et al. (1996) [35]	$\sigma(n,p) = 1830(N-Z+1)\exp\left[-50.70(N-Z+1)/A\right]$	14.5
Broeders & Konobeyev (2006) [36]	$\sigma(n,p) = \pi r_0^2(A^{1/3}+1)^2\exp[A^{0.5}(-4.4785(N-Z+1)/A+ + 0.047174Z/A^{1/3}-0.27407)]$	14.5

Table 2. **Theoretical, evaluated and semi-empirical cross sections for ^{69,71}Ga(n, 2n) and ^{75}As(n, 2n) reactions**

Source	σ(n, 2n), mb			Energy, MeV
	^{69}Ga	^{71}Ga	^{75}As	
EMPIRE [8]	740.370	962.850	901.370	14.5
TALYS [9]	756.288	1028.63	1053.980	14.5
ALICE ASH [10]	968.446	1212.070	1113.950	14.0
ENDF/B-VII.1	885.973	970.290	1056.360	14.5
TENDL-2015	830.176	1038.440	1037.830	14.5
JEFF-3	815.168	949.997	-	14.5
JENDL-4	-	-	1019.050	14.7
Tel et al. (2008) [33]	650.434	1092.260	978.161	14.7
Lu and Fink (1971) [29]	802.229	1010.130	997.970	14.8
Konno et al. (1993) [34]	851.758	1200.530	1119.580	14.5

Table 3. **Theoretical, evaluated and semi-empirical cross sections for ^{69,71}Ga(n, p) and ^{75}As(n, p) reactions**

Source	σ(n, p), mb			Energy, MeV
	^{69}Ga	^{71}Ga	^{75}As	
EMPIRE [8]	57.461	18.504	28.212	14.5
TALYS [9]	30.030	16.140	25.28	14.5
ALICE ASH [10]	69.140	44.480	62.15	14.0
ENDF/B-VII.1	37.354	14.218	24.025	14.5
TENDL-2015	31.340	16.993	20.637	14.7
JEFF-3	32.110	22.260	-	14.5
JENDL-4	-	-	18.290	
Tel et al. (2003) [32]	24.485	24.485	17.601	14.7
Kasuage et al. (1996) [35]	40.987	40.987	21.214	14.5
Broeders and Konobeyev (2006) [36]	36.710	36.710	18.690	14.5

4. Results and discussion

In the present work, cross section theoretical calculations were carried out for the ^{69}Ga(n, 2n)^{68}Ga, ^{71}Ga(n, 2n)^{70}Ga, ^{69}Ga(n, p)^{69}Zn, ^{71}Ga(n, p)^{71}Zn, ^{75}As(n, 2n)^{74}As and ^{75}As(n, p)^{75}Ge reactions by using three model codes (EMPIRE 3.2 [8], TALYS 1.6 [9] and ALICE/ASH for the Geometry-Dependent Hybrid (GDH) model [10]) for incident neutron energies up to 20 MeV. The most commonly used statistical models, the Weisskopf - Ewing (WE) [15] and Hauser - Feshbach (HF) [11], were implemented in these three model codes.

Figs. 1 - 6 show the cross section theoretical calculations results obtained from EMPIRE 3.2 [8], TALYS 1.6 [9] and ALICE/ASH (GDH) [10] codes, along with evaluated data from ENDF/B-VIII.0 (2018), JEFF-3.2 (2014), JENDL-4.0 (2012) and TENDL-2015 libraries and experimental data adopted from EXFOR database [37]. The present results were also compared with semi-empirical data (see Table 1), which were calculated by Tel et al. (2003, 2008) [32, 33], Lu and Fink (1971) [29], Konno et al. (1993) [34], Kasuage et al. (1996) [35], Broeders and Konobeyev (2006) [36]. The comparisons between the results of the present work, the evaluated data and the semi-empirical formulae results in the 14 - 15 MeV region are also presented in Tables 2 and 3. For each of the studied reactions, the results will be separately discussed in detail below.

4.1. ^{69}Ga(n, 2n)^{68}Ga reaction

The cross section of the ^{69}Ga(n, 2n)^{68}Ga reaction is presented in Fig. 1 for neutron energies up to 20 MeV, while comparisons around 14.5 MeV are given in Table 2. As seen from Fig. 1, theoretical calculations obtained with EMPIRE 3.2 [8], TALYS 1.6 [9] and ALICE/ASH (GDH) [10] are generally in agreement with the evaluated nuclear data from JENDL-4.0u2 (2012), TENDL-2015, JEFF-3.2 (2014) and ENDF/B-VIII.0 (2018) and with the experimental data from EXFOR between 10 and 20 MeV. However, theoretical calculations with the ALICE code reproduce the experimental data much better than the other codes. Moreover, semi-empirical cross sections around 14 - 15 MeV obtained by the formulae of Konno et al. (1993) [34], of Lu and Fink (1971) [29] and of Tel et al. (2008) [33] are seen slightly higher from both evaluated data and theoretical calculations.

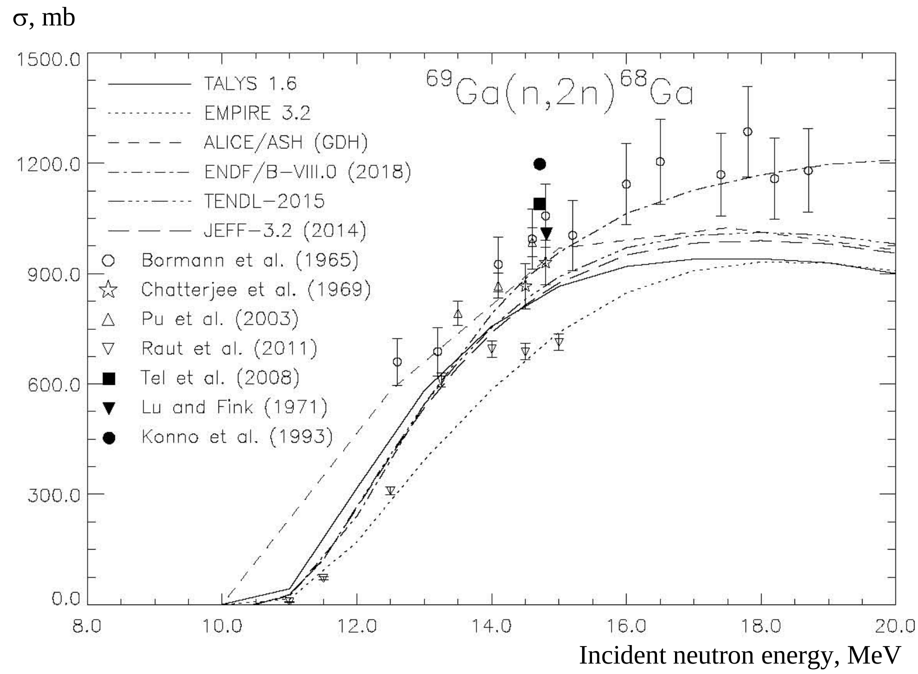

Fig. 1. Cross section of the ^{69}Ga(n, 2n) reaction.

4.2. ^{71}Ga(n, 2n)^{70}Ga reaction

The cross section of the ^{71}Ga(n, 2n)^{70}Ga reaction is shown in Fig. 2. The theoretical calculations results present a quite good agreement with both evaluated and experimental data from 10 to 20 MeV. Due to the fact that the experimental data are discrepant and present large uncertainties, all the theoretical model codes give acceptable and satisfying results. More specifically, as shown in Fig. 2 and Table 2, the results obtained with the ALICE/ASH (GDH) code [10] give almost the same cross sections values to those of empirical data of Konno et al. (1993) [34] and to the experimental data by Jishan et al. (2005) from EXFOR [37]. In addition, the cross section curve of TALYS 1.6 [9] agrees with the dataset of Luo et al. (2012) and with the empirical data from Tel et al. (2008) [33]. Regarding the EMPIRE 3.2 [8] results, the cross section values are similar to the empirical data of Lu and Fink (1971) [29] around 14.5 MeV neutron energy, while they are also very close to the ENDF/B-VIII.0 (2018) evaluated data.

4.3. ^{69}Ga(n, p)^{69}Zn reaction

The cross section of the ^{69}Ga(n, p)^{69}Zn reaction is shown in Fig. 3 for neutron energies up to 20 MeV, while comparisons around 14.5 MeV are given in Table 3. The results of the EMPIRE 3.2 [8] and ALICE/ASH (GDH) [10] codes overestimate the experimental data, especially over 5 MeV, whereas the cross section curve obtained with TALYS 1.6 [9] underestimates them, especially above 10 MeV. Moreover, the centroid of the theoretically calculated cross section curves lies in lower energies (around 11 - 13 MeV) compared to the centroid indicated by the experimental data (around 14 MeV). However, between the three model codes, the TALYS 1.6 [9] is the one that gave the most satisfying reproduction of the cross section, since it presents an agreement with the data by Bormann et al. [38]. Moreover, the empirical data introduced by Tel et al. (2003) [33], by Kasuagai et al. (1996) [18], Broeders and Konobeyev (2006) [36], indicate that the cross section lies at lower values compared to the EMPIRE and ALICE curves and closest to the TALYS one. Furthermore, the evaluated data of the TENDL-2015 and JEFF-3.2 (2014) are in agreement with the results obtained with TALYS, while the ENDF/B-VIII.0 library (2018) gives higher cross section values.

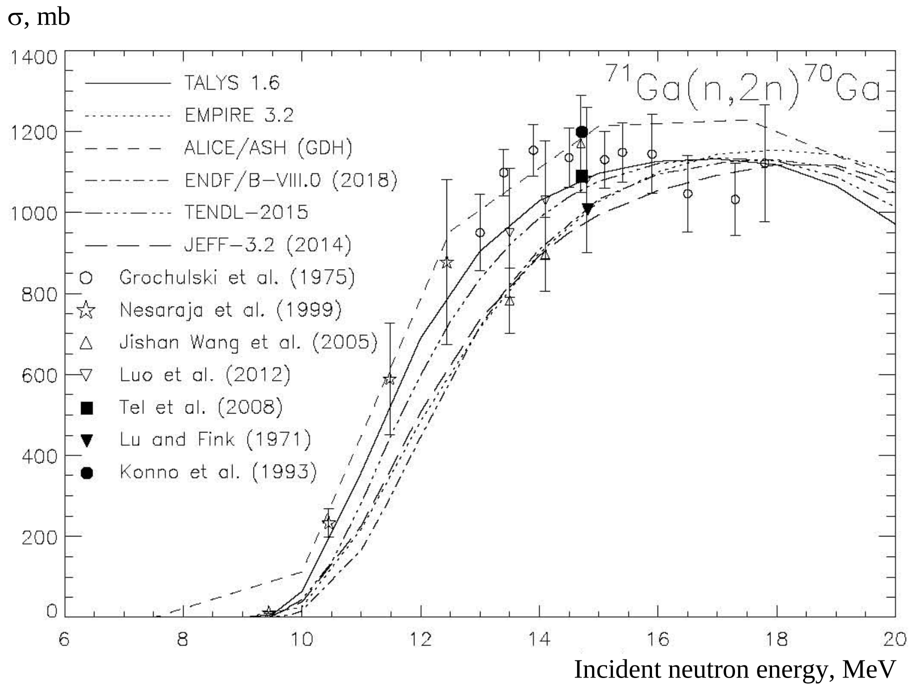

Fig. 2. Cross section of the ^{71}Ga(n, 2n) reaction.

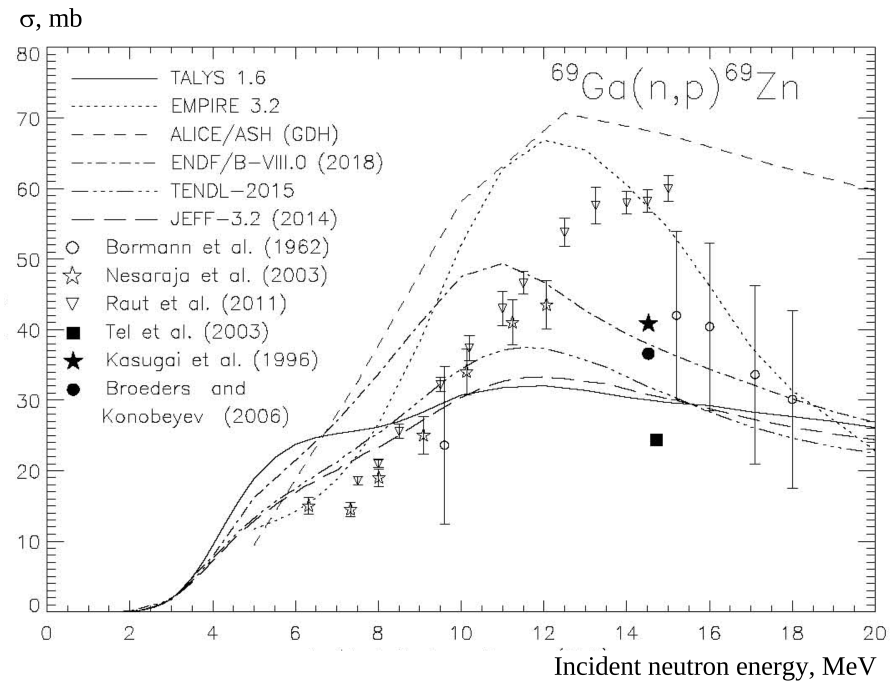

Fig. 3. Cross section of the ^{69}Ga(n, p) reaction.

4.4. ^{71}Ga(n, p)^{71}Zn reaction

The theoretical calculations results for the cross section of the ^{71}Ga(n, p)^{71}Zn reaction are shown in Fig. 4, along with evaluated and semi-empirical data (see also Table 3). The results obtained with the EMPIRE 3.2 [8] and TALYS 1.6 [9] codes give a very satisfying reproduction of existing in literature experimental data and evaluations. On the contrary, the results of the ALICE code and the empirical data introduced by Kasugai et al. (1996) [27] and Broeders and Konobeyev (2006) [36] seem to significantly overestimate the cross section.

4.5. ^{75}As(n, 2n)^{74}As reaction

The results for the cross section of the ^{75}As(n, 2n)^{74}As reaction are presented in Fig. 5. As can be seen in Fig. 5 and Table 2, the results obtained with TALYS 1.6 [9] and ALICE/ASH (GDH) [10] codes are in very good agreement not only with evaluated data of JENDL-4.0u2 (2012), TENDL-2015, JEFF-3.2 (2014) and ENDF/B-VIII.0 (2018) libraries, but also with existing experimental data. Moreover, the results of the EMPIRE 3.2 [8] code agree with existing experimental datasets and both TALYS and ALICE cross section curves above 16 MeV, but in the 10 - 16 MeV energy region they slightly underestimate the cross section. Furthermore, the empirical data of Tel et al. (2008) [33] and of Lu and Fink (1971) [29] are closest to the lower experimental data points (Raut et al. [37]) and to the EMPIRE curve, while the data point by Konno et al. (1993) [34] lies closest to the TALYS curve. Due to the fact that the results obtained with the ALICE code slightly overestimate the cross section in the low energy region (10 - 12 MeV), the TALYS curve is chosen for giving the most satisfactory results for this reaction channel over the whole energy range.

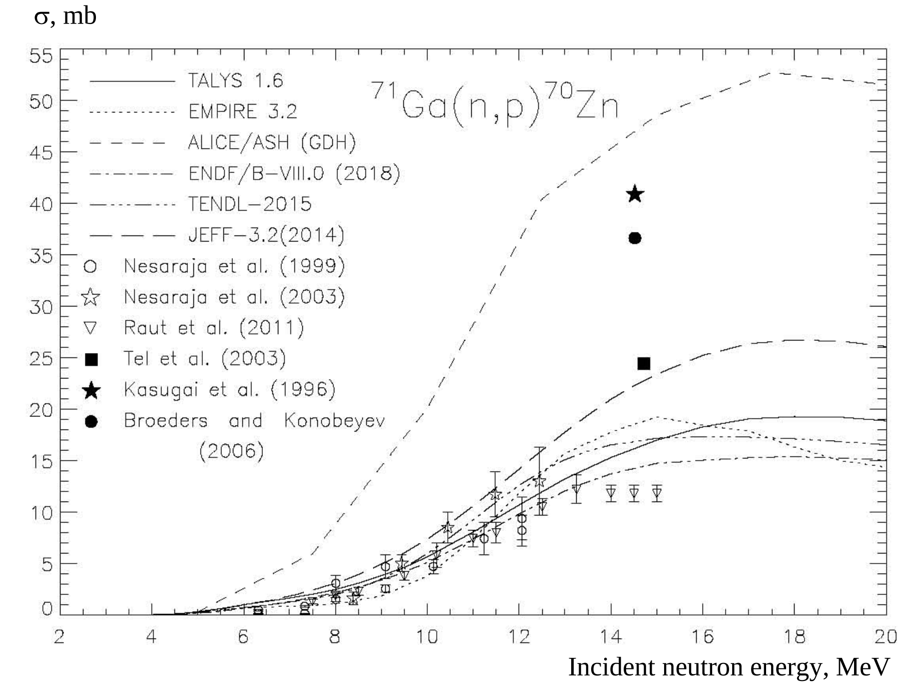

Fig. 4. Cross section of the ^{71}Ga(n, p) reaction.

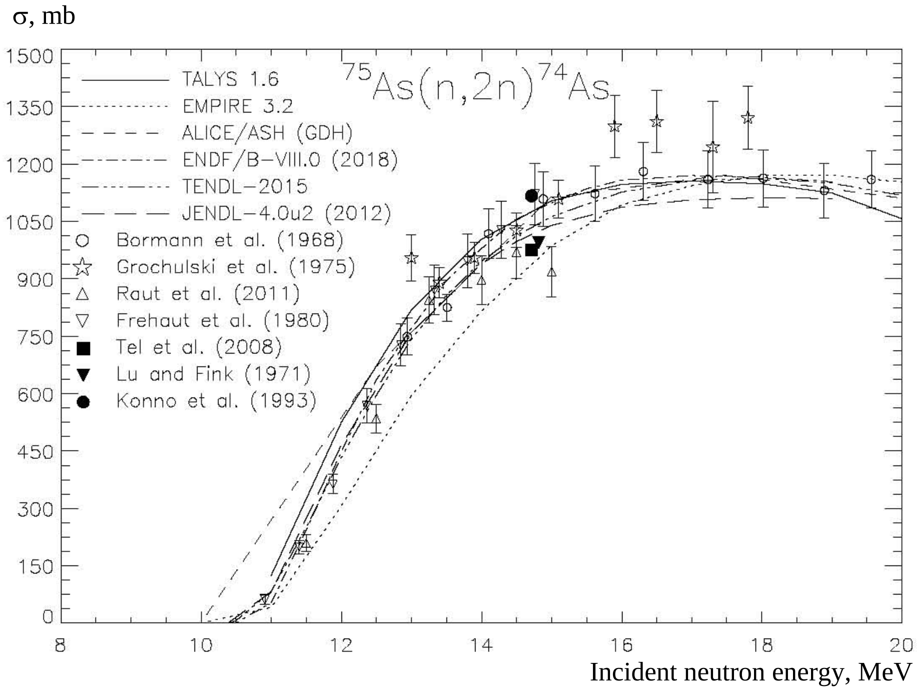

Fig. 5. Cross section of the ^{75}As(n, 2n) reaction.

4.6. $^{75}As(n, p)^{75}Ge$ reaction

The cross section of the $^{75}As(n, p)^{75}Ge$ reaction is shown in Fig. 6 for neutron energies up to 20 MeV. As can be seen in Fig. 6 and Table 3, the results obtained with EMPIRE 3.2 [8] and TALYS 1.6 [9] codes are in quite good agreement with both experimental and evaluated data of ENDF/B-VII.1, TENDL-2015 and JENDL-4 libraries. The semi-empirical data by Tel et al. (2003) [32], Kasugai et al. (1996) [35], Broeders and Konobeyev (2006) [36], although they agree with the lowest experimental data in the 14 - 15 MeV region, they give low cross section values compared to the EMPIRE and TALYS results. Moreover, the results obtained with the ALICE/ASH (GDH) [10] code present large differences with the other model codes, the evaluations and the experimental datasets. Obviously, for this reaction channel, the EMPIRE curve gives the better reproduction of the experimental data.

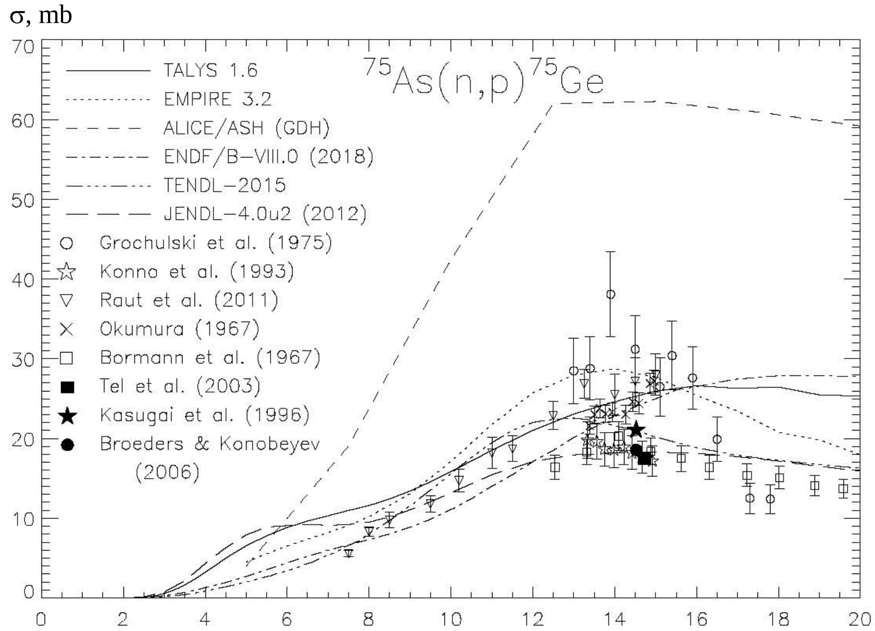

Fig. 6. Cross section of the $^{75}As(n, p)$ reaction.

5. Summary and conclusions

Cross section theoretical calculations were carried out for the $^{69}Ga(n, 2n)^{68}Ga$, $^{71}Ga(n, 2n)^{70}Ga$, $^{69}Ga(n, p)^{69}Zn$, $^{71}Ga(n, p)^{71}Zn$, $^{75}As(n, 2n)^{74}As$ and $^{75}As(n, p)^{75}Ge$ reactions for incident neutron energies up to 20 MeV. The calculations were performed by using three nuclear model codes, namely the EMPIRE 3.2 [8], TALYS 1.6 [9] and ALICE/ASH (GDH) [10] ones. The present results were compared with experimental nuclear data found in literature (EXFOR) [37] and with evaluated nuclear data from the JENDL-4.0u2 215 (2012), TENDL-2015, JEFF-3.2 (2014) and ENDF/B-VIII.0 (2018) libraries. Moreover, the results were also compared to some semi-empirical data (see Tables 1, 2 and 3).

Concerning the (n, 2n) reactions on ^{69}Ga, ^{71}Ga and ^{75}As, the results are presented in Figs. 1, 2 and 5 respectively. As can be seen in these Figures, in general terms, the cross section theoretical calculations results obtained by means of EMPIRE, TALYS and ALICE codes present a quite good agreement not only with experimental and semi-empirical data, but also with evaluations. In each reaction channel, probably one code can be selected for giving the most satisfactory results, but all the codes give reasonable cross section values.

Regarding the (n, p) reactions on ^{69}Ga, ^{71}Ga and ^{75}As, the situation is more complicated. The results are presented in Figs. 3, 4 and 6 respectively and as can be seen, the cross section values obtained with the ALICE code significantly overestimate the existing experimental data and the evaluations in all reaction channels. Moreover, especially in cases of ^{69}Ga and ^{75}As, the existing experimental data are discrepant and have large uncertainties. Therefore, many cross section curves with large differences in both shape and height can be acceptable. In the case of $^{71}Ga(n, 2n)$ reaction channel, in which the experimental data present an obvious trend, the latter is followed by both the EMPIRE and TALYS cross section curves.

Concerning the semi-empirical data, the cross section values for the (n, 2n) reaction channels are in agreement with theoretical calculations, evaluations and existing experimental data. The same holds for the ^{75}As(n, p) reaction cross section, but the semi-empirical values for the other two studied (n, p) reaction channels increase the discrepancies in the cross section.

Therefore, the (n, p) reaction cross sections on ^{69}Ga, ^{71}Ga and ^{75}As need further investigation. Firstly, more accurate experimental data is needed, in order to create a clear trend in the cross section shape. Then, it will be possible to implement a better theoretical parameterrization by means of the EMPIRE, TALYS and ALICE codes.

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РОЗРАХУНКИ ПЕРЕРІЗІВ (n, 2n) ТА (n, p) РЕАКЦІЙ ДЛЯ ЯДЕР ^{69,71}Ga І ^{75}As ДО 20 МеВ

Вивчалися перерізи нейтронно-індукованих реакцій ^{69,71}Ga(n, 2n), ^{69,71}Ga(n, p), ^{75}As(n, 2n) та ^{75}As(n, p) для енергій до 20 МеВ. Три теоретичних коди (EMPIRE 3.2, TALYS 1.6 і ALICE/ASH) використовувалися для модельних розрахунків на основі теорій Вайскопфа - Івінга і Хаузера - Фешбаха. Теоретичні розрахунки порівнювалися: з результатами, отриманими за деякими емпіричними формулами, розробленими в різних дослідженнях; з оціненими наборами ядерних даних (JENDL-4.0u2 (2012), TENDL-2015, JEFF-3.2 (2014), ENDF/B-VIII.0 (2018)); з наявними в літературі експериментальними даними.

Ключові слова: ядерні реакції, ^{69,71}Ga, ^{75}As, TALYS 1.6, EMPIRE 3.2, ALICE/ASH, поперечний переріз.

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РАСЧЕТЫ СЕЧЕНИЙ (n, 2n) И (n, p) РЕАКЦИЙ ДЛЯ ЯДЕР ^{69,71}Ga И ^{75}As ДО 20 МэВ

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Изучались сечения нейтронно-индуцированных реакций ^{69,71}Ga(n, 2n), ^{69,71}Ga(n, p), ^{75}As(n, 2n) и ^{75}As(n, p) для энергий до 20 МэВ. Три теоретических кода (EMPIRE 3.2, TALYS 1.6 и ALICE/ASH) использовались для модельных вычислений на основе теорий Вайскопфа - Ивинга и Хаузера - Фешбаха. Теоретические вычисления сравнивались: с результатами, полученными по некоторым эмпирическим формулам, разработанным в разных исследованиях; с оцененными наборами ядерных данных (JENDL-4.0u2 (2012), TENDL-2015, JEFF-3.2 (2014), ENDF/B-VIII.0 (2018)); с существующими в литературе экспериментальными данными.

Ключевые слова: ядерные реакции, ^{69,71}Ga, ^{75}As, TALYS 1.6, EMPIRE 3.2, ALICE/ASH, поперечное сечение.

Надійшла 08.08.2018
Received 08.08.2018