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ORIGINAL PAPER

Calculation of 14–15 MeV (*n, d*) Reaction Cross Sections Using Newly Evaluated Empirical and Semi-empirical Systematics

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Abstract In this study, we have investigated the asymmetry term effect for the (*n, d*) reaction cross sections at 14–15 neutron incident energy. It has been discussed the odd–even effect and the pairing effect considering binding energy systematic of the nuclear shell model for the new experimental data and new cross section formulae developed by Tel et al. for (*n, d*) reactions. We have determined different parameter groups by the classification of nuclei into even–even, even–odd and odd–even for (*n, d*) reactions cross sections. The obtained empirical and semi-empirical formulae by fitting two parameters for (*n, d*) reactions were given. By using the new cross sections formulae for (*n, d*) reactions the obtained results have been discussed and compared with the available experimental data.

Keywords (*n, d*) Cross section · Empirical and semi-empirical formulae · Hybrid reactor

Introduction

The neutron scattering cross sections and the neutron emission differential data have a critical importance on fusion reactor and in the fusion–fission hybrid reactors. These data can be extensively used for the investigation of the structural materials of the fusion reactors, radiation damage of metals and alloys, tritium breeding ratio, neutron multiplication and nuclear heating in the components. Especially, in the fusion–fission hybrid reactor, tritium self-sufficiency must be maintained for a commercial power plant.

The hybrid reactor is a combination of the fusion and fission processes. The fusion plasma is surrounded with a blanket made of the fertile materials (U^{238} or Th^{232}) to convert them into fissile materials (Pu^{239} or U^{233}) by transmutation through the capture of the high yield fusion neutrons [1–4]. The fertile materials may also undergo a substantial amount of nuclear fission, especially, under the irradiation of the high energetic 14.1 MeV-(D, T) neutrons. For self-sustaining (D–T) fusion driver tritium breeding ratio should be greater than 1.05. So, working out the systematics of (*n, t*) and (*n, d*) reaction cross sections is of great importance for the definition of the excitation function character for the given reaction taking place on various nuclei at energies up to 20 MeV. Additionally, obtained data from various techniques are necessary to develop more nuclear theoretical calculation models in order to explain nuclear reaction mechanisms and the properties of the excited states for different energy ranges.

In the present study, first only empirical formula of the (*n, d*) cross sections was obtained at the energy range of 14–15 MeV by using fitting procedure. Second, three different parameter groups by the classification of nuclei into even–even, even–odd, odd–even for (*n, d*) reaction cross

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sections have been determined. In this way, it has been discussed odd–even effect and basic nucleon–nucleus interaction considering the new experimental data and the new semi-empirical cross section formulae have been developed for (*n, d*) reactions. The current obtained results have also been investigated and compared with the other theoretical and experimental results proposed in early studies.

Empirical Systematic for 14–15 MeV Neutron Reaction Cross Sections

The neutron incident energy around 14–15 MeV is enough to excite the nucleus for the reactions such as (*n, p*), (*n, d*), (*n, 2n*), (*n, t*) and (*n, α*). Furthermore, the experimental cross section data of neutron around 14–15 MeV energy and particle emission spectra have a profound importance for understanding the binding energy systematics, the basic nucleon–nucleus interaction, nuclear structure and refined nuclear models.

Therefore, many more experiments have been carried out to obtain and detect neutrons for different energy ranges. For an instance, the method of energy measurement by means of velocity determination is a widely used technique and known as time of flight (TOF) [5]. The systematic experimental studies for the cross sections of (*n, charged particle*) such as $\sigma(n, p)$ and $\sigma(n, \alpha)$ at 14–15 MeV have been studied over the years for a large number of nuclei [6–12]. Moreover, applications of statistical and thermodynamical methods to the calculation of nuclear process for heavy nuclei go back to the fundamental work of Weisskopf and Ewing [13, 14]. On the other hand, a number of empirical and semi-empirical formulae with different parameters for cross sections calculations of the reactions (*n, p*), (*n, t*), (*n, α*) and (*n, 2n*) at the different neutron energies has also been proposed by several authors [15–17] and Tel et al. [18] suggested using these new experimental data to reproduce a new empirical formula of the cross sections of the (*n, p*) reactions. This formula depends on the asymmetry parameter, $s = (N - Z)/A$, and has the pairing effect on the binding energy systematics of nuclear shell model. Tel et al. also obtained a new appropriate coefficient by using this formula for (*n, 2n*), (*n, α*), (*n, d*) and (*n, t*) reactions [18–21].

Recently, nuclear data files have been prepared to study the neutron transport, nuclear heating and gas production, and radiation damage for materials irradiated by fast neutrons [22, 23]. These data files include the information about total cross sections, elastic and inelastic cross sections for threshold reactions, energy and angular distributions for secondary neutrons, protons and α-particles. However, nuclear models are frequently needed to provide the estimations of neutron-induced reaction cross sections, especially when experimental data are scarce or very difficult to perform. If the calculations on nuclear models are carried out using global parameters that have not been sufficiently validated by the experimental data, the obtained numerical results can be quite unreliable. The calculations employed to various model codes have shown that the results may vary depending on the codes and input parameters when no experimental data are available. Furthermore, a large number of experimental data have been published on the (*n, charged particle*) and (*n, 2n*) reaction cross sections induced by 14–15 MeV neutrons [22, 23]. According to previous reports [6–12] the cross sections for many nuclei significantly vary with the mass number *A*, neutron number *N* and proton number *Z* of the target nucleus. In addition, the attributable effects to the asymmetry parameter, $s = (N - Z)/A$, as well as to the isotopic, isotonic and odd–even properties of nuclei have been observed in the data.

The empirical cross sections of reactions induced by fast neutrons can be approximately expressed as follows,

$$\sigma(n,x) = C\sigma_{\mathrm{ne}} \exp\left[as\right] \tag{1}$$

where σ_{ne} is the neutron non-elastic cross section, and the coefficients *C* and *a* are the fitting parameters determined from least-squares method for different reactions. The non-elastic cross sections have been measured intensely for many nuclides in the MeV range, enabling us to find out their variation with atomic mass. The neutron non-elastic cross section is given by πr^2, where *r* is the nuclear radius and

$$\sigma_{\mathrm{ne}} = \pi r_0^2 (A^{1/3} + 1)^2 \tag{2}$$

where, $r_0 = 1.2 \times 10^{-13}$ cm.

Equation 1 represents the product of two factors, each of which might be assigned to a stage of nuclear reaction within the framework of the statistical model of nuclear reactions. The exponential term represents the escape of the reaction products from a compound nucleus. It has a strong $(N - Z)/A$ dependence implied by Eq. 1. This case has already been shown by Betak et al. [24] for neutron-induced reaction cross sections. There are also several formulae describing the isotopic dependence of cross sections for different reactions at neutron energy of 14.5 MeV. The measured cross sections exhibit a large gradient for the lighter masses ($Z \leq 30$) with increasing asymmetry parameter and then become almost constant for medium and heavy mass nuclei (starting from $A \leq 100$).

The best fitting can be obtained with the new free parameters in order to provide the minimum value of the following expression,

$$\chi^2 = \frac{1}{N}\sum_{i}^{N}\left(\frac{\sigma_{\mathrm{exp}}^{i} - \sigma_{\mathrm{cal}}^{i}}{\Delta\sigma_{\mathrm{exp}}^{i}}\right)^2 \tag{3}$$

where $\sigma_{\mathrm{exp}}^{i}$ and $\sigma_{\mathrm{cal}}^{i}$ are the experimental and the calculated cross sections, respectively, and $\Delta\sigma_{\mathrm{exp}}^{i}$ is the error associated with $\sigma_{\mathrm{exp}}^{i}$. Details on the results of the best fitting parameters and the values of χ^2 can be found for (*n, p*), (*n,* α), (*n, 2n*), (*n, d*) and (*n, t*) reactions in Refs. [18–21, 25].

Results and Discussions

Empirical and semi-empirical formulae are applied for the creation of systematic studies. Empirical expressions contain the exponential dependence of cross sections upon the number of neutrons and protons in nuclei. The empirical formulae use the evaporation model and ignore an important role of the pre-equilibrium mechanism of particle emission for medium and heavy nuclei. But the semi-empirical systematics are based on the use of analytical expressions for calculation of particle emission within the frame of pre-equilibrium exciton and evaporation models.

The odd–even and the nucleon binding energy systematics have been compared with the (*n, d*) measured cross sections with the empirical fits as shown in Fig. 1. The (*n, d*) experimental data include only (*n, d*) cross sections and does not include (*n, np*) or (*n, pn*) cross sections. In these reactions, it can be also seen that the reaction cross sections decrease by the increasing of the asymmetry parameter (Figs. 1–5). According to Levkovskii's formula [6], the proton and alpha emission probabilities increase with increasing relative proton number. The same relation can also be expected for *d, t* and *n* emissions. Besides, pre-equilibrium processes are important mechanisms in nuclear reactions induced by light projectiles with incident energies above 10 MeV [26–28]. The pre-equilibrium reaction effects strongly depend on the asymmetry parameter. Particularly, in the region I (*A* = 40–62), the (*n, p*) reaction is possible with compound process whereas this reaction is possible with pre-equilibrium process in region III (*A* = 90–160). Moreover, in the intermediate region II (*A* = 63–89) this reaction is also governed by both processes in the regions I and III [15]. In Figs. 2–5, reaction cross sections were classified according to odd–even properties by depending upon asymmetry parameter. As it can be obviously seen from Figs. 2–5, the reaction cross sections separate from each other (with relative to odd–even properties) according to the raising of asymmetry parameter. This separation can be observed mostly for (*n, d*) reactions. This case shows a strong pairing effect by depending up on the target nuclei mass number (*A*).

Detailed investigations for (*n, p*), (*n,* α) and (*n, 2n*) reaction cross sections have been performed in previous studies [18–21]. In the present study, we have only investigated the (*n, d*) reaction cross sections at the energy of 14–15 MeV in three different groups by using Tel et al. formula as can be seen in Figs. 3–5. As can be clearly seen from Figs. 1 and 2, the (*n, d*) reaction cross sections

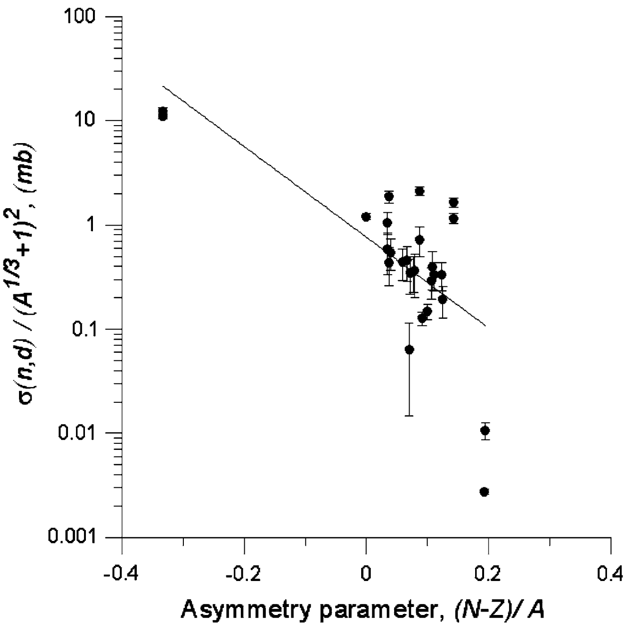

Fig. 1 The experimental points were fitted with $\sigma_{\mathrm{empirircal}}(n, d) = 0.76(A^{1/3} + 1)^2 \exp(-10.025s)$ and correlation coefficient was determined as $R^2 = 0.49$. Experimental data were taken from the EXFOR file

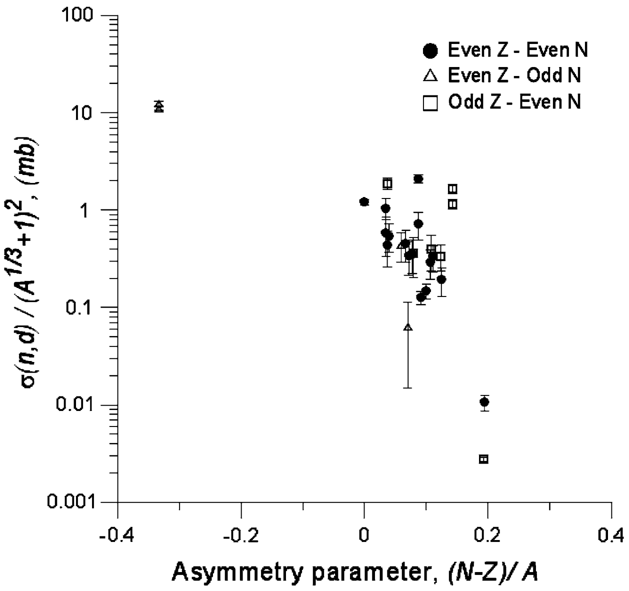

Fig. 2 Systematic of (*n, d*) reaction cross sections (in mb) for even-Z, even-*N*; even-Z, odd-*N*; odd-Z, even-*N* nuclides induced by 14–15 MeV neutrons. Experimental data were taken from the EXFOR file

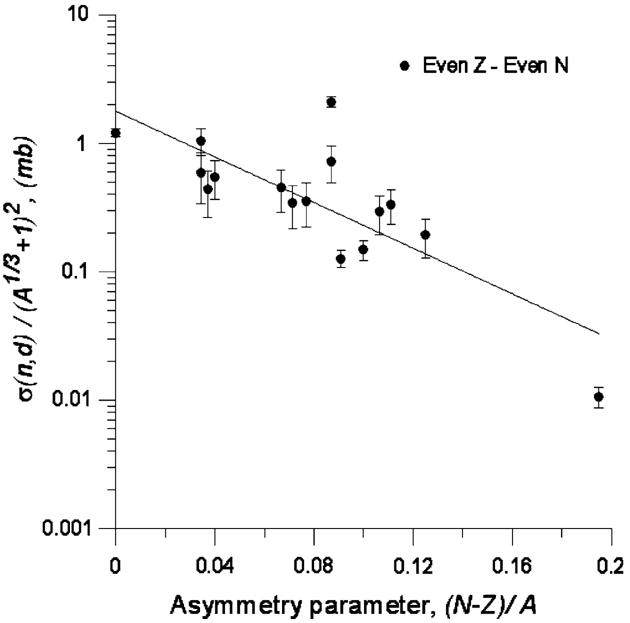

Fig. 3 Systematic of (*n, d*) reaction cross sections (in mb) for even-*Z*, even-*N* nuclides induced by 14–15 MeV neutrons. The experimental points were fitted with $\sigma(n, d) = 1.77(A^{1/3} + 1)^2 \exp(-20.46s)$ and correlation coefficient was determined as $R^2 = 0.62$. Experimental data were taken from the EXFOR file

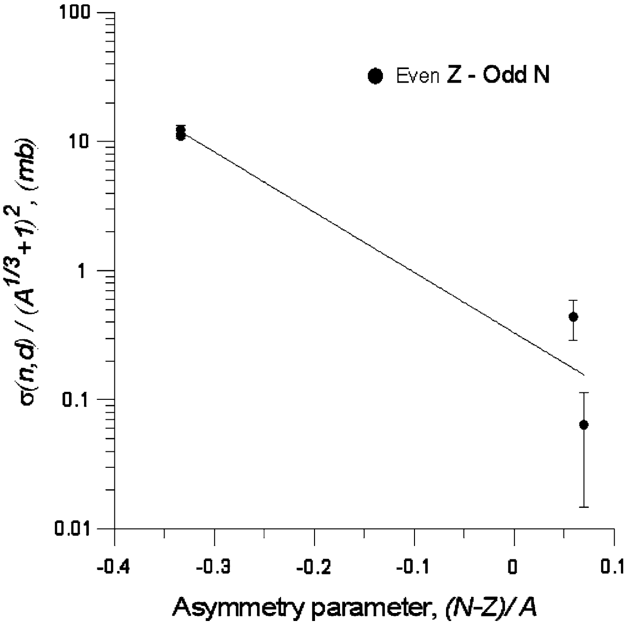

Fig. 4 Systematic of (*n, d*) reaction cross sections (in mb) for even-*Z*, odd-*N* nuclides induced by 14–15 MeV neutrons. The experimental points were fitted with $\sigma(n, d) = 0.33(A^{1/3} + 1)^2 \exp(-10.74s)$ and correlation coefficient was determined as $R^2 = 0.92$. Experimental data were taken from the EXFOR file

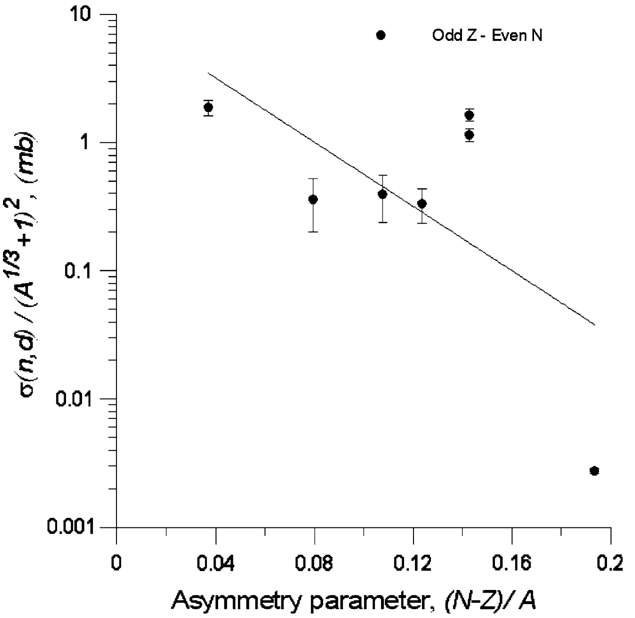

Fig. 5 Systematic of (*n, d*) reaction cross sections (in mb) for odd-*Z*, even-*N* nuclides induced by 14–15 MeV neutrons. The experimental points were fitted with $\sigma(n, d) = 1.77(A^{1/3} + 1)^2 \exp(-20.46s)$ and correlation coefficient was determined as $R^2 = 0.41$

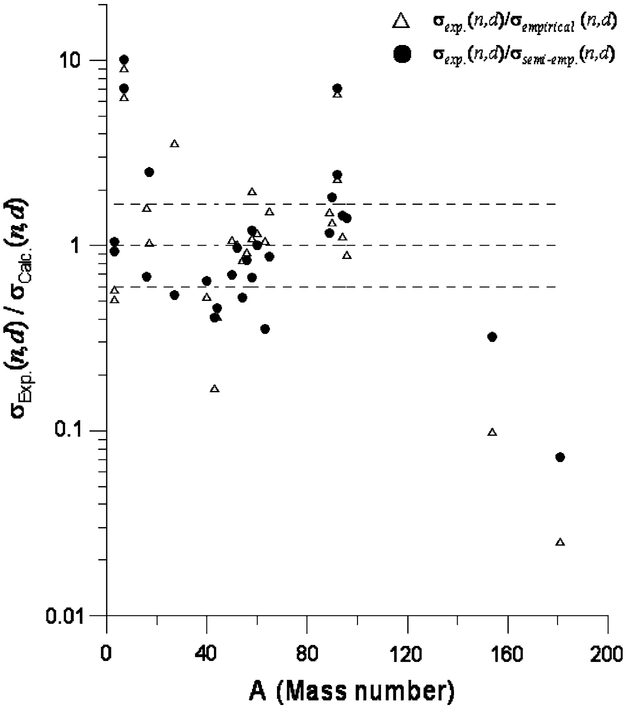

Fig. 6 Ratios of the (*n, d*) experimental cross sections to the cross sections calculated with semi-empirical formulae developed in this work

separate from each other due to increasing of asymmetry parameter. Therefore, we could not perform a good fitting for this case. However, for the (*n, d*) cross sections values, a good fitting was achieved by considering the even–even, even–odd and odd–even correction (Figs. 3–5). We have determined three different parameter groups by the

Table 1 The coefficients C and a, and the empirical and semi-empirical formulae for (n, d) reactions

Z	N	C	a	$\sigma(n, d) = C\sigma_{ne} \exp[as]$	R^2
All nuclei		0.76	−10.025	$\sigma_{\text{empirical}}(n, d) = 0.76(A^{1/3} + 1)^2 \exp(-10.025s)$	0.49
Even	Even	1.77	−20.46	$\sigma_{\text{semi-empirical}}(n, d) = 1.77(A^{1/3} + 1)^2 \exp(-20.46s)$	0.62
Even	Odd	0.33	−10.74	$\sigma_{\text{semi-empirical}}(n, d) = 0.33(A^{1/3} + 1)^2 \exp(-10.74s)$	0.92
Odd	Even	10.12	−28.85	$\sigma_{\text{semi-empirical}}(n, d) = 10.12(A^{1/3} + 1)^2 \exp(-28.85s)$	0.41

classification of nuclei into even–even, even–odd and odd–even for (n, d) reactions.

We have used the number of 27 experimental (n, d) cross sections data for different nuclei taken from Refs. [22, 23] for fitting procedure. The nuclei used in this study have mass numbers of $A = 3$–181, atomic numbers of $Z = 2$–73 and neutron numbers of $N = 1$–108. In Figs. 3–5, we have introduced three formulae by fitting two parameters for each formula presented by considering the pairing effect of the nuclear shell model. For this purpose, the three different groups by the classification of nuclei into even–even, even–odd and odd–even for these reaction cross sections parameters depending on asymmetry have been also determined.

The coefficients C and a were determined by least-squares fitting method the empirical and the semi-empirical formulae obtained by fitting two parameters for (n, d) reactions are given in Table 1 and also in Figs. 1–5, respectively. Besides, the comparison of the cross sections calculated with the empirical and semi-empirical formulae with the experimental (n, d) reaction cross sections for 14–15 MeV incident neutrons are given in Table 2 and also in Fig. 6, respectively.

When the more experimental data for the neutron scattering and emission differential cross sections have been obtained by using the new technology, it can be explained more reliable results and developed more nuclear reaction

Table 2 The comparison of the cross sections calculated with the empirical and semi-empirical formulae with the experimental (n, d) reaction cross sections for 14–15 MeV incident neutrons

Target	Reaction products	Half life and decay mode	Threshold energy (MeV)	Q value (MeV)	Excitation energy (MeV)	σ_{exp} (mb)	$\Delta\sigma_{\text{exp}}$ (mb)	empirical formula (mb)	Semi-empirical formula (mb)
^{3}He	^{2}H+^{2}H	Stable	4.3626	−3.2689	11.3311	66	3.2	128.1	70.63
^{3}He	^{2}H+^{2}H	Stable	4.3626	−3.2689	11.3311	74	5	128.1	70.63
^{7}Li	^{6}He+^{2}H	806.7 ms (β^-)	8.8660	−7.7514	6.8486	14	1.5	1.54	1.392
^{7}Li	^{6}He+^{2}H	806.7 ms (β^-)	8.8660	−7.7514	6.8486	9.8	1.1	1.54	1.392
^{16}O	^{15}N+^{2}H	Stable	10.5275	−9.9028	4.6972	15		9.413	21.978
^{17}O	^{16}N+^{2}H	7.13 s (β^-)	12.2428	−115.556	−100.956	5.6	1.9	5.37	2.237
^{27}Al	^{26}Mg+^{2}H	Stable	6.272583	−6.0465	8.5535	30	4	8.386	55.626
^{40}Ar	^{39}Cl+^{2}H	56 m (β^-)	10.5642	−10.3041	8.5535	2.9	0.5	5.447	4.478
^{44}Ca	^{43}K+^{2}H	22.3 h (β^-)	10.1678	−9.9396	4.6604	2.6	0.4	6.268	5.667
^{43}Ca	^{42}K+^{2}H	12.4 h (β^-)	8.6499	−8.4515	6.1485	1.3		7.656	3.163
^{50}Cr	^{49}V+^{2}H	330 d (EC)	7.5158	−7.3669	7.2330	12	4	11.163	17.169
^{52}Cr	^{51}V+^{2}H	Stable	8.4408	−8.2799	6.3200	8	3	7.87	8.233
^{54}Fe	^{53}Mn+^{2}H	3.7 My (EC)	6.7529	−6.6289	7.9710	10	4	11.975	18.995
^{56}Fe	^{55}Mn+^{2}H	Stable	8.1027	−7.9592	6.6408	8	3	8.647	9.580
^{58}Ni	^{57}Co+^{2}H	271 d (EC)	6.0515	−5.9479	8.6521	14	6	12.758	20.785
^{60}Ni	^{59}Co+^{2}H	Stable	7.4311	−7.3081	7.2919	11	4	9.407	10.953
^{58}Ni	^{57}Co+^{2}H	271 d (EC)	6.0515	−5.9479	8.6521	25	6	12.758	20.785
^{63}Cu	^{62}Ni+^{2}H	Stable	3.9603	−3.8978	10.7022	9	4	8.5	25.41
^{65}Cu	^{64}Ni+^{2}H	Stable	5.3100	−5.2288	9.3712	10	4	6.507	11.408
^{89}Y	^{88}Sr+^{2}H	Stable	4.8994	−48.4444	−33.8444	10	3	6.57	8.542
^{90}Zr	^{89}Y+^{2}H	Stable	6.1987	−6.1299	8.4701	10	3	7.494	5.487
^{92}Mo	^{91}Nb+^{2}H	700 y (EC)	5.29445	−5.2369	9.3630	22	7	9.66	9.104
^{96}Mo	^{95}Nb+^{2}H	Stable	7.1474	−7.0730	7.5269	6	2	6.754	4.278
^{92}Mo	^{91}Nb+^{2}H	Stable	5.2945	−5.2369	9.3630	64	6	9.662	9.104

Experimental data were taken from Refs. [22, 23]

mechanisms and nuclear models. As a result, the precise knowledge of the systematic for different neutron-induced reactions is of great importance in the account of the understanding the binding energy systematics of the nuclear shell model. Also, the present kind of studies lead to improve and clarify the binding energy systematic of the nuclear shell model and the estimation of unknown data for the development of nuclear reaction theories.

Summary and Conclusions

In this article, we have discussed the odd–even effect and the pairing effect considering binding energy systematic of the nuclear shell model for the new experimental data. We have determined different parameter groups by the classification of nuclei into the even–even, the even–odd and the odd–even for (*n, d*) reactions cross sections. The obtained semi-empirical formulae by fitting three parameters for the (*n, d*) reactions were given and the following conclusions can be summarized as follows:

1. The (*n, d*) reaction cross sections for 14–15 MeV decrease by the increasing of the asymmetry parameter.
2. The deuterium emission probabilities increase with increasing relative proton number.
3. The pre-equilibrium reaction effects strongly depend on asymmetry parameter for the (*n, d*) cross sections.
4. A good fitting of the (*n, d*) cross section values was achieved by considering the pairing correction.
5. The semi-empirical formulae are better than the empirical formulae for (*n, d*) cross sections. For understanding the (*n, d*) reaction systematics and the other nuclear reaction mechanisms it is need to develop semi-empirical formulae.

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