

New Evaluated Semi-Empirical Formula Using Optical Model for 14–15 MeV (n, t) Reaction Cross Sections

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Abstract In the next century the world will face the need for new energy sources. Nuclear fusion can be one of the most attractive sources of energy from the viewpoint of safety and minimal environmental impact. Fusion will not produce CO₂ or SO₂ and thus will not contribute to global warming or acid rain. Achieving acceptable performance for a fusion power system in the areas of economics, safety and environmental acceptability, is critically dependent on performance of the blanket and diverter systems which are the primary heat recovery, plasma purification, and tritium breeding systems. Tritium self-sufficiency must be maintained for a commercial power plant. The hybrid reactor is a combination of the fusion and fission processes. For self-sustaining (D-T) fusion driver tritium breeding ratio should be greater than 1.05. So working out the systematics of (n, t) reaction cross-sections are 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. In this study, we have calculated non-elastic cross-sections by using optical model for (n, t) reactions at 14–15 MeV energy. We have investigated the excitation function character and reaction Q -values depending on the asymmetry term effect for the (n, t) reaction cross-sections.

We have obtained new coefficients for the (n, t) reaction cross-sections. We have suggested semi-empirical formulas including optical model nonelastic effects by fitting two parameters for the (n, t) reaction cross-sections at 14–15 MeV. 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 and new cross-sections formulas (n, t) reactions developed by Tel et al. We have determined a different parameter groups by the classification of nuclei into even–even, even–odd and odd–even for (n, t) reactions cross-sections. The obtained cross-section formulas with new coefficients have been discussed and compared with the available experimental data.

Keywords Optical model · (n, t) Cross-section · Tritium · Semi-empirical formulas

Introduction

Nuclear fusion is one of the most attractive long term energy options. There is an essentially unlimited fuel supply, deuterium from the ocean and tritium from transmutation of lithium using neutrons produced in the D-T fusion reaction [1]. In the hybrid reactor the fusion plasma is surrounded with a blanket made of the fertile materials (U²³⁸ or Th²³²) to convert them into fissile materials (Pu²³⁹ or U²³³) by transmutation through the capture of the high yield fusion neutrons [2–5]. 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. Tritium self-sufficiency must be maintained for a commercial power plant. For self-sustaining (D-T) fusion driver tritium breeding ratio should be greater than 1.05.

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So, working out the systematics of (n, t) 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.

Neutron irradiation produces significant changes in the mechanical and physical properties of each of structural fusion material systems raising feasibility questions and design limitations. A focus of the research and development effort is to understand these effects, and through the development of specific compositions and microstructures, produce materials with improved and adequate performance [1, 5]. The neutron scattering cross-sections and the emission differential data have a critical importance on fusion reactor (and in the fusion–fission hybrid reactor) neutronics. 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, neutron spectrum, and reaction rate in the blanket and neutron dosimetry. There are several new technological applications on the fields of fast neutrons such as accelerator driven incineration/transmutation of the long-lived radioactive nuclear wastes into short-lived or stable isotopes [6, 7]. Especially, in accelerator driven subcritical systems for fission energy production and/or nuclear waste transmutation as well as in intermediate-energy accelerator driven neutron source, ions and neutrons with energies beyond 20 MeV, the upper limit of existing data files that were produced for D-T fusion applications, will interact with materials. As well, there can be found several biomedical applications i.e., production of radioisotopes and cancer therapy.

Because of above mentioned cases, it is needed to form new data about the cross-sections of nuclear reactions for the energy up to 20 MeV [8, 9]. Therefore, more many 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) [10]. 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. 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.

In this study, we have investigated the excitation function character and reaction Q -values depending on the asymmetry term effect for the (n, t) reaction cross-sections at 14–15 neutron incident energy. We have calculated

non-elastic cross-sections using optical model for (n, t) reactions. We have obtained new coefficients for the (n, t) reaction cross-sections at 14–15 MeV energy. We have suggested new semi-empirical formulas including optical model nonelastic effects by fitting two parameters for the (n, t) reaction cross-sections at 14–15 MeV. The coefficients were determined from by least-squares fitting method. 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 and new cross-sections formulas (n, t) reactions developed by Tel et al. We have determined a different parameter groups by the classification of nuclei into even–even, even–odd and odd–even for (n, t) reactions cross-sections. The obtained cross-section formulas with new coefficients have been discussed and compared with the available experimental data.

Optical Model Non-Elastic Cross Section Calculations

The non-elastic part of the interaction between the incident particle and the target nucleus manifest itself as the reaction cross-section. As a first approximation this interaction is described by an optical potential, the imaginary part of which leads to a finite reaction cross-section. In literature the projectile–target interaction for target nuclei over the periodic chart has been given in terms of global optical parameter-sets [11]. The reaction cross-sections generated using these global parameters are employed in several further calculations. In the statistical evaporation theory and the pre-equilibrium model the break-up of the total reaction cross-section into partial modes involving the emission of one or more particles is described by emission rate expressions which contain the cross-sections for the inverse processes involving the emitted particle as a function of energy [12, 13]. The cross-section for the inverse process is the optical reaction cross-section of the excited residual nucleus with the emitted particle as the projectile. This is approximated as the optical nucleus with the emitted particle as the projectile. This is approximated as the optical reaction cross-section between the residual nucleus in its ground state and the emitted particle. Thus optical reaction cross-sections are required for the incident channel at the projectile energy and for the exit channels over the energy range of the emitted particles. The statistical evaporation theory is a widely used description for reactions at low energies. At energies in the range of several tens of MeV the pre-equilibrium models have been successful. Reaction cross-sections are also used in intranuclear-cascade calculations [14] and in the calculation of the nuclear reaction efficiency correction for detectors [15].

Usually the optical reaction cross-sections at all the required energies and particle-target combinations are obtained by a numerical solution of the Schrödinger equation for several partial waves. This involves a large amount of computation time. Also, where more than one global optical potential appears in the literature for the same projectile it is quite laborious to repeat the calculations for each of the sets to see the effect on the final results. The form of the optical potential is [16],

$$U(r, E) = -U_N(r, E) + V_c(r) + U_{so}(r) \tag{1}$$

where V_c is the Coulomb potential due to a uniformly charged sphere with radius r_c , U_{so} is the spin-orbit potential and U_N is the complex central potential taken as,

$$U_N(r, E) = V_R(E)f(x_R) + i[W_V(E)f(x_V) + W_S(E)g(x_S)] \tag{2}$$

where $f(x_R) = [1 + \exp(x_R)]^{-1}$ and $x_R = (r - r_RA^{1/3})/a_R$, $g(x_S) = -4\frac{df(x_S)}{dx_S}$ (Woods–Saxon derivative) or $\exp(-x_S^2)$ (Gaussian).

Here x_V and x_S are defined in the same manner with appropriate radius parameters r_S , r_V and diffuseness parameters a_S , a_V . The spin-orbit potential U_{so} is, given by,

$$U_{SO}(r) = \lambda_\pi^2(l.\sigma)\frac{1}{r} \frac{d}{dr} f(x_{SO}) V_{SO} \tag{3}$$

Using this form of the potential several extensive analyses of differential elastic, polarization and reaction cross-section data have been carried out by various workers resulting in global parameter sets [11, 17].

Systematic for Neutron Reaction Cross Sections at 14–15 MeV

The reaction cross-sections 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 [18]. On the other hand, a number of empirical and semi-empirical formulas 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 [19–22] and Tel et al. [23] 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 systematic of nuclear shell model. Tel et al. [23–29] obtained a new appropriate coefficient by using this formula for $(n, 2n)$, (n, α) , (n, d) and (n, t) reactions. Tel et al. [30] also have investigated the asymmetry term effect for the $(p, n\alpha)$ reaction cross-sections and they have obtained

new coefficients for the $(p, n\alpha)$ reactions at 24.8 and 28.5 MeV energies. Although these obtained parameters by Tel et al. provide a means of fitting a number of such cross-sections at 14–15 MeV, there are some cross-sections which deviate substantially from the obtained fit results. In the lately work, Hadizadeh and Grimes [31] examine straightforward extensions of the model to see if the fit can be improved.

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 systematic are based on the use of analytical expressions for calculation of particle emission within the frame of pre-equilibrium exciton and evaporation models. According to previous reports [21, 22, 32, 33] 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,

$$\sigma(n, x) = C\sigma_{ne} \exp[as] \tag{4}$$

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

$$\sigma_{ne} = \pi r_0^2(A^{1/3} + 1)^2 \tag{5}$$

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

Equation 4 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. 4. 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 $A \leq 100$). 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. [23–29].

Results and Discussions

In Fig. 1, we have shown the asymmetry parameter values by depending up on the target nuclei mass number- A used in this work. As can be obviously seen from Fig. 1, the asymmetry parameter values have changed from 0.025 to 0.23 between $A = 46$ and 209. The asymmetry parameter values exhibit a gradient and they are increasing with increasing the target nuclei mass number- A from the lighter masses nuclei to heavier mass nuclei. In Figs. 2 and 3, we have shown the asymmetry parameter values by depending up on the (n, t) reaction Q -values and excitation energy used in this work at 14–15 MeV. And also, we have calculated non-elastic cross-sections by using optical model for (n, t) reactions at 14–15 MeV energy in Fig. 4. As can be obviously seen from Figs. 2 and 3, the reaction Q -values and excitation energy values exhibit a gradient and they are increasing with increasing the asymmetry parameter values from the lighter masses nuclei to heavier mass nuclei.

In Fig. 5, the (n, t) reaction cross-sections were classified according to odd–even properties by depending up on asymmetry parameter. As can be obviously seen from Fig. 5, the (n, t) reaction cross-sections separate with each other (with relative to odd–even properties) with the raising of asymmetry parameter. This case shows a pairing effect by depending up on the target nuclei mass number- A . Since there is not enough experimental data for the (n, t) reactions, it has been determined two different parameter groups by the classification of nuclei into the even Z –even

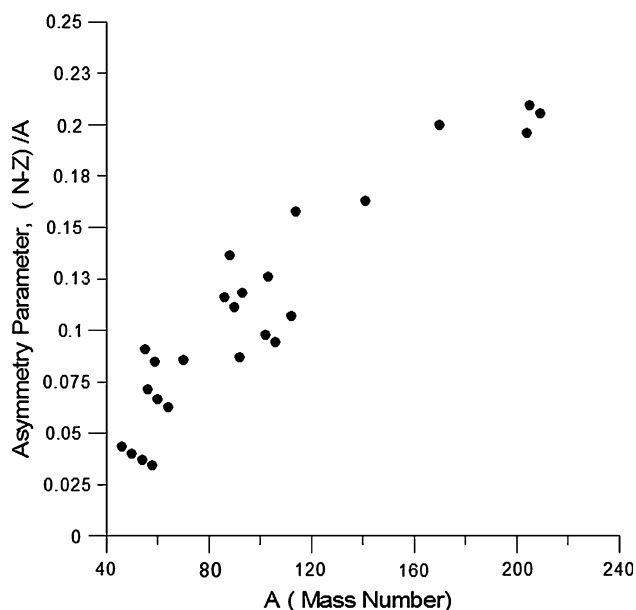


Fig. 1 Asymmetry parameter values for the target nuclei mass number- A used in this work

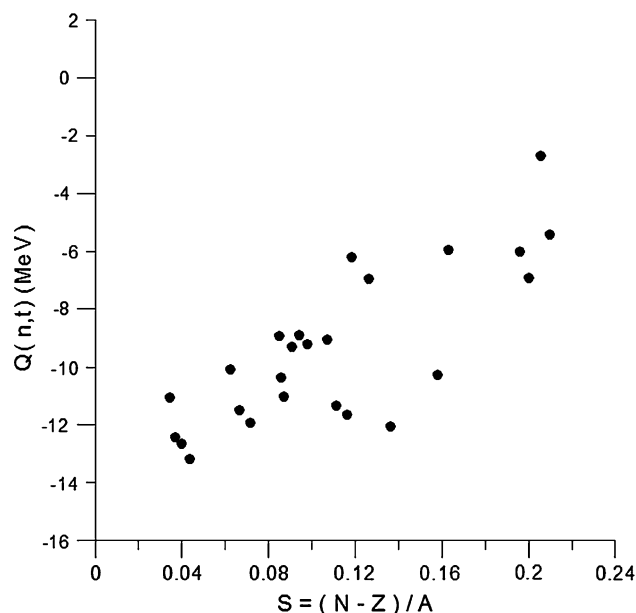


Fig. 2 (n, t) Reaction Q -values by depending up on asymmetry parameter

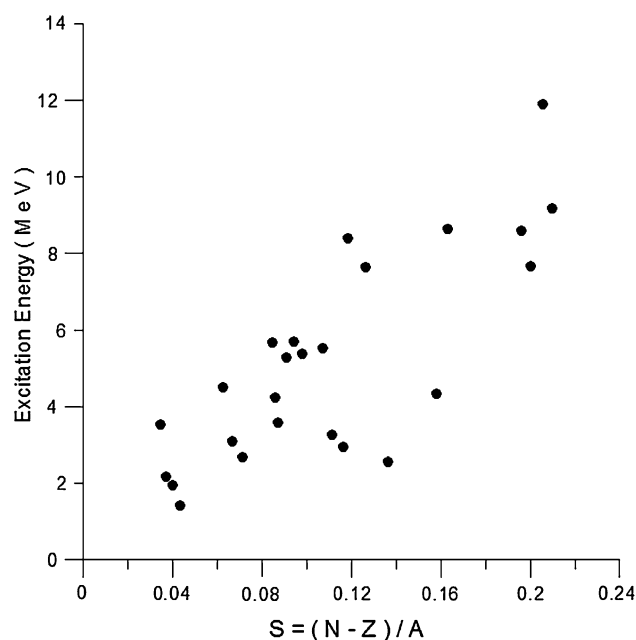


Fig. 3 Compound nucleus excitation energies by depending up on asymmetry parameter

N (for even- A) and odd Z –even N (for odd- A). As it can be clearly seen from Fig. 4, the (n, t) reaction cross-sections separate with each other due to increasing of the asymmetry parameter.

Detailed investigations for (n, p) , (n, α) , $(n, 2n)$, (n, d) , $(n, {}^3\text{He})$ and (n, t) reaction cross-sections have been performed in previous studies [23–29]. In the present study, we have calculated non-elastic cross-sections by using

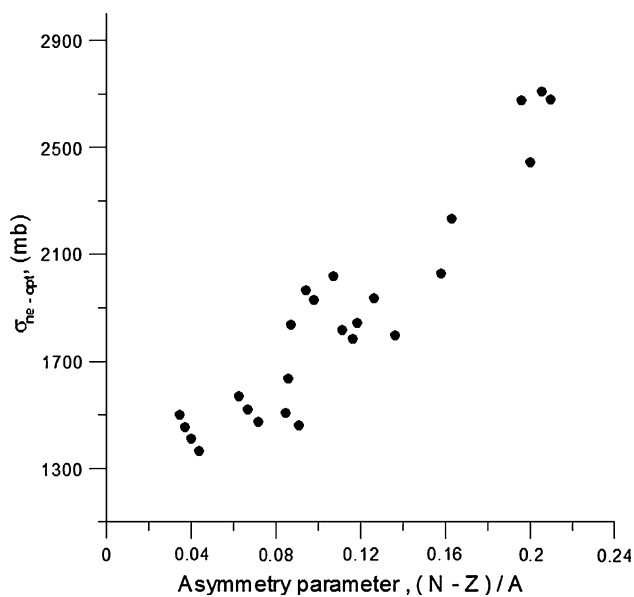


Fig. 4 Optical model neutron non-elastic cross-section by depending up on asymmetry parameter

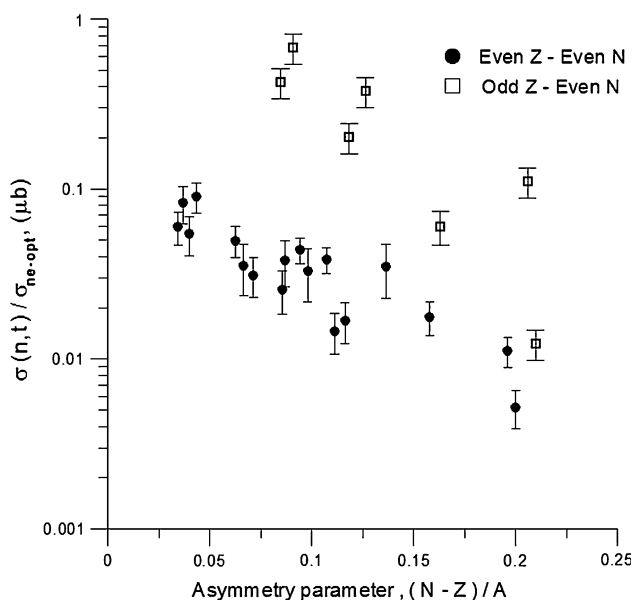


Fig. 5 Systematic of (n, t) reaction cross-sections (in μb) for even-Z, even-N; odd-Z, even-N nuclides induced by 14–15 MeV neutrons. Experimental data were taken from Refs. [8, 9, 35]

optical model for (n, t) reactions at 14–15 MeV energy in Table 1 and also we have suggested that the semi-empirical cross-sections of reactions induced by neutron can be approximately expressed as follows,

$$\sigma(n, t) = C\sigma_{\text{ne-opt}} \exp[as], \tag{6}$$

where x represents particles of the reaction produced. The coefficients C and a are the fitting parameters determined

from the least-squares method. The $\sigma_{\text{ne-opt}}$ represents the optical model neutron non-elastic cross-section. In this work, the $\sigma_{\text{ne-opt}}$ neutron non-elastic cross-sections were obtained by using the optical potential parameters of Ferrer et al. [17]. The neutron non-elastic cross-section calculations have been made in the framework of the optical model using SCAT 2 computer code [34].

We have used the number of 25 experimental (n, t) reaction cross-sections data taken from Refs. [8, 9, 35] for fitting procedure. We have used the nuclei which their mass numbers change from $A = 46$ to 209, the atomic numbers change from $Z = 22$ to 83 and also the neutron numbers change from $N = 24$ to 126. Firstly, the fitting parameters of empirical formula have been determined for all target nuclei having mass number for the (n, t) reactions cross-sections at 14–15 MeV (Fig. 6; Table 2). Secondly, we have determined two different fitting parameter groups by the classification of the target nuclei into even–even and odd–even (Figs. 7, 8; Table 2). The comparison of the first fitting and the second fitting reaction cross-section formulae shows that the second formulae proposed in our study give better description of experimental data. From Table 2, it can be seen that there is a better correlation because the R^2 is higher than the first fitting procedure. The maximum R^2 of the second formula provide more close results to experimental data. The second formula includes the odd–even (and even–even) nuclei the pairing correction and this formula has been taken into consideration to be the non-elastic cross-sections using optical model. The coefficients C and a were determined by the least-squares fitting method. The obtained by fitting the two parameter for the (n, t) reactions and R^2 values are given in the Table 2 and also in Figs. 6, 7 and 8, 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 mechanisms and nuclear models. As a result, the present kind of studies leads 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 paper, we have calculated non-elastic cross-sections by using optical model for (n, t) reactions at 14–15 MeV energy. We have suggested semi-empirical formulas including optical model nonelastic effects by fitting two parameters for the (n, t) reaction cross-sections at 14–15 MeV. We have discussed the odd–even effect and

Table 1 The comparison of calculations empirical and semi-empirical formulas with experimental for (n, t) reactions 14–15 MeV incident neutrons

Target	Reaction products	Half life-residual nucleus and decay mode	Threshold energy (MeV)	Q -value (MeV)	Excitation energy (MeV)	$\sigma_{\text{ne-opt}}$ optical model non-elastic cross-section (mb)	All nuclei fitted empirical formula (μb)	Even-even and odd-even fitted semi-empirical formula (μb)	σ_{exp} (μb)	$\Delta\sigma_{\text{exp}}$ (μb)
^{46}Ti	$^{44}\text{Sc} + ^3\text{H}$	3.93 h (EC)	13.475	-13.185	1.415	1,364.07	106.52	78.56	123	25
^{50}Cr	$^{48}\text{V} + ^3\text{H}$	16 d (EC)	12.918	-12.662	1.938	1,410.81	113.23	84.92	77	20
^{55}Mn	$^{53}\text{Cr} + ^3\text{H}$	Stable	9.475	-9.304	5.296	1,461.60	78.54	733.84	990	198
^{54}Fe	$^{52}\text{Mn} + ^3\text{H}$	5.59 d (EC)	12.657	-12.425	2.175	1,454.97	119.53	90.94	121	30
^{56}Fe	$^{54}\text{Mn} + ^3\text{H}$	312 d (EC)	12.143	-11.928	2.672	1,474.35	92.37	59.56	46	12
^{59}Co	$^{57}\text{Fe} + ^3\text{H}$	Stable	9.079	-8.926	5.674	1,507.20	85.02	872.95	640	128
^{58}Ni	$^{56}\text{Co} + ^3\text{H}$	78.8 d (EC)	11.259	-11.066	3.534	1,500.48	125.78	96.87	90	20
^{60}Ni	$^{58}\text{Co} + ^3\text{H}$	70.8 d (EC)	11.698	-11.504	3.096	1,520.66	98.92	65.25	54	18
^{64}Zn	$^{62}\text{Cu} + ^3\text{H}$	9.73 m (EC)	10.243	-10.084	4.516	1,568.61	105.44	70.97	78	16
^{70}Ge	$^{68}\text{Ga} + ^3\text{H}$	68.1 m (EC)	10.504	-10.355	4.245	1,634.69	91.51	55.08	42	12
^{86}Sr	$^{84}\text{Rb} + ^3\text{H}$	32.9 d (EC)	11.788	-11.652	2.948	1,782.65	78.44	40.76	30	8
^{88}Sr	$^{86}\text{Rb} + ^3\text{H}$	18.8 d (EC)	12.195	-12.053	2.547	1,798.41	67.55	31.87	63	22
^{90}Zr	$^{88}\text{Y} + ^3\text{H}$	106.6 d (EC)	11.473	-11.346	3.254	1,818.07	83.32	44.39	26.5	7
^{93}Nb	$^{91}\text{Zr} + ^3\text{H}$	Stable	6.263	-6.196	8.404	1,844.30	79.88	490.98	37	74.4
^{92}Mo	$^{90}\text{Nb} + ^3\text{H}$	14.6 h (EC)	11.148	-11.027	3.573	1,838.35	101.91	60.98	70	21
^{103}Rh	$^{101}\text{Ru} + ^3\text{H}$	Stable	7.019	-6.950	7.651	1,935.96	78.77	428.80	730	146
^{102}Pd	$^{100}\text{Rh} + ^3\text{H}$	20.8 h (EC)	9.310	-9.219	5.381	1,930.31	98.06	55.63	64	22
^{106}Cd	$^{104}\text{Ag} + ^3\text{H}$	69.2 m (EC)	8.984	-8.899	5.701	1,967.30	102.90	59.42	86.5	15
^{114}Cd	$^{112}\text{Ag} + ^3\text{H}$	3.14 h (b-)	10.366	-10.275	4.325	2,028.51	64.30	27.35	36	8
^{112}Sn	$^{110}\text{In} + ^3\text{H}$	69.1 m (EC)	9.146	-9.064	5.536	2,017.50	95.40	51.80	77.5	13
^{141}Pr	$^{139}\text{Ce} + ^3\text{H}$	137.2 d (EC)	5.989	-5.946	8.654	2,234.17	67.97	210.35	134	30
^{170}Er	$^{168}\text{Ho} + ^3\text{H}$	46.6 d (b-)	6.967	-6.926	7.674	2,446.31	55.65	19.33	12.7	3.2
^{205}Tl	$^{203}\text{Hg} + ^3\text{H}$	12.2 d (EC)	5.456	-5.429	9.171	2,680.55	56.47	85.62	33	6.6
^{204}Pb	$^{202}\text{Tl} + ^3\text{H}$	12.2 d (EC)	6.034	-6.005	8.595	2,676.77	62.80	22.23	30	6
^{209}Bi	$^{207}\text{Pb} + ^3\text{H}$	Stable	2.698	-2.685	11.915	2,708.82	58.89	94.96	300	60

Experimental data were taken from Refs. [8, 9, 35]

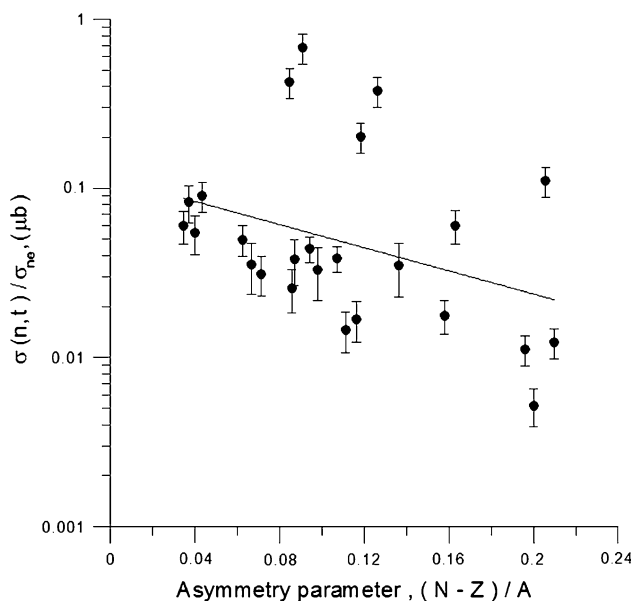


Fig. 6 The experimental points were fitted with $\sigma(n, t)_{\text{empirical}} = 0.11\sigma_{\text{ne-opt}} \exp[-7.88s]$ and correlation coefficient was determined as $R^2 = 0.13$. Experimental data were taken from Refs. [8, 9, 35]

the pairing effect considering binding energy systematic of the nuclear shell model. We have determined a different parameter groups by the classification of nuclei into even-even and odd-even for (n, t) reactions cross-sections. The obtained empirical formulas by fitting two parameters for the (n, t) reactions were given and the following conclusions can be summarized as follows:

- The asymmetry parameter increases with increasing relative mass number.
- The (n, t) reaction Q -values and the excitation energy of compound nucleus increase with increasing the asymmetry term.
- The optical model non-elastic cross-sections increase with increasing the asymmetry term.
- The (n, t) reaction cross-sections decrease by the increasing of the asymmetry parameter.
- A good fitting of the (n, t) cross-section values was achieved by considering the pairing correction.
- The semi-empirical formulas better than the empirical formulas for (n, t) reaction cross-sections.

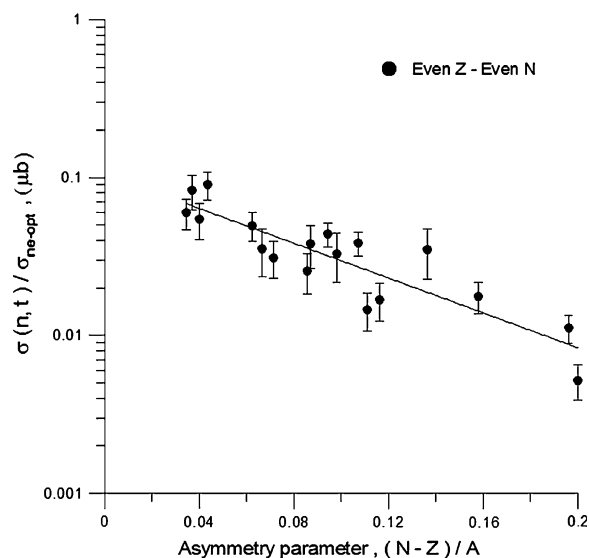


Fig. 7 Systematic of (n, t) reaction cross-sections (in μb) for even-Z, even- N nuclides induced by 14–15 MeV neutrons. The experimental points were fitted with $\sigma(n, t)_{\text{semi-empirical}} = 0.10\sigma_{\text{ne-opt}} \exp[-12.69s]$ and correlation coefficient was determined as $R^2 = 0.78$. Experimental data were taken from Refs. [8, 9, 35]

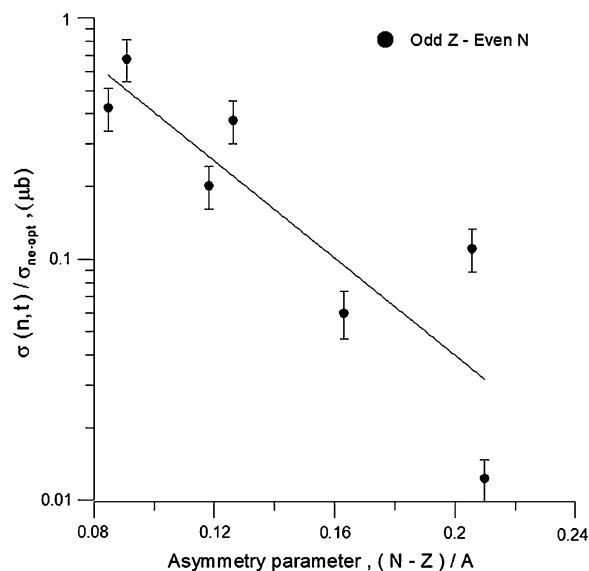


Fig. 8 Systematic of (n, t) reaction cross-sections (in μb) for odd-Z, even- N nuclides induced by 14–15 MeV neutrons. The experimental points were fitted with $4.13\sigma_{\text{ne-opt}} \exp[-23.18s]$ and correlation coefficient was determined as $R^2 = 0.74$. Experimental data were taken from Refs. [8, 9, 35]

Table 2 The coefficients C and a , and the empirical and semi-empirical formulas for (n, t) reactions

C	a	$\sigma(n, x) = C\sigma_{\text{ne-opt}} \exp[as]$	R^2
0.11	-7.88	$\sigma(n, t)_{\text{empirical}} = 0.11\sigma_{\text{ne-opt}} \exp[-7.88s]$ All nuclei	0.13
0.10	-12.69	$\sigma(n, t)_{\text{semi-empirical}} = \begin{cases} 0.10 \sigma_{\text{ne-opt}} \exp[-12.69s] & \text{Even Z - Even N} \\ 4.13 \sigma_{\text{ne-opt}} \exp[-23.18s] & \text{Odd Z - Even N} \end{cases}$	0.78
4.13	-23.18		0.74

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