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**SOME CRITERIA FOR SELECTION OF EVALUATED
THRESHOLD REACTION EXCITATION FUNCTIONS**

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Some criteria for selection of evaluated threshold reaction excitation functions.

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ABSTRACT. Some empirical systematics of excitation function shapes and cross sections of neutron induced threshold reactions at the maximum of excitation functions are described.

Introduction.

There are many works devoted to the investigation of the neutron cross section systematics of threshold reactions in the 14-15 MeV neutron energy region. For reactions with outgoing charged particles the main idea of these systematics is an exponential dependence of 14-15 MeV incident neutron cross sections on parameter $(N-Z)/A$. These systematics are very important for prediction of cross sections. Among the early works, in which the systematics were realized, the works of V.Levkovsky, D.Gardner, S.Qaim should be mentioned first of all.

However, some works were made to analyze shapes of excitation functions and cross sections at its maxima. The important results have been obtained by H.Vonach in the work /2/ for $(n,2n)$ reaction. The similarity of $(n,2n)$ excitation function shapes for heavy nuclei ($A > 100$) was shown and universal excitation function and systematics of the peak cross sections were proposed. In the works /3, 4/ Yu.Trofimov proposed relations for evaluation of (n,p) reaction cross sections at the maxima of the excitation functions and for determination of the neutron energy corresponding to the maxima.

In the present paper some systematics and systematical trends for parameters, which characterize the threshold reaction excitation functions, are described. These empirical systematics are based on experimental data and can be used for an evaluation and a selection of more reliable excitation functions among those which have no experimental data and are calculated on the base of theoretical models.

The following values are considered as parameters of nuclear reaction excitation functions: reaction threshold, difference of thresholds of main and competing reactions (for example, (n,p) and (n,np)), cross section at the maximum of excitation function and position of the maximum on neutron energy scale. The shape of excitation functions is considered also as a parameter.

As far as these parameters are connected with atomic nucleus characteristics (mass number A , nuclear charge Z , neutron excess $(N-Z)$) it appeared to be possible in some cases to find quantitative relations between the parameters mentioned above and A , Z , $(N-Z)$. It allows to make consistent evaluation of cross sections of the isotopes of a given group on the base of experimental cross section data for other isotopes which have the same characteristics.

The systematics for (n,2n) and (n,3n) reaction excitation function were published in the work /1/ and in this paper only brief results with some additions and corrections are given. The main purpose of this paper is to describe systematics of excitation function parameters for (n,p), (n,a), (n,np) reactions.

1. The (n,2n) and (n,np) - reactions.

The value of cross section in the maximum of (n,2n) reaction excitation function depends essentially on interrelation of (n,2n) and (n,np) reaction energies ($Q_{n,2n}$ and $Q_{n,np}$, respectively). Let us consider two cases: $Q_{n,2n} \leq Q_{n,np}$ and $Q_{n,2n} > Q_{n,np}$.

1.1. $Q_{n,2n} \leq Q_{n,np}$.

The maximum (top) cross sections of the (n,2n)-reaction excitation functions are determined by the following equation /1/:

$$\sigma_{\text{top}} = 65.4 A^{2/3}, \text{ mb}, \quad (1)$$

where A is atomic mass number.

This maximum (top) value is reached in the neutron energy region of 5 - 8 MeV (in the most cases 6-7 MeV) above the reaction thresholds. The analysis of experimental and theoretical excitation functions shows that this equation is reasonable for any A, if the condition $Q_{n,2n} \leq Q_{n,np}$ is fulfilled. In the range of $A \approx 50 - 210$, where there are enough experimental data this is proved quite well. But in the range of $A < 50$ there are no experimental data near maximum of (n,2n) reaction excitation functions and comparison with theoretical curves can be only used. In Fig.1-4 some examples are given for nuclides with $A=18-40$. It is seen that the maximum values of theoretical excitation functions calculated using STAPRE code /2 /are close to the values obtained from the equation (1).

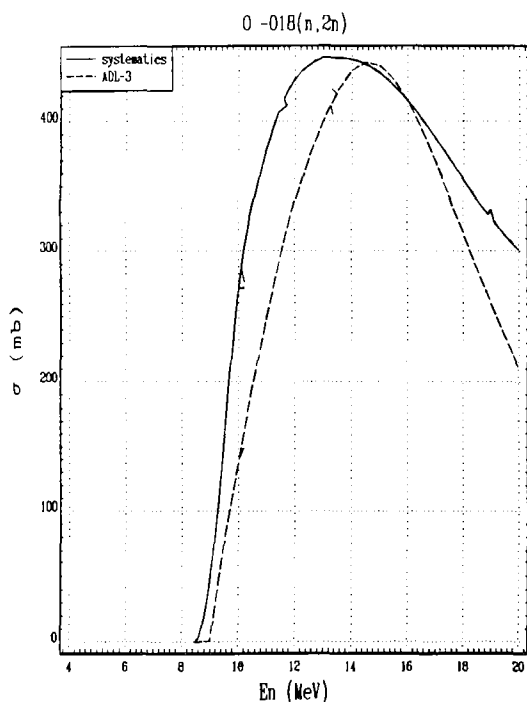


Fig.1. The $^{18}\text{O}(n,2n)^{17}\text{O}$ reaction.

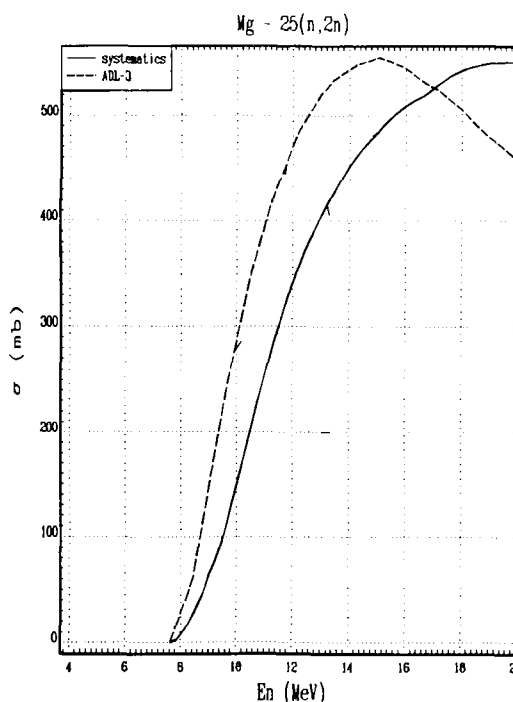
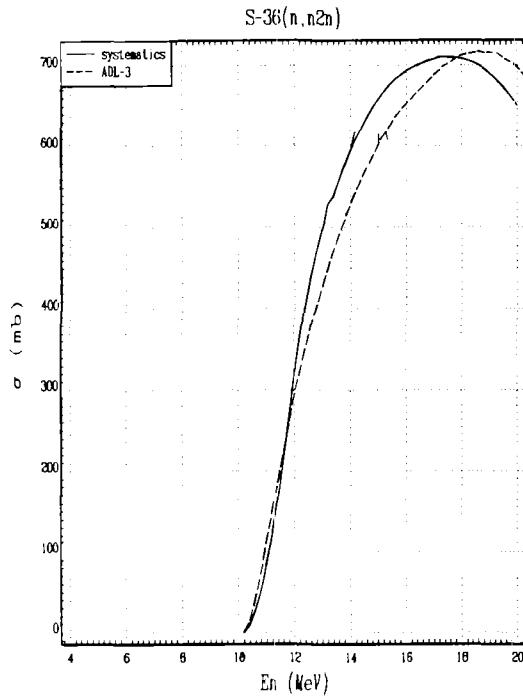
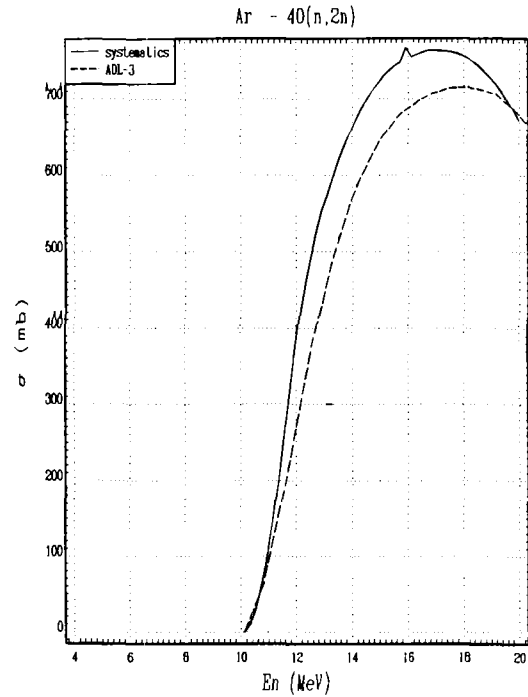


Fig.2. The $^{25}\text{Mg}(n,2n)^{24}\text{Mg}$ reaction.

Fig.3. The $^{36}\text{S}(n,2n)^{35}\text{S}$ reaction.Fig.4. The $^{40}\text{Ar}(n,2n)^{39}\text{Ar}$ reaction.

1.2. The $(n,2n)$ -reaction excitation functions in the neutron energy region from the threshold to the maximum of excitation functions are similar and can be described by the normalized excitation function in scales $(\sigma/\sigma_{\max} - \Delta E/\Delta E_{\max})$ (Table 1), where σ_{\max} - cross section at the maximum, $\Delta E = E - E_{\text{th}}$, E_{th} - threshold energy, $\Delta E_{\max} = E_{\max} - E$, E - neutron energy, E_{\max} - neutron energy at the maximum of excitation function and corresponds to $(n,3n)$ reaction threshold.

If $Q_{n,2n} < Q_{n,np}$, the σ_{\max} is equal to σ_{top} (see eq.1).

If $Q_{n,2n} > Q_{n,np}$, then σ_{\max} is determined from experimental data or from other considerations however the shape of excitation function is described by the same normalized function.

Table 1. Normalized excitation function of $(n,2n)$ -reaction

$\Delta E/\Delta E_{\max}$	σ/σ_{\max}	$\Delta E/\Delta E_{\max}$	σ/σ_{\max}
0.05	0.03	0.50	0.81
0.10	0.09	0.55	0.85
0.15	0.18	0.60	0.88
0.20	0.30	0.65	0.91
0.25	0.42	0.70	0.93
0.30	0.53	0.75	0.95
0.35	0.60	0.80	0.97
0.40	0.68	0.85	0.98
0.45	0.75	0.90	0.99

In the work/4/ the following relation was given for calculation of (n,2n) reaction excitation functions in the energy region from the (n,2n) reaction threshold up to the (n,3n) reaction threshold:

$$\sigma = \sigma_{\max} (\Delta E / \Delta E_m)^{1.35} \exp[1.4(1 - \Delta E / \Delta E_m)], \quad (2)$$

This relation gives a reasonable result but the normalized function (Table 1) is better adjusted to experimental data (especially near threshold) and recommended for the use instead of the relation.

1.3. $Q_{n,2n} > Q_{n,np}$

In this case the (n,2n) cross section in the maximum of the excitation function is below the values, calculated from the equation (1), and the difference is determined by contribution of the (n,np) reaction cross section at the same neutron energy. At this condition the maxima both reaction excitation functions lies near 20 MeV and the sum of the (n,2n) reaction cross section and the (n,np) reaction cross section is approximately equal to σ_{top} .

$$\sigma_{\text{top}} \approx \sigma_{n,2n} + \sigma_{n,np} \quad (3)$$

In this case ($Q_{n,2n} > Q_{n,np}$) the $Q_{n,3n}$ is above ~20 MeV.

In the Fig. 5 one can see the (n,2n) and (n,np) reaction excitation functions of ^{58}Ni evaluated on the base of experimental data.

The values of (n,2n) and (n,np) reaction cross sections at the maximum of its excitation functions can be evaluated as 80 and 870 mb, respectively. In the sum it gives 950 mb that is close to 978 mb, predicted by equation (1) for σ_{top} .

The ^{58}Ni (n,np) reaction excitation function, plotted in Fig.5, in the energy range above Coulomb barrier can be approximated by the normalized function(see Table 2).

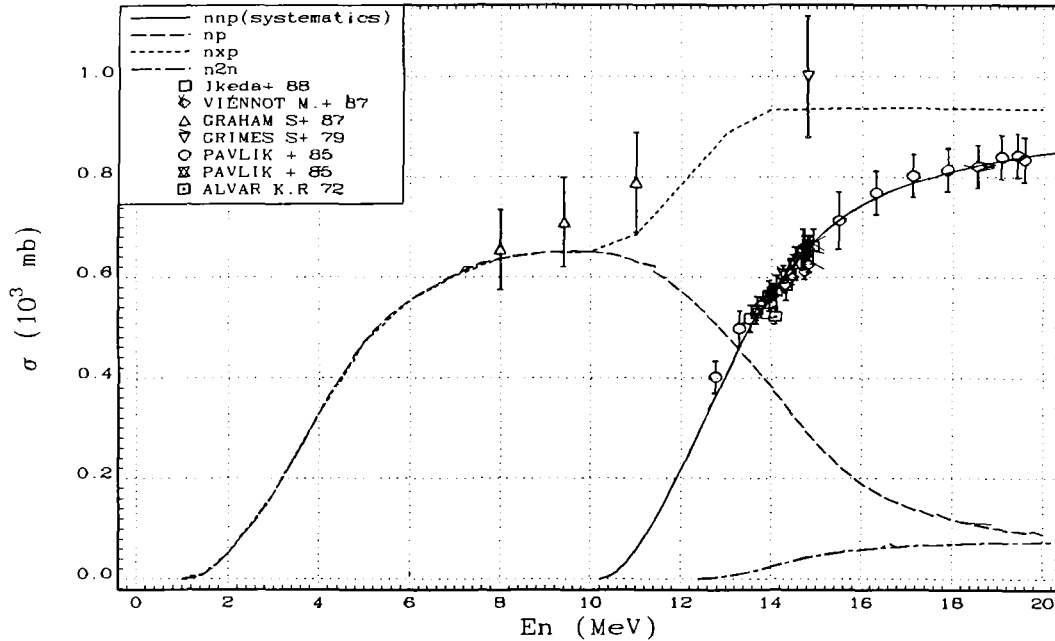


Fig.5. The (n,2n), (n,p), (n,np) and (n,xp) reactions on ^{58}Ni .

Table 2. Normalized excitation function of (n,np)-reaction.

$\Delta E / \Delta E_{\max}$	σ / σ_{\max}	$\Delta E / \Delta E_{\max}$	σ / σ_{\max}
0.05	0.04	0.50	0.88
0.10	0.14	0.55	0.90
0.15	0.26	0.60	0.92
0.20	0.40	0.65	0.94
0.25	0.53	0.70	0.955
0.30	0.64	0.75	0.965
0.35	0.73	0.80	0.975
0.40	0.79	0.85	0.980
0.45	0.84	0.90	0.990

The sum of (n,np) and (n,p) reaction excitation functions (see Fig.5) gives the (n,xp) reaction excitation function. As one can see there is a reasonable agreement with the experimental (n,xp) reaction cross sections measured by S.Grimes et al/6 /and S.Saraf et al/ 7 /.The (n,p) reaction excitation function was evaluated on the base of reliable experimental data.

1.4. If $Q_{n,2n} > Q_{n,np}$ there is a systematic trend in the dependence of the (n,2n) reaction cross section in the maximum excitation function (about 20-22 MeV) on the value $\Delta Q = Q_{n,2n} - Q_{n,np}$ for isotopes with the same (N-Z).

In this case the (n,2n) reaction cross section at the maximum of the excitation function decreases with the increase of ΔQ . It is clearly observed in the chains of isotopes:

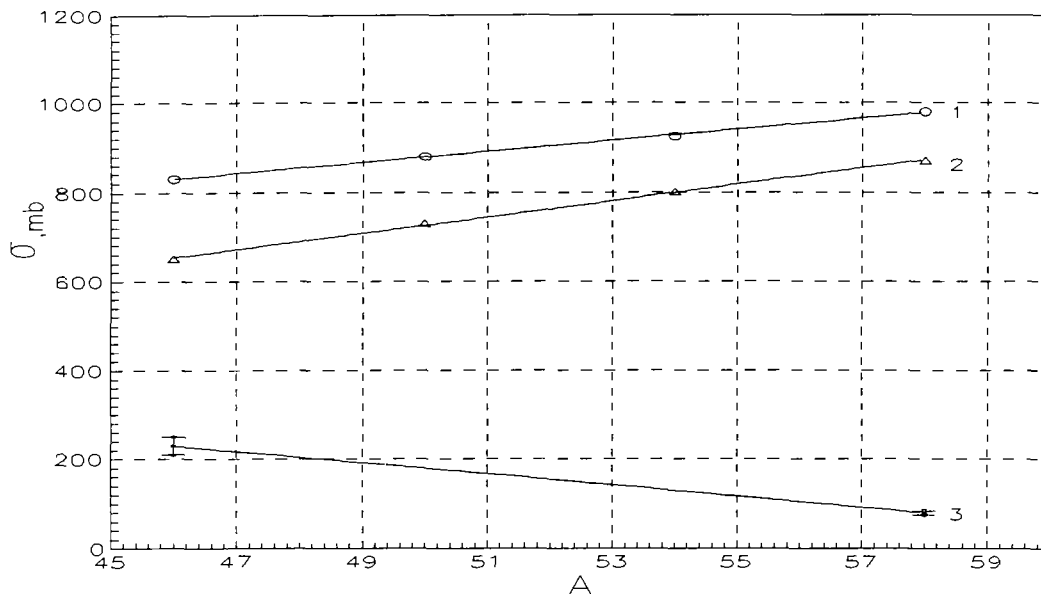
- ^{19}F , ^{23}Na , ^{27}Al , ^{31}P , ^{35}Cl , ^{39}K (N-Z=1),
- ^{46}Ti , ^{50}Cr , ^{54}Fe , ^{58}Ni (N-Z=2),
- ^{55}Mn , ^{59}Co , ^{63}Cu (N-Z=5).

Although there are no reliable experimental data for the chain of isotopes ^{12}C , ^{14}N , ^{16}O , ^{20}N , ^{24}Mg , ^{28}Si , ^{36}Ar and ^{40}Ca (N-Z=0), the existing experiments and some model calculations indicate on decreasing the cross sections with growth of ΔQ .

The approach above described for ^{58}Ni and the mentioned systematic trend can be used for consistent evaluation (n,2n) and (n,np) reaction cross sections of the isotopes with the same (N-Z).

In the Fig.6 there are curve for $\sigma_{\text{top}}(n,2n)$ of ^{46}Ti , ^{50}Cr , ^{54}Fe , ^{58}Ni , evaluated values for (n,2n) reaction cross sections of ^{54}Fe and ^{58}Ni and for (n,np) reaction cross section of ^{58}Ni at the maximum of excitation functions. The evaluation was made by extrapolation of experimental data from the energy region below 20 MeV up to the energy region at the maximum of excitation functions.

We can draw line through the points of (n,2n) cross sections for ^{46}Ti and ^{58}Ni , predict (n,2n) reaction cross sections for ^{50}Cr , ^{54}Fe at the maximum excitation functions and subtracting the (n,2n) cross sections (curve 2) from the $\sigma_{\text{top}}(n,2n)$ (curve 1) to obtain the (n,np) cross sections (curve 3) for the isotopes mentioned.



T Fig.6. The $(n,2n)$ and (n,np) reactions cross sections at maximum of excitation functions against mass number A: 1 - $\sigma_{\text{top}}(n,2n)$, 2 - $\sigma(n,np)$, 3 - $\sigma(n,2n)$.

In Fig. 7-9 the (n,np) reaction excitation functions, evaluated on the base of so obtained maximum cross sections and the normalized function (see Table 2) are given in comparison with the (n,xp) reaction cross sections, measured in the works /6-8/.

One can see that the sum of evaluated (n,p) and (n,np) reaction cross sections agrees with (n,xp) reaction cross sections within uncertainties of experimental data.

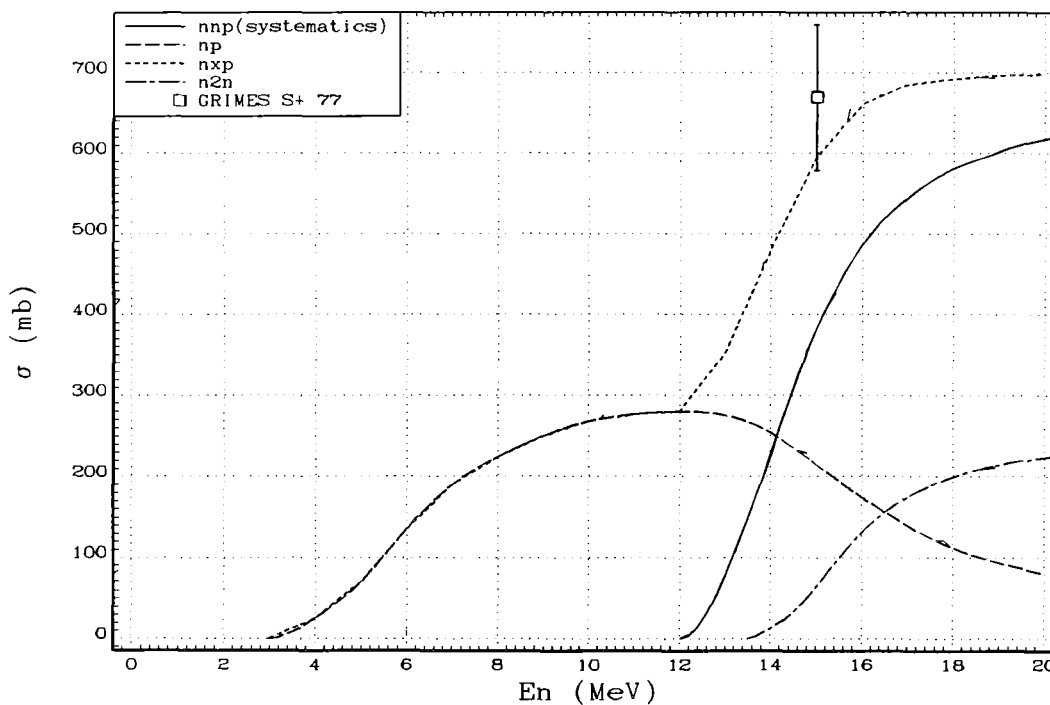


Fig.7. The $(n,2n)$, (n,p) , (n,np) and (n,xp) reactions on ^{46}Ti .

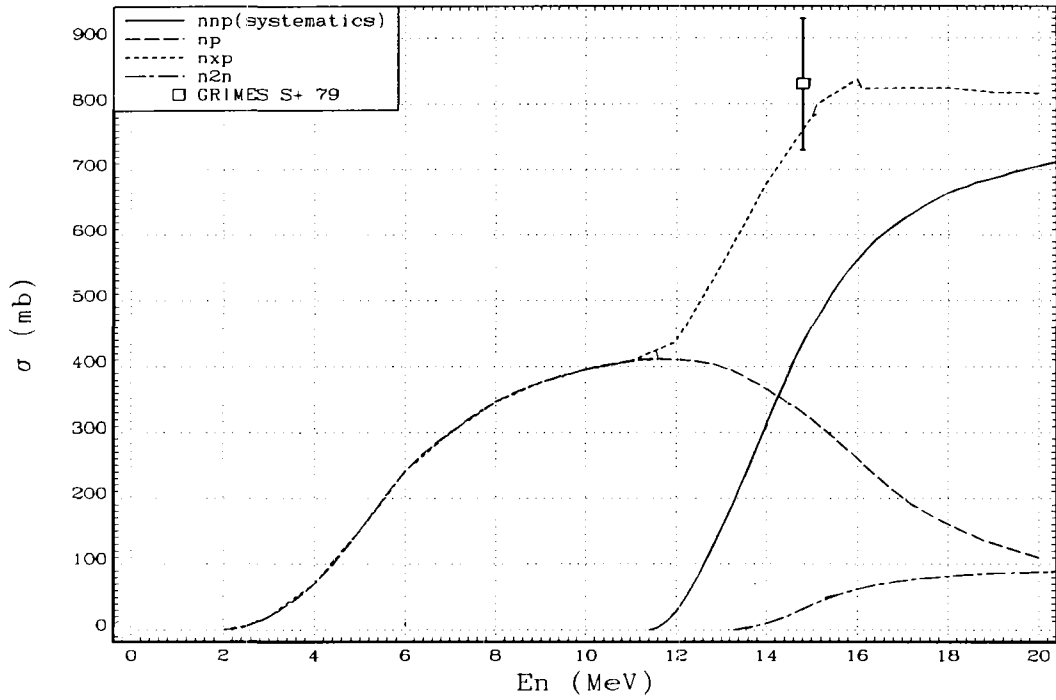


Fig.8. The (n,2n), (n,p), (n,np) and (n,xp) reactions on ^{50}Cr .

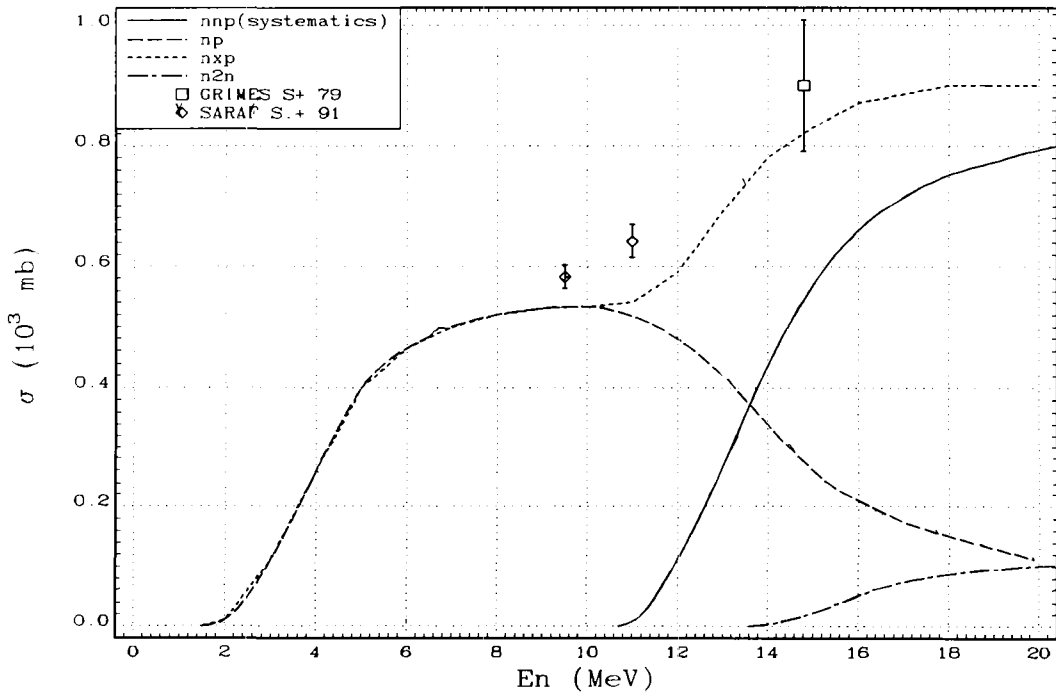
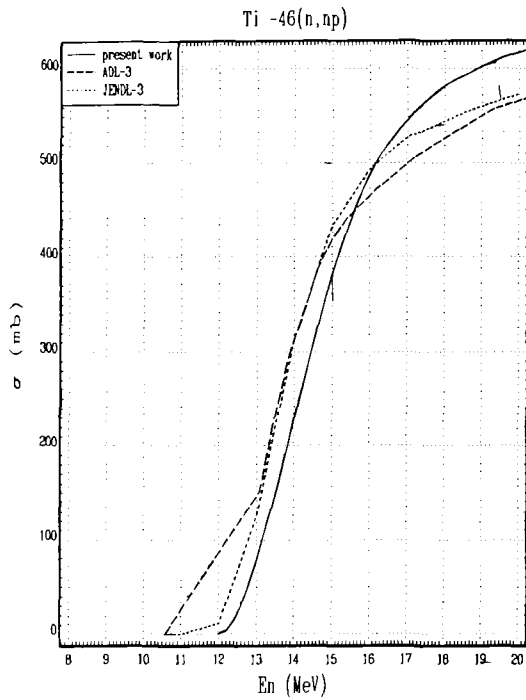
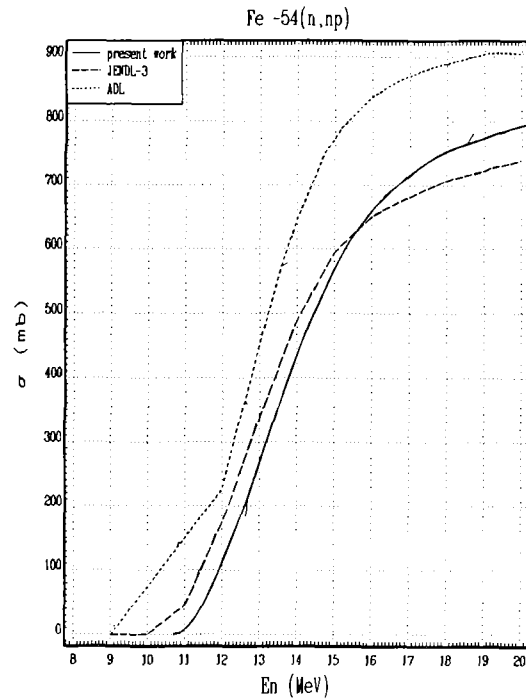


Fig.9. The (n,2n), (n,p), (n,np) and (n,xp) reactions on ^{54}Fe .

A comparison of evaluated (n,np) reaction excitation functions with theoretical curves calculated by STAPRE code/2/ shows close agreement in shapes (see Fig. 10 and-11).

Fig.10. The $^{46}\text{Ti}(n,np)$ reaction .Fig.11. The $^{54}\text{Fe}(n,np)$ reaction..

2.The (n,3n) reaction.

The shapes of the (n,3n) reaction excitation functions are similar in the neutron energy region from the threshold up to the neutron energy at the maximum of the excitation function (at 10-11 MeV above the threshold) and can be approximated by the equation:

$$\sigma = \sigma_{\max} (\Delta E / \Delta E_m)^{3.3} \cdot \exp[3.3(1 - \Delta E / \Delta E_m)], \quad (4)$$

where ΔE and ΔE_m are counted from the (n,3n) reaction threshold, σ_{\max} is determined by the equation:

$$\sigma_{\max} \approx 10 A \text{ mb}, \quad (5)$$

where A is atomic mass number.

These equations describe (within experimental uncertainties) the available experimental (n,3n) reaction excitation functions. The use of the equations for taking into account of (n,3n) reaction competition in calculations of (n,2n) reaction excitation function gives the results for (n,2n) reaction cross section which agree very well with experimental data.

In Fig.12-13 the (n,2n) and (n,3n) reaction cross sections calculated on the base of the systematics above described are given for ^{197}Au and ^{209}Bi . It was proposed that ΔE_m for (n,3n) reaction excitation functions is equal to 10 Mev. This value was determined from the experimental data for (n,3n) reaction cross sections in the energy region from the threshold up to 26 MeV, available from the measurements of L.Veeser et al./9/ and B.Bayhurst et al./10/.

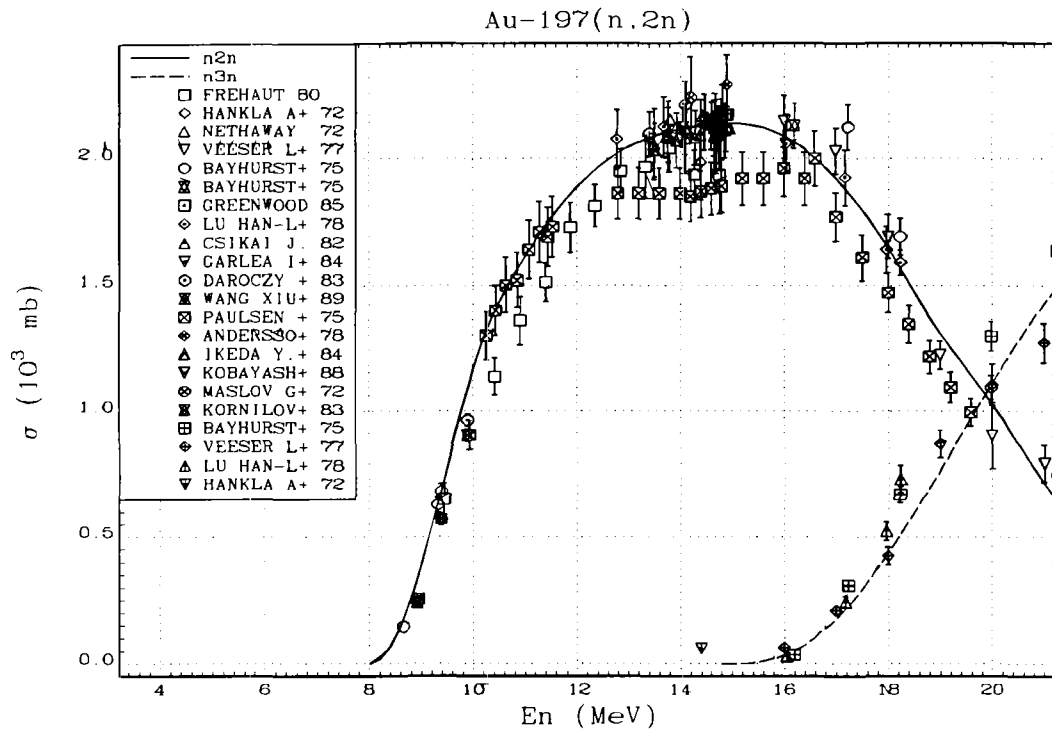


Fig.12. The (n,2n) and (n,3n) reactions on ^{197}Au .

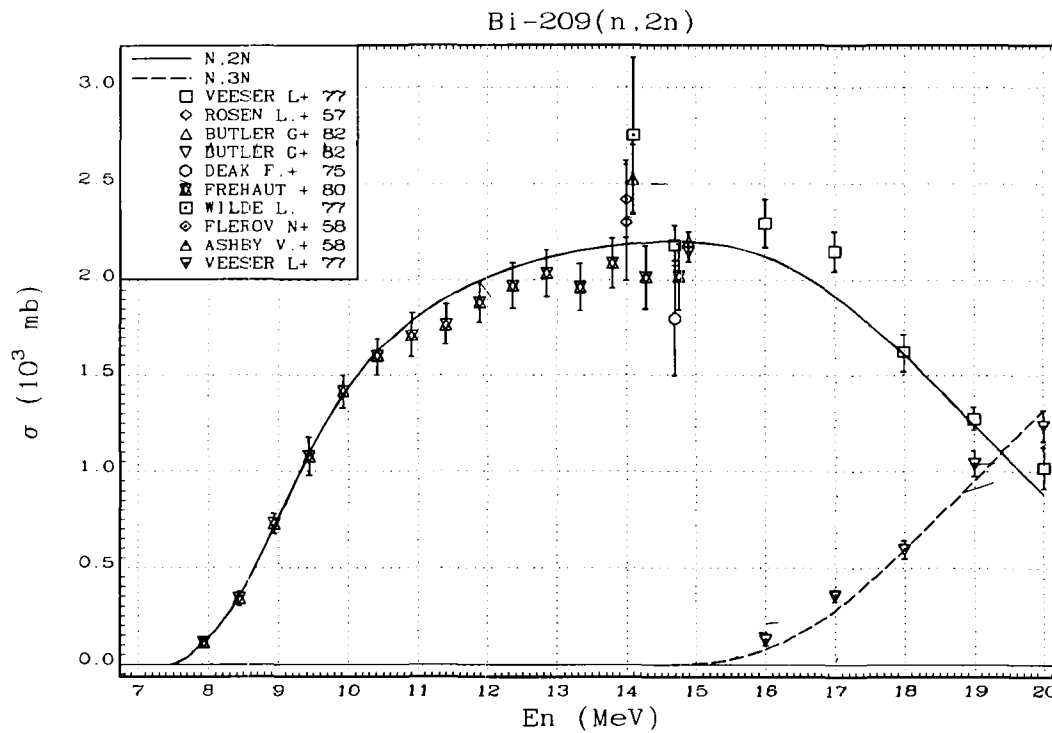


Fig.13. The (n,2n) and (n,3n) reactions on ^{209}Bi .

3. The (n,p) and (n,a) - reactions.

3.1. The maximum of (n,p) - reaction cross sections for the isotopes of a given element decreases exponentially. Within the spread of experimental data the value of $\ln\sigma_{n,p}^{\max}$ decreases linearly as a function of (N-Z) or A. In Fig.14, for example, the dependences of $\ln\sigma_{n,p}^{\max}$ on neutron excess (N-Z) are given for isotopes of elements with Z=20-30.

For the different elements these linear dependences are practically parallel and equidistant (this was pointed by D.Gardner in 1962 for 14.5 MeV neutrons). However with the increasing of Z a slope of the lines decreases.

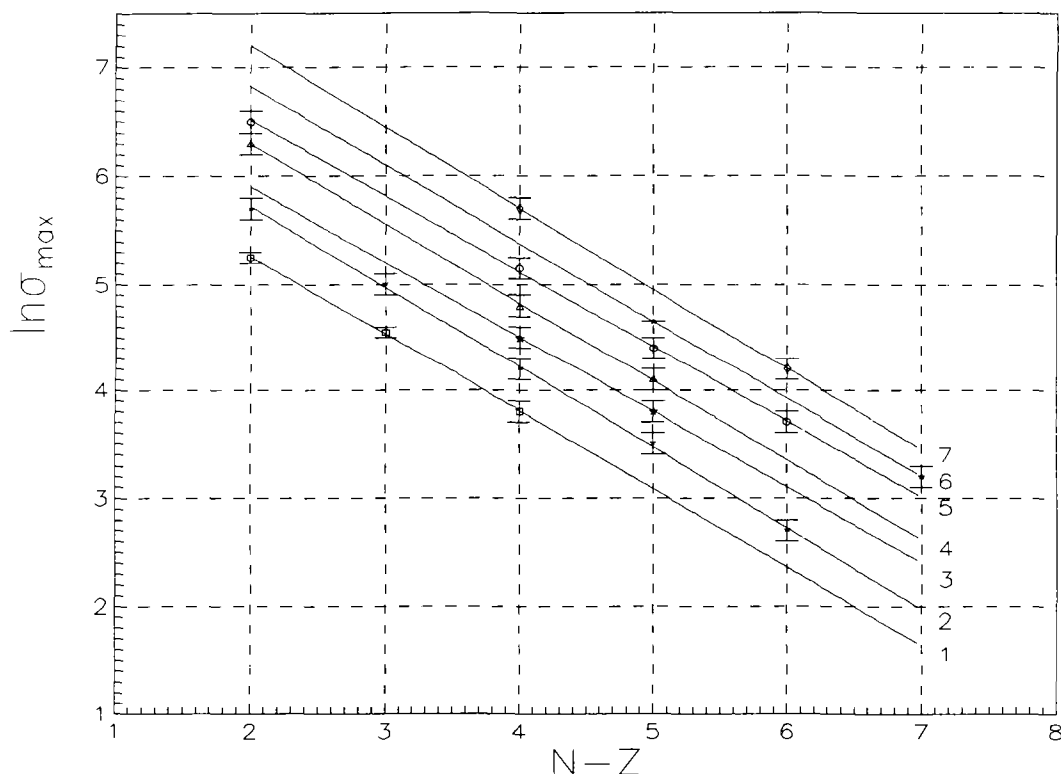


Fig.14. The (n,p) reaction cross sections at maximum of excitation functions against neutron excess (N-Z). 1-Ca, 2-Ti, 3-Cr, 4-Fe, 5-Ni, 6-Cu, 7-Zn.

The value $\ln\sigma_{n,p}^{\max}$ increases also practically linearly as a function of Z for the isotopes with the same (N-Z)(Fig.15). These dependences for different elements seem to be also parallel and equidistant.

Those systematics are proved for the mass numbers from 10 to 100 and for (N-Z) = 0 -15.

There are not so many reliable experimental data to determine the cross sections at the maximum of excitation function with high accuracy, however in several cases one can observe an effect of splitting the lines as a result of different values of $\Delta Q=(Q_{nnp}-Q_{np})$.

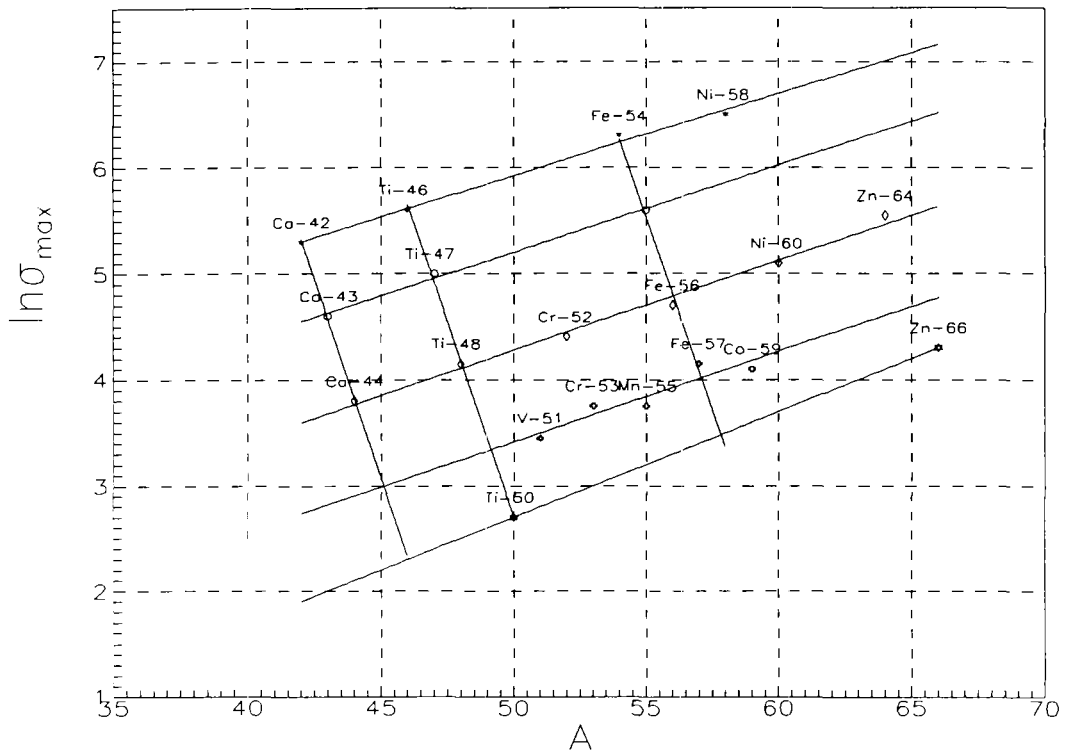


Fig.15. The (n,p) reaction cross sections at the maximum of the excitation functions against mass number A .

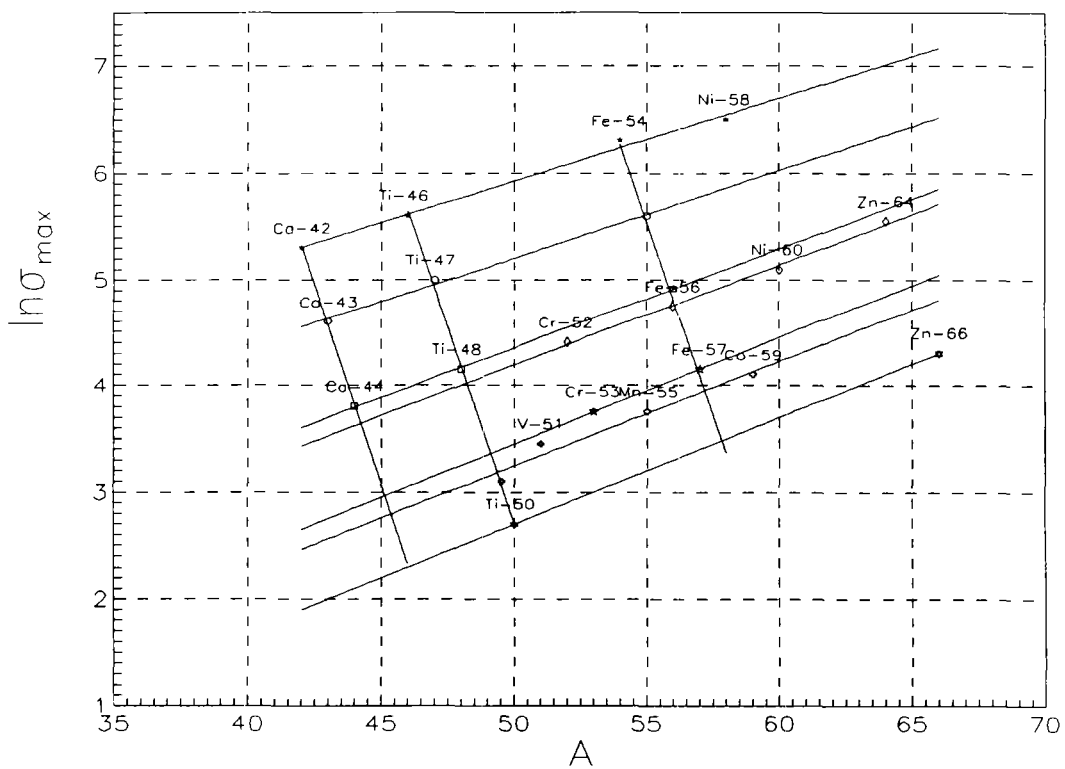


Fig.15a. The (n,p) reaction cross sections at the maximum of the excitation functions against mass number A .

In Fig.15a one can see the maximum of (n,p) reaction cross sections for isotopes with $(N-Z)=5$. For the ^{53}Cr and ^{57}Fe isotopes the values of $(Q_{\text{nnp}} - Q_{\text{np}})$ are equal to 8.5 MeV and 8.7 MeV, respectively, and for the ^{51}V and ^{55}Mn isotopes - 6.4 MeV and 6.2 MeV. It seems to be a reason why there are two close but different lines.

The same picture is for ^{48}Ti and ^{64}Zn ($\Delta Q=8.2$ and 7.9 MeV) and ^{52}Cr , ^{56}Fe , ^{60}Ni ($\Delta Q=7.3, 7.3, 7.5$ MeV, respectively). The isotopes with the same ΔQ lies on the same line. There are no accurate experimental data for other chains, but it seems that the effect is less for heavier isotopes. In any case for Zr and Mo isotopes the experimental data available did not allow to reveal it for certain.

An intercomparison of experimental (n,p) reaction excitation functions shows that the shapes of these functions are similar for the isotopes with the same $(N-Z)$ (see Fig.16). The excitation functions, plotted on Fig.16, were evaluated independently for every isotope on the base of quite reliable experimental data, normalized to the same cross section at the maximum of excitation functions and shifted to the same position of the maxima.

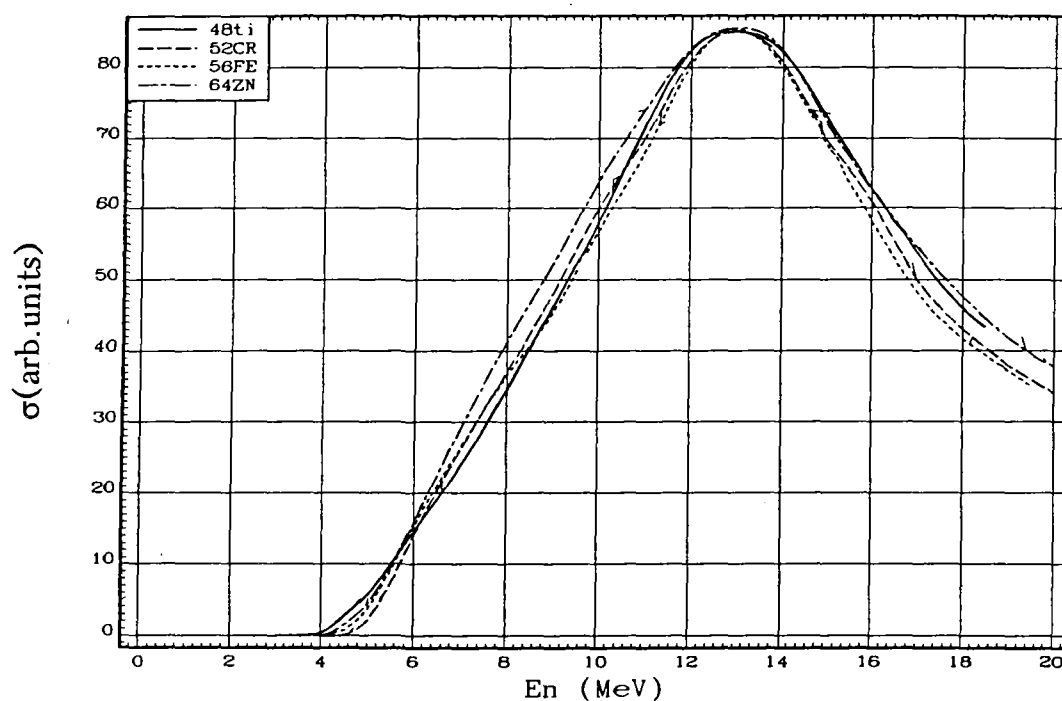


Fig.16. The normalized (n,p) reaction excitation functions for isotopes with $(N-Z)=4$.

For many other isotopes one can observe the same similarity. There are not enough experimental data to determine the limits of such systematics. However in those cases where there are no structure in excitation functions near threshold one should consider a good measured (n,p) reaction excitation function of any isotope as first approximation for excitation functions of the isotopes with the same neutron excess $(N-Z)$ and with scarce or contradictory experimental data. Together with the systematics of the maximum (n,p) reaction cross sections it

allows to predict with acceptable uncertainty the the excitation functions of isotopes, for which the experimental data are absent.

As far as a position of the maxima of the (n,p) reaction excitation functions above $E_{th}+Q_C$ (where Q_C is Coulomb barrier) is proportionally to the value of $(Q_{nnp}-Q_{np})$, where Q_{nnp} and Q_{np} are reaction energies of (n,np) and (n,p) reactions, respectively, it is useful to compare these values for different isotopes in the process of selection and evaluation of the (n,p) reaction excitation functions.

3.2. There are no enough experimental information to evaluate reliably the (n,α) - reaction cross sections in the maximum of the excitation functions. However the available experimental data allows to propose that the maximum cross section of (n,α) - reaction excitation function for the isotopes of a given element decreases exponentially and within of the spread of experimental data the value $\ln\sigma_{n,\alpha}^{max}$ decreases practically linearly as a function of A or $(N-Z)$.

For the different elements these dependences are almost parallel and equidistant. The dependence of $\ln\sigma_{n,\alpha}^{max}$ as a function of Z is more weak in comparison with similar dependence for (n,p) reaction cross sections and for adjacent isotopes with the same $(N-Z)$ these values are approximately equal although in more wide range one should notice the increasing of the cross sections. It seems the dependences of $\ln\sigma_{n,\alpha}^{max}$ for the different $(N-Z)$ to be parallel.

The shapes of the (n,α) -reaction excitation functions are similar for the isotopes with the same $(N-Z)$ (see Fig.17).

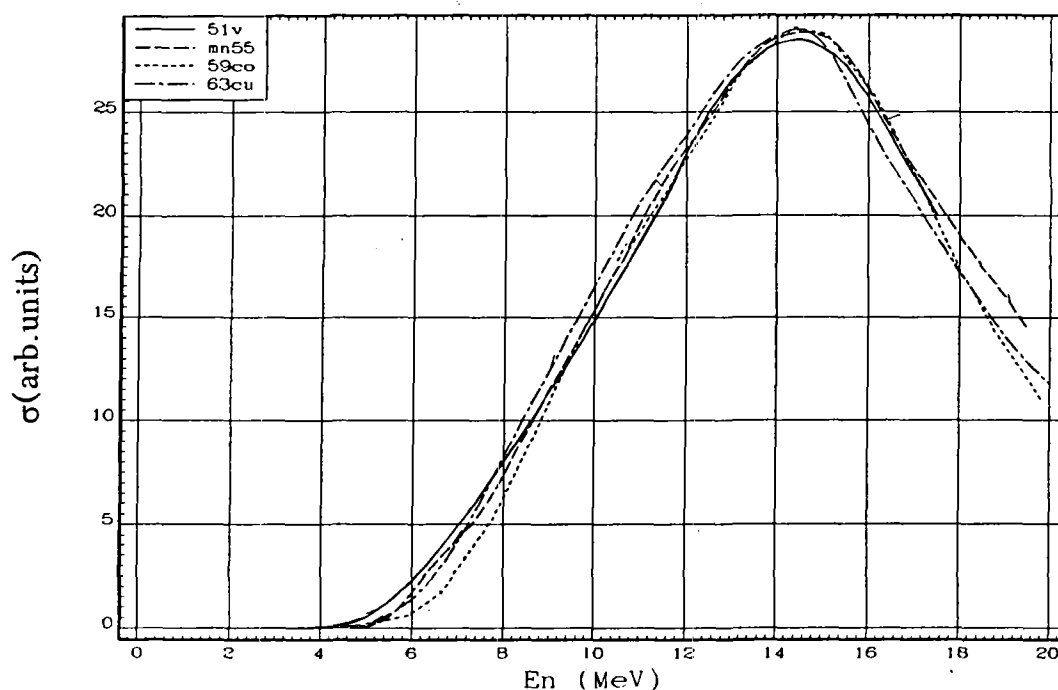


Fig.17. The normalized (n,α) reaction excitation functions for isotopes with $(N-Z)=5$.

These curves are also evaluated independently for each isotopes on the base of experimental data and are normalized to the same cross section maximum and shifted to the same position of the maxima.

Conclusion.

The existing systematics play important role in evaluation and prediction of threshold reaction cross sections in the neutron energy range of 14-15 MeV and are also used for normalization of theoretical excitation functions.

The systematics, described in this paper, allow to expand the number of parameters, which can be used for evaluation of cross sections and selection of theoretical excitation functions, and thus to provide more reliable evaluated data in the whole energy range from the reaction threshold up to 20 MeV.

However, a further work is needed to determine more exactly predictive possibilities of these systematics and limits of its application.

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