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Comparison of Threshold Reaction Cross Sections for the Ti, V, Cr, Fe, Ni, Cu and Zn Isotopes from Evaluated Data Libraries

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Abstract

Evaluated excitation functions for various threshold reactions on Ti, V, Cr, Fe, Ni, Cu and Zn isotopes are compared to reveal discrepancies between different nuclear data libraries. The recommended excitation functions for (n,p), (n,np), (n,α) and (n,2n) reactions, evaluated on the basis of empirical systematics, are given for comparison to facilitate selection of a more reliable data. The available experimental data are also plotted.

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COMPARISON OF THRESHOLD REACTION CROSS SECTIONS FOR THE TI, V, CR, FE, NI,CU AND ZN ISOTOPES FROM EVALUATED DATA LIBRARIES.

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ABSTRACT

Evaluated excitation functions for various threshold reactions on Ti, V, Cr, Fe, Ni, Cu and Zn isotopes are compared to reveal discrepancies between different nuclear data libraries. The recommended excitation functions for (n,p), (n,np), (n,) and (n,2n) reactions, evaluated on the basis of empirical systematics, are given for comparison to facilitate selection of a more reliable data. The available experimental data are also plotted.

Most of the excitation functions in the evaluated data libraries are calculated on the basis of theoretical models with the parameters adjusted to the experimental data available. However, because of the differences in models and codes, input parameters, and experimental data used for the adjustment there are large discrepancies in evaluated data, available in different evaluated data libraries, even for the isotopes and reactions of great importance for technological applications. We have compared all evaluations of threshold reaction excitation functions for Ti, V, Cr, Fe, Ni, Cu, Zn isotopes which are available in the libraries BROND-2 /1/, ENDF/B-VI /2/, JEF-2 /3/, JENDL-3 /4/, ADL-3 /5/, and EAF-97 /6/.

To facilitate the selection of the most reliable excitation functions from these libraries we propose our recommended curves which result from the empirical systematics without using any theoretical model calculations. These systematics are based on the analysis of the experimental data. Because our evaluation method is independent from the model calculations we consider the theoretical excitation functions which are in closer agreement with our recommended excitation functions as more reliable.

The recommended excitation functions were evaluated on the basis of the systematics developed in the works /7-10/. Below, the essential features of those systematics and evaluation procedure of our recommended curves are given.

1. The shapes of (n,2n) reaction excitation functions are similar in the energy region from the (n,2n) threshold up to the (n,3n) reaction threshold.

For $Q_{n2n} < Q_{nnp}$ the maximum values (σ_{top}) of (n,2n) reaction cross sections are determined by the relation

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

where A is the atomic mass number.

For $Q_{n,2n} > Q_{n,np}$ the (n,2n) cross section in the maximum of the excitation function is lower than the values calculated using Eq. 1, and the difference is determined by the contribution of the (n,np) reaction cross section at the same neutron energy. The maximum of both reaction excitation functions lies near $E_n=20$ MeV and the sum of the (n,2n) and (n,np) reaction cross sections is approximately equal to σ_{top}

$$\sigma_{\rm top} \approx \sigma_{\rm n,2n} + \sigma_{\rm n,np}, \qquad (2)$$

providing the value of $Q_{n,3n}$ is above ~20 MeV.

The (n,2n) cross section in the energy region from the threshold up to the maximum of excitation function (i.e. up to the (n,3n) reaction threshold) was calculated using universal normalized excitation function (see /7-10/) in scales ($\sigma/\sigma_{max} - \Delta E/\Delta E_{max}$). Here σ_{max} is cross section at the maximum, $\Delta E=E-E_{th}$, E_{th} - threshold energy, $\Delta E_{max}=E_{max}-E_{th}$, E is a neutron energy, and E_{max} - neutron energy at the maximum of (n,2n) excitation function.

The (n,2n) cross section in the energy region above the (n,3n) reaction threshold was calculated by subtracting the (n,3n) reaction cross section from the σ_{top} (n,2n).

2. The shapes of (n,3n) reaction excitation functions are similar in the energy region between the threshold and the energy of the maximum of the excitation function and can be approximated by the equation

$$\sigma = \sigma_{\max} \left(\Delta E / \Delta E_m \right)^{3.3} \cdot \exp[3.3(1 - \Delta E / \Delta E_m)].$$
(3)

Here ΔE and ΔE_m are counted from the (n,3n) reaction threshold.

The maximum value (σ_{max}) of (n,3n) reaction excitation function are determined by relation σ_{max} (n,3n) = 10A [mb].

It was proposed that ΔE_m for (n,3n) reaction excitation functions is equal to 10 MeV. This value was determined from available experimental data.

3. The shapes of (n,p) reaction excitation functions are similar for the isotopes with the same (N-Z).

The maximum (n,p) reaction cross sections decrease linearly as a function of A for the isotopes of a given element and increase linearly as a function of Z for the isotopes with the same (N-Z).

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

The maximum (n,α) reaction cross sections decrease linearly as a function of A for the isotopes of a given element and increase linearly as a function of Z for the isotopes with the same (N-Z).

5. The position of the maximum of (n,p) excitation function relative to the threshold is proportional to the difference $(Q_{nnp} - Q_{np})$.

6. The position of the maximum of (n,α) reaction excitation function relative to the threshold is proportional to the difference $(Q_{nn\alpha} - Q_{n\alpha})$.

In conclusion we should like to note that we are far from considering our recommended curves as the most accurate. However, our recommendations are based on the systematic trends, which were extracted from analysis of available experimental data. Our point of view is that they describe better the physics of the processes. We propose that the curves which deviate considerably from our recommendations should be checked. It is very probable that some of them are wrong.

Acknowlegement

We express our thanks to Dr. M. Herman for support and editing the text.

Some comments to the Figures:

1. In Figures 1, 17, 20, 24, 34 and 35 the evaluated data for (n,np) reaction are plotted. The experimental data by Grimes and Saraf are given for comparison. One should keep in mind that these data are the sums of the (n,p) and (n,np) reaction cross sections.

2. In many Figures the number of evaluated curves is less than the number of their abbreviations in the legend field. It means that the data in some libraries are the same. Very often the libraries EAF-97 and JEF-2 contain the data taken from other libraries. We indicate this in the List of Figures and in captions to the figures.

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Fig.1. Cross section of 46 Ti(n,np) 45 Sc reaction.



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Fig.36. Cross section of ${}^{56}Fe(n,\alpha){}^{53}Cr$ reaction.



Fig.37. Cross section of 57 Fe(n,2n) 56 Fe reaction. EAF-97 = JEF-2.2.



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Fig.56. Cross section of ${}^{63}Cu(n,\alpha){}^{60}Co$ reaction.



Fig. 57. Cross section of ${}^{65}Cu(n,p){}^{65}Ni$ reaction.



Fig.58. Cross section of ${}^{65}Cu(n,\alpha){}^{62}Ni$ reaction.



Fig.59. Cross section of ${}^{64}Zn(n,2n){}^{63}Zn$ reaction. EAF-97 = ADL-3.



Fig.60. Cross section of ${}^{64}Zn(n,\alpha){}^{61}Ni$ reaction.



Fig.61. Cross section of ${}^{66}Zn(n,p){}^{64}Cu$ reaction.



Fig.62. Cross section of ${}^{66}Zn(n,\alpha){}^{63}Ni$ reaction.



Fig.63. Cross section of ${}^{67}Zn(n,2n){}^{66}Zn$ reaction. EAF-97 = ADL-3.



Fig.64. Cross section of ${}^{67}Zn(n,p){}^{67}Cu$ reaction. EAF-97 = ADL-3.







Fig.66. Cross section of ${}^{68}Zn(n,p){}^{68}Cu$ reaction.



Fig.67. Cross section of ${}^{68}Zn(n,\alpha){}^{65}Ni$ reaction. EAF-97 = ADL-3.



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