Analysis of the cross sections of the formation of nuclei in isomeric states in $(\mathrm{n,p})$ reactions
Анализ сечений образования ядер в изомерных состояниях в $(\mathrm{n,p})$ реакциях

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Проведён анализ надёжности доступных экспериментальных и оценённых данных по сечениям трёх $(\mathrm{n,p})$ ядерных реакций с образованием ядер в долгоживущих изомерных состояниях. Данный анализ мотивирован недавними результатами измерений, выполненных в НИЦ «Курчатовский институт», на нейтронах с энергиями, близкими к 14 МэВ. Продемонстрирована возможность использования программного комплекса TALYS-1.9 для оценки сечений упомянутых реакций.

Analysis of the reliability of available experimental and evaluated data on cross sections for three $(\mathrm{n,p})$ reactions leading to the formation of isotopes in isomeric metastable states is performed. This examination is motivated by recent measurements carried out with neutrons with energies of about 14 MeV at the NRC "Kurchatov Institute". The possibility of using the TALYS-1.9 software package in order to evaluate cross sections of mentioned reactions is demonstrated.

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Introduction

In nuclear facilities suitable for controlled thermonuclear fusion reaction $\mathrm{d} + \mathrm{t} \to {}^4\mathrm{He} + \mathrm{n}$ neutrons with an energy of 14.1 MeV are formed. These neutrons interact with the nuclei of atoms of construction materials of said facilities and, in particular, nuclei in metastable (isomeric) states are formed as a result. They decay with the emission of high-energy γ-rays, which should be taken into account while designing these facilities. Therefore, numerical evaluations of cross sections of these reactions are of interest.

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Recently, measurements of the rate of nuclei formation in isomeric states in several reactions initiated by neutrons with energies near 14 MeV have been made at the NRC "Kurchatov Institute" [1]. The measured rates can be compared to the calculated rates of the corresponding reactions using their cross sections. This article discusses currently available data, both measured and estimated, on cross sections of three reactions, $^{58}\mathrm{Ni}(\mathrm{n,p})^{58\mathrm{m}}\mathrm{Co}$, $^{90}\mathrm{Zr}(\mathrm{n,p})^{90\mathrm{m}}\mathrm{Y}$, and $^{91}\mathrm{Zr}(\mathrm{n,p})^{91\mathrm{m}}\mathrm{Y}$, studied in [1].

Analysis Method

According to [1], the cross sections of the formation of nuclei in isomeric states are rather poorly represented in the nuclear databases. In particular, the cross sections for the three $(\mathrm{n,p})$ reactions mentioned above are available only in TENDL-2021 (TALYS Evaluated Nuclear Data Library) [2]. The data provided by this library are obtained via TALYS-1.9 [3] software package calculations. There exist various programs that permit simulation of nuclear reactions with standardised parameters from the Reference Input Parameter Library (RIPL) [4]. However, the data presented in TENDL-2021 is typically obtained with some of parameters different from those included in the RIPL.

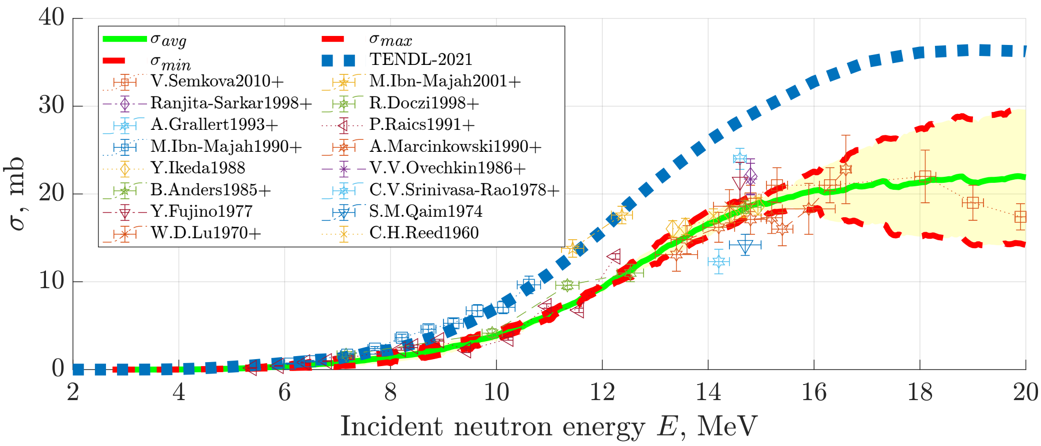

Figure 1. Formation cross section of isomeric (m) state in the $^{91}\mathrm{Zr}(\mathrm{n,\ p})^{91\mathrm{m}}\mathrm{Y}$ reaction as a function of incident neutron energy.

Figures 1, 2, and 3 show cross sections estimates from TENDL-2021 and experimental data of these cross sections taken from the EXFOR [5] database. It can be seen that the estimates agree well with the experimental points for the cases of $^{90\mathrm{m}}\mathrm{Y}$ and $^{58\mathrm{m}}\mathrm{Co}$ isomers formation, but in the case of $^{91\mathrm{m}}\mathrm{Y}$ isomer the estimate lies well above the points. That is why we performed additional calculations using TALYS-1.9. Main advantages of TALYS-1.9 package is that it is open-source, free and well documented. We evaluated cross sections for three $(\mathrm{n,p})$ reactions of interest with incident neutron energy up to 20 MeV.

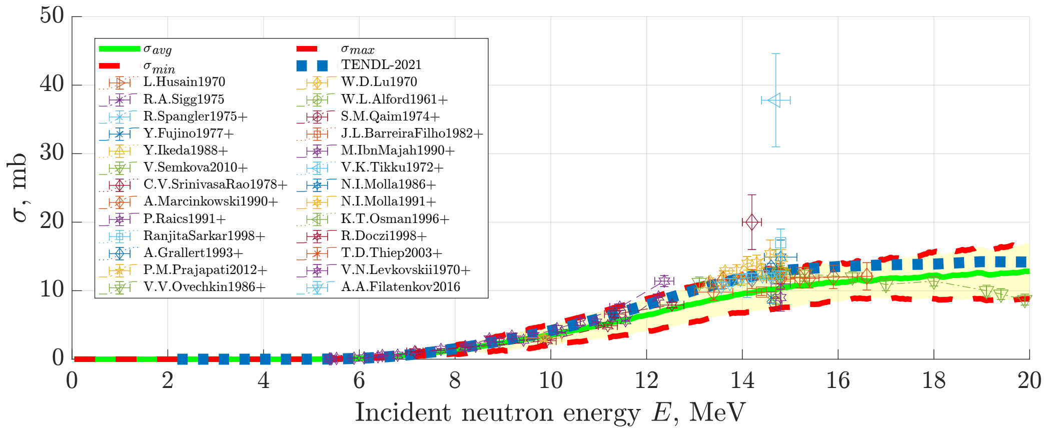

Figure 2. Formation cross section of isomeric (m) state in the ^{90}Zr(n, p)$^{90\text{m}}$Y reaction as a function of incident neutron energy.

These reactions undergo the formation of excited compound nuclei which makes calculations of cross sections highly sensitive to the chosen model of density of excited levels. The TALYS-1.9 package includes 6 models for level density. The first 3 of them are Composite Gilbert-Cameron Model [6], The Back-Shifted Fermi Gas Model [7] and Generalised Superfluid Model [8, 9]. The next 3 models are based on various combinatorial calculations, the reliability of which is not more than that of the previous 3 models.

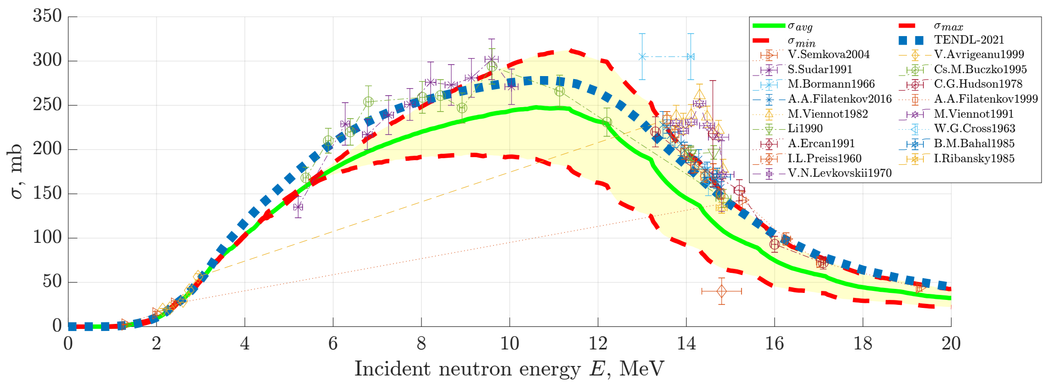

Figure 3. Formation cross section of isomeric (m) state in the ^{58}Ni(n, p)$^{58\text{m}}$Co reaction as a function of incident neutron energy.

Results and Discussion

For the first 3 level density models the corresponding cross sections $\sigma_1(E)$, $\sigma_2(E)$ and $\sigma_3(E)$ for each of the aforementioned reactions were calculated (with all model parameters taken from the RIPL). These cross sections are functions of incident neutron energy E varying from threshold to 20 MeV. After comparing the results with the EXFOR data it turned out that none of the three models had advantage over the others. At the same time, it was found that the arithmetic mean

$$\sigma_{avg}(E) = \frac{\sigma_1(E) + \sigma_2(E) + \sigma_3(E)}{3} \qquad (1)$$

of these cross sections considered agrees well with experimental data. It can be said that in the case of ^{91m}Y the function $\sigma_{avg}(E)$ is significantly closer to the experimental points than the TENDL-2021 estimate, whereas in the case of ^{58m}Co it is farther away from the points than the TENDL-2021 estimate, but not by much.

In addition, it was discovered that in two (formation of isomers ^{91m}Y and ^{90m}Y) of the three cases considered, the observed spread of experimental points correlates well with a value

$$\Delta\sigma_{avg}(E) = \max\left\{\epsilon_{12}(E), \epsilon_{23}(E), \epsilon_{31}(E)\right\}, \qquad (2)$$

where $\epsilon_{ij}(E) = |\sigma_i(E) - \sigma_j(E)|$. The function $\Delta\sigma_{avg}(E)$ can be interpreted as an uncertainty of the theoretical prediction of the cross section due to limitations of our understanding of mechanisms of nuclear reactions. Indeed, the corridor between $\sigma_{min} = \sigma_{avg} - \Delta\sigma_{avg}$ and $\sigma_{max} = \sigma_{avg} + \Delta\sigma_{avg}$ in two cases mentioned above includes the majority of experimental points. In particular, in the energy range of 14–15 MeV, the proportion of such points is 60 % and 77 %, respectively.

Conclusion

We have analysed three specific (n, p) reactions that result in the creation of metastable nuclei in isomeric states. Our goal was to determine the reliability of the available estimates for the relevant cross sections. We have demonstrated that the TENDL-2021 estimates are not consistent with experimental data from EXFOR for all reactions considered. We have also shown that reasonable estimates for cross sections can be obtained by the means of TALYS-1.9 software package using parameters of nuclear models from the RIPL only. The results of the calculations performed this way are in good agreement with the available experimental data.

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