Cross-section Calculations of ^{175}Lu(n,p)^{175}Yb reaction for production of medically important radioisotope ^{175}Yb

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Abstract. Ytterbium-175 (^{175}Yb) is considered suitable for the preparation of therapeutic radiopharmaceuticals due to its decay characteristics ($T_{1/2}$ = 4.18 d). In this study, the reaction cross section via the (n, p) reaction for ^{175}Yb was theoretically calculated using Lutetium-175 (^{175}Lu) as the target material. Neutrons with energies up to 50 MeV were considered, taking into account all nuclear reaction mechanisms. The Q-value for the neutron-induced reaction is 312 keV. The produced ^{175}Yb can be converted back to the parent stable nuclei ^{175}Lu through beta decay (100%), with no co-produced impurities remaining during the production of ^{175}Yb. This makes it suitable for the preparation of potential radiotherapeutic and imaging agents. The deterministic codes EMPIRE-3.2.3 and TALYS-2.0 were used in this study with their default models as well as optimized models. Experimental data were also included for comparison from the EXFOR data library. Major newly evaluated nuclear data libraries such as ENDF, JEFF, and TENDL were used for comparison. The results were found to be comparable with some discrepancies.

1 Introduction

Radioisotopes play a critical role in medical diagnosis and therapy. Depending on their decaying properties, radionuclides are classified as diagnostic and therapeutic radioisotopes. Positron emission tomography (PET) and single-photon emission computed tomography (SPECT) are the two forms of emission tomography that use the diagnostic radioisotopes [1]. In the present study, the neutron-induced excitation functions of the medically important ^{175}Yb radionuclide are calculated.

In the current study, Lutetium-175 (^{175}Lu) target was considered for the production of Ytterbium-175 (^{175}Yb) with energies ranging from the threshold value to 50 MeV. For the production of ^{175}Yb, the Q-value for the neutron-induced reaction is 312 keV and, its half-life makes it feasible for easy transportation to remote locations from production sites to nuclear medicine sites. It is suitable for therapeutic purposes with β- emission (mean energy 113keV, maximum energy 470 keV) as well as for diagnostic purposes for SPECT imaging with electromagnetic radiation emission (396.3 keV and 282.5 keV). The TALYS-2.0 [2] and EMPIRE-3.2.3 [3] codes were chosen to calculate the production cross-sections of the ^{175}Yb radionuclides produced through the (n, p) reaction. The calculations were conducted using the Hauser-Feshbach statistical model, incorporating default and various expressions. Nuclear level density models and gamma-ray strength functions in the codes were also tested to estimate the desired cross sections. Decay data and data related to the reaction is given in Table 1.

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Table 1. Decay data

Target	Product nucleus	$T_{1/2}$	E_{level} (keV)	Jπ	Decay mode	Final product
^{175}Lu	^{175}Yb	4.18 d	0.0	7/2-	β-: 100 %	^{175}Lu
^{175}Lu	^{175}Yb	68. ms	514.9	1/2-	IT: 100 %	^{175}Yb

The results obtained in this study are compared with the results available in the EXFOR database published by different authors and the newly released evaluated data from ENDF [4], JEFF [5], JENDL [6], BROND-3.1 [7], TENDL-2019, TENDL-2021, and TENDL-2023 [8].

2 Theoretical calculations

The popular deterministic modular programs TALYS-2.0 and EMPIRE-3.2.3 have been used to compute the neutron induced reaction cross sections in this work. These calculations were employed to theoretically understand the measured cross section results for the production of ^{175}Yb. The calculations were performed in the neutron energy range up to 50 MeV incident on a ^{175}Lu target via the ^{175}Lu(n, p) reaction (Q = 312 keV). They employ reaction parameters taken from the RIPL database [9]. They also consider compound, pre-equilibrium, and direct reaction mechanisms based on various model parameters as a function of projectile energies.

In both codes, the default optical model potential of spherical type with and without MSD is utilized for the calculation of inelastic scattering to collective levels in the neutron incident channel. For comparison, the Coupled Channel (CC) and distorted wave Born approximation (DWBA) methods are also used in the EMPIRE-3.2.3 calculations by using the keywords “direct” = 1 & 3 options, respectively.

Both codes can also perform calculations in the compound nucleus calculations.

For the TALYS-2.0 code, we explored six level density models using keyword “ldmodel” and ten E1 gamma-ray strength functions using keyword “strength”.

In the EMPIRE code calculations for the ^{175}Lu target, keyword “ompot” for the optical model potential (“ompot” = -587) selects RIPL Han Yinlu (RIPL number 587) data up to 20 MeV, and then the default option Koning and Delaroche are executed for the calculations.

In the code, six level density models and seven gamma-ray strength functions were utilized for the prediction of the cross-sections using keywords “levden” and “gstrfn” respectively.

3 Results and discussions

The neutron induced nuclear reaction cross sections up to 50 MeV for the ^{175}Lu target were calculated. The calculations were performed using well-known TALYS and EMPIRE codes, first with default nuclear models and then with other possible models. The results are compared with the latest versions of nuclear data libraries and published experimental data. Both theoretical codes included several models, including optical model potentials, nuclear level densities, and gamma-ray strength functions as mentioned in the heading above.

Among all the nuclear model calculations, for comparison, we chose only the results of default models, along with those models that gave the maximum and minimum cross-section values (labeled by codes, detailed model names, and keywords in the following figures). The figures also show experimental data points from various studies (labeled by year and author) [10-14]. These points represent the measured cross-sections at different neutron energies utmost 14.8 MeV. The different colored lines and some data points represent theoretical models and evaluated nuclear data libraries used to describe the neutron induced reactions for the ^{175}Lu (n, p) reaction.

In the Fig. 1, it is mentioned that the spherical type optical model potential predicted approximately 20% higher values than both the CC type and DWBA calculated values. Additionally, in the CC type, the excitation function is comparable to DWBA but is found up to approximately 42 MeV.

In Fig. 2, experimental data points [10-14] and the different colored lines of newly evaluated nuclear data libraries are shown. The latest experimental data [10] and old experimental data [13, 14] presented in the current work's reaction agree with the ENDF/B-VII.1

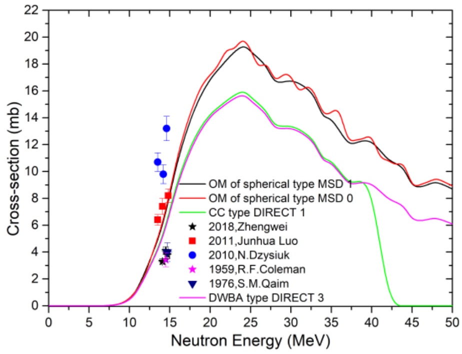

Figure 1. EMPIRE-3.2.3 calculations for optical model potentials.

and BROND-3.1 libraries, as well as with the calculated gamma strength function using the keyword “gstrfn”= 0 in the EMPIRE-3.2.3 code, which is discussed in next section. The remaining experimental data agree with various nuclear model calculations in the codes. Among the nuclear data libraries, TENDL-2023 presented results with the maximum cross-section values.

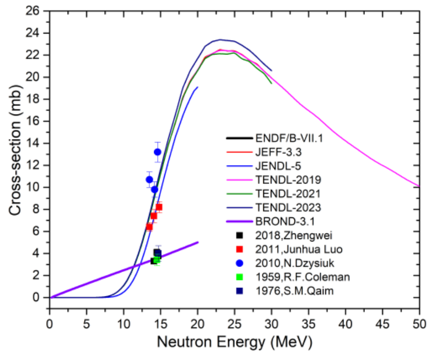

Figure 2. Cross-section for comparison of nuclear data libraries and experimental data.

Figure 3 shows the TALYS-2.0 and EMPIRE 3.2.3 codes predicted data for the level density models.

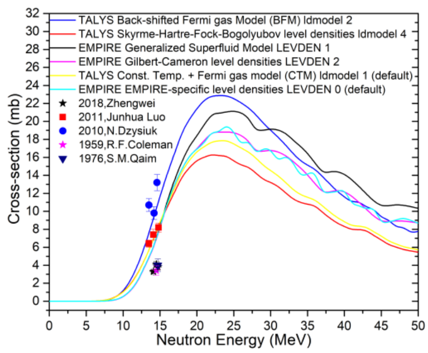

Figure 3. Cross-section for comparison of level density models with experimental data.

As shown in the graph, in the TALYS code, Back-shifted Fermi gas Model (BFM) calculated the maximum and highest values at 22.86 mb, while the Skyrme-Hartree-Fock-Bogolyubov level densities from numerical tables calculated the minimum at 16.33 mb. In the EMPIRE code, among the level density models, the Generalized Superfluid Model calculated the maximum at 21.31 mb, and CT+EGSM calculated the minimum at 18.80 mb.

Among the gamma-ray strength functions in the TALYS-2.0 code, the Brink-Axel Lorentzian model calculated a maximum of 18.51 mb, while the Goriely T-dependent HFB model calculated a minimum of 17.26 mb. In the EMPIRE-3.2.3 code, the SLO standard Lorentzian model calculated a maximum of 19.64 mb, and the EGLO enhanced generalized Lorentzian (Uhl-Kopecki) model calculated a minimum of 8.25 mb. These results, along with the default model results, are shown with the experimental data in Fig. 4. The graph also illustrates that gamma emission strongly contributed to the cross-section values as calculated in the TALYS-2.0 code. Interestingly, the result predicted by "gstrfn" = 0 (EGLO enhanced generalized Lorentzian Uhl-Kopecki) in the EMPIRE-3.2.3 code agrees with both the new and old experimental data [10, 13, 14] and the data taken from the ENDF/B-VII.1 [4] and BROND-3.1 [7] libraries. The experimental result [11] agreed well with the other model results while [12] remained higher even higher than all the model results.

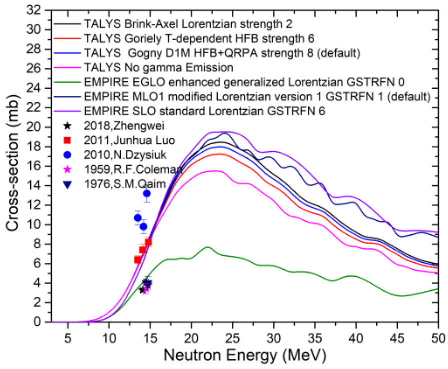

Figure 4. Cross-section for comparison of gamma-ray strength functions with experimental data.

4 Conclusion

In this article, we compared cross sections for the ^{175}Lu(n,p)^{175}Yb reaction predicted by nuclear models in EMPIRE-3.2.3 and TALYS-2.0 nuclear reaction codes, nuclear data libraries, and with the experimental data. In all calculated results, the cross sections are almost similar at lower energies regardless of the models used and start to deviate at high projectile energies. The cross-section generally increases with neutron energy then decreases. This trend is indicative of a resonance behavior, where neutrons interact strongly with the nucleus at specific energies.

The presented results showed that optical model potential types, different level density models, and gamma-ray strength functions affected the calculations.

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