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Systematic study of $(n,^{3}He)$ nuclear reaction and calculation of excitation functions with TALYS code

Defended on 21 /06 /2023 in front of the jury composed of:

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Dedication

To my loving family,

This thesis is dedicated to you with immense gratitude, for your unwavering support, encouragement. Your belief in me, even when I doubted myself, has been an unwavering source of strength that propelled me forward.

To my parents, thank you for your endless sacrifices, boundless patience, and unconditional love. Your unwavering faith in my abilities has been the cornerstone of my success. Your constant presence and guidance have instilled in me the values of perseverance and determination.

To my siblings, you have been my pillars of strength, my confidants, and my biggest cheerleaders. Your unwavering support and belief in my abilities have given me the confidence to pursue my dreams relentlessly.

To my friends, thank you for your constant companionship, laughter, and understanding. I am grateful for the countless hours spent together, both in study and in leisure, for the camaraderie that sustained me during challenging times.

Lastly, I dedicate this thesis to all those aspiring minds who dare to dream, who believe in the power of knowledge.

With deepest love and gratitude,
ILYAS FERHAT

Thanks

This thesis is realized at Mohamed Boudiaf university of Msila.

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Ilyas Ferhat

Contents

Chapter I:

Neutron reactions and theoretical models

Chapter II:

Talys nuclear code

Chapter III:

Systematic study (n,3He) and Function excitation obtained with Talys code

Introduction

The (n, ^{3}He) nuclear reaction involves the collision of a neutron with a target nucleus, resulting the emission of a helium-3 nucleus. This reaction is important in both fundamental nuclear physics and practical applications, such as in the production of tritium for nuclear fusion reactors. However, there still much to be learned about the (n, ^{3}He) reaction, including its dependence on target nuclei and neutron energies. The (n, ^{3}He) reaction is a specific type of neutron reaction where the collision of a neutron with a target nucleus, resulting the emission of a helium-3 nucleus (a stable isotope of helium as ^{4}He) and a gamma ray. This reaction has several important features that make it a useful tool for both fundamental nuclear physics research and practical applications. In recent years, there have been significant developments in our understanding of the (n, ^{3}He) reaction and its applications. Advances in computational methods and experimental techniques have allowed for more precise measurements of reaction cross-sections and a better understanding of the underlying nuclear physics.

In this work, we performed a systematic study of the (n, ^{3}He) reaction across a range of target nuclei and neutron energies vary from 10 MeV to 40 MeV. We used the TALYS, which is a widely nuclear reaction simulation code, to calculate the excitation functions for this reaction. These excitation functions describe the probability of the reaction occurring at different energies and can be used to predict the behavior of the reaction in various experimental conditions.

We used the TALYS code to perform calculations of the (n,^{3}He) reaction on a range of target nuclei, including ^{31}P ,^{41}K , ^{45}Sc, ^{59}Co, ^{63}Cu, ^{75}As, , ^{93}Nb, ^{133}Cs, ^{142}Ce , ^{159}Tb , ^{169}Tm , ^{181}Ta,^{187}Re. We varied the neutron energy in our calculations from 14 MeV to 15 MeV, covering a range of energies relevant to both fundamental nuclear physics and practical applications. To validate our calculations, we compared them to available experimental data from the EXFOR database. The EXFOR database contains a comprehensive collection of experimental nuclear reaction data from various sources, including accelerator-based experiments, nuclear reactors, and cosmic rays.

The (n,^{3}He) reaction is a critical process in neutron reactions, with important applications in nuclear physics and engineering. Its relatively height threshold energy and cross-section make it a useful tool for studying the properties of atomic nuclei and for practical applications such as neutron spectroscopy and tritium production. Ongoing research and development in this field hold great promise for future advancements in both fundamental science and practical applications.

The primary objective is to investigate the reaction mechanism and to gain a deeper understanding of the (n,^{3}He) nuclear reaction mechanism. Another important objective is to calculate the excitation functions for the (n,^{3}He) reaction. Our study scopes to improve nuclear reaction modeling by comparing the calculated excitation functions with experimental data, the study aims to assess the performance and accuracy of the TALYS code in predicting the (n,^{3}He) reaction. This evaluation will help identify areas where the current models may need improvement, leading to refinements and advancements in nuclear reaction modeling. We enhance nuclear energy research: The systematic study of the (n,^{3}He) reaction has implications for nuclear energy research. By improving our understanding of the reaction mechanism and obtaining accurate excitation functions, the study can provide valuable input for reactor design, fuel optimization, and nuclear waste management.

This manuscript is divided to three chapter. In the first one we define the cross section, we explorer different reaction induced by a thermal or rapid neutron, we view theoretical models used in reaction description, in the second chapter we present TALYS nuclear code with its output and input files, we present too experimental and evaluated nuclear library used by researchers and customers. In the third chapter we show experimental and evaluated data concerning (n, ^{3}He) which included in TALYS code, we propose our semi empirical function with 3 free parameters to reproducing (n, ^{3}He) reaction cross sections, in the chapter with comparison we evaluate data included in TALYS code especially its limited power in such reaction, in the second step we control the quality of our proposed formula, at last we finish with conclusion by underling the few data observed of (n, ^{3}He) reaction in the TALYS code and the utility of systematic study.

Chapter I

Neutron reactions and theoretical models

Neutron reactions are processes that involve the interaction of neutrons with atomic nuclei. These reactions play a critical role in many areas of nuclear physics and engineering, including nuclear energy production, nuclear medicine and fundamental nuclear physics research. In this chapter we present (n,^{3}He) reaction which signed by neutron capture and the production of ^{3}He, the reaction scenario: compound nucleus formation, compound nucleus decay, emission of helium-3 and energy transfer, excitation, at last we present theoretical models used in the description of nuclear reaction.

I.1. (n, ^{3}He) neutron reaction

Neutron reactions can implicate a wide range of phenomena, including: the emission of various particles, the creation of new isotopes, and the release of energy in the form of gamma rays, one of nuclear reaction observed around neutron source is the (n, ^{3}He) reaction, it is a useful reaction in applications such as neutron spectroscopy, where the energy spectrum of neutrons is measured to gain information about the structure of atomic nuclei. The (n, ^{3}He) reaction also has applications in nuclear energy production. In nuclear fusion reactors, tritium is one of the fuels used to produce energy. Tritium can be produced through the (n, ^{3}He) reaction by irradiating a target material with neutrons. This reaction is also used in the production of neutron detectors, where the emitted ^{3}He can be detected to measure the intensity of neutron radiation.[1]

The most significant features of the (n, ^{3}He) reaction is that it can be initiated by relatively low-energy neutrons for the reason of its relatively low threshold energy equal to 0.82 MeV. Another important feature of the (n, ^{3}He) reaction is its cross-section, which is a measure of the probability of the reaction occurring at a given energy. The cross-section for this reaction depends on both the target nucleus and the neutron energy. This dependence can be used to study the properties of atomic nuclei, such as their size and shape, and to investigate the behavior of neutrons in various materials.

I.2. (n, ^{3}He) reaction mechanism

The (n, ^{3}He) nuclear reaction involves the interaction of a neutron with a target nucleus, resulting in the production of a helium-3 nucleus (^{3}He) and the release of energy. Understanding the reaction mechanism is crucial for interpreting experimental data, predicting reaction outcomes, and investigating the underlying nuclear structure and dynamics involved. The (n, ^{3}He) reaction mechanism can be described as follows:

1. Neutron capture and compound nucleus formation: The incident neutron is captured by the target nucleus, forming a compound nucleus in an excited state. This process involves the absorption of the neutron by the target nucleus, leading to the addition of a neutron to the nucleus's atomic mass.
2. Compound nucleus decay: The compound nucleus formed in the previous step undergoes various decay processes. The compound nucleus can decay by emitting a variety of particles, including protons, alpha particles, gamma rays, and in the case of the (n, ^{3}He) reaction, a helium-3 nucleus.
3. Emission of helium-3: In the (n, ^{3}He) reaction, the compound nucleus releases a helium-3 nucleus along with other reaction products. The emitted helium-3 nucleus carries away the excess energy and angular momentum resulting from the reaction.[1]
4. Energy transfer and excitation: During the reaction, energy is transferred between the incident neutron and the target nucleus. The neutron imparts energy to the target nucleus, promoting it to an excited state. The excitation energy is then distributed among the reaction products, including the helium-3 nucleus and any other emitted particles.
5. Reaction cross section: The reaction cross section is a key parameter that characterizes the likelihood of the (n, ^{3}He) reaction occurring for a given incident neutron energy. The cross section depends on factors such as the target nucleus properties, neutron energy, and the reaction mechanism. It provides valuable information about the reaction rate and the probability of the (n, ^{3}He) reaction taking place.

Theoretical models, such as the Hauser-Feshbach formalism, are often employed to describe the (n, ^{3}He) reaction mechanism. These models consider various nuclear structure properties, such as level densities, optical potentials, and transmission coefficients, to calculate the excitation functions and predict the reaction outcomes. Computational codes like TALYS utilize these theoretical models to simulate the (n, ^{3}He) reaction and provide predictions for excitation functions [2]

I.3. Nuclear reaction cross section

Nuclear reactions are fundamental processes that occur when atomic nuclei interact with each other or with other subatomic particles. These reactions play a crucial role in various areas of science and technology, including nuclear physics, astrophysics, nuclear energy, and medicine. Understanding nuclear reactions is essential for interpreting experimental data, predicting reaction outcomes, and exploring the properties of atomic nuclei.[2]

In the context of nuclear reactions, cross sections are key parameters that quantify the likelihood of a particular reaction occurring. The cross section represents the effective area that a target nucleus presents for an incident particle to interact and initiate a reaction. It is expressed in units of area typically barns, with $1barn = 10^{-24}cm^2$ and is proportional to the reaction rate.

The cross section for a nuclear reaction depends on several factors, including the nature of the reactants, their energy, and the reaction mechanism. The energy dependence of the cross section is particularly important as it provides information about the reaction dynamics and the energy thresholds required for the reaction to take place.

The theoretical description of nuclear reactions and the calculation of cross sections often involve models such as the Hauser-Feshbach formalism, the statistical model, and the direct reaction model. These models consider nuclear properties, such as level densities, optical potentials, and scattering theory, to calculate the cross sections for various reaction channels .[1]

Experimental studies play a vital role in determining nuclear cross sections. These experiments involve bombarding target nuclei with particles or other nuclei and measuring the resulting reaction products. By systematically varying the incident particle energy, researchers can obtain cross-section data as a function of energy, providing valuable information about the reaction mechanism and energy dependence.

Several experimental techniques are employed to measure nuclear cross sections, including the activation method, in-beam measurements, and scattering experiments. These techniques involve detecting and analyzing the reaction products using detectors, such as solid-state detectors, gas detectors, or scintillation detectors. [2]

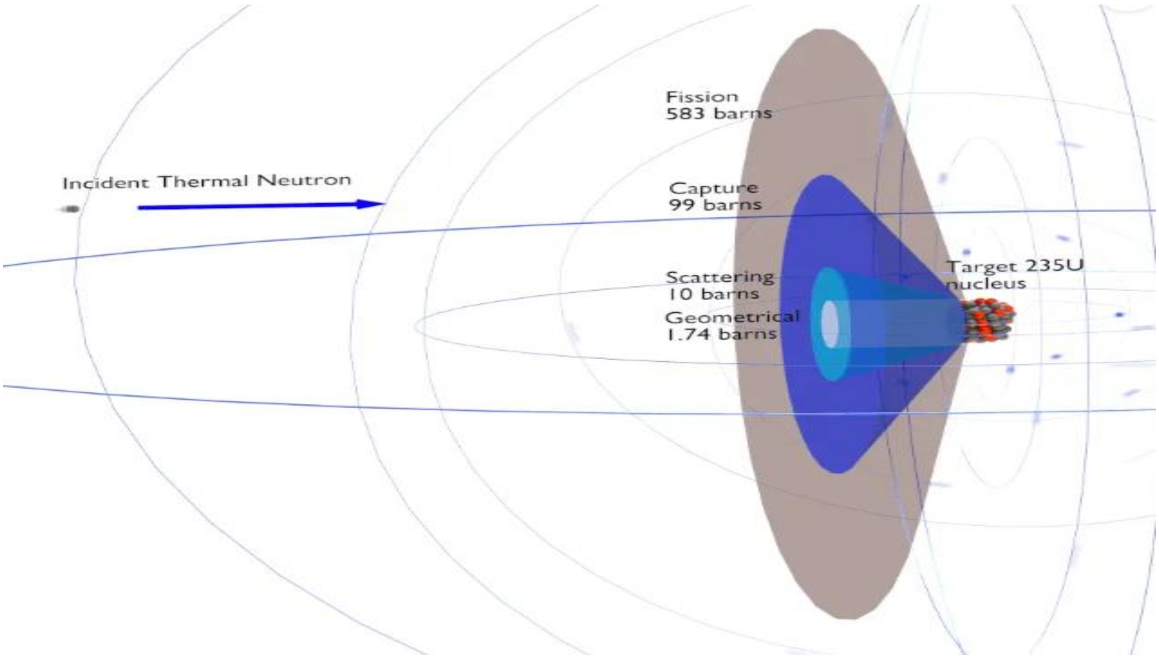


Figure I.1: Concept of cross section

I.3.1 Microscopic cross section

The microscopic cross section is a fundamental quantity in nuclear physics that quantifies the probability of a specific particle-matter interaction at the microscopic level. It represents the effective target area per unit volume for a particular nuclear reaction. The microscopic cross section is dependent on various factors, including the incident particle energy, the characteristics of the target nucleus, and the specific interaction mechanism being considered (e.g., scattering, absorption, or fission). It is typically expressed in units of area and is denoted by the symbol Σ. The determination of microscopic cross sections often involves theoretical models, such as the Hauser-Feshbach formalism, or experimental measurements using particle accelerators and detectors. Accurate knowledge of the microscopic cross section is essential for understanding and predicting the behavior of nuclear reactions.

I.3.2 Macroscopic cross section

The macroscopic cross section is a fundamental parameter used in the field of nuclear physics to describe the interaction of particles with matter at a macroscopic scale. It represents the effective interaction area per unit volume of the material and is a measure of the likelihood of particle-matter interactions occurring. The macroscopic cross section is obtained by multiplying the microscopic cross section by the density of the material. It is expressed in units of area per unit volume, typically in barns per centimeter (b/cm). This parameter is crucial for understanding the attenuation of particle beams as they traverse through materials, as it determines the overall probability of interactions along the path length. The macroscopic cross section is utilized in various applications such as radiation shielding design, nuclear reactor calculations, and radiation transport simulations. Accurate knowledge of the macroscopic cross section allows scientists and engineers to effectively analyze and predict the behavior of particle interactions in complex systems, contributing to the advancement of nuclear science and technology.

I.4. (n, ^{3}He) nuclear reaction experience

Experimental studies play a crucial role in validating and refining the understanding of the (n, ^{3}He) reaction mechanism. By comparing experimental data with theoretical predictions, researchers can improve the accuracy of reaction models, gain insights into nuclear structure properties, and enhance our understanding of the dynamics involved in the (n, ^{3}He) reaction.

The (n, ^{3}He) nuclear reaction, which involves the interaction of a neutron with a helium-3 nucleus, presents certain challenges when attempting to perform experimental measurements. There are several reasons why the (n, ^{3}He) reaction is considered relatively difficult to be studied experimentally.

Firstly, the availability of intense and well-characterized neutron beams is a crucial requirement for conducting (n, ^{3}He) experiments. Neutrons with specific energies and intensities need to be produced and accurately controlled to initiate the reaction. Generating such neutron beams can be technically demanding and requires specialized facilities, such as nuclear reactors or particle accelerators. Secondly, the detection of the reaction products in (n, ^{3}He) experiments poses a significant challenge. The reaction typically produces a helium-3 nucleus (^{3}He) and a proton as the reaction products. Detecting and distinguishing these particles from background noise and other particles in the experimental setup requires sophisticated detection systems with high efficiency and excellent energy resolution. Developing and operating such detectors can be complex and time-consuming.

Moreover, the (n, ^{3}He) reaction is characterized by a relatively low cross section compared to some other nuclear reactions. This means that the probability of the reaction occurring is relatively low, making it challenging to measure accurately. As a result, long measurement times or high-intensity neutron beams are often required to accumulate a sufficient number of reaction events for meaningful data analysis.

Furthermore, the (n, ^{3}He) reaction is strongly dependent on the incident neutron energy. Achieving precise control and measurement of neutron energies across a wide energy range adds another layer of complexity to experimental studies. Calibrating and validating the neutron energy spectrum is essential to accurately determine the cross section and understand the reaction dynamics. Overall, the (n, ^{3}He) nuclear reaction presents experimental challenges due to the need for intense and well-characterized neutron beams, the difficulty in detecting the reaction products, the low cross section, and the energy dependence of the reaction. Overcoming these challenges requires sophisticated experimental setups, specialized detection systems, and careful control of experimental parameters. However, despite the difficulties, experimental investigations of the (n, ^{3}He) reaction are valuable for understanding nuclear structure, reaction dynamics, and applications in fields such as nuclear energy, astrophysics, and fundamental research.

I.4.1 Experimental Challenges and Potential Solutions for Studying the (n, ^{3}He) Nuclear Reaction in Algeria

Studying the (n, ^{3}He) nuclear reaction experimentally in Algeria may present additional challenges specific to the research environment and available resources. Here are some factors that could contribute to the experimental challenges in Algeria:

1. Limited Neutron Sources: Algeria may have limited access to intense and well-characterized neutron sources, such as research reactors or particle accelerators, which are essential for generating the required neutron beams for the (n,^{3}He) reaction. The availability of such facilities could significantly impact the feasibility and accessibility of conducting experimental studies.
2. Infrastructure and Funding: The infrastructure and funding for nuclear physics research in Algeria might be limited compared to countries with well-established research programs. Insufficient resources can hinder the development and operation of experimental setups, including neutron beam lines, target systems, and detector arrays, which are necessary for studying the (n, ^{3}He) reaction.
3. Detector Systems and Expertise: The availability of sophisticated detector systems and the expertise required to operate them could be limited in Algeria. Detecting and characterizing the reaction products (helium-3 nuclei and protons) with high efficiency and precision is crucial for studying the (n, ^{3}He) reaction. Lack of access to state-of-the-art detectors and trained personnel could pose challenges in conducting the experiments.
4. Collaboration Opportunities: Collaborations with international research institutions and facilities play a crucial role in advancing experimental studies in nuclear physics. Limited opportunities for collaboration with renowned research groups, which might possess specialized expertise, infrastructure, and funding, could further impede the progress of (n, ^{3}He) reaction studies in Algeria.
5. Experimental Support and Access: The availability of technical support, equipment, and dedicated experimental facilities within Algeria could impact the ability to conduct (n, ^{3}He) experiments. Limited access to specialized research laboratories, data analysis software, and experimental support services may add logistical challenges and require researchers to overcome technical barriers independently.

It's important to note that while these challenges may exist, they can be mitigated through international collaborations, research networks, and initiatives aimed at supporting scientific research and infrastructure development. Governments, scientific institutions, and funding agencies can play a crucial role in providing support and resources to facilitate experimental studies, including those related to the (n, ^{3}He) nuclear reaction, in Algeria.

I.5. Nuclear reaction models

Nuclear reactions are complex processes. Understanding the behavior of nuclear reaction is important steps scientists have developed several nuclear reaction models to explain describe and predict nuclear reactions .[2] [5]

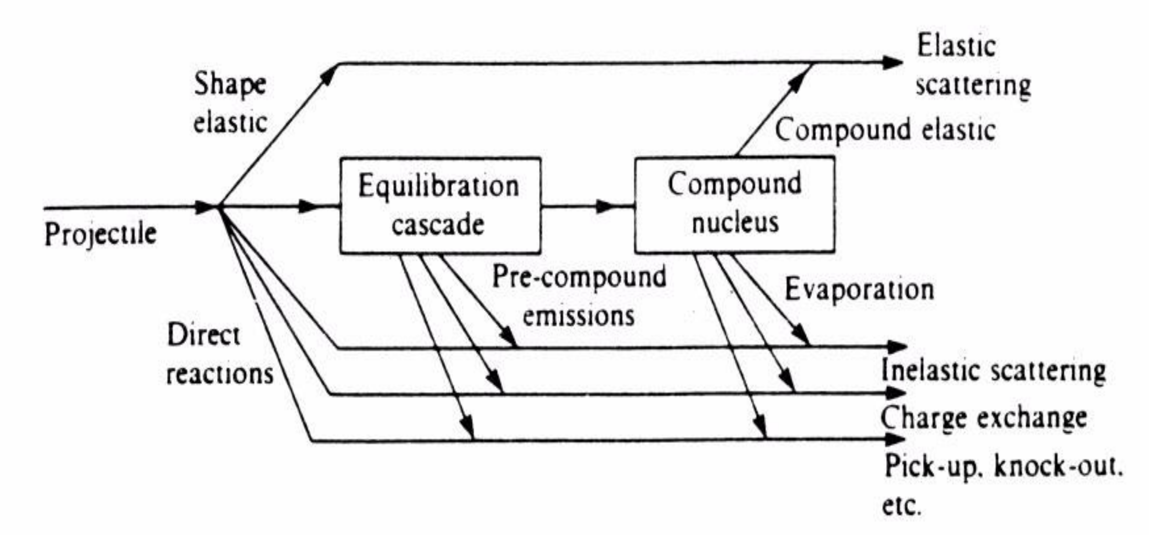


Figure I.2: Nuclear reaction models

a. The compound nucleus model

The compound nucleus model is one of the most widely used nuclear reaction models in nuclear physics. It describes a process where a projectile particle collides with a target nucleus, and a compound nucleus is formed. The compound nucleus is in an excited state and can decay by emitting particles or gamma rays, depending on its energy level. The compound nucleus model assumes that the compound nucleus has reached thermal equilibrium, meaning that the internal energy of the nucleus is evenly distributed among its constituent nucleons. This allows the model to predict the properties of the decay products based on the initial energy and angular momentum of the collision. While the model has its limitations one of the key advantages of the compound nucleus model is that it can be applied to a wide range of nuclear reactions giving heavy nuclei and high energies. The model assumes that the formation of the compound nucleus is a rapid process compared to the timescale of the decay, so that the compound nucleus is effectively at rest during the decay process [1].

The compound nucleus model also takes into account the quantum mechanical nature of the nuclear interactions. The wave functions of the colliding particles are described using Schrödinger's equation, and the interactions between the particles are described using a potential well. The compound nucleus model is particularly useful for predicting the behavior of fission, where the compound nucleus splits into two fragments with a large release of energy. It is also useful for predicting the properties of excited states in atomic nuclei.

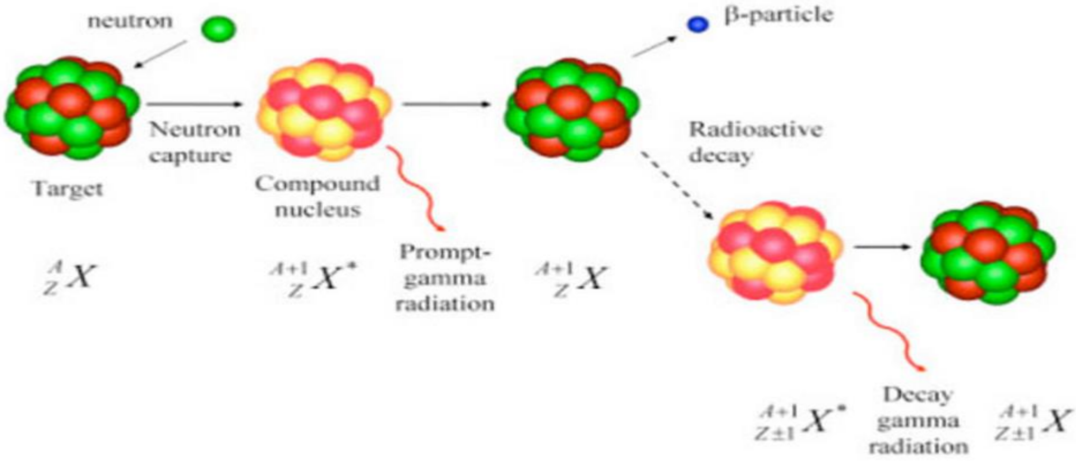


Figure I.3: The compound nucleus model is appropriate for neutron capture reaction

The Hauser-Feshbach model is a theoretical model used to calculate the cross sections of nuclear reactions. It is based on the assumption that the excited compound nucleus formed in a nuclear reaction is in thermal equilibrium with its environment, which allows the use of statistical mechanics to describe its behavior. The compound nucleus is assumed to undergo a sequence of decays, which can include emission of particles, gamma rays, or fission. The probability of each decay pathway is determined by the properties of the initial and final states of the compound nucleus, as well as the properties of the outgoing particles.[1]

The Hauser-Feshbach model has been successfully used to calculate the cross sections of a wide range of nuclear reactions, including neutron capture reactions, alpha-particle capture reactions, and fission reactions. However, the accuracy of the model is limited by several assumptions, including the assumption of thermal equilibrium and the neglect of direct reactions. Improvements to the model have been proposed to account for these effects, but they are still an active area of research in nuclear physics.

b. The direct reaction model

The direct reaction model is a nuclear reaction model that describes the interaction between a projectile particle and a target nucleus without assuming the formation of a compound nucleus. In this model, the projectile particle interacts directly with one or more nucleons in the target nucleus, without forming a long-lived intermediate compound state. The direct reaction model is particularly useful for predicting the behavior of reactions involving light nuclei and low energies, where the compound nucleus formation process is unlikely to occur. The model can provide insights into the details of the nuclear interaction at the nucleon level, and can be used to study the structure of atomic nuclei and the dynamics of nuclear reactions.

One of the key assumptions of the direct reaction model is that the reaction takes place through a one-step process, where the incoming projectile scatters off one or more nucleons in the target nucleus and produces one or more outgoing particles. The model assumes that the interactions between the particles are described by a potential well, and that the reaction cross-section can be calculated using a combination of the wave functions of the particles and the potential well.

The direct reaction model can also take into account the effects of nuclear deformation and shell structure, which can play important roles in determining the behavior of nuclear reactions. For example, the model can be used to study the effects of pairing correlations on the transfer of nucleons between target and projectile nuclei.

The limitation of the direct reaction model is that it can be difficult to accurately describe the detailed interactions between the particles in the nuclear potential well. In addition, the model may not be suitable for describing reactions involving heavy nuclei or high energies, where the compound nucleus formation process may play a more significant role. Despite these limitations, the direct reaction model remains an important tool in the study of nuclear reactions, and has been used to make important contributions to our understanding of the structure and behavior of atomic nuclei.

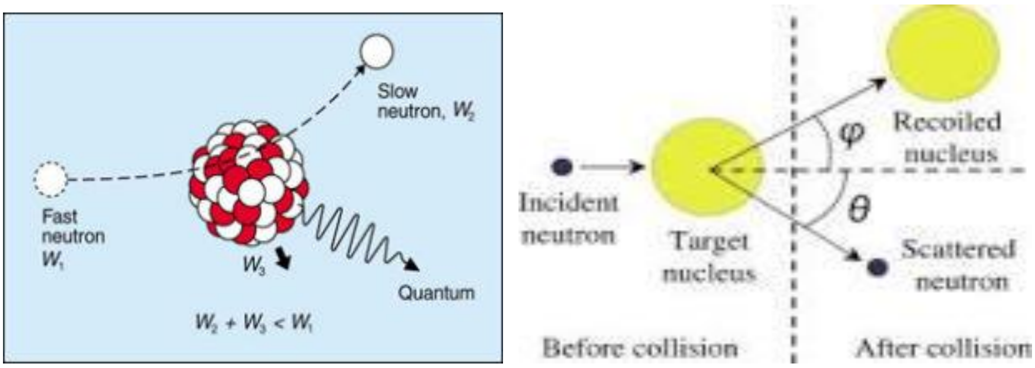


Figure I.4: the direct reaction model is appropriate for elastic and inelastic diffusion

c. The optical model

The optical model is a widely used nuclear reaction model that describes the scattering of particles, such as neutrons or protons, off atomic nuclei. The model assumes that the target nucleus is a smooth, continuous potential well that can be described by an optical potential. The optical potential is a complex-valued potential that describes the interaction between the projectile particle and the target nucleus. It takes into account the effects of nuclear structure and the finite range of the nuclear force. The real part of the potential represents the mean field interaction between the projectile and the target nucleus, while the imaginary part represents the absorption of the projectile particle as it interacts with the nucleus. The optical model assumes that the target nucleus is in its ground state and that the scattering takes place at a low enough energy so that the target nucleus is not excited to a higher energy state. The model also assumes that the scattering is elastic, meaning that the projectile particle retains its identity after the collision. The optical model can be used to predict the scattering cross section of neutrons or protons off a target nucleus at a range of incident energies. It can also be used to study the structure of atomic nuclei, as the shape of the optical potential depends on the properties of the target nucleus .[1]

One of the strengths of the optical model is its ability to provide a quantitative description of the scattering process. The model can be used to extract information about the nuclear structure and the properties of the nuclear force, such as the range and strength of the force.

However, the optical model also has its limitations. For example, it assumes a static potential well, and does not take into account the effects of nuclear excitations or the possibility of inelastic scattering. In addition, the model may not be suitable for describing reactions involving heavy nuclei or high energies, where other models such as the compound nucleus model or the direct reaction model may be more appropriate.

Overall, the optical model is an important tool in the study of nuclear reactions and the structure of atomic nuclei. Its ability to provide a quantitative description of scattering processes has made it a valuable tool in many areas of nuclear physics and nuclear engineering.

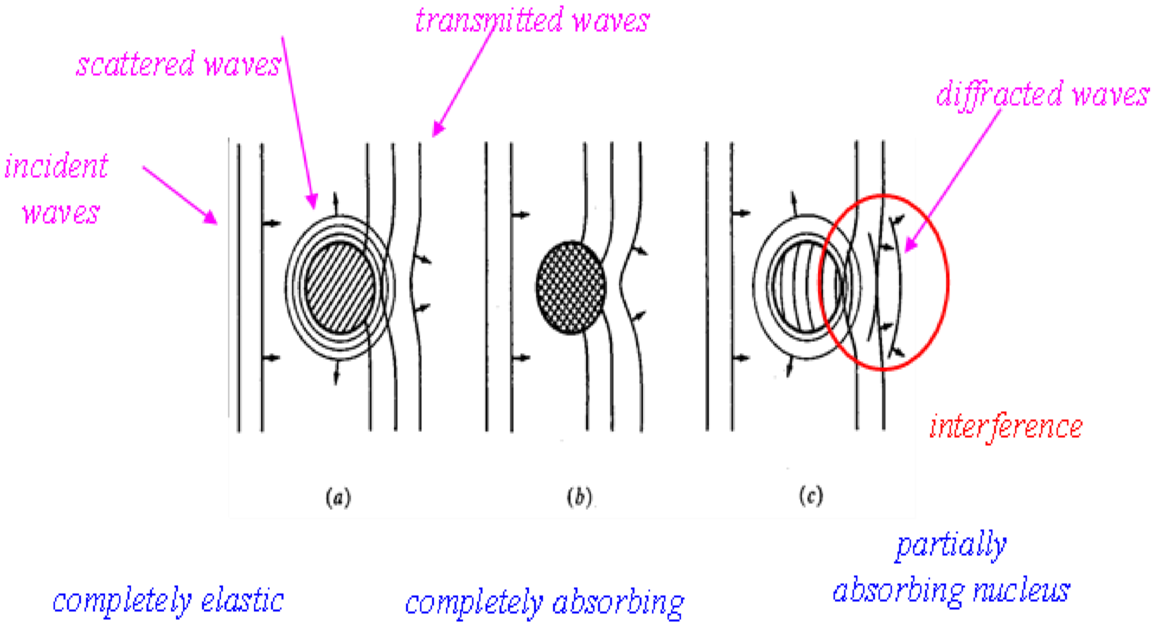


Figure I.5: incident wave , diffracted wave, transmitted wave and scattered wave used for particles description in optical model

d. The pre-equilibrium model

The pre-equilibrium model is a theoretical model used to describe nuclear reactions where the compound nucleus is not in thermal equilibrium. In these reactions, the incident particle interacts with a nucleon in the target nucleus, causing it to be excited to a high-energy state. The excited nucleon then undergoes a series of interactions before reaching a state of equilibrium with the surrounding nucleons.

The pre-equilibrium model assumes that the initial excited state of the nucleon is not in thermal equilibrium, and that the interactions that lead to the final equilibrium state occur through a series of non-equilibrium steps. The model is based on the concept of a pre-equilibrium emission stage, in which particles are emitted from the excited nucleon before it reaches thermal equilibrium. This stage is followed by an equilibrium emission stage, in which particles are emitted from the compound nucleus in thermal equilibrium.

The pre-equilibrium model is particularly useful for describing reactions involving high-energy particles, such as neutron-induced reactions, and has been used to calculate the cross sections for a wide range of nuclear reactions. The model takes into account a number of factors, including the initial excitation energy of the nucleon, the angular momentum of the incoming particle, and the level density of the target nucleus.

The pre-equilibrium model is an important tool for understanding the dynamics of nuclear reactions, and has been used to study a wide range of phenomena, including the production of isotopes in stars, the behavior of nuclear fuels in nuclear reactors, and the effects of radiation on biological systems. However, the accuracy of the model is limited by a number of assumptions, including the assumption of statistical equilibrium and the neglect of direct reactions. Improvements to the model have been proposed to address these limitations, but they remain an active area of research in nuclear physics.

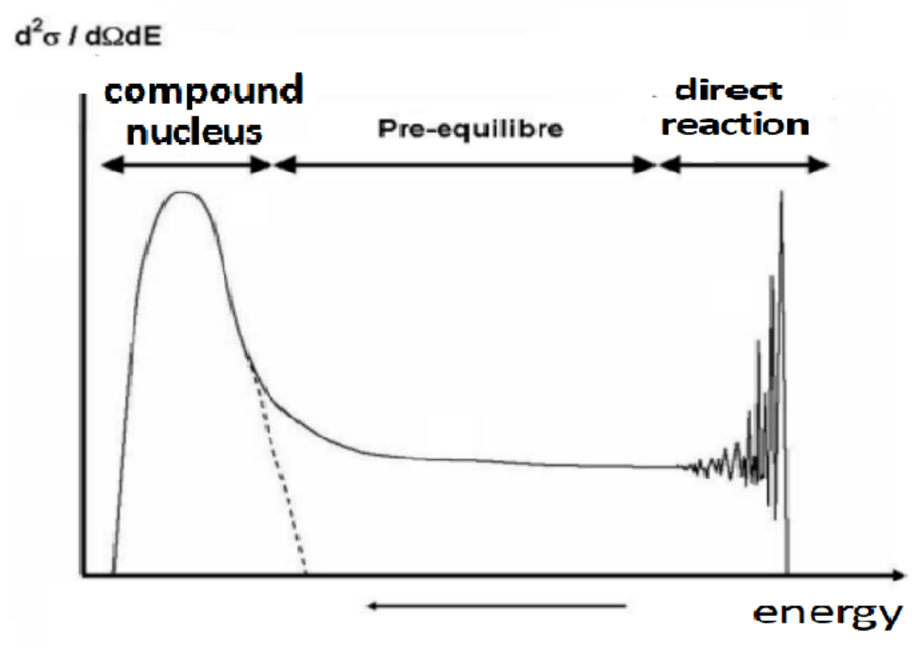


Figure I.6: double differential cross section for nuclear reaction models, pre-equilibrium model, optic model and compound nucleus model

Chapter II

Talys nuclear code

II.1. Overview of the TALYS Code

The TALYS (TALYS based Nuclear Model) code is a widely used nuclear reaction simulation tool that incorporates various nuclear reaction models to calculate reaction cross sections and related quantities. It provides a comprehensive framework for the theoretical analysis and prediction of nuclear reactions, enabling researchers to simulate and interpret the behavior of atomic nuclei under different conditions.

TALYS is designed to handle a wide range of reactions involving both stable and unstable target nuclei, as well as incident particles such as neutrons, protons, alpha particles, and other light ions. It offers a versatile platform for investigating reactions induced by different particles across a broad energy spectrum.

The code incorporates several state-of-the-art reaction models, each tailored to specific energy regimes and reaction types. These models include the Hauser-Feshbach model, the exciton model, the pre-equilibrium model, and the direct reaction model. Each model treats different aspects of nuclear reactions and is selected based on the specific characteristics of the reaction being studied.

TALYS takes into account various input parameters, such as nuclear structure information, level densities, optical model potentials, and decay properties, to provide a comprehensive description of the nuclear reaction dynamics. It allows users to input these parameters manually or extract them from libraries and databases, ensuring flexibility and accuracy in the calculations.

The code employs advanced mathematical algorithms and computational techniques to solve the underlying equations governing the reaction models. These algorithms efficiently handle complex calculations, including the determination of cross sections, energy distributions, angular distributions, and decay properties.

One of the key strengths of TALYS is its user-friendly interface, which enables researchers to easily define the reaction system, select the desired reaction model, and set the necessary input parameters. It provides graphical tools for visualizing and analyzing the results, allowing users to interpret the simulation outcomes and compare them with experimental data.

TALYS has found widespread application in various fields, including nuclear astrophysics, reactor design, nuclear data evaluation, and fundamental nuclear physics research. It has been utilized to study reactions relevant to nuclear energy production, nucleosynthesis in stellar environments, medical isotope production, and radiation damage assessment.

In summary, the TALYS code is a versatile and powerful tool for simulating nuclear reactions. It integrates various reaction models, incorporates user-defined input parameters, and employs advanced computational techniques to calculate reaction cross sections and related quantities. Its user-friendly interface and broad applicability make it a valuable asset for researchers studying nuclear reactions and their applications.

II.2. Input parameters and Model Selection in TALYS

When using the TALYS code for nuclear reaction simulations, several input parameters need to be specified to accurately describe the reaction system and select the appropriate reaction models. These parameters play a crucial role in determining the calculated cross sections. Here are some key input parameters and considerations for model selection in TALYS:

- Target nucleus: The target nucleus is the nucleus that is bombarded by the incident particle. The user can specify the atomic number, mass number, and isotope of the target nucleus.
- Projectile: The projectile is the incident particle that interacts with the target nucleus. The user can specify the atomic number, mass number, and energy of the projectile.
- Incident Particle Energy: The energy of the incident particle, such as a neutron or a proton, is a crucial input parameter. It determines the energy available for the reaction and influences the reaction dynamics. The energy range should be selected based on the specific objectives of the study and the energy regime relevant to the reaction being investigated.
- Excitation energy: The excitation energy of the compound nucleus formed after the reaction is an essential input parameter. The user can specify the excitation energy, or TALYS can calculate it based on the incident energy and the target and projectile masses.
- Reaction Channel Selection: The desired reaction channel needs to be specified in TALYS. This includes specifying the type of particles involved in the reaction, such as neutron-induced, proton-induced, or alpha-induced reactions. The specific reaction channel determines the appropriate reaction models to be employed in the simulation.

- Reaction Mechanism Models: TALYS offers various reaction models, as discussed earlier, including the Hauser-Feshbach model, pre-equilibrium model, exciton model, direct reaction model, and optical model. The selection of the appropriate model(s) depends on factors such as the energy range, target nucleus, and reaction type. The models can be chosen based on previous experimental data, theoretical expectations, or a combination of both.
- Model Parameters: Each reaction model in TALYS has associated parameters that need to be specified. These parameters control the behavior of the reaction models and may include level densities, optical model potentials, decay properties, and other relevant quantities. These parameters can be determined from experimental data or theoretical calculations. Sensitivity analysis can be performed to investigate the impact of varying these parameters on the calculated results.
- Reaction type: The user can specify the reaction type, such as (n, p), (n, alpha), (n, 2n), etc.
- Model selection and parameters: As discussed earlier, TALYS incorporates several nuclear reaction models. The user must select the appropriate model(s) based on the energy regime and reaction type of interest. Additionally, the user can adjust the associated parameters for each model to improve the accuracy of the simulation.

After specifying the input parameters, TALYS performs a simulation to calculate the cross section and other reaction properties. The user can visualize and analyze the results using the code's output files and visualization tools.

The selection of the appropriate model(s) is crucial to obtaining accurate and reliable results. The user should consider several factors, such as the energy regime, reaction type, and available experimental data, when selecting the model(s). The TALYS code provides default settings for the model parameters, but the user should adjust them based on the available experimental data and knowledge of the reaction mechanism.

It is essential to note that nuclear reactions are complex phenomena, and accurate predictions may require more sophisticated models beyond those available in TALYS. The user should consider the limitations of the code and the assumptions underlying the models when interpreting the results.

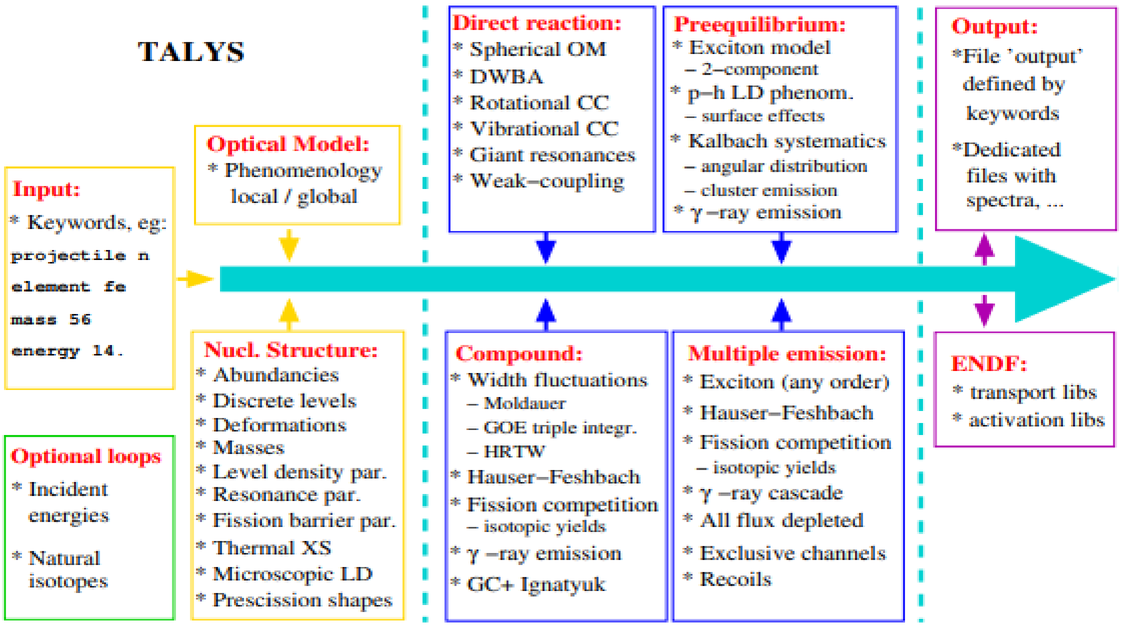
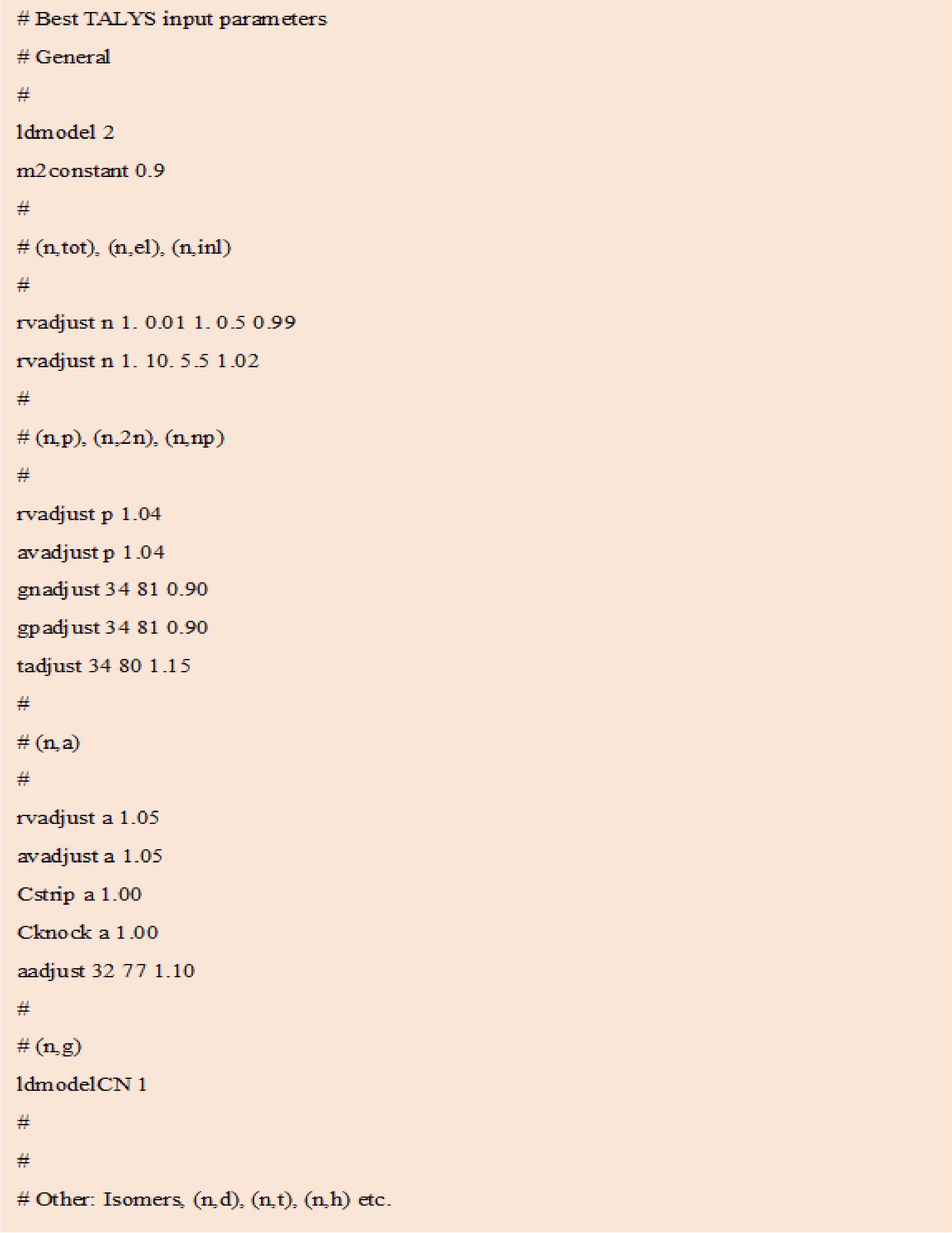


Figure II.1: Nuclear models in TALYS

II.2. 1 Best TALYS input parameters

This feature serves to ensure the reproducibility of previously obtained results in nuclear reaction analysis using TALYS. It facilitates the organization of input files and directories, preventing scattering and enabling a comprehensive collection of the best TALYS input parameter files. This comprehensive collection allows for a high-quality description of nuclear reactions on all nuclides simultaneously, particularly when multiple individuals are involved in the work or when generating a complete nuclear data library through scripting. By setting the keyword "best y" in the input file, one can obtain optimal results using a seemingly default input file.

To maintain the organization of adjusted optical model, level density, and other parameters, the talys/structure/best directory stores all relevant information. The subdirectories within this directory should use the full isotope names in the format (a1,i3.3) or (a2,i3.3), with the first character of the element symbol in upper case. Examples of valid sub directories include Yb174/, F019/, Be009/, and U235/. Within these sub directories, the sets of best parameters are saved using the filename format zZZZaAAAS.best, where ZZZ and AAA represent the Z and A of the nuclid in i3.3 format, and S denotes the particle symbol (e.g., g, n, p, d, t, h, or a). This strict naming procedure is essential for software that employs TALYS for nuclear data evaluation purposes. As an illustration, we provide the example of the best parameters for neutrons incident on 80Se, found in the file talys/structure/best/Se080/n-Se080.talys.



```
# Best TALYS input parameters
# General
#
ldmodel 2
m2constant 0.9
#
# (n,tot), (n,el), (n,inl)
#
rvadjust n 1. 0.01 1. 0.5 0.99
rvadjust n 1. 10. 5.5 1.02
#
# (n,p), (n,2n), (n,np)
#
rvadjust p 1.04
avadjust p 1.04
gnadjust 34 81 0.90
gpadjust 34 81 0.90
tadjust 34 80 1.15
#
# (n,a)
#
rvadjust a 1.05
avadjust a 1.05
Cstrip  a 1.00
Cknock a 1.00
aadjust 32 77 1.10
#
# (n,g)
ldmodelCN 1
#
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
```

Figure II.2: Best TALYS input parametrs.

II.3. Additional Output and Information in TALYS

TALYS generates a diverse range of output files that offer detailed information and insights into nuclear reactions. The calculated cross-sections provide quantitative data on the probability of different reaction channels occurring as a function of energy. These cross-sections help researchers understand the reaction rates and probabilities associated with specific processes.

The angular distributions provided by TALYS describe the scattering patterns and angular correlations of the reaction products. They give valuable information about the direction and spread of outgoing particles, shedding light on the underlying reaction mechanisms [5].

Energy spectra produced by TALYS offer a comprehensive view of the energy distribution among the reaction products. They enable researchers to analyze the kinematics and energy deposition characteristics of the reaction, helping to identify specific features such as prominent peaks or broadening effects.

The level schemes provided in the output files present the nuclear structure of the target and product nuclei involved in the reaction. They include energy levels, spins, parities, and other relevant properties. These level schemes allow for a deeper understanding of the nuclear excitations and their influence on the reaction dynamics.

Decay properties calculated by TALYS provide information about the decay behavior of excited nuclear states and reaction products. This includes decay branching ratios, lifetimes, and other decay characteristics. Such information is essential for studying radioactive decays, isomeric transitions, and other related phenomena.

Resonance parameters calculated by TALYS highlight resonant behavior in the system. They include resonance energies, widths, spin-parity assignments, and their contributions to the reaction cross-sections. Resonance parameters are crucial for understanding resonance phenomena and their impact on reaction rates.

In addition to these main results, TALYS may generate additional output files related to nuclear structure, reaction mechanisms, optical model parameters, nuclear level densities, and more. These additional details provide researchers with a wealth of information for analyzing and interpreting the results of their nuclear reaction simulations. It's worth noting that the output files generated by TALYS may vary depending on the specific version and configuration of the code. Consult the TALYS documentation or refer to official sources for comprehensive information on the output files and their interpretation in the context of your research or application.

By analyzing the output files generated by TALYS, researchers gain valuable insights into the underlying physics of nuclear reactions. The output allows for comparisons with experimental data, the validation of theoretical models, and a deeper understanding of nuclear processes in various applications.

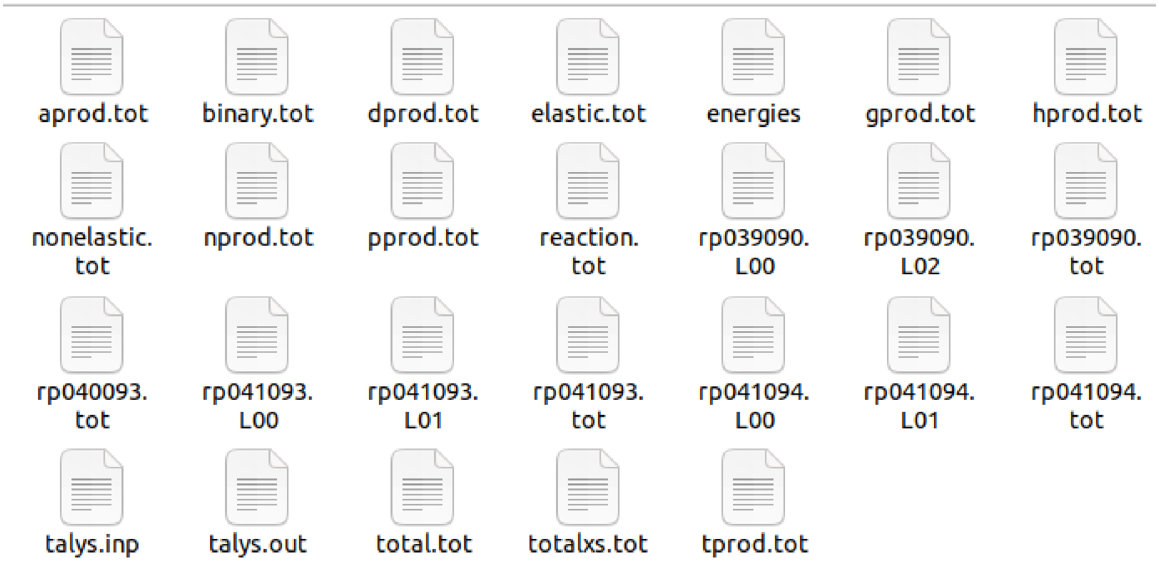
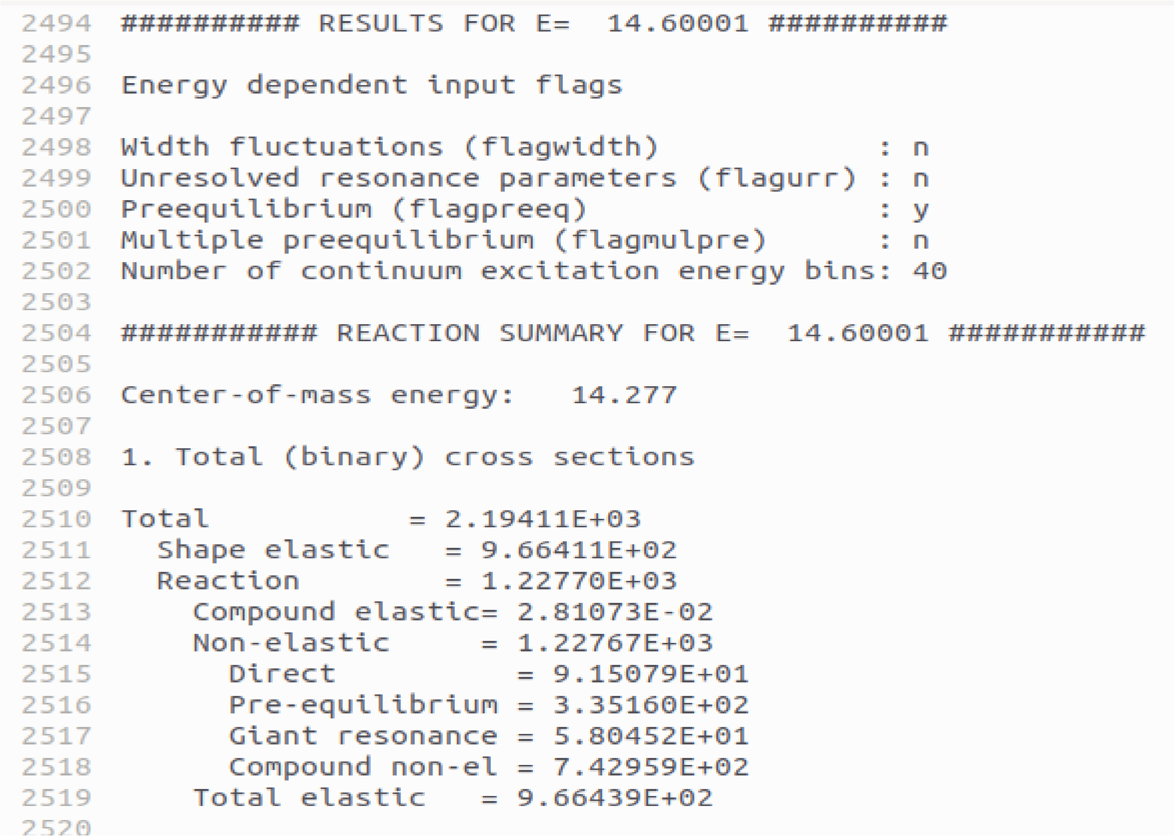
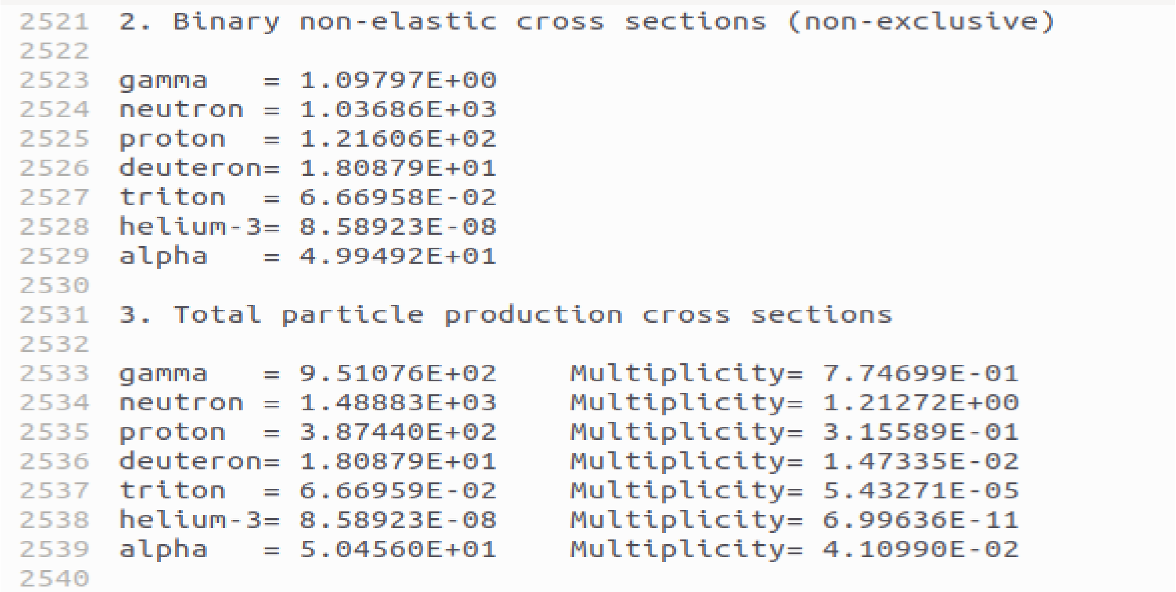


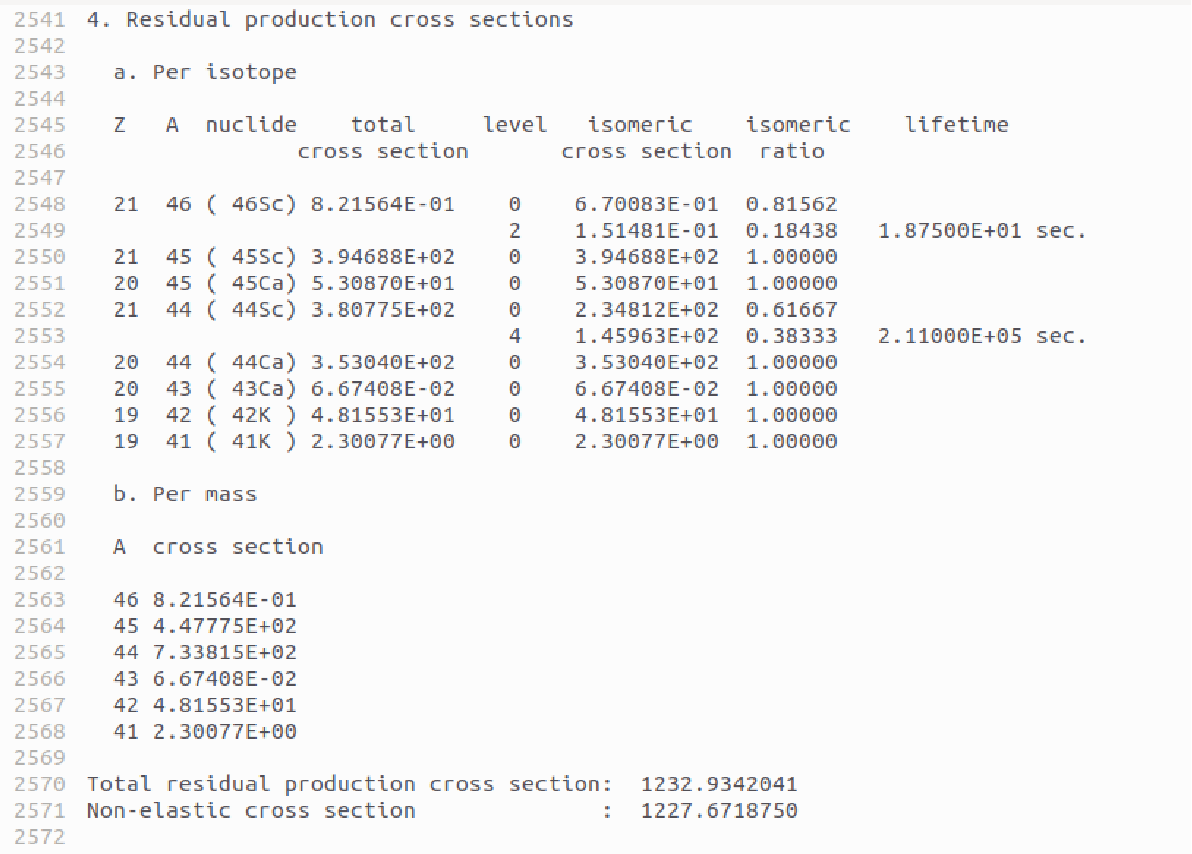
Figure II.3: Talys output files



```
########## RESULTS FOR E=  14.60001 ##########

Energy dependent input flags

Width fluctuations (flagwidth)            : n
Unresolved resonance parameters (flagurr) : n
Preequilibrium (flagpreeq)                : y
Multiple preequilibrium (flagmulpre)      : n
Number of continuum excitation energy bins: 40

########### REACTION SUMMARY FOR E=  14.60001 ###########

Center-of-mass energy:   14.277

1. Total (binary) cross sections

Total           = 2.19411E+03
  Shape elastic   = 9.66411E+02
  Reaction        = 1.22770E+03
    Compound elastic= 2.81073E-02
    Non-elastic     = 1.22767E+03
      Direct          = 9.15079E+01
      Pre-equilibrium = 3.35160E+02
      Giant resonance = 5.80452E+01
      Compound non-el = 7.42959E+02
    Total elastic   = 9.66439E+02

```



```
2. Binary non-elastic cross sections (non-exclusive)

gamma    = 1.09797E+00
neutron  = 1.03686E+03
proton   = 1.21606E+02
deuteron= 1.80879E+01
triton   = 6.66958E-02
helium-3= 8.58923E-08
alpha    = 4.99492E+01

3. Total particle production cross sections

gamma    = 9.51076E+02    Multiplicity= 7.74699E-01
neutron  = 1.48883E+03    Multiplicity= 1.21272E+00
proton   = 3.87440E+02    Multiplicity= 3.15589E-01
deuteron= 1.80879E+01    Multiplicity= 1.47335E-02
triton   = 6.66959E-02    Multiplicity= 5.43271E-05
helium-3= 8.58923E-08    Multiplicity= 6.99636E-11
alpha    = 5.04560E+01    Multiplicity= 4.10990E-02

```



```
4. Residual production cross sections

  a. Per isotope

  Z   A  nuclide    total     level   isomeric    isomeric    lifetime
                cross section       cross section  ratio

  21  46 ( 46Sc) 8.21564E-01    0     6.70083E-01  0.81562
                                2     1.51481E-01  0.18438   1.87500E+01 sec.
  21  45 ( 45Sc) 3.94688E+02    0     3.94688E+02  1.00000
  20  45 ( 45Ca) 5.30870E+01    0     5.30870E+01  1.00000
  21  44 ( 44Sc) 3.80775E+02    0     2.34812E+02  0.61667
                                4     1.45963E+02  0.38333   2.11000E+05 sec.
  20  44 ( 44Ca) 3.53040E+02    0     3.53040E+02  1.00000
  20  43 ( 43Ca) 6.67408E-02    0     6.67408E-02  1.00000
  19  42 ( 42K ) 4.81553E+01    0     4.81553E+01  1.00000
  19  41 ( 41K ) 2.30077E+00    0     2.30077E+00  1.00000

  b. Per mass

  A  cross section

  46 8.21564E-01
  45 4.47775E+02
  44 7.33815E+02
  43 6.67408E-02
  42 4.81553E+01
  41 2.30077E+00

Total residual production cross section:  1232.9342041
Non-elastic cross section              :  1227.6718750

```

Figure II.4: Extract from the talys.out file

II.4 Validation and Benchmarking of TALYS Code

The accurate prediction of nuclear reaction cross-sections and excitation functions is essential for various applications in nuclear physics and related fields. The TALYS (TALys-based Evaluated Nuclear Data Estimation Suite) code is widely used for nuclear reaction modeling, but its predictions must be rigorously validated against experimental data to ensure reliability. This chapter focuses on the validation and benchmarking of the TALYS code, assessing its performance in reproducing experimental results for (n,^{3}He) reactions.

- Experimental Database Selection

To validate the TALYS code, a comprehensive and diverse experimental database for (n,^{3}He) reactions is essential. The selection process involves identifying relevant studies, including those published in scientific journals, conference proceedings, and evaluated nuclear reaction databases. Considerations are given to the energy range, target nuclei, and available cross-section measurements.

- Comparison Methodology

A systematic and quantitative comparison between TALYS predictions and experimental data is crucial for assessing the code's accuracy. The comparison methodology should account for uncertainties in both the experimental measurements and the TALYS calculations. This may involve statistical analysis, such as chi-square tests or the calculation of root-mean-square deviations, to determine the agreement between the predicted and measured cross-sections.

- Sensitivity Analysis

A sensitivity study is done to see how sensitive TALYS predictions are to different input factors. In order to do this study, it is necessary to repeatedly change important factors including nuclear level densities, optical potentials, and decay modes while watching how these changes affect the final cross-sections. The most important parameters and how they affect the precision of the TALYS predictions can be determined with the aid of sensitivity plots and correlation analysis.

- Benchmarking Against Experimental Data

The benchmarking process involves comparing the TALYS-calculated excitation functions with the selected experimental data points. This comparison should be performed across a range of neutron energies and for multiple target nuclei to obtain a comprehensive assessment of the code's performance. The benchmarking process should consider the statistical significance of the agreement/discrepancy between the calculated and measured cross-sections.

- Discussion of Results

The results obtained from the validation and benchmarking process are discussed, focusing on the strengths and weaknesses of the TALYS code. Discrepancies between the calculated and measured cross-sections are analyzed, and potential sources of error or model deficiencies are identified. This discussion may lead to recommendations for code improvements or modifications to enhance its predictive capabilities for (n,^{3}He) reactions.

- Uncertainty Estimation

The estimation of uncertainties associated with the TALYS calculations is crucial for providing a realistic assessment of the code's reliability. Uncertainties in input parameters, such as nuclear structure data, optical potentials, and model parameters, are propagated through the calculations to obtain the uncertainties in the predicted cross-sections. Statistical methods, such as Monte Carlo simulations, may be employed to quantify the uncertainties and provide confidence intervals for the calculated excitation functions.

- Limitations and Future Directions

The limitations and potential areas of improvement for the TALYS code are discussed, highlighting any challenges encountered during the validation process. Suggestions for future research and development are provided, such as the incorporation of more sophisticated reaction models or improved treatment of nuclear structure effects. Additionally, recommendations for expanding the experimental database for (n,^{3}He) reactions are made to further enhance the validation process [8].

II.5 The EXFOR Experimental Database

The EXFOR Experimental Database is a comprehensive and widely recognized resource in the field of nuclear reaction data. It serves as a repository of experimental nuclear reaction data obtained from a diverse range of measurements conducted worldwide. The database covers a vast array of nuclear reactions, including reactions induced by particles such as protons, neutrons, alpha particles, and heavy ions. The EXFOR database contains detailed information on reaction cross sections, angular distributions, energy spectra, and other relevant observables, providing valuable data for nuclear physicists, researchers, and reactor designers. It plays a crucial role in benchmarking theoretical models, validating simulations, and facilitating the development of nuclear data evaluations. The EXFOR database is continuously updated, maintained, and expanded by an international collaboration of experts, ensuring its relevance and reliability for a wide range of applications in nuclear science and engineering.

One remarkable aspect of the EXFOR database is its emphasis on data quality and reliability. The included data undergoes rigorous scrutiny and validation processes, ensuring that only high-quality, peer-reviewed experimental results are incorporated. This meticulous curation enables researchers and scientists to have confidence in the accuracy and precision of the data they retrieve from EXFOR.

II.5.1 Exploring the Richness of Data in the EXFOR Experimental Database

Accessing experimental data from EXFOR is straightforward through its website, available at https://www-nds.iaea.org/exfor/

Some notable types of data included in the EXFOR database are:

- Reaction Cross Sections: The database provides detailed information on the cross sections of nuclear reactions, which quantifies the probability of a particular reaction occurring. These cross sections are crucial for understanding reaction rates and can help predict the behavior of nuclear systems.

- Angular Distributions: Angular distributions describe the directional properties of emitted particles or fragments resulting from a nuclear reaction. This data provides insights into the angular momentum and conservation laws governing the reaction process.

- Energy Spectra: Energy spectra capture the distribution of energies of particles or fragments involved in a nuclear reaction. These spectra reveal important details about energy transfer, excitation levels, and decay processes, aiding in the analysis and interpretation of reaction dynamics.

- Polarization Measurements: The EXFOR database also includes polarization measurements, which indicate the degree of alignment or orientation of particles involved in a reaction. Polarization data provides additional information about spin-dependent interactions and can shed light on underlying nuclear forces.

- Fission Yield Data: The database contains fission yield data, which characterizes the distribution of products resulting from nuclear fission reactions. This information is essential for reactor design, nuclear fuel management, and understanding the behavior of fissile materials.

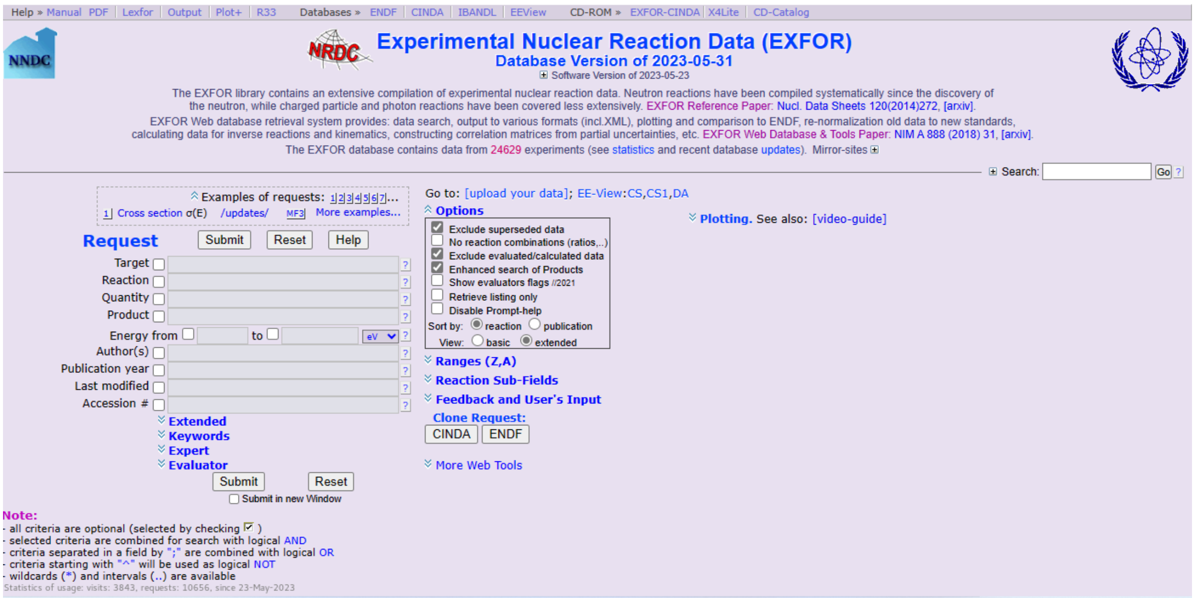
- Experimental Details: The EXFOR database includes comprehensive experimental details associated with each measurement, such as the type of particle beam used, target nucleus, laboratory conditions, and measurement techniques. These details enable researchers to assess the experimental setup and reproduce results.

II.5.2 Principles of EXFOR

The EXFOR Experimental Database is built upon several key principles that guide its structure and operation. These principles ensure the consistency, reliability, and usability of the database for the nuclear physics community. Some of the fundamental principles of EXFOR include:

- Standardization: The EXFOR database follows a standardized format for organizing and presenting nuclear reaction data. This format ensures consistency across entries and facilitates the comparison and analysis of different measurements.
- Data Quality Assurance: The EXFOR database places a strong emphasis on data quality. It includes rigorous review processes to ensure that the data included is reliable, well-documented, and validated. This helps maintain the integrity of the database and builds trust among researchers.

- ➢ Accessibility: The EXFOR database aims to be easily accessible to researchers and scientists. It is made available through various platforms and tools, allowing users to efficiently retrieve and analyze the data. Open access policies are often implemented to promote widespread usage and collaboration.
- ➢ Metadata and Documentation: The EXFOR format includes comprehensive metadata and documentation for each entry. This includes information about the measurement, experimental setup, uncertainties, and references to relevant publications. These details enable users to understand the context and background of the data and facilitate proper citation and attribution.
- ➢ Collaboration and Community Involvement: The EXFOR database is a result of international collaboration and cooperation among researchers, institutions, and data centers. It encourages contributions from the global nuclear physics community and actively seeks input to improve and expand the database. This collaborative approach ensures that the database reflects the diverse range of experiments and measurements conducted worldwide.
- ➢ Continuous Updates: The EXFOR database is continuously updated with new experimental data as it becomes available. This ensures that the database remains current and reflects the latest advancements in nuclear reaction research. Regular updates also allow for the incorporation of improved analysis techniques and methodologies.



Experimental Nuclear Reaction Data (EXFOR)

Database Version of 2023-05-31

⊞ Software Version of 2023-05-23

The EXFOR library contains an extensive compilation of experimental nuclear reaction data. Neutron reactions have been compiled systematically since the discovery of the neutron, while charged particle and photon reactions have been covered less extensively. EXFOR Reference Paper: Nucl. Data Sheets 120(2014)272, [arxiv].

EXFOR Web database retrieval system provides: data search, output to various formats (incl.XML), plotting and comparison to ENDF, re-normalization old data to new standards, calculating data for inverse reactions and kinematics, constructing correlation matrices from partial uncertainties, etc. EXFOR Web Database & Tools Paper: NIM A 888 (2018) 31, [arxiv].

The EXFOR database contains data from 24629 experiments (see statistics and recent database updates). Mirror-sites ⊞

Go to: [upload your data]; EE-View:CS,CS1,DA

Options

☑ Exclude superseded data
☐ No reaction combinations (ratios,..)
☑ Exclude evaluated/calculated data
☑ Enhanced search of Products
☐ Show evaluators flags //2021
☐ Retrieve listing only
☐ Disable Prompt-help
Sort by: ● reaction ○ publication
View: ○ basic ● extended

Plotting. See also: [video-guide]

☐ Submit in new Window

Note:
- all criteria are optional (selected by checking ☑)
- selected criteria are combined for search with logical AND
- criteria separated in a field by ";" are combined with logical OR
- criteria starting with "^" will be used as logical NOT
- wildcards (*) and intervals (..) are available

Statistics of usage: visits: 3843, requests: 10656, since 23-May-2023

Figure II.5: EXFOR database interface

Chapter III

Systematic study (n,^{3}He) and Function excitation obtained with Talys code

In the third Chapter, we explorer evaluated and measured (n,^{3}He) reactionfunction excitation using the Talys code and systematic study. taken neutron with energy from 14 MeV to 15 MeV we present (n,^{3}He) reaction function excitation for the following reactions :^{31}P(n, ^{3}He)^{29}Al, ^{41}K(n, ^{3}He)^{39}Cl, ^{45}Sc(n, ^{3}He)^{43}K, ^{59}Co(n, ^{3}He)^{57}Mn, ^{63}Cu(n, ^{3}He)^{61}Co,^{75}As(n, ^{3}He)^{73}Ga, ^{93}Nb(n, ^{3}He)^{91}Y ^{103}, ^{133}Cs(n, ^{3}He)^{131}I , ^{142}Ce(n, ^{3}He)^{140}Ba, ^{159}Tb(n, ^{3}He)^{157}Eu, ^{169}Tm(n, ^{3}He)^{167}Ho , ^{181}Ta(n, ^{3}He)^{179}Lu , ^{187}Re(n,^{3}He)^{185}Ta.

Furthermore, the chapter includes a systematic study, where we a propose a semi-empirical (n,^{3}He) cross-section formula, which based on This pre equilibrium model to calculate the cross-sections of the (n,^{3}He) reaction for 13 target nucleus. Experimental data are used to fix free parameters of the proposed expression. Statistical parameters Σ and χ^2 are used to verify the quality of the systematic formula and to compare it to previous formula. In the last step we use our formula to regenerate (n, ^{3}He) reaction function excitation.

III.1 Talys nuclear code

The Talys code is a powerful tool for simulating nuclear reactions and calculating excitation functions. It incorporates various theoretical models and experimental data to accurately predict the behavior of the (n,^{3}He) reaction. In this chapter, we explore the capacity of the Talys code to calculate the (n,^{3}He) function excitation for a specific energy range.

Lastly, the chapter concludes with a comprehensive comparison and discussion of the calculated (n,^{3}He) function excitation and the proposed semi-empirical cross-section function. Any discrepancies, trends, or noteworthy observations are examined, and their implications for understanding the (n,^{3}He) reaction and nuclear processes are discussed.

Overall, this chapter provides a detailed analysis of the (n,^{3}He) function excitation obtained using the Talys code, along with the systematic study of a proposed semi-empirical cross-section function. The comparison and discussion of these results contribute to our understanding of the (n,^{3}He) reaction and facilitate further advancements in the field of nuclear reactions.

A	**Z**	**Energie (MeV)**	$\sigma_{\mathrm{exp}} \pm \Delta\,\sigma_{\mathrm{exp}}$ **(μb)**
31	15	14.7	13 ± 6.5
41	19	14.6	6 ± 3
45	21	14.6	8.6 ± 4
59	27	14.6	4.6 ± 2.1
63	29	14.6	4 ± 2
75	33	14.6	3.5 ± 1.9
93	41	14.6	3.1 ± 1.5
133	55	14.7	5 ± 3
142	58	14.7	3.3 ± 1.3
159	65	14.6	4.6 ± 1.8
169	69	14.6	4 ± 2
181	73	14.6	3.4 ± 1.5
187	75	14.6	4 ± 3

Table III.1: (n, 3He) experimental cross sections at the incident neutron energy of 14.6 MeV.

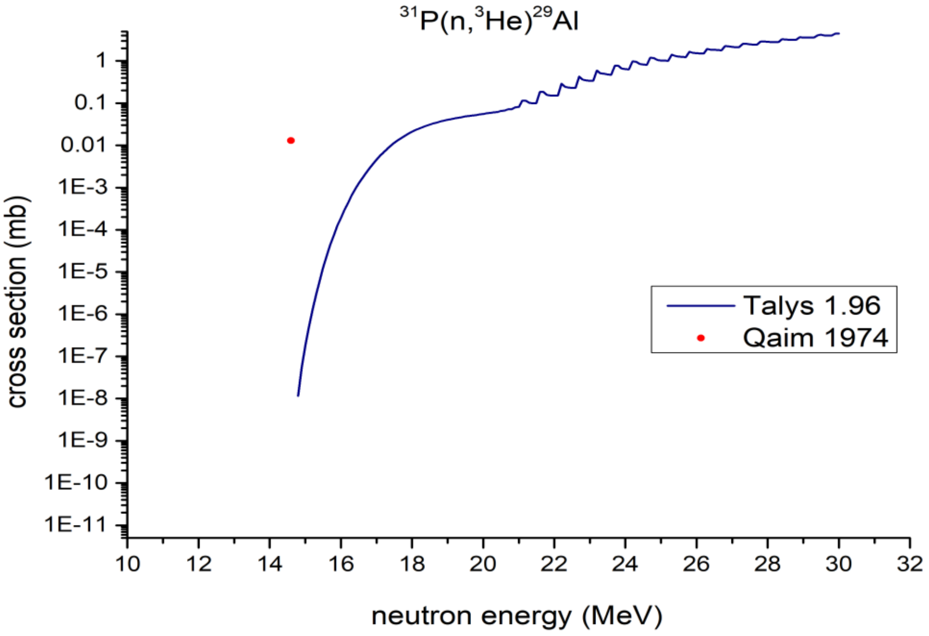


Figure III.1: Measured and evaluated ^{31}P (n, ^{3}He)^{29}Al reaction cross section obtained with Talys code.

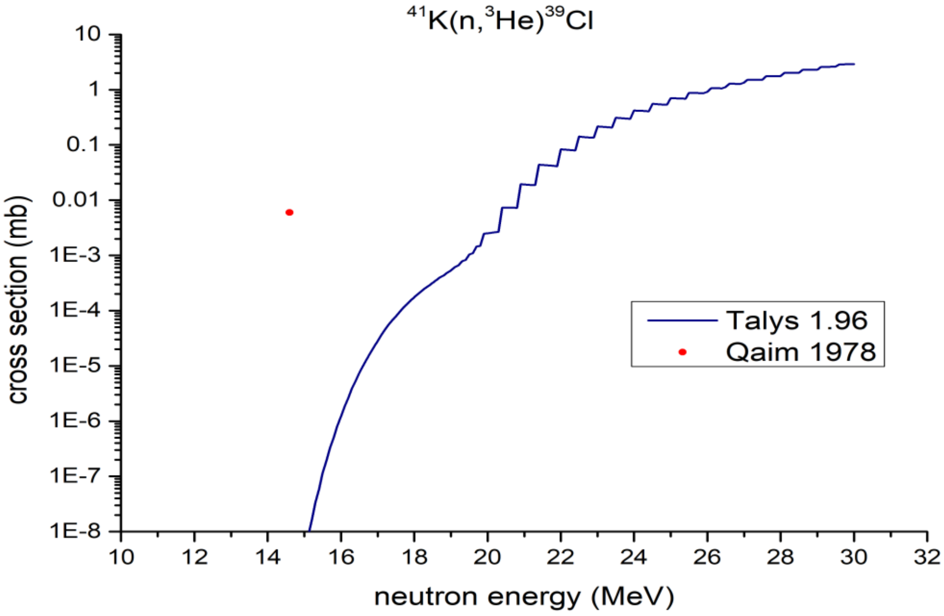


Figure III.2: Measured and evaluated ^{41}K (n, ^{3}He) ^{39}Cl reaction cross section obtained with Talys code.

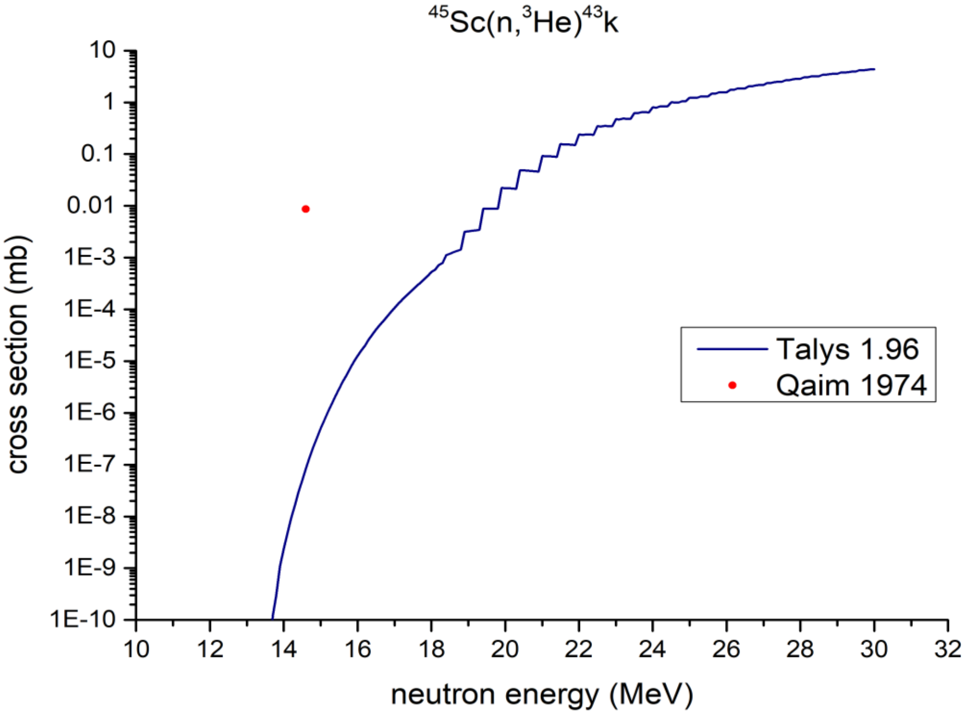


Figure III.3: Measured and evaluated ^{45}Sc (n, ^{3}He)^{43}K reaction cross section obtained with Talys.

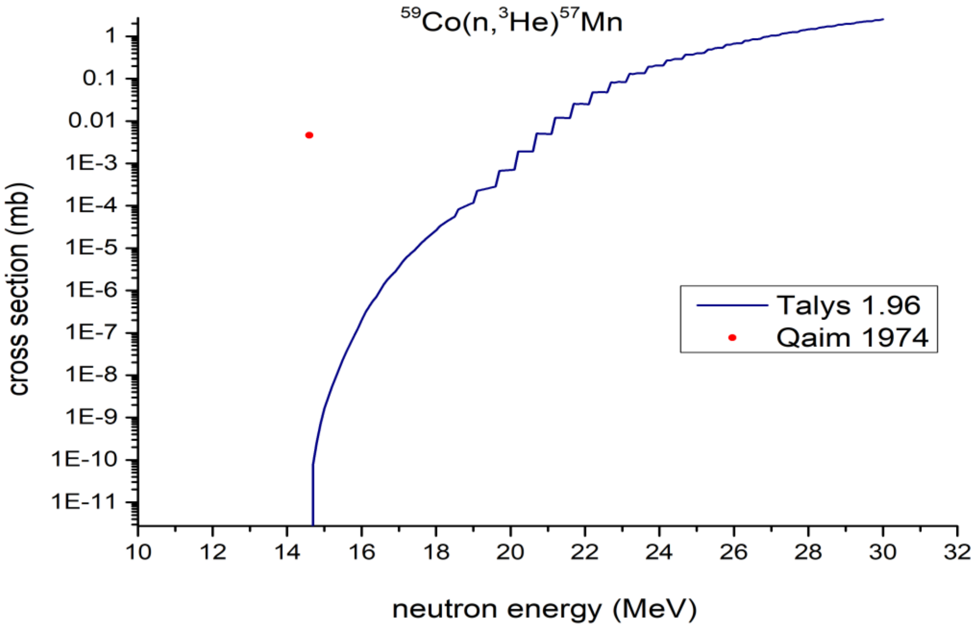


Figure III.4: Measured and evaluated ^{59}Co (n, ^{3}He)^{57}Mn reaction cross section obtained with Talys.

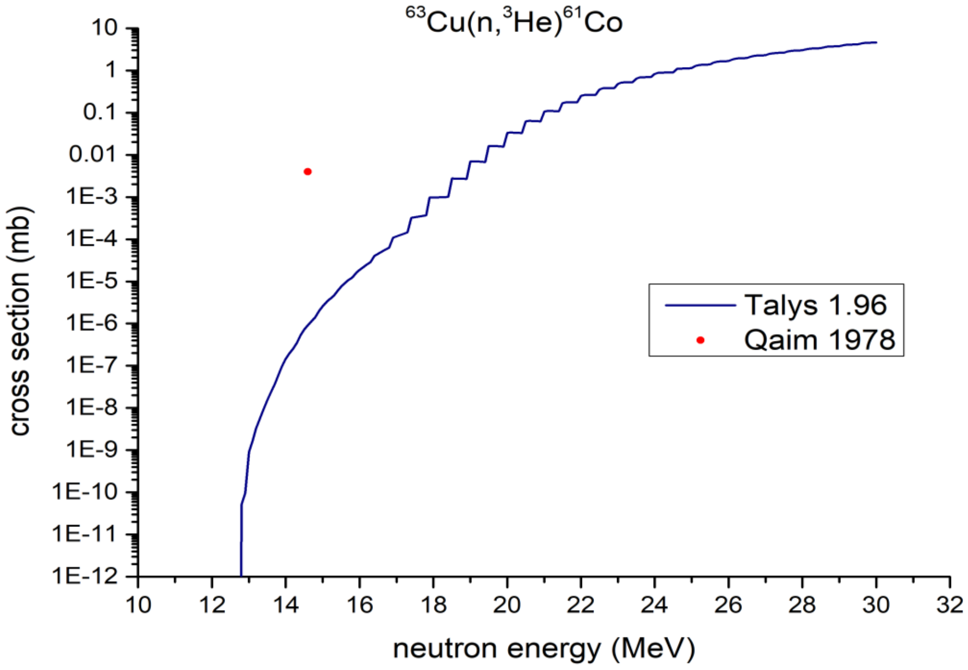


Figure III.5: Measured and evaluated ^{63}Cu (n, ^{3}He)^{61}Co reaction cross section obtained with Talys.

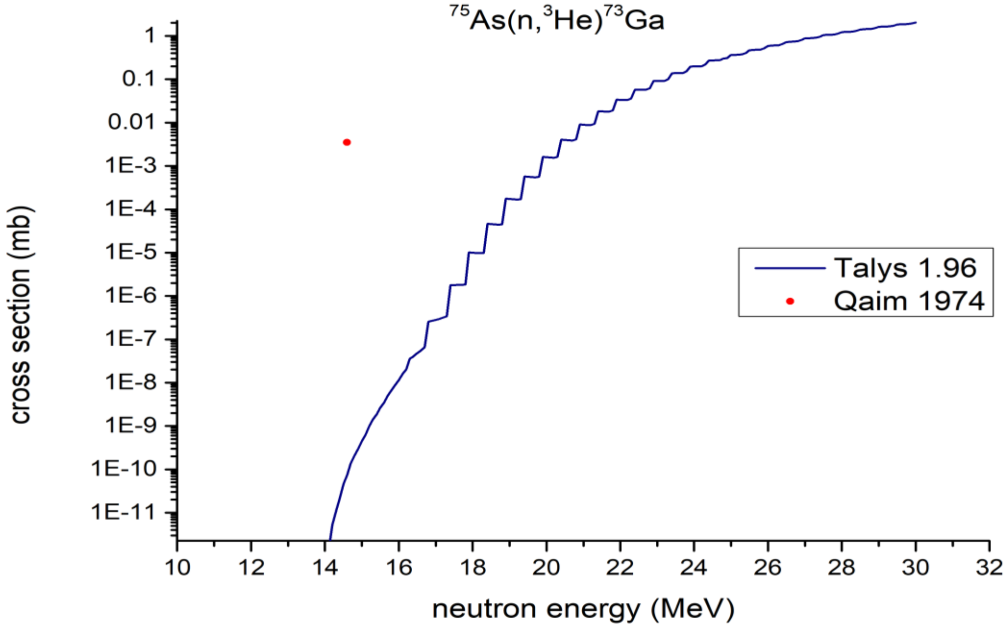


Figure III.6: Measured and evaluated ^{75}As (n, ^{3}He)^{73}Ga reaction cross section obtained with Talys.;

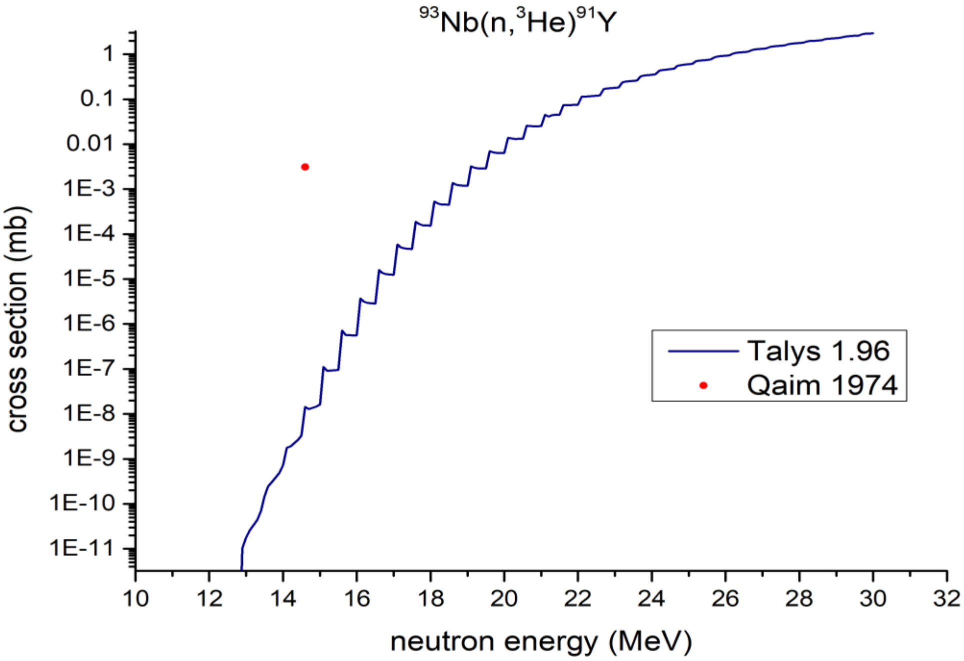


Figure III.7: Measured and evaluated ^{93}Nb (n, 3He)^{91}Y reaction cross section obtained with Talys.

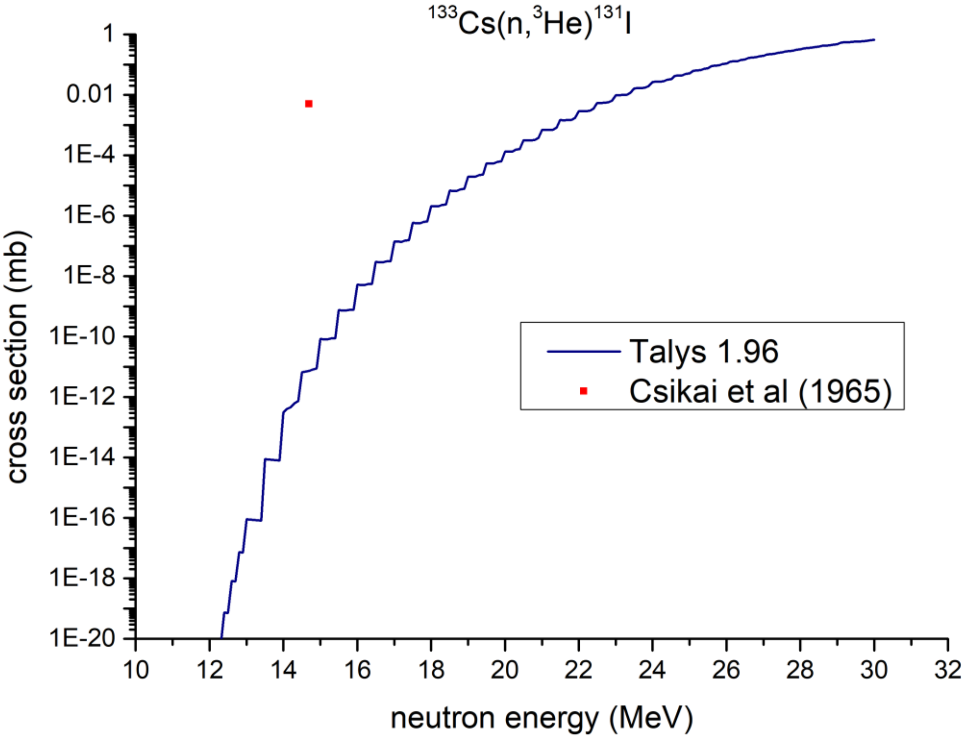


Figure III.8: Measured and evaluated ^{133}Cs (n, ^{3}He)^{131}I reaction cross section obtained with Talys.

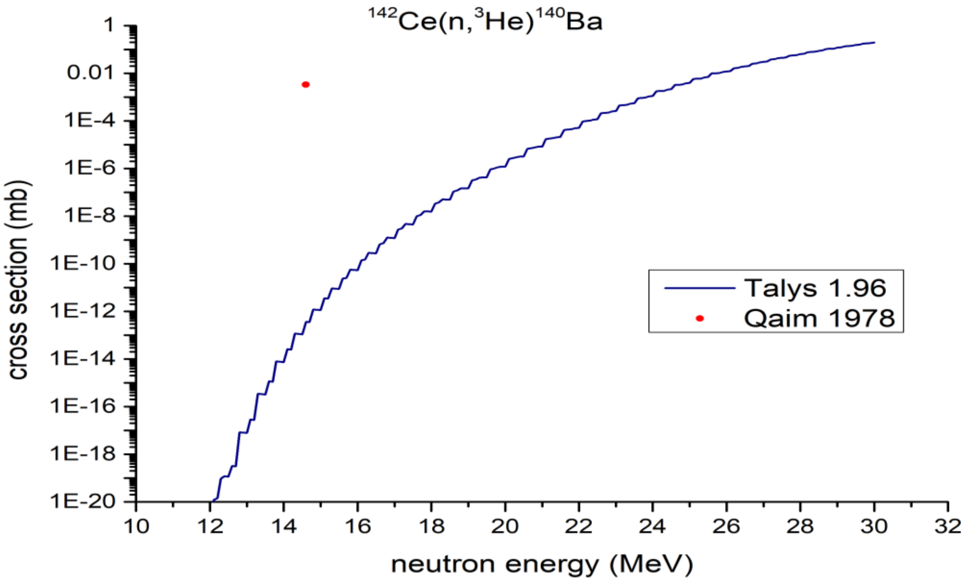


Figure III.9: Measured and evaluated ^{142}Ce (n, ^{3}He)^{140}Ba reaction cross section obtained with Talys.

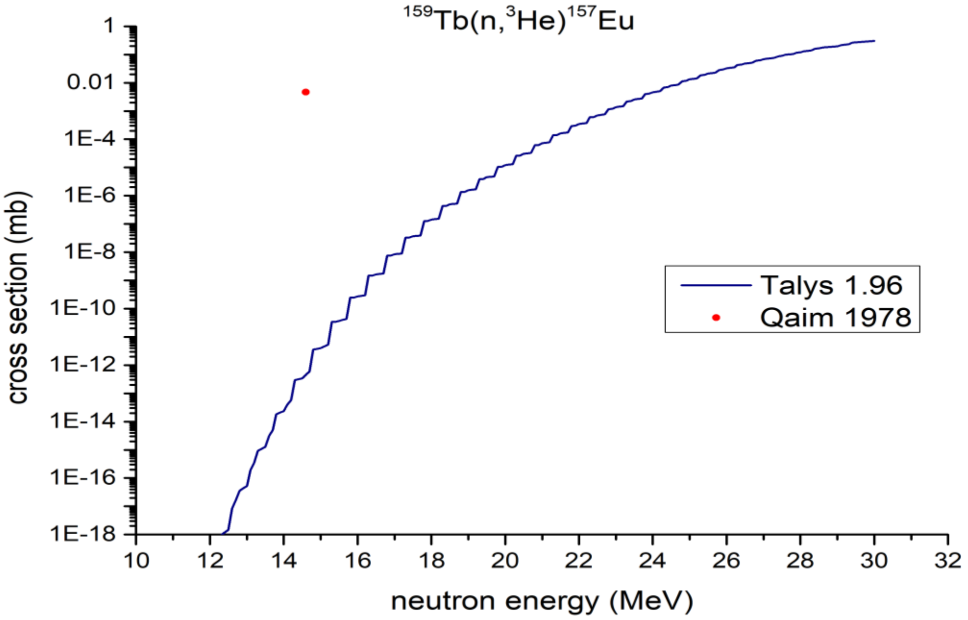


Figure III.10: Measured and evaluated ^{159}Tb (n, ^{3}He)^{157}Eu reaction cross section obtained with Talys.

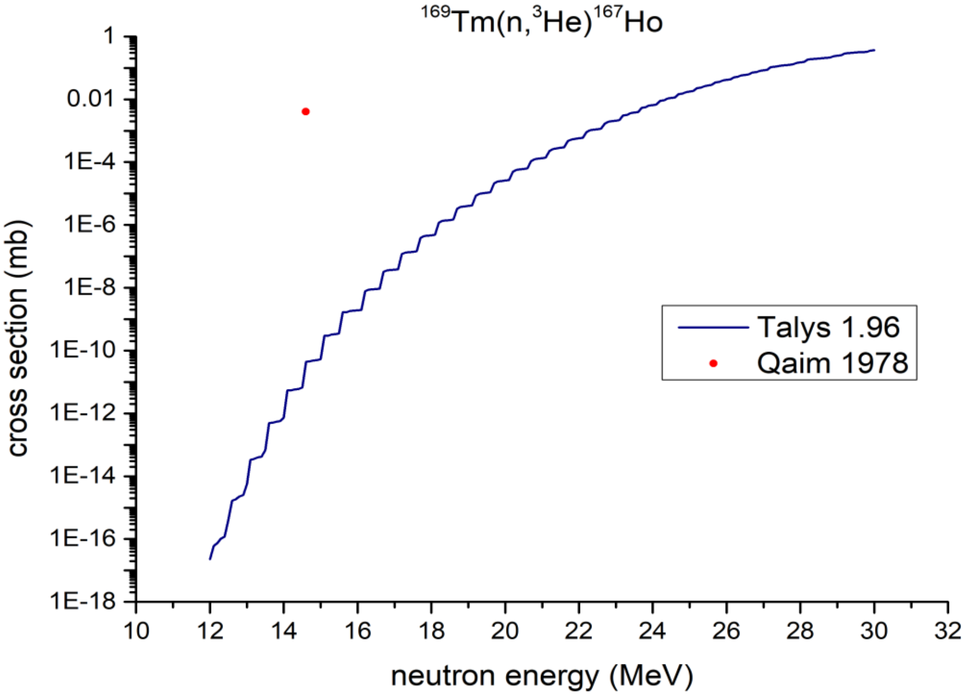


Figure III.11: Measured and evaluated ^{169}Tm (n, ^{3}He)^{167}Ho reaction cross section obtained with Talys.

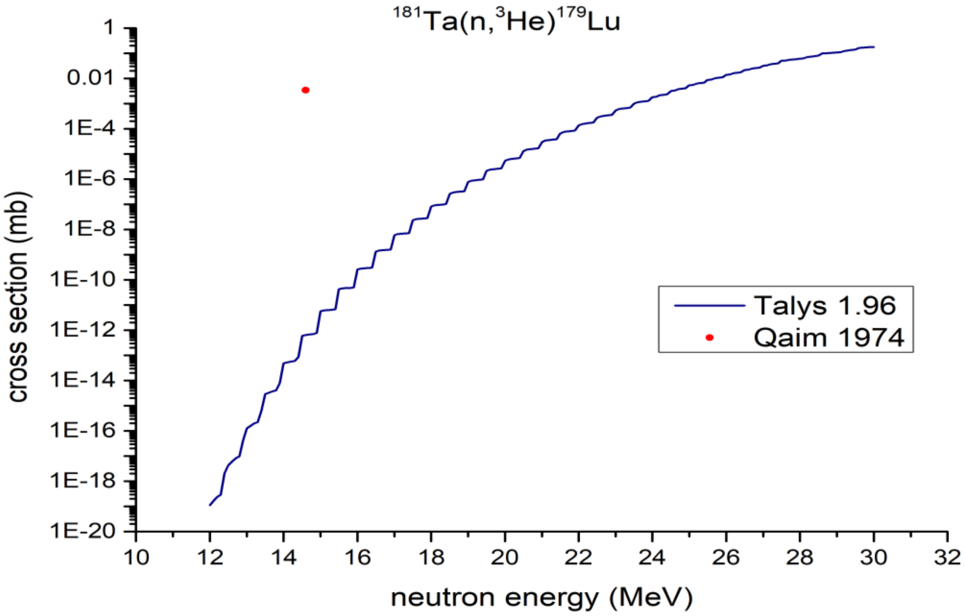


Figure III.12: Measured and evaluated ^{181}Ta (n, ^{3}He)^{179}Lu reaction cross section obtained with Talys.

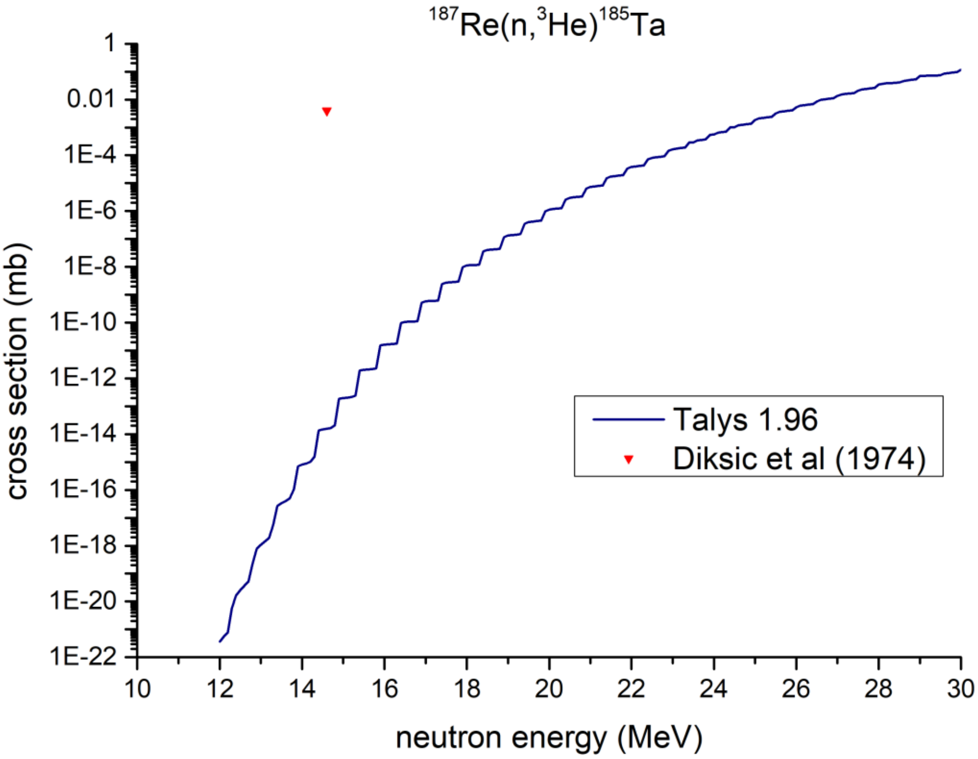


Figure III.13: Measured and evaluated ^{187}Re (n, ^{3}He)^{185}Ta reaction cross section obtained with Talys.

III.1.1 Results and discussion

In first step, we can conclude tha the code contains a few experimental data correct for a few targets (<20) and for a fixed value of neutron's energy (14, 6 MeV or 14,7 MeV).

The Talys code gives (n, ^{3}He) function excitation for neutron energies between 14 MeV and 15 MeV with a great difference between evaluated and experimental data.

Also for calculated (n, ^{3}He) function excitations, the code shows limits, the reason of these limits is the features related to the (n,^{3}He) reaction like: difficulty of the experience and the low probability of its realization.

III.2 Systematic study

The goal of this systematic study is to propose a cross-section function that can estimate the (n,^{3}He) cross-section for a wide range of energies or target nuclei. The proposed semi-empirical cross-section function would include parameters that are adjusted to fit the experimental data.

III.2.1 Semi-empirical formula proposed for calculating the cross section of the neutron reaction (n,3He)

From 1960 only measured (n, ^{3}He) reaction cross sections at 14.6 MeV for 13 elements ($31 \leq A \leq 187$). The difficulty of measure in nuclear reactor is the reason of this poor data. For that the systematic (n, ^{3}He) reaction cross section is used to reproduce measured data and predict unmeasured data. Evaporation and pre-equilibrium models are used in previous (n, ^{3}He) systematics to find empirical and semi-empirical formulae which describe correctly (n, ^{3}He) reaction. These formulae contain free parameters fixed with fitting experimental data, several calculations has succeed to reproduce measured (n, ^{3}He) reaction cross sections at 14.6 MeV. We cite the studies given by: Nehaoua, Yiğit, Yettou and Belgaid, Broeders and Konobeyev, Qaim, Bölükdemir et al , Atasoy and Dokmen, and Lishan and Yuling . Using pre equilibrium model, we can propose the following formula:

$$\sigma^{pre}_{^3He} = \pi r_0^2 \left(A^{1/3}+1\right)^2 A^{\alpha_3} \left(\alpha_1 \left(\frac{N-Z+1}{A}\right) + \alpha_2\right)^{15} \ldots\ldots\ldots\ldots \text{(III.1)}$$

A an Z are respectively the mass number and the charge number,r_0 is nucleus radius equal to 1.3 fm, α_i are free parameters fixed to have the minimum values of χ^2 and Σ.

III.2.2 Statistical parameters Σ and χ^2

The three parameters of eq. (III.1) are fixed by fitting experimental (n, ^{3}He) cross section reaction at 14.6 MeV, the valuation is released for 13 nuclei with$31 \leq A \leq 181$, we try to obtain the minimum values of statistical parameters: Σ and χ^2 are respectively defined as:

$$\Sigma = \sum_{i=1}^{N} \left(\frac{\sigma_i^{exp} - \sigma_i^{cal}}{\Delta\sigma_i^{exp}}\right)^2 \ldots\ldots\ldots\ldots \text{(III.2)}$$

$$\chi^2 = \frac{\Sigma}{(N-M)} \ldots\ldots\ldots\ldots \text{(III.3)}$$

where σ_i^{cal} is the calculated cross section, σ_i^{exp} and $\Delta\sigma_i^{exp}$ are respectively the $\sigma_{(n,\ ^3He)}$ experimental data and the corresponding error. N is the number of experimental data (equal to 13) and M is the number of free parameters in proposed formulas (M=3).

In this work we use (n, ^{3}He) experimental reaction excitation function for 13 elements ($31 \leq A \leq 187$), taken from EXFOR database and measured by: by Qaim , Csikai and Szalay and Dikšič et al., Pepelnik et al.

Table **III.1** contains the experimental data at 14.6 MeV and 14.7 MeV. We calculated the cross section of (n, ^{3}He) reaction as well and statistical parameters using an algorithm written in Python language in Jupyter Notebook (Annex).

III.2.3 Comparison with previous systematics

We compare our proposed formula with ones proposed by: Nehaoua, Yiğit, Yettou and Belgaid, Broeders and Konobeyev (with 2 and 3 free parameters), and Qaim given respectively:

$$\sigma_{(n,\,^3He)} = \pi r_0^2 \left(A^{1/3} + 1\right)^2 A^{\alpha_3} (\alpha_1 \left(\frac{N-Z+1}{A}\right) + \alpha_2)^{\alpha_4}. \tag{III.4}$$

$$\sigma_{(n,\,^3He)} = \alpha_1 \left(A^{1/3} + 1\right)^2 \exp(-\alpha_2 Q_{(n,\,^3He)}). \tag{III.5}$$

$$\sigma_{(n,\,^3He)} = \alpha_1 \left(A^{1/3} + 1\right)^2 \exp\left(\alpha_2 \left(\frac{Z-1}{A^{1/3}}\right) + \alpha_3 \left(\frac{Z-1}{A}\right)^3\right). \tag{III.6}$$

$$\sigma_{(n,\,^3He)} = \pi r_0^2 \left(A^{1/3} + 1\right)^2 A^{\alpha_3} (\alpha_1 \left(\frac{N-Z+1}{A}\right) + \alpha_2)^3. \tag{III.7}$$

$$\sigma_{(n,\,^3He)} = \pi r_0^2 \left(A^{1/3} + 1\right)^2 A^{-1/3} (\alpha_1 \left(\frac{N-Z+1}{A}\right) + \alpha_2)^3. \tag{III.8}$$

$$\sigma_{(n,\,^3He)} = \alpha_1 \left(A^{1/3} + 1\right)^2 \exp(-\alpha_2 \frac{N-Z}{A}). \tag{III.9}$$

where r_0 is equal to 1.3 fm, α_i are free parameters fixed to have the minimum values of χ^2 and Σ. $Q_{(n,3He)}$ is the $(n,\,^3$He) reaction energy.

III.2.4 Results and discussion

The results of excitation function for 13 target studied are presented in Figures III.14, and III.15. Table III.2 presents statistical values for our proposed formula and previous empirical and semi empirical formulae, free parameters which fixed with fitting experimental (n, ^{3}He) cross section data presented in table III.2. Σ and χ^2 values are presented for each formula.

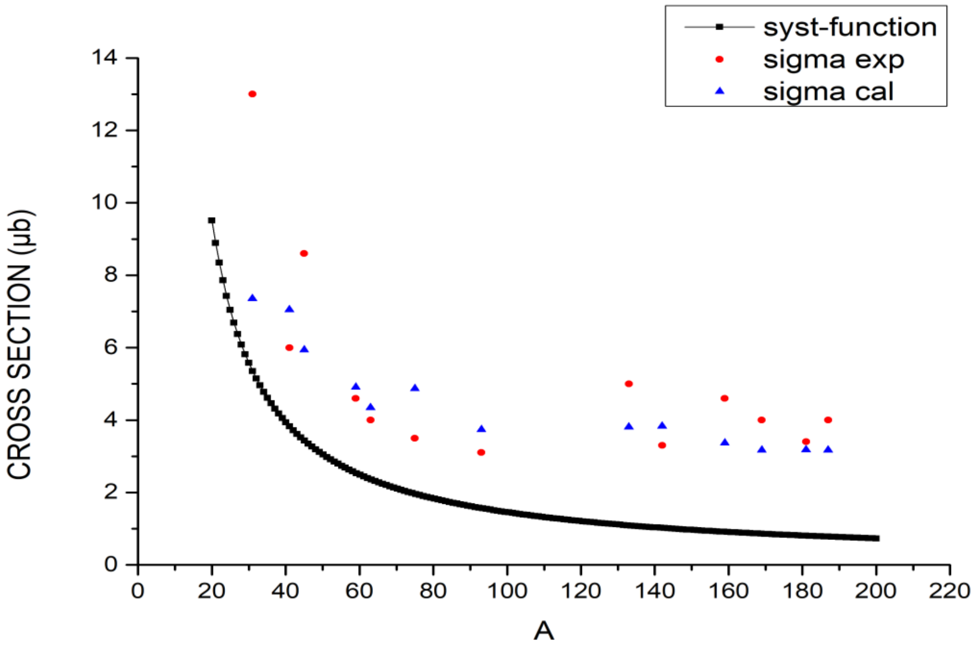


Figure III.14: experimental and calculated cross section of the (n, ^{3}He) reaction in function of mass number A for the 13 atoms taken in the study.

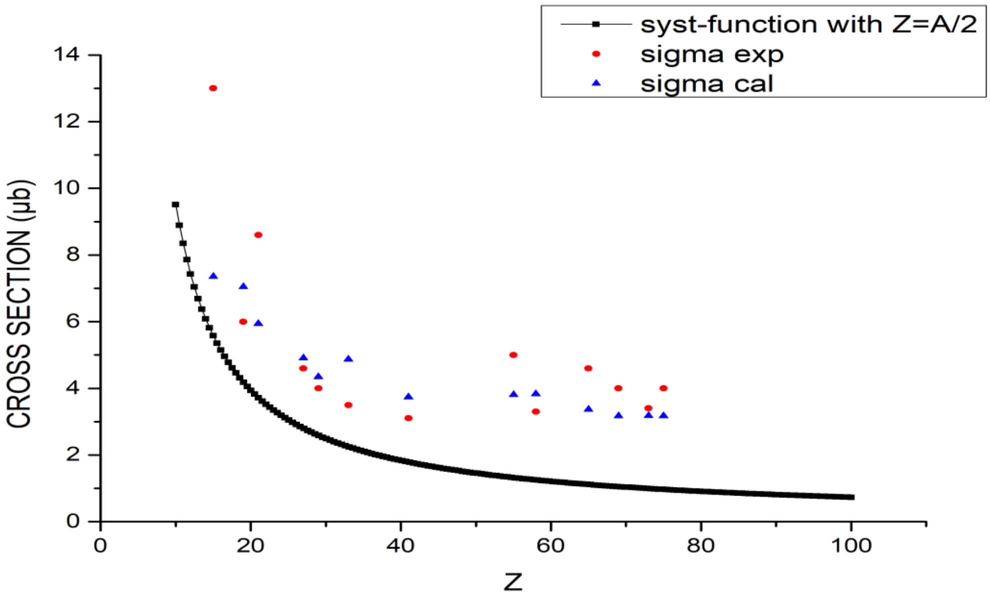


Figure I.15: experimental and calculated reaction (n, ^{3}He) cross section function of charge number Z for 13 atoms taken in the study.

Formula	eq.	Σ	χ^2	Parameters
This work	(III.1)	3.08	0.31	α_1=3.1683.10^{-1}μb, α_2=6.2143.10^{-1}μb, α_3 =-1.5
Nehaoua	(III.4)	7.45	0.83	$\alpha_1 = 2.1136 \times 10^{-2}$ μb, α_2= 9.8232×10^{-1} μb, $\alpha_3 = 1.62$, $\alpha 4 = 374.23$
Yigit	(III.5)	10. 23	0.93	α_1=0.0042 μb,α_2=0.375
Yettou et al.	(III.6)	13.26	1.32	α_1=5.583.10^2 μb,α_2=-0.42631 μb,α_3=-61.492
Broeders et al.	(III.7)	15.1	1.51	α_1=1.6534 μb,α_2=0.15257 μb,α_3=-2.3
Broeders et al.	(III.8)	20.8	1.89	α_1=5.8701.10^{-3} μb,α_2=1.7378.10^{-2} μb,
Qaim	(III.9)	21.8	1.99	α_1=8.475.10^{-2} μb,α_2=-1.6467

Table III.2: Σ and χ^2 values are presented for each formula and it's free parameters.

III.2.5 Comparison and discussion

In this study to compare the quality of our formula we calculate statistical parameters Σ and $\chi 2$ values for 13 nuclei ($31 \leq A \leq 187$), using data presented in table 1 we find that formula given by eq. (III.1) with three parameters reduces the difference between experimental and calculated (n, ^{3}He) cross section, Σ and χ^2 have the minimum values equal to 3.08 and 0.31 respectively which are lower than values obtained in previous studies. The semi empirical formula given by eq. (III.1) decreases significantly the difference between experimental and calculated (n, ^{3}He) cross section, Σ and χ^2 have the least values.

III.2.6 Conclusion

The difficulty of measure in nuclear reactor is the reason of this poor data. For that the systematic (n, ^{3}He) reaction cross section is used to reproduce measured data and predict unmeasured data. Evaporation and pre-equilibrium models are used in previous (n, ^{3}He) systematics to find empirical and semi-empirical formulae which describe correctly (n, ^{3}He) reaction. These formulae contain free parameters fixed with fitting experimental data, several calculations has succeed to reproduce measured (n, ^{3}He) reaction cross sections at 14.6 MeV.

The study concerns the following reactions:

^{31}P(n, ^{3}He)^{29}Al, ^{41}K(n, ^{3}He)^{39}Cl, ^{45}Sc(n, ^{3}He)^{43}K, ^{59}Co(n, ^{3}He)^{57}Mn, ^{63}Cu(n, ^{3}He)^{61}Co, ^{75}As(n, ^{3}He)^{73}Ga, ^{93}Nb(n, ^{3}He)^{91}Y ^{103},^{133}Cs(n, ^{3}He)^{131}I ,^{142}Ce(n, ^{3}He)^{140}Ba, ^{159}Tb(n, ^{3}He)^{157}Eu, ^{169}Tm(n, ^{3}He)^{167}Ho , ^{181}Ta(n, ^{3}He)^{179}Lu , ^{187}Re(n,^{3}He)^{185}Ta.

In this work we use pre-equilibrium ^{3}He particle emission and regenerate (n, ^{3}He) reaction cross section at 14,6 MeV. We have proposed formula with three parameters which given as:

$$\sigma^{pre}_{^3He} = \pi r_0^2 \left(A^{1/3} + 1\right)^2 A^{-1.5} \left(3.1683.\,10^{-1} \left(\frac{N-Z+1}{A}\right) + 6.2143.\,10^{-1}\right)^{15} \text{. .... (III.10)}$$

Compared to previous studies the three parameters formula gives the lowest χ^2=0.31 value of and assure best fit. These results demonstrate the domination of the pre-equilibrium process to direct and evaporation process in ^{3}He particle emission.

Z	A	E$_n$ (MeV)	$\sigma_i^{exp} \pm \sigma\Delta_i^{exp}$ (µb)	σ_i^{calc} (µb)	Σ
15	31	14.6	13.±6.5	7.35	0.765
19	41	14.6	6. ±3.	7.05	0.123
21	45	14.6	8.6±4.	5.94	0.441
27	59	14.6	4.6±2.1	4.91	0.021
29	63	14.6	4. ±2.	4.34	0.029
33	75	14.6	3.5±1.9	4.87	0.518
41	93	14.6	3.1±1.5	3.74	0.181
55	133	14.7	5. ±3.	3.81	0.156
58	142	14.6	3.3±1.3	3.83	0.168
65	159	14.6	4.6±1.8	3.37	0.470
69	169	14.6	4. ±2.	3.17	0.171
73	181	14.6	3.4±1.5	3.18	0.022
75	187	14.6	4.±3.	3.17	0.076

Table III.3: show calculated (n, ^{3}He) cross section obtained with formula given in eq (III.1) and the corresponding *Σ* value.

Conclusion

The objectives of the study on the systematic study of the (n,^{3}He) nuclear reaction and calculation of excitation functions using the TALYS code are as follows:

to investigate the reaction mechanism, to calculate excitation functions and to improve nuclear reaction modeling by comparing the calculated excitation functions with experimental data

The study aims to assess the performance and accuracy of the TALYS code in predicting the (n, 3He) reaction. This evaluation will help identify areas where the current models may need improvement, leading to refinements and advancements in nuclear reaction modeling.

Overall, the objectives of this study aim to deepen our understanding of the (n,3He) nuclear reaction, improve the accuracy of nuclear reaction modeling, contribute to nuclear data evaluations, and advance research in nuclear energy applications.

In first step, we can conclude that Talys nuclear code contains a few experimental data correct for a few targets (<20) and for a fixed value of neutron's energy varing from 14, 6 MeV to 14,7 MeV. For calculated (n, ^{3}He) function excitations, the code shows limits, the reason of these limits is the features related to the (n, ^{3}He) reaction like: difficulty of the experience and the low probability of its realization. Also The Talys code gives (n, ^{3}He) function excitation for neutron energies between 14 MeV and 15 MeV with a great difference between evaluated and experimental data. The proposed formula with three parameters is written as:

$$\sigma_{^3He}^{pre} = \pi r_0^2 \left(A^{1/3} + 1\right)^2 A^{-1.5} \left(3.1683.\,10^{-1} \left(\frac{N-Z+1}{A}\right) + 6.2143.\,10^{-1}\right)^{15}$$

Our results show that the excitation functions for the (n,3He) reaction exhibit a strong dependence on both the target nucleus and neutron energy.

Using our semi empirical formula, We good agreement between our calculations and available experimental data in most cases. Our study provides valuable information on the behavior of the (n,^{3}He) reaction across a range of target nuclei and neutron energies. The excitation functions we calculated can be used to predict the behavior of the reaction in various experimental conditions, such as in neutron spectroscopy experiments or in the production of tritium for nuclear fusion reactors.

Annex

python code to calculate the cross section from semi empirical formula Proposed and sigma

```
import math
import numpy as np

r_0= 1.3e-13 #convert from fm to cm

E=13  # number of particles

α_1=3.1683e-1
α_2=6.2143e-1
α_3=-1.5

# data (A,N,Z) A: mass number N:number of neutrons Z: number of protons

data=[(31,16,15),(41,22,19),(45,24,21),(59,32,27),(63,34,29),(75,42,33),(93,52,41),
(133,78,55),(142,84,58),(159,94,65),(169,100,69),(181,108,73),(187,112,75)]

σ_exp =np.array ([13,6,8.6,4.6,4,3.5,3.1,5,3.3,4.6,4,3.4,4]) # the experimental values of
the cross section

Δσ_exp =np.array([6.5,3,4,2.1,2,1.9,1.5,3,1.3,1.8,2,1.5,3]) #experimental errors


def calculate_cross_section(A, N, Z, α_1, α_2, α_3, r_0):
    term1 = math.pi * r_0**2
    term2 = (A**(1/3) + 1)**2
    term3 = A**α_3
    term4 = (α_1 * ((N - Z + 1) / A) + α_2)**15
    cross_section = term1 * term2 * term3 * term4 * 1e30 #convert from cm² to μb
    return cross_section

def calculate_sigma(σ_exp, σ_calculated, Δσ_exp):
    sum_squared_diff = sum(((σ_exp[i] - σ_calculated[i]) / Δσ_exp[i])**2 for i in
range(E))
    return sum_squared_diff
```

```
σ_calculated = [calculate_cross_section(A, N, Z, α_1, α_2, α_3, r_0) for A, N, Z in data]

σ_sigma = calculate_sigma(σ_exp, σ_calculated ,Δσ_exp)

sigma=((σ_exp - σ_calculated) / Δσ_exp)**2


print("cross section =",σ_calculated)

print ("sigma=",sigma)

print ("sigma_total",σ_sigma)

print("\n**************************************************\n")


print('\x1b[6;30;42m' + ' THE END ' + '\x1b[0m')
```

```
cross section = [6.823340648801321, 6.5969827000156, 5.651610569496894, 4.765268080691931, 4.26657089765826, 4.749365679149384, 3.7479833337933486, 3.8440149371715955, 3.867365124647587, 3.442554729286158, 3.2666844401551995, 3.274292959692681, 3.2726358763856354]


sigma= [ 0.90298511 , 0.0395987 , 0.54331251 , 0.00619355 , 0.01776501 , 0.43238632 , 0.1866144 , 0.14847794 , 0.19047526 , 0.41348134 , 0.13443793 , 0.00702323 , 0.05878429]


sigma_total 3.0815355829090025


**************************************************


THE END
```

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Abstract

Our work focused (n, ^{3}He) nuclear reaction cross section, in the first step we present data available of this reaction in Talys code. In the second state a new three parameters formula is proposed to calculate (n, ^{3}He) nuclear reaction cross section at 14.6 MeV, this semi-empirical systematic reduces parameters taken in previous proposed formulae which increase the contribution of pre-equilibrium ^{3}He particle emission. ^{3}He particle emission in reaction induced by neutron. To check the formula's quality we compare obtained cross section with measured ones. The formula obtained in this work has a good fitting with the lowest value of statistical parameters Σ and χ^2 equal respectively to 3.08 and 0.31

Résumé

Dans ce travail, nous avons mené une étude systématique pour reproduire des fonctions d'excitation des réaction neutronique (n, ^{3}He) proches des données expérimentales de EXFOR, la formule semi empirique proposée est basée sur le modèles de pré-équilibre, elle contient trois paramètres libres pour avoir le minimum des paramètres statistiques Σ et χ^2. En parallèle, on a vérifié les données expérimentales et évaluées du code de simulation nucléaire Talys pour les 13 cibles étudiées, on a ramarque un enorme manque de données pour la réaction neutronique (n, ^{3}He) à 14,6 MeV, ainsi une divergence entre les données calculées et les données expérimentales.