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Original Research Article

Investigation of Nuclear Property of Protactinium-231 for Reactor Fuel Application Using the Coupled-Channel Optical Model Code for Energy up to 20 MeV

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ABSTRACT

In this study, we investigated the neutron-induced fissile isotopes of Protactinium-231 using the Coupled-Channeled Optical Model code (OPTMAN) up to 20 MeV. The research was driven by the growing demand for nuclear reactor fuels. Protactinium-231, a naturally occurring radionuclide with significant fuel potential, is found in nearly 100% abundance. When subjected to neutron bombardment, Protactinium-231 can yield fissile materials suitable for use as reactor fuel. We performed computations using two different approaches: The Potential Expanded by Derivatives (PED), which incorporates the Rigid-Rotor Model (RRM) treating nuclei as rigid vibrating spheres while considering nuclear volume conservation, and the Rotational Model Potentials (RMP), which accounts for the Soft-Rotator Model (SRM) treating nuclei as deformable, rotating spheres. Each set of calculated data was compared with data retrieved from the Evaluated Nuclear Data File (ENDF), and a high level of agreement was observed. In all cases, the threshold energies were found to be ≤ 4 MeV for both PED and RMP. Notably, the results obtained from the RMP approach exhibited closer agreement with the retrieved data than those from the PED approach.

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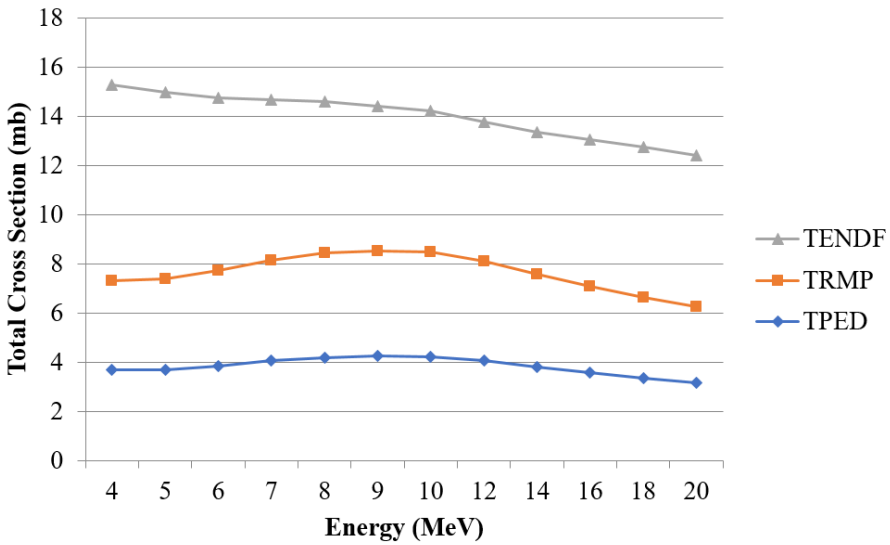
GRAPHICAL ABSTRACT



1. INTRODUCTION

The needs for Fissile isotopes of uranium are due to their practical applications. These isotopes or materials can be used as fuel in nuclear reactors of both power plants and research reactors, as they can be split by neutrons in a self-sustaining nuclear chain reaction. The amount of energy released during these reactions is large enough to generate electricity. Aside from being used as nuclear reactor fuels, fissile materials can undergo fission reaction processes. They are the key components of nuclear weapons or other nuclear explosives devices. Those mostly used in nuclear weapons are highly enriched uranium (uranium-235 and plutonium-239). However, this study is for nuclear research reactor application. As such, we should focus on nuclear reactor fuels [1-5]. It is pertinent to search for alternative fuel means in some isotopes that are radioactive aside the uranium-235 and plutonium-239. We may recall that the two most important fissile materials normally used as fuels are uranium-235 and Plutonium-239. These are weapon-grade materials that can also be used as reactor fuels. Uranium 235 is a natural isotope of uranium with an abundance of 0.72%. This concentration is very small. Nuclear physicists have made efforts to increase this concentration through the enrichment process. However, due to the prevalent need for reactor fuels, we ought to seek alternative isotopes that can be used as fuels [6-10]. The fissile materials Plutonium-239 and uranium-233, which do not occur in nature, are produced by the transmutation of uranium-238 and thorium-232, respectively. These materials are called fertile materials. For fuel cycles using plutonium-239 and uranium-233 as fuel, irradiation of uranium-238 and thorium-232 in the fuel blanket and reprocessing to extract the plutonium-239 and uranium-233 become important steps in the cycle [11-13]. Plutonium-239 is not a natural isotope of plutonium. It is bred from the naturally occurring uranium-238 whose natural abundance is 99.9%. Uranium-238 is irradiated by fast neutrons to produce Uranium-239 and this Uranium-239 can undergo a radioactive decay to produce Plutonium-239. Plutonium-239 just like Uranium-235 is a fissile material. The Plutonium-239 can then be bombarded with high-speed neutrons. When a Plutonium nucleus absorbs one such free neutron, it splits into two fission fragments. This

fission releases heat as well as neutrons, which in turn splits other plutonium nuclei present, freeing still more neutrons. As this process is repeated, it becomes a self-sustaining chain reaction, yielding a steady source of energy, chiefly in the form of heat transported from the reactor core by a liquid sodium coolant to a system of heat exchange. This system utilizes heat to produce steam for a turbine that drives an electric generator [14-17]. Uranium-233 is a fissile isotope of uranium bred from thorium-232 as part of the thorium fuel cycle. Uranium-233 was investigated for use in nuclear weapons and as reactor fuel. It has been successfully used or tested in experimental nuclear reactors and has been proposed for much more or wider use as nuclear fuel. It has a half-life of 160,000 years [18]. Uranium-233 is produced by neutron irradiation of thorium-232. When thorium-232 absorbs a fast neutron, it becomes thorium-233 with a half-life of 22 minutes. After 22 minutes, thorium-233 decay by alpha to protactinium 231 with a half-life of 27 days, and beta decays to uranium 233. Just like uranium-235 and plutonium 239, protactinium-231 has been proposed to be used as nuclear fuel as asserted above [19]. Therefore, protactinium-231 being naturally occurring isotope, is a breeder fissile material [20]. A research was conducted by Avrigeanu and Avrigeanu (2019) [21] on the analysis of neutron bound states of ^{208}Pb by a dispersive optical model potential, in their research, they discussed the effect of dispersive-

$$W_D(E) = A_D\left[\frac{(E-E_F)^{-2}}{(E-E_F)^{-2}+(B_D)^2} - \exp\left(-\lambda_D(E-E_F)\right)\right] \quad (1)$$

Where, A_D, B_D, and λ_D are constants (undetermined), E and E_f are Proton and femi energy, respectively.

Another utilized energy (dependence) for the surface (imaginary) term has been pointed out by Naik *et al.* (2021) [22] Naik *et al.* (2020) [23], as follow:

correction terms on the calculation of bound-state energies and finally reported that, the derived ^{208}Pb root mean square radius shows good agreement with measured data. Another research was carried out by Avrigeanu and Avrigeanu *et al.* (2021) [24] on the dispersive optical model description of nucleon scattering on Pb–Bi isotopes and reported that the new potential is shown to give a very good description of nucleon scattering data on near-magic targets ^{206,207}Pb and ^{209}Bi. This work investigates the effects of excitation in neutron induced fissile isotopes of protactinium-231 for 20 MeV using Coupled-Channels Optical Model OPTMAN Code with adjustment for soft and rigid rotation of the nucleus.

2. EXPERIMENTAL

2.1. Theory

The current optical potential encompasses corrections (relativistic) as reported by Avrigeanu and Avrigeanu (2022) [25] and expanded by Avrigeanu and Avrigeanu *et al.* (2018) [26].

Surface variation $W_D(E)$ and potential for volume absorption $W_V(E)$ can wisely be presented in terms of energy which could be suitable for the dispersive optical model analysis [27, 28]. The most utilized energy (dependence) for the surface (imaginary) term has been pointed out by Avrigeanu and Avrigeanu *et al.* (2023) [29], as follow:

$$A_{D,V} = W_{D,V}^{DISP}\left[1 + (-1)Z' + 1\frac{C_{wiso,wviso}N-Z}{W_{D,V}^{DISP}\quad A}\right]. \quad (2)$$

Where, $W_{D,V}^{DISP}$ and $C_{wiso,wviso}$ are constants (undetermined), and also A, N, and Z are mass, neutron and atomic number, respectively.

Utilized energy (dependence) for the volume (imaginary) term has been confirmed in studies of nuclear matter theory by Gopalakrishna *et al.* (2018) [30].

$$W_V(E) = A_V\frac{(E-E_F)^2}{(E-E_F)^2+(W_V^{DISP})^2} \quad (3)$$

Where, A_V and W_V^{DISP} are constants (undetermined), and also E and E_f are proton and femi energy, respectively [31-32].

2.2. METHODOLOGY

The OPTMAN code for this work was downloaded from the IAEA website at http://nds-IAEA.org. The optical model code OPTMAN was chosen because it can study nucleon interactions with light-mass, medium-mass, and heavy-mass nuclei for a broad range of energy up to 200 MeV. In addition, it has a Soft-Rotator model in addition to its Rigid-Rotator model, which improves the precision of the even-even nuclide.

The selection of the appropriate record cards and switches determines how the code will run when the software has been successfully installed using the G-FOTRAN compiler. Record cards that describe input data are themselves described by switches for the description of the model. The "va" executable file is used to invoke each calculation's input data and is produced using the Windows command

The code is executed immediately the command "va" is issued, the input file name is requested and supplied, the output file name is requested and supplied, and the enter key is pushed. The OPTMAN code computation was based on Equations (1) to (6).

3. RESULTS and DISCUSSION

The results obtained from the computer software (OPTMAN Code) based on the Equations (1) to (6) for Rotational Model Potential (RMP) which accounts for Soft-Rotator Model and Potentially Expanded by Derivatives (PED) accounts for Rigid-Rotor Model by calculating the neutron-induced Total Potentially Expanded by Derivatives (TPED), Total Rotational Model Potential (TRMP), Reaction Potentially Expanded by Derivatives (RPED), Reaction Rotational Model Potential (RRMP), Elastic Potentially Expanded by Derivatives (EPED), and Elastic Rotational Model Potential (ERMP) cross section reactions for ^{231}Pa is presented in Table 1:

Table 1. Results obtained for Soft and Rigid-Rotor Model for Protactinium-231 (^{231}Pa)

	Cross Section (Reaction)			Cross Section (Elastic)			Cross Section (Total)		
Energy (MeV)	**RPED**	**RRMP**	**RENDF**	**EPED**	**ERMP**	**EENDF**	**TPED**	**TRMP**	**TENDF**
4	1.81	1.76	0.87	1.78	1.87	4.43	3.59	3.63	5.30
5	1.66	1.62	0.80	1.95	2.07	4.24	3.61	3.69	5.04
6	1.63	1.59	0.88	2.14	2.29	3.80	3.77	3.88	4.68
7	1.65	1.61	1.55	2.32	2.48	3.34	3.97	4.09	4.89
8	1.66	1.62	1.82	2.45	2.62	2.96	4.11	4.24	4.78
9	1.65	1.61	1.69	2.52	2.68	2.71	4.17	4.29	4.40
10	1.63	1.58	1.55	2.53	2.67	2.58	4.16	4.25	4.13
12	1.58	1.53	1.35	2.41	2.50	2.56	3.99	4.03	3.91
14	1.56	1.52	1.31	2.19	2.24	2.74	3.75	3.76	4.05
16	1.57	1.54	1.63	1.94	1.97	2.96	3.51	3.51	4.59
18	1.58	1.56	1.73	1.72	1.73	3.13	3.30	3.29	4.86
20	1.57	1.56	1.70	1.53	1.54	3.22	3.10	3.10	4.92

To compare the obtained results from this study with retrieved data (TENDF), charts for the computation of the excitation function for the cross-section (Total), cross-section (Reaction), and cross-section (Elastic) of ^{231}Pa are plotted and presented in Figures 1, 2, and 3.

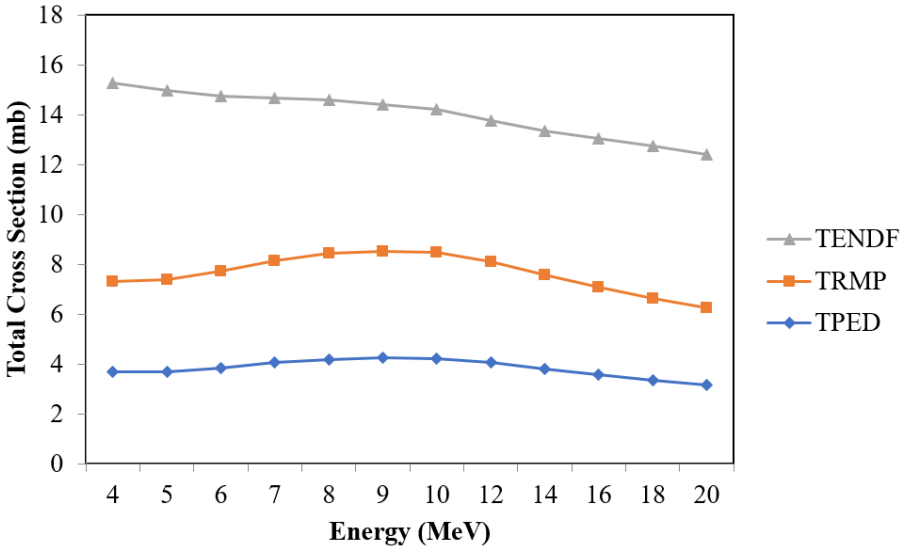


Fig1. Cross-section of Protactinium-231 (^{231}Pa)

According to Fig 1, the excitation function of the total cross section induced by neutrons in ^{231}Pa displays a consistent pattern: An escalation from 4 to 9 MeV followed by a decline from 9 to 20 MeV. Notably, the outcomes derived from the Total Rotational Model Potential (TRMP) exhibit a higher degree of concurrence with the data obtained from the Thermal Neutron-Induced Fission Data File (TENDF), in comparison to the outcomes produced by the Total Potential Expanded by Derivatives (TPED).

In addition, the impact of rotational excitation becomes more conspicuous, with the Rotational Model Potential emerging as the optimal approach for effectively accounting for this phenomenon.

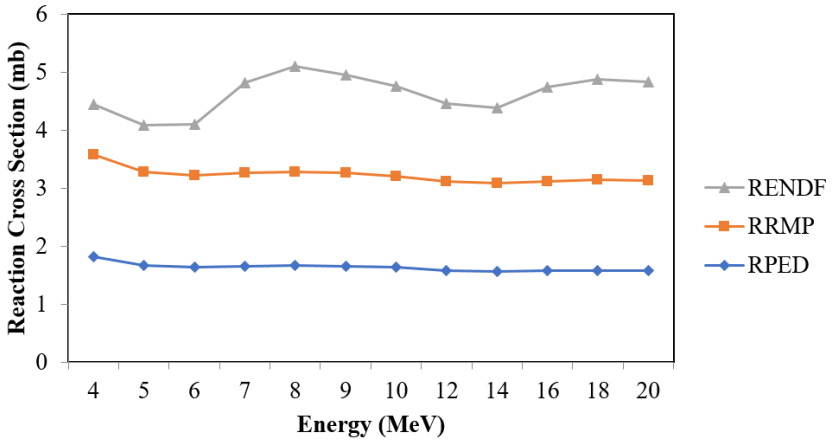


Fig 2. Reaction Cross-section of Cross Section of Protactinium-231 (^{231}Pa)

As depicted in Fig 2, the excitation function of Protactinium-231 exhibits a noteworthy alignment between the Potential Expanded by Derivatives (RPED) and the Rotational Model Potential (RRMP), particularly within the energy range of 4-6 MeV, as evidenced by the congruence with the established reference data (RENDF). This alignment suggests that the threshold energy for neutron-induced reactions in both RPED and RRMP lies at ≤ 4 MeV.

However, a marked disparity arises between the calculated PED values and the established ENDF standard data within the energy span of 6-12 MeV.

Notably, the results derived from the Rotational Model Potential exhibit superior accord with the reference data (RENDF) when contrasted with the outcomes obtained from the Potential Expanded by Derivatives.

This underscores the capacity of the Rotational Model Potential to effectively characterize the dynamic alterations in the nuclear structure brought by rotation.

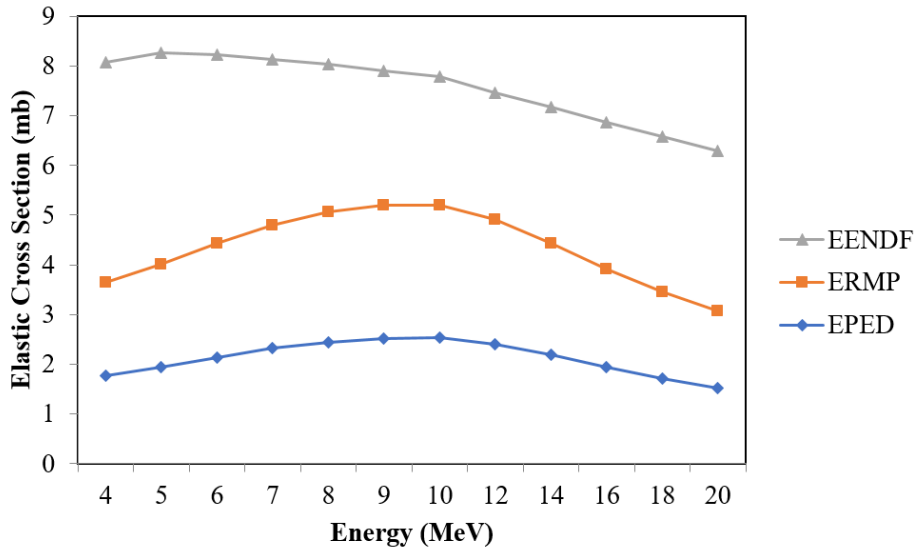


Fig 3. Elastic Cross-section of Protactinium-231 (^{231}Pa)

As demonstrated in Fig 3, a noteworthy correspondence is evident in neutron-induced elastic scattering between the Potential Expanded by Derivatives (EPED) and the Rotational Model Potential (ERMP), specifically within the energy intervals of 4 to 6 MeV and 10 to 20 MeV, where alignment with the retrieved reference data (EENDF) is observed. However, a lack of consensus emerges between EPED and the established EENDF standard data within the energy span of 6 to 9 MeV.

This discrepancy underscores the efficacy of the Rotational Model Potential, which incorporates the soft-Rotor model of the Coupled-channels Optical Model, in effectively elucidating the impact of excitation-induced rotation on neutron capture. Notably, this approach exhibits a stronger concurrence with the reference data (EENDF), solidifying its suitability for describing the intricate interplay between rotation and neutron interactions.

5. CONCLUSION

We employed the Coupled-Channel Optical Model code, OPTMAN, to explore the effects of neutron-induced fissile isotopes of Protactinium-231. Optical model computations were conducted using two distinct approaches: The Coupled-

Channel Rotational Model Potential (CC-RMP), which characterizes the Soft-Rotor model treating nuclei as either soft rotational spheres or deformed nuclei, and the Potential Expanded by Derivatives (CC-PED), which corresponds to the Rigid-Rotor Model, treating nuclei as rigid vibrating spheres while accounting for nuclear volume conservation.

In our computations for both PED and RMP, we observed that the energies in agreement with the established reference data (ENDF) were consistently at 4 MeV. Notably, the results derived from the Rotational Model Potential (RMP) generally exhibited higher values and demonstrated superior agreement with the standard ENDF data compared to those obtained from the Potential Expanded by Derivatives (PED). Additionally, when examining elastic scattering cross sections, it became evident that the values were generally higher for 231Pa when utilizing both PED and RMP, and they displayed better alignment with the retrieved ENDF data. Furthermore, we observed a trend where Odd-A nuclides tended to have higher cross-section values compared to Even-A nuclides. This characteristic can be attributed to the oddness in both proton (Z) and neutron (N) numbers, which tends to lower the nuclear binding energy, rendering odd nuclei less stable and more prone to fission. Consequently, all odd-A nuclei considered in this study may be particularly promising for reactor fuel applications, with the exception of materials that are fissionable but not fissile. In light of these findings, it is recommended that the suitability of the odd-A nuclei explored in this research for use as reactor fuel be further investigated and tested.

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