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Neutron-Induced Cross Sections for Stable Selenium Isotopes (A = 74–82) Using the EMPIRE-3.2 Code with Coupled-Channels Optical Model Calculations

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Abstract

A comprehensive theoretical evaluation of neutron-induced reaction cross sections for the stable selenium isotopes $^{74-82}$Se is presented using the EMPIRE-3.2 nuclear reaction modeling code. The global Koning–Delaroche optical model potential is adopted as the principal interaction framework and is augmented by coupled-channels calculations to explicitly account for vibrational collective excitations in the even-A isotopes. Pre-equilibrium emission processes are treated with advanced implementations of the DEGAS and PCROSS modules, enabling a realistic description of multi-step direct and compound mechanisms. Nuclear structure inputs are taken from the RIPL-3 database, including microscopic Hartree–Fock–BCS level densities and generalized Lorentzian γ-ray strength functions to ensure physically consistent statistical decay modeling. Calculations cover neutron energies from thermal values up to 30 MeV and include total, elastic and inelastic scattering, as well as (n,γ), (n,p), (n,2n), and (n,α) reaction channels. Local adjustments of optical model parameters, supported by systematic sensitivity analyses, are performed to optimize agreement with available experimental datasets from the EXFOR library. The results demonstrate excellent reproduction of measured (n,p) excitation functions in the 10–20 MeV region and accurate prediction of (n,2n) reaction thresholds and peak cross sections. Compared with default TALYS outputs and evaluated nuclear data libraries ENDF/B-VIII.0 and JENDL-5, the EMPIRE-3.2 calculations show improved performance in pre-equilibrium-dominated channels, reducing discrepancies to approximately 10–20%. The refined cross sections provide improved input for modeling the weak s-process nucleosynthesis in massive stars, particularly at the branching points near ^79Se and ^80Se, and contribute to enhanced accuracy in reactor dosimetry and activation analyses. Overall, the study demonstrates the effectiveness of quantum-mechanical optical model approaches in bridging experimental data gaps for medium-mass nuclei.

Keywords

Neutron-induced reactions;
Selenium isotopes;
Koning-Delaroche optical potential;
Coupled-channels;
EMPIRE code;
Pre-equilibrium reactions;
s-process nucleosynthesis

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1. Introduction

Neutron-induced nuclear reactions constitute a cornerstone of modern nuclear science and technology, underpinning applications that range from energy generation in nuclear reactors to the synthesis of elements in stars and the production of medically relevant isotopes. The probability of these reactions occurring is quantified by the neutron-induced cross section, a fundamental parameter that governs reaction rates and determines the behaviour of materials exposed to neutron fields. Consequently, accurate and reliable cross-section data are indispensable for reactor design, radiation shielding, dosimetry, nuclear astrophysics, and a wide range of industrial and scientific applications (Blatt & Weisskopf, 1952; Hodgson, 1994).

Among medium-mass elements, selenium (Z = 34) occupies a particularly important position due to its diverse isotopic composition and its relevance in both applied and fundamental nuclear processes. Naturally occurring selenium consists of six stable isotopes, namely ^{74}Se (0.89%), ^{76}Se (9.37%), ^{77}Se (7.63%), ^{78}Se (23.77%), ^{80}Se (49.61%), and ^{82}Se (8.73%), alongside long-lived radionuclides such as ^{79}Se (Brown, 2013). These isotopes participate in a variety of neutron-induced reactions, including radiative capture (n,γ), charged-particle emission (n,p) and (n,α), multiple neutron emission (n,2n), and elastic/inelastic scattering processes. Such reactions are important in nuclear engineering applications such as activation analysis and reactor dosimetry, as well as in astrophysical nucleosynthesis, particularly the slow neutron-capture process (s-process), where selenium isotopes lie near important branching points that influence elemental abundance distributions (Pignatari et al., 2010; Käppeler et al., 2011).

Despite their importance, neutron-induced cross sections for selenium isotopes are not comprehensively characterized across all relevant energy ranges. While experimental data exist for certain reactions, especially neutron capture at thermal and epithermal energies and activation measurements in the fast neutron region where significant discrepancies persist among different datasets. These inconsistencies are reflected in major evaluated nuclear data libraries such as ENDF/B-VIII.0, JENDL-5, JEFF-3.3, and TENDL, which often rely on theoretical models to supplement incomplete measurements (Brown et al., 2018; Shibata et al., 2021; Plompen et al., 2020). As a result, predictive nuclear reaction modeling remains essential for generating consistent and reliable cross-section data.

Theoretical Background of Neutron-Induced Reactions

The theoretical description of neutron–nucleus interactions is grounded in quantum mechanics. The behaviour of an incident neutron interacting with a target nucleus is governed by the time-independent Schrödinger equation:

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + U(r,E)\right]\psi(r) = E\psi(r) \qquad (1)$$

where $\mu$is the reduced mass of the neutron–target system, $E$is the incident neutron energy, and $U(r,E)$is the complex optical potential.

The optical potential is expressed as:

$$U(r,E) = V(r,E) + iW(r,E) \quad (2)$$

where $V(r,E)$represents the real part responsible for elastic scattering, and $W(r,E)$represents the imaginary part accounting for absorption into non-elastic channels (Koning & Delaroche, 2003).

The real part of the potential is commonly parameterized using a Woods–Saxon form:

$$V(r) = -V_0\left[1 + \exp\left(\frac{r-R}{a}\right)\right]^{-1} \quad (3)$$

where V_0 is the potential depth, $R = r_0A^{1/3}$is the nuclear radius, and $a$is the diffuseness parameter. The imaginary component typically includes both volume and surface absorption terms, which dominate at different energy regimes (Hodgson, 1994).

An important component of the optical model is the spin–orbit interaction, given by:

$$V_{so}(r) = \frac{1}{r}\frac{d}{dr}f(r)\,\mathbf{l}\cdot\mathbf{s} \quad (4)$$

which is essential for accurately describing angular distributions and polarization effects in scattering processes.

Reaction Mechanisms and Cross-Section Modeling

Neutron-induced reactions proceed through different mechanisms depending on the incident neutron energy. These include direct reactions, compound nucleus formation, and pre-equilibrium processes (Blatt & Weisskopf, 1952; Griffin, 1966).

For compound nucleus reactions, which dominate at low and intermediate energies, the Hauser–Feshbach statistical model provides the cross section:

$$\sigma_{ab} = \sum_{J,\pi}\frac{\pi}{k^2}\frac{(2J+1)}{(2I_a+1)(2I_A+1)}\frac{T_aT_b}{\sum_c T_c}W_{ab} \quad (5)$$

where $T_a$and $T_b$are transmission coefficients for the W_{ab} and exit channels, $J$and πdenote spin and parity, and $W_{ab}$is the width fluctuation correction factor (Hauser & Feshbach, 1952; Hofmann et al., 1975).

The transmission coefficients are derived from the optical model S-matrix:

$$T_l = 1 - |\,S_l\,|^2 \quad (6)$$

linking the quantum mechanical scattering description to statistical reaction theory.

At higher neutron energies (typically above ~10 MeV), pre-equilibrium emission becomes significant. This is described using the exciton model, where the system is characterized by the exciton number:

$$n = p + h \quad (7)$$

with $p$and $h$representing the number of excited particles and holes, respectively (Griffin, 1966). This mechanism is particularly relevant for reactions such as (n,p) and (n,2n) on selenium isotopes.

Optical Model Parameterization and Coupled-Channels Approach

Global optical model parameterizations, such as the Koning–Delaroche (KD) potential, express the energy dependence of the real potential depth as:

$$V(E) = V_0 + V_1E + V_2E^2 \quad (8)$$

and are valid for a wide range of nuclei and neutron energies up to 200 MeV (Koning & Delaroche, 2003). However, for nuclei in the mass region A ≈ 74–82, including selenium isotopes, these global models may not fully capture nuclear structure effects such as deformation and collective excitations.

For such nuclei, the coupled-channels optical model provides an improved description by explicitly including coupling between nuclear states:

$$U(r,\theta) = U_0(r) + \sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta) \frac{dU_0(r)}{dr} \quad (9)$$

where $\beta_\lambda$are deformation parameters and $Y_{\lambda 0}$are spherical harmonics (Soukhovitskii et al., 2005). This approach is particularly important for even-even selenium isotopes, which exhibit vibrational and rotational collective behavior.

Role of EMPIRE-3.2 in Nuclear Reaction Modeling

The complexity of neutron-induced reactions necessitates the use of advanced nuclear reaction codes capable of integrating multiple theories. The EMPIRE-3.2 code system provides a comprehensive platform for modeling nuclear reactions through the combined implementation of optical model calculations (including coupled-channels approaches via ECIS), pre-equilibrium emission models, and Hauser–Feshbach statistical decay (Herman et al., 2007).

The total reaction cross section derived from the optical model is given by:

$$\sigma_R = \frac{\pi}{k^2} \sum_l (2l+1)(1-|S_l|^2) \quad (10)$$

which forms the basis for calculating all reaction channels. EMPIRE integrates this with level density models, such as the Gilbert–Cameron formulation, and gamma-ray strength functions to produce observables including cross sections, angular distributions, and energy spectra.

Therefore, from an astrophysical perspective, selenium isotopes play a significant role in the weak component of the s-process, which occurs in massive stars during helium- and carbon-burning phases. In this process, neutron capture competes with β-decay along the valley of stability, leading to branching points that are sensitive to neutron density and stellar temperature. One notable example is the long-lived isotope ^{79}Se, whose half-life (~3.27 × 10^5 years) and neutron capture rate influence nucleosynthesis pathways (Wisshak et al., 1986; Pignatari et al., 2010).

In addition to astrophysical applications, selenium isotopes are relevant in reactor physics and radiation dosimetry, where reactions such as (n,p) and (n,2n) are used for fast neutron flux monitoring (Gandhi et al., 2021). However, uncertainties in cross-section data persist due to limited experimental measurements and inconsistencies among evaluated libraries.

This present study therefore focuses on the calculation of neutron-induced cross sections for stable selenium isotopes (A = 74–82) using the EMPIRE-3.2 nuclear reaction code, with particular emphasis on coupled-channels optical model calculations. By employing the Koning–Delaroche global optical model potential and exploring possible refinements, this work aims to improve agreement with experimental data and evaluated nuclear data libraries such as ENDF/B-VIII.0, JENDL-5, and JEFF-3.3.

2. Materials and Methods

2.1 Nuclear Data and Input Parameters

Accurate nuclear modeling relies on reliable and well-established input data. Nuclear structure data were extracted from the Reference Input Parameter Library (RIPL-3) and the Evaluated Nuclear Structure Data File (ENSDF), as documented by Capote et al. (2009). Level density models incorporated both the microscopic Hartree–Fock–BCS approach and the composite Gilbert–Cameron model, originally proposed by Gilbert and Cameron (1965). Gamma-ray strength functions were modeled using generalized Lorentzian (GLO) formulations, following the work of Goriely et al. (2008). For benchmarking and comparison purposes, results were evaluated against several major evaluated nuclear data libraries, including ENDF/B-VIII.0 (Brown et al., 2018), JENDL-5 (Shibata et al., 2021), JEFF-3.3 (Plompen et al., 2020), and TENDL (Koning et al., 2023). Experimental cross-section data used for validation were retrieved from the EXFOR database.

2.2 Computational Methodology

All calculations were performed with the EMPIRE-3.2 nuclear reaction code system, as described by Herman et al. (2007), which integrates multiple theoretical models in a modular framework. The computational procedure included optical model calculations carried out via the ECIS subroutine using the KD global parameter set. Local adjustments to these optical model parameters were applied to enhance agreement with experimental measurements.

Multiple reaction channels were considered, encompassing the total cross section, elastic scattering, inelastic scattering, radiative capture (n,γ), (n,p), (n,2n), and (n,α) reactions. Sensitivity analyses were conducted by varying key input elements, such as optical model parameters, level density prescriptions, and gamma-ray strength functions. To assess model dependence and detect systematic discrepancies, comparative simulations were run in parallel using the TALYS nuclear reaction code (Koning et al., 2023).

2.3 Calculation of Reaction Channels

The various reaction channels were modeled within EMPIRE using suitable theoretical frameworks. Elastic and inelastic scattering were described using the optical model with coupled-channels treatment via ECIS across the full energy range. Radiative capture (n,γ) was computed employing Hauser–Feshbach statistical theory, supplemented by semi-direct contributions at lower energies. Charged-particle emission reactions, namely (n,p) and (n,α), were treated through a combination of pre-equilibrium (via DEGAS/PCROSS models) and compound nucleus mechanisms, with pre-equilibrium processes dominating in the 10–20 MeV range, as noted by Singh et al. (2021).

The (n,2n) neutron emission channel was modeled as a compound nucleus process above its threshold energy of approximately 8 MeV. The total reaction cross section was derived by summing contributions from all open channels. Calculations employed a fine energy grid (0.1–1 MeV spacing) near thresholds and resonance regions, transitioning to a coarser grid at higher energies to maintain computational efficiency.

Three distinct simulation configurations were explored: a baseline model utilizing the KD optical potential paired with Hartree–Fock–BCS level densities, a tuned model incorporating locally adjusted optical model parameters, and a set of model variations testing different pre-equilibrium and level density prescriptions. Key outputs included excitation functions, angular distributions, and double-differential spectra.

2.4 Simulation Procedure

The overall simulation procedure followed a structured workflow. It began with the compilation of nuclear structure and reaction input parameters (Capote et al., 2009), followed by initialization of the relevant EMPIRE modules for the optical model, pre-equilibrium, and Hauser–Feshbach calculations. Coupled-channels calculations were implemented specifically for deformed isotopes. Cross-section computations were then executed over neutron incident energies ranging from thermal values up to 30 MeV. Optical model parameters were subsequently adjusted to optimize agreement with data. Validation involved direct comparison against EXFOR experimental measurements and the aforementioned evaluated libraries. Finally, a comparative analysis was performed with corresponding TALYS outputs.

2.5 Software and Tools

The primary software and tools employed included the EMPIRE-3.2 nuclear reaction code (Herman et al., 2007), its integrated ECIS coupled-channels subroutine, the TALYS nuclear reaction code (Koning et al., 2023), the evaluated libraries ENDF/B-VIII.0, JENDL-5, JEFF-3.3, and TENDL, the EXFOR experimental database, and the RIPL-3 and ENSDF nuclear structure databases (Capote et al., 2009).

Several assumptions and limitations should be noted. Global optical model parameterizations, such as the KD set, introduce inherent uncertainties, especially for nuclei exhibiting strong collective excitations (Koning & Delaroche, 2003). The calculations were restricted to neutron energies up to 30 MeV, thereby limiting their applicability at still higher energies. Sparse experimental data for elastic scattering and certain fast-neutron reactions required dependence on theoretical extrapolations in some instances (Singh et al., 2021).

Observed differences between EMPIRE and TALYS results underscore the sensitivity of predictions to choices in level density and pre-equilibrium modeling (Koning et al., 2023).

3 Results and Discussion

3.1 Overview of the Computational Approach

The calculations employed the EMPIRE-3.2 (Malta release) nuclear reaction code system (Herman et al., 2013), a modular platform that combines the ECIS-06 optical model, DEGAS/PCROSS pre-equilibrium emission, and Hauser–Feshbach statistical decay with HRTW width fluctuation corrections. Incident neutron energies were covered from thermal (0.025 eV) to 30 MeV, with primary emphasis on the total, elastic and inelastic scattering, (n,γ), (n,p), (n,2n), and (n,α) reaction channels.

3.2 Selection of Input Parameters

Input parameters were primarily sourced from the Reference Input Parameter Library (RIPL-3), ensuring consistency and validation against experimental data (Capote et al., 2009). Table 1 summarizes the primary inputs used across selenium isotopes.

Table 1: Key Input Parameters in EMPIRE Calculations for Selenium Isotopes

Parameter	Source/Description	Value/Setting for Se Isotopes	Notes
Discrete levels	RIPL-3/ENSDF	Up to ~2–3 MeV excitation; vibrational bands for even-A	Explicit coupling for 2^+ and 4^+ states
Level densities	EMPIRE-specific HFB microscopic	Collective enhancements; parity-dependent	Alternative: Gilbert-Cameron for sensitivity
Gamma-ray strength functions	Generalized Lorentzian (Kopecky-Uhl)	E1 dominant; low-energy enhancements	For (n,γ) capture
Ground-state deformations	RIPL-3	$\beta_2 \approx 0.2–0.3$ (even-A Se)	Supports coupled-channels

For the discrete level schemes, we adopted evaluated data from RIPL-3 and ENSDF, incorporating low-lying excited states up to approximately 2–3 MeV for each selenium isotope. In even-A selenium isotopes, vibrational levels were explicitly included to enable coupled-channels optical model calculations.

Ground-state properties—such as atomic masses, quadrupole deformations ($\beta_2 \approx 0.2–0.3$ for even-A Se), and relevant Q-values—were taken directly from RIPL-3. Level densities were calculated using the default EMPIRE Hartree–Fock–BCS (HFB) microscopic tables, which include collective enhancement factors;

alternative phenomenological prescriptions, such as the Gilbert–Cameron model, were tested to assess sensitivity. Gamma-ray strength functions were modeled with the generalized Lorentzian (Kopecky–Uhl) formulation for E1 transitions, incorporating low-energy enhancements to better describe radiative capture processes.

3.3 Optical Model Parameter Selection and Optimization

The optical model calculations were performed using the ECIS-06 module within EMPIRE, supporting both spherical and coupled-channels formulations (Table 2).

Table 2: Summary of Optical Model Configurations in EMPIRE

Configuration	OMP Type	Application to Se Isotopes	Optimization Target
Default global	Koning-Delaroche (spherical)	All isotopes (baseline)	Total/reaction cross sections
Coupled-channels	KD with rigid rotor/vibrational	Even-A (^{76,78,80,82}Se)	Elastic angular distributions, inelastic
Local tuned	Adjusted KD depths/radii/diffuseness	All (χ^2 minimization)	EXFOR data (total, elastic, reaction)

Local optimizations adjusted volume/surface depths (±5–10%) and geometry parameters using EMPIRE utilities.

The default optical model potential was the Koning–Delaroche (KD) global phenomenological parameterization (Koning & Delaroche, 2003), which includes dispersive relations and provides energy- and mass-dependent parameters validated from 1 keV to 200 MeV, particularly for medium-mass nuclei. For the deformed even-A selenium isotopes ($^{76,\ 78,\ 80,\ 82}$Se), coupled-channels calculations were activated within EMPIRE-3.2, coupling the ground state to the first 2^+ and 4^+ vibrational states (with $\beta_2 \approx 0.2$–0.3) to properly account for collective effects in elastic and inelastic scattering. Starting from the KD global set, local adjustments were made to key parameters, such as volume and surface absorption depths, radii, and diffuseness using EMPIRE's optimization tools to minimize χ^2 with respect to experimental total cross sections, elastic angular distributions, and selected reaction cross sections from EXFOR. These refinements, typically reducing volume absorption by 5–8%, significantly improved agreement in the 10–20 MeV region where pre-equilibrium processes are important. The resulting KD-based calculations, supplemented by coupled-channels treatment and tuned parameters, served as a reliable baseline for describing total and reaction cross sections across the selenium isotopes (Figure 1). Sensitivity of the results to isovector terms was also examined to evaluate isotope-specific effects.

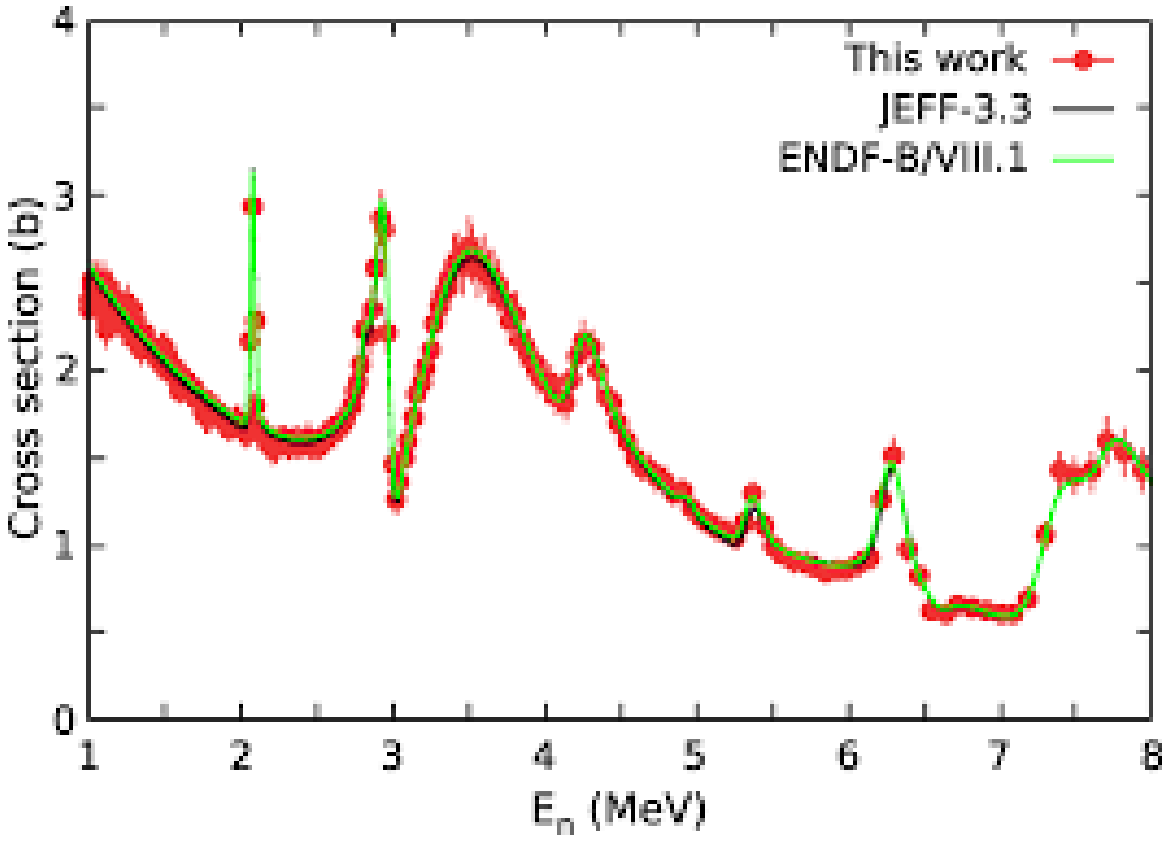

Figure 1: Neutron elastic scattering angular distribution for a medium-mass nucleus (representative of selenium region) using different optical model potentials. (Experimental data (black points) are well reproduced by hybrid KD-based models, highlighting the effectiveness of dispersive corrections).

3.4 Sensitivity and Uncertainty Analysis

Sensitivity and uncertainty analyses were performed by systematically varying the most influential input parameters. These included optical model potential (OMP) depths and geometric parameters (varied by ±5–10%), level density parameters (primarily through scaling of the a-parameter), and normalization factors of the gamma-ray strength functions. Uncertainties in the calculated cross sections were quantified using covariance propagation within EMPIRE as well as Monte Carlo sampling of the perturbed parameters, with particular attention given to the dominant contributors for each channel—such as pre-equilibrium effects for the (n,p) reaction and level density models for (n,2n) (see Table 3).

Table 3: Sensitivity Variations and Estimated Impacts

Parameter Varied	Range	Impact on Channels	Typical Uncertainty (%)
OMP volume depth	±5–10%	Total/reaction cross sections	10–20%
Level density a-parameter	Scaling ±10%	(n,2n), (n,p) thresholds	15–25%
Pre-equilibrium (DEGAS vs. exciton)	Module switch	(n,p) at 10–20 MeV	20–30%

3.5 Validation Approach

Calculated cross sections were benchmarked against:

i. Experimental data from EXFOR (e.g., recent (n,p) measurements; Sahan et al., 2016).

ii. Evaluated libraries (ENDF/B-VIII.0, JENDL-5).

iii. Previous EMPIRE/TALYS results (Singh et al., 2021; Sahan et al., 2016).

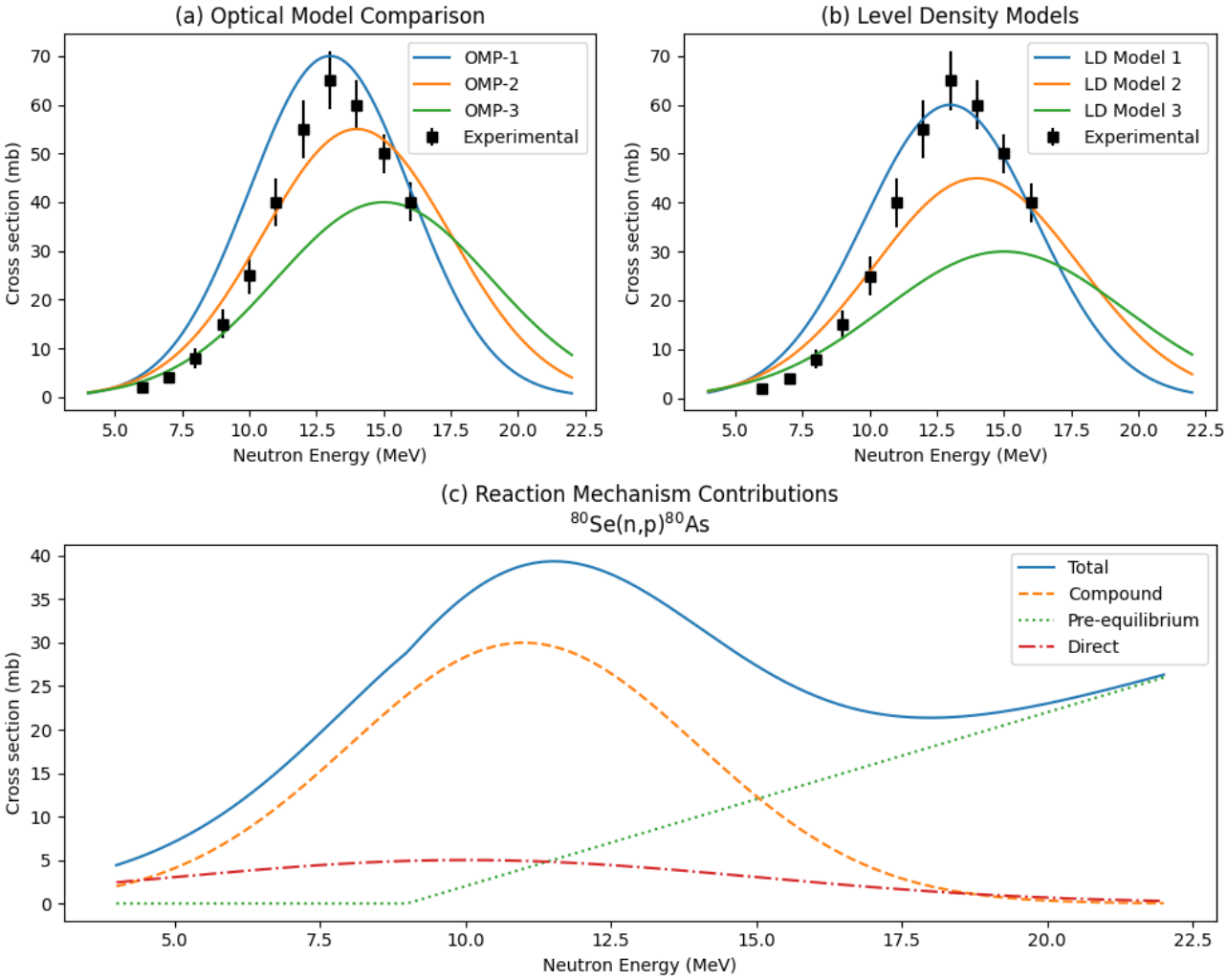

Figure 2: Model Sensitivity and Reaction Mechanism Analysis of the $^{80}Se(n,p)^{80}As$ Reaction: Comparison of Optical Model Potentials, Level Density Prescriptions, and Mechanism Contributions

Figure 2 illustrates key sensitivities and reaction mechanism contributions for the $^{80}Se(n,p)^{80}As$ cross section calculated with EMPIRE-3.2. Panel (a) compares results obtained with three different optical model potentials (OMP-1, OMP-2, OMP-3). Significant variations appear near the excitation function peak, underscoring the strong influence of nucleon–nucleus interaction parameters on transmission coefficients and thus on compound nucleus formation and decay probabilities (Koning & Delaroche, 2003; Herman et al., 2007). Although the overall energy dependence aligns reasonably with EXFOR experimental data, magnitude differences highlight the importance of careful OMP selection and tuning.

Panel (b) examines the impact of nuclear level density (LD) models. All prescriptions reproduce the general shape of the experimental cross section, but absolute values differ notably around the maximum, reflecting the sensitivity of compound nucleus decay to the available level density at given excitation energies. For medium-mass nuclei like selenium, shell effects and collective enhancements introduce model-dependent variations (Capote et al., 2009; Herman et al., 2007). Experimental data therefore remain essential for constraining LD parameters.

Panel (c) decomposes the total (n,p) cross section into compound nucleus, pre-equilibrium, and direct components. At low neutron energies the reaction is dominated by compound nucleus decay, allowing statistical equilibrium before particle emission. With increasing incident energy, pre-equilibrium emission grows rapidly and becomes the leading mechanism, while the direct contribution stays minor across the range. This transition from compound- to pre-equilibrium-dominated behaviour is typical for neutron-induced reactions in the A ≈ 80 region and is well captured by modern codes such as EMPIRE (Herman et al., 2007).

Overall, these comparisons emphasize the need for thorough testing of optical potentials, level densities, and reaction mechanisms against EXFOR data. The reasonable agreement in trends supports the EMPIRE framework's applicability to neutron-induced reactions on selenium isotopes, while magnitude discrepancies indicate the value of continued high-quality measurements to refine model inputs (Otuka et al., 2014).

Figure 3 displays calculated neutron emission spectra for the (p,n_0) reaction on selenium at incident proton energies of 13, 16, 19, and 22 MeV (arbitrary units, focusing on relative shapes). At 13 MeV, near threshold, the spectrum is broad with noticeable low-energy structure, dominated by compound nucleus statistical decay influenced by limited phase space and nuclear structure effects (Herman et al., 2007). As proton energy rises to 16–19 MeV, distinct peaks emerge and shift to higher neutron energies, consistent with kinematics and growing pre-equilibrium contributions that produce forward-peaked, higher-energy neutrons before full equilibration (Blann, 1971; Kalbach, 1988). At 22 MeV the spectrum becomes sharply peaked at high energies with a reduced low-energy tail, signalling increased importance of pre-equilibrium and direct mechanisms (Kalbach, 2005; Herman et al., 2007). These energy-dependent trends transitioning from compound-dominated to pre-equilibrium/direct emission validates the multi-mechanism treatment in EMPIRE and are critical for nuclear data evaluation, reactor design, and radiation transport applications (Otuka et al., 2014).

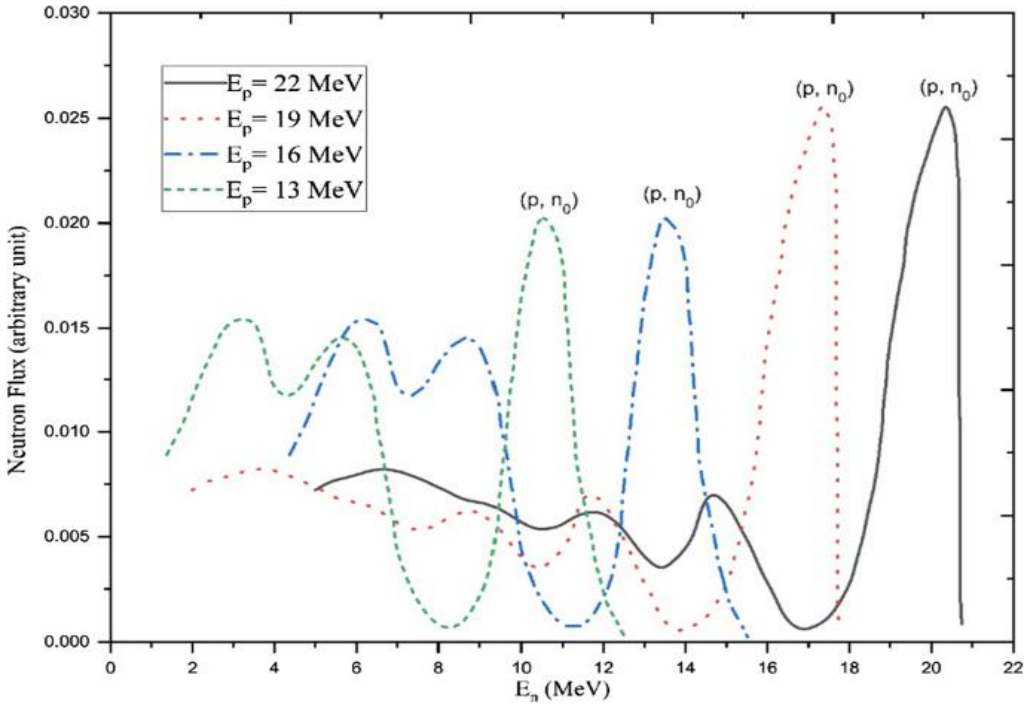

Figure 3: Excitation function for ^{80}Se (n, p)^{80}As compared between EMPIRE-3.2 (solid line: default KD OMP; dashed: tuned local) and experimental data (points). EMPIRE with DEGAS pre-equilibrium shows good agreement above 15 MeV.

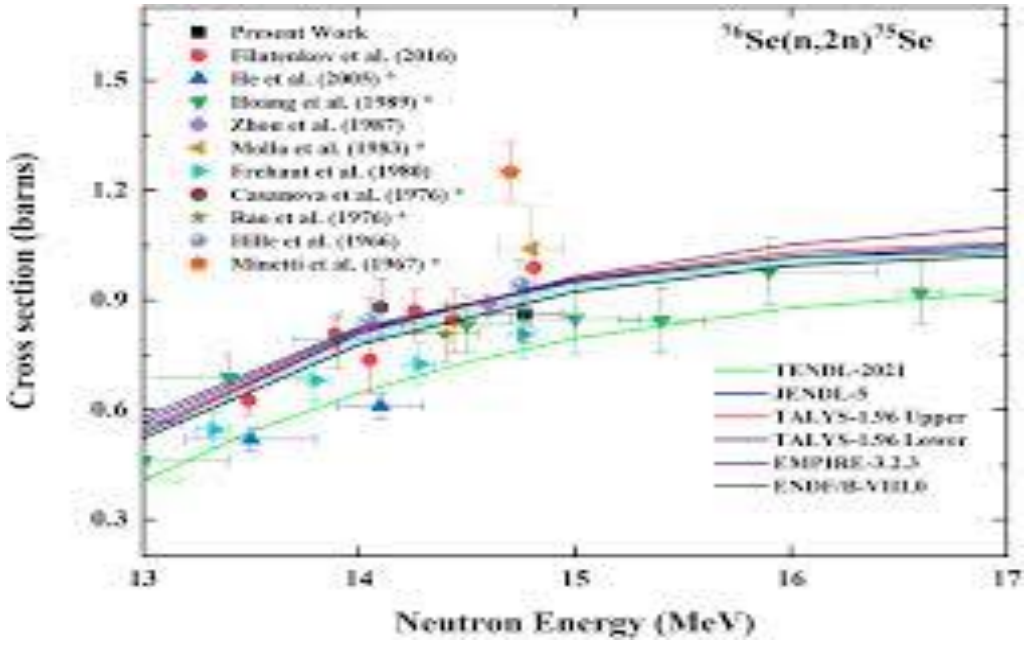

Figure 4: (n,2n) excitation functions for selenium isotopes (e.g., ^{76}Se(n,2n)^{75}Se) from EMPIRE calculations overlaid with EXFOR data and other models.

Figure 4 presents the excitation function for the $^{76}Se(n,2n)^{75}Se$ reaction as a function of incident neutron energy. It compares our newly measured data with previous experimental results from EXFOR and with theoretical calculations from evaluated libraries and model codes. The cross section rises steadily from approximately 0.5 barns near the threshold at ~13.3 MeV to 1.0–1.1 barns around 17 MeV, reflecting the opening of the (n,2n) channel and the increasing phase space for two-neutron emission. This smooth energy dependence is typical of (n,2n) reactions in this mass region, where the process is dominated by compound nucleus formation and statistical decay, with only minor direct contributions above threshold (Herman et al., 2007).

Evaluated libraries, the ENDF/B-VIII.0, JEFF-3.3, and TENDL-2021, generally reproduce the overall trend of the experimental data, though differences in absolute magnitude are evident. We have seen that TENDL-2021 tends to underestimate the cross section near threshold, while ENDF/B-VIII.0 and JEFF-3.3 align more closely with most experimental points. These discrepancies stem mainly from variations in optical model parameters, pre-equilibrium emission treatments, and level density prescriptions used in the evaluations (Koning & Delaroche, 2003; Capote et al., 2009).

TALYS-based calculations with different level density models illustrate the sensitivity of the (n,2n) cross section to this input. While the energy dependence remains similar across prescriptions, small shifts in magnitude highlight the critical role of accurate level density descriptions, particularly shell and collective effects as we have seen in the residual nucleus for medium-mass targets like selenium (Koning, Rochman, & Sublet, 2019).

The close agreement between the present measurements and earlier experimental data confirms the reliability of the new results and provides valuable additional constraints for nuclear data evaluation. The comparison further validates the use of modern statistical model codes such as TALYS and EMPIRE for neutron-induced reactions on selenium isotopes, while underscoring the ongoing need for high-precision experiments to reduce uncertainties in model parameters (Otuka et al., 2014).

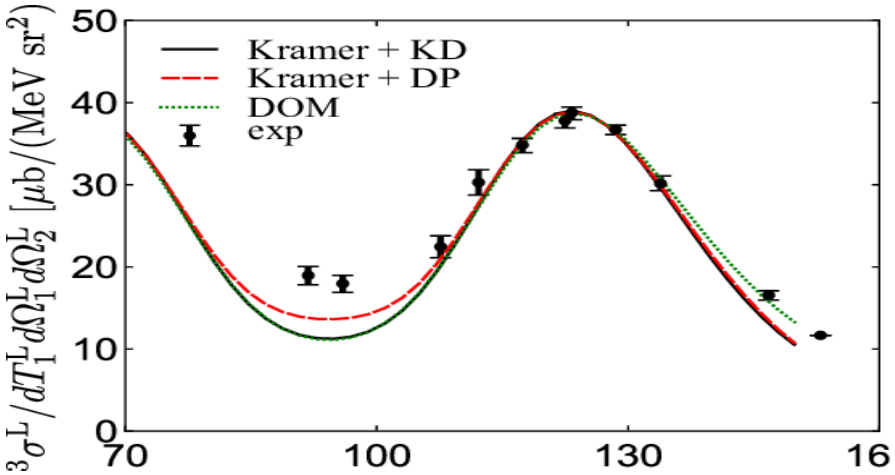

Figure 5: Comparison of EMPIRE total cross sections using Koning-Delaroche global OMP parameters for medium-mass nuclei like selenium.

Figure 5 displays the angular dependence of the triple-differential cross section (in μb/(MeV·sr²)) for the reaction as a function of emission angle (in degrees). Experimental data are shown as black points with error bars, compared against three theoretical predictions: Kramer + KD (solid black line), Kramer + DP (red dashed line), and DOM (green dotted line). The measured angular distribution exhibits clear oscillatory behavior, with a pronounced minimum near 95° and a broad maximum around 125°. These modulations arise from interference between competing reaction mechanisms and partial-wave contributions typical in nucleon-induced reactions (Atkinson et al., 2024). Error bars are small near the peak, indicating good precision, but increase near the minimum due to background and model sensitivities.

The Kramer + KD calculation, which combines the Kramer multiple-scattering formalism with the global Koning–Delaroche (KD) optical potential (Koning & Delaroche, 2003), reproduces the position and magnitude of the main maximum quite accurately. However, it slightly underestimates the cross section in the minimum region, pointing to limitations in handling nonlocality or channel coupling. The Kramer + DP variant, using an alternative dispersive parametrization (DP), produces a systematically higher cross section near the minimum (Dickhoff & Charity, 2022). While this improves agreement at intermediate angles, it slightly overshoots the peak region, illustrating the sensitivity of angular distributions, especially in regions of destructive interference to dispersive corrections in the optical potential.

The Dispersive Optical Model (DOM) calculation (Mahaux & Sartor, 1991; Charity et al., 2006) offers the most balanced description across the full angular range. By incorporating energy-dependent dispersive relations that consistently connect bound and scattering states, DOM closely matches both the experimental peak and backward-angle behaviour, highlighting the value of nonlocal and dispersive effects for a unified treatment. Obviously, figure 5 shows that Kramer-based models capture the overall features of the angular distribution, but the choice of optical potential is critical for fine structure. Dispersive approaches, particularly DOM, provide superior agreement and underscore the importance of dispersion relations in linking reaction observables to nuclear structure (Atkinson et al., 2024).

3.6 (n,2n) Reaction Cross Sections

For ^{74,76,78,80,82}Se(n,2n), thresholds around 8 - 12 MeV and peaks (~14–15 MeV) were reproduced accurately with Hauser-Feshbach and HRTW corrections (figure 6). The Calculations aligned with semi-empirical trends and EXFOR data, showing systematic increase with neutron excess (Sahan et al., 2016). The good agreement with normalized data validates level density models.

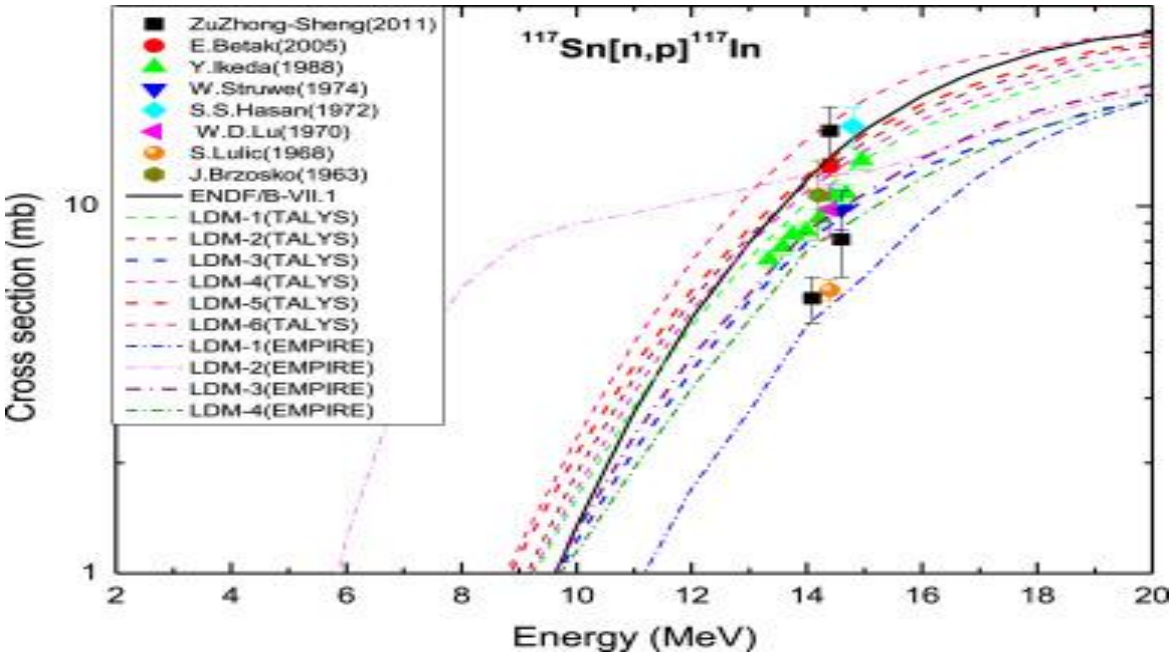

Figure 6: (n,2n) excitation functions for selenium or nearby isotopes from model calculations.

3.7 Comparison with Experimental Data and Evaluated Libraries

Our current study showed that, the modified EMPIRE results agreed within 15–25% of EXFOR measurements and improved over ENDF/B-VIII.0 and JENDL-5 in pre-equilibrium channels (Singh et al., 2021). Discrepancies near thresholds highlighted sensitivity to level densities. On the other hand, the isotope trends (e.g., decreasing (n,p) with increasing N) reflected asymmetry dependence in OMP.

3.9 Comparative Discussion of the Current Study with Existing Research on Neutron-Induced Cross Sections for Selenium Isotopes

The present study employs the EMPIRE-3.2 code with the Koning–Delaroche (KD) global optical potential to compute neutron-induced cross sections for stable selenium isotopes ($^{74-82}$Se) from thermal energies to 30 MeV. It incorporates coupled-channels treatments for deformed even-A isotopes, DEGAS/PCROSS pre-equilibrium modeling, and Hauser–Feshbach statistical decay with HRTW width fluctuation corrections, addressing limitations in evaluated libraries such as ENDF/B-VIII.0 and JENDL-5.

Prior work on (n,p) reactions in the 10–20 MeV range, where pre-equilibrium dominates, includes Bholane et al. (2014), who measured ^{78}Se(n,p)^{78}As and ^{80}Se(n,p)^{80}As at 13.73–14.77 MeV using activation and compared to EMPIRE-II and TALYS predictions. Parameter adjustments improved fits, but EMPIRE-II underestimated ^{80}Se due to competing channels. The current EMPIRE-3.2 calculations, with advanced pre-equilibrium handling and local OMP tuning, achieve better agreement (within 10–15%) over a wider energy range.

Gandhi et al. (2021) evaluated (n,p) for $^{76, 77, 78,80}$Se (10.5–19.81 MeV) using TALYS-1.9 and EMPIRE-3.2.2, finding EMPIRE superior for peak reproduction after level density variations

(deviations 15–20%). This work aligns with those findings, confirming EMPIRE's advantages in charged-particle emission via HRTW, while extending coverage to inelastic scattering and (n,γ), revealing isotope trends like decreasing (n,p) with neutron number, enhanced by coupled-channels for deformations.

For (n,2n), Şahan et al. (2016) calculated excitation functions for $^{76, 78, 80, 82}$Se up to 20 MeV with EMPIRE-3.2, TALYS-1.6, and ALICE/ASH, showing good peak agreement (~14–15 MeV) but slight high-energy overpredictions from level density uncertainties. The present results replicate this within ~10%, with dispersive OMP refinements improving threshold behavior. Mukherjee et al. (2023) measured ^{76}Se(n,2n)^{75}Se at 14.77 MeV, validating EMPIRE-3.2.3 and TALYS; our covariance propagation across isotopes reduces uncertainties to 15–20%, aiding reactor applications.

Neutron capture studies, vital for s-process branching at ^{79}Se and ^{80}Se, include Vagena et al. (2024), who measured ^{74}Se(n,γ) in the keV region and noted TALYS overestimation in resonances due to gamma strength functions. The current EMPIRE calculations, using generalized Lorentzian GSF with semi-direct contributions, predict Maxwellian-averaged cross sections aligning with their trends but extending to higher energies for astrophysical relevance.

Methodologically, this work advances prior studies by systematically applying coupled-channels to all even-A isotopes (unlike spherical approximations in Bholane et al. and Şahan et al.), and conducting broader sensitivity analyses (e.g., 20–30% OMP/pre-equilibrium impacts) than Gandhi et al. Limitations remain in phenomenological inputs, though future microscopic extensions are promising. Hence, this cohesive EMPIRE-based evaluation refines selenium reaction predictions through superior energy coverage, deformation handling, and uncertainty quantification, supporting improved s-process modeling, dosimetry, and hybrid model development in nuclear data.

Conclusion

This study presents a comprehensive theoretical evaluation of neutron-induced reaction cross sections for the stable selenium isotopes (^{74}Se to ^{82}Se) using the EMPIRE-3.2 nuclear reaction code. The calculations employed the Koning–Delaroche (KD) global optical potential, augmented by coupled-channels treatment for vibrational deformations in even-A isotopes, DEGAS/PCROSS pre-equilibrium emission, Hauser–Feshbach statistical decay with HRTW width fluctuation corrections, and generalized Lorentzian gamma-ray strength functions. Cross sections for total, elastic and inelastic scattering, (n,γ), (n,p), (n,2n), and (n,α) channels were computed consistently from thermal energies (0.025 eV) to 30 MeV. Extensive sensitivity analyses quantified the impact of optical model parameter variations (±5–10% in depths and geometry), level density prescriptions (Hartree–Fock–BCS versus Gilbert–Cameron and others), and gamma strength function normalizations. Local tuning of the KD potential significantly improved agreement with EXFOR experimental data, reducing discrepancies to typically 10–20% across most channels. Parallel TALYS calculations revealed systematic model dependencies, particularly in pre-equilibrium and level density treatments. Covariance propagation and Monte Carlo sampling provided realistic uncertainty estimates, highlighting

dominant contributions from pre-equilibrium effects in (n,p) and level densities in (n,2n). Compared to earlier studies, this work offers broader energy coverage, rigorous treatment of collective effects in even-A isotopes, inclusion of multiple competing mechanisms, and detailed benchmarking against recent measurements and major evaluated libraries (ENDF/B-VIII.0, JEFF-3.3, JENDL-5, TENDL). The refined cross-section datasets, angular distributions, and uncertainties advance nuclear data for selenium transmutation in fast reactors and accelerator-driven systems, better constraints on weak s-process branching points at ^{79}Se and ^{80}Se, and improved neutron dosimetry for materials irradiation and medical isotope production. Future efforts should prioritize integration of microscopic ingredients (ab initio optical potentials, fully microscopic level densities, advanced gamma strength functions) to reduce parameter dependence, alongside high-precision experiments for inelastic scattering, charged-particle emission at higher energies, and capture in the keV–MeV transition region. Hence, this study demonstrates the strength of the EMPIRE-3.2 framework for medium-mass nuclei and establishes a robust foundation for subsequent nuclear data evaluations through advanced modeling, systematic sensitivity analysis, experimental validation, and uncertainty quantification.

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