

Forward modeling approach to nuclear reaction cross sections: Applications in neutron inelastic scattering

J. M. Gordon ^{1,*} B. L. Goldblum ^{1,2} D. L. Bleuel³ C. A. Brand ^{1,3} J. A. Brown ¹ T. A. Laplace ¹
T. S. Nagel ¹ and L. A. Bernstein^{1,2}

¹*Department of Nuclear Engineering, University of California, Berkeley, California 94720, USA*

²*Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

³*Lawrence Livermore National Laboratory, Livermore, California 94550, USA*



(Received 18 August 2025; revised 4 December 2025; accepted 2 February 2026; published 3 April 2026)

The development of nuclear reaction models for the production of evaluated nuclear data has traditionally been performed by comparing measured cross sections with predictions from reaction model codes whose physical input parameters are adjusted to obtain the best agreement between measured and modeled results. To more directly probe reaction model inputs, this work introduces a forward modeling approach to experimental reaction cross-section determination, where the most important physical input parameters to reaction model calculations are obtained via χ^2 minimization between measured and calculated observables. This was demonstrated using data collected by the Gamma Energy Neutron Energy Spectrometer for Inelastic Scattering (GENESIS) at the 88-inch cyclotron at Lawrence Berkeley National Laboratory, a detection array consisting of organic liquid scintillators and high-purity germanium (HPGe) detectors. Using a broad-spectrum neutron beam and a 99.98%-enriched ^{56}Fe target, GENESIS was used to perform a simultaneous measurement of ^{56}Fe γ -ray production cross sections and secondary neutron energy and angle distributions. The results of the forward modeling approach to the determination of energy-differential γ -ray production cross sections for the yrast $4^+ \rightarrow 2^+$ and $6^+ \rightarrow 4^+$ transitions, as well as eight other off-yrast transitions, were compared against those obtained using conventional techniques, and the results are in good agreement. In addition to discrete γ -ray yield total scattered neutron energy-angular distributions as a function of incident neutron energy were also obtained using forward modeling and found to agree with evaluated data, with the exception of elastic scattering at small angles. The fitted reaction model parameters obtained through forward modeling were also used to calculate the cross section for the unobserved $(n, 2n)$ reaction; excellent agreement with the current evaluation was obtained, providing a validation of the predictive capabilities of the forward model approach. This work bridges the gap between nuclear data experiment and evaluation by providing a new means for extracting inelastic neutron-scattering cross sections and neutron-induced γ -ray production data while directly probing reaction model physics.

DOI: [10.1103/wdzh-ybzf](https://doi.org/10.1103/wdzh-ybzf)

I. INTRODUCTION

The generation of an evaluated nuclear data file for neutron-induced reaction cross sections on a given isotope starts with the collection of relevant experimental data. Measurements to obtain these data are commonly conducted by observing the yield of secondary particles of energy, E' , produced via the interaction of a neutron beam of energy, E_n , and intensity, $\phi(E_n)$, with a target of a known number of atoms, N_T . Mathematically, this is given by

$$\sigma(E_n, \theta_i) = \frac{Y_{\text{obs}}(E_n, \theta_i) - Y_{\text{bkg}}(E_n, \theta_i)}{\epsilon(E', \theta_i)\phi(E_n)N_T}, \quad (1)$$

where $\sigma(E_n, \theta_i)$ is the neutron-induced reaction cross section θ_i is the angle at which the secondary particle is detected with efficiency $\epsilon(E', \theta_i)$, and Y_{bkg} is the amount of background in the observed yield Y_{obs} . The quality of an individual measurement is assessed based on specific criteria, such as the validity of the experimental methods and the completeness of the description of the associated uncertainties.

However, measurements often contain gaps: some reaction channels may lack data, the incident energy range coverage may be limited, the description of secondary particle distributions may be incomplete, etc. As a result, nuclear reaction models are used to calculate the missing information following an adjustment of the model parameters based on the available data [1]. Recent work by the Cross Section Evaluation Working Group on the development of templates of expected measurement uncertainties [2] underscores one of the key difficulties in the generation of evaluated nuclear data libraries: the reconciliation of experiments at various facilities employing a wide range of measurement modalities (e.g., γ -ray spectroscopy [3], neutron spectrum unfolding [4])

*Contact author: jmgordon@berkeley.edu

providing differing, but ostensibly complementary, pictures of the same reacting system. The current approach, using reaction models to explain existing data, is useful in interpreting experimental results, but also limited in that *posthoc* model parameter tuning may result in compensating errors, potentially restricting the ability of the model to extrapolate to new reaction channels or unmeasured energy ranges.

A leading approach to addressing this challenge involves tuning reaction model parameters against a number of high-quality experimental datasets, including both energy- and angular-differential data. For example, the evaluated nuclear data library, TENDL [5], is generated by tuning TALYS reaction model parameters to experimental data, which are then validated against differential databases such as EXFOR [6] and integral benchmark datasets like those in the International Criticality Safety Benchmark Evaluation Project handbook [7]. To further assess the quality of evaluated nuclear data libraries, the quasidifferential measurements of Rensselaer Polytechnic Institute provide a valuable means of validation [8]. In this approach, a white neutron source is made incident on a thick target in which multiple scattering occurs [9]. The scattered-neutron energy distributions as a function of angle are then compared against Monte Carlo *N*-Particle (MCNP) simulations [10,11] performed using various evaluated nuclear data libraries [8,9,12].

To more directly link the nuclear reaction theory and experimental data, this work introduces a forward modeling approach in which nuclear reaction model parameters are optimized using experimental data generated from a setup that allows for the simultaneous observation of multiple reaction channels. In this approach, a trial cross section is calculated from a set of model parameters. This is then convolved with the detector response, taking into account the neutron beam intensity and number of target atoms, to provide a prediction of the secondary particle yield. By adjusting the reaction model parameters until the difference between the calculated and observed yields is minimized, the cross section for the observed reaction channels can be determined. Additional information on unobserved channels is also obtained due to the codependence of reaction channels inherent in the reaction model physics.

To validate this technique, a measurement was conducted using the Gamma Energy Neutron Energy Spectrometer for Inelastic Scattering (GENESIS), an experimental platform that couples high-purity germanium (HPGe) detectors with an array of EJ-309 pulse-shape-discriminating organic liquid scintillators [13]. An ^{56}Fe target was irradiated with a broad-energy neutron beam produced at the 88-inch cyclotron at Lawrence Berkeley National Laboratory (LBNL) [14] to enable the simultaneous measurement of secondary γ rays and scattered neutrons arising from neutron-induced reactions. Here, ^{56}Fe was used as the target nucleus given the abundance of literature data (see Table IX of Ref. [15] for measurements before 2018 and [4,16,17] for more recent work). Additionally, ^{56}Fe was the focus of the Collaborative International Evaluated Library Organization (CIELO) project whose evaluation was published in 2018 [15] for inclusion in the release of ENDF/B-VIII.0 [18]. The neutron beam, ^{56}Fe target, and GENESIS detectors, calibration procedures, and detector

efficiencies are described in Sec. II. Section III details the construction of the data products. Section IV describes the two analysis methods used to extract neutron-induced reaction cross sections from the GENESIS data, an inverse approach akin to that outlined in Eq. (1) and the forward modeling method. Section V provides the results of the data analysis with comparisons to previous measurements and the findings of the CIELO project as included in the ENDF/B-VIII.0 evaluation. Concluding remarks are given Sec. VI.

II. EXPERIMENTAL METHODS

A general description of the GENESIS array is provided in Gordon *et al.* [13]; the specific experimental details for the ^{56}Fe measurement will be presented here. Neutrons were produced by colliding a 14 MeV $^2\text{H}^+$ beam with a 3.5-mm-thick carbon target mounted to a Faraday cup in the 88-inch cyclotron vault at LBNL with readout electronics to record the average beam current in 1 s intervals. The neutrons were then collimated via a tapered, 60-cm-long copper cylinder with an inner radius of 0.33 to 0.6 cm and an outer radius of 7.62 cm before passing through a 5-cm-radius iron beam pipe penetrating a 2.44-m-thick wall separating the experimental area from the neutron production zone.

The neutron flux spectrum was monitored using the scatter time-of-flight (sTOF) spectrometer [19]. The sTOF spectrometer was positioned 2.704 m downstream of the center of the GENESIS array. The temporal structure of the deuteron beam was determined using sTOF and found to be roughly Gaussian distributed with a full-width-at-half-maximum (FWHM) of 6.1 ns. The absolute energy-differential efficiency of sTOF was determined using GEANT4 [20] with the Shielding Physics List and the G4NDL library based on ENDF/B-VII.1 [21]. The energy-integral neutron flux was validated using foil activation analysis. Four activation foils were fielded at the ^{56}Fe target position (i.e., in the center of the GENESIS array). The 1-mm thick foils were, in order of upstream to downstream, zirconium (13.0024 g), nickel (17.2187 g), indium (14.369 g), and aluminum (5.3187 g). Each foil was a 5.08-cm-diameter cylinder of standard density. The foils were irradiated for 2 hours and then placed in front of a calibrated HPGe detector [22] to measure the activation product yields. For the Zr foil, activation via $^{90}\text{Zr}(n, 2n)$ was negligible due to the 12.1 MeV neutron energy threshold. Using the cross sections and associated uncertainties from IRDFF-II [23] and the neutron spectrum measured by sTOF (for neutron energies ≥ 1.73 MeV), the indium, nickel, and aluminum activation foils yielded an average integrated flux at the target location of $(2.94 \pm 0.09) \times 10^9 \text{ n sr}^{-1} \mu\text{C}^{-1}$. The analysis of the sTOF data using the GEANT4-calculated efficiency yielded an integrated flux at the sTOF detector location of $(2.858 \pm 0.008) \times 10^9 \text{ n sr}^{-1} \mu\text{C}^{-1}$, in agreement with the foil activation data within 1σ . The GEANT4-normalized sTOF neutron flux spectrum is shown in Fig. 1. The uncertainty on the neutron flux spectrum is a quadratic sum of the statistical uncertainty in the measurement and the statistical uncertainty of the efficiency simulation.

The scattering target was $9.7653 \pm 0.0001 \text{ g}$ [24], 99.98% enriched in ^{56}Fe . The target was an ellipse with a major radius

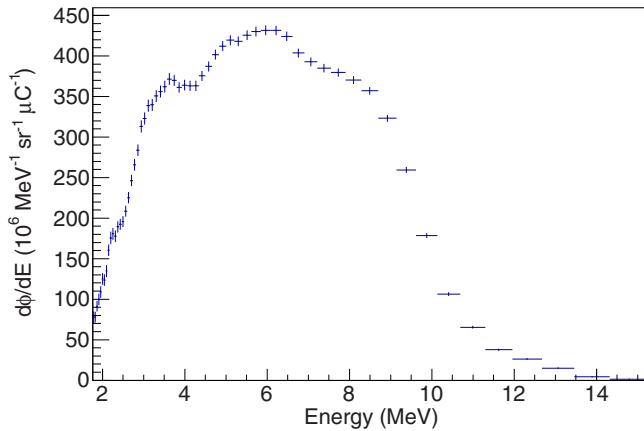


FIG. 1. Neutrons per MeV per steradian per microCoulomb from the interaction of a 14 MeV $^2\text{H}^+$ beam with a 3.5-mm-thick carbon target measured by the sTOF detector. The x -error bars represent a bin width set as $\sigma/3$ of the incoming neutron TOF resolution. The y -error bars represent a quadratic sum of the statistical uncertainty in the measurement and the statistical uncertainty of the efficiency simulation.

of 3.6 cm, a minor radius of 1.75 cm, and an average thickness of 0.60 ± 0.04 mm [25]. The ^{56}Fe target was suspended in the center of the GENESIS array using a copper bar and a thin nylon string, 7.365 m from the neutron-production target at an angle of 50.3° relative to the neutron beam. The incident neutron energy-dependent multiple scatter probability was calculated via Monte Carlo sampling of the Lib80x ACE file library [26] based on the ENDF/B-VIII.0 [18] library as described in Ref. [25]. The energy-dependent probability was multiplied by the neutron flux spectrum measured using sTOF to yield an energy-integrated multiple-scattering probability of $2.235 \pm 0.007\%$ (stat.).

Beam-on-target data were taken for 67.70 hours at an average current of $8.82 \mu\text{A}$. Data were also taken with the ^{56}Fe target removed (“blank”) for 4.53 hours at an average current of $9.54 \mu\text{A}$. Fast neutrons that scattered off the ^{56}Fe target and into the HPGe crystals can produce discrete γ rays via inelastic scattering that overlap in energy with discrete γ rays from ^{56}Fe , especially the 847.15 keV γ ray from ^{76}Ge , which is close in energy to the 846.77 keV γ ray from ^{56}Fe , and the 1039.506 keV level in ^{70}Ge , close in energy to the 1037.83 keV γ ray from ^{56}Fe . To investigate the amount of contamination in the discrete $^{56}\text{Fe}(n, n') \gamma$ -ray yields from these reactions on Ge isotopes, a 0.723-mm-thick, 5.03 cm $\times$ 6.36 cm rectangular Be target was also fielded for a total of 6.68 hours at an average $^2\text{H}^+$ beam current of $9.54 \mu\text{A}$. The copper bar from which the ^{56}Fe target was suspended was used to hang the Be target and was also present in the blank run.

Two Eurisys twofold segmented HPGe CLOVER detectors were fielded. One HPGe detector (“CLOVER 0”) was placed at 91.4° relative to the neutron beam at a radial distance of 20.05 cm from the center of the ^{56}Fe target. The other HPGe detector (“CLOVER 1”) was placed at 49.3° relative to the neutron beam at a radial distance of 26.83 cm from the

center of the target. The CLOVER leaves were connected to a single Mesytec MDPP-16 module [27] configured with the standard charge-integrating preamplifier (SCP) firmware [28]. Also present in the GENESIS array were 16, 5.08 cm diameter by 5.08 cm high right cylindrical EJ-309 organic liquid scintillators [29] for neutron detection. These were connected to an MDPP-16 module with the charge-to-digital convertor (QDC) firmware [30]. Every detector was allowed to generate a trigger, which was fed to an external or gate and propagated back to the Mesytec boards to ensure temporal synchronicity. The signal from the cyclotron radio-frequency (rf) generator was passed through a constant fraction discriminator and then passed into the second trigger input on the Mesytec boards to allow for timing of events against the $^2\text{H}^+$ beam pulses. The list-mode data from the Mesytec boards were processed into a custom data structure representing a general event topology wherein events from all three boards within the same event window ($2.88 \mu\text{s}$) were associated. These associated events, which can include any number of intra- or interdetector coincidences, were also associated with a set of rf timestamps and a global timestamp to allow for time-dependent gain calibrations across the entire experiment.

The detectors were calibrated using the methods described in Ref. [13], which will be briefly summarized here. The timing resolution and offset parameters, the latter required to translate measured time differences into real time differences, were measured using $\gamma\gamma$ coincidences from an encapsulated ^{252}Cf source. The average timing resolution (represented by the standard deviation of a Gaussian fit to the time difference distributions) for a CLOVER leaf and EJ-309 detector was 3.3 ± 0.1 ns and 0.333 ± 0.012 ns, respectively. The time offset relative to the cyclotron rf signal, used to calculate the incoming neutron time-of-flight (TOF), was measured via the arrival time in a single EJ-309 detector of photons originating from the collision of the $^2\text{H}^+$ beam with the carbon break-up target which underwent Compton scattering in the ^{56}Fe target.

The amplitude-dependent trigger probability [13] was measured with a $10.45 \mu\text{Ci}$ ^{152}Eu source. The gain calibration, energy resolution, and efficiency of the HPGe CLOVER detectors were determined using a $0.916 \mu\text{Ci}$ ^{152}Eu point source positioned in the center of the detector array. The measured efficiency from this source geometry was compared with a calculation using the GEANT4 model described in Refs. [13,25]. The measured and simulated efficiencies agreed in the energy range of 121.8 to 1408.0 keV to within 1.9% for CLOVER 0 and 3.4% for CLOVER 1. Figure 2 shows the efficiency for the two CLOVER detectors operating in total detection mode, calculated using the GEANT4 model and a source geometry equivalent to the ^{56}Fe target. The uncertainty of the efficiency at 846.8 keV, 4.35% for CLOVER 0 and 4.21% for CLOVER 1, was dominated by the uncertainty in the amplitude-dependent trigger probability.

The gain calibration and light yield resolution of the 16 EJ-309 detectors were determined using the methods described in Refs. [13,25]. In brief, plots of the neutron TOF versus analog-to-digital converter channel number were generated from data taken with an encapsulated ^{252}Cf source. The GEANT4 model was used to generate simulated neutron

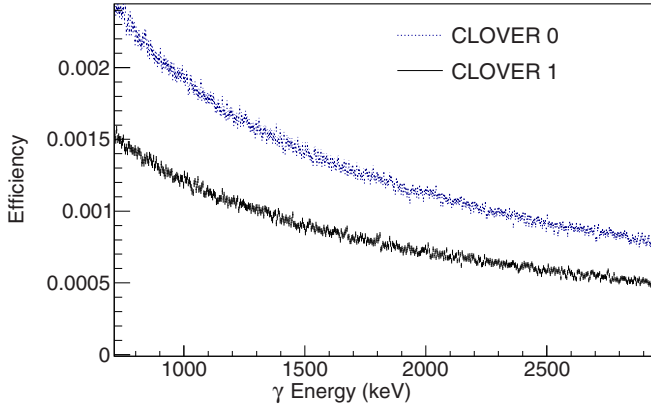


FIG. 2. Efficiency of the CLOVER detectors operated in total detection mode for an isotropic source of γ rays, uniformly distributed in energy, emitted from the ^{56}Fe target calculated using a GEANT4 model of the GENESIS array.

TOF versus proton light yield curves, where the simulated proton energy deposited was converted to light using an EJ-309 proton light yield relation based on prior measurements from Brown *et al.* [31] and Laplace *et al.* [32], fitted with the light yield model of Yoshida *et al.* [33] in accordance with the methods described in Ref. [34]. These simulated neutron TOF versus proton light yield curves were compared with the experimental data following a linear gain scaling and convolution of the simulation output with the heteroskedastic light yield resolution function [35]. Optimal linear gain scaling and detector resolution parameters that minimized the χ^2 between the measured and simulated data were then obtained. The uncertainties and covariances between these fitted parameters were used to generate uncertainties in the detector response via Monte Carlo methods [13].

III. DATA PRODUCTS

The event topologies considered for further analysis included those with $n \geq 1$ intra-CLOVER events and/or $n = 1$ EJ-309 events. Neutron- γ coincidences were explored, but due to the low statistics, a quantitative analysis of the coincident data was not pursued. Regardless, the γ -ray and neutron data are complementary as they arise from the same nuclear reactions and must be interpreted as such. Section III A describes the data products derived from the CLOVER detectors. Section III B describes the data products derived from the EJ-309 detectors.

A. Gamma rays

Due to the temporal spacing between successive deuteron beam pulses ($T_{RF} = 169.2563$ ns) and the distance from the breakup target to the ^{56}Fe scattering target (7.365 ± 0.005 m), the measured arrival time of a neutron that produced an observed discrete γ ray was uncertain by n cyclotron rf periods, a phenomenon known as frame overlap [36]. Instead of proceeding with the analysis in neutron TOF space, the measured

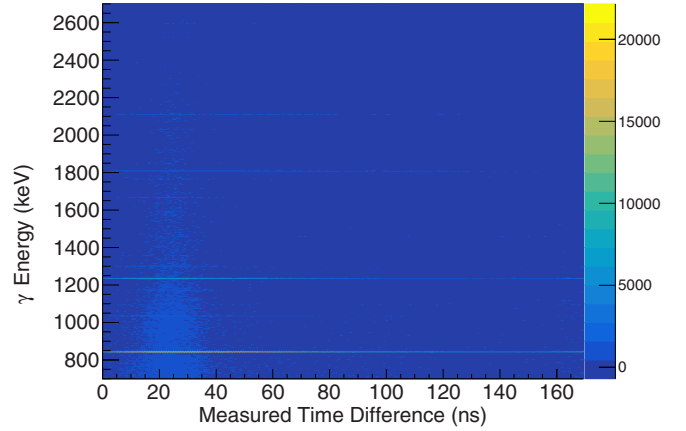


FIG. 3. Two-dimensional histogram of γ -ray energy as a function of measured time difference for a single CLOVER detector at 49.3° relative to the neutron beam. The spectrum gathered with the ^{56}Fe target present in the center of the GENESIS array was subtracted from the spectrum gathered with a Be target in the same location, scaled to the ^{56}Fe target-in data by the ratio of the integrated charge.

time difference Δt was used [19]. Here,

$$\Delta t = t_i - t_{\gamma_i} - t_{RF}, \quad (2)$$

where t_i is the calibrated detection time of a γ ray in the i th detector, t_{γ_i} is the travel time of the γ ray from the target to the i th CLOVER detector, and t_{RF} is the time corresponding to the cyclotron rf signal. The data from each CLOVER detector operating in total detection mode were compiled into histograms of the calibrated γ -ray energy versus the measured time difference, where for each event, Δt was shifted by an integer number of rf periods to ensure that all events fell within a window spanning $\Delta t = \{0, T_{RF}\}$. Figure 3 shows the γ -ray energy as a function of the measured time difference for CLOVER 1 arising from neutron-induced events on the ^{56}Fe target, with background subtracted using the Be data. The ratio of the integrated charge (measured at the carbon breakup target) for each dataset served as the scaling factor for the subtraction. Prominent in Fig. 3 are the horizontal bands corresponding to the production of characteristic γ rays following neutron inelastic scattering on ^{56}Fe . The 846.8, 1037.8, 1238.3, and 1810.8 keV are the strongest populated across the measured time difference domain. Also prominent is the broad-energy feature from roughly 18 to 30 ns corresponding to photons generated in the breakup target that underwent Compton-scattering in the ^{56}Fe target.

The yield from the discrete γ rays emitted following inelastic scattering was computed for 12.1-ns-wide bins of the two-dimensional (2D) background-subtracted histogram shown in Fig. 3. A Gaussian distribution plus a linear background term was fitted to each γ -ray peak. The centroid of each peak was fixed based on the known γ -ray energy, and the width was fixed based on the HPGe resolution measured with the ^{152}Eu point source. The yield of the 846.8 keV γ ray in CLOVER 1 (positioned at 49.3° with respect to the incoming neutron beam) as a function of measured time difference is plotted in Fig. 4.

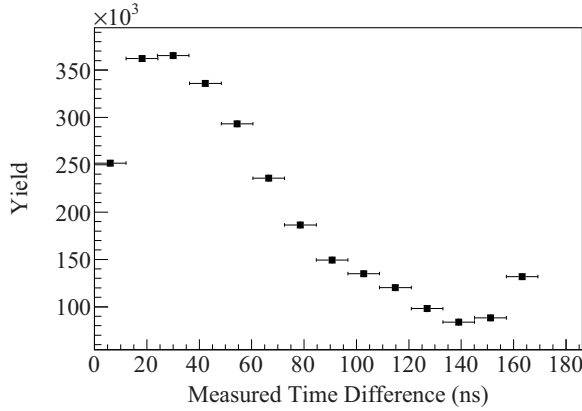


FIG. 4. Yield of the 846.8 keV ($2_1^+ \rightarrow \text{G.S.}$) transition in ^{56}Fe as a function of measured time difference for HPGe CLOVER 1 operating in total detection mode and positioned at 49.3° relative to the incident neutron beam.

B. Neutrons

For the organic scintillator data, the measured time difference was given by

$$\Delta t' = t_i - t_{RF}, \quad (3)$$

where t_i is the calibrated detection time of a neutron in the i th detector and t_{RF} is the time corresponding to the cyclotron rf signal. Given that the amount of energy lost by the neutron in the target via elastic or inelastic scattering is unknown, the measured time difference does not directly correspond to a set of degenerate incident neutron energies as is the case with the γ -ray data. Rather, the measured time difference $\Delta t'$ represents the degenerate sum of the incident and outgoing neutron TOF. The data from each organic scintillator detector were processed into a 2D histogram of light yield versus measured time difference. To select neutron events, a dual constraint was applied on the light yield and the pulse shape discrimination metric, the latter evaluated using charge integration via a tail-to-total technique. Data from the ^{56}Fe target and the blank were processed separately, and the ratio of the integrated charge for each dataset was used as a scaling factor to perform background subtraction.

Figure 5 shows the background-subtracted 2D histogram of light yield versus measured time difference for an EJ-309 detector located 70.0 cm from the center of the GENESIS array and 13.1° relative to the neutron beam. The dominant wedge-shaped feature is the detector response primarily from elastically scattered neutrons. Elastically scattered high-energy neutrons from the most recent deuteron pulse appear at high light yield and for measured time differences greater than 150 ns. Elastically scattered low-energy neutrons from two previous deuteron pulses appear at light yields below 1 MeVee and between 0 and 80 ns. The shelf from 1 to 6 MeVee at approximately 20 ns is due to the majority of the neutron flux (see Fig. 1) being between 3 MeV (≈ 140 ns) and 8.5 MeV (≈ 15 ns). The lack of a clear feature arising from inelastic scattering to, i.e., the first-excited state ($E_{ex} = 846.8$ keV) is due to the energy resolution of the

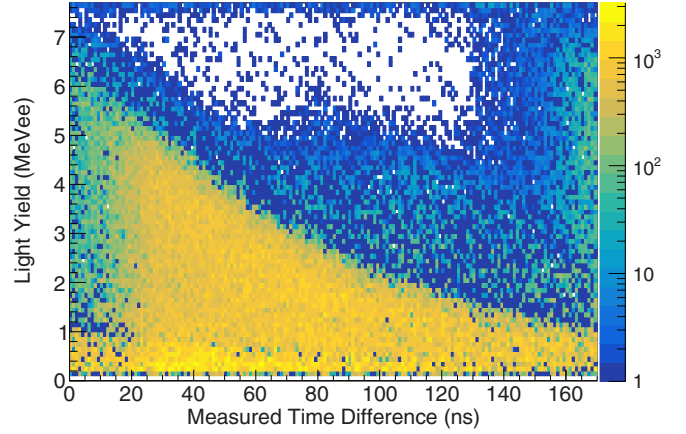


FIG. 5. Light yield versus measured time difference for neutrons scattered by the ^{56}Fe target in the center of the array and detected by a single EJ-309 detector positioned 70.0 cm from the target and 13.1° relative to the neutron beam.

detector and the relative weakness of the inelastic scattering compared with elastic scattering at this forward angle.

IV. ANALYSIS

Two approaches to the analysis of the γ -ray data were pursued. Section IV A describes the traditional inverse approach, which was used to provide a basis for comparison and benchmarking. Section IV B introduces the forward modeling method as a new means for extracting nuclear reaction cross sections from experimental data.

A. Inverse approach

For the inverse approach using GENESIS at the 88-inch cyclotron, the neutron energy contributing to the yield of a specific γ ray in a given measured time difference bin is uncertain due to frame overlap. As such, Eq. (1) cannot be directly applied except in those cases in which the reaction energy threshold physically prohibits lower energy neutrons from contributing to the γ -ray yield. For ^{56}Fe , all γ rays except the 846.8 keV transition either have energy regions that satisfy this condition or are completely free from frame-overlap-induced degeneracy.

To quantify the number and energy of the neutrons contributing to the observed yield in each measured time difference bin, the neutron flux spectrum measured by the sTOF spectrometer (shown in Fig. 1) was mapped into a 2D space of measured time difference versus incident neutron energy. This flux matrix, $\Phi(E_n, \Delta t)$, was then convolved with a Gaussian distribution representing the timing resolution of the system, which was a quadratic sum of the resolution of the CLOVER detectors (3.3 ns) and the temporal spread of the deuteron beam (6.1 ns). Figure 6 shows the flux matrix, where the elements represent the number of neutrons per μC per steradian of a given neutron energy arriving at the ^{56}Fe target with a given measured time difference. Each band in the matrix corresponds to a deuteron beam pulse from the cyclotron. The width of the bins in the x and y dimensions

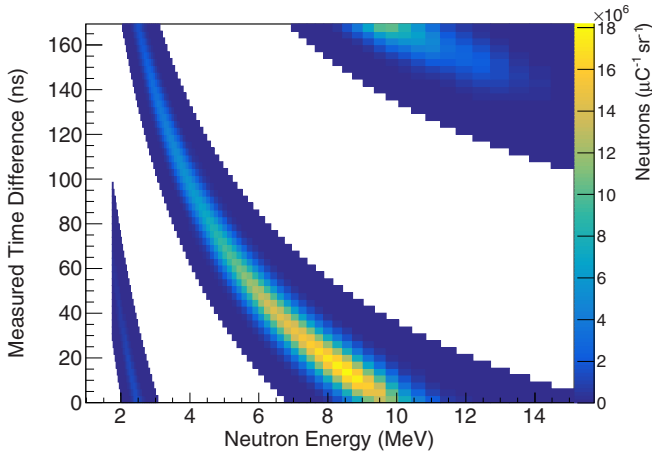


FIG. 6. Two-dimensional representation of the sTOF measured neutron flux showing the number and energy of the neutrons contributing to the total neutron flux in a given measured time difference bin. Each x and y bin is 3.03 ns in width. The color scale indicates the number of neutrons per steradian per μC of $^2\text{H}^+$ beam incident on the break-up target. The flux measured by sTOF was convolved with the timing resolution of the $^2\text{H}^+$ beam (6.1 ns) and the resolution of the CLOVER detectors (3.3 ns).

is 3.03 ns. A similar matrix, $V_\Phi(E_n, \Delta t)$, was constructed where the value of each matrix element is the corresponding uncertainty in the neutron flux.

To compute the neutron flux, $\phi(E_n)$, needed for Eq. (1) for a given γ -ray production cross section with an energy threshold of E_{thresh} , the total number of neutrons from $E_n \geq E_{\text{thresh}}$ in each row of the flux matrix was computed. If the yield from any one of the deuteron pulses comprised $\geq 98\%$ of the neutrons, that measured time difference bin was considered for the inverse analysis. The mean neutron energy was calculated by constructing a cumulative distribution function in neutron energy corresponding to the contributing deuteron beam pulse. The spread in neutron energy was calculated as the range containing the central 68% of the neutron flux.

An additional consideration necessary to integrate the cross section computed with Eq. (1) is the angular distribution of the emitted γ rays as a function of incident neutron energy. In general, γ rays emitted following a compound neutron inelastic scattering interaction have an angular distribution of the form

$$W(\theta) = \sum_k^{J_i} a_{2k}(E_n, L) P_{2k}(\cos \theta), \quad (4)$$

where θ is the angle of emission of the secondary γ ray relative to the incident neutron beam, J_i is the total angular momentum of the initial state, L is the multipolarity of the transition, and a_{2k} are incident neutron energy-dependent weighting factors for the Legendre polynomials P_{2k} [37]. In principle, the weighting factors can be found by fitting measured angular distributions. However, in this case, the placement of the CLOVER detectors during the ^{56}Fe experiment did not provide angular coverage sufficient to accurately infer the angular distributions. Additionally, the experimental

values of these weighting factors for most of the observed γ rays are not available. It has been shown that a measurement of $\Delta J = 2$ γ -ray transitions at 55° can be scaled by a constant factor, independent of the actual values of a_2 and a_4 , to compute the angle-integrated cross section [38]. Using the data of Beyer *et al.* [39] and Savin *et al.* [40], the latter of which are summarized in Ref. [41], an assumption that the CLOVER detector centered at 49.3° obtains this same scaling factor introduces a systematic bias of approximately 3%. The results of this analysis approach for γ -ray production cross sections in regions of measured time difference that do not suffer from frame overlap will be presented in Sec. V.

B. Forward modeling

For the forward modeling approach, a minimization routine was employed to determine the cross section that best matches the observed data. To facilitate this comparison, a model was developed that projects the calculated cross section into the space corresponding to that observed using the GENESIS array (see, e.g., data illustrated in Fig. 4 or Fig. 5). The calculated secondary particle yield for a specific detector D , Y_{model}^D , is given by

$$Y_{\text{model}}^D(\Delta t, E_{\text{det}}, \theta) = \mathbf{R}_D \Phi(E_n, \Delta t) S(E_n, E', \theta), \quad (5)$$

where $S(E_n, E', \theta)$ is the source term that describes the distribution of secondary particles produced from interactions with neutrons of energy, E_n , and emitted from the scattering target with energy, E' , and angle, θ , relative to the incident neutron beam. The flux matrix $\Phi(E_n, \Delta t)$ defined above (see Fig. 6) relates the incoming neutron energy to the measured time difference Δt . Here, $\mathbf{R}_D$ is the detector response matrix, which transforms the initial energy and angle of the secondary particle into the observables measured by detector D :

$$\mathbf{R}_D : (E', \theta) \rightarrow (E_{\text{det}}, \theta).$$

Specifically, $\mathbf{R}_D$ describes how the reaction product distributions are transported from the ^{56}Fe target to a specific detector and then mapped into the measured data product space according to the detector response, with E_{det} (i.e., the energy of the simulated detector observable) corresponding to the γ -ray energy E_γ for the HPGe detectors or the scintillator light yield L for the neutron detectors.

To quantify agreement between the observed and modeled data, a χ^2 statistic was defined for each detector:

$$\chi_D^2 = \sum_i \frac{[Y_{\text{obs}}(\Delta t_i) - Y_{\text{model}}(\Delta t_i)]^2}{\sigma_{\text{obs}}(\Delta t_i)^2 + \sigma_{\text{model}}(\Delta t_i)^2}, \quad (6)$$

where $Y_{\text{obs}}(\Delta t_i)$ is the measured secondary particle yield as a function of measured time difference Δt_i , Y_{model} is the calculated secondary particle yield, σ_{obs} is the uncertainty in the measured yield, and σ_{model} is the uncertainty in the modeled yield due to uncertainties in the measured neutron flux and the detector response matrix. For the γ -ray data, the χ^2 statistic was calculated for each γ ray observed by the HPGe CLOVER detector at 49.3° , summing over the i measured time difference bins. For the neutron data, the χ^2 statistic was calculated for detectors located at angles of 13.1° , 30.6° ,

and 51.7° relative to the neutron beam and a two-dimensional summation was performed over the i measured time difference bins and l light yield bins. The EJ-309 detectors at larger angles were not considered due to limited statistics in the background-subtracted spectra. The end result of the minimization was a set of model parameters used to calculate cross sections that best fit the observed data. The uncertainties on the obtained model parameters were used to calculate uncertainties on the cross sections reflective of the uncertainties on the experimental data (see Sec. IV B 2). The minimization routine and computation of parameter uncertainties will be described following a discussion of the source term modeling and construction of the modeled data products.

1. Construction of modeled data products

The nuclear reaction model code TALYS-1.96 [42,43] was used with the Koning-Delaroche neutron optical model potential (nOMP) [44] to generate the cross sections for the forward model. Based on the results of large studies conducted comparing the various level densities [45] and γ -ray strength functions [46], the Gilbert and Cameron [47] plus Fermi gas [48] level density and the simplified modified Lorentzian (SMLO) [49] γ -ray strength function were used for all calculations reported in this work.

The expected γ -ray yields as a function of measured time difference, $Y_{\text{model}}(\Delta t)$, were calculated by first scaling the γ -ray production cross sections $\sigma_\gamma(E_n)$ for the 11 observed transitions by the areal density of ^{56}Fe atoms in the scattering target, n_T ; the solid angle subtended by the target, Ω ; and the integrated $^2\text{H}^+$ current I to get the source term, $S(E_n)$. These source terms were then multiplied by the flux matrix $\Phi(\Delta t, E_n)$ and then the response function R_D . For the HPGe CLOVER detector at 49.3° , the response function was described by a set of scalar values, the calculated efficiencies for detection of a given γ -ray energy, ϵ_γ . The calculated γ -ray yield was then given by

$$Y_{\text{model}}(\Delta t) = \epsilon_\gamma \Omega I n_T \Phi(\Delta t, E_n) \sigma_\gamma(E_n). \quad (7)$$

Figure 7 shows the observed and calculated yield of the $4_1^+ \rightarrow 2_1^+$ 1238.3 keV γ ray for CLOVER 1 (positioned at 49.3° with respect to the incoming neutron beam). The cross section was calculated using TALYS-1.96 with keyword `best y`, which directs TALYS to a set of files containing optimized input keyword values determined based on evaluations against experimental data [50]. The uncertainties on the modeled yields are due to the uncertainty in the neutron flux, the uncertainty in the CLOVER efficiency, the uncertainty in the target thickness, and the ^{56}Fe target multiple-scattering probability, all added in quadrature.

The response matrices for the EJ-309 detectors were calculated using a benchmarked GEANT4 model of the array (see Ref. [13] for details on the model construction and benchmarking). The simulation was run using an isotropic neutron source launched from a geometry equivalent to the ^{56}Fe scattering target with a uniform energy distribution from 0 to 20 MeV. The energy deposited in each scintillator volume was converted into light yield L in units of MeVee using the procedure outlined in Sec. II. A 2D matrix, $R_D(E_n', \theta_n, L)$, was

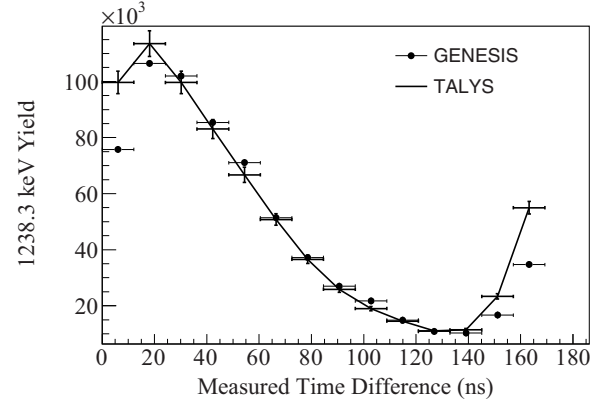


FIG. 7. Yield of the 1238.3 keV γ -ray from the $4_1^+ \rightarrow 2_1^+$ transition in ^{56}Fe as a function of measured time difference. The data points were measured with CLOVER 1 (49.3°) in the GENESIS array and are compared with the γ -ray production cross section calculated using TALYS-1.96 with keyword `best y` convolved with the flux matrix.

built for each detector. This matrix maps the neutron energy (discretized into a 0.4-MeV-wide bins) and angle relative to the neutron beam axis (discretized into b bins of 2° width) into light yield in each detector (in l bins). The response matrix is then given by

$$R_D^T = \begin{pmatrix} R(E'_0, \theta_0, L_0) & R(E'_0, \theta_0, L_1) & \dots & R(E'_0, \theta_0, L_l) \\ R(E'_0, \theta_1, L_0) & R(E'_0, \theta_1, L_1) & & \vdots \\ \vdots & & & \\ R(E'_1, \theta_0, L_0) & & & \\ R(E'_1, \theta_1, L_0) & & & \\ \vdots & & \ddots & \\ R(E'_a, \theta_b, L_0) & \dots & & R(E'_a, \theta_b, L_l) \end{pmatrix}. \quad (8)$$

To represent the absolute efficiency of the detector, this matrix was scaled by the number of source neutrons in the GEANT4 calculation. A similar matrix, $V_{RD}(E_n', \theta_n, L)$, was constructed that represents the uncertainty on the response due to the uncertainty on the light yield resolution and detector threshold. These were derived from the uncertainties on the fitted linear gain factor and resolution parameters obtained via the scintillator calibration procedure [13].

A visual representation of the matrix is shown in Fig. 8 for an EJ-309 detector positioned 70.0 cm from the center of the ^{56}Fe target and at 13.1° relative to the incident neutron beam. The detected light yield spectra as a function of initial scattered-neutron energy are shown for four different initial scattered-neutron angles. The response is strongest for the scattered neutrons with an initial momentum directed at the detector [Fig. 8(a), $10^\circ \leq \theta \leq 12^\circ$]. Small-angle scatters on the 70.0 cm of air between the ^{56}Fe target and the detector lead to a response at least one order of magnitude weaker for neutrons with initial scattered-neutron angles between 20° and 22° [Fig. 8(b)]. The response at even greater angles [Figs. 8(c)

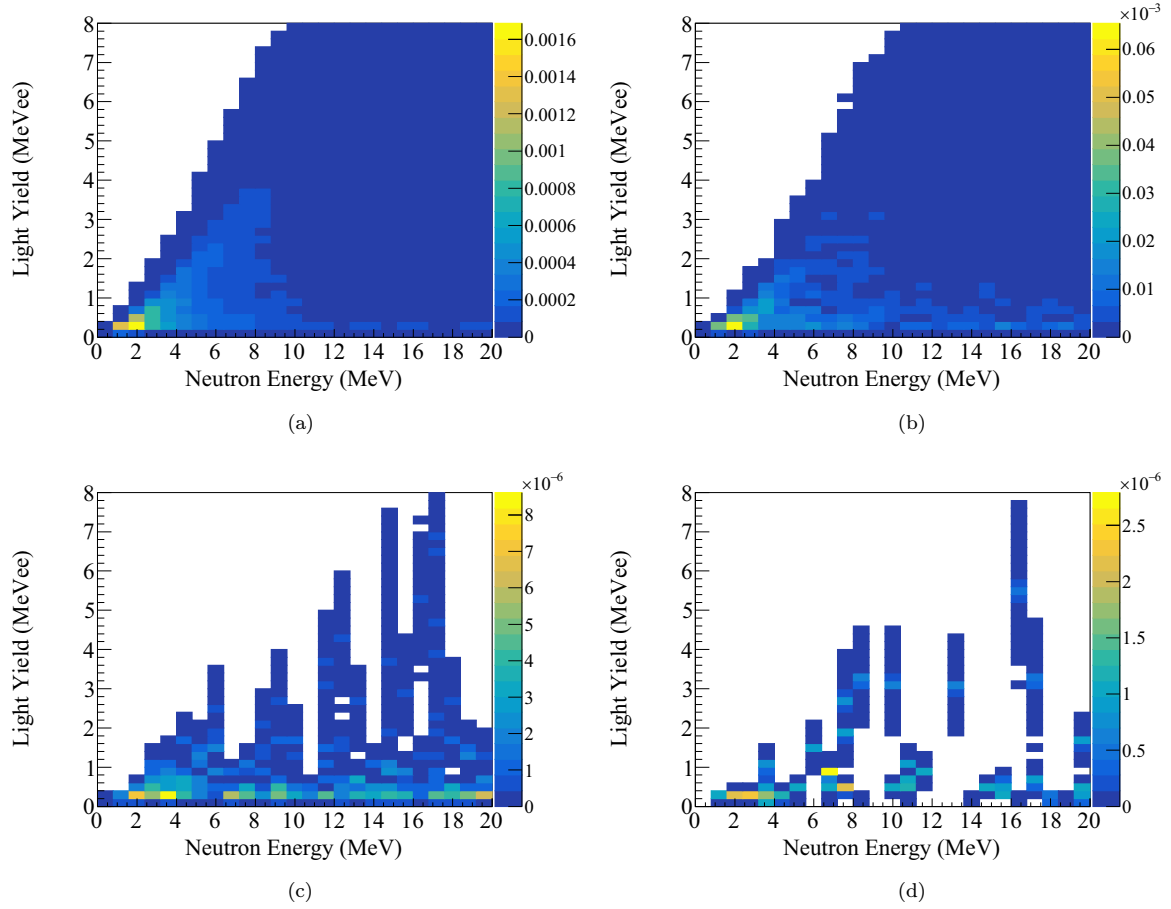


FIG. 8. Visual representation of a portion of the neutron response matrix [Eq. (8)] calculated with GEANT4 for a single EJ-309 detector at 13.1° relative to the incident neutron beam for neutrons emitted from a source geometry equivalent to the ^{56}Fe target with various initial angles. The majority of the response comes from neutrons with initial momenta pointed at the detector [Fig. 8(a)], but some response is obtained from small-angle scatters along the 70.0 cm flight path [Fig. 8(b)]. The response for neutrons with angles much different than the detector angles [Figs. 8(c) and 8(d)] is orders of magnitude lower. (a) $10 - 12^\circ$, (b) $20 - 22^\circ$, (c) $90 - 92^\circ$, and (d) $160 - 162^\circ$.

and 8(d)] is minimal, due mainly to large-angle scatters on other detectors (e.g., the CLOVER detectors) and the support structure.

The secondary neutron energy-angle distributions as a function of incident neutron energy from TALYS were processed into a matrices $S_i(\theta, E_n)$ for each outgoing neutron energy E'_i , with the rows corresponding to incoming neutron energy and the columns corresponding to outgoing neutron angle. These matrices were scaled by the number of ^{56}Fe atoms in the scattering target, the scattering target solid angle, and the integrated current and multiplied by the flux matrix $\Phi(E_n, \Delta t)$ to yield matrices $S_i(\theta, \Delta t)$. These matrices describe the angular distribution of the scattered neutrons as a function of the incoming measured time difference for a given scattered-neutron energy. To translate these matrices into the measured time difference space obtained with the experimental data (as shown in Fig. 5, i.e., the sum of incoming and scattered TOF $\Delta t'$), permutation matrices $\mathcal{T}_i^D$ were constructed to cycle the rows of a matrix $\mathcal{S}$ based on the scattered-neutron TOF for a given EJ-309 detector D . These matrices were then concatenated into a single matrix $\mathcal{S}^D$ that describes the full scattered-neutron energy-angle distribution

as a function of the total measured time difference:

$$\mathcal{S}_D(E', \theta, \Delta t') = \{\mathcal{T}_0^D \mathcal{S}_0 \quad \mathcal{T}_1^D \mathcal{S}_1 \quad \dots \quad \mathcal{T}_a^D \mathcal{S}_a\}. \quad (9)$$

The transpose of this matrix was then multiplied by the response matrix to generate modeled light yield versus measured time difference histograms $Y_{model,D}(\Delta t, L)$. A similar source matrix, $V_{SD}(E', \theta, \Delta t)$, was also constructed that represented the uncertainty due to the neutron flux and target characteristics. The uncertainty on the model yield for a given measured time difference Δt_i and light yield L_j was computed as

$$V_Y^D(\Delta t_i, L_j)^2 = \sum_{\alpha, \beta}^{a, b} [V_{RD}(E'_\alpha, \theta_\beta, L_j) \mathcal{S}_D^T(\Delta t_i, E'_\alpha, \theta_\beta)]^2 + [R_D(E'_\alpha, \theta_\beta, L_j) V_{SD}^T(\Delta t_i, E'_\alpha, \theta_\beta)]^2. \quad (10)$$

Figure 9 shows the measured and modeled light yield spectra for measured time differences between 20 and 22 ns for a single EJ-309 detector at 13.1° with respect to the incoming neutron beam. The source term was generated using TALYS-1.96 with keyword `best y`.

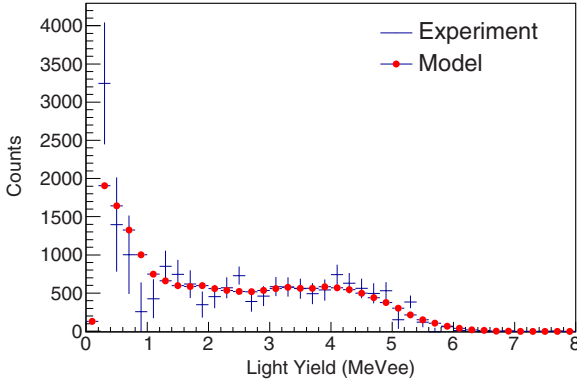


FIG. 9. Light yield spectrum (blue crosses) for measured time differences between 20–22 ns from a single EJ-309 detector at 13.1° relative to the neutron beam. Also shown is the prediction of the forward model (red circles), with secondary neutron energy-angle distributions calculated using TALYS-1.96.

2. Forward modeling with Minuit2

The Minuit2 minimization library [51] was used to determine the optimal values of the TALYS keywords. This was accomplished via the ROOT C++ application programming interface [52]. At each step in the algorithm, a new TALYS input file was created based on the current location in parameter space (the mutable TALYS keywords) and used to calculate new data products. The χ^2 value calculated between the observed and modeled data [Eq. (6)] was passed to the minimizer to continue the parameter search. The uncertainties and covariance of the TALYS parameters at the minimum were derived from the matrix of second derivatives of the χ^2 function (i.e., the Hessian matrix), calculated via Minuit2. These uncertainties are proportional to the quadratic sum of the modeled and experimental uncertainties [53], i.e., the statistical uncertainties of the γ -ray and neutron measurements, the neutron flux, and the systematic uncertainties of the detector response functions [see Eq. (6)].

To limit the number of parameters included in the minimization, one-dimensional scans of relevant TALYS input keywords were conducted against the γ -ray and neutron singles data. The scans were conducted by varying one keyword from its allowed minimum to maximum value in 50 equidistant steps and calculating the χ^2 statistic. The rest of the keywords were set using the keyword `best y`.

All keywords affecting parameters in the nOMP were evaluated against the neutron data from the EJ-309 detectors positioned at 13.1°, 30.6°, and 51.7° with respect to the incident neutron beam. Those that showed $\geq 10\%$ difference in the minimum and maximum χ^2 values were considered for the multidimensional minimization. These keywords are listed in Table I. The parameters relating to the pre-equilibrium model in TALYS-1.96 were not considered because the influence of this reaction mechanism on the observed yields is minimal due to the low flux of neutrons above 10 MeV.

All keywords that affected the level density and γ -ray strength function were evaluated against the γ -ray singles data. Twelve keywords were found to have a $\geq 10\%$ difference between the minimum and maximum χ^2 values across the

TABLE I. TALYS keywords used for secondary neutron energy and angle forward modeling. The range of values over which the keyword was sampled and the percent difference in the minimum and maximum χ^2 values obtained are also provided.

Parameter	Initial value	Range	Variation (%)
avadjust n	1.0	[0.5,2.0]	80.6
awdadjust n	1.0	[0.1,10.0]	15.4
d1adjust n	1.0	[0.2,5.0]	21.1
d2adjust n	1.0	[0.2,5.0]	16.7
d3adjust n	1.0	[0.2,5.0]	19.7
elwidth	0.5	[10 ⁻⁶ , 100.0]	80.1
rvadjust n	1.0	[0.5,2.0]	94.1
rvsoadjust n	1.0	[0.5,2.0]	14.1
rwdadjust n	1.0	[0.5,2.0]	94.2
v1adjust	1.0	[0.2,5.0]	54.9
v2adjust	1.0	[0.2,5.0]	43.1
w2adjust	1.0	[0.2,5.0]	13.6

range. This list of twelve was further down-selected as some of the keywords pertain to parametrized expressions of other adjustable keywords. The keywords ultimately included in the full minimization are provided in Table II.

The overall scheme for analyzing the ^{56}Fe GENESIS data in the forward modeling approach is presented in Fig. 10. First, the optimal nOMP parameters were found based on a minimization against the neutron data with the parameters pertaining to the level density (LD) held fixed at their best y values. These optimal parameters were then used as fixed parameters in a second minimization against the γ -ray data where the LD parameters were allowed to vary. Finally, a third minimization was performed using both types of experimental data and using the previously converged upon parameters as seeds to find a minimum in the combined-parameter space and to calculate the uncertainties and covariances of all the parameters listed in Tables I and II. All minimizations were performed with keyword `best y`, which was included in the TALYS input file before the list of mutable parameters. Following this third minimization loop, the optimal parameters and the covariance matrix were used to generate cross sections and secondary neutron distributions with uncertainties via Monte Carlo techniques.

TABLE II. TALYS keywords for γ -ray production forward modeling. The range of values over which the keyword was sampled and the percent difference in the minimum and maximum χ^2 values obtained are also provided.

Parameter	Initial value	Range	Variation (%)
alimit 26 56	8.07484	[1.0,100.0]	80.9
Pshiftadjust 26 56	0.0	[-10.0,10.0]	33.6
s2adjust 26 56	1.0	[0.1,10.0]	64.1
Tadjust 26 56	1.0	[0.1,10.0]	34.9

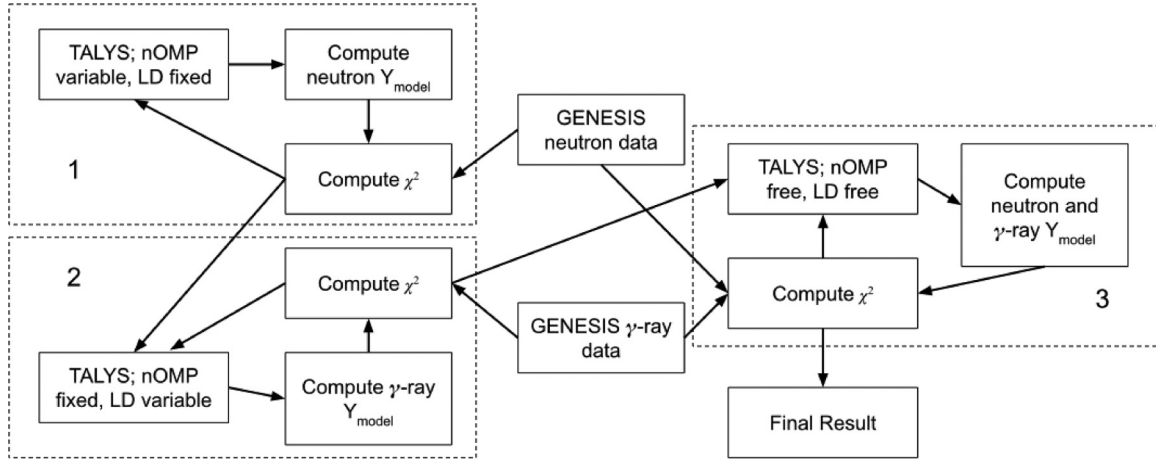


FIG. 10. Flow chart for the forward modeling analysis. Three separate minimizations are performed: (1) First, nOMP parameters are varied to find a best fit against the neutron light yield as a function of measured time difference distributions. (2) The best-fit nOMP parameters are held constant while LD parameters are varied to find the best fit using the γ -ray production data. (3) Previous parameters are used as seeds to calculate the best-fit parameters, uncertainties, and covariances against the combined neutron and γ -ray data.

V. RESULTS

The nOMP parameters converged upon in the forward model minimization are listed in Table III. The “adjust” keywords in TALYS are values that are used to scale default parameters. Most of the values in Table III indicate adjustments of nOMP parameters of less than 5% with the majority being $<1\%$. This is expected given the wealth of historical data on ^{56}Fe and its inclusion in the deduction of optimal parameters of the Koning-Delaroche nOMP [44]. The parameters d_1 , d_2 , and d_3 are found in the energy-dependent well depth for the imaginary, surface-central part of the Koning-Delaroche nOMP. The adjusted values yielded an increase of on average 2% in the well-depth between 0 and 14.9 MeV. This part of the nOMP is the second strongest contributor to the total potential in this energy range, but is a factor of approximately 6.5 to 10 times weaker than the real, volume-centered potential.

Figure 11 shows the ^{56}Fe neutron elastic-scattering cross section calculated using the TALYS parameters that were

found to provide a best fit to the GENESIS neutron data (labeled “GENESIS Forward”). Also shown is the ENDF/B-VIII.0 cross section and associated uncertainties [18]. The GENESIS results plotted in Fig. 11 and all subsequent figures in this section are available at [54]. Overall, the two cross sections agree within uncertainty, with the TALYS cross section lying approximately 10% higher for neutron energies ≥ 10 MeV. The resolution of the GENESIS array precludes observation of the resonance structures in the cross section. Additionally, TALYS is a statistical reaction model code and cannot predict the resonance cross sections. For measurements on nuclei with resonances that can be resolved with the time resolution achievable using the GENESIS array, the TALYS output would need to be adjusted to include those features, or another reaction model would be required.

Figure 12 shows the cross section for neutron inelastic scattering to the first-excited state in ^{56}Fe ($E_{ex} = 846.8$ keV, $J^\pi =$

TABLE III. Optimal values for TALYS keywords when compared against GENESIS secondary neutron energy or angle data.

Keyword	Value
avadjust n	0.9767(5)
awdadjust n	0.9935(8)
d1adjust n	1.034(2)
d2adjust n	1.0847(7)
d3adjust n	0.998(2)
elwidth	0.3004(2)
rvadjust n	1.0010(1)
rvsoadjust n	0.9998(1)
rwadjust n	1.0123(3)
v1adjust n	1.03(1)
v2adjust n	0.999(6)
w2adjust n	1.000(2)

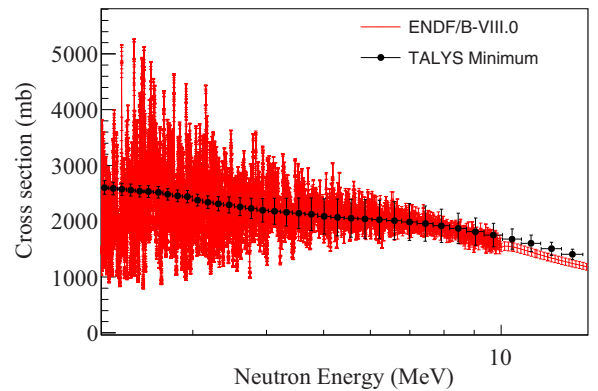


FIG. 11. ^{56}Fe neutron elastic-scattering cross section calculated using TALYS-1.96 with input parameters found through a minimization of the GENESIS neutron singles data against a convolution of the TALYS secondary neutron energy or angle distributions with the GEANT4-calculated detector response functions. Also plotted is the cross section and associated uncertainties from ENDF/B-VIII.0.

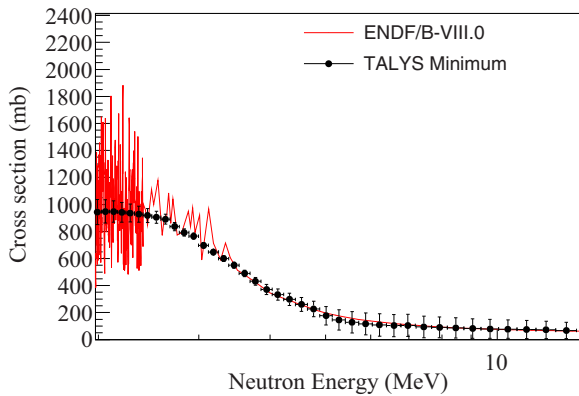


FIG. 12. Cross section for neutron inelastic scattering to the first-excited state in ^{56}Fe ($E_{ex} = 846.8$ keV) calculating using TALYS-1.96 with input parameters found through a minimization of the GENESIS neutron singles data against a convolution of the TALYS secondary neutron energy or angle distributions with the GEANT4-calculated detector response functions. Also plotted is the cross section and uncertainties from ENDF/B-VIII.0.

2^+). The cross section and uncertainty obtained via the TALYS calculation with the optimal parameters in Table III agree well with the cross section from ENDF/B-VIII.0 [18] across the entire energy range examined in this work. Again, resonance structures are not resolved.

Figure 13 shows the angle-differential ^{56}Fe neutron elastic-scattering cross section at the three neutron detector angles used in the forward modeling. The cross section for the detector at 51.7° agrees well with ENDF/B-VIII.0 across the entire energy range, though as the angle decreases or becomes shallower, the agreement worsens. The Minuit2 gradient descent algorithm is not guaranteed to find a global minimum, and the complexity of the angular distribution of elastic scattering was not well constrained by the detector placements used in this experiment.

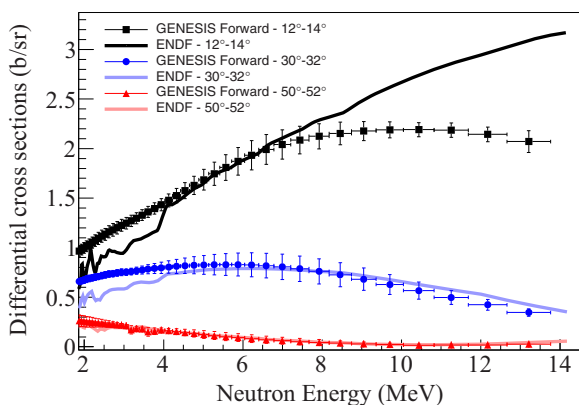


FIG. 13. Angle-differential elastic-scattering cross section calculated using TALYS-1.96 with the parameters from the forward model at the three angles corresponding to the three EJ-309 detectors used in the forward modeling. The data are compared with the cross sections from ENDF/B-VIII.0. The resonance structure apparent in the ENDF/B-VIII.0 data is not captured by the TALYS cross sections.

TABLE IV. Optimal values for TALYS keywords obtained using forward modeling with the GENESIS γ -ray production data.

Keyword	Value
Pshiftadjust 26 56	$-0.0631(2)$
Tadjust 26 56	$1.2314(1)$
alimit 26 56	$7.9978(1)$
s2adjust 26 56	$1.0333(1)$

The ^{56}Fe γ -ray production cross sections obtained using both the forward model and inverse analysis techniques are presented in Figs. 14 and 15. The results labeled “GENESIS Inverse” show the γ -ray production cross sections obtained via the inverse approach using data from CLOVER 1 at 49.3° . The γ -ray production cross sections obtained using best-fit parameters via forward modeling (labeled “GENESIS Forward”) and TALYS cross sections calculated using default parameters with keyword best (labeled “TALYS”) are also shown. These are compared with measurements from Negret *et al.* [3], Dickens *et al.* [56], and Beyer *et al.* [55]. These data were rebinned to match the energy-bin structure of the flux matrix to facilitate comparisons in measured time difference space. This bin structure was also used for the comparisons against GENESIS data in neutron energy space. These three measurements were conducted using the standard inverse approach described in Eq. (1). The best-fit parameters from the forward modeling of the γ -ray data are presented in Table IV, along with the uncertainties on the parameters. As with the nOMP parameters, it is expected that the parameters included in the minimization against the γ -ray yield data would be close to default values.

Overall, good agreement was obtained between the GENESIS cross sections obtained using the inverse technique and the literature data, with a few exceptions. For γ -rays with neutron energy regions not impacted by frame overlap up to the highest neutron energies available with the 14 MeV thick target deuteron breakup (TTDB) beam, the cross sections extracted with the inverse approach disagree with the literature above 12 MeV. The neutron flux in this energy range is small and the correspondingly high uncertainties on the determination of the flux and the counting statistics of the γ -ray yield are reflected in the cross sections uncertainties. Excellent agreement is obtained with the results of both the forward and inverse analysis techniques presented in this work and the selected literature data for the 1238.3 keV transition [Fig. 14(a)]. Similar agreement is obtained for the 2094.9 keV transition (Fig. 14(b)) and the 2273.2 keV transition [Fig. 14(c)] except above 7 MeV, where the forward model yields a higher cross section than the inverse method. Two of the three observed transitions available for analysis with the inverse approach that originate from a 2^+ state [Figs. 14(d) and 14(e)] exhibit similar behavior, where the results of the inverse analyses and the literature data both disagree with the forward model exclusively from 5 to approximately 8 MeV. Negret *et al.* [3] report similar disagreements for these transitions between their measurements and fully microscopic TALYS-1.6 calculations, indicating a deficiency

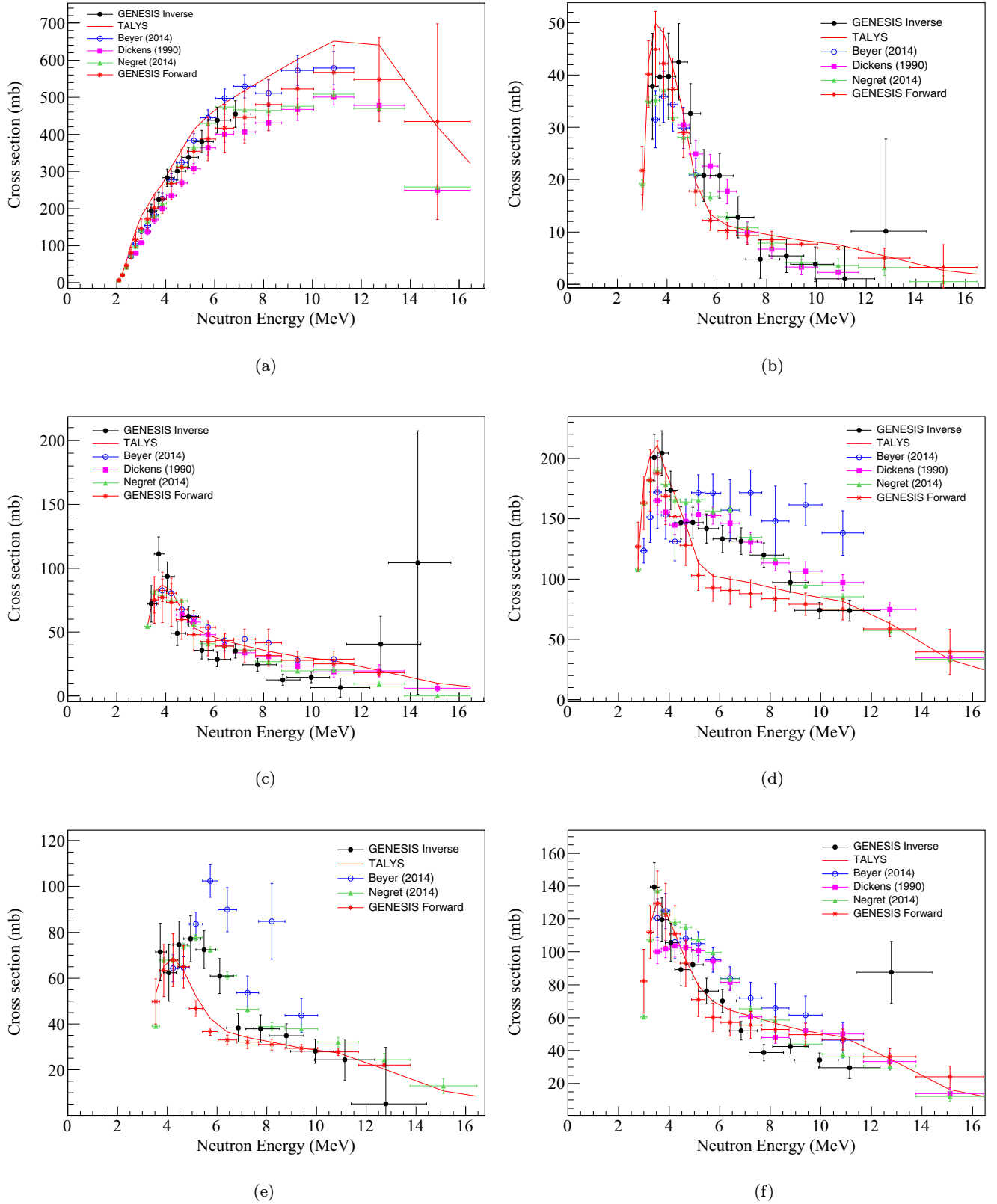


FIG. 14. Gamma-ray production cross sections for the $^{56}\text{Fe}(n, n'\gamma)$ reaction. The filled black circles were obtained using the backward analysis method, and the red filled circles are from a TALYS-1.96 calculation using the input parameters obtained with the forward modeling. The red line is the default TALYS-1.96 cross section with keyword `best y`. Also plotted are rebinned data from Beyer *et al.* [55], Negret *et al.* [3], and Dickens *et al.* [56]. (a) 1238.3 keV ($4_1^+ \rightarrow 2_1^+$) γ -ray, (b) 2094.9 keV ($0_1^+ \rightarrow 2_1^+$) γ -ray, (c) 2273.2 keV ($1_1^+ \rightarrow 2_1^+$) γ -ray, (d) 1810.8 keV ($2_2^+ \rightarrow 2_1^+$) γ -ray, (e) 2523.1 keV ($2_4^+ \rightarrow 2_1^+$) γ -ray, and (f) 2113.1 keV ($2_3^+ \rightarrow 2_1^+$) γ -ray.

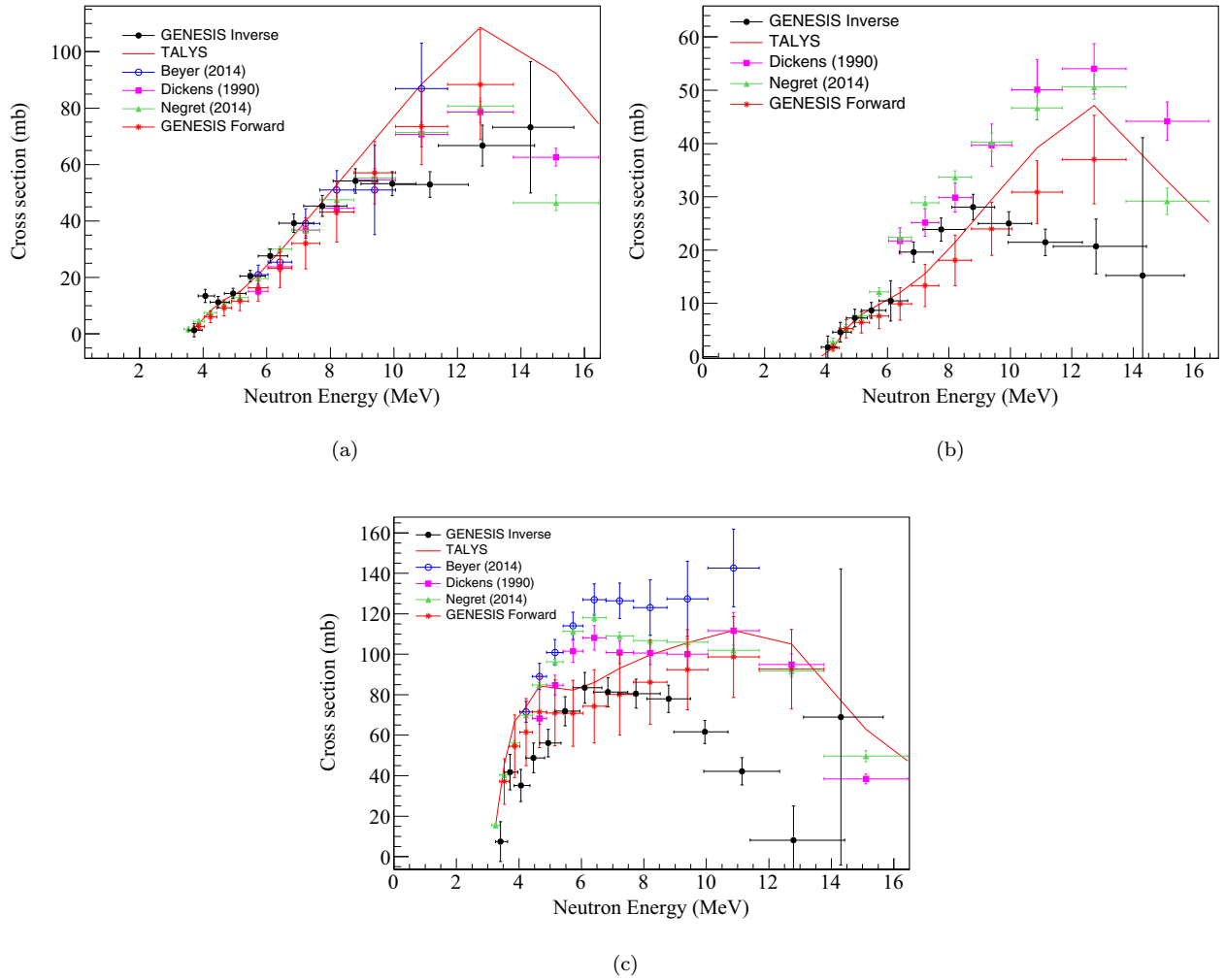


FIG. 15. Gamma-ray production cross sections for the $^{56}\text{Fe}(n, n'\gamma)$ reaction. The black circles were obtained using the backward analysis method, and the red circles are from a TALYS-1.96 calculation using the input parameters obtained with the forward modeling. The red line is the default TALYS-1.96 cross section with keyword `best γ`. Also plotted are rebinned data from Beyer *et al.* [55], Negret *et al.* [3], and Dickens *et al.* [56]. (a) 1303.4 keV ($6_1^+ \rightarrow 4_1^+$) γ -ray, (b) 1670.8 keV ($6_2^+ \rightarrow 4_1^+$) γ -ray, and (c) 1037.8 keV ($4_2^+ \rightarrow 4_1^+$) γ -ray.

in the reaction modeling not strictly dependent on the choice of optical model. The third $J_i = 2^+$ transition accessible with the inverse technique [Fig. 14(f)] diverges from this pattern and obtains consistency across the GENESIS data from 5 to 7 MeV, and not with the literature.

The γ rays from levels with $J^\pi = 6^+$ [Figs. 15(a) and 15(b)] also show some disagreement between the results from the forward model and inverse approach, and with the literature data at higher neutron energies, more so for the off-yrast transition. In Fig. 15(a), the data obtained in this work using both the forward and inverse approaches agree with the literature except at 11 MeV where the inverse approach disagrees. In Fig. 15(b), the inverse approach agrees with the literature up to 9 MeV before diverging, whereas the forward model agrees up to approximately 6 MeV. Above 6 MeV, the forward model is systematically lower than the literature. Given the relative strength of the 1670.8 keV production cross section and the correspondingly low counting statistics available for the forward-model χ^2 computations, it is unlikely that

the gradient descent was able to access regions of `s2adjust` 26 56 that could have yielded better agreement. The γ -ray production cross section calculated using both approaches for $E_\gamma = 1037.8$ keV [Fig. 15(c)] is systematically lower than the literature data for neutron energies above 5 MeV. Additionally, the values obtained with the inverse method diverge significantly from the forward model above 9 MeV. The first-excited state in ^{70}Ge is at 1039.506 keV, giving rise to a triangular feature in the spectrum, and a peak that overlaps with the 1037.8 keV peak from ^{56}Fe . This contaminating peak is removed via background subtraction using the Be target data, but given the relative lack of background data, the resulting spectrum may still contain some residual contamination, which would bias both analysis methods.

Figure 16 shows the γ -ray production cross section for the yrast $2^+ \rightarrow 0^+$, $E_\gamma = 846.8$ keV transition. Due to the threshold of this reaction, analysis via the inverse approach was not possible, though the forward modeling approach allowed for a determination of the cross section. However, because

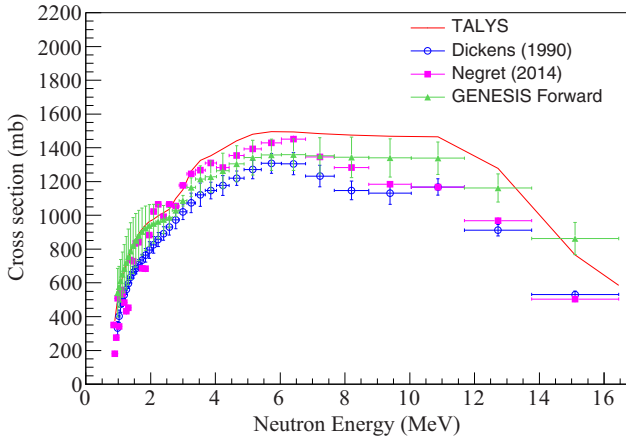


FIG. 16. Cross section for the production of the 846.8 keV ($2_1^+ \rightarrow 0_0^+$) γ -ray. The green triangles are from a TALYS-1.96 calculation using the input parameters obtained via forward modeling. The red line is the default TALYS-1.96 cross section with keyword *best* y. Also plotted are rebinned data from Negret *et al.* [3] and Dickens *et al.* [56].

the cross section was determined using the statistical nuclear reaction models employed by TALYS, the resonance structure observed in the data from Dickens *et al.* and Negret *et al.* was not reproduced. Overall, better agreement is obtained with the resolution-broadened data of Negret *et al.* below 3 MeV. Between 3 and 6 MeV, the forward model results in a cross section that is roughly halfway between the two literature measurements shown. The forward model retains more strength in this γ -ray production pathway above 8 MeV than these selected literature measurements.

The correlation matrix between the 16 TALYS keywords used in the forward model is represented in Fig. 17. The strongest correlations or anticorrelations are between the v_i parameters and between the d_i parameters. These keywords affect, respectively, the incident energy-dependent multipliers for the nOMP well depths of the real volume-central potential

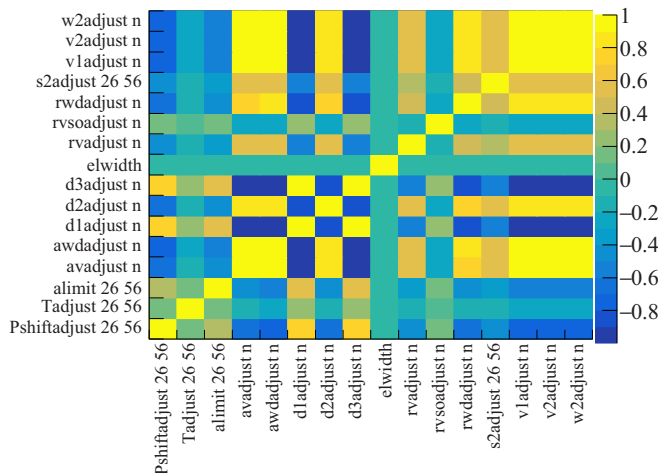


FIG. 17. Correlation matrix for TALYS keywords used in the forward model.

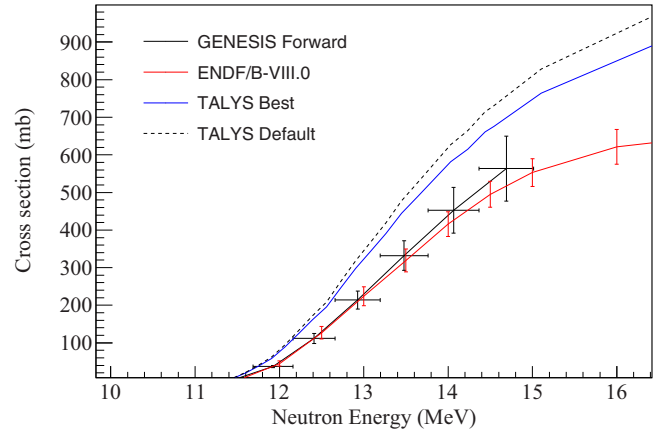


FIG. 18. Cross section for the $^{56}\text{Fe}(n, 2n)$ reaction calculated using TALYS-1.96 with TALYS default parameters (black dashed line), TALYS best (blue solid line), and with parameters found using a forward model applied to the GENESIS data (black data points). Also shown is the $^{56}\text{Fe}(n, 2n)$ cross section from ENDF/B-VIII.0 (red points).

and the imaginary surface-central potential, respectively. The presence of strong anticorrelation across various parameters is also notable. The diffuseness of the radial parts of these potentials (*avadjust n* and *awdadjust n*) also correlates both with each other and the functional forms of the energy-dependent well depths. These correlations underscore the need for the inclusion of multiple reaction channels, beyond those observed with GENESIS, when performing any kind of nuclear reaction model evaluation.

The secondary neutrons or γ -rays from the $^{56}\text{Fe}(n, 2n)$ reaction were not observed with sufficient yield to be included in the forward modeling analysis. However, the TALYS parameters found through minimization against the secondary γ rays and neutrons from elastic and inelastic scattering observed in this work were used to calculate a cross section for the $(n, 2n)$ reaction channel. Figure 18 provides the result of this calculation performed using the best-fit reaction model parameters obtained through forward modeling with uncertainty based upon the covariance matrix (labeled “GENESIS Forward”). The results are in excellent agreement with the $^{56}\text{Fe}(n, 2n)$ ENDF/B-VIII.0 cross section.

The calculated $^{56}\text{Fe}(n, 2n)$ cross section obtained using parameters extracted via the forward modeling approach demonstrates significantly improved agreement with the ENDF/B-VIII.0 cross section as compared with the result of TALYS calculations performed using default or “best” parameters. This improvement arises because the best-fit parameters obtained through forward modeling, specifically parameters related to the nOMP and nuclear level density that are important for prediction of the partial γ -ray cross sections and neutron energy-angle distributions observed in this work, are also important for the accurate calculation of the $^{56}\text{Fe}(n, 2n)$ reaction cross section. That is, the observation of secondary γ rays and scattered neutrons from elastic and inelastic scattering provides sufficient constraint for the extraction of reaction model parameters governing the behavior

of the unobserved $(n, 2n)$ reaction channel to enable an improvement in this cross-section calculation. It should be noted that the $^{56}\text{Fe}(n, 2n)$ cross section calculated using parameters obtained from the GENESIS forward model analysis is not merely a scale factor of the TALYS calculation (e.g., the cross section calculated using best-fit parameters is 29.9% lower than the TALYS best result at 12 MeV and 22.9% at 14 MeV). The Koning-Delaroche nOMP [44] was adopted in this work with no additional energy-dependent parameter adjustments. This suggests that the energy dependence of the level density and real and imaginary components of the volume-central, surface-central, and spin-orbit potentials in the Koning-Delaroche nOMP is sufficient to capture the energy dependence of the cross section and extrapolate beyond the observed energy range.

VI. SUMMARY

The construction of evaluated nuclear data libraries, which serve as essential inputs to deterministic and stochastic models of nuclear technologies spanning application spaces including reactors, aerospace, medicine, and nonproliferation, is fundamentally challenging due to the variety of experimental modalities, generally tailored to specific reaction channels, the varying quality of individual measurements, and, critically, the lack of data for every reaction channel across the relevant neutron energy range. Additionally, given that reaction cross sections are seldom measured directly—what is measured are the products of certain reactions, modulated by various experimental factors, from which cross sections are deduced—there is sufficient reason for a new analysis paradigm of experimental nuclear reaction data. The forward modeling approach introduced in this work, where parametrized nuclear reaction models are used to generate cross sections that, when convolved with validated response functions describing the experimental apparatus, yield data products that can be directly compared with observations, is one possibility for that new framework.

The GENESIS array consists of a combination of HPGe detectors and organic liquid scintillators, enabling the simultaneous measurement of the energy and angular distributions of both scattered neutrons and secondary γ rays following the interaction of a pulsed, broad-spectrum neutron beam within a thin target. An experiment with an isotopically enriched ^{56}Fe target was performed. A forward model, based on a GEANT4 model of the GENESIS array and the nuclear reaction code TALYS-1.96, was used to determine 11 γ -ray production cross sections and scattered neutron energy-angle distributions. The γ -ray production cross sections obtained with this method are in general agreement with previous measurements and with the results of a standard inverse analysis, with a few notable exceptions. The scattered neutron distributions extracted using forward modeling show general agreement with the evaluated data, excluding the elastic-scattering angu-

lar distributions at small scattering angles. The disagreements observed in the γ -ray production and secondary neutron data could be due to limitations in the nuclear reaction model used, the presence of local minima in the 16-dimensional parameter space of the forward model, and/or suboptimal HPGe and organic liquid scintillator placement. Given the relatively higher statistics for the 846.8 and 1238.3 keV transitions, these data exert a disproportionately larger influence on the forward modeling minimization process. However, even with these transitions excluded from the simultaneous minimization, it is not possible to obtain a global set of reaction model input parameters that demonstrates agreement with the data extracted using the inverse approach over the full energy range examined in this work. This suggests that there may be insufficient degrees of freedom within TALYS for the selected nOMP and level density and γ -ray strength function parametrizations to accurately describe the underlying physics. Future work will investigate the use of local potentials, coupled channels calculations, and alternate reaction model codes (e.g., CoH [57], YAHFC [58], etc.) in the forward modeling framework. Despite these limitations, the best-fit reaction model parameters extracted using the forward modeling technique yielded a significant improvement in the calculated $^{56}\text{Fe}(n, 2n)$ cross section (even though these data were not directly observed using the GENESIS array), compared with that obtained using the default and “TALYS best” parameters. This suggests that, although the selected TALYS models may not fully capture all aspects of the data, the forward modeling framework can still enhance the predictive power of the calculations.

ACKNOWLEDGMENTS

The authors are grateful for discussions with James Bevins and Juan Manfredi at the Air Force Institute of Technology. This work was performed under the auspices of the U.S. Department of Energy (DOE) by Lawrence Berkeley National Laboratory under Contract No. DE-AC02-05CH11231, Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344, and the Defense Threat Reduction Agency under Grant No. HDTRA1033292. This work was supported in part by the U.S. DOE National Nuclear Security Administration through the Nuclear Science and Security Consortium under Award No. DE-NA0003996, the U.S. DOE National Nuclear Security Administration Office of Defense Nuclear Nonproliferation R&D through the LB23-GammaProdXSwthGENESIS-PD3Ob project, the U.S. DOE Office of Nuclear Energy Nuclear Energy University Program (NEUP), and the U.S. DOE Office of Nuclear Energy, Nuclear Energy Advanced Modeling and Simulation (NEAMS) program.

DATA AVAILABILITY

The data that support the findings of this article are openly available [54].

[1] M. Herman, D. Brown, R. Capote, M. Chadwick, W. Haack, J. Hutchinson, T. Kawano, D. Neudecker, G. Palmiotti, M.

Salvatores, P. Talou, A. Trkov, and M. White, *Ann. Nucl. Energy* **163**, 108494 (2021).

- [2] D. Neudecker, A. M. Lewis, E. F. Matthews, J. Vanhoy, R. C. Haight, D. L. Smith, P. Talou, S. Croft, A. D. Carlson, B. Pierson, A. Wallner, A. Al-Adili, L. Bernstein, R. Capote, M. Devlin, M. Drosge, D. L. Duke, S. Finch, M. W. Herman, K. J. Kelly, *et al.*, *EPJ Nuclear Sci. Technol.* **9**, 35 (2023).
- [3] A. Negret, C. Borcea, P. Dessagne, M. Kerveno, A. Olacel, A. J. M. Plompen, and M. Stanoiu, *Phys. Rev. C* **90**, 034602 (2014).
- [4] E. Pirovano, R. Beyer, M. Dietz, A. R. Junghans, S. E. Müller, R. Nolte, M. Nyman, A. J. M. Plompen, M. Röder, T. Szücs, and M. P. Takacs, *Phys. Rev. C* **99**, 024601 (2019).
- [5] A. Koning, D. Rochman, J.-C. Sublet, N. Dzysiuk, M. Fleming, and S. van der Marck, *Nucl. Data Sheets* **155**, 1 (2019), special Issue on Nuclear Reaction Data.
- [6] N. Otuka, E. Dupont, V. Semkova, B. Pritychenko, A. Blokhin, M. Aikawa, S. Babykina, M. Bossant, G. Chen, S. Dunaeva, R. Forrest, T. Fukahori, N. Furutachi, S. Ganesan, Z. Ge, O. Gritzay, M. Herman, S. Hlavač, K. Katō, B. Lalremruata, *et al.*, *Nucl. Data Sheets* **120**, 272 (2014).
- [7] Nuclear Energy Agency, International handbook of evaluated criticality safety benchmark experiments, Tech. Rep. No. 7645 (Organisation for Economic Cooperation and Development, Paris, France, 2022-2023).
- [8] A. Daskalakis, E. Blain, B. McDermott, R. Bahrn, Y. Danon, D. Barry, R. Block, M. Rapp, B. Epping, and G. Leinweber, *Ann. Nucl. Energy* **110**, 603 (2017).
- [9] F. Saglime, Y. Danon, R. Block, M. Rapp, R. Bahrn, G. Leinweber, D. Barry, and N. Drindak, *Nucl. Instrum. Methods Phys. Res., Sect. A* **620**, 401 (2010).
- [10] J. E. Sweezy, T. E. Booth, F. B. Brown, J. S. Bull, R. A. Forster, III, J. T. Goorley, H. G. Hughes, III, R. L. Martz, R. E. Prael, A. Sood, A. J. Zukaitis, R. C. Little, H. R. Trellue, M. C. White, M. B. Lee, and S. M. Girard, MCNP - A general Monte Carlo N-particle transport code, Version 5 - Volume 1: Overview and theory, Tech. Rep. No. LA-UR-03-1987 (Revised 2/1/2008) (Los Alamos National Laboratory, Los Alamos, NM, USA, 2003).
- [11] D. B. Pelowitz, J. T. Goorley, M. R. James, T. E. Booth, F. B. Brown, J. S. Bull, L. J. Cox, J. W. Durkee, Jr., J. S. Elson, M. L. Fensin, R. A. Forster, III, J. S. Hendricks, H. G. Hughes, III, R. C. Johns, B. C. Kiedrowski, R. L. Martz, S. G. Mashnik, G. W. McKinney, R. E. Prael, J. E. Sweezy, *et al.*, MCNP6 User's Manual, Tech. Rep. No. LA-CP-13-00634 (Los Alamos National Laboratory, Los Alamos, NM, 2013).
- [12] D. P. Barry, G. Leinweber, R. C. Block, T. J. Donovan, Y. Danon, F. J. Saglime, A. M. Daskalakis, M. J. Rapp, and R. M. Bahrn, *Nucl. Sci. Eng. (La Grange Park, IL, U. S.)* **174**, 188 (2013).
- [13] J. Gordon, J. Batchelder, L. Bernstein, D. Bleuel, C. Brand, J. Brown, B. Goldblum, B. Frandsen, T. Laplace, and T. Nagel, *Nucl. Instrum. Methods Phys. Res. Sect. A* **1061**, 169120 (2024).
- [14] M. Kireeff Covo, R. Albright, B. Ninemire, M. Johnson, A. Hodgkinson, T. Loew, J. Benitez, D. Todd, D. Xie, T. Perry, L. Phair, L. Bernstein, J. Bevins, J. Brown, B. Goldblum, M. Harasty, K. Harrig, T. Laplace, E. Matthews, A. Bushmaker, *et al.*, *Measurement* **127**, 580 (2018).
- [15] M. Herman, A. Trkov, R. Capote, G. Nobre, D. Brown, R. Arcilla, Y. Danon, A. Plompen, S. Mughabghab, Q. Jing, G. Zhigang, L. Tingjin, L. Hanlin, R. Xichao, L. Leal, B. Carlson, T. Kawano, M. Sin, S. Simakov, and K. Guber, *Nucl. Data Sheets* **148**, 214 (2018).
- [16] Z. Ilic, E. Mauerhofer, C. Stieghorst, Z. Révay, M. Rossbach, T. Randriamalala, and T. Brückel, *J. Radioanal. Nucl. Chem.* **325**, 641 (2020).
- [17] N. Fedorov, D. Grozdanov, Y. Kopatch, T. Tretyakova, I. Ruskov, V. Skoy, I. Dashkov, F. Aliyev, S. Dabylova, C. Hramco, A. Kumar, A. Gandhi, D. Wang, E. P. Bogolyubov, D. I. Yurkov, and the TANGRA Collaboration, *Eur. Phys. J. A* **57**, 194 (2021).
- [18] D. Brown, M. Chadwick, R. Capote, A. Kahler, A. Trkov, M. Herman, A. Sonzogni, Y. Danon, A. Carlson, M. Dunn, D. Smith, G. Hale, G. Arbanas, R. Arcilla, C. Bates, B. Beck, B. Becker, F. Brown, R. Casperson, J. Conlin, *et al.*, *Nucl. Data Sheets* **148**, 1 (2018).
- [19] J. M. Gordon, B. L. Goldblum, J. A. Brown, T. A. Laplace, J. C. Batchelder, D. L. Bleuel, C. A. Brand, B. Buckley, A. Georgiadou, C. J. Henderson, T. S. Johnson, J. W. Lee, K. Myers, T. S. Nagel, J. R. Sebastian, A. S. Voyles, and L. A. Bernstein, *Phys. Rev. C* **111**, 044608 (2025).
- [20] S. Agostinelli, J. Allison, K. Amako, J. Apostolakis, H. Araujo, P. Arce, M. Asai, D. Axen, S. Banerjee, G. Barrand, *et al.*, *Nucl. Instrum. Methods Phys. Res. Sect. A* **506**, 250 (2003).
- [21] E. Mendoza and D. Cano-Ott, Update of the Evaluated Neutron Cross Section Libraries for the GEANT4Code, Tech. Rep. No. INDC(NDS)-0758 (International Atomic Energy Agency, 2018).
- [22] D. L. Bleuel, L. Bernstein, R. Marsh, J. Morrell, B. Rusnak, and A. Voyles, *Appl. Radiat. Isot.* **170**, 109625 (2021).
- [23] A. Trkov, P. Griffin, S. Simakov, L. Greenwood, K. Zolotarev, R. Capote, D. Aldama, V. Chechev, C. Destouches, A. Kahler, C. Konno, M. Košťál, M. Majerle, E. Malambu, M. Ohta, V. Pronyaev, V. Radulović, S. Sato, M. Schulc, E. Šimečková, *et al.*, *Nucl. Data Sheets* **163**, 1 (2020).
- [24] AL204 Analytical Balance, Mettler Toledo (2024).
- [25] J. M. Gordon, Simultaneous measurements of secondary gamma rays and neutrons from fast neutron scattering on ^{56}Fe with GENESIS, Ph.D. thesis, University of California, Berkeley, 2023.
- [26] J. Conlin, W. Haeck, D. Neudecker, D. Parsons, and M. White, Release of ENDF/B-VIII.0-Based ACE Data Files, Tech. Rep. No. LA-UR-18-24034 (Los Alamos National Laboratory, Los Alamos, NM, 2018).
- [27] A. Ruben, P. Bender, P. Chowdhury, P. L. Kerr, F. Lüke, G. Montermann, A. M. Rogers, and R. Schneider, A new, versatile, high-performance digital pulse processor with application to neutron/gamma-ray pulse-shape discrimination in scintillator detectors, *Proc. Nima_Sorma Xvii* (2018).
- [28] MDPP-16 SCP/RCP, Mesytec (2022), https://www.mesytec.com/products/datasheets/MDPP-16_SCP-RCP.pdf.
- [29] Neutron/Gamma PSD EJ-301, EJ-309, Eljen Technology (2021), <https://eljentechnology.com/products/liquid-scintillators/ej-301-ej-309>.
- [30] Software Module MDPP-16-QDC, Mesytec (2022), https://www.mesytec.com/products/datasheets/MDPP-16_QDC.pdf.
- [31] J. A. Brown, B. L. Goldblum, T. A. Laplace, K. P. Harrig, L. A. Bernstein, D. L. Bleuel, W. Younes, D. Reyna, E. Brubaker, and P. Marleau, *J. Appl. Phys.* **124**, 045101 (2018).
- [32] T. Laplace, B. Goldblum, J. Bevins, D. Bleuel, E. Bourret, J. Brown, E. Callaghan, J. Carlson, P. Feng, G. Gabella, K. Harrig, J. Manfredi, C. Moore, F. Moretti, M. Shinner, A. Sweet, and Z. Sweger, *J. Instrum.* **15**, P11020 (2020).

- [33] S. Yoshida, T. Ebihara, T. Yano, A. Kozlov, T. Kishimoto, I. Ogawa, R. Hazama, S. Umehara, K. Mukaida, K. Ichihara, Y. Hirano, I. Murata, J. Datemichi, and H. Sugimoto, *Nucl. Instrum. Methods Phys. Res. Sect. A* **622**, 574 (2010).
- [34] T. Laplace, B. Goldblum, J. Brown, G. LeBlanc, T. Li, J. Manfredi, and E. Brubaker, *Mater. Adv.* **3**, 5871 (2022).
- [35] G. Dietze and H. Klein, *Nucl. Instrum. Methods Phys. Res.* **193**, 549 (1982).
- [36] K. Harrig, B. Goldblum, J. Brown, D. Bleuel, L. Bernstein, J. Bevens, M. Harasty, T. Laplace, and E. Matthews, *Nucl. Instrum. Methods Phys. Res. Sect. A* **877**, 359 (2018).
- [37] E. Sheldon and D. M. V. Patten, *Rev. Mod. Phys.* **38**, 143 (1966).
- [38] L. Mihailescu, L. Olah, C. Borcea, and A. Plompen, *Nucl. Instrum. Methods Phys. Res. Sect. A* **531**, 375 (2004).
- [39] R. Beyer, M. Dietz, D. Bemmerer, A. R. Junghans, T. Kögler, R. Massarczyk, S. Müller, K. Schmidt, R. Schwengner, T. Szücs, M. P. Takács, and A. Wagner, *Eur. Phys. J. A* **54**, 58 (2018).
- [40] M. V. Savin, A. V. Livke, Y. Y. Nefedov, M. S. Shvetsov, A. G. Zvenigorodskii, and A. I. Blokhin, *J. Nucl. Sci. Technol. (Abingdon, U. K.)* **37**, 748 (2000).
- [41] A. Hurst, L. Bernstein, T. Kawano, A. Lewis, and K. Song, *Nucl. Instrum. Methods Phys. Res. Sect. A* **995**, 165095 (2021).
- [42] A. Koning, S. Hilaire, and M. Duijvestijn, in *Proceedings of the International Conference on Nuclear Data for Science and Technology*, edited by O. Bersillon, F. Gunsing, E. Bauge, R. Jacqmin, and S. Leray (EDP Sciences, Nice, France, 2008), pp. 211–214.
- [43] A. Koning, S. Hilaire, and S. Goriely, *Eur. Phys. J. A* **59**, 131 (2023).
- [44] A. Koning and J. Delaroche, *Nucl. Phys. A* **713**, 231 (2003).
- [45] S. Goriely, A.-C. Larsen, and D. Muecher, *Phys. Rev. C* **106**, 044315 (2022).
- [46] S. Goriely, P. Dimitriou, M. Wiedeking, T. Belgia, R. Firestone, J. Kopecky, M. Krticka, V. Plujko, R. Schwenger, S. Siem, H. Utsunomiya, S. Hilaire, S. Peru, Y. Cho, D. Filipescu, N. Iwamoto, T. Kawano, V. Varlamov, and R. Xu, *Eur. Phys. J. A* **55**, 172 (2019).
- [47] A. Gilbert and A. Cameron, *Can. J. Phys.* **43**, 1446 (1965).
- [48] H. A. Bethe, *Phys. Rev.* **50**, 332 (1936).
- [49] V. A. Plujko, I. M. Kadenko, E. V. Kulich, S. Goriely, O. I. Davidovskaya, and O. M. Gorbachenko, in *Proceedings of Workshop on Photon Strength Functions and Related Topics — PoS(PSF07)* (Proceedings of Science, Prague, Czech Republic, 2008).
- [50] A. Koning, S. Hilaire, and S. Goriely, *TALYS-1.96/2.0: Simulation of Nuclear Reactions* (Vienna, Austria, 2021).
- [51] F. James and M. Winkler, Minuit 2 (2024), <https://root.cern.ch/root/html/doc/guides/minuit2/Minuit2.pdf>.
- [52] R. Brun and F. Rademakers, *Nucl. Instrum. Methods Phys. Res. Sect. A* **389**, 81 (1997).
- [53] F. James, *The Interpretation of Errors*, CERN Geneva, Switzerland (2004), Vol. 532, p. 533.
- [54] J. M. Gordon *et al.*, (2026) <https://doi.org/10.5061/dryad.rv15dv4p5>.
- [55] R. Beyer, R. Schwengner, R. Hannaske, A. Junghans, R. Massarczyk, M. Anders, D. Bemmerer, A. Ferrari, A. Hartmann, T. Kögler, M. Röder, K. Schmidt, and A. Wagner, *Nucl. Phys. A* **927**, 41 (2014).
- [56] J. Dickens, J. Todd, and D. Larson, Cross sections for production of 70 discrete-energy gamma rays created by neutron interactions with ^{56}Fe for E_n to 40 MeV: Tabulated Data, Tech. Rep. No. ORNL/TM-11671 (Oak Ridge National Laboratory, Oak Ridge, TN, 1990).
- [57] T. Kawano, P. Talou, M. B. Chadwick, and T. Watanabe, *J. Nucl. Sci. Technol. (Abingdon, U. K.)* **47**, 462 (2010).
- [58] W. E. Ormand, Monte Carlo Hauser-Feshbach computer code system to model nuclear reactions: YAHFC, Tech. Rep. No. LLNL-TR-824700 (Lawrence Livermore National Laboratory (LLNL), Livermore, CA, 2021).