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Thermal Capture and Gamma Emission

Summary Report of the IAEA Consultants' Meeting

IAEA Headquarters, Vienna, Austria

23-25 October 2023

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1. Introduction

The Consultants Meeting on Thermal Capture and Gamma Emission began with the election of meeting officials (chair and rapporteur) followed by opening remarks given by the NDS Section Head, Arjan Koning (AK) and the Scientific Secretary of the meeting, Roberto Capote (RC). AK discussed the need for new evaluators and mentioned the US Department of Energy (DOE) Office of Science (SC) Program Manager Keith Jankowski's upcoming initiative aimed at training new younger evaluators. This new initiative will be proposed in a future Funding Opportunity Announcement (FOA) in FY24 (with funding to commence in FY25) where it is intended for current data evaluators and senior researchers working in areas of relevance to nuclear data to team together with identified younger researchers. The goal is to train younger researchers to become full time nuclear data evaluators at the conclusion of the training program. Roberto Capote (RC) described the need for new EGAF (Evaluated Gamma-ray Activation File) applications and his plan to develop a road map in this direction. RC also highlighted needs for possible new measurements of the total radiative thermal neutron capture cross section (σ_0).

2. Participants' Presentation Summaries

Participants' presentations are available at: CM Thermal Capture and Gamma Emission 2023

2.1. Spectroscopy database for PGAA, *Z. Révay*

It was mentioned that many tasks stemmed from the first Consultants' Meeting, however, it was suggested that such a plan was too ambitious and not all tasks were completed. This is understandable in part due to the pandemic.

ZR highlights important questions that need to be addressed in Prompt Gamma Activation Analysis (PGAA) for the development of a corresponding database: peak fitting (in particular, asymmetric peaks and their effects associated with larger detectors); non-linearity in energy calibrations; and high-energy efficiencies. ZR says that new data is needed for the development of a new database, and that this will require a full-time effort from a new postdoctoral researcher. RC suggests the IAEA may be able to help with the fulfillment of this role.

The γ-ray data for the new database initiative will be analyzed using the HYPERMET γ-ray spectroscopy software package which can reliably handle the various components of the peak shapes observed in (n,γ) measurements: baseline (linear, polynomial); peak-dependent background (step, tail); peak shape (Gaussian, left-skew from incomplete charge collection, right-skew from pile-up effects). ZR also describes the functional form used in the fitting procedure. A few representative plots are shown by ZR illustrating the shape of prompt peaks: examples are shown for high count- rate and high-energy measurements. The individual peak components are shown in comparison to the measured data and reveal how the peak shape is dependent upon both energy and count rate. We may expect high count-rate peaks to deviate significantly from a purely Gaussian distribution. ZR asks if any other modern methodologies used to describe peak shapes could also be considered.

A representative efficiency-calibration curve obtained using HYPERMET is also presented: Here one absolute radioactive source (usually ^{152}Eu) is used as a normalization source and other radioactive sources are calibrated relative to it: ^{133}Ba, ^{207}Bi, and ^{241}Am are used in the fit shown. Additionally, reaction sources (important for high-energy γ lines) that are commonly used in (n,γ) measurements are also shown in the presented fit: N(n,γ), Cl(n,γ), and Cr(n,γ). Collectively, these sources cover an energy range E_γ = 50keV − 11MeV. It is pointed out that because all high-energy data is derived from the same source [N(n,γ)], a change in source may result in a corresponding change in derived results. The radioactive sources only go up to around ~ 2.5 MeV, and the reaction sources provide higher-energy coverage. However, with consideration to the sources presented, there is a gap between about 9 − 11 MeV. TB will discuss this in his talk.

A representative energy calibration is also presented with a discussion of linear and non-linear components; crystal-spectrometer data from ^{152}Eu(n,γ) and ^{35}Cl(n,γ) are presented. ZR shows non-linearity problems at high energy. There are instability issues in this region due to a lack of data points cf. much more data at lower energy allowing for a better-constrained fit. RC suggests using splines to describe high-energy non-linearity of the energy-calibration curve. AT says that although splines force the data to go through the points but may not be a physical solution. ZR is open to adoption of cubic-spline interpolation methods.

The next part of the presentation involves a discussion of measurements beginning with a description of the use of the relative standardization method. ZR explains how this method utilizes comparator which negates the need for absolute measurements of quantities such as flux, etc., because many terms cancel upon taking ratios. It is also explained how the relative standardization approach helps reduce uncertainties. RC asks about the unique H-standard. ZR mentions that he uses the H γ-ray line at 2223 keV as the primary comparator line in relative measurements. Thus, the unique normalization partial γ-ray production cross section σ_γ(H; 2223 keV) = 0.3326 b±0.2% is used as the reference line for measurements. It is noted that should the standard value for H change, then all results would need to be scaled accordingly. David Bernard (participating remotely) provides a PRL reference for the cross section σ_γ(H; 2223 keV) = 0.3349(5) b [Phys. Rev. Lett. **115**, 13201]. However, that is a single value and the adopted value used for standardization of 0.3326 b comes from evaluations (ENDF/B-VIII uses a value of 0.3327(69) b).

ZR presents some information on the flux at the Budapest PGAA facility (thermal and cold fluxes and background count rates) and mentions that the larger detector at the FRM-II PGAA facility may have a bigger problem with peak-shape asymmetry due to incomplete charge collection. The PGAA instrumentation is reviewed, and it is suggested that elements with $Z > 30$ will be performed at the FRM-II.

In a discussion of the analysis/evaluation procedure ZR begins by providing a breakdown of the uncertainties associated with the measured quantities (flux, efficiency, etc.). All terms needed for absolute-method determinations are first presented and discussed, followed by the relative standardization methodology. ZR shows how the relative approach results in cancellation of terms common to both the standard and measured sample resulting in a smaller overall uncertainty. The relative standardization method is similar to the k_0 method. RC asks if other standards besides H are also used. ZR says *"yes"*, e.g., Cl, but emphasizes that everything ultimately traces back to H, i.e., the γ-ray production cross section for the Cl lines is deduced relative to H. Corrections to prompt γ-ray spectra are also described including radioactive-decay line corrections and self-attenuation corrections from neutron self-shielding and γ-ray self-absorption. For γ rays the linear absorption mass-attenuation coefficient (μ/ρ) is taken from the XCOM database (NIST). The uncertainty propagation is then discussed in detail, and it is mentioned that statistical uncertainties dominate the deduced cross sections but small systematic uncertainties, e.g., uncertainties associated with the comparator line from H, also need to be identified and combined appropriately. ZR also mentions that lines with relative uncertainties of less than 0.1% are not included in the database, based on a dynamic range of 10^{-4}. The dynamic range is based on peak counts relative to the associated Compton continuum. It is noted that there are, however, many weaker peaks. RC asks if this limit is reasonable for certain applications, e.g., modeling the complete detector-response spectrum? For analytical applications, however, this limit is probably fine for prompt γ rays. ZR suggests it is possible to go to lower relative uncertainties of < 0.1% in certain situations over energy ranges where there are many peaks, e.g., ~ 5 MeV in Fe.

An overview of the library measurements is presented: Elemental spectra to obtain relative positions and intensities of the γ-ray lines; absolute scale determination for the energy calibration; standardization methodology to establish an absolute intensity scale. Although the ultimate comparator is still H, a set of well-established standards can also be used: C, N, O, F, S, Cl, Fe (Au). For the low-energy region (10 keV − 1 MeV) a LEPS detector (low-energy photons) with superior resolution over this region is used. Decay measurements should be linked to the k_0 database. ZR has already performed around 300 measurements at the FRM-II; these are mainly elemental measurements of natural samples although some measurements with separated isotopes have also been performed. ZR is willing to share the data

with colleagues. ZR also provides an historical overview of cold PGAA library measurements in the period from 2004-2023, with several new measurements having been performed recently in Garching (FRM-II). ZR highlights new features of the library: (1) New standardization for several elements and the observed non-1/*v* behaviour in Sm is found to be different in Budapest and Garching; (2) Non-characteristic lines are completely omitted. Because there are too many interferences at certain energies these lines are not suitable for and cannot be used for identification purposes. A list of compound samples used in a new set of standardization measurements at the Budapest Neutron Centre (BNC) is also presented. Finally, ZR presents a few slides illustrating differences in deduced cross sections based on thermal (around 20% higher) and cold beams due to resonances in the non-1/*v* isotopes. ZR uses Sm to illustrate this observation but suggests it is likely to be an issue for all non-1/*v* isotopes (those with Westcott *g*-factors that deviate significantly from unity at the respective temperature). This seems plausible given that the decay of the compound nucleus to final set of states is dependent on the energy given to the system in the entrance channel.
During questions, VP asks how you can exclude efficiency from relative measurements since γ-ray energies are generally different. ZR shows a covariance method for determination of energy-dependent efficiency ratios.

2.2. Pile Oscillator Thermal Neutron Capture Cross Sections, *V. Pronyaev*

This work is motivated by a need for renormalization of pile-oscillator measurements. Pile- oscillator measurements were not included in the comparison of results from measurements of thermal-capture cross sections performed by different methods. These measurements of thermal Maxwellian spectrum-averaged capture cross sections were done mostly for natural elements in the 1950s and 1960s and the results show a large spread. The use of the original published data may lead to a strong bias in the evaluations. A comprehensive analysis of the data before the evaluation will require detailed consideration of the condition of the measurements, introducing possible corrections and renormalization to the latest standards. However, this is practically impossible for many of the 1950s era results.

VP shows a comparison of the ratio of Mughabghab's Adopted evaluated cross sections to the original pile-oscillator measurements. Results are presented for many cases with $Z < 85$ and show a statistically significant deviation from unity in many of these cases. The renormalization of the pile oscillator data was performed by Rick Firestone (RF) using a least-squares fitting procedure; the results from this procedure were written-up in an IAEA technical report [1]. The ratio plots used in this presentation were also taken from this report. VP shows the pile oscillator spread in data in comparison with spread of data measured by other methods relative to Mughabghab's evaluation:

- Pile Oscillation (for 53 datasets of the available 467);
- Activation (de Corte);
- Activation (Farina Arbocco);
- Prompt Gamma Activation Analysis;
- Time of Flight;
- Accelerator Mass Spectrometry.

VP then describes the method of pile oscillator data renormalization. The method of renormalization and data treatment is different from what is commonly used in the evaluation procedures. The common method includes the following options: renormalization of the data to the latest standards, introduction of corrections if needed, the increase of the outlaying data uncertainties or USU approach to outlaying data treatment. There is often very little information on the adopted standards and conditions of the measurements. The normalization coefficient *N* is the same for all pile oscillator cross sections of different elements published in one work/article. The value of *N* is obtained from an average over all reaction cross sections in a least-squares-adjustment to the Adopted values in the Mughabghab's evaluation. Normalized values given in column *"Average"* in Table 2 of Ref. [1] can be considered as a type of combined evaluation of pile oscillator results and Mughabghab's evaluation based on the results of all other measurement methods.

VP shows results of data renormalization for a few specific cases: Ag, ^{56}Fe, and ^{55}Mn. The renormalized values are shown in comparison to the pile oscillator cross sections prior to renormalization, whereupon significant differences can be seen in some cases.

The pile oscillator renormalization procedure eliminates some systematic deviations relative to the Adopted values of Mughabghab and the approach can generally correct outlying data by increasing associated uncertainties. The combined evaluation of the renormalized pile oscillator data together with Mughabghab's data or experimental data that contributes to Mughabghab's Adopted value may result in some instances of double counting the same experimental data in the evaluation. The pile oscillator renormalization covers 360 results documented in the report [1]. These data can be used as benchmarks for isotopic evaluations of thermal neutron capture cross sections obtained with different measurement methods.

RC suggests the analysis of the pile oscillator renormalization is a good starting point, but needs more investigation. RC also states that it is not always entirely clear how Mughabghab arrived at his Adopted values. David Brown (DB) replies that Mughabghab lists pile oscillator measurements when relevant and that such values would likely be taken into consideration. However, VP counters that it seems unlikely Mughabghab took these pile oscillator results into account, based on his experience from working with him. David Bernard (DBE) says at CEA they only show C/E values to validate evaluations (for actinides, absorbing or structural materials) and not thermal or epithermal cross sections (because of the Westcott *g*-factor uncertainties) DBE also asks about reactivity comparison to reference values. David Brown (DB) asks if it is possible to repeat some pile oscillator measurements and maybe attempt to tease out systematic errors that were never documented. Andrej Trkov (AT) replies that he is doubtful about new measurements being fielded due to a lack of experience in the field. RC suggests highlighting some discrepancies first rather than repeating well-known measurements. AT wants to know what the biggest outliers are; VP says he can provide a list. Boris Pritychenko (BP) mentions that many old results are presented without uncertainties. In EXFOR he suggests this number may be approximately 15% of the results. BP also asks if Rick Firestone (RF) considered data without uncertainties. RC responds that RF only used data with reported associated uncertainties. VP asks if there could be any additional pile oscillator reports available in the NNDC library. BP replies that it would take time to locate any such reports as they are not available online. RC will follow up to see what RF used, and also try and source any additional PDF documentation regarding pile oscillator reports.

2.3. Unfolding radiative capture γ-ray spectra to determine total capture cross section, *T. Belgya*

TB lists and describes the γ-ray sources used in efficiency and non-linearity calibrations of the Budapest PGAA facility:

- Certified calibration sources for absolute efficiencies: ^{241}Am, ^{133}Ba, ^{137}Cs, ^{214}Bi, ^{60}Co, ^{152}Eu, ^{22}Na, ^{226}Ra;
- Home made sources for improving shape: ^{110m}Ag, ^{57}Cd, ^{24}Na, ^{182}Ta and many more;
- Higher energy accelerator sources: ^{56}Co, ^{66}Ga;
- Prompt γ primary sources based on basic physic principles: H(n,γ), for high energy N(n,γ) up to 10.83 MeV;
- Secondary high-energy prompt γ sources calibrated with primary sources: Cl(n,γ), Cr(n,γ), S(n,γ), Ti(n,γ).

The simplest set of γ-ray sources to cover the region from the 50 keV to 10.8 MeV energy range: ^{241}Am, ^{152}Eu, ^{226}Ra, and N(n,γ) with the nitrogen target preferably in the form of Urea.

TB describes the γ-ray intensity balance method for the calibration reaction ^{14}N(n,γ)^{15}N. This method uses a χ^2-minimization to deduce an inverse efficiency. The intensities used in the intensity balance of the levels can also be normalized to cross sections provided internal conversion coefficients are also considered. TB shows four different efficiency curves and compares to earlier intensity results. To obtain these results the calibration source information was loaded into Hypermet-PC, but the nitrogen

data was changed in each case according to the appropriate ^{14}N(n,γ)^{15}N calibration data. TB suggests that new γ-ray intensity data from high-energy nitrogen sources influences PGAA measurements. TB shows cumulative energy-weighted intensity sum results for ^{27}Al(n,γ) obtained by using new intensities of the high-energy calibration standard. ZR points out that there may be some issues with efficiency calibrations at the Budapest PGAA facility. The calibration problems at the Budapest PGAA facility are highlighted and TB presents a list of several sources that are used for efficiency and non-linearity evaluation of the PGAA detector. From 2020 the Hyperlab routine is used; the 2023 evaluation also used Hypermet-PC. TB summarizes recommendations for N(n,γ) primary source data set usage: the new intensity dataset published by *"Belgya"* performs better in describing high-energy efficiencies (E_γ > 2 MeV); because two intensity datasets (*"Jurney"* and *"Belgya"*) were used the high-energy partial γ-ray cross section, and should be corrected; check the Cl and S secondary sources dependence on N data used for efficiency calibration. TB and ZR disagree on certain methods and practices for normalization of data. TB points out another problem with the detector system in that the BGO-suppression shield was not working well and needs to be sent away for service. The BGO problem is evident from prominent Ge(n,γ) lines in the capture-γ spectra; these lines are strongly suppressed in the corresponding spectra from earlier measurements.

The unfolding of γ-ray spectra is also described by TB. Here, TB explains the unfolded spectra can be useful for many applications including nuclear model calculations; development of photon strength function (PSF) models; γ-decay heat calculations of nuclear reactors; modeling origin of the elements in nuclear astrophysics; oil-well logging. Unfolding γ-ray spectra reveals useful quantities such as the average number of photons per fission ($\overline{M}_\gamma$) and the average total energy per fission ($E_{\gamma,\mathrm{tot}}$). From these two quantities, the mean photon energy can then be deduced as $\epsilon_\gamma = E_{\gamma,\mathrm{tot}}/\overline{M}_\gamma$. TB showed some examples of unfolded γ-ray spectra in comparison to different measurements and remarked that they agree well within uncertainties. The unfolded γ-ray spectrum is described as a measured γ-ray spectrum that is corrected for background, impurity, decay, random coincidences and finally corrected for the detector response function. A detector response function is the response of a detector for a mono-energetic γ-ray source which can be measured. Because there are only a limited number of such sources, Monte Carlo simulations are used to cover the entirety of the measured energy range. Spectra are presented showing results of Geant4 calculations used to simulate the detector response. Simple spectra were used to establish detector-parameter adjustments. Simulated high-statistics node spectra were also presented where the Oslo Method was used for interpolation. TB presents spectra illustrating the unfolding process step by step, using gold as an example: removal of background components followed by detector-response correction. The measured and unfolded γ-ray spectra for the ^{197}Au(n,γ)^{198}Au reaction are presented and compared. TB also shows the efficiency-corrected standardized spectrum for this reaction from which the corresponding set of partial γ-ray production cross sections can be deduced for this reaction. TB further explains and shows γ-ray multiplicity as a function of E_γ and cumulative energy-weighted cross section as a function of E_γ, including expressions for deduction of these quantities. To summarize, TB suggests the PGAA library should be revised for partial γ-ray production cross sections for transitions above 2 MeV, and the effect on changes to the efficiency calibration due to various dependencies needs to be studied further.

During questions, ZR mentions that he would like to combine Budapest and Garching measurements. Again, ZR reiterates that he will need help from a postdoctoral researcher in such an activity. RC asked about how best to characterize the continuum. TB responded by showing some simulated spectra cf. unfolded spectra paying attention to the continuum region.

2.4. Neutron direct capture, compilation of thermal capture values, and astrophysical neutron capture results, *Yi Xu*

YX's talk covers three topic areas:

1.) Calculation of neutron direct capture cross sections at thermal incident energies.
2.) (Re)-compilation of thermal neutron capture cross sections.
3.) Extension of neutron capture results towards astrophysical energies.

Two reaction mechanisms, the compound-nucleus reaction and the direct reaction, contribute to the total neutron-capture cross section. The compound-nucleus reaction is usually the important one and its cross section generally calculated with the Hauser-Feshbach model. For topic (1), YX developed a direct capture model based on the perturbation theory and suggests direct capture should be investigated systematically using this approach. The direct-capture code takes into account all electric dipole ($E1$), electric quadrupole ($E2$), magnetic dipole ($M1$) transitions. TB asked how the $E1$ and $M1$ matrix elements were calculated. YX uses a potential model to solve the Schrödinger Equation. Emanuel Chimanski (EC) comments that direct capture results from the overlapping of projectile wave functions with bound states in the $A + 1$ nucleus, and uncertainties in spectroscopic amplitudes can present significant challenges.

For verification of the model, YX compares his calculations with published direct-capture results for ^{122}Sn$(n,\gamma)^{123}$Sn and ^{132}Sn$(n,\gamma)^{133}$Sn for which there is good agreement. YX has performed a set of direct-capture calculations for 91 isotopes over 15 elements. YX first presents some results for ^{16,17,18}O and ^{19}F. Dave Brown (DB) says that the ^{17}O evaluation is not accurate and that all the resonances above the separation energy are included as if they are discrete states; this is true for ENDF, JEFF, and JENDL libraries. The whole evaluation is wrong according to DB. Roberto Capote (RC) comments that because ^{17}O is a minor isotope it is not necessarily a major concern. DB then says that the "screw-up" is in the fast region, but the thermal part is clearly messed up as well and comments that he cannot understand the thought-process behind the evaluation. Andrej Trkov (AT) suggests the background component could be included in File 3 of ENDF; RC responds it may not be straightforward and R-matrix calculations are needed. DB says with LRF=7 it is possible to handle direct capture properly. Ian Thompson (IT) is preparing some trial evaluations to take advantage of this, but it needs special MTs for capture to specific states. These MTs were not approved for ENDF/B-VIII.1. DB also mentions that we have a trial ^{207}Pb evaluation that exercises their MTs from Amanda Lewis (AL). This evaluation does not take advantage of LRF=7; GNDS already handles direct γ rays.

The results for direct neutron capture cross sections at thermal energies are next shown for the calcium isotopes. As before, YX breaks up and presents the direct and total neutron capture cross sections from Mughabghab's Atlas of Neutron Resonances and compares these values with the relevant ENDF library and the direct capture calculations. YX comments that there is good agreement between Mughabghab's Atlas (2018 version) and the present direct capture calculations for the closed-shell nucleus ^{40}Ca. In some other cases it may be worth considering parameter adjustment (neutron optical model and spectroscopic factor) to match the values in Mughabghab's Atlas. In the presentation of the chromium and manganese results, YX notes that the calculated direct capture cross section is significantly larger than the experimental data for ^{52}Cr and ^{54}Cr. RC suggests that the impact of direct capture is bigger near magic numbers due to shell-structure effects. The iron results presented generally show favourable comparisons. YX also presents calculated direct- capture cross-section results for cobalt, copper, nickel, zinc, zirconium, tin, tungsten, lead, and uranium isotopes. Boris Pritychenko (BP) suggests that Mughabghab would have used a simple analytical formalism to extract the direct-capture contribution from the total-capture cross section.

YX summarizes topic (1):

- For most nuclei, the preliminary direct capture results are reasonable, indicating that the direct capture is (and should be) lower than the total capture data from databases: ENDF, INDEN, JENDL, JEFF, etc.
- The five exceptions in this study are ^{41}Ca, ^{52}Cr, ^{54}Cr, ^{204}Pb, and ^{208}Pb, of which the calculated direct capture is larger than the total capture. Further analysis is needed.
- Relative approximate contribution from the direct capture (DIC) to the total capture:
  - DIC contribution < 10%: 38 in 91 studied nuclei
  - DIC contribution in 10 − 50%: 23 in 91 studied nuclei
  - DIC contribution in 50 − 90%: 19 in 91 studied nuclei
  - DIC contribution > 90%: 11 in 91 studied nuclei

- Comparison with the direct capture (treated as hard-sphere scattering) or background capture (direct capture + sub-threshold contribution) is compiled in Mughabghab (2018). In this Atlas, direct capture or background capture (at 0.0253 eV) are available for 55 nuclei among the 91 studied nuclei. For 50 of these 55 nuclei, the difference between the direct (or background) capture of the Atlas and the present direct capture is less than a factor of 10.

Regarding topic (2), YX has built a database of thermal neutron-capture cross sections including Westcott *g*-factors:

- Thermal neutron-capture data are extracted from EXFOR and recompiled.
- *g*-factor is included (taken from the latest version of database, perhaps use an average value in future?).
- Experimental method is presented.
- Pile oscillator data are NOT included.
- The database currently encompasses $Z = 1$ to $Z = 70$. The rest will be finished soon.

YX shows a representative portion of the database entries.

Regarding topic (3), extension of neutron-capture cross-section results into the astrophysical regime, YX suggests there is a need to develop a database providing neutron-capture data at astrophysical energies, similar to that of thermal capture. For astrophysical purposes, both experimental data and theoretical predictions are required. Existing sources of experimental data can be leveraged including the Bao2000 compilation, NETEGEN (ULB), and KADoNiS. YX mentions that KADoNiS only contains measured data and post-KADoNiS measured data are compiled from EXFOR and literature. BP advises against using KADoNiS because it is no longer being maintained and that there is an alternative new library developed at Frankfurt that should be considered instead: the ASTrophysical Rate and rAw data Library (ASTRAL). The ASTRAL library also only contains experimental data. Arjan Koning (AK) mentions that he uses KADoNiS with corrected gold standard and all values are reduced by around 5 − 6%, accordingly. For the theoretical predictions, YX suggests leveraging the TENDL-astro, BRUSLIB, and REACLIB libraries, for example.
YX further mentions that for the theoretical prediction, the key issue is to find the *"optimal"* nuclear structure inputs for the neutron-capture calculations. At present, the optimal sets of nuclear structure inputs are:

- Nuclear mass: AME2020 experimental masses and HFB-31 theoretical masses.
- Optical potential: Woods-Saxon or JLMB [2, 3].
- Level density: Constant-temperature or HFB combinatorial [4].
- Photon strength function:SMLO or D1M-QRPA [5].

YK presents MACS data at $kT = 30$ keV and explains how it can be used to verify and optimize nuclear structure inputs by finding the minimum of the f_{rms}:

$$f_{\mathrm{rms}} = \exp\left(\frac{1}{N_{\mathrm{expt}}}\sum_{i=1}^{N_{\mathrm{expt}}}\left(\ln\frac{\sigma_i^{\mathrm{calc}}(kT=30\ \mathrm{keV})}{\sigma_i^{\mathrm{expt}}(kT=30\ \mathrm{keV})}\right)^2\right)^{1/2}, \quad (1)$$

where N_{expt} is the number of experimental data points. Here, calculations with different structure inputs are compared with experimental compilations of Bao2000 and KADoNiS, and the optimal set of nuclear structure inputs with the minimum f_{rms} can be obtained.

2.5. A new open-source Python library for handling neutron-capture γ-ray data from EGAF, *A. Hurst*

This presentation by AH is comprised of two parts: (i) a short talk describing the original Evaluated Gamma-ray Activation File (EGAF) and its transition to a modern open-source library, pyEGAF; (ii) a software demonstration briefly exploring some of the features and capabilities of pyEGAF.

AH briefly overviews the EGAF library and the source data based on thermal (n,γ) measurements carried out at the Budapest Research Reactor and mentions where the library can be obtained. Next, AH explains the need for modernization of the library and provides a high-level overview of the pyEGAF project. This project is available on GitHub and can be obtained by cloning the repository:

```
git clone https://github.com/AaronMHurst/python_egaf.git
```

The project has also been deployed to the Python Package Index (PyPI) repository server and can be installed from there using:

```
pip install pyegaf
```

AH notes and refers to extensive documentation describing this work including the README (on GitHub), the DESCRIPTION (on PyPI), a corresponding reference article [6], and the supporting docstrings for all classes and methods of the pyEGAF library. The pyEGAF library is bundled with all 245 original ENSDF-formatted EGAF datasets along with RIPL and JSON translated versions of each dataset; 735 datasets in total. AH shows the translated representative JSON schema in comparison to the original ENSDF-formatted file using a snippet of the ^{28}Si$(n,\gamma)^{29}$Si file as an example. Additionally, AH shows a corresponding RIPL format for the same capture-γ dataset.

AH summarizes the *"talk"* part of the presentation by explaining where the source data is taken from: (n,γ) datasets from EGAF; S_n and S_p from AME2020; Adopted σ_0 values from the Atlas of Neutron Resonances (earlier editions from 1981 and 1984). The suite of Python modules that has been developed for this project are designed to interact with the JSON schema and the project comes shipped with over 200 unit tests and Jupyter Notebooks to help demonstrate the utility of pyEGAF. AH further mentions future work that he would like to carry out regarding this project including the incorporation of additional data into the existing EGAF library; principally, transition multipolarities and γ-ray mixing ratios that will allow for the determination and the inclusion of BrIcc-calculated internal conversion coefficients.

In the second part of the presentation, AH runs through some Jupyter Notebooks to give a flavour of the pyEGAF library and its utility in the analysis of thermal neutron-capture γ-ray data. These notebooks are available from the afore mentioned online repositories. Andrej Trkov (AT) called attention to be careful with the source of the total capture cross section values listed. He added that the total capture cross section displayed could come from a slightly different incident energy where $1/v$ scaling and g-factor corrections were employed. AT discussed the necessary corrections. RC mentioned that benchmarks tend to be very sensitive to capture due to their experimental setup. It was discussed to consider including the evaluated total capture cross section into pyEGAF, this would be consistent with ENDF library. AH agrees this could be done.

2.6. Epithermal neutron dosimetry, *A. Trkov*

JSI-CEA collaboration aims to find monitors sensitive to the epithermal energy range for cross-section validation in this region. This collaboration work (2017 − 2019) involves using (n,γ) reactions for epithermal neutron dosimetry using boron-based filters. AT notes that very few nuclear reactions are sensitive specifically to the epithermal range and there is a need for candidate reactions with strong resonances at high energies. The use of boron filters, e.g., BN, B_4C, $^{10}B_4C$, shifts the sensitivity to the epithermal energy regime and also suppresses the thermal peak. AT shows a plot illustrating the median energy of different monitors from a sensitivity study of profiles for IRDFF-II reactions. AT refers to a NIMA article [7] where a systematic study was conducted to identify candidate reactions suitable for

epithermal neutron dosimetry. These are mainly inelastic reactions but also some capture. AT lists several capture reactions that would be suitable for this purpose and mentions the criteria that must be satisfied for their consideration together with an observable energy shift under a BN filter:

- Suppression of the thermal part of the spectrum;
- Median energy shifts by 1 keV measurable via γ-ray spectroscopy;
- Suitable product (compound-nucleus) half life (a few minutes to a few days);
- Sufficiently high γ-ray emission probability;
- Solid sample material compatible with irradiation.

A few examples of different boron filters are presented, each having a different concentration of ^{10}B: BN (weakest); B_4C; $^{10}B_4C$ (strongest). All samples are measured in the same filter geometry; in the examples presented: filter height (closed) = 13 mm, filter diameter = 13 mm, cavity height = 5 mm, cavity diameter = 5 mm. AT mentions that using the same filter preserves the sample location under irradiation. The samples shown are from an experimental campaign performed in December 2018 with cutoff at progressively higher energies.

AT then presents some MCNP calculations (and fits) of filter transmission functions for each of the filters. The results show shifts to progressively higher energies for each filter: $^{10}B_4C > B_4C >$ BN. Validation and characterization of the calculated spectra (parametrization/fitting of the filter transmission functions) was accomplished using ^{197}Au(n,γ) and ^{238}U(n,γ) data.

AT presents the tabulated results from the work carried out on epithermal neutron dosimetry measurements for the three different boron filters. AT comments that the results related to IRDFF-II validation evidence encompassing measurements of Au, U, Mn, Th, and Na have already been published [8], while a paper is currently in preparation on results for new candidate reactions. Roberto Capote (RC) mentions that he wants the spectra. Tamas Belgya (TB) asks why the difference between measured and calculated spectra is so large for ^{64}Ni(n,γ). AT suggests it is due to lots of uncertainties (he will take a look at the paper). RC mentions that ^{197}Au and ^{238}U are used to define the flux and also mentions that he defines the epithermal region up to 10 keV. TB counters that he considers epithermal to be defined up to 200 keV. RC suggests the fast region is well-characterized from ^{252}Cf fission. AT mentions that ^{238}U data are in good agreement, but also notes that in general there is a lot of spread in results − some are in good agreement, other less so. AT announces that they will repeat some experiments since they have a well-characterized setup. AT also says with Cd they can pin down the resonance integral but warns that some definitions of resonance integral may differ, e.g., AT suggests that Mughabghab's Atlas uses a type of analytical definition that is inconsistent with his method. Boris Pritychenko (BP) disagrees with AT's definition of the resonance integral; BP suggests the definition used in the Atlas is a general definition. RC says we can disagree on definitions but not what is measured. AT then says only the first few resonances contribute and a cutoff needs to be defined. Furthermore, AT says that whenever the resonance integral is being used it needs to be defined how it is being used. RC says he would prefer not to discuss resonance integrals any further as it takes the focus away from the purpose of the meeting. RC does suggest, however, that we could consider another meeting to discuss this further. This is agreed upon. AT begins to wrap up proceedings and says he will provide the spectra based on new measurements in addition to a published paper. RC reiterates that he wants the spectra used for the calculation. AT mentions that ^{241}Am(n,γ) and ^{237}Np(n,γ) are the important reactions. For ratio measurements it is useful to include ^{197}Au(n,γ) and ^{238}U(n,γ). AT also proposes a generalized description of the Westcott g-factor as a ratio of the spectrum-averaged cross section up to 0.5 eV to the thermal cross section based on a numerical integration (compare to the standard definition involving the Maxwellian distribution); AT will provide a list of nuclides that have been measured.

2.7. Status of neutron capture gamma-ray production in translated ENDF/B-VIII.0 GNDS files and remediation actions, *E. Chimanski*

EC begins his presentation with a discussion of applications of neutron-capture γ-ray data, e.g., compact neutron sources for nondestructive assay and planetary nuclear γ-ray spectroscopy. Both capture γ rays and γ rays from inelastic neutron scattering play an important role in these applications. Although γ-ray production from the energy region of interest is expected to be dominated by $(n,n'\gamma)$, as neutrons downscatter (moderation) the capture-γ signal may ultimately play a significant role upon thermalization. EC displays a list of prioritized isotopes categorized by application and materials containing the isotopes (or elements) of interest.

EC explains that there are generally two different types of use cases for the evaluated γ-ray production libraries:

(i) *Traditional*. Single-detector applications that produce coarse binned spectra or high-resolution γ-ray spectroscopy allowing for identification of characteristic lines. For this use case we *just need to fix the evaluations.*

(ii) *Event-by-event*. Multiple-detector systems that record events in coincidence that enable projections of coincident-gated $\gamma-\gamma$ events that occur within a prompt time window. In this case we *need to re-think the API and decide what data should be stored, e.g., complete cascade information.*

We are reminded by EC that the γ-ray production data in ENDF is not perfect(!). Neutron-induced reactions need to be correctly modeled incorporating all experimental knowledge available. To help focus efforts EC has produced a gap analysis [9] to help identify some of the key deficiencies in the γ-ray data libraries. Here, EC has made a comparison of level schemes between ENDF, RIPL, and ENSDF, and compared primary γ rays in ENDF, ENSDF, and EGAF. EC emphasizes that there is no easy way to verify the capture-γ spectrum above thermal-incident neutron energies.

EC describes a triage of the data to help assess the γ-ray deficiencies in ENDF/B-VIII.0:

- 144 targets with no photon data for capture in ENDF;
- 11 with primary and discrete photons;
- 161 with only discrete photons − these could be either primary or secondary γ rays because they have not been flagged;
- Most isotopes in ENDF do not have flagged primary transitions separately but seem to include them all into the discrete type (or in the *"continuum"*).

EC further notes that the number of photons in ENDF is in overall good agreement with ENSDF up to $A = 80$ and between $150 \leq A \leq 210$ and shows plots to illustrate these points. Flagging gammas (primary or secondary) as appropriate will help fix some of the afore mentioned issues. EC also notes that not every isotope present in ENSDF is included in ENDF (ENDF prioritize applications and near stability). EC highlights some problems with the γ-ray spectra in ENDF by showing a few select examples:

- ^{31}P(n,γ): ENDF does not flag primaries or secondaries;
- ^{65}Cu(n,γ): Primaries have been included as part of the continuum; many secondaries are missing in ENDF and some have been misassigned;
- ^{197}Au(n,γ): ENDF only includes a continuum spectrum; there are no primaries and secondaries have been folded into the continuum;
- $^{230,232-240}$U(n,γ): ENDF is restricted to mostly continuum spectra for the U isotopes.

EC summarizes his observations of the ENDF/B-VIII.0 photon spectra and suggests that because some isotopes already have a *complete* γ-ray spectrum reported in ENSDF or EGAF we should include as much experimental information as possible and fill the gaps with simulated spectra where needed. This raises the question whether we need to decide what isotopes are considered to have a complete set of thermal-capture γ rays and which cases do we need to provide simulated spectra?

The issue of completeness is addressed by EC by comparison of primaries and ground-state feeding transitions with independent measurements of the [adopted] total thermal neutron-capture cross section (σ_0).

Plots showing the ratio of (i) summed primary γ-ray cross sections, or (ii) summed ground-state-feeding γ-ray cross sections to σ_0 help reveal completeness as well as gaps in the data:

- Ratios statistically consistent with 1 imply completeness;
- Ratios < 1 imply missing data;
- Ratios > 1 are not physical and implies a problem with either the partial γ-ray cross section data or σ_0 value.

This comparison is best performed using EGAF since it contains absolute partial γ-ray cross sections whereas ENSDF (and therefore, CapGam) only has relative intensities. EC presents a list classifying isotopes according to completeness and notes that some fixes will be easier than others, with some of the easy, i.e., complete isotopes suitable for *"copy and paste jobs"*. EC also mentions that we need to be careful with EGAF data for low abundance isotopes as there may be inaccuracies and suggests that ENSDF and EGAF need to be merged/reconciled to help improve overall completeness of libraries.
Next, EC describes the data processing chain to help understand the fixing strategy, essentially: ENDF library → processed file → simulation input. Simulations based on the ENDF-6 formatted library are restricted to singles γ-ray simulations, while inclusion of the representative GNDS library into the data processing workflow also allows for coincident $\gamma - \gamma$ simulations. Additionally, GNDS can be used to generate the ENDF-6 formatted library in the conventional workflow. EC explains ENDF currently has myriad ways to handle and store the γ data:

- *"Old way"*
  - MF12−Multiplicity; MF14−angular distributions; MF15−energy distributions (contin- uum);
  - Cannot correlate energy/angle (but no one uses this anyway);
  - Primary γ rays flagged in MF12; capture γ rays do not have a limit associated with 40 discrete low-lying levels;
  - Branching ratio table.
- *"New way"*
  - All γ-ray data stored in MF6;
  - Correlated energy-angle information;
  - Primary γ rays flagged in MF6 (but interpolation is painful for processing codes);
  - No branching ratios.

EC comments that we need the branching ratio information and GNDS provides a suitable solution since it can readily handle associated levels and branching ratios for all γ-ray transitions within a nucleus. Tamas Belgya (TB) asks about the handling of levels from different reactions. Roberto Capote (RC) suggests that *"all"* levels should be included. EC and Aaron Hurst (AH) comment that a reaction-specific set of levels may be a more useful way handling things when modeling said reaction. RC replies this may cause problems for coupled-channels calculation if there is inconsistency between the levels used.

EC briefly describes the use of pyEGAF in the analysis of capture-γ data and its utility for incorporation of experimental data into new libraries. EC also discusses a new formatting code, the GRIN-formatter, which can read RIPL files and JSON-formatted ENSDF datasets or DICE- BOX/RAINIER simulated cascade γ data with primaries taken from EGAF. RC comments that we should not be competing with a Hauser-Feshbach code. EC says this allows for storing of all the levels. RC replies this would make the file far too big, and it would be better just to use level density models, i.e., to treat the continuum in terms of the level density. EC presents results on ^{28}Si(n,γ) illustrating a well-balanced decay scheme and notes that the ENDF library is in good shape other than correctly labeling the currently unflagged primaries. EC mentions this fix is an example of low-hanging fruit and there are others that fall into this category. EC also shows how the calculation often breaks down if attempting to model the primaries with level density and photon strength function models rather than using experimental data. The modeled data compares poorly with the actual experimental data and EC notes that it best to use experimental data wherever possible and only model what is needed. EC also presents ^{16}O(n,γ) and ^{32}S(n,γ) as some further examples of *"treated"* datasets.

EC briefly describes the extrapolation from thermal-incident neutron energies to higher-incident neutron energies. Often, part of the spectrum follows the $1/v$ law as the capture cross section falls off rapidly with

higher-incident energies. EC summarizes a few of the isotopes currently being worked on.

EC notes there are similarities in γ-ray cascades observed in the same compound nucleus whether it is produced via (n,γ) or $(n,n'\gamma)$ and ponders two different approaches for rebuilding the cascade: (1) Assume each cascade in the continuum comprises two γ rays in total; or (2) Account for all γ rays in the continuum and, therefore, all associated levels and branching ratios. EC reports that approach number (1) is unrealistic and produces demonstrably poor results cf. ^{238}U(n,γ). Although approach number (2) works much better, as shown for ^{238}U(n,γ), RC is concerned that this approach is impractical owing to the excessively large file size that would be generated even for medium-mass nuclei.

EC points out that the Geant4 implementation of γ-ray emission from thermal (n,γ) is limited, e.g., Geant4 does not distinguish between primaries and secondaries even when the ENDF library does, there are no γ-ray correlations, energy is not conserved on an event-by-event basis, and these problems impact the γ-ray multiplicity. EC discusses the utilization of MCGIDI++, a component of the GIDI+ open-source software package, as an event generator within Geant4. This method enables the generation of cascades directly in a Geant4 simulation using GNDS files, thereby minimizing information loss due to file format translations and providing a more accurate event-by-event depiction of the underlying physics.

Finally, EC summarizes by emphasizing a need for additional independent measurements of capture cross sections as well as more partial cross sections in addition to EGAF. The RIPL-formatted EGAF decay schemes are being used to make evaluated level schemes from thermal neutron capture. Datasets from EGAF with complete sets of primaries and secondaries can be sourced and properly formatted into ENDF, when incomplete theory can be used to simulate the missing component of the decay scheme, e.g., the ^{32}S(n,γ) work that was presented. A NIMA article will be written to demonstrate the Geant4/G4LEND problems and highlight the impact and improvement of Geant4/MCGIDI. EC also points out that he is looking into machine-learning approaches for the prediction of primary γ rays but this work is at a preliminary stage.

2.8. ENDF/B-VIII.1β2 Library Nuclear Astrophysics Testing, *B. Pritychenko*

BP briefly describes the nuclear reaction data workflow, essentially: Experiment → Compilation (EXFOR) → Evaluation (ENDF) → Applications. BP mentions that ENDF contains evaluated (recommended) cross sections, spectra, angular distributions, fission product yields, thermal neutron scattering, and photoatomic and other data with an emphasis on neutron-induced reactions. The ENDF library evaluations are based on theoretical calculations normalized to experimental data with the exception of neutron resonance region, where priority is given to experimental data.

BP states that the ENDF/B-VIII.1 library is currently a work in process. BP also mentions that thermal cross section values have been Doppler broadened at T = 293.16 K in the ENDF/B-VIII.1 library.

BP comments that ENDF/B-VIII.1 and JENDL-5 often show significant differences between the libraries, e.g., there is a factor of almost 50 difference between the libraries for ^{240}U, and there is a similar situation between the calculated and measured capture cross section in ^{88}Zr. Recent measurements confirm the large thermal cross section in ^{88}Zr but disagree on the resonance integral. BP suggests that these cases highlight issues at thermal energies when no experimental data is available.

Next, BP describes the implementation of Westcott g-factors in ENDF/B-VIII.1β2. The Westcott g-factor, g_ω, is defined as the ratio of the Maxwellian averaged cross section to the 2200 ms^{-1} (thermal) cross section:

$$g_\omega = \frac{\sigma(\text{Maxw})}{\sigma(2200)} \qquad (2)$$

BP mentions that g_ω for ENDF/B-VIII.1β2, JEFF-3.3, JENDL-5, BROND-3.1, and CENDL-3.2 libraries have been calculated. Resonance integrals are also calculated and the analysis is in progress.

The ENDF/B-VIII.1β2 library will also contain calculated Maxwellian-averaged cross sections (MACS). BP explains how the MACS values are calculated. The ENDF/B-VIII.1β2 MACS (kT = 30 keV) data compare well with the [preferred] ASTRAL database:

https://exp-astro.de/astral/

BP shows a plot illustrating the good agreement between the MACS values from the ENDF/B- VIII.1β2 library and the ASTRAL database. BP explains that a recent re-analysis of the ^{197}Au standard cross section by the international evaluation of neutron cross-section standards revealed problems with systematic errors. This issue has been recognized leading to revised values based on the new standard, e.g., the KADoNiS database. The ENDF/B-VIII.1β2 MACS analysis has revealed several findings. The analysis of the ratios shows agreements in most cases and strong deviations in ^{13}C, ^{34,36}Ar, and ^{196}Hg,3and minor deviations in ^{40}Ca, ^{64}Ni, ^{120}Te, and ^{126,129}Xe cases. The analysis of the EXFOR database shows that there are no experimental data for ^{36,38}Ar and ^{126}Xe above the thermal region, and the observed differences are due to issues with theoretical modeling. For ^{129}Xe and ^{196}Hg, ASTRAL results are based on single measurements. In ^{40}Ca we need to consider three contradictory measurements and choices of ENDF and ASTRAL evaluators. BP also discusses stellar nucleosynthesis work using the ENDF/B-VIII.1β2 library.

In his outlook, BP announces that the ENDF/B library is the most comprehensive evalu- ated nuclear data library for applications developed by Cross Section Evaluation Working Group (CSEWG) and that the ENDF/B-VIII.1β2 library has great potential in nuclear astrophysics applications. Roberto Capote (RC) mentions that KADoNiS has problems because it is not always clear whether it is using experimental or calculated data. RC also asks whether all isotopes are present in the KADoNiS/ASTRAL databases and mentions that, as an example, ^{56}Fe is missing from one of the libraries.

2.9. Proposal for ENDF format − use MT=900-999 for primary gammas, *I. Thompson*

In collaboration with Sofia Quaglioni (SQ)

IT describes primary γ-ray production in 2-body kinematics and mentions that we need a way to distinguish between primary and secondary γ-ray production. We also need to establish correlations between coincident primary and secondary γ rays. IT also comments on ENDF format complications in that the MT=102 format must describe both primary and secondary γ rays. The primaries have energies that rise with incident projectile energy, while the secondaries have energies that are fixed and are independent of the projectile energy.

IT mentions that historically MT102 has traditionally been used in ENDF for capture reactions: 2-body reactions for particle products exist for light projectiles *n, p, d, t, h, a*, but not for gammas. MT102 is different from other summing channels MT4, MT103, MT104, MT105, MT106, and MT107 for *n, p, d, t, h* and *a*, respectively, as these can be the sum of 2-body channels. In this proposal it is suggested to adopt MT= 900-998 for the first 99 discrete primary γ rays and use MT= 999 as a continuum channel for any further primaries. IT proposed this convention at the MiniCSEWG meeting held at LLNL in April 2023. Backward compatibility needs to be demonstrated prior to adoption and this proposal will not be ready in time for the release of ENDF/B-VIII.1. However, this new system should still be useful for experimentalists, evaluators, and users of nuclear data.

A list of ENDF libraries for some light isotopes was presented by IT along with their associated primary γ-ray statistics. These light isotopes will have primaries added in via the GRIN project. All are candidates for conversion to MT= 900-999 to describe the primary γ rays. Consultant Meeting participants David Brown (DB), Emanuel Chimanski (EC), and Aaron Hurst (AH) are part of this effort.

Below are new MT definitions that are being suggested for adoption in the ENDF library for the description of all primary gammas in accordance with:

- MT900: Production of primary γ, leaving residual in the ground state;
- MT901: Production of primary γ, leaving residual in the 1st excited state;
- MT902: Production of primary γ, leaving residual in the 2nd excited state;
- …….
- MT998: Production of primary γ, leaving residual in the 98th excited state;
- MT999: Production of primary γ in the continuum not included in the above discrete representation.
- MT102: Radiative capture: production of one or more gammas (photons) plus a residual. Redundant: sum of MT=900-999, if they are present.

These definitions will need to be added to the ENDF-6 manual Appendix B. IT also recommends as a policy to reconstruct current MT= 102 with distributions, for backward compatibility.

The next question is how to specify the secondary gammas. IT suggests the following permutations:

1) By transition probability arrays with MF= 12 data (the preferred way perhaps).
2) Separately for each discrete MT channel (900-998).
3) In a continuum distribution for MT channels, MT999.

IT says that all primary gammas MT900-998 are 2-body channels and MT= 999 can be used in situations where primary channels are unknown or if data only gives a continuum. MT= 102 can now be derived from the new channels.

Adoption of this new system for describing primaries will require future updates to the processing and transport codes in order to handle the new MT numbers. It is noted that the processing software FUDGE will need to be developed to convert MT= 102 to MT= 900-998,999 using GNDS. Additionally, FUDGE will need to reconstruct MT102 from 900-999 for backward compatibility. Some testing has been done to this effect on ENDF/B-VIII.0 versions of n+^{6,7}Li,^{10,11}B,^{12}C. Demonstration files are available. Published ENDF evaluations can have both MT= 102 and MT= 900-999 as long as the policy is defined to avoid double counting cf. MT103-107 for charged particles. Roberto Capote (RC) comments that the discrete levels are ordered, but they are not necessarily all fed by primary gammas. We need to ensure internal consistency for all reactions.

In summary, IT suggests there will soon be an explicit description of primary capture-γ data from 2-body reaction channels. No change is needed for GNDS 2.0, only for the ENDF-6 format. A relativistic kinematic treatment is required. Resonance parameters should give a separate channel for each MT= 900-998. Reich-Moore *"absorption"* should no longer be used to give summed capture γ rays. Processing and transportation codes will need to be modified to handle the new MT numbers. If gamma-then-particle emission, particle resonance width has to be assumed zero (discrete) if MT=900-998, MT=999 is fine. For example, the ^{5}He resonance in $d + t \rightarrow \gamma + (^5\text{He} \rightarrow ^4\text{He} + n)$.

3. Discussion

3.1. Validation of prompt gammas

Roberto Capote (RC) leads a discussion on the validation of prompt γ-ray data. This discussion is centered on a recent publication in Radiation Physics and Chemistry, *"Measurement of prompt gamma production from neutron capture on manganese"* [10]. In this work a manganese bath is used for neutron calibration with a ^{252}Cf spontaneous fission source inside the Mn + H_2O bath. This setup is viewed by a shielded HPGe detector and stilbene scintillator to measure the γ leakage spectrum of the manganese bath. Pulse shape discrimination was used to distinguish γ and neutron events measured by the scintillator. RC mentions that in this experiment most of the capture events are due to thermal neutron capture from moderated neutrons. MCNP simulations of the experiment performed using the ENDF/B-VIII.0 and JEFF-3.3 libraries showed significantly discrepant results for the prompt γ production. RC states that strange artifacts were also identified in the libraries. INDEN updated data for γ production on ^{55}Mn was also tested and showed a significant improvement compared to the original ENDF/B-VIII.0 data. RC notes that the IAEA developed an evaluation of the γ production data for ^{55}Mn(n,γ) based on the prompt

γ-ray data in EGAF plus a continuum contribution from a statistical-model Hauser-Feshbach calculation using EMPIRE. An adjustment to the manganese prompt γ production tables based on the IAEA evaluation using the EGAF data shows much better agreement with the measurement. RC suggests that further improvements could be achieved through adjustments to other data sources, e.g., S and O data. Maurie-Laure (ML) is working on new benchmarks, but these are proprietary projects. RC asks about the normalization of the EGAF cross section data compared to the old ^{55}Mn(n,γ) data and presents an IAEA technical document showing the evaluation of prompt neutron-capture γ-ray data (INDC(NDS)-0810,2020). Emanuel Chimanski (EC) mentions that he is aware of this work and will provide some notes on it. It is further discussed that the application cannot be described by EGAF data alone and continuum data is also needed.

3.2. Final session

In the final session there is a short discussion concerning beam profiles at the Budapest Research Reactor and the FRM-II. It is mentioned that the peak flux of a cold beam will be downshifted with respect to a pure Maxwellian spectrum, e.g., at the FRM-II, the cold flux is around 4 times higher than the thermal flux. Is this the same for the Budapest Reactor when operating with the cold source? It is also mentioned that comparator measurements are best performed using a cold beam because at this temperature we are generally much further away from resonances and so Westcott g_ω-factor corrections are not usually required.

Next follows a fairly lengthy discussion on the g_ω-factor for ^{56}Fe(n,γ): 1.00 or 1.049(5); what is the origin of g_ω = 1.049(5)? Upon discussing the σ_0 value for ^{56}Fe(n,γ), Roberto Capote (RC) states that the *"best"* value should be around 2.57 b cf. Mughabghab's Atlas. However, Rick Firestone's (RF) paper on the thermal neutron capture cross section for ^{56}Fe(n,γ) [11] is somewhat at odds with this result giving a value σ_0 = 2.394(19) b. RF did not assume a g_ω-factor correction in his work. Although, there was additional speculation that this result may have been obtained assuming standardization using elemental cross sections. This could explain the discrepancy given the natural abundance of ^{56}Fe is 91.743%, thus, after *"correcting for abundance"* we would find $\sigma_0 = 2.394 \times (100.0/91.743) = 2.61$ b, which brings us back into much closer agreement with the adopted result. We will need to check with RF and confirm this result.

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APPENDIX: Deliverables

Summary of expected deliverables

I. Updated version of the PGAA ATLAS (end of 2024)

The database will contain the following information:

Elem	Z	E(gamma)	DE	Sigma	DSigma
H	1	2223.259	.001	3.33E-01	7.00E-04
H	1	6250.200	.100	4.92E-04	2.50E-05
LI	3	477.580	.040	1.55E-03	9.00E-05
LI	3	6769.500	.300	1.50E-03	1.20E-04
LI	3	7246.700	.300	2.40E-03	3.00E-04
LI	3	980.480	.040	4.10E-03	1.40E-04
LI	3	1051.810	.050	4.10E-03	1.20E-04
LI	3	2032.300	.020	3.87E-02	1.20E-03

The library will represent an update of the current file that contains ~31k lines for all elements ranging from H to U.
Cross sections are expected to be relative to the hydrogen capture cross section (or selected secondary standards – e.g., N, Cl, etc)
This database will be available online and will be described in a technical paper to be submitted to the J. Radioanal. Nucl. Chem.
The purpose of this database is to be used for analytical purposes.

Actions:
Use the HyperLabs Software - A new concept for gamma-ray spectrometry software (hlabsoft.com) to process about 600 16K measured PGAA spectra which should include background spectra.
Corresponding energy and efficiency calibrations will be provided.

- For that purpose the IAEA will hire a consultant with the goal to process those spectra and calculate the TPA as well as undertake the identification of the observed peaks.
  The consultant will work closely with experts Z. Revay and T. Belgya for training on spectrum processing and during the actual processing.
- Identification of single and DE peaks as well as of target impurities is needed to simplify the analysis.
- The IAEA will purchase one commercial version of the HyperLabs Software - A new concept for gamma-ray spectrometry software (hlabsoft.com)

II. New EGAF-II file derived from the updated PGAA ATLAS, split by isotopes and containing identified primary/secondary PG lines (end of 2025)

The journal for the publication of the new EGAF-II database is still to be determined.

- The updated gamma list should be consistent with latest adopted ENSDF level scheme for energies and intensities.
- There are going to be placement problems (not all peaks could be IDs).
- Check reconstructed thermal capture XS vs recommended.

III. Provide updated nglist_a.dat file with flagged primary transitions (January 2024 – A. Hurst)

- Check feasibility of listing ALL (adopted) ENSDF transitions to the GS;
- Check with EMPIRE the list of transitions that can be calculated for a few selected targets.

IV. Development of the code for ID of primary/secondary/isotopes and GS transitions using the adopted ENDSF scheme and the given new PGAA subset of peaks/intensities

- TB & ZR to release a preliminary "updated" peak list for two elements;
- AH to develop an algorithm to identify primary/secondary and GS transitions starting from adopted ENSDF evaluation using pyEGAF as the starting point;
- Could be transferred to a post-doc for posterior EGAF-II database creation.

V. Produce a comprehensive compilation of vetted thermal capture XS, document it in a paper to be submitted to ADNDT (to be published in November 2024)

Sources:

- Compilation of EXFOR measurements (excluding pile oscillation measurements) by Xu Yi. Data should be corrected to the latest monitor data.
- Compilation of pile oscillation measurements in the INDC(USA)-0109 by R. Firestone plus selected updates.
- Table 5.1 of the EGAF (IAEA technical report STI/PUB/1263) plus updated Rick's publications (W, Fe??, etc)
- Mughabghab latest compilation provided by BNL (D. Brown).
- K0 derived values provided by A. Trkov.
- Values adopted in R-matrix evaluations from existing Nuclear Data Libraries (JEFF,JENDL,ENDF/B, CENDL?).
- New data available (if any).

Annex 1

IAEA Consultancy Meeting on Thermal Capture and Gamma Emission

23 – 25 October 2023
IAEA, Vienna
MOE07 (virtual component)

ADOPTED AGENDA

Monday, 23 October (10:00 am – 6:00 pm, open 09:45 Vienna time)

10:00	**Opening of the meeting,** A. Koning / NDS Section Head **Election of Chair and Rapporteur(s), adoption of Agenda**	
	Welcome and introduction, R. Capote Noy / Scientific Secretary	
10:30	**Participants' Presentations** (~60' each w/ discussion)	
	Z. Revay	New standardization measurements for the upgraded PGAA spectroscopy database
	V. Pronyaev	Pile Oscillator Thermal Neutron Capture Cross Sections
Lunch Break		
	T. Belgya	Unfolding radiative capture γ-ray spectra to determine total capture cross section
	Y. Xu	Neutron direct capture, compilation of thermal capture values, and astrophysical neutron capture results
	A. Hurst	A new open-source Python library for handling neutron-capture γ-ray data from EGAF
	Discussion	*Coffee breaks as needed*

Tuesday, 24 October (10:00 am – 6:00 pm)

10:00	**Participants' Presentations** cont' (~60' each w/ discussion)	
	A.Trkov	Epithermal neutron dosimetry
	E. Chimanski	Status of neutron capture γ-ray production in translated ENDF-VIII.0 GNDS files and remediation actions
Lunch Break		
	B. Pritychenko (remote)	ENDF/B-VIII.1beta2 Library Nuclear Astrophysics Testing
	S. Quaglioni (remote)	Proposal for ENDF format: Use MT=900-999 for primary gammas
	Discussion	*Coffee breaks as needed*

19:00 Dinner at a restaurant (separate information)

Wednesday, 25 October (10:00 am – 5:00 pm)

10:00	**Technical discussions and drafting of the meeting summary report**
Lunch Break	
	Technical discussions and drafting of the meeting summary report cont'
	Closing of the meeting
	Coffee breaks as needed

Annex 2

IAEA Consultancy Meeting on Thermal Capture and Gamma Emission

23 – 25 October 2023
IAEA, Vienna

PARTICIPANTS

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