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THERMAL CAPTURE AND PROMPT CAPTURE GAMMA DATABASES

Summary Report of the IAEA Technical Meeting
IAEA Headquarters, Vienna, Austria
23 – 27 May 2022

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October 2023

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ABSTRACT

A summary is given of the IAEA Technical Meeting on Thermal Capture and Prompt Capture Gamma Databases. The program to compile and evaluate thermal capture cross sections is discussed. An update of the prompt gamma activation database EGAF is planned. Technical discussions and the resulting work plan are summarized, along with planned actions.

October 2023

Contents

1. Introduction

A Technical Meeting (TM) on Thermal Capture and Prompt Capture Gamma Databases was organised at the IAEA in Vienna on 23-27 May 2022, devoted to neutron thermal capture and prompt gamma activation analysis data. Roberto Capote, who served as Scientific Secretary, defined the goals of the meeting: i) to review the status of thermal capture cross sections and move toward producing a recommended set of IAEA values, ii) to discuss the update of the IAEA EGAF database. He also highlighted the needs of PGAA data for planet and prompt gamma spectrometry, geology, nuclear security, archeology, etc.

The technical meeting was held at the IAEA HQ in Vienna and attended by ten international experts. The meeting was opened by Arjan Koning, Section Head of NDS. R. Firestone (Massachusetts General Hospital, Boston, USA) was elected Chairman of the meeting, and B. Prytichenko (BNL, USA) and D. Rochman (PSI, Switzerland) agreed to act as rapporteurs. The adopted Agenda is attached as Appendix 1, as well as the list of participants and their affiliations (Appendix 2). Links to participants' presentations are given in Appendix 3.

2. Presentation Summaries

2.1. Calibrations for prompt gamma activation analysis (PGAA) and ways of neutron cross section measurements, T. Belgya

After an outline of the basic principles of the Prompt Gamma Activation Analysis (PGAA), the efficiency and energy calibrations of the PGAA experimental facility placed at about 35 m from the core of the Budapest Research Reactor was presented. The cold neutrons are guided with a so-called curved super-mirror neutron guide to the sample. The curving helps to reduce the high energy direct neutron and gamma radiation to obtain very-low background for the measuring system. At the PGAA station a Compton and lead-shielded HPGe detector measures the energy and intensity of the γ-rays deexciting the cold neutron irradiated sample's nuclei, which is used to determine the average elemental composition of the sample. γ-ray production cross section σ_γ can also be determined relative to a monitor isotope. Recalibration of the intensities in the spectrum to σ_γ makes it possible to determine the γ-ray neutron capture cross section σ_0 for ${}^{1}/_{v}$ nuclei. Five different ways to calculate σ_γ will be presented. Results for simple and complicated decay-scheme nuclei will be shown to demonstrate the capabilities of the method.

<u>Discussion:</u>

Neutron capture or (n,γ) - PGAA. Thermal neutrons, so kinetic energy is negligible compared to the binding energy of a nucleus. Discussion on instrumentation, system shielding, characterization and calibration. Russian made 10 MW research reactor in Budapest. Cold flux is 10^8 n/cm^2/sec thermal equivalent. The thermal neutron flux is 10^{14} n/cm^2/sec in the core. PGAA activation station, 23% HPGe at the NIPS and 27% HPGe at the PGAA stations. Detector efficiency calibration: ε=R/AP, R measured rate, A neutron capture rate, P emission probability. The average absolute efficiency is 0.2% at 100 keV, mostly because of geometry. They mostly use relative efficiency. Linear energy calibration is corrected for non-linearity. Cross-over transitions are the problem (two gammas are interpreted as one, true and random coincidences): relatively low count rates help. True coincidences are below 0.1%. The comparator method is used to measure partial γ-ray production cross sections for 1/v samples. For nuclei with 1/v cross section, the shape of the flux energy dependence does not count because it reduces to neutron number in the integral of average cross section (it applies to mostly light elements because the heavier ones may have resonances at low energy which can change the 1/v dependence). From γ-ray production cross sections it is possible to estimate the total capture cross section. As examples of Fe cross sections are shown in the neutron capture Atlas which presents high uncertainties. In experiments on CERN's highly enriched samples brought to Budapest by Frank Gunsing, we measured the $^{54}Fe(n,\gamma)$ reaction which was shown as an example. Significant improvement of the total cross section uncertainties was achieved using the crossing intensity sums (CIS) of the complete decay scheme constructed by Rick Firestone from the Budapest data. After proper renormalization of the intensities to partial gamma-ray production cross sections the CIS values give the total capture cross section. If the CIS values are giving the same constant, then the decay scheme is well balanced. Another example was shown for the $^{27}Al(n,\gamma)^{28}Al(\beta^-)$ cumulative energy-weighted intensity sum that gives the same total capture cross section as it comes out from the 1778 keV gamma ray production cross section. New efficiency deviates from the Jurney's measurements by 5% at high energy. Another method for calculation of the total capture cross section can be made using the response function corrected radiation capture spectrum. For demonstration calculation results are presented for the $^{197}Au(n,\gamma)^{198}Au$ reaction. Response function capture corrected spectra for $^{113}Cd(n,\gamma)^{114}Cd$: calculated and measured, multiple transition contributions. Importance of Photon Strength Functions.

2.2. Spectroscopy database for prompt gamma activation analysis, Z. Revay

Please see presentation (Appendix 3).

Discussion:
Prompt Gamma activation analysis is very linear, peak area/efficiency and time (for a given energy). Partial gamma-ray production cross section: $\sigma_\gamma = P_\gamma$ * theta* sigma. 1969-1970: MIT, 1981 Lone table (cross sections * relative intensity), 1993 IAEA-Lone table, 1995 Tuli database.
Determination of Partial cross section - relative method. A1/e1/A2/e2 = n1*sigma1/n2*sigma2. Relative efficiency: A/(eff*t)=a*Pg. For low-energy neutrons (s wave), the angular distribution is isotropic, relative method works. Comparator earlier – Cl, now hydrogen. Relative method is insensitive to systematic errors, uncertainties cancel out. 20 MW reactor in Budapest, 2*10**14 n/cm2/sec. Neutron guides are not very good, flux is low. Pure slow neutrons. Compton supressed HPGe, background is reduced by a factor of 10. Cold neutron flux went up from 2.5*10**6 to 1.5*10**8 n/cm2/sec from 1997 to 2009; background went from 3 to 10 cps. 20 MW in Garching, 10**15 n/cm2/sec, it is 95% enriched U while Budapest is low enriched. 1997-1998 establishment of PGAA data library. 2002-2004 Handbook and Atlas [1], 2012-2021 new measurements for the library, 2021 updated library. Calibration issues: efficiency, non-linearity, peak shape, … efficiency curve 30 keV-11 MeV. Is it possible to link this database to the decay database. Measurements of elements in Budapest across the periodic table. TECDOC in 2007 [2], 2004 Handbook of PGAA. Atlas and catalog: 100 lines/element. Samples of light elements: D2O (92%), …. A few elements are still missing Cs, Tl, …. Data Library is in an Excel file: a) Li, Be, C, O, F, Cr, Co, Ru, Ce, Pr, Nd; b) Sm,Gd,Tb,Er,Yb,Ta(digi), Ta(book), W, Re, Tl. Final goal is a chemical analysis. Evaluation with Hyperlab. Sensitivity to elements is within a few percents. Differences in new and old measurements/Mughabghab could be as large as 100%.

References:

[1] See: https://www-nds.iaea.org/ngatlas2/
[2] Database of Prompt Gamma Rays from Slow Neutron Capture for Elemental Analysis, Report STI/PUB/1263, IAEA, Vienna (2007), see: https://www.iaea.org/publications/7030/database-of-prompt-gamma-rays-from-slow-neutron-capture-for-elemental-analysis

2.3. What is the real cross section (k_0) value of Na-24? A case study, Z. Revay

Please see presentation (Appendix 3).

2.4. Thermal capture cross sections for evaluated libraries: selection, validation and recommendation, D. Rochman

Please see presentation (Appendix 3).

Discussion:

Capture cross sections are deduced from resonance parameters. Roberto clarified that cross sections are not deduced from resonance parameters, they are rather related to resonance integrals. Arjan took over for ^{151,152}Sm. Order of adoption of thermal cross sections: Kayzero [1], Mugh2018 [2], Sukhoruchkin [3], Mugh2006 [4], RIPL [5], KADONIS [6], EXFOR [7]. Andrej pointed out that SIGMA1 should be run for thermal cross sections. Remarks on libraries comparison, k0, … How are we using this information??? Andrej is using k0 to validate cs because k0 are measured well. Andrej has an EXCEL file of the k0 database and ENSDF emission probabilities. Franz derived cs using updated emission probabilities. 8,892 isotopes of interest.

References:

[1] See: http://www.kayzero.com/

[2] S.F. Mughabghab, Atlas of Neutron Resonances, 6th Edition, 2018.

[3] S.I. Sukhoruchkin, Z.N. Soroko, Low Energy Neutron Physics - Tables of Neutron Resonance Parameters (H. Schopper, Ed.), 2004.

[4] S.F. Mughabghab, Atlas of Neutron Resonances, 5th Edition, 2006.

[5] R. Capote, et al, Nucl. Data Sheets **110** / Issue 12 (2009) 3107.
see: https://www.sciencedirect.com/science/article/pii/S0090375209000994?via%3Dihub

[6] See: https://exp-astro.de/kadonis1.0/

[7] N. Otuka, et al., Nucl. Data Sheets **120** (2014) 272.
see: https://www.sciencedirect.com/science/article/pii/S0090375214005171?via%3Dihub

2.5. Atlas of Neutron Resonances: Status of the Atlas, D. Brown

An update on the status of the Atlas of Neutron Resonances (a.k.a. *Atlas*) was provided, the comprehensive compilation of neutron resonance parameters and properties. The *Atlas*, which is a direct descendent of the famous BNL-325 series of "Barn Books", had been maintained by Dr. Said Mughabghab from the 1970s until his passing in the summer of 2018. Sadly, Dr. Mughabghab passed away mere months after the publication of the 2018 edition of the Atlas of Neutron Resonances. After Dr. Mughabghab had passed away, preservation of the *Atlas* fell to a small team of scientists at the National Nuclear Data Center who, with a small army of students, sought to further develop the *Atlas* and the set of software tools that are used to generate the *Atlas* documents. Six products of these student projects are outlined in the following:

1. Documented the *Atlas* electronic file format, released in a lab report (BNL-212201-2019-INRE), available from OSTI.gov.
2. Developed a simple pythonic API to simplify working with the *Atlas* electronic files. Using this, D. Brown was able to extract the thermal capture cross section data from the *Atlas* as a simple to use JSON file or as text output. These files were shared with the participants of the Technical Meeting.
3. With the API, students identified and corrected over 239 typos.
4. Building on IAEA Memo 4C-3/401 (3 May 2016), the NNDC attempted to match *Atlas* bibliography to EXFOR/NSR. This is still work in progress.
5. Developed a more statistically robust, mathematically sound and well documented approach to extract mean resonance spacings and capture widths. Although "rough edges" remain in the analysis, some striking observations were already apparent.
6. Developed a machine learning approach to reclassify the L and J assignments of resonances, with impressive success rates using *Atlas* and generated test data.

The NNDC will continue cleaning up the *Atlas* and are developing a long-term stewardship plan to continue the *Atlas* compilation effort. This plan potentially includes open sourcing the electronic files and python API and/or joining the *Atlas* compilation work to the Evaluated Nuclear Structure Data File (ENSDF) project.

Discussion:
Three essential readings: Atlas, JEFF-18, Lane & Thomas. Donald Hughes (1915-1960). BNL-325 (1955). Said Mughabghab passed away in 2018. Atlas has many issues like resonance parameters given using different R-matrix formalisms (e.g., Multi-level Breit-Wigner vs. Reich-Moore) vs. actual R-matrix. Students discovered 239 typos. Methodology used by Said not documented. Average widths and spacings can be extracted from empirical cumulative distributions. How to fit a distribution of delta functions? Problems with degrees of freedom may indicate issues with Reich-Moore and Hauser-Feshbach. Attempts to correlate degrees of freedom with energies. Study of spacings and capture widths. Brookhaven resonance reclassifier. Machine learning to reclassify the resonances. Questions about Atlas instrumentation by Pronyaev. Dave says that not all Said's results are reproducible. Dave does not understand the origin of Said's thermal cross sections.

2.6. Deconstructing the photon strength, R. Firestone

Please see presentation (Appendix 3).

Discussion:
Capture gamma contribute to photon strength (proportional to level density times populated by E1).
New level density model, fitted on the CT level density model (CT-JPI): fit level with the same spin and parity, and leads to the same temperature, +/- 5%, up to 10 MeV.
Extract D0 from the CT-JPI model.
Compared to RIPL, results are generally consistent.
Valid up to spin 6.
Photon strength function: at the GDR, the strength function is not simply an increase of a gamma-strength.
Shell gap: increase in level density, leading to the GDR; no collectivity effect.
GDR cross section is proportional to the increase of level density mass.
The GDR is completely described to first order as a function of A and beta2 (deformation).
Created a gamma-ray strength database (n,γ).
Conclusion: Spin-dependent level densities were obtained, g-ray strengths determined up to 30 MeV from the CT-JPI level density model

Discussion on Pile oscillation measurements. Rick renormalized these original data with new standards [1], and 90% of the time, the new data agreed with the Atlas [2].

This Rick report + the atlas + PGAA + k_0 + Sukhoruckhin + exfor (exfor table) is the base for our recommendation. Then we can use evaluated libraries for cross checking.
Question: element and isotopes, what to do?

References:

[1] R.B. Firestone, IAEA Report INDC(USA)-109, Oct 2021,
see: https://nds.iaea.org/publications/indc/indc-usa-0109/
[2] S.F. Mughabghab, Atlas of Neutron Resonances, 6th Edition, 2018.

2.7. Analysis of observed distributions of the measured thermal neutron capture cross-sections, V. Pronyaev, S.A. Badikov

The origins of large differences observed in the measurements of thermal neutron capture cross sections for isotopes were presented and discussed based on different measurement methods: activation, prompt gamma analysis, time of flight and accelerator mass spectrometry. The pile oscillation method was not considered because extremely old standards were used for mostly natural element measurements. Without consideration of clear outlaying data, often without assigned experimental uncertainties given, the maximal spread of the measurements done by these four methods is in the range of 3.5% and the average difference is 1.5%. This leads to the conclusion that depending on the nuclides there is a preferred method. The activation method can only be applied to nuclei with ground and metastable states, which have radiation decay characteristics convenient for the measurements. The PGAA method is preferable for light nuclides with A < 40, where practically all gamma transitions can be observed. The TOF method can be applied to all stable or long-lived nuclides in ground or metastable state but requires the appropriate (difficult) normalization. The AMS method can be used for measurements of very low capture cross sections, which are difficult to measure by other methods, but only on a few (AMS) nuclides.

Few simple one-parametric statistical models, which evaluate the uncertainties of cross sections or their ratios considering the distribution of the results were employed. The results of evaluations using these models have shown that the uncertainties of measurements are often strongly underestimated. The assigned uncertainties of many activation and PGAA measurements are less than 1%. An estimate with simple models predicts that the unrecognized source of uncertainties may contribute an average of 2 – 4% uncertainty in activation measurements.

Discussion:

Analysis of observed (n,γ) thermal cross section.

1st part: CRP on PGAA , 2006. Conclusion: differences with the Atlas (report from 2003).

Study based on activation, prompt gamma, TOF, AMS.

Activation: two sets de Corte and Farina Arbocco: good agreement.

Example of ^{9}Be(n,γ), ^{23}Na(n,γ): some time dependence, ^{54}Fe(n,γ) (AMS uncertainty 4-5%); ^{108}Pd, ^{139}La, ^{209}Bi, ^{210m}Bi, ^{235}U.

Detail on ^{23}Na(n,γ) PGAA: 2 groups of data 487 vs. 504 mb. For (n,tot), 519 mb, or 524, or 541 mb.

Consistency between all methods: histogram of comparison: data within +/- 11% for 245 data, with many additional outliers.

USU: 4-6 % (unknown sources of uncertainties).

Conclusion: average spread of data introduced by different methods of measurements can be roughly estimated to be 1.3%.

2nd part: Development of a statistical model for consistency between measurements and the Atlas.

Example for ^{23}Na: re-evaluated (n,γ); same for ^{139}La.

Proposed an estimation of Arbocco uncertainties (originally 1.4%, and increased to 5 %) and De Corte (higher than 1, changed to 2.9%).

Discussion: The method does not consider the experimental uncertainties. It produced uncertainties from statistical distributions. Certainly, USU are there. How large is USU?

2.8. The use of the ENDF library for stellar nucleosynthesis and applied studies, B. Pritychenko

On August 17, 2017, two gravitational wave detection stations in Washington and Louisiana, USA, observed a strong signal that was not seen at the third station in Italy. Using this information scientists were able to find the exact position in the sky where the neutron stars' merger (GW170817) took place. For the first time in the history of science, the astrophysical site of the r- or rapid neutron

capture process was found and observed. This discovery generated tremendous enthusiasm in a broad scientific community and triggered a reanalysis of the existing models and underlying data.
Traditionally, the nuclear astrophysics models used neutron capture Maxwellian-averaged cross-sections (MACS) from KADoNiS (Karsluhe Astrophysical Database of Nucleosynthesis in Stars). Approximately 65% of the KADoNiS MACS values were produced using a single measurement of the ^{197}Au(n,gamma) cross-section in Karlsruhe. A recent reanalysis of gold cross sections by the International Evaluation of Neutron Cross Sections Standards project at the IAEA demonstrated that the Karlsruhe gold measurements are 5-7% lower than world data imply. The IAEA project results were incorporated in the latest release of the ENDF/B-VIII.0 library in 2018.
These developments created a unique opportunity to apply the ENDF/B-VIII.0 data to nuclear astrophysics modeling. The neutron library was Doppler broadened to reconstruct the resonance region of energies that are of interest to nuclear astrophysics, and MACS and astrophysical reaction rates were calculated. The obtained MACS were used to deduce the solar system r-process abundances using a classical model. The obtained results agreed well with the previous findings of Arnold et al. and Arlandini et al. The same model was applied to process the KADoNIs data and 20-30% deviations in r-process abundances were found. The ENDF/B-VIII.0 astrophysical reaction rates were used to produce the reliable REACLIB fits in the 0.01-10 GK range of temperatures.
The current work found potential deficiencies in ^{138}Ba and ^{140}Ce neutron capture cross-sections and the strong need for ^{198}Au evaluation in the ENDF/B-VIII.0 library. The present collection of codes and gained knowledge will be used to estimate thermal neutron cross sections and resonance integrals from the world's collection of evaluated libraries.

Discussion:
ENDF for Astro and applied studies;
Astrophysics, prediction of abundancy;
ENDF for r-process calculations;
MACS Au-197 differs between Kadonis and B80 = standard (582+/- 9 vs 620 +/- 11 mb). Kadonis is not correct. New Kadonis: 612 +/- 6 mb (due to Cu backing and spectrum);
Benford's law.

2.9. Some comments on compilation of thermal capture data, Y. Xu

The potential model is used for the direct reaction contribution to the neutron capture reaction. The allowed electric dipole (E1), electric quadrupole (E2) and magnetic dipole (M1) transitions are considered. The nuclear structure ingredients involved in the calculation are determined from experimental data whenever available, and if not, from global microscopic nuclear models. A systematic study for about 6400 nuclei with Z in the ranges from 8 to 102 (lying between the proton and neutron drip lines) shows that the direct capture cross section is proportional to the number of levels available below the neutron threshold and decreases with decreasing neutron separation energies. The potential model is shown to provide a fair agreement between the predicted radiative neutron capture cross section and the experimental data as well as the previous calculations for the targets in a wide range of mass. The E2 and M1 components are usually negligible with respect to the E1 contribution, but they can dominate the direct capture rate for about several hundred nuclei.
Furthermore, the direct capture model is specifically used for thermal neutron capture and neutron capture data evaluation. For some isotopes (e.g., Fe-56 and Ba-137), the direct capture cross sections at the thermal energy compiled in the Atlas2018 are well reproduced by the model. In particular, the ^{138}Ba(n,γ) calculated thermal cross section is 355 mb, which is very close to 375 in Mugh2018 [1]. However, this case is the best agreement among several cases. The direct capture model is expected to provide the neutron direct capture cross sections for nuclear data evaluated files, which is particularly useful to define the background contribution in R-matrix analyses of measured yields for nuclear data evaluation.

Additionally, a comprehensive compilation of experimental thermal neutron capture data is proposed, which can be considered in future evaluations. A compilation of the experimental neutron capture Maxwellian averaged cross sections (MACS) in the energy range of astrophysics interest is ongoing.

Discussion:
Three topics were suggested:

(1) Neutron Direct Capture at Thermal Energies
Direct capture was not systematically investigated down to the thermal energy range, so we propose to calculate the neutron direct capture cross sections down to the thermal energy range for some important elements. For the first round, we consider O, F, Ca, Mn, Fe, Co, Ni, Cu, Zn, Sn, Pb, and U. Meanwhile, the direct capture computer code was updated and extended to adopt the nucleon direct capture (ELI-NP, Romania) based on the perturbation theory, including all the electric dipole, electric quadrupole and magnetic dipole contributions. This computer code can be used to perform the calculations where various nuclear ingredients are required. In particular, the spectroscopic factors should be carefully selected. The calculations shall be finished in 2023, and a paper is in preparation.

(2) (Re-)compilation of Thermal Neutron Capture Data
The experimental thermal neutron capture cross sections are (re-)compiled. The main sources are EXFOR and new publications that have not been included in EXFOR yet. Evaluated data in EXFOR should be discarded as well as pile oscillation data already used by Firestone in his compilation (INDC(USA)-0….) The g-factor is compiled. The experimental method is compiled. This will be done for all available targets in EXFOR, and should be finished in 2023.

(3) Possible Compilation/Evaluation of Nuclear Astrophysics Data
The possible compilation of neutron capture in the astrophysical energy range is proposed. The starting point is the compilation of MACS at kT = 25, 30 keV. The data source includes EXFOR, Bao2000, and the results compiled in NETGEN and its updates. We should stress the differences between the ongoing compilation versus the NETGEN or Kadonis compilations. A further consideration would be the calculation of MACS for the nuclei of which the experimental MACS is not available, which is planned for 2024. This needs the well-determined nuclear ingredients.

There are also a few other open questions.
Vivian: For the study of the determination of nuclear ingredients (here the neutron optical model potential), how about the comparison between the results deduced from the neural network method and the conventional fitting results? Y. XU: From our studies, the answer is that, the results obtained from the two methods are quite close to each other.
Andrej suggested to add direct capture calculations to ENDF with a faked MT number. Y. XU: Agreed. We shall discuss the technical details.

References:
[1] S.F. Mughabghab, Atlas of Neutron Resonances, 6th Edition, 2018.

2.10. Gaps and inconsistency in ND for MSR applications, D. Roubtsov

D. Roubtsov (Canadian Nuclear Laboratories, Canada) delivered a presentation titled “Gaps and Inconsistency in ND for MSR applications: Notes on Thermal Data for Thermal Scattering Laws”. The developers of thermal scattering data ($S(\alpha,\beta)$ data) use the thermal elastic cross sections σ_s for normalization of $S(\alpha,\beta)$ and the thermal radiative capture cross sections σ_γ to calculate the total cross sections as a function of the incident neutron energy E in the thermal energy region, $\sigma_t(E)$. The sources of these data (thermal cross sections and their uncertainties) are the evaluated nuclear data (ND) libraries, Atlas of Neutron Resonances by S.F. Mughabghab (shorted as Atlas), and nuclear data compilations used by different Neutron Optics (NO) groups. For many nuclides, the consistency in the evaluated $\sigma_\gamma \pm \Delta\sigma_\gamma$ among the different ND libraries, different Atlas editions, and NO data is reasonable/acceptable, and the differences can be traced back to the original publications and EXFOR data records. However, the consistency in the evaluation of $\sigma_s \pm \Delta\sigma_s$ together with the asymptotic behaviour of $\sigma_s(E)$ at $E \rightarrow 0$ ($T = 0$ K) is worse in comparison with $\sigma_\gamma \pm \Delta\sigma_\gamma$ and $\sigma_\gamma(E)$ (at $E \rightarrow 0$), and the origin of the differences is more difficult to trace back. For a few nuclides important for the Molten Salt Reactor development, D. Roubtsov demonstrated the differences in σ_s and good consistency in σ_γ. In particular, the following nuclides were discussed in detail: ^{6}Li, ^{7}Li, ^{23}Na, K, and C. For future studies, it was proposed to estimate and compare the sensitivity coefficients of the neutron multiplication factor (k_{eff}) to the thermal cross sections σ_s and σ_γ in modeling of the thermal critical assemblies with significant amount of ^{7}Li, ^{23}Na, and K.

Discussion*:*
Notes on Thermal Data for Thermal Scattering Laws.
^{7}LiOH is used for providing pH balance in PWR coolants with boric acid used for excess reactivity control. In MSR, LiF=^{7}LiF with ^{7}Li enrichment, say, >99.95%.
Sodium, NaF. Sodium is more like a scatterer at thermal energy. Danila evaluated data himself, new numbers agree with Atlas [1], JEFF-3.3 matches, JENDL is not, issues with ENDF/B-VIII.0. Potassium, KF in MSR. Mostly, 39,41K isotopes. In thermal spectrum, potassium is a neutron absorber. Danila evaluated potassium himself, and added more data compared to Atlas ((n,α) and (n,p) thermal reactions). Moderators in MSR: Graphite in MSR. Fine grains, ultra-fine graphite, isostatic graphite. Liquid moderator is proposed: D_2O, NaOH, … to avoid problems with graphite. Notes on C: to introduce isotopes and get rid of natural carbon.

References:
[1] S.F. Mughabghab, Atlas of Neutron Resonances, 6th Edition, 2018.

2.11. On the use of reaction rate measurements in filtered neutron beams, A. Trkov

Please see presentation (Appendix 3).

Discussion*:*
Difficult to determine the neutron spectrum in the epithermal region, no monitors. Shift the energy to the epithermal with a Boron filter. Filtered neutron spectra with targets inside Boron boxes. Use boron of different thickness and composition: BN, B4C and enriched B4C used at the TRIGA reactor.
Develop new monitors. CEA-JSI collaboration, Boron Nitride filters, obtained BC and enriched boron (BN, B_4C,$^{10}B_4C$). ^{94,96}Zr(n,γ) cs with resonances. Use boron filters to measure reaction rates in natural zirconium. Measured vs. calculated reaction rates in ^{94}Zr:

Filter	E_median [eV]	Ratio	Diff. from meas. [%]
$^{10}B_4C$	2000	4.6447	-24.4
B_4C	100	3.8731	-19.6
BN	20	3.7015	-19.7

Analysis suggests a 25% decrease in the epithermal capture cross sections.

Irradiation of ^{94}Zr (1st resonance in the few keV range), in combination with ^{96}Zr. The goal is to see the deviation from 1/v from the reactor spectrum.
Perform MCNP and analytical expression for the filtered neutron beam.
Calculated ratio is smaller than measured: need to increase the RRR by 25%. Is that reasonable for ^{94}Zr for the first resonance?

3. Additional Discussions

Start with prompt gamma activation analysis (PGAA): Partial gamma-ray production cross sections for analytical purpose. PGAA is going to be selected, the best gamma-rays for analytical purpose. A revision of what was done before. The previous database contains 6,000 gamma lines.

How to define the full spectra?? The IAEA will provide additional funding or find someone to process. If we want to put spectra in evaluated file, we need spectra of that element.

Spectra for comparison purposes. The first priority are monoisotopic elements because they are directly usable. Full list of peaks, the deconvoluted spectra (peaks + continumum). Issue the list of facilities: Munich, Budapest, Rez, NIST (difficult), WSU (PNNL), KAERI, Malaysia, Vietnam, … Discussion on Schlumberger presentation in CSEWG 2019: modeling gamma-rays for oil and space exploration. How to represent the data and store the multiplicity and normalize to one. Andrej Trkov placed the whole spectrum in File 6 for manganese, a document was published. Can we adopt the measured spectra instead of the EMPIRE calculations?

Maxw *λ**2 = Gw corrected for spectrum.
Andrej Trkov: Calculate temperature dependent Westcott factors for various libraries (ENDF/B-VIII.0, JENDL-5.0, JEFF-3.3, TENDL). Using spectrum from Zolt Revay. Reactor spectra exist in IRDFF+Budapest+Munich, spectrum depends on particular irradiation channel. PGAA chapter closed.

Maxwellian spectrum: g factor =(Mawx sigma)/sigma.
Non-Maxwellian Cold neutron Reactor spectrum: g factor = (Non-Maxw sigma)/ sigma.

4. Recommendations

4.1. Prompt Gamma Activation Analysis

The continuity of such facilities is recommended (neutron guide: Budapest, Munich, NIST JAERI (to be checked)).

Number 1: Z. Revay will provide the database of partial gamma ray production cross sections for analytical applications (not comprehensive, selected, not enough to extract a cross section) based on measurements at the Munich reactor. The database will be released together with the publication submitted to the peer-reviewed journal (e.g., Atomic Data and Nuclear Data Tables). New table: subset or corrected compared to 2004 version (6000 lines, no complete decay schemes, or single individual transition).

Number 2: full prompt gamma activation analysis (PGAA) list of peaks (Z.Revay & T. Belgya).
Need to be in a shape for an evaluated file.
Need to process the raw data (is it possible? Provide raw and processed data?)

In the shape of cross sections (it exists: complete spectra were analysed)
This list of peaks is comprehensive, with the background removed. No continuum is provided. This second list includes the first one (number 1). New peaks will be provided.
Below Ca and including Pb: Rick offers to provide gamma-rays: mostly complete decay scheme. Two sets: comprehensive (Budapest) and gamma lines (almost) complete (Rick). See the comment further down below about Ca.

Number 3: Finally, for monoisotopic elements (something close to what goes in the file, for instance for elements mentioned by Marie Laure Mauberg from Schlumberger – H, Cl, Si, K, Fe, Ca, Ti, Al, S, Mg):

provide the deconvoluted spectra (peaks plus continuum). This is possible for data which is not Compton suppressed.

Note: These spectra are available for selected cases only (most of available comprehensive spectra are Compton suppressed). Depending on the benchmarks, we may ask for further measurements of these spectra (T. Belgya). MnSo4 and FeSo4 measurements have been already undertaken at Rez, CZ [1-4].

Need to know what has to go into the ENDF file, be careful with the format.
The main difference between B68 and B80 is the measured data vs calculated gamma (empire). So, for the future: put the EGAF data plus a calculated background.
This is only for thermal. For higher energy, we can use calculated spectra.
Formatting issues to be done: description.

Full energy peak (unfolded spectrum); convoluted spectra, multiplicity, normalized to 1.
Complete information, and test combination number 2 and 3, how this performs in different applications. What is the impact of the continuum?
Z. Revay offers to repeat for the most important isotopes with suppressed and not suppressed Compton measurements, to help understand the background.
In the case of minor isotopes: it is difficult to assign gamma lines to the main one (eg Cd113), or to another isotope (from the experimental processing).

Number 4: Rick: evaluation of the prompt gamma data leading to “Photon strength for (n,g) as a function of multipolarity”, across many isotopes. May provide PGAA thermal cross section for element lighter than Ca and a few other ones, including isomers.

Number 5: Z. Revay: do we need Westcott generalized G factors? For instance for Sm?
We provide the g-factor for a specific library, or if a spectra is provided by Budapest (cold neutrons), the g-factor can also be calculated.
We need the spectrum from Budapest and Munich, and then the g-factors can be calculated at the IAEA.
B. Pritychenko offered to calculate the g-factor temperature dependent from various libraries.

^{197}Au is the most important case where the correction from the g-factor is needed. Z. Revay was presenting a PGAA value to be corrected for the experimental spectrum to understand consistency with the neutron standard.
R. Firestone: proposed to deliver gamma ray in coincidence with resonance (higher than thermal neutron energies), measured by TOF, in the 70s.

4.2. Thermal (n,g) cross sections at room temperature

What source to consider?
Two requirements: traceable to original values AND updated to the current standards.
Important: avoid repetition (e.g., double counting from EXFOR and k0 for instance).

Consistency checks:
- Evaluated elemental cross section (derived from isotopic data) should agree with elemental cross section.
- Evaluated thermal capture cross section should be consistent with measured (evaluated from ToF) total cross section data AND elastic cross section (e.g., from neutron optics).

Total cross section could be derived from evaluated libraries (assuming that evaluations considered are all transmission data).

1st class (for direct evaluation)

- Neutron activation data: we use only k0, Excel table from A. Trkov, might differ from the published k0 values (Nudat-2.6 could be checked in the table).
  Assessment of systematic uncertainty of K0 is required.
- Beyond k0, (neutron activation with gamma production) limited review of activation measurements to retrieve additional information (e.g., in EXFOR) on a case by case basis. The IAEA will take care of this review.
- PGAA thermal capture. Previous CRP report as a source "Database of prompt gamma rays from slow neutron capture for elemental analysis" STI/PUB/1263, 2007 (pages 59-74: tables of cross sections). These values will be updated by Z. Revay by the end of 2022 (Z. Revay).
- Pile oscillation data: Rick report [5] with corrections, for element and some isotopes. Firestone checked the original publications.
- What is left from EXFOR: unsorted source of experimental information, can be repeated in other sources.

Resonance Tables from Koning were extracted from EXFOR [6] and could be used to check EXFOR completeness (do not use Mughabghab 2006 [7] values compiled in EXFOR (no experimental data)). Do not use derived data.

Check experimental data used in Atlas (as provided by Dave Brown) vs our sources to find potentially missing or repeated references/corrections.

2nd class (for comparison with the outcome of the 1st class)

- Atlas 2006 [7], 2018 [8], Sukhoruchkin [9], compilation by J. Kopecky [10].

References:

[1] T. Czakoj, M. Koštal, et al., Nucl. Eng. Technology **54** (2022) 3824.
[2] T. Czakoj, M. Koštal, et al., Radiat. Phys. Chem. **202** (2023) 110542.
[3] T. Czakoj, M. Koštal, et al., EPJ Web of Conferences **253** (2021) 04014.
[4] T. Czakoj, M. Koštal, et al., Radiat. Prot. Dosimetry **198** (2022) 698.
[5] R.B. Firestone, IAEA Report INDC(USA)-109, Oct 2021,
see: https://nds.iaea.org/publications/indc/indc-usa-0109/
[6] A. Koning, D. Rochman, Resonancetables-1.0, IAEA(NDS)-234, 2020
See: https://www-nds.iaea.org/publications/nds/iaea-nds-0234/
[7] S.F. Mughabghab, Atlas of Neutron Resonances, 5th Edition, 2006.
[8] S.F. Mughabghab, Atlas of Neutron Resonances, 6th Edition, 2018.
[9] S.I. Sukhoruchkin, Z.N. Soroko, Low Energy Neutron Physics - Tables of Neutron Resonance Parameters (H. Schopper, Ed.), 2004.
[10] See: https://www-nds.iaea.org/RIPL-1/gamma/recommended/kopecky_dat.htm

Appendix 1

IAEA Technical Meeting on Thermal Capture and Resonance Integral Data

23 – 27 May 2022
IAEA, Vienna

ADOPTED AGENDA

Monday, 23 May (10:00 am – 5:30 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)	
	T. Belgya	Calibrations for prompt gamma activation analysis (PGAA) and ways of neutron cross section measurements
	Z. Revay	Spectroscopy database for prompt gamma activation analysis
Lunch Break		
	D. Rochman	Thermal capture cross sections for evaluated libraries: selection, validation and recommendation
	D. Brown	Atlas of Neutron Resonances: Status of the Atlas
	Discussion	

Tuesday, 24 May (10:00 am – 5:30 pm)

10:00	**Participants' Presentations** cont' (60' each w/ discussion)	
	R. Firestone	Deconstructing the photon strength
	V. Proniaev, S.A. Badikov	Analysis of observed distributions of the measured thermal neutron capture cross-sections
Lunch Break		
	B. Pritychenko	The use of the ENDF library for stellar nucleosynthesis and applied studies
	A. Trkov	On the use of reaction rate measurements in filtered neutron beams
	D. Roubtsov	Gaps and inconsistency in ND for MSR applications
	Y. Xu	Some comments on compilation of thermal capture data
	Discussion	

Wednesday, 25 May (10:00 am – 5:30 pm)

10:00	**Technical discussions and recommendations on thermal capture cross sections**
Lunch Break	
	Technical discussions and recommendations on thermal capture cross sections (cont')

19:30 Dinner at a restaurant (separate information)

Thursday, 26 May (10:00 am – 5:30 pm)

10:00	**Technical discussions and recommendations on PGAA**
Lunch Break	
	Drafting of the meeting summary report

Friday, 27 May (10:00 am – 3:00 pm)

10:00	**Drafting of the meeting summary report**
	Closing of the meeting

Appendix 2

IAEA Technical Meeting on Thermal Capture and Resonance Integral Data

23 – 27 May 2022
IAEA, Vienna

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Appendix 3

Presentations

#	Author	Title	Link
1	T. Belgya	Calibrations for prompt gamma activation analysis (PGAA) and ways of neutron cross section measurements	PDF
2	D. Brown	Status of the Atlas	PDF
3	R. Firestone	Deconstructing the Photon Strength	PDF
4	B. Pritychenko	The use of the ENDF library for stellar nucleosynthesis and applied studies	PDF
5	V. Pronyaev	Analysis of observed distributions of the measured thermal neutroncapture cross-sections	PDF
6	Zs. Revay	What is the real cross section (k_0) value of Na-24?	PDF
7	Zs. Revay	Spectroscopy database for PGAA	PDF
8	D. Rochman	Thermal capture cross sections for evaluated libraries: selection, validation and recommendation	PDF
9	D. Roubtsov	Gaps and Inconsistency in ND for MSR applications	PDF
10		Some useful references of neutron optics methods, data, etc.	PDF
11	A. Trkov	On the Use of Reaction Rate measurements in Filtered neutron beams	PDF
12	Y. Xu	Neutron capture and nuclear astrophysical data	PDF

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