INDC International Nuclear Data Committee

NEUTRON DATA STANDARDS
Summary Report of the IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria
18 – 21 October 2022

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Vienna, Austria

August 2023

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ABSTRACT
A Technical Meeting on Neutron Data Standards was held from 18 to 21 October 2022 with the objective to review recent work and facilitate the coordination of work towards the next release of the Neutron Data Standards. The topics discussed included the review of data of recent experimental campaigns, ongoing evaluation work, the proposal of cross section integrals as references, improvements of evaluation methodology as well as ongoing code developments. 27 participants from eight Member States took part in the meeting. A list of recommendations and actions was issued to coordinate the next steps.

August 2023
Contents

1. INTRODUCTION .............................................................................................................................................. 7

2. PRESENTATION SUMMARIES ......................................................................................................................... 7

   2.1. Searches for structure in the n-p total scattering cross section, A.D. Carlson (NIST, USA) .......... 7

   2.2. Recent R-matrix work at Los Alamos on the light-element standard cross sections, G. Hale, M.W. Paris (LANL, USA) ........................................................................................................ 8

   2.3. Toward maximization of synergy between experiment and R-matrix theory - Recent works with the AMUR code, S. Kunieda (JAEA, Japan) .............................................................. 8

   2.4. Measuring the $^{235}$U(n,f)/$^6$Li(n,t) cross section ratio measurement in the NIFFTE fission TPC, M. Anastasiou (LLNL, USA) ......................................................................................................... 9

   2.5. Proposal of improving the $^{10}$B neutron standards, I. Duran (USC, Spain) ................................. 9

   2.6. Measurement of the cross section of $^{235}$U(n,f) induced by high-energy neutrons relative to n-p elastic scattering performed at the n_TOF facility at CERN, A. Manna (INFN, Italy). 13

   2.7. $^{235}$U, $^{238}$U neutron capture at thermal and sub-thermal neutron energies, A. Walther (HZDR, Germany) ........................................................................................................................................ 14

   2.8. Extending the integral references for ToF (n,tot) and (n,g) measurements in fission targets reactions and its relations with the Standard Thermal Neutron Constants, I. Duran (USC, Spain). 16

   2.9. About USU treatment in gmapy, Georg Schnabel (IAEA) ................................................................. 21

   2.10. Impact of SACS measurements on the standards evaluations, R. Capote (IAEA) ...................... 22

   2.11. Gmapy developments, G. Schnabel (IAEA) ....................................................................................... 22

   2.12. What can be improved in the new update of the Standards?, V. Pronyaev ................................. 23

   2.13. Test of nuclear-data evaluation for $^{239}$Pu(n,f) and $^{238}$U(n,f) cross sections using G-HyND, H. Iwamoto (JAEA, Japan) ........................................................................................................ 25

   2.14. Fission cross section measurement of $^{232}$Th, $^{235}$U and $^{238}$U relative to n-p scattering at CSNS Back-n, Y. Chen (IHEP, China) ...................................................................................................... 25

   2.15. High accuracy, high resolution $^{235}$U(n,f) cross section from n_TOF (CERN) from 18 meV to 170 keV, S. Amaducci (INFN, Italy) ................................................................. 25

   2.16. Recovering Mannhart's $^{252}$Cf(sf) PFNS evaluation, Denise Neudecker, et al. ......................... 26

3. RECOMMENDATIONS ........................................... 27

   3.1. Measurement campaigns ........................................... 27

   3.2. Evaluation work ......................................................... 27

   3.3. Extension of GMApy and the GMA database ......................................................... 27

4. ACTIONS ......................................................................................................................................................... 28

   4.1. Experimental data ......................................................... 28

   4.2. Evaluation methodology and uncertainty quantification ......................................................... 28

   4.3. Code development ......................................................... 28

APPENDIX I: ADOPTED AGENDA .................................................................................................................... 29

APPENDIX II: PARTICIPANTS ......................................................................................................................... 31

APPENDIX III: PRESENTATION LINKS ........................................................................................................... 33
1. INTRODUCTION

Arjan Koning, the Head of the IAEA Nuclear Data Section, opened this meeting on the topic of the Neutron Data Standards and welcomed all participants. Afterwards, Roberto Capote, co-host of the meeting, elaborated on essential topics that need to be addressed within this meeting in order to determine necessary activities for the preparation of the next release of the Standards, such as the consideration of SACS measurements as an ingredient in the Standards evaluation process and the treatment of Unrecognized Sources of Uncertainty (USU). Georg Schnabel, who served as the IAEA meeting host, briefly went through the proposed agenda. He asked participants for their consent to record the meeting to help with the preparation of the meeting report; the consent was given unanimously.

Allan Carlson was appointed Chair of the meeting and Denise Neudecker agreed to act as rapporteur.

The hybrid meeting took place 18-21 October 2022 and was attended by 27 participants (7 in-person, 20 remote) from eight member states, with daily convening times 2pm to 6pm CET. The adopted agenda can be found in Appendix I, the participants’ list in Appendix II and links to participants’ presentations in Appendix III.

2. PRESENTATION SUMMARIES

Summaries of participants’ presentations are given below, including their most important statements and conclusions. Full versions of the individual presentations are available in Appendix III of this report.

2.1. Searches for structure in the n-p total scattering cross section, A.D. Carlson (NIST, USA)

In 1969, Hrehuss and Czibok [1] analyzed several hydrogen total cross section data sets. Their work indicated to them that there is structure in the cross section. This led to an NBS linac measurement by Schwartz, et al. [2]. They found there is no apparent structure in the cross section. They investigated the publication by Hrehuss and Czibok and found they had used several total cross-section sets, but emphasized the Nereson and Darden data [3]. They assumed that data had been obtained with uncertainties of 0.5% to 1%, but they had been obtained with 10% uncertainty, so only the appearance of structure was observed.

More recently (2005), an apparent problem with hydrogen scattering was observed. Chatzidimitriou-Dreismann, et al. [4] saw an apparent drop in that cross section of about 40% in the eV energy region [4]. Moreh, et al. [5] then made measurements at RPI indicating the effect is not there [5]. They noted that the previous work had neglected the effect of the neutron attenuation in the relatively thick samples, thus possibly creating an artificial anomaly.

References:
2.2. Recent R-matrix work at Los Alamos on the light-element standard cross sections, G. Hale, M.W. Paris (LANL, USA)

We summarized the progress of R-matrix analyses for the \(^7\)Li and \(^{13}\)C systems using the EDA code at Los Alamos. The \(^7\)Li analysis includes 6 channels, and data for 9 different reactions at energies corresponding to incident neutrons up to 8 MeV. More than 6500 data points are being fitted with a chi-squared per degree of freedom of 1.65, although the analysis has not yet reached a true minimum (zero-gradient point) of the \(\chi^2\) surface. The main point was to show how well the present analysis agrees with the differential cross section measurements of Bai et al. [1] for the \(^6\)Li(n,t)\(^4\)He reaction at energies between 1 eV and 3 MeV. These data indicate the presence of negative-parity resonances above about 1.8 MeV that affect the values of the integrated cross section at lower energies in the standards range.

Recent work on reactions in the \(^{13}\)C system includes new measurements of elastic and inelastic n+\(^{12}\)C differential cross sections by Ramirez (Vanhoy) et al. [2] up to 7 MeV incident neutron energy. The agreement with these data is quite good and required increasing \(l_{\text{max}}\) in the n+\(^{12}\)C*(2\(^+\)) channel from 1 to 3. Overall, the fit to more than 8100 data points in the analysis has a chi-squared per degree of freedom of 1.48.

The status of other light-element standards was reviewed, including the need for additional work on n-p scattering up to 200 MeV, and a new analysis for the \(^{11}\)B system that includes new experimental data for the n+\(^{10}\)B, and possibly for the \(\alpha +.^3\)Li, reactions at energies up to a few MeV.

References:

2.3. Toward maximization of synergy between experiment and R-matrix theory - Recent works with the AMUR code, S. Kunieda (JAEA, Japan)

The AMUR code [1] is a multi-channel/multi-level R-matrix analysis code which is based on the formalism of Wigner and Eisenbud [2], except for the radiative capture reaction that is based on the Reich-Moore approximation [3]. The code is able to search resonance parameter values and the covariance matrix with the Kalman filtering method [4].

In an effort to simulate experimental conditions, the code was extended to enable the calculation of angular distributions of cross-sections with the energy resolution of the incident particles. This new option was applied to the evaluation of neutron cross-section on \(^{19}\)F in a resolved resonance range for JENDL-5 [5]. He emphasized that the new evaluation gives better results on the neutronics simulation than those reached with the previous library. It was essentially because the angular distribution of the elastic and in-elastic scattering cross-sections was estimated by taking into account the feature of resonant reaction. He suggested that such an approach could be useful for a more elaborate evaluation of light-nuclei in the neutron standards. He also proposed a new method for describing the non-resonant process in the R-matrix theory that is associated with additional background poles which are exclusively given to the incident particles. This approach may be relevant for the simultaneous analysis of different reactions, which share the same compound nuclei.

References:
2.4. Measuring the $^{235}\text{U}(n,f)/^{6}\text{Li}(n,t)$ cross section ratio measurement in the NIFFTE fission TPC, M. Anastasiou (LLNL, USA)

Neutron-induced fission cross sections are typically measured as ratios, relative to a well-known cross section standard. The $^{235}\text{U}(n,f)$ is a well measured standard, often used as a reference on cross section ratio measurements of other actinides. However, some light particle reactions are also well-known and their use as reference can provide information to remove shared systematic uncertainties that are present in an actinide-only ratio measurement. The NIFFTE collaboration’s fission time projection chamber (fissionTPC) is a charged particle tracker designed for precision measurements of neutron-induced fission reactions. Detailed 3D track reconstruction of the reaction products enables evaluation of systematic effects and corresponding uncertainties which are less directly accessible by other measurement techniques. A recent measurement of the $^{235}\text{U}(n,f)$ using as a reference the light-ion standard $^{6}\text{Li}(n,t)$ reaction was conducted with the fissionTPC at the Los Alamos Neutron Science Center. Preliminary data of the $^{235}\text{U}(n,f)/^{6}\text{Li}(n,t)$ measurement were presented, focusing on the identification of the $^{6}\text{Li}(n,t)$-reaction events in the fissionTPC, and on the newly developed anode timing method for neutron time of flight determination. Analysis on the correction factors (selection efficiency, wraparound, etc) included in the cross section ratio calculation is still on-going, before reporting on the final $^{235}\text{U}(n,f)/^{6}\text{Li}(n,t)$ cross section ratio result.

LLNL-ABS-842272: This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

2.5. Proposal of improving the $^{10}\text{B}$ neutron standards, I. Duran (USC, Spain)

The evaluation accuracy of any nuclear-reaction cross section relies on the quality of the experimental datasets being analyzed. But the quality of the experimental datasets ultimately relies on the precision of the standards used as reference.

Historically, the principal international nuclear standards were a few constants at thermal point (in the TNC table). However, these TNC including (n,f), (n,g) and (n,el) reactions cannot be directly measured with the required low uncertainty. These thermal values are strongly correlated with each other and the consideration of an additional USU (Unknown Systematic Uncertainty) is beneficial to make the statistical analysis with GMA more robust. Big improvements have been made in the last decade, after the IAEA launched an international project for the “Maintenance of the Neutron Cross Standards”, adopting from ENDF/B an upgraded version of the GMAP code. The TNC set has a special treatment in the R-matrix procedure together with the specific neutron cross sections of light elements (H, $^{4}\text{Li}$ and $^{10}\text{B}$), so that the final uncertainties of the whole matrix rely on their accuracy.

New inputs are needed to increase the quality of this international effort and one of the most sensitive points is the standard value at thermal point of the $^{10}\text{B}(n,\alpha)$ reaction.

Allan Carlson, in his article in Metrologia [1], said:

“Using the standard it is not necessary to make a direct measurement of the neutron fluence. However, then it is necessary to measure the standards very accurately since any measurement relative to a standard is limited in accuracy to that of the standard.”

“An idealized standard should have the following characteristics:

- It should be possible to use the nuclide in elemental form, be chemically inert and not radioactive.
• It should be easy to fabricate into various shapes.
• It should be readily available; not expensive.
• It should have few (or no) other channels that could cause interference with the reaction of interest.

….

• Monotopes are preferred.

….

• In the standards energy region, the cross section should be large with a minimal amount of structure.”

$^{10}$B+n reactions fulfil these requirements! Moreover:

- $^{10}$B(n,α) is standard from 25.3 meV to 1 MeV.
- Its cross section shape follows perfectly the $1/\nu$ law up to at least 5 eV so we can use its mathematical parametrisation:

$$\sigma(\nu) = \sigma_0 \cdot (\nu / 0.0253)^{-0.5}$$

and its exact integral in the thermal energy region (20 to 60 meV) is easily obtained:

$$I = \sigma_0 \cdot (0.06^{0.5} - 0.02^{0.5}) / (0.0253^{0.5} \cdot 0.5)$$

The standard $^{10}$B(n,α) thermal value in NDS18 [1] is 3844(31) b and so the integral I is 127.1(1.0) b·eV. These uncertainties in the Standards are dominated by USU (0.8%), which is relatively high if one considers that we are looking for a primary standard. In any case, the $^{10}$B(n,α) thermal value is tightly tied to the $^{235}$U(n,f) value in such a way that any improvement in the $^{10}$B(n,α) accuracy will produce a decrease of the TNCs’ associated uncertainties.

$^{10}$B+n reactions at thermal and epithermal energies show only three channels: one is the elastic scattering, and the other two are neutron capture followed by either an alpha emission or the emission of an alpha and a gamma.

These two alpha channels can be evaluated as one single reaction – $^{10}$B(n,α) – as their Q-values are close to each other (2.70 and 2.31 MeV respectively) so that the detection efficiency of both alphas is very similar. On the other hand, the elastic channel cross section is very low (around 2.2(0.5) b), and hence does not interfere with the alphas’ channels.

Concerning the effect of impurities in the sample, their only effect at these energies should be in the (n,el) channel, which can be considered as negligible.

Moreover, natural boron is composed of two isotopes: $^{10}$B (19.9%) and $^{11}$B(80.1%). The $^{11}$B total cross section is dominated by the (n,el) one of 5.1(2) b and without any contribution to the alpha channels. This means that for an accurate measurement the samples must be enriched in $^{10}$B, but also that the knowledge of final concentration of $^{11}$B does not notably limit the experiment accuracy.

All in all, the correction by the different elastic channels in a (n,tot) measurement should contribute with less than about 7(3) b, leading to an uncertainty component at the thermal point below 0.08% when the (n,α) cross section is obtained by subtracting the (n,el) from the (n,tot) cross section.

Considering these aspects of the $^{10}$B+n reactions, a transmission experiment can help to reduce the uncertainty of the $^{10}$B(n,α) cross section in the thermal range. Moreover, the total cross section in the thermal range is large and its shape perfectly known without any significant deviation from the $1/\nu$ law up to around 20 eV. I am therefore proposing to adopt $^{10}$B(n,tot) in the thermal region as reference, because it is very close to Allan Carlson’s definition of an “idealized standard”, and such a transmission experiment should provide an absolute measurement that can be done at several facilities all around the world. My suggestion is for the IAEA NDS group to promote an international inter-comparison.
campaign for absolute measurements the $^{10}$B(n,tot) cross section in the thermal range. Obviously, performing experiments at different facilities will lead to a better knowledge of systematic errors, thus reducing USU.

The scheme of a possible $^{10}$B(n,tot) experimental setup for an international inter-comparison campaign for measuring the $^{10}$B(n,tot) cross section in the thermal range (Fig 1) should include a filter box with capacity for several $^{10}$B foils – in order to allow measuring the beam attenuation for several sample thicknesses as well as to make the in-beam boron mass more uniformly distributed – and a flux monitor that could be either a Si detector with $^{10}$B to detect (n,$\alpha$), a Li-glass detector or any other kind of high-efficiency ionization chamber. Both the samples and the beam monitor would have to cover the whole beam profile.

Every detector to be used as beam monitor has its own detection efficiency, $\varepsilon$, which is known with a certain uncertainty, but the impact of this source of uncertainty can be eliminated by doing relative-attenuation measurements as described in the following.

In the thin-sample approximation, for any sample thickness, $x$, the initial neutron flux, $\Phi$, is attenuated:

$$\Phi' = \Phi \cdot \exp[-\mu \cdot x]$$

with the attenuation coefficient being: $\mu = \sigma_t \cdot \rho \cdot N_A / A$,
where $\sigma_t$ is the $^{10}$B(n,tot) cross section, $\rho$ is the density, $A$ the mass number, and $N_A$ the Avogadro’s number (multiplied by $10^{-28}$ to get $\sigma_t$ in barn).

Let $R(En)$ be the counting rate in the beam flux monitor without any sample in the filter box, and $R'(En)$ the reduced one when a thin sample (of thickness $x$) is added. Obviously, these counting rates depend on the efficiency of the flux monitor as well as the beam flux, but doing the quotient $R'(En) / R(En)$, both $\Phi$ and $\varepsilon$ cancel and we have:

$$R'(En) / R(En) = \exp[-\mu \cdot x] = \exp[-\sigma_t(En) \cdot \rho \cdot x \cdot N_A / A] = \exp[-C \cdot \sigma_t(En)]$$

where $C$ is a constant, so that the quotient of the counting rates only depends on $\sigma_t(En)$. Inverting the ratio, we have:

$$R(En) / R'(En) = \exp[C \cdot \sigma_t(En)]$$

Further rearranging this equation yields the cross section:

$$\sigma_t(En) = (1 / C) \cdot \ln[R(En) / R'(En)]$$

(1)

This $^{10}$B(n,tot) cross section so becomes an absolute measurement that, eventually, can reach uncertainties below 1%. It can be proposed as an absolute reference which should, moreover, improve the $^{10}$B(n,$\alpha$) standard, and thus other standards related to it.
The cross-section uncertainty – even though small – is dominated by both the sample parameters and the accuracy of the En calibration, provided that the statistical uncertainty of the counting rates stays small enough.

It is worth mentioning that the fact of assuming the well-known 1/v behaviour of the $^{10}$B(n,tot) cross section allows to extrapolate from points measured at higher energies (potentially well above the 20-60 meV thermal range) to the thermal point, thus leading to lower statistical uncertainties.

Once adopted, the 1/v behaviour for the $^{10}$B(n,a) XS, it becomes easy to obtain integral values (between limits $E_1$ and $E_2$ [in eV]) that will depend only on the $\sigma_t(th)$ thermal value:

$$I_2 = 2 \cdot \sigma_t(th) \cdot (\sqrt(E_2) - \sqrt(E_1)) \cdot \sqrt(0.0253)$$

then, the $^{10}$B(n,tot) cross section at thermal point:

$$\sigma_t(th) = I_2 / (2 \cdot (\sqrt(E_2) - \sqrt(E_1)) \cdot \sqrt(0.0253))$$

where $I_2$ is the integral value obtained by adding, in the $E_1$ to $E_2$ energy interval, consecutive bins of $\sigma_t(En)$ experimentally obtained from Eq (1). It is important to mention that this feature of the boron cross section is not shared by the (n,f) cross section of the actinides, which do not accurately exhibit the 1/v behaviour, especially for incident energies above 60 meV.

The final goal is to improve the standard value of $^{10}$B(n,a) with its thermal value in NDS18 [2] being 3844(31) b. Some evaluated libraries still show the former NDS09 [3] value of 3842.4. The only high-resolution experimental file in EXFOR (Prosdocimi 1967 [4]) reports a value of 3836(9) b, and the value obtained by fitting in the thermal energy range assuming the 1/v behaviour is 3835(5) b.

Therefore, it is of interest to improve the $^{10}$B(n,a) standard, i.e. to reduce its uncertainty, and the value obtained from (n,tot) - (n,el) should give a more precise knowledge of this standard.
References:

2.6. Measurement of the cross section of $^{235}\text{U}(n,f)$ induced by high-energy neutrons relative to n-p elastic scattering performed at the n_TOF facility at CERN, A. Manna (INFN, Italy)

Neutron cross section standards are fundamental ingredients for both measurements and evaluations of neutron-induced reaction cross sections. This is the case of $^{235}\text{U}(n,f)$ cross section: one of the most important standard cross sections at thermal neutron energy and between 0.15 MeV and 200 MeV. No measurement exists for neutron energies above 200 MeV. This led to a request for new measurements of $^{235}\text{U}(n,f)$ cross section relative to the neutron-proton elastic scattering cross section. The n_TOF facility at CERN offers the possibility to study such reaction thanks to the wide neutron energy spectrum available in its experimental area, from thermal to 1 GeV. A dedicated measurement campaign was then carried out to provide accurate and precise cross-section data of the $^{235}\text{U}(n,f)$ reaction in the energy region from 10 MeV to 450 MeV.

The experimental apparatus consisted of three flux and two fission detectors, thus allowing to simultaneously record the fission events as well as the neutrons flux impinging on the $^{235}\text{U}$ samples, as a function of the neutron energy. More in detail, the experimental signature of fission reactions was obtained by detecting the fission fragments (FFs) originating from the nuclear reactions in $^{235}\text{U}$. In one of the two fission detectors, i.e., the Parallel Plate Avalanche Counters (PPACs), both fragments were recorded in coincidence, while the working principle of the Parallel Plate Ionization Chamber (PPFC) was based on the detection of one fragment only.

This different detection scheme results in a different detection efficiency, which is, on average some 60% for PPAC and near 100% for PPFC. On the other hand, because of the different gas pressure, construction properties and applied electric field, the response of the two detectors to the $\gamma$-flash made PPFC suitable to cover neutron energies up to 150 MeV, while PPACs could reach 1 GeV.

The other section of the detection setup, i.e., the neutron flux detectors, was especially developed for this measurement (by the Istituto Nazionale di Fisica Nucleare (INFN), and by the Physikalisch-
Technische Bundesanstalt (PTB)). The detection principle of n-p scattering events relies on the use of a counter telescope for the discrimination of the protons originating from the polyethylene sample (hence the name "recoil protons telescope" (RPT)). The measurement of the neutron flux through the n-p scattering events required an extensive background measurement and characterization (also through Monte Carlo simulations) to estimate the impact of the reactions induced by neutrons on the carbon, contained in the polyethylene target.

The redundancy of the apparatus allows cross-checking between systems in the low energy region (up to about 150 MeV) in order to verify and have confidence in the cross section obtained at higher energies. In the presentation, the analysis of the PPAC chambers, with particular focus on the study of its efficiency, was presented together with the analysis of the RPTs developed by INFN.

From these data, the $^{235}$U(n,f) cross section was determined and represents, at this time, the unique measure in the neutron energy region from 10 to 450 MeV.

2.7. $^{235}$U, $^{238}$U neutron capture at thermal and sub-thermal neutron energies, A. Wallner (HZDR, Germany)

The recommended – highly precise – cross-section value for $^{235}$U neutron capture at thermal energies is largely based on the difference from total and competing cross sections of $^{238}$U. Despite its importance and high cross-section (100 barn), direct measurements of (n,γ) are rare and exhibit large uncertainties. The reason is the difficulty to measure the characteristic radiation of the reaction product $^{236}$U within a dominant fission background. Furthermore, the decay rate of $^{236}$U is very low due to its long half-life of 23.4 Myr.

The $^{235}$U capture cross section may potentially exhibit a deviation from a pure 1/v-behaviour around thermal energies. Additional energy dependent data are required to provide information about the cross section and of α, i.e., the capture-to-fission ratio. Measurements at different beam temperatures directly provide the shape of the correction factor as a function of energy.

We present new experimental data to determine this cross section in different neutron fields to evaluate its energy dependence in the low energy region. We applied a combination of (1) activation technique with (2) subsequent accelerator mass spectrometry (AMS) measurements through direct atom counting of the reaction products off-line after the activations [1]. AMS does not suffer from the molecular isobaric (same mass) interferences that limit the sensitivity of conventional low-energy mass spectrometers. The main quantity measured in AMS is the isotope ratio of the reaction product relative to the target nuclide, e.g. the conversion ratio $^{236}$U/$^{235}$U for $^{238}$U(n,γ)$^{236}$U. Here, we present highly precise capture data by applying a multi-isotope spike method to minimize systematic uncertainties.

By utilizing different neutron fields we mapped the energy dependence of the capture cross section in six activations from thermal to ultra-cold energies: activations had been performed at a number of neutron producing facilities: Uranium samples had been activated with cold neutrons at BNC Budapest, with an almost pure Maxwellian spectrum at room temperature at BR1 (SCK/CEN in Mol), with cold neutrons at FRM-2 (Munich, 2 samples), and at ILL (Grenoble, 2 samples) and with very cold neutrons again at ILL. We applied AMS for counting the number of produced radionuclides directly after the activations. This technique represents a completely independent method compared to online methods (detecting the associated prompt radiation) or decay counting methods.
Chart of nuclides showing the relevant isotopes used for AMS measurements. The reaction product of $^{235}\text{U}(n,\gamma)$ is $^{236}\text{U}$ which was measured relative to $^{238}\text{U}$ and $^{233}\text{U}$, a well-known amount of a spike added to the sample after the irradiation. Using natural uranium samples allowed to measure in parallel also $^{238}\text{U}(n,\gamma)$. Here, AMS measured the decay product of the reaction product $^{239}\text{U}$, this is $^{239}\text{Pu}$ which was quantified relative to another spike, $^{242}\text{Pu}$, also added to the sample after the activation. The isotope ratio $^{236}\text{U}/^{239}\text{Pu}$ therefore represents the cross-section ratio of $^{235}\text{U}(n,\gamma)/^{238}\text{U}(n,\gamma)$.

Uranium samples of natural isotopic composition were used. The high sensitivity of AMS required only very small sample masses (30-50 mg of natural U) and short irradiation times. Our method, being independent from the fission channel, allows for an accurate direct value of this important cross section in the low energy region. The capture cross section of $^{235}\text{U}(n,\gamma)$ was measured, however, not only absolute (using e.g. Au as fluence monitor), but importantly also relative to $^{238}\text{U}(n,\gamma)$.

AMS determines the isotope ratio $^{236}\text{U}/^{235}\text{U}$ directly, completely independent of the sample mass. The U pellets were completely dissolved after the irradiations and spiked with well-known amounts of $^{233}\text{U}$ and $^{242}\text{Pu}$. We use $^{233}\text{U}$ as a proxy for absolute $^{238}\text{U}$ atom counting and as a reference for the stoichiometry via $^{233}\text{U}/^{238}\text{U}$ ratios. They allow to measure in parallel additional reactions, $^{238}\text{U}(n,\gamma)^{239}\text{Np}^\rightarrow^{239}\text{Pu}^\rightarrow^{239}\text{Pu}$ and allow for isotope ratio measurements in AMS.

Pu was separated from the U matrix and Pu-oxide powder produced. The remaining uranium fraction will be converted into U-oxide powder for analyses by AMS. The reaction products $^{236}\text{U}$, $^{239}\text{Pu}$ were counted to $^{235}\text{U}$ (and $^{238}\text{U}$) and $^{242}\text{Pu}$ as isotope ratios $^{236}\text{U}/^{235}\text{U}$, $^{239}\text{Pu}/^{242}\text{Pu}$ respectively, by AMS at VERA (Univ. of Vienna).

The cross-section ratio of $^{235}\text{U}$ and $^{238}\text{U}$ capture can also be expressed by the isotope ratio of the reaction products and the natural abundance of $^{235}\text{U}$ and $^{238}\text{U}$, completely independent of the neutron fluence. Based on experience with previous AMS measurements of actinides and neutron cross sections, we expect a final uncertainty in the isotope ratio of <2%.

First preliminary results are shown in Fig. 2. Expressed as isotope ratios $^{236}\text{U}/^{239}\text{Pu}$ for the various activations.


\[ \frac{N_{236}(^{235}\text{U}(\gamma))}{N_{239}(^{238}\text{U}(\gamma))} \]

\[ \frac{^{236}\text{U}}{^{239}\text{Pu}} = \frac{^{235}\text{U}}{^{238}\text{U}} \times \frac{\sigma_{\text{U}}(\gamma)}{\sigma_{\text{Pu}}(\gamma)} = \frac{0.7204}{99.274} \times \frac{99}{2.08} = 0.2681 \]

**FIG. 2.** Preliminary results for the measured AMS quantity, the isotope ratio \(^{236}\text{U}/^{239}\text{Pu}\), reflecting the cross section ratio of \(^{235}\text{U}(\gamma)/^{238}\text{U}(\gamma)\).

References:

2.8. Extending the integral references for ToF (n,tot) and (n,g) measurements in fissile targets reactions and its relations with the Standard Thermal Neutron Constants, I. Duran (USC, Spain)

**Part I. Integrals I** (thermal range)

Historically, the principal international standards are a few constants at thermal point (the TNC table), that include (n,f), (n,g) and (n,el) cross sections for the four main fissile actinides. But, as a matter of fact, there are experimental problems to perform measurements with neutrons having exactly the thermal point energy of 25.3 meV, and many experimental datasets are loosely normalized due to lack of a good reference to the thermal point. Therefore, it should be useful to provide, first, integral values in the thermal energy range (from 20 to 60 meV) and, second, high-accuracy reference data in the Resolved Resonance Region (RRR) at energies above a few 1eV, which for many experimental setups are more easily reachable than the thermal point.

A previous work was dedicated to propose as reference or standard new integral data on (n,f) for the fissile major actinides: \(^{233}\text{U},^{235}\text{U},^{236}\text{Pu}\) and \(^{241}\text{Pu}\). In this work the same procedure has been applied to the (n,tot) experimental data, and the corresponding (n,g) constants have been deduced from the equation: (n,g) = (n,tot) − (n,f) − (n,el), where the (n,el) constants are obtained from the literature. In the first part of this report the thermal-energy region results are commented, and in the second those corresponding to the integrals in the RRR, which may help to renormalize the EXFOR datasets before being used for an evaluation.

It must be understood that the goal of this work is not to improve the TNC, but to obtain the integral values in the standard energy intervals. Comparison with the TNC values is performed throughout this report to check the coherence of this analysis.
For the fissile actinides, high-resolution experiments on the (n,g) reaction (radiative capture) are scarce and without the high quality required to obtain cross section values to be recommended as references. On the other hand, there are much better high resolution data related to the (n,tot) reaction from transmission experiments. Therefore, I deduce the (n,g) cross section values from the (n,tot) analysis, subtracting the corresponding values of both (n,f) and (n,el) reactions.

The (n,f) thermal cross sections were studied in a previous work [1], so that in this work I have taken those values. The (n,tot) thermal cross sections have been newly obtained from the analysis of the experimental datafiles retrieved from EXFOR, just in the same way those of (n,f) were obtained (see [1]). The σ(n,el) values, in the next table, have been adopted from those in the TNC table, slightly modified taking into account the very limited information in EXFOR as well as the values given by the three main evaluated libraries, and those compiled by Mughabghab and by Divadeenam:

TABLE 1. THE (n,el) CROSS SECTIONS AT THERMAL POINT

<table>
<thead>
<tr>
<th>σ(n,el) [b]</th>
<th>U-233</th>
<th>U-235</th>
<th>Pu-239</th>
<th>Pu-241</th>
</tr>
</thead>
<tbody>
<tr>
<td>This work</td>
<td>12.4(0.5)</td>
<td>14.3(0.4)</td>
<td>8.0(0.8)</td>
<td>11.5(1.5)</td>
</tr>
<tr>
<td>TNC table</td>
<td>12.2(0.7)</td>
<td>14.1(0.2)</td>
<td>7.8(1.0)</td>
<td>11.9(2.6)</td>
</tr>
<tr>
<td>Mughabghab</td>
<td>12.7</td>
<td>14.2</td>
<td>7.9</td>
<td>8.9</td>
</tr>
<tr>
<td>Divadeenam</td>
<td>12.6</td>
<td>14.0</td>
<td>7.3</td>
<td>9.1</td>
</tr>
</tbody>
</table>

It is worth mentioning that the evaluated values of (n,el) are strongly correlated with (n,tot) and (n,f). Therefore, due to the high uncertainties in the (n,el) cross section data, a certain trade-off is allowed when looking for values of both (n,el) and (n,g) to be close to the TNC ones. For 233U there is agreement between the evaluations and TNC, even if a value slightly higher is suggested by Divadeenam. For 235U, the analysis here done of the (n,tot) thermal value is pointing to a (n,el) value higher than the one adopted by the standard TNC, staying within the quoted uncertainty; among the evaluated libraries there is a big spread and so the here adopted value of 14.3 b seems to be conservative, being coincident with two of the three experimental values compiled by Divadeenam. For 239Pu the here evaluated (n,el) value of 8.0 b is compatible with Mughabghab and the mean value of the evaluated libraries, though slightly greater that in the TNC. For 241Pu the here evaluated (n,el) value of 11.5 b is around 30% higher than the compiled ones, lying closer to the TNC one.

Table 2 shows the new cross-section results in the thermal energy range, and their comparison with those from the TNC table (the TNC (n,tot) values are found by summing (n,f), (n,el) and (n,g)).

TABLE 2. NEW CROSS SECTION RESULTS IN THE THERMAL ENERGY RANGE AND COMPARISON WITH THE TNC VALUES

<table>
<thead>
<tr>
<th></th>
<th>σtot</th>
<th>I1tot</th>
<th>Ratiotot</th>
<th>σfis</th>
<th>I1fis</th>
<th>Ratiosfis</th>
<th>σel</th>
<th>I1el</th>
<th>Ratiosel</th>
<th>σg</th>
<th>I1g</th>
<th>Ratiosg</th>
</tr>
</thead>
<tbody>
<tr>
<td>U3</td>
<td>590.2(1.7)</td>
<td>19.47(07)</td>
<td>30.31(17)</td>
<td>533.0(0.7)</td>
<td>17.53(10)</td>
<td>30.40(25)</td>
<td>12.4(0.5)</td>
<td>0.492(20)</td>
<td>25.9(1.0)</td>
<td>44.8(1.9)</td>
<td>1.45(12)</td>
<td>30.8(1.6)</td>
</tr>
<tr>
<td>TNC</td>
<td>590.1(2.5)</td>
<td>533.0(2.2)</td>
<td>12.2(0.7)</td>
<td>44.9(0.9)</td>
<td>3.14(10)</td>
<td>31.9(1.9)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0%</td>
<td>0%</td>
<td>+1.6%</td>
<td>-0.2%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>U5</td>
<td>700.7(1.3)</td>
<td>22.49(01)</td>
<td>31.16(19)</td>
<td>586.1(2.6)</td>
<td>18.78(08)</td>
<td>31.20(27)</td>
<td>14.3(0.4)</td>
<td>0.568(19)</td>
<td>25.54(1.8)</td>
<td>100.3(2.7)</td>
<td>3.14(10)</td>
<td>31.9(1.9)</td>
</tr>
<tr>
<td>TNC</td>
<td>700.9(1.9)</td>
<td>587.3(1.4)</td>
<td>14.1(0.2)</td>
<td>99.5(1.3)</td>
<td>0.8%</td>
<td>3.14(10)</td>
<td>31.9(1.9)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0%</td>
<td>-0.2%</td>
<td>+1.4%</td>
<td>+0.8%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pu9</td>
<td>1028.7(1.1)</td>
<td>35.21(02)</td>
<td>29.21(18)</td>
<td>751.0(1.9)</td>
<td>25.41(05)</td>
<td>29.56(13)</td>
<td>8.0(0.8)</td>
<td>0.315(32)</td>
<td>25.81(5.2)</td>
<td>269.7(2.4)</td>
<td>9.48(18)</td>
<td>28.45(77)</td>
</tr>
</tbody>
</table>
Concerning the (n,tot) integral values in the thermal region, I1 in Table 2, they have been obtained by the same procedure as used for the (n,f) integrals as described in [1]. It is worth noting that for the (n,tot) reaction, good enough experimental datafiles are retrieved from EXFOR for every nuclei, which have produced accurate values for both the I1 integral and the thermal cross section consistent with the TNC standards. In conclusion, the I1 (n,tot) values quoted in Table 2 are reliable enough to be taken as reference for evaluation purposes.

The I1 values for (n,el) in Table 2 have been obtained using the thermal point values quoted in Table 1, and taking into account the small slope of the cross-section function on a lin-lin scale from the main evaluated libraries. As the (n,el) cross section behaviour is so flat, the uncertainty of the I1 integrals comes directly from those of the thermal point values.

\[
\begin{array}{cccccccccccc}
| \text{TNC} | \sigma_{\text{tot}} & I1_{\text{tot}} & \text{Ratio}_{\text{tot}} & \sigma_{\text{fis}} & I1_{\text{fis}} & \text{Ratio}_{\text{fis}} & \sigma_{\text{el}} & I1_{\text{el}} & \text{Ratio}_{\text{el}} & \sigma_{\text{g}} & I1_{\text{g}} & \text{Ratio}_{\text{g}} \\
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pu1 | 1392.1 & 45.87 & 30.35 & 1018.9 & 34.05 & 29.93 & 11.5 & 0.453 & 25.5 & 361.7 & 11.38 & 31.78 \\
| TNC | 1398 & 45.87 & 30.35 & 1024 & 34.05 & 29.93 & 11.5 & 0.453 & 25.5 & 361.7 & 11.38 & 31.78 \\
\end{array}
\]

Note: $\sigma_{\text{xx}}$ [b] are the values of the cross section at thermal point; $I1_{\text{xx}}$ [b-eV] are the integral values in the thermal energy range between 20 to 60 meV; the ratio $\sigma_{\text{xx}} / I1_{\text{xx}}$ [eV-1] is shown in every third column. The uncertainties between parenthesis are those coming from (n,tot), (n,f) and (n,el) experimental values as standard deviations, propagated without taking into account their covariances.

The new (n,tot) thermal cross sections obtained in this work are in very close agreement with the TNC table (their differences are shown in percent, every third line). The worst case is $^{241}$Pu with a mere 0.4%. It is important to note that these new (n,tot) values have been obtained from a limited set of experimental data, in accordance with the analysis procedure described in [1]; only those datafiles in EXFOR having point-data with high energy resolution have been selected, and few outliers have been discarded.

When comparing the (n,f) thermal values –taken from [1] – with those in the TNC table, they are systematically lower, though their differences are small, remaining well below the uncertainties quoted there. The worst case is again that of $^{241}$Pu, but its percentage difference is still as low as 0.5%.

On the other hand, comparing the (n,el) thermal cross sections with those in TNC table, their differences appear to be relatively high, being positive for $^{233}$U, $^{235}$U and $^{239}$Pu, and negative (around -3.5%) for $^{241}$Pu (see Table 2). It is worth noting, nevertheless, the disagreements between the TNC table and the evaluated libraries, which also show significant differences between each other. This is the weakest point in the combined analysis of the thermal neutron constants, because the elastic scattering of neutron at thermal energies is not easily measured with precision and so the experimental datafiles are scarce and not very accurate. As the (n,g) cross section values are here deduced after the (n,tot) analysis -subtracting then the corresponding values of both (n,f) and (n,el) reactions – the resulting (n,el) cross section is negatively correlated with the corresponding (n,g) cross section. Nevertheless, the absolute value of the (n,el) cross sections is much lower than that of the (n,f) and (n,g) ones, and its effect on the final (n,g) cross section, as quoted in Table 2, is not so high.

Although the aim of this work is not to criticize the standard TNC values, it is worth commenting on the fact of having values for $^{241}$Pu which are systematically bigger than the ones found in this work. Moreover, the $^{241}$Pu values in the TNC table have too high uncertainties which propagate to (n,tot). These too high uncertainties, mainly for (n,f), are not consistent with the ones found in this work, coming from a reduced set of experimental values.

Cross-section integral references in the thermal energy region.

Concerning the (n,tot) integral values in the thermal region, I1 in Table 2, they have been obtained by the same procedure as used for the (n,f) integrals as described in [1]. It is worth noting that for the (n,tot) reaction, good enough experimental datafiles are retrieved from EXFOR for every nuclei, which have produced accurate values for both the I1 integral and the thermal cross section consistent with the TNC standards. In conclusion, the I1 (n,tot) values quoted in Table 2 are reliable enough to be taken as reference for evaluation purposes.
Finally, the \( I_1 \) values for the \((n,g)\) capture reaction are deduced from the \((n,tot)\) \( I_1 \) integrals, subtracting then the corresponding values obtained for both \((n,f)\) and \((n,el)\) reactions. In Table 3, their corresponding ratios \( \sigma(n,g) \) over \( I_1(n,g) \) are shown, being compared with different evaluations.

**TABLE 3. COMPARISON OF \((n,g)\) THERMAL \( \sigma \) AND \( I_1 \) (AND ITS RATIOS) WITH MAIN EVALUATED LIBRARIES.**

<table>
<thead>
<tr>
<th>( \sigma / I_1 \ (n,g) )</th>
<th>U-233</th>
<th>U-235</th>
<th>Pu-239</th>
<th>Pu-241</th>
</tr>
</thead>
<tbody>
<tr>
<td>This work</td>
<td>44.8 / 1.45 = <strong>30.9</strong></td>
<td>100.3 / 3.14 = <strong>31.9</strong></td>
<td>269.7 / 9.48 = <strong>28.4</strong></td>
<td>361.7 / 11.4 = <strong>31.7</strong></td>
</tr>
<tr>
<td>ENDF8</td>
<td>42.3 / 1.41 = <strong>30.0</strong></td>
<td>99.4 / 3.17 = <strong>31.4</strong></td>
<td>270.1 / 9.63 = <strong>28.1</strong></td>
<td>363.0 / 11.4 = <strong>31.8</strong></td>
</tr>
<tr>
<td>JEFF3.3</td>
<td>45.3 / 1.51 = <strong>30.0</strong></td>
<td>99.6 / 3.20 = <strong>31.1</strong></td>
<td>271.4 / 9.72 = <strong>27.9</strong></td>
<td>363.0 / 11.4 = <strong>31.8</strong></td>
</tr>
<tr>
<td>JENDL4</td>
<td>45.3 / 1.51 = <strong>30.0</strong></td>
<td>98.7 / 3.09 = <strong>31.9</strong></td>
<td>271.5 / 9.71 = <strong>27.8</strong></td>
<td>363.0 / 11.4 = <strong>31.8</strong></td>
</tr>
</tbody>
</table>

The main conclusion concerning the capture cross sections found in this work in the thermal energy range \((20 – 60 \text{ meV})\) is the good agreement with the TNC values (see Table 2), but there are also small differences when compared with the values obtained from the evaluated libraries, which are, however, still compatible with the quoted uncertainties, with the remarkable exception of the ENDF8 evaluation of the \(^{233}\text{U}(n,g)\), which shows a 6% lower value for \( \sigma \) and 3.5% lower for the \( I_1 \) integral. Conversely, the JEFF3.3 (and JENDL4) values for \(^{233}\text{U}(n,g)\) are higher by 1%. Nevertheless, all the ratios \( \sigma(n,g) \) over \( I_1(n,g) \) show a reasonable behaviour, although there is room for improvement in the evaluations. These evaluations may be improved by taking into account that the \( I_1 \) integral values are coming from a cross section that has a well-defined behaviour (linear in the thermal energy range in log-log scale, as for the \((n,f)\) ones shown in [1].

According to this, the \((n,g)\) thermal cross section values presented here are reliable with the \(^{235}\text{U}(n,g)\) case (+0.8%) showing the biggest difference to TNC, but still well inside the 1.3% uncertainty quoted in the TNC table. Therefore, the corresponding \( I_1 \) values can be recommended as reference for normalization purposes.

It is noteworthy that everything is pointing to a low value in the ENDF8 evaluation of the \(^{233}\text{U}(n,g)\) cross section all along the thermal range.

In order to check the consistency of the \((n,g)\) data reported herein, the \( \alpha \)-values (defined as \( \sigma(n,g) / \sigma(n,f) \) at thermal point) obtained in this work are shown in Table 4 compared to those in the TNC table and with other references found in literature.

**TABLE 4. COMPARISON OF \( \alpha \)-VALUES**

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>U-233</strong></td>
<td>0.0841(31)</td>
<td>0.0842(17)</td>
<td>0.0784(32)</td>
<td>0.0861(21)</td>
<td></td>
</tr>
<tr>
<td><strong>U-235</strong></td>
<td>0.1711(54)</td>
<td>0.1694(22)</td>
<td>0.1691(35)</td>
<td>0.1697(29)</td>
<td>0.1690(35)</td>
</tr>
<tr>
<td><strong>Pu-239</strong></td>
<td>0.3591(41)</td>
<td>0.3586(35)</td>
<td>0.3595(42)</td>
<td>0.3555(57)</td>
<td></td>
</tr>
<tr>
<td><strong>Pu-241</strong></td>
<td>0.3550(44)</td>
<td>0.3537(79)</td>
<td>0.3533(71)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Note:** Std Deviation (shown between parenthesis) comes from the uncertainties in Table 2.

The good agreement with the last NDS18 [2] table of the TNC can be seen, even if the data are showing much bigger uncertainties, which can be explained with the \((n,g)\) values having been obtained indirectly, dragging the uncertainties found in \((n,tot), (n,f)\) and \((n,el)\). It should be noted that the \((n,tot)\)
and (n,f) values –with their uncertainties– come from the analysis of ample experimental data, while (n,el), conversely, suffers from a lack of good experimental support. Nevertheless, the agreement of α-values is a proof of the consistency of the data in Tables 1 and 2.

Part II. Integrals I3 (RRR)

The use of cross section integrals as reference in the RRR (Resolved Resonance Region) is of great importance to normalize high-resolution datafiles. The energy intervals here used for the (n,tot) and (n,g) integrals are the same as those chosen for the (n,f) integrals in [1]. For the selected experiments measuring (n,tot), a renormalization has been done according to their historical records, as was done in the thermal range. Once every experiment is renormalized, their I3 value is calculated as in [1], and the mean value is used as the I3 value here proposed for the (n,tot) reaction in the RRR.

Concerning the integrals for (n,el) in the RRR, the experimental datafiles retrieved from EXFOR are limited to three experiments for 233U, 235U and 241Pu, and hence the evaluated libraries are based on the resonance parameters derived from very few experimental data. The systematic uncertainties are expected to be high, close to 10%, but their effect on the (n,g) values will be low because of the small (n,el) cross section, compared to (n,tot) and (n,f).

In Table 5 the I3 values found in this work are summarized, as well as their ratio over their corresponding values of I1. The I3 values for (n,tot) come from the numerical integrals of the experimental datasets once renormalized, whereas the here proposed I3 values for (n,g) have been obtained after subtracting the (n,f) and (n,el) from the (n,tot) integral. Taking into consideration the large uncertainties, they compare well with the mean value of those obtained by integrating the data retrieved from the evaluated libraries. This relative agreement is better for uranium than for plutonium, which seems to suffer from the effect of contamination from 242Pu and 241Am, which is not always properly accounted for in the evaluations.

TABLE 5. NEW VALUES OF INTEGRALS I3 AND THEIR RATIOS WITH I1

<table>
<thead>
<tr>
<th>(n,tot)</th>
<th>I1_renorm</th>
<th>I3_renorm</th>
<th>I3 / I1</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-233</td>
<td>19.5(0.1)</td>
<td>871.2(2.5)</td>
<td>44.8</td>
</tr>
<tr>
<td>U-235</td>
<td>22.5(0.1)</td>
<td>375.0(10)</td>
<td>16.7</td>
</tr>
<tr>
<td>Pu-239</td>
<td>35.2(0.1)</td>
<td>1834(38)</td>
<td>52.1</td>
</tr>
<tr>
<td>Pu-241</td>
<td>45.9(0.1)</td>
<td>2235(94)</td>
<td>48.7</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(n,g)</th>
<th>I1_proposed</th>
<th>I3_proposed</th>
<th>I3 / I1</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-233</td>
<td>1.45(12)</td>
<td>100(9)</td>
<td>68.5</td>
</tr>
<tr>
<td>U-235</td>
<td>3.14(12)</td>
<td>95(11)</td>
<td>30.1</td>
</tr>
<tr>
<td>Pu-239</td>
<td>9.48(17)</td>
<td>673(39)</td>
<td>71.5</td>
</tr>
<tr>
<td>Pu-241</td>
<td>11.38(47)</td>
<td>775(98)</td>
<td>67.4</td>
</tr>
</tbody>
</table>

Note: The Std Devs (between parenthesis) have been found propagating the Std Devs quoted for the (n,tot), (n,f) and (n,el) without covariances.

Conclusions

The cross sections of both (n,tot) and (n,g) reactions integrated in wide energy ranges have been studied, looking for integral values that could be agreed as IAEA Standard or Reference values eventually. The values of I1 (thermal energy range) and I3 (RRR) with their ratios to the thermal-point value are provided for the four fissile actinides.

When trying to obtain the (n,g) values of the cross section integral values directly from the experimental datafiles retrieved from EXFOR, they show problems with sample impurities and background suppression. This fact leads to the conclusion that much better results are obtained when they are obtained by subtracting the (n,f) and (n,el) cross sections from the (n,tot) one.
This study shows that the analysis of the \((n,\text{tot})\) experimental data produces very good results – as there are good enough experimental datafiles in EXFOR – and so we can conclude that those results showed in Tables 2 and 5 are worth being taken as IAEA References for evaluation purposes.

Concerning the \((n,\text{el})\) results it can be seen that their uncertainties are too high to be taken as references, due to the lack of good experimental support. These uncertainties are strongly correlated with those coming from the other neutron reactions, and are negatively correlated with the \((n,\text{g})\) ones. This is the weakest point in assessing the \((n,\text{g})\) integrals in this work, indicating a need for new measurements of neutron elastic scattering for the four actinides.

References:
[1] I. Duran, R. Capote, P. Cabanelas, Accepted for publication in Nucl. Data Sheets (submitted 2022)

2.9. About USU treatment in gmapy, Georg Schnabel (IAEA)

In a recent paper R. Capote, et al., addressed the topic of unrecognized sources of uncertainty (USU) in the context of nuclear data evaluation [1]. Even the most diligent care in the assessment of potential error contributions associated with an experimental setup may not guarantee that all error contributions have been identified and considered. A visual signature of USU are datasets obtained from experiments at different institutions and times which are incompatible considering their uncertainties. Therefore, the presence of USU cannot be excluded and should be accounted for in an evaluation procedure so that small inconsistencies in the data do not deteriorate estimates while at the same time shrinking evaluated uncertainties to unreasonable small values.

This presentation elaborated on an approach to account for USU, which has already been tentatively implemented in the gmapy code package [2]. The starting point was the insight that the well-known formulas to perform the Generalized Least Squares (GLS) method can be obtained by employing the maximum likelihood (ML) principle, if we assume a multivariate normal distribution with known covariance matrix for the measurement process. The ML principle states in this context that we should choose the values of the unknown model parameters (or cross sections in the case of the neutron standards) so that the likelihood of the actually measured values becomes maximal. The introduction of USU means that we abandon the assumption of a completely known covariance matrix. This entails that we cannot use the GLS formulas anymore to arrive at a solution, but we can nevertheless employ the ML principle as it is more general. It was shown how the idea of unknown components in the experimental covariance matrix can be formalized and it was discussed how the necessary optimization to implement the ML principle can be achieved algorithmically.

The presentation concluded with a suggestion on the specific modelization of the USU error components in the neutron data standards project:

- Data points are split into groups according to their energy region;
- The points of each dataset in each energy group are associated with an additional normalization factor (a dataset covering several energy regions can therefore have multiple normalization factors).

Roughly speaking, USU uncertainties entering the experimental covariance matrix are then computed for each energy group based on the estimated normalization factors for each dataset. More precisely, the estimation of USU uncertainties according to the ML principle is an iterative process were cross sections and USU uncertainties are estimated self-consistently, as an adjustment of USU uncertainties affects the evaluated cross sections and, vice-versa, adjustments to evaluated cross sections have an impact on the estimation of USU uncertainties.
2.10. Impact of SACS measurements on the standards evaluations, R. Capote (IAEA)

A new evaluation of spectrum averaged cross sections (SACS) of $^{235}$U, $^{238}$U, and $^{239}$Pu measured in the $^{252}$Cf(sf) reference neutron field is presented and found to be consistent with the original Mannhart SACS evaluation in IRDF-2002. The comprehensive vetted experimental database that includes SACS ratio and absolute SACS measurements of major actinides is being used to update the SACS database employed as input of the new GMApy code to derive the Neutron Standards.

An update of the current neutron standards based on Time Projection Chamber (TPC) shape data, a new comprehensive uncertainty quantification, and revised SACS experimental database is proposed which result in a 0.7% increase of the evaluated $^{239}$Pu(n,f)/$^{235}$U(n,f) cross-section ratio in the 1–5 MeV energy region. The increase is due to a 0.3% reduction of the standard $^{235}$U(n,f) cross section and a 0.4% increase of the $^{239}$Pu(n,f) reference cross section in the 1–5 MeV energy region. Those changes are well within estimated USU fission cross-section uncertainties of 1.2% but are relevant for the evaluated mean values.

2.11. Gmapy developments, G. Schnabel (IAEA)

The development of a new analysis code called gmapy [1] has been initiated in 2020 with the objective to become eventually a modern replacement of the GMA code based on the methodology as outlined in [2], which was used in the past for about 40 years for evaluations in the neutron data standards project. Even though GMA is efficient, established and has been extensively tested, it is not easily maintainable or extensible due to a complex code flow with readability traded for execution speed. This optimization was certainly necessary in the 1980s due to the very limited processing power of computers, but nowadays we have much faster computers and can forsake some optimization for the sake of code readability. Furthermore, the development of a successor to GMA in Python – the most popular programming language for data science tasks at present – makes the code accessible to a broader audience with potential benefits for the neutron data standards project in the future. At this stage, gmapy is robust and has been proven to be backwards compatible with GMA. The backwards compatibility has been proven by various tests to confirm the functional equivalence of GMA and gmapy, such as:

- End-to-end tests: Both codes are run on the complete standards database and the equivalence of results is verified;
- Unit tests: Test cases were written to check many individual modules of the new code in isolation (e.g., reading of the database, algorithm to fit cross sections, etc.);
- Divergence tests: Some bugs in GMA that were fixed in gmapy lead to small deviations in the results, which were quantified in test cases as well.

Relying on an extensive suite of test cases, gmapy was improved over GMA by the removal of some minor glitches and the implementation of methodological improvements. Noteworthy, the iterative Generalized Least Squares ((GLS) algorithm has been replaced by a customized Levenberg-Marquardt [3, 4] algorithm with convergence checking to ensure that (numerically) the best solution is found. Furthermore, an adaptive integration routine based on Romberg’s method [5] has been implemented to ensure an accurate consideration of spectrum-averaged cross sections (SACS). Furthermore, the possibility to include measurements that represent ratios of SACS has been implemented in the new code. The code is open-source and available on GitHub [1].

References:
Related to the developments of gmapy, the presentation also addressed the modernization of the format of the neutron data standards database, which serves as input for the GMA and gmapy code. The complete database has been successfully converted to a JSON format, which can be readily read by most programming languages. This development represents another effort to make the standards project future-proof and ensures that valuable experimental information collected and revised over decades will remain easily accessible in the future. The merits of a new database format were also exemplified by the introduction of a covariance matrix on the $^{252}$Cf spontaneous fission spectrum and its use in a tentative evaluation with gmapy.

Finally, efforts to make the impact of new data and code developments on evaluation results traceable were summarized. A repository has been created on GitHub with the neutron standards database given in the version used for the preparation of the standards 2017 [6] and in a version updated with new and revised experimental data [7,8]. This repository has been prepared to work together with the Data Version Control (DVC) [9] package to facilitate reproducible studies of evaluation scenarios based on specific versions of gmapy in combination with specific versions of the standards database with potentially some manipulations on the data, such as the removal of datasets.

References:
[8] D. Neudecker, V. Pronyaev, L. Snyder, Including $^{238}$U(n,f)/$^{235}$U(n,f) and $^{239}$Pu(n,f)/$^{235}$U(n,f) NIFFTE fission TPC Cross-sections into the Neutron Data Standards Database, Report LA-UR-21-24093, 2022. https://www.osti.gov/biblio/1788383

2.12. What can be improved in the new update of the Standards?, V. Pronyaev

Possible updates in the Standards evaluation based on the use of the Python version of the GMA code (GMAPy), developed by G. Schnabel, were considered. GMAPy provides more options for the GLSQ fit and more freedom in the processing of experimental data. The proposal includes:

- The fixing of the external thermal neutron constants (TNC) evaluation for microscopic 0.0253 eV point values, as done by G. Noguere, should be included in the final standards evaluation. This evaluation should be included in the combined GMAPy fit to inform the evaluation of other cross sections while keeping the TNC fixed. This will exclude a reverse influence of the results of high-energy cross section evaluation at the TNC.
The use of the results of R-M fit for $^{235}$U(n,f) with inclusion of the latest TOF experimental data for all reaction channels and TNC constants as constraints in the evaluation of the ratio of fission cross section integral between 7.8 and 11 eV and the thermal value. This ratio with the evaluated uncertainties should be added to the GMAPy fit. The result of the fission integral R-M fit should be fixed as the standard value. This will exclude a reverse influence of the results of the cross-section measurements for higher energy at the TNC.

The introduction of new energy nodes for cross section presentation in the energy range between 1 keV and 100 keV. It is proposed to use 20 nodes per decade, equidistant on a lethargy ($\log(En)$) scale. The structures observed in the cross sections, which are not standards in this energy range, could be better accounted for, and high-resolution TOF measurements will be reduced to the resolution close to the one of measurements with constant neutron energy beams.

The use of a new approach to account for $^{252}$Cf(s.f.) neutron spectrum averaged cross sections (SACS) in the fit. SACS can be evaluated independently by GMAPy, similar to the suggestion for TNC. These pre-evaluated values and covariance matrix of their uncertainties could be used as the evaluated parameters in the GMAPy combined standards fit. For this, the $^{252}$Cf spectrum at new energy nodes and their covariance matrix of uncertainties could also be used as evaluated parameters. The integration of the spectrum with the cross sections for new nodes could be done in the GMAPy. This approach allows to account for the spectrum uncertainty in the cross section adjustment procedure.

The development of a new traceable and practical approach for the work with the outlying data. The chi-square per degree of freedom in the fit with the data in the GMA database is about 4 and it requires the search and work with the outlying experimental points. The ad hoc procedure, which was used in the previous standards evaluation, consists in the increase of the uncertainties for the outlying points (relative “true” values). In the iterative fitting procedure, in each iteration the posterior obtained in the previous iteration is used as the a priori evaluation in the current iteration. Additionally, the one-group estimation of the Unrecognized Source of Uncertainties (USU) contribution was added to the evaluated covariances.

A new approach proposed by G. Schnabel introduces a statistical estimate of additional multi-group variances to the experimental data sets during their fit. By this, the one group USU variances used before in the standards evaluation as additional uncertainty to the final evaluated data, can be replaced by the estimated multi-group USU variance associated with the experimental data used in the GMA fit.

Another simple ad hoc approach for practical implementation allows to construct the USU covariances for each experimental data set that contains outlying points in the process of the evaluation. The approach is based on the use of population statistics for biases between “true” evaluated and experimental values. The iterative procedure should be used for the determination of “true” values. This approach replaces the treatment of outlying data in the previous standards evaluation. As for previous treatment of outlying data, it is not clear, to which extent the statistical nature (distribution) can be assigned to the bias between the “true” evaluated and experimental data point. The criteria for determination of values containing USU in the case of multivariate data should also be fixed.

The procedure of experimental data reduction to the energy nodes applied in the evaluation (DAT code) should be used in each iteration. Usually, one iteration is enough to obtain good consistency between the shape of evaluated data applied for interpolation of the experimental points to the nodes and the shape of a posteriori evaluation.

The energy node at 235 keV should be added to the $^{239}$Pu(n,f) GMAPy evaluation. It was missed in the GMA data.

The analysis of the uncertainties done by D. Neudecker for $^{239}$Pu and $^{235}$U fission cross sections should be extended to other reactions and ratios in the GMA database.

The results of multivariate absolute cross section (or ratio) measurements, which are outliers due to normalization problems should be used in the GMAPy evaluation as the shape type of data.
The TUD/KRI results of absolute cross section measurements for fission cross sections done with the associated particle method and already included in the GMA database can be trusted as they have been independently verified in the JENDL-5 evaluation of actinides fission cross sections.

2.13. Test of nuclear-data evaluation for natPb(n,f) and 238U(n,f) cross sections using G-HyND, H. Iwamoto (JAEE, Japan)

Hiroki Iwamoto briefly introduced his code G-HyND [1,2], and reported the test results of nuclear data evaluation for the natPb(n,f) and 238U(n,f) cross sections using this code. The G-HyND code is a nuclear-data estimation code which is based on the Gaussian process regression model. Although this code has no capability to estimate correlations between related reactions, it enables us to estimate cross sections together with their uncertainty information as a function of incident particle energies. In an attempt to evaluate nuclear data, this code is partially used in the evaluation of JENDL-5 [3].

In his presentation, he demonstrated that this code can estimate the natPb(n,f) and 238U(n,f) cross sections by means of the Gaussian process regression model, which are consistent with the IAEA neutron standards. On the other hand, he also noted that the uncertainty information estimated by his code was quite different from that evaluated in the IAEA neutron standards. In the future, it may be necessary to investigate differences in uncertainty evaluation results due to evaluation methodologies.

References:

2.14. Fission cross section measurement of 232Th, 235U and 238U relative to n-p scattering at CSNS Back-n, Y. Chen (IHEP, China)

In the presentation, we first gave a brief introduction to the CSNS and Back-n facility. Then the experimental setup was shown, which mainly consists of a fission chamber (named as FIXM) and a proton recoil telescope (PRT). The 232Th, 235U and 238U samples were mounted in the FIXM for measuring the neutron-induced fission events. PRT was used for extracting the neutron flux by measuring the n-p scattering on a low-density polythene foil. For the measurement of 232Th(n,f) cross sections, both 235U(n,f) and n-p scattering were used as references. For the determination of the 235, 238U(n,f) cross sections, merely n-p scattering was used as reference. Since the beam profile and the samples’ homogeneities have not been well characterized yet, this work was normalized to the evaluation data as a shape measurement. The measured 232Th(n,f) cross sections from 1 to 300 MeV, and the 235, 238U(n,f) cross sections from 10 to 66 MeV were shown.

2.15. High accuracy, high resolution 235U(n,f) cross section from n_TOF (CERN) from 18 meV to 170 keV, S. Amaducci (INFN, Italy)

The presentation summarized the final result of the 235U(n,f) cross section measurement, performed at n_TOF between 18 meV and 170 keV, relative to the standards 6Li(n,t) and 10B(n,α). For this measurement a dataset with high resolution has been recently released and included in EXFOR (entries 23453013 and 23453014). The resonance analysis performed up to 200 eV confirms the correctness of the changes introduced by ENDF/B-VIII and JEFF-3.3 libraries, which are on average in good agreement with the n_TOF data. However, a kernel analysis demonstrated that some local discrepancies are still present, which leaves room for improvement upon the existing evaluations. In particular, both libraries seem to underestimate the uranium-235 fission cross section in the energy range between 1 and 100 keV. With respect to previous experiments, the n_TOF data are in reasonable agreement.
2.16. Recovering Mannhart’s $^{252}\text{Cf(sf)}$ PFNS evaluation, Denise Neudecker$^1$, D. Brown$^2$, A.D. Carlson$^3$, M.J. Grosskopf$^1$, K.J. Kelly$^1$, B. Pritychenko$^2$, S. Vander Wiel$^1$

$^1$ Los Alamos National Laboratory, USA
$^2$ Brookhaven National Laboratory, USA
$^3$ National Institute of Standards and Technology, USA

The $^{252}\text{Cf(sf)}$ prompt fission neutron spectrum (PFNS) evaluated by W. Mannhart [1] is an important Neutron Data Standard. Unfortunately, its input was lost and is no longer available:

- Some of the input experimental data are not even in the EXFOR database [2] at the time this document was presented. For instance, the data sets of Boettger [3] and Maerten [4] are not in EXFOR. N. Otsuka compiled the latter, and put in a request to compile those of Boettger. Also, when one extracts and compares the data termed “Lajtai” in Ref. [1] to those in EXFOR, it seems more likely that the data used for Mannhart’s evaluation actually are those authored by Dyachenko [5] in EXFOR.
- It is unclear what exact data points were rejected by Mannhart from Boldemann’s data [6].
- The covariances used as input for the evaluation were augmented by Mannhart’s expert judgment and his private communication with the authors. Therefore, the experimental uncertainties are not the same as reported by experimentalists.
- The executable of Mannhart’s evaluation code is available internally at the IAEA, but the source code was lost. However, calculating spectrum-averaged cross sections with Mannhart’s code yields the same results as the GMA code. So, we trust that Mannhart correctly implemented GLS, and that the missing code is a minor obstacle in reproducing his evaluation.

The Department of Energy Office of Science project AIACHNE (AI/ML Informed cAlifornium CHi Nuclear data Experiment) strives to design and execute a differential $^{252}\text{Cf(sf)}$ PFNS experiment to reduce uncertainties in the standard evaluation. As a first step, we will reproduce Mannhart’s evaluation to the best of our ability. The AIACHNE team will use this as a means to counter-check our own code sets and assumptions on the experiment. But, at the same time the Standards project benefits by recovering part of the input data for one of their evaluations. In a second step, we plan to update the evaluation by:

- Revising preliminary data sets that Mannhart used for his evaluation by the final published version;
- Extending the evaluation with data sets that have been measured since the new evaluation;
- Treating all data as shape data.

This work requires an in-depth review of all pertinent experimental data and estimating their uncertainties. Allan Carlson joined the EUCLID team to this end. We will also work with Georg Schnabel on implementing the data into GMA as well as a code-comparison across the AIACHNE and the Standards project.

References:
3. RECOMMENDATIONS

The following recommendations were issued during the meeting. They are grouped by the categories measurements, evaluation work, and code and database development.

3.1. Measurement campaigns

It is recommended to:

- promote new measurements of $^{239}\text{Pu}/^{235}\text{U}(n,f)$ at 14 MeV to reduce uncertainties and to sort out inconsistencies among the available datasets. These measurements should be included in the NEA Nuclear Data High Priority Request List.

3.2. Evaluation work

It is recommended to:

- extend the $^1\text{H}(n,n)$ evaluation up to 100 MeV;
- use the R-matrix fit of TOF data with TNC constraints for the evaluation of the fission cross section integral value in the resonance range. This integral value should be recommended as the standard value and used in the GMAPy fit of the high-energy data;
- extend the revision of the experimental data uncertainties using templates for all reactions;
- to include SACS information in future standards evaluations and to study the impact of uncertainties on the spectrum in an evaluation exercise;
- analyze and compare practical approaches for introducing the treatment of Unrecognized Sources of Uncertainty (USU) as a capability into the GMAPy code;
- treat outlying absolute multivariate experimental data as shape type in the fitting with GMAPy;
- use the pre-evaluated values of $^{252}\text{Cf}$ SACS with spectral weights as evaluated parameters in the GMAPy fit.
- It is recommended to review the $^{239}\text{Pu}/^{235}\text{U}$ absolute ratios for their normalization and decide whether they should be only used as shape data;

3.3. Extension of GMAPy and the GMA database

It is recommended to:

- modify the energy mesh below 100 keV at 20 nodes per decay equidistant in lethargy scale in the GMA database;
- add the missing 235 keV node point for the $^{239}\text{Pu}(n,f)$ cross section;
- use an iterative an approach to perform the reduction of experimental data to the energy nodes using the shape of the a posteriori evaluation;
- extend GMAPy to be able to deal with uncertainties in spectra.
4. ACTIONS

This section lists the actions agreed upon during the meeting and their assignments to participants.

4.1. Experimental data

*Actions for the standards committee:*
- Discuss strategy to include TNC in new analysis;
- Review 14-MeV absolute $^{239}$Pu(n,f) cross sections and remove outlying or otherwise unsuitable datasets;
- Final TUD/KRI result of absolute fission cross section measurement: two different versions in standards and JENDL-5.0: decide which data to use and review;
- Include work of Ignacio for I1 and I3.

*D. Neudecker:*
- Revisit the $^{252}$Cf PFNS datasets;

*V.G. Pronyaev, G. Schnabel:*
- Add $^{239}$Pu energy point at 235 keV.

*G. Noguerre:*
- Revise the Axton database, as already done by Peter Schillebeeckx for the Geel data.

4.2. Evaluation methodology and uncertainty quantification

*H. Iwamoto, G. Schnabel:*
- Compare the evaluation method employed in the Neutron Data Standards project (GLS) to Gaussian process regression.

*G. Schnabel, S. Badikov, V.G. Pronyaev*
- Consider different techniques for an estimation of the USU contribution, especially regarding $^5$U, $^9$U, and $^{235}$U.

*S. Kunieda:*
- Investigate and develop a reasonable and feasible method to account for experimental covariance matrices in R-matrix evaluations.

4.3. Code development

*G. Schnabel*
- Implement USU determination in the GMAPy code package
- Implement renormalization algorithm on PFNS ($\chi$)-values and covariances;
- Implement possibility to allow for several spectra (e.g., $^{252}$Cf, $^{235}$U);
- Create a modern readable format for the GMA database.
## APPENDIX I: ADOPTED AGENDA

### ADOPTED AGENDA

#### Tuesday 18 October (14:00 – 18:00, open 13:45 Vienna time)

<table>
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<tr>
<th>Time</th>
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<tbody>
<tr>
<td>14:00</td>
<td>Opening of the meeting&lt;br&gt;Election of Chair and Rapporteur(s), discussion of Agenda</td>
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<tr>
<td>14:20</td>
<td>Participants’ Presentations (with discussion)&lt;br&gt;Break as needed</td>
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<tr>
<td></td>
<td>A. Carlson&lt;br&gt;A Search for Structure in the n-p total scattering cross section</td>
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<td>G. Hale&lt;br&gt;Recent R-matrix work at Los Alamos on the light-element standard cross sections</td>
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<td>S. Kunieda&lt;br&gt;Toward maximization of synergy between experiment and R-matrix theory</td>
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<td></td>
<td>M. Anastasiou&lt;br&gt;The $^{235}$U(n,f)/$^6$Li(n,t) cross section ratio measurement in the NIFFTE fission TPC</td>
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#### Wednesday 19 October (14:00 – 18:00, open 13:45 Vienna time)

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<td></td>
<td>I. Duran&lt;br&gt;Extending the integral references for ToF (n,tot) and (n,g) measurements in fissile targets reactions and its relations with the Standard Thermal Neutron Constants</td>
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<td></td>
<td>A. Manna&lt;br&gt;Measurement of the cross section of $^{235}$U(n,f) induced by high-energy neutrons relative to n-p elastic scattering performed at the n_TOF facility at CERN</td>
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<td>A. Wallner&lt;br&gt;AMS versus TOF - a complementary or alternative method</td>
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Dinner at a restaurant downtown (separate information)

#### Thursday 20 October (13:00 – 18:00, open 12:45 Vienna time)

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<tr>
<td></td>
<td>R. Capote&lt;br&gt;Experimental spectrum average cross sections in $^{252}$Cf(sf) neutron field and its impact on evaluation and UQ of neutron standards</td>
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<td></td>
<td>G. Schnabel&lt;br&gt;gmapy developments</td>
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<tr>
<td></td>
<td>I. Duran&lt;br&gt;Proposal of an improved $^{10}$B standard</td>
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<td>V. Pronyaev&lt;br&gt;What can be improved in new update of the Standards?</td>
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#### Friday 21 October (13:00 – 18:00, open 12:45 Vienna time)

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<tr>
<td></td>
<td>D. Neudecker&lt;br&gt;Recovering Mannhart’s $^{252}$Cf(sf) PFNS evaluation</td>
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<td>H. Iwamoto&lt;br&gt;Test of nuclear-data evaluation for nat_Pb(n,f) and $^{238}$U(n,f) cross sections using G-HyND</td>
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<td>Y. Chen&lt;br&gt;Fission cross section measurement of $^{232}$Th, $^{235}$U and $^{238}$U relative to n-p scattering at CSNS Back-n</td>
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<td>S. Amaducci&lt;br&gt;High accuracy high resolution $^{235}$U(n,f) cross section from n_TOF (CERN) from 18 meV to 170 keV</td>
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<td>G. Schnabel&lt;br&gt;About USU treatment in gmapy</td>
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## APPENDIX II: PARTICIPANTS

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<tr>
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# APPENDIX III: PRESENTATION LINKS

<table>
<thead>
<tr>
<th>#</th>
<th>Author</th>
<th>Title</th>
<th>Link</th>
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<tbody>
<tr>
<td>1</td>
<td>A. Carlson</td>
<td>Searches for Structure in the n-p Total Scattering Cross Section</td>
<td>PDF</td>
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<tr>
<td>2</td>
<td>G. Hale</td>
<td>Recent R-matrix Work at Los Alamos on Light-Element Standard Cross Sections</td>
<td>PDF</td>
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<tr>
<td>3</td>
<td>S. Kunieda</td>
<td>Toward maximization of synergy between experiment and R-matrix theory - Recent works with AMUR code</td>
<td>PDF</td>
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<td>4</td>
<td>M. Anastasiou</td>
<td>The $^{235}$U(n,f)$^{6}$Li(n,t) cross section ratio measurement in the NIFFTE fission TPC</td>
<td>PDF</td>
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<td>5</td>
<td>I. Duran</td>
<td>Extending the integral references for ToF (n,tot) and (n,g) measurements in fissile targets reactions and its relations with the Standard Thermal Neutron Constants</td>
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<td>A. Manna</td>
<td>Measurement of the cross section of $^{235}$U(n,f) induced by high-energy neutrons relative to n-p elastic scattering performed at the n_TOF facility at CERN</td>
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<td>7</td>
<td>A. Wallner</td>
<td>U-235, U-238 neutron capture at thermal and sub-thermal neutron energies</td>
<td>PDF</td>
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<td>R. Capote</td>
<td>Experimental spectrum average cross sections in $^{252}$Cf(sf) neutron field and its impact on evaluation and UQ of neutron standards</td>
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<td>G. Schnabel</td>
<td>gmapy developments</td>
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<td>I. Duran</td>
<td>Proposal of improving the B10 neutron standards</td>
<td>PDF</td>
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<td>V.G. Pronyaev</td>
<td>What can be improved in new update of the Standards?</td>
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<td>D. Neudecker</td>
<td>Recovering Mannhart’s $^{252}$Cf(sf) PFNS evaluation</td>
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<td>H. Iwamoto</td>
<td>Test of nuclear data evaluation for $^{208}$Pb n,f ) and $^{238}$U( n,f ) cross sections using G-HyND</td>
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<td>Y. Chen</td>
<td>Fission cross section measurement of $^{232}$Th, $^{235}$U and $^{238}$U relative to n-p scattering at CSNS Back-n</td>
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<td>15</td>
<td>S. Amaducci</td>
<td>High accuracy, high resolution 235U(n,f) cross section from n_TOF (CERN) from 18 meV to 170 keV</td>
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