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EVALUATION AND RECOMMENDATION OF PHOTON STRENGTH FUNCTION DATA

Summary Report of the IAEA Consultants' Meeting
IAEA Headquarters, Vienna, Austria
28 Nov – 1 Dec 2022

Stephane Goriely
Université Libre de Bruxelles
Brussels, Belgium

Mathis Wiedeking
iThemba LABS
Cape Town, South Africa

Paraskevi Dimitriou
International Atomic Energy Agency
Vienna, Austria

July 2023

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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or to:
Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

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ABSTRACT

A Consultant's Meeting was held to discuss the evaluation and recommendation of Photon Strength Function data following the completion of the Coordinated Research Project on the same topic in 2019. Participants discussed progress in measurements, models, systematic studies of the data, as well updates of the IAEA PSF database, and agreed on actions to maintain the database current and provide recommended PSF data. A summary of the discussions and agreed actions are provided in this report.

July 2023

Contents

1. Introduction

The study of photon strength functions (PSF) lies at the heart of understanding the interaction between electromagnetic radiation and atomic nuclei. PSF are average quantities that describe the probability of a nuclear transition occurring through the emission or absorption of a photon. Accurate determination of PSF is important for nuclear structure as well as for the modelling of nuclear reactions relevant to nuclear astrophysics, nuclear energy, nuclear medicine, and other applications.

An IAEA Coordinated Research Project (CRP) that ran from 2016 to 2019, produced a Reference Database for Photon Strength Functions [1]. The database comprises a compilation of all available and published PSF data that were extracted from experimental photoneutron cross sections, neutron capture data (average resonance capture, direct resonance capture and thermal capture data), charged--particle reactions, inelastic proton scattering, and (γ,γ) data. The CRP also recommends two global models that were verified and validated following a well-defined procedure within the CRP, namely the D1M+QRPA [2] and SMLO [3]. One of the tasks of the CRP was to evaluate and recommend the best PSF data in cases where multiple measurements exist or where the data are discrepant. Three such evaluations were performed; however, they were not conclusive mainly due to lack of a full uncertainty analysis of the experimental data.

The evaluation of available PSF data remains an open issue that requires contributions from experimentalists, theorists, and nuclear data experts. Additionally, the IAEA PSF database needs to be maintained up to date and as comprehensive as possible. To best serve the user community, the data and models should be disseminated online from a user-interactive retrieval interface and by means of web-based APIs, in a format that can be easily understood and used.

To address these open issues, the IAEA organized a Consultants' Meeting on Photon Strength Function Data, from 28 November to 1 December 2022. The meeting was hybrid and was attended by the following experts: S. Goriely (Belgium), S. Jongile (S. Africa), J. Kopecky (Netherlands), M. Krticka (Czech Rep.), S. Siem (Norway), R. Schwengner (Germany), M. Wiedeking (S. Africa), and IAEA staff P. Dimitriou and A. Koning. The meeting was opened by the Head of the Nuclear Data Section, A. Koning, and an introduction to the goals of the meeting was presented by the scientific secretary, P. Dimitriou.

Summaries of the presentations are given in Section 2, a summary of the discussions is provided in Section 3, a template of the proposed experimental data file is given in Section 4, and the conclusions are presented in Section 5. A list of actions is given in the Appendix. The agenda and participants list are given in Annex 1 and 2, respectively. The presentations can be found on the meeting website: https://www-nds.iaea.org/index-meeting-crp/PSFmeeting2022/.

References:

[1] S. Goriely, P. Dimitriou, M. Wiedeking, et al., The European Physical Journal A **55** (2019) 172.
[2] S. Goriely, S. Hilaire, S. Péru, K. Sieja, Phys. Rev. C **98** (2018) 014327.
[3] S. Goriely, V. Plujko, Phys. Rev. C **99** (2018) 014303.

2. Presentation Summaries

2.1. NDS PSF-Database 2019, J. Kopecky

The following deliverables have been sent to NDS or presented at the meeting:

1. Validation of the PSF-2019 database described in report INDC(NDS)-0868 (2022);
2. Extended <6.5 MeV> comparison with all PSF entries, sent as a mail insert;
3. The slide contribution: SF-CRP_JUKO_0112022_short.ppt;
4. Three files with graphical comparisons: ATLAS_OSLO_final+.docx; ATLAS_NRF+PG_final+.docx; ATLAS_NG_final+.docx.

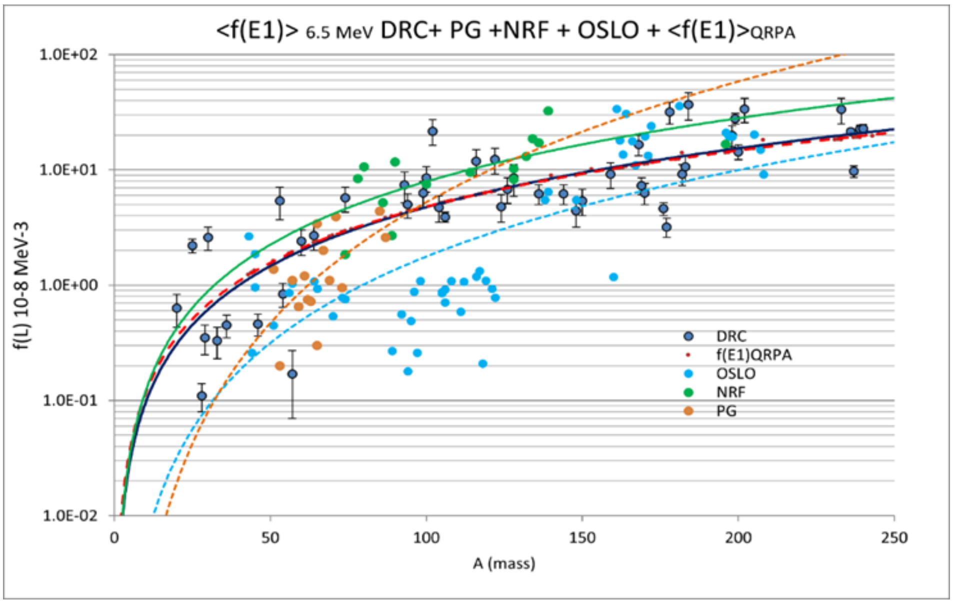

FIG. 2.1. Latest Version: Comparison between the E1 experimental DRC, PG, NRF and OSLO data, with the <<f(E1)>> systematics curve, all data has been averaged within the (6.5±0.5) MeV bin.

Note the remarkable agreement between the DRC and theoretical systematic predictions (the blue and red dotted curves are almost identical) in Fig. 2.1. The power trend fit is applied for other data, as an eye guiding tool. The NRF data (green points) show a reasonable agreement with the E1 systematics, the PG are in a limited A region (51 < A < 87) and are systematically lower which makes the power prediction (brown dotted curve) useless and finally the OSLO data (light blue points) show a sharp step dependence between data below and above A ~ 150 and the power curve is certainly not a proper fit.

2.2. Update on MSC, TSC and DICEBOX, M. Krticka

An update on three topics was presented: (i) development of the DICEBOX code, (ii) recent results from the two-step gamma cascade (TSC) experiments and (iii) recent results from multi-step gamma cascade (MSC) experiments. (i) DICEBOX: There have been no major changes in the code since it was made available on the IAEA web page. A small error was found a few weeks after publication and was fixed. (ii) TSC: No new data have been published on two-step cascades since 2019 (according to the presenter's knowledge). (iii) MSC: A summary of measurements published (or submitted) and results since 2019 were presented. This included data on gamma cascades (and results on the gamma-ray strength functions) in ^{196}Pt, ^{168}Er, and ^{96}Zr from data measured with the DANCE detector – the paper on ^{168}Er is currently in the review process, results on the other two isotopes have been published. Results for ^{168}Er are similar to those from other well-deformed rare-earth nuclei. The strength function in Pt shows a large “enhancement” for gamma ray energies near 6 MeV. In addition, results on gamma-ray strength functions from analysis of data on three uranium isotopes measured with the Total Absorption Calorimeter of the n_TOF experiment at CERN were also summarized. This experiment could serve as a “verification” of the experimental technique using the DANCE detector as data were acquired at a different facility with a different detector system. Fully consistent results have been obtained from both the detection setups.

2.3. Shape Method, M. Wiedeking

The Shape method [1] is a novel approach to obtain the slope of the Nuclear Level Density (NLD) and photon strength function (PSF) in the absence of neutron resonance spacing data. The method utilizes concepts from the average resonance proton capture approach and from the ratio and X2 methods [2], however, the identification of gamma-ray lines from discrete levels has been replaced with identification using diagonals in a particle-gamma matrix. The diagonals are directly related to the first-generation (or primary) matrix provided by the Oslo method. Cuts on excitation energy allow the identification of primary transitions to the low-lying levels as determined by the diagonals. The diagonals may appear in three variants containing either final states with the same spin and parity, or two or more specific final states or, in case of high-level density, many final states with a corresponding average final level energy and spin/parity.

For each excitation energy bin and for each pair of diagonals two data points are obtained which are internally normalized. This procedure is repeated for many different excitation energy bins yielding an equivalent number of pairs of data. These are then sewn together using a logarithmic interpolation. The robustness of the Shape method has been demonstrated for ^{56}Fe, ^{92}Zr and ^{164}Dy [1].

Most recently, the Shape method has been applied to nine Nd isotopes and a brief review of this work [3] was provided. Guttormsen et al. were able to determine the spin distribution through the determination of side-feeding into yrast states. It was shown that the spin distribution for (p,p’) and (d,p) reactions is greatly reduced over the intrinsic spin distribution. This leads to a reduction in slope for the NLD and PSF of affected nuclei. The Shape method was then applied and provided additional constraints by confirming the reduction in slopes.
One of the appealing aspects of the Shape method is that it can be applied to the same set of experimental data as that used to extract the NLD and PSF with the Oslo method. This is highly beneficial when the Shape method is used to specifically constrain the slope for the NLD and PSF from the Oslo method since it avoids unnecessary additional systematic uncertainties which would arise from different experiments.

References:

[1] M. Wiedeking, M. Guttormsen, A.C. Larsen et al., Phys. Rev. C **104** (2021) 014311.
[2] M. Wiedeking, L.A. Bernstein, M. Krtička, et al., Phys. Rev. Lett. **108** (2012) 162503.
[3] M. Guttormsen, K.O. Ay, M. Ozgur, et al., Phys. Rev. C **106** (2022) 034314.

2.4. Photon Strength Function Update on theoretical developments, S. Goriely

New theoretical developments on photon strength functions (PSF) since 2019 have been published. These concern essentially in-depth microscopic studies beyond the QRPA approximation and include methods like the Second RPA, Finite Fermi System theory, quasi-phonon model, equation of motions, both within the non-relativistic and relativistic mean-field framework, as well as more fundamental approaches like the shell and ab-initio models. These theoretical developments are only applied to a few specific cases and help to better understand the physics but can hardly be used for nuclear applications at the present time. An important development also concerns the calculation of the de-excitation strength from excited states. This was already available for light nuclei from shell model calculations and is now being developed within the QRPA approach by the Bruyeres-le-Chatel (France) group.

Only one new large-scale model including both E1 and M1 channels has been made available since 2019. This is a Skyrme-HFB plus QRPA spherical calculation based on the BSk27 Skyrme force. The QRPA calculation has been corrected including energy shift, spectrum broadening and deformation effects to reproduce at best the photodata. Additionally, a temperature dependence has been added to describe the de-excitation strength. Results for the E1 PSF can be found in Ref. [1]. The M1 PSF is in the process of being published. Since such a QRPA M1 calculation assumes spherical symmetry, it only describes the spin flip component and needs to be complemented by the M1 scissors mode for deformed nuclei, as for example described by the SMLO model, as well as by the M1 upbend when dealing with the de-excitation strength. Both the resulting E1 and M1 PSF have been compared with experimental data from the 2019 PSF library, namely, the photodata, ARC/DRC data, M1 scattering data, average radiative width data, and Maxwellian-averaged cross sections. They still need to be compared with Oslo, NRF and (p,γ) data as well as tested on multistep cascade data. After that, the BSk27+QRPA model could potentially be proposed as an alternative to the existing recommended and extensively tested PSF models, namely SMLO and D1M+QRPA.

References:

[1] Y. Xu, S. Goriely, E. Khan, Phys. Rev. C **104** (2021) 044301.

3. Summary of Discussions

- The systematic comparison of Photon Strength Function (PSF) data among each other and with models has revealed the following:
  - In certain measurements, the PSF may depend on the structure of the initial state, therefore it should be provided as a function of incident energy and spin-parity of the initial state in addition to the photon energy E_γ.
  - Understanding the fluctuations in the low-energy capture cross-section and PSF data could provide insight in disentangling the spin-parity dependence.
  - In analyzing thermal capture data, it is important to introduce corrections for missing transitions (weak ones). This can be done by comparing with nuclear level density models.
- PSF data collection: new data have been compiled for 33 new nuclei (since the release of the database in 2019):
  - Oslo data: ^{59,60,63}Ni, ^{116,120,124}Sn, ^{127}Sb, $^{142,144\text{-}151}$Nd, ^{151,153,155}Sm, ^{179}Hf, ^{192}Os;
  - β-Oslo method: ^{93}Sr, ^{74}Zn;
  - NRF method: ^{54}Fe, ^{66}Zn, ^{76}Ge, ^{87}Rb, ^{120}Sn, ^{206}Pb;
  - (p,p’) data from RCNP: ^{112,114,116,118,120,124}Sn.
- New method: measurements of (γ,$\gamma\gamma$) and (p,$\gamma\gamma$) from the University of Cologne can be used to extract (γ,abs) cross sections, and hence PSF. They should be considered for inclusion in the database.
- Open data, FAIR data and data preservation: in accordance with the FAIR (findable, accessible, interoperable and reusable) principles for sharing experimental data, as well as the need to preserve all the experimental information in the long term, including raw data, there were discussions on how and where these data could be stored for long-term purposes, as well as the kind of metadata that would be needed to ensure this data are findable and reusable. The raw data in reference were the primary gamma-matrices from Oslo measurements. Options that were discussed included local repositories maintained by the Oslo group and repositories maintained by the IAEA.

- Clarification of the relevance of thermal (n,γ) data of Groshev et al.(1968, 1969) extracted by the spectrum fitting method for the PSF database by J. Kopecky

  [Sec. note: Action 1 (see final table) completed before the end of meeting]

  The main active period of the Groshev group at the Kurchatov Institute of Atomic Energy in Moscow was 1956 - 1970. It was the first group which systematically measured the thermal cross sections and gamma ray transitions and spectra. For the gamma ray detection, the NaI - detectors and the Compton and pair magnetic spectrometers were used. The use of high-resolution Ge(Li) detectors started after 1968 with a limited amount of data in the period 1969 – 1971.

  There are many references from that period, primarily in Russian with translations in the Soviet Journal of Nuclear Physics. This double publication makes the search often difficult. Compilations of measured data (g-ray transitions and sg; no PSF values) were collected in compendium reports:

  Compendium I for Z ≤ 46 (Pd), G.A. Bartholomew et al., Nuclear Data Sheets (Section A), Vol. 3 (1967) p.367.

  Compendium II for 46 < Z < 67 (Ag - Ho), L.V. Groshev et al., Nuclear Data Tables (Nuclear Data Sect A), Vol. 5 (1968) p.1.

  Compendium III for 67 < Z < 94 (Er – Pu), L.V. Groshev et al., Nuclear Data Tables (Section A), Vol. 5 (1969) p.243.

  The collaboration between the Groshev and Chalk River groups (G.A. Bartholomew) continued, and after 1970 the Canadian group took over and became the leader in this field and included the Photon Strength Functions survey in Advances in Nuclear Physics (M. Baranger, E. Vogt, Eds), Vol. 7, Chapter 4, p. 229, as G.A. Bartholomew et al., Gamma-Ray Strength Functions in a compilation of methods and results.

  Conclusion: The capture data of Groshev have been superseded by many new measurements with better experimental tools and/or data analysis and there is no need to include them in the recent database. However, some PSF conclusions from Bartholomew's compilation may be individually considered.

  Remarks on the thermal capture databases:

  1. The standard compilation (with Eg, Ig, Jfp in partial format) is available in the NDS PGAA database (section EGAF).
  2. The present PSF THC database includes a selection of the recent individual references (also EGAF entries if needed) and the final outputs are partial PSF values. This database covers all light mass (A < 70) targets and only some relevant heavier ones to complete the PSF analysis with the superior DRC and ARC data.
  3. The extension to heavier target nuclides may be considered, if found necessary.

- Comment to Pt contribution and discussed plot of Milan Krticka which has initiated the Groshev search episode
  Firstly, a comparison with OSLO data:

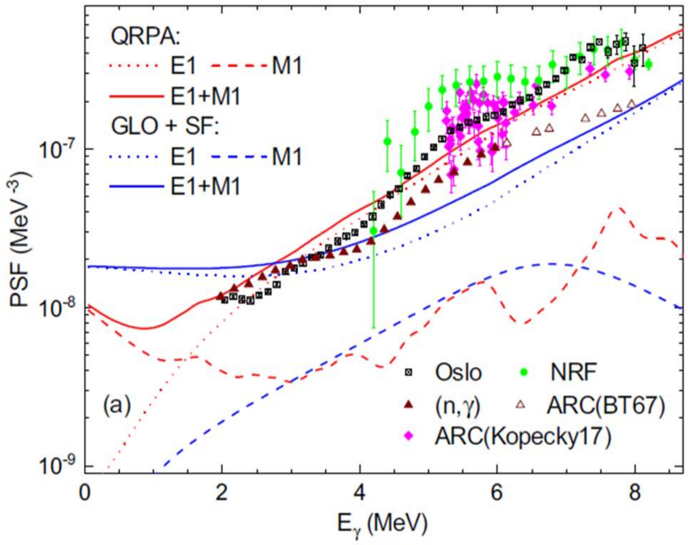

FIG 3.1. PSF data for ^{196}Pt compared with model calculations (D1M+QRPA and SMLO). For details see presentation by M. Krticka (https://www-nds.iaea.org/index-meeting-crp/PSFmeeting2022/).

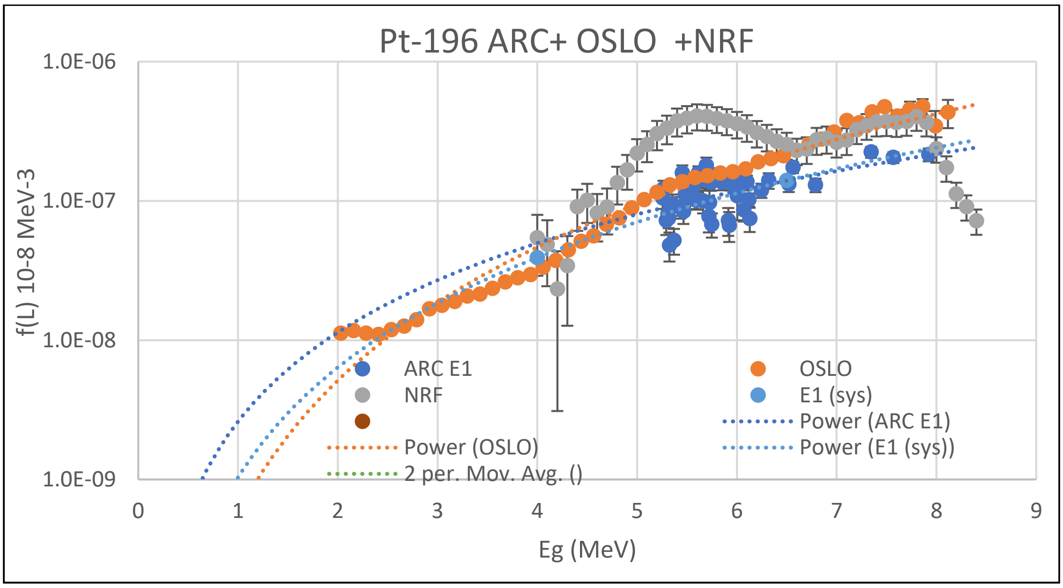

FIG 3.2. PSF data for ^{196}Pt compared with E1 systematics from ARC/DRC PSF data evaluation.

Note on plots: theoretical predictions are disregarded, and focus is only on the experimental points. The ARC19, OSLO and NRF data reasonably agree in both plots, there is a small difference in the NRF data, but the trend remains. The blue and red curves in Fig. 3.2 are trend power fits to ARC and OSLO data. The dashed curve is the f(E1) systematics.
The (n,γ) data in Fig. 3.1 are discussed further:

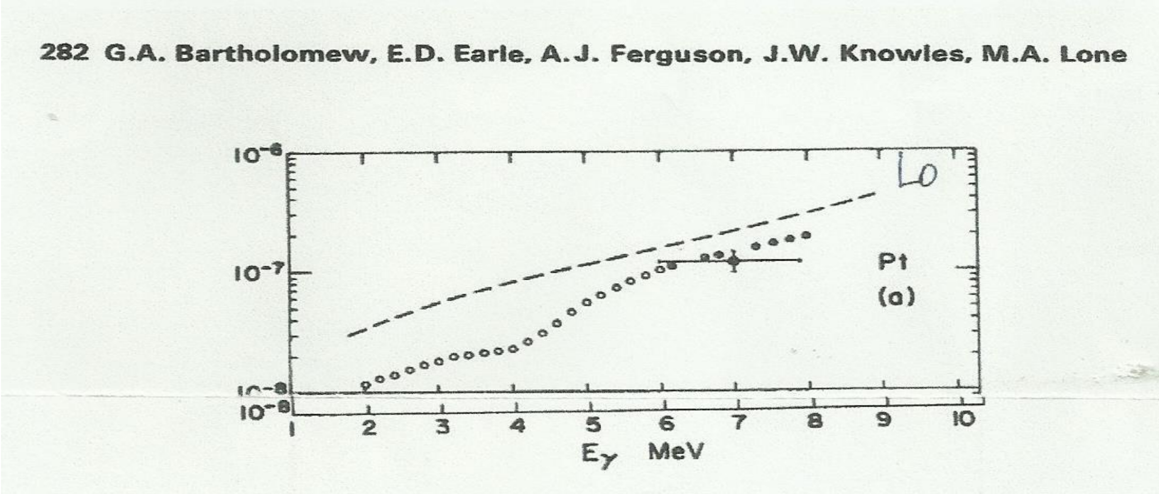

FIG 3.3 Original figure from Bartholomew et al. from which PSF data for ^{196}Pt in Fig.3.1 were extracted.

Explanation of Bartholomew's figure:

- The dashed curve is a standard Lorentzian.
- The open circles below 6 MeV have been derived from L.V. Groshev et al. (Sov. J. of Nucl. Physics 5 (1969) 563), using the spectrum fitting method developed at Chalk River by Aslam Lone, see in Advances in Nuclear Physics (M. Baranger, E. Vogt, Eds), Vol. 7, Chapter 4 p. 229, G.A. Bartholomew et al., Gamma-Ray Strength Functions) and specifically on page 259. Thus, they are not directly measured data points, but according to Aslam Lone: The PSF may be obtained by calculating the shape of spectral distribution with different trial strength functions until good agreement is achieved with the observed shape.
- The half-filled points are from Bollinger and Thomas boron ARC data from 1967.
- The solid point is the DRC average bin <6 – 8 MeV> value from C. Samour et al., Nuclear Physics A 121 (1968) 65.

4. Experimental data template

General requirements for submitting experimental derived PSF data sets for inclusion in the PSF database were agreed upon. The following experimental and/or model-dependent information should be provided along with the experimental PSF data:

1) Experimental uncertainty budget
2) Model-dependent uncertainties
3) Additional constraints
    a. Oslo method
        i. Normalization constraints (D_0, Γ_γ)
        ii. Shape method
    b. NRF
        i. NLDs and PSFs used initially in the cascade simulation
    c. (p,p')
    d. (p,γ)
        i. Normalization
    e. ARC/DRC/THC
        i. Normalization constraints (D_0, Γ_γ)
        ii. Completeness of decay scheme (THC)
    f. Photonuclear – tbd
4) Any additional measurement-specific constraints enhancing the reliability of the data.

5. Conclusions

Meeting participants discussed upcoming updates of the IAEA PSF database since its release in 2019, as well as the new model developments. A new independent method of validating the shape of the Oslo PSF data, namely the Shape Method, and its potential, was discussed. The importance of fluctuations and nuclear structure effects, especially for low-energy capture measurements, was emphasized. A new interactive and user-friendly interface for retrieving PSF data was presented.

Participants agreed to hold an online meeting on 14 March 2023 to monitor progress in the agreed assignments. An in-person meeting was decided to be held in October 2023.

All participants emphasized the usefulness and effectiveness of regular in-person meetings for the success of the project on evaluation and recommendation of PSF data.

APPENDIX

Actions from PSF meeting. In red are revisions made on 14 March 2023 (online meeting)

No	Responsible	Action	Deadline
1	Jura Kopecky	Clarify relevance of thermal (n,γ) data of Groshev et al (1968,1969) extracted by spectrum fitting method for the PSF database and update the database accordingly	31 Dec 2022 Done
2	Milan Krticka	Clarify whether the PSF data in Bartholomew's review paper should be added to the PSF database (related to Action #1)	31 Dec 2022 Done
3	Mathis Wiedeking	Systematic comparison of PSF data averaged over 1 MeV bins across the measured photon energy range, as a function of A, Z, N, N-Z, β_2, to identify trends and/or outliers: (n,γ), OM, NRF, (p,γ), (p,p'), photonuclear (in relevant energies)	14 March 2023 To be done pending #7
4	Mathis Wiedeking, Sunniva Siem, Ronald Schwengner, Jura Kopecky et al.	Investigate outliers found in Action #3 for possible experimental or model-dependent effects	31 July 2023 Pending #3
5	Stephane Goriely	Provide theoretical estimates in 1 MeV energy bins using the D1M+QRPA and SMLO models to compare with data systematics from Action #3	14 March 2023 Done
6	All	Use experimental data template to submit PSF data to the PSF database	Continuous [starting 1 Dec 2022]
7	Mathis Wiedeking, Vivian Dimitriou	Update of the PSF database	31 Dec 2022 Done a) Add HIgS data b) Add Oslo data (6-7 datasets) c) Check database by 1st May 2023
8	Mathis Wiedeking, Sunniva Siem, Vetle Ingeberg	Review multiple OM measurements of the same nuclide using different reactions and recommend data for evaluation	14 March 2023 New deadline: 30 June 2023
9	Mathis Wiedeking, Sunniva Siem, Vetle Ingeberg	Apply Shape Method on ^{96}Mo and ^{196}Pt to confirm the shape and normalization and compare with the other methods	18 Sep 2023 ^{106}Cd assigned to PhD student ^{96}Mo: may not be suitable data ^{196}Pt to be looked into / Ongoing

APPENDIX

No	Responsible	Action	Deadline
10	Mathis Wiedeking, Sunniva Siem, Vetle Ingeberg	Review all OM data and assign a quality indicator according to the agreed criteria outlined in the data template (full exp. uncertainty budget; model-dependent uncertainties; constraints (D_0,Γ_γ) and Shape Method)	18 Sep 2023
11	Mathis Wiedeking	Assess high-energy OM data to remove spurious effects due to low number of discrete states in energy resolution window	14 March 2023 Done
12	Mathis Wiedeking	Clarify with responsible person the normalization of the HIγS data to the ELBE data and the treatment of uncertainties	14 March 2023 Done
13	Mathis Wiedeking	Clarify with P. von Neuman Cosel the model dependencies associated with the PSF extracted from (p,p') data	14 March 2023 Follow-up email to be sent
14	Milan Krticka, Stephane Goriely	Test the new microscopic PSF model based on BSk27+QRPA with MSC spectra	14 March 2023 Ongoing - plan to complete by June 2023
15	Vivian Dimitriou	Contact Vladimir Plujko about updating the photonuclear PSF database	5 Dec 2022 In discussion
16	Arjan Koning Vivian Dimitriou	Convert the (γ,abs) evaluated data in the IAEA/PD-2019 library from ENDF-6 to simple x,y(±Δy) tabular form. Make these tables available on PD-2019 website	31 Dec 2022 Done ASAP
17	Vetle Ingeberg, Vivian Dimitriou	Collect and archive all raw data associated with the OM PSF measurements in a publicly available repository using suitable format – explore formats and repository	14 March 2023 Continue discussion
18	Sandile Jongile, IAEA-NDS	Create a new user-friendly interface for the PSF data retrieval allowing for search filters, different options for downloading the data, plotting capabilities, and reference search.	31 Dec 2023 [possibly extend by 3 months]
19	Vivian Dimitriou	Contact A. Tonchev about ^{206}Pb strengths for the PSF database	31 March
20	Jura Kopecky	Complete re-analysis of thermal neutron capture data for light nuclides (A<70)	18 September 2023
		Next meeting at IAEA	9-11 October 2023

ANNEX 1

IAEA Consultancy Meeting on the Evaluation and Recommendation of Photon Strength Function Data

28 Nov – 1 Dec 2022, IAEA, Vienna, CO234 (virtual component)

ADOPTED AGENDA

Monday, 28 November (10:00 – 17:00, open 09:45 Vienna time)

	Morning coffee at Nuclear Data Section (+ cookies)	
10:00 – 10:15	**Opening: Welcome** A. Koning / NDS Section Head	
	Election of Chair and Rapporteur(s), Adoption of Agenda	
10:15-12:30	**Participants' Presentations**	
	V. Dimitriou	Introduction – Goal and Scope of meeting
	J. Kopecky	PSF database: Systematic comparison of the Oslo vs the Neutron Capture method
	M. Wiedeking	Status of compilations – updates
12:30 -14:00	***Lunch***	
14:00 – 17:00	**Participants' Presentations cont'd**	
	M. Wiedeking	Shape method
	S. Siem	Developments in the Oslo method
	M. Krticka	Developments in the TSC and/or DICEBOX
		Coffee breaks as needed

Tuesday, 29 November (10:00 – 17:00, open 09:45 Vienna time)

09:00 – 12:30	**Presentations cont'd & Roundtable discussion**	
	S. Goriely	PSF Model developments
	A. Koning	PSFs in TALYS
	Roundtable discussion	
	1. Experimental methods	
	2. Evaluation - recommendation of PSFs	
	3. Models	
12:30 -14:00	***Lunch***	
14:00 – 17:00	**Roundtable discussion cont'd**	
		Coffee breaks as needed

18:30 Dinner at restaurant (separate information)

Wednesday, 30 November (10:00 – 17:00, open 09:45 Vienna time)

09:00 – 12:30	**Roundtable discussion:** PSF database interface
12:30 -14:00	***Lunch***
14:00 – 17:00	**Roundtable discussion:** Meeting recommendations
	Drafting of the meeting summary report
	Coffee breaks as needed

19:00 Dinner at restaurant (separate information)

Thursday, 1 December (10:00 – 17:00, open 09:45 Vienna time)

Mini Consultants' Meeting on New CRP (2024+)	
09:00 – 12:30	**New CRP on Nuclear Level Densities: goal, scope, work programme, participation**
12:30	**Closing of the meeting**
	Coffee break as needed

ANNEX 2

IAEA Consultancy Meeting on the Evaluation and Recommendation of Photon Strength Function Data

28 Nov - 1 Dec 2022

IAEA (hybrid)

PARTICIPANTS

Country		Name	Surname	Affiliation	Email
BELGIUM		Stephane	GORIELY	Université Libre de Bruxelles	stephane.goriely@ulb.be
CZECH REPUBLIC	🎧	Milan	KRTICKA	Charles University in Prague	rticka@ipnp.mff.cuni.cz
	🎧	Frantisek	BECVAR	Charles University in Prague	becvarfrank@icloud.com
GERMANY	🎧	Ronald	SCHWENGNER	Helmholtz-Zentrum Dresden-Rossendorf	rs@hzdr.de
NETHERLANDS		Iura	KOPECKY	JUKO Research	juko@planet.nl
NORWAY	🎧	Sunniva	SIEM	University of Oslo	sunniva.siem@fys.uio.no
SOUTH AFRICA		Mathis	WIEDEKING	iThemba Lab for Accelerator Based Sciences	m.wiedeking@ilabs.nrf.ac.za
	🎧	Sandile	JONGILE	iThemba Lab for Accelerator Based Sciences	sandilej@tlabs.ac.za
INT. ORGANIZATION		Paraskevi (Vivian)	DIMITRIOU	International Atomic Energy Agency	p.dimitriou@iaea.org
		Arjan	KONING	International Atomic Energy Agency	a.koning@iaea.org

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria
E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://nds.iaea.org