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EVALUATION OF PHOTON STRENGTH FUNCTION DATA

Summary Report of the IAEA Consultants' Meeting
IAEA Headquarters, Vienna, Austria
9 – 11 Oct 2023

Prepared by

Mathis Wiedeking
iThemba LABS
Cape Town, South Africa
Lawrence Berkeley National Laboratory
Berkeley, CA, USA

Paraskevi Dimitriou
International Atomic Energy Agency
Vienna, Austria

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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 Consultants' Meeting was held to discuss the evaluation and recommendation of Photon Strength Function data. 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.

March 2024

Contents

1. Introduction

Photon Strength Functions (PSFs) are fundamental nuclear parameters that describe the excitation and deexcitation of a nucleus by electromagnetic radiation at high excitation energies where nuclear levels overlap. The precise determination of PSFs is important, not only for understanding nuclear structure, but also for modelling nuclear reactions relevant to basic science and various applications, including nuclear astrophysics, nuclear energy, nuclear medicine, and more.

The IAEA Coordinated Research Project (CRP) F41032 which ran from 2016 to 2019 generated a Reference Database of Photon Strength Functions [1] comprising all available experimentally derived PSFs. In addition, the CRP also recommended two global models that were verified and validated [1], namely the D1M+QRPA [2] and SMLO [3].

As a follow-up activity, the IAEA is coordinating an effort to update the database and assess the quality of the available PSF data, by inferring systematic trends and performing evaluations. The goal is to provide the best values with valid uncertainty quantification to the user community. In parallel, a user-friendly retrieval interface based on web-based APIs is under development to facilitate the dissemination of the experimental and calculated PSFs.

To this end, the first Consultants' Meeting was held in late 2022 [4]. The 2nd IAEA Consultants' Meeting on Evaluation of Photon Strength Functions was held from 9 to 11 October 2023 to monitor the progress in these efforts. The meeting was hybrid and was attended by the following experts: S. Goriely (Belgium), O. Gorbachenko (Ukraine), V. Ingeberg (Norway), S. Jongile (S. Africa), J. Kopecky (Netherlands), M. Krticka (Czech Rep.), V. Plujko (Ukraine), S. Siem (Norway), R. Schwengner (Germany), M. Wiedeking (S. Africa), and IAEA staff A. Koning who, as NDS Head, opened the meeting, and P. Dimitriou, the scientific secretary, who gave a short introduction and set out the goals.

Presentation summaries are given in Section 2, a summary of the discussions is provided in Section 3, and the conclusions are presented in Section 4. A list of actions is given in the Appendix, and the agenda and participants list are given in Annex 1 and 2, respectively. Participants' presentations can be found on the meeting website: https://conferences.iaea.org/event/365/

References

[1] S. Goriely, P. Dimitriou, M. Wiedeking, et al., Eur. Phys. J. A **55** (2019) 172.
[2] S. Goriely, S. Hilaire, M. Girod, et al., Phys. Rev. Lett. **102** (2009) 242501.
[3] S. Goriely, V. Plujko, Phys. Rev. C **99** (2018) 014303.
[4] IAEA report INDC(NDS)-0869, 2023, https://www-nds.iaea.org/publications/indc/indc-nds-0869/

2. Presentation Summaries

2.1. "Neutron capture today" = description of actions and results from the report INDC(NDS) – 0886 (2023), J. Kopecky (JUKO Research)

The PSF extracted for the low mass A < 70 targets have been revisited, improved, and delivered to the Nuclear Data Section as an update to the 2019 IAEA PSF database [1]. The available information on direct capture (DC) contributions to neutron-capture reactions in this energy and mass region has been surveyed and the DC contribution to the total E1 and M1 primary strength has been determined.

Primary data: The improvements in recent thermal neutron capture measurements have been acknowledged and tested in detail for the case of ^{57}Fe. The main improvement is the extension of the low-energy gamma detection limit close to zero energy. The primary transitions were revised according to the improved decay schemes which are far more complete in both transitions and spin-parity assignments. This completeness of the decay schemes makes it possible to directly study the strength in the low energy "upbend" region instead of extrapolating the shape of the PSFs resulting from earlier obtained systematics. Preliminary comparisons of the different PSF experimental data suggest that the low-energy derived PSF data need to be re-analysed in conjunction with the high-quality thermal capture (THC) data.

Secondary data: The wealth of secondary transitions placed in the decay scheme with strong spin-parity assignments of similar accuracy as the primaries, allows us to study PSF data using the decay of bound levels with Ex < Bn. This is a novel approach that gives insight into the behaviour of the PSF not only with respect to the photon energy but also as a function of Ex energy with Ex lower than the maximum Ex=Einc+Bn. This method is still being tested.

References

[1] S. Goriely, P. Dimitriou, M. Wiedeking, et al., Eur. Phys. J. A **55** (2019) 172.

2.2. Update on theoretical photon strength functions, S. Goriely (ULB)

Following the actions agreed at the first Consultants' Meeting, the below points have been presented:

- theoretical estimates in 1 MeV energy bins using the D1M+QRPA and SMLO models have been sent in December 2022 to use them in the comparison with data systematics.
- the new microscopic photon strength function (PSF) model based on BSk27+QRPA have been sent to Milan Krticka in order to test the model prediction on multi-step cascade data. The conclusions are that for spherical nuclei the agreement is satisfactory, but the inclusion of SMLO M1 scissors model component for deformed nuclei leads to deviations that could be improved (see Section 2.3).
- A meeting with Jura Kopecky took place in July 2023 to discuss the extraction of PSF from thermal capture data and compare the predictions with theoretical predictions.
- The library 2023 has been tested for possible typos or mistakes. These have been communicated at the present Consultants' meeting.

Finally new developments in theoretical mean-field plus QRPA calculations of the de-excitation PSF made in collaboration with CEA/DAM (Bruyères le Chatel) were presented for the specific case of ^{98}Mo. The E1 and M1 de-excitation strength was extracted and compared with the photoabsorption PSF for different initial excitation energies. TALYS was accordingly updated to accommodate E1 and M1 PSFs that depend on both the photon energy and the initial excitation energy. The application of the newly determined ^{98}Mo de-excitation PSF in the calculation of the ^{97}Mo(n,g)^{98}Mo cross section was illustrated.

2.3. Comparison of BSK27 interaction with MSC data, M. Krtička (Charles Univ. Prague)

A new parametrization of the Skyrme force, called BSK27, has been recently proposed and a QRPA calculation of the PSF with this parametrization has been made by Stephane Goriely. To test the consistency of this parametrization, and especially of its M1 component, with experimental data, simulations of multi-step-cascade (MSC) spectra following resonance neutron capture have been performed. We compared simulated and experimental spectra from 17 different isotopes. For some of them, spectra from resonances of different spin and parity are available. 15 out of these 17 nuclei have already been checked earlier against predictions based on D1M Gogny interaction parametrization [1]. MSC spectra for two additional nuclei, ^{168}Er [2] and ^{196}Pt [3], have been published after the D1M tests were performed. The comparison to D1M predictions can be found in the respective publication for these two isotopes.

The QRPA calculation of PSFs with the Skyrme force is made with the spherical basis. This means that there is no strength corresponding to the orbital motion, i.e., no scissors mode contribution in the M1 PSF. The scissors mode parameterization from the SMLO model has thus been adopted although we indicated in our PSF review [4] that this scissors mode parameterization is likely not to be fully appropriate. However, possible combination of the low-energy M1 strength from D1M – which in general showed better agreement with MSC spectra than the SMLO one [4] with the BSK27 M1 at higher energies is difficult as we would need to match two curves originating from calculations.

It has been found that for spherical, or almost spherical nuclei (Mo and Cd isotopes), the reproduction of experimental MSC spectra with simulations is rather good if we talk about a global model that is not adjusted for a particular nucleus. However, there are some problems with reproduction of the MSC spectra in deformed nuclei. This is evidently due to the properties of the scissors' mode (mentioned above). Attempts to systematically shift the energy of the scissors mode and change its strength have been made. A reproduction of MSC spectra in several deformed nuclei was then better, but this was not always the case. In general, simulations with D1M force reproduced experimental spectra better.

In the case of ^{196}Pt, the reproduction is not acceptable with any QRPA PSF model. This is evidently due to triaxiality of this isotope. A strong resonance-like structure is typically seen in the decay of nuclei with A between about 190 and 205 at energy near 5.5 MeV. This structure is not predicted by any of the models tested so far.

References

[1] M. Krtička, et al., Phys. Rev. C **99** (2019) 044308.
[2] I. Knapová, et al., Phys. Rev. C **107** (2023) 044313.
[3] N. Simbirtseva, et al., Phys. Rev C **101** (2020) 024302.
[4] S. Goriely et al., Eur. Phys. J. A **55** (2019) 172.

2.4. Report on actions from previous meeting, M. Wiedeking (iThemba LABS & LBNL)

Over the last year, experimental PSF data extracted from the Oslo, (p,p'), NRF (including HIγS) methods were collected and forwarded to the IAEA for inclusion in the database update.

Three PSF numerical data for ^{197}Au, ^{198}Au and ^{195}Pt could not be retrieved and instead the published figures have been forwarded to the IAEA for digitization.

Currently, two ^{51}Ti data sets from the Oslo and beta-Oslo method are missing and we are in the process of obtaining these data sets.

Clarifications on the treatment of model and/or method uncertainties and normalizations were received for the HIγS and (p,p') data.

A quality indicator has been assigned to each Oslo method data set with 1 being the lowest and 5 the highest quality indicator. The quality indicator considers the following:

- Have all experimental uncertainties, including $\Gamma\gamma$ and D0 uncertainties, been included?
- Are full model uncertainties included?
- Are $\Gamma\gamma$ and D0 external normalization parameters available?
- Has the Shape Method been applied to the data?
- Has the work been published after 2014 following the Oslo Method software update?

A total of 172 data sets were considered and the quality indicators are distributed as follows:

- Quality Indicator 1: 67 data sets;
- Quality Indicator 2: 28 data sets;
- Quality Indicator 3: 26 data sets;
- Quality Indicator 4: 45 data sets;
- Quality Indicator 5: 3 data sets.

Oslo method measurements were reviewed to find suitable data for potential evaluation where the same nuclides were populated in different reactions. These are:

- $(^{3}He,^{3}He)^{162}Dy$ and $(^{4}He,^{4}He)^{162}Dy$
- $(^{3}He,^{3}He)^{161}Dy$ and $(^{4}He,^{4}He)^{161}Dy$
- $(d,d)^{181}Ta$ at 12.5 MeV and 15 MeV and $(^{3}He,^{3}He)^{181}Ta$

A systematic comparison of PSF data from the various methods averaged over 1 MeV bins across the measured photon energy range, as a function of A, Z, N, N-Z, and β_2, as well as separating the data for even-even, even-odd, odd-odd nuclei was presented. The goal is to identify trends and/or outliers.

2.5. PSF database – status and next steps, P. Dimitriou (IAEA)

A summary of the efforts undertaken at the IAEA to maintain the PSF database up to date and coordinate the various joint activities was given. One such activity involves the creation of a new user-friendly interface for the PSF database. The design of the database was proposed and the implementation by S. Jongile in collaboration with L. Marian (IAEA) is closely supervised with regular meetings and progress assessments. Finally, a new approach to evaluating the experimentally derived PSF data is proposed.

2.6. Development of a PSF Database, S. Jongile (iThemba LABS)

The Photon Strength Function (PSF) Interface was presented. The new interface stands as a robust web application explicitly crafted for the extraction, management, and presentation of PSF data currently available. This interface centralizes data primarily sourced from .dat and .readme files available on the IAEA's Photon Strength Function (PSF) webpage.

The highlights of this project are the enhanced query and visualization capabilities, features notably absent from the original webpage. The system is designed to upload data into a structured database, organizing information derived from both .dat files and associated README files. In doing so, the application ensures that every .dat file is paired with its corresponding .readme, melding the primary data, and metadata with its contextual backdrop.

Offering users an interactive platform, the interface facilitates database searches using specific fields like A (mass number), Z (proton number), Multipolarity, and method. Such queries give detailed visual representations, ranging from expansive data overviews to details on individual records. These visualizations, in the manner of graphs, present the data in an intuitive and comprehensible manner. Once a query is executed, users are presented with a dynamic table that encapsulates their search results. This table, augmented with column-specific search functionalities, provides users with the flexibility to refine and reorder their results, ensuring a streamlined browsing experience.

In conclusion, the Photon Strength Function Interface is an integral component of a larger initiative. While the current focus is on experimental data, future phases of the project will encompass theoretical data as well in addition to other enhancements.

3. Technical Discussions

3.1. Quality indicators

After the presentation of the quality indicators assigned to the OM PSF data, participants discussed the possibility to extend this assessment and assignment of quality indicators to the PSF data extracted from the other methods.

(n,γ) data: Jura Kopecky will look into how quality indicators could be assigned to DRC, ARC and THC PSFs.

Photonuclear data: it was agreed that PSFs should also be extracted from the evaluated photonuclear cross sections in the new IAEA Photonuclear Data Library 2019 that was released in 2020 [1]. These extracted PSFs should be considered as recommended PSFs in the corresponding energy region. It was agreed that after extracting these “recommended” PSFs, they should be compared with the experimentally derived PSFs for validation. Quality indicators could then be assigned to the experimental PSFs depending on how well they agreed with the “recommended” PSFs.

NRF data: Ronald Schwengner should be contacted about the possibility of assigning quality indicators to the experimentally derived PSF data. Mathis Wiedeking to contact Ronald Schwengner.

(p,γ) data: the lack of information concerning the experimental data and model uncertainties should automatically yield a quality indicator of 1 (lowest) for all compiled data.

(p,p’) data: as more such measurements are becoming available for extracting PSF data, it should be clarified if the most recently published data should be considered of the highest quality.

3.2. Evaluation of PSFs

The possibility to evaluate PSF data should be investigated for the few cases where we have (p,p’) data (^{96}Mo, even-even Sn isotopes, ^{208}Pb). In addition to statistical uncertainties, systematic uncertainties as well as correlations should be considered. Evaluation should be performed for E1, M1 and E1+M1 data. Evaluators of IAEA (Capote, Schnabel) to be contacted to advise on how to proceed with evaluation using no-model approach and Bayesian inference.

Hold a meeting with experimentalists at the Oslo Workshop (27 to 31 May 2024) to prepare for detailed discussions with evaluators at the time of the CNR*24 workshop at the IAEA (8 to 12 July 2024).

3.3. Data file format

Add a compiler field to the data files in addition to the author field. The author field should include the full reference of the original publication. The compiler field should include the name(s) of the persons who extracted the PSF data and compiled them in an appropriately formatted data file for inclusion in the PSF database.

Adopted style for author reference: follow EPJA referencing style as in the PSF 2019 publication [1]. Action on M. Wiedeking: generate appropriate datafiles for OM, NRF, pp PSF data. Action on V. Dimitriou: generate appropriate datafiles for pg, ARC, DRC, and THC PSF data. Action on O. Gorbachenko to do the same for the photonuclear PSF datafiles.
Extensions used to identify the various PSF datafiles corresponding to the same isotope, multipole strength and method should be uniform across the database. V. Dimitriou and M. Wiedeking to propose a global scheme applicable to all the PSF datafiles. Possible exceptions could be the

photonuclear datafiles due to the shear number of files already generated using year of publication and first three letters of author's name to distinguish the files.

3.4. New PSF database interface

The following additions/modifications were proposed:

- Add min and max energy infilter and table,
- Larger fonts in plots,
- Standard scientific log scale in plot,
- Add year in table,
- Add file name with hyperlink to readme file,
- Use filename in plot legend,
- Use filename in table,
- In the individual plots include all available information.

References

[1] S. Goriely, P. Dimitriou, M. Wiedeking, et al., Eur. Phys. J. A **55** (2019) 172.

4. Conclusions

Meeting participants discussed delivery and outcome of the actions assigned at the previous meeting and developments related to the new interactive interface of the PSF database. They agreed that while studying systematic global trends in the data is useful for revealing outliers and biases in the PSFs extracted from the different methods, the evaluation of the various PSF data and recommendation of best values for the user community should be the goal of the effort. New assignments were made to complete the systematic comparison of the different data, the assessment of the data with quality indicators, and to initiate discussions on the evaluation of the PSF data. Efforts will be made to complete the new PSF retrieval interface by the next meeting scheduled for autumn 2024.

Participants agreed to meet at both the Oslo and CNR* workshop in 2024 to monitor progress.

.

Appendix: List of Actions

Actions revised on 10 October 2023

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)	31 October 2023 Include all methods in same plots for comparisons. Prepare the plots and share with group.
4	All	Investigate outliers found in Action #3 for possible experimental or model-dependent effects	15 January 2024 At dedicated Online meeting
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 in the PSF database	Continuous
7a	Mathis Wiedeking, Vivian Dimitriou	Update of the PSF database	01 Dec 2023 Upload of July 2023 submissions and corrections.
7b	Vivian Dimitriou Mathis Wiedeking	Address issues in the datafiles reported at October 2023 meeting	01 Dec 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 Done
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	31 Dec 2024 ^{106}Cd assigned to PhD student ^{96}Mo: not suitable data ^{196}Pt to be looked into
10a	Mathis Wiedeking, Sunniva Siem, Vetle Ingeberg	Review all OM data and assign a quality indicator according to the agreed criteria outlined in data template (full exp. uncertainty budget; model-dependent uncertainties; constraints (D_0,Γ_γ) and Shape Method)	18 Sep 2023 Done

No	Responsible	Action	Deadline
10b	Mathis Wiedeking	Discuss with Oslo group to make quality indicator spreadsheet publicly available	15 December 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
13a	Mathis Wiedeking	Clarify with P. von Neuman Cosel the model dependencies associated with the PSF extracted from (p,p') data	14 March 2023 Done
13b	Mathis Wiedeking	Include clarifications for (p,p') and HIgS data in readme files.	15 December 2023
14	Milan Krticka, Stephane Goriely	Test the new microscopic PSF model based on BSk27+QRPA with MSC spectra	14 March 2023 Done
15a	Vivian Dimitriou	Contact Vladimir Plujko about updating the photonuclear PSF database	05 Dec 2022 Done
15b	Vladimir Plujko Oleksandr Gorbachenko	Update photonuclear PSF	15 December if possible else 31 March 2024.
16	Arjan Koning	Convert the (γ,abs) evaluated data in the IAEA/PD-2019 library from ENDF-6 to simple x,y($\pm\Delta$y) tabular form.	31 Dec 2022 Done
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	Continue discussion
18a	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 Done
18b	Sandile Jongile Ludmila Marian IAEA-NDS	Release beta-version for public testing	31 January 2024
19	Vivian Dimitriou	Contact A. Tonchev about ^{206}Pb strengths for the PSF database Contact Johan Isaak on how to extract PSF from cross sections.	31 March 2023 Done 31 December 2023
20	Jura Kopecky	Complete re-analysis of thermal neutron capture data for light nuclides (A<70)	18 September 2023 Done

No	Responsible	Action	Deadline
21	Vivian Dimitriou Mathis Wiedeking Oleksandr Gorbachenko	Include compiler field with compiler name in addition to author and publication field in the datafiles.	15 December 2023
22	Mathis Wiedeking	Include previously discarded data files	31 March 2024
23	Mathis Wiedeking	Update OM readme files with information for pre-2013 cases	15 December 2023
24	Jura Kopecky	Quality Indicators DRC, ARC and THC	31 March 2024
25	Vladimir Plujko Oleksandr Gorbachenko	Investigate and compare PSF extracted from evaluated photonuclear data. Identify problems/difficulty and obtain quality indicator.	31 March 2024
26	Ronald Schwengner	Quality indicators for NRF measurements. Wiedeking to contact RS.	31 March 2024
27	Stephane Goriely	Obtain absolute value of PSF for ^{51}Mn in (p,g) reactions with TALYS.	15 November 2023
28	Mathis Wiedeking	For (p,p') is the first and last data set of the same quality?	15 December 2023
29	Vivian Dimitriou Sandile Jongile	Provide file a booklet (file) for all available methods and nuclei.	31 January 2024
30	Vetle Ingeberg Mathis Wiedeking Vivian Dimitriou Jura Kopecky	Harmonise datafiles for identification. and come up with scheme for OM files. For p,g and ARC DRC	15 December 2023 15 January 2024
31	All	Online meeting prior to Oslo workshop for review of actions.	08 April 2024

ANNEX 1

IAEA Consultancy Meeting on the Evaluation of Photon Strength Function Data

9 – 11 October 2023
IAEA, Vienna
MOE10 (virtual component)

ADOPTED AGENDA

Monday, 9 October (10:00 – 17:00, open 09:45 Vienna time)

	Morning coffee at Nuclear Data Section	
10:00 – 10:15	**Opening and Welcome A. Koning / NDS Section Head**	
	Election of Chair and Rapporteur(s), Adoption of Agenda	
10:15-13:00	**Participants' Presentations**	
	J. Kopecky	"Neutron capture today" = description of actions and results from the INDC(NDS)-0886 (2023) *tbp*
	S. Goriely	Update on theoretical photon strength functions
	M. Krticka	Update on PSFs from coincidence measurements following neutron capture
13:00 -14:30	***Lunch***	
14:30 – 17:00	**Participants' Presentations cont'd**	
	M. Wiedeking	Report on assignments
	V. Dimitriou	Review of assignments and next steps
		Coffee breaks as needed

18:30 Dinner at a restaurant (separate information)

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

10:00 – 12:30	**Roundtable discussion**
	1. Experimental methods – assessment
	2. Evaluation – method ?
	3. Systematics
	4. Updating the database
12:30 -14:00	***Lunch***
14:00 – 17:00	**Roundtable discussion cont'd**
	Coffee breaks as needed

Wednesday, 11 October (9:00 – 12:10, open 08:45 Vienna time)

09:00 – 12:00	**New PSF retrieval platform**	
	S. Jongile	Presentation and discussion
12:00	**Closing of the meeting**	
		Coffee break as needed

ANNEX 2

IAEA Consultancy Meeting on the Evaluation of Photon Strength Function Data

9 - 11 October 2023
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 Prague	krticka@ipnp.mff.cuni.cz
GERMANY		Ronald	SCHWENGNER	Helmholtz-Zentrum Dresden-Rossendorf	rs@hzdr.de
NETHERLANDS		Jiri	KOPECKY	JUKO Research	juko@planet.nl
SOUTH AFRICA		Mathis	WIEDEKING	iThemba Lab for Accelerator Based Sciences Lawrence Berkeley National Laboratory	m.wiedeking@ilabs.nrf.ac.za mwiedeking@lbl.gov
		Sandile	JONGILE	iThemba Lab for Accelerator Based Sciences	s.jongile@ilabs.nrf.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
		Ludmilla	MARIAN	International Atomic Energy Agency	l.marian@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