

Nuclear Data Newsletter



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Contents			
From the Section Head	1	NDS Meeting Reports	3
Announcements	2	Selected Charts, Reports and Documents	7
Computer Codes, Data Libraries and Web News	3	In Memoriam	7

From the Section Head

It seems a long time ago, but it was mid-January (which in Vienna means fog and a few degrees above zero, day after day), when we organized our biennial Technical Meeting on Anti-neutrino spectra applications. This meeting, coordinated by Vivian Dimitriou, enjoyed a large attendance, both in person and virtual.

We held a Consultancy Meeting on Level densities. A few world experts were invited to discuss the set-up of a level density Coordinated Research Project that we will start next year.

The major event from our Atomic and Molecular Data Unit this year was the 21st meeting on Atomic Processes in Plasmas. This is a biennial conference focusing on the fundamental physics of various plasmas across a wide range of densities and plasmas (from industrial and medical plasmas up to conditions relevant to nuclear fusion energy research). There were 127 participants from 30 countries.

The Nuclear Reaction Data Centre network held its annual meeting to discuss the compilation aspects of the EXFOR database. In recent years, there seems to be an increased interest in the EXFOR database outside the NRDC community, and this gave rise to discussions on the accessibility of the EXFOR data in different forms. Several efforts to make EXFOR computationally readable are now underway.

The Nuclear Data Section will undergo some personnel changes as the following two topics will make clear.

This Newsletter contains a summary of several EXFORrelated products that are currently being released. They are the result of an effort by Viktor Zerkin, who will retire at the end of October, in making the EXFOR database available to users in more different ways.

New approaches for streamlining nuclear reaction data through the nuclear data pipeline were addressed in a Consultancy Meeting on GNDS/FUDGE/TAGNDS, where in particular the changes required in the TALYS output to make it suitable for further automation and Artificial Intelligence (AI) applications were addressed. This was coordinated by Jean-Christophe Sublet in what will be one of his final meetings for the Section, as he will retire at the end of November.

The above two items also mean that those interested should keep an eye on the IAEA vacancy site!

A Consultancy Meeting was held for a Comprehensive European Plan to Acquire and Curate Nuclear Data. One of the outcomes of the meeting will be a side event at the General Conference (25-29 September 2023) on the importance of nuclear data for various technological applications. I will report about that in the next Newsletter.

All the best!

Arjan Koning, SH-NDS

Announcements

Dr Roberto Capote Noy honored with Oppenheimer Coin



Mr William Hayward Tobey and Dr Roberto Capote Noy with the Oppenheimer coin

Roberto Capote Noy received the Oppenheimer coin in an award ceremony on 12 April 2023. The coin was awarded by Mr Thomas Mason, Director of Los Alamos National Laboratory (LANL) and handed over by Mr William Hayward Tobey, Director of the LANL Office of National Security and International Studies.

The Oppenheimer coin stands for highest accomplishments in scientific excellence and technical leadership and was awarded in acknowledgement of the organization and coordination of the IAEA International Nuclear Data Evaluation Network (INDEN), and its contribution to the US evaluated nuclear data libraries, which are used worldwide. With Dr Capote Noy's ability to bring experts together along with his research expertise, the IAEA Nuclear Data Section projects - INDEN, IAEA standards and reactor dosimetry have advanced the US and international research goals in nuclear criticality safety and non-proliferation.

We congratulate him on this prestigious award.

High Honor for Syed M. Qaim



Professor Syed M. Qaim of the Forschungszentrum Jülich (FZJ) and University of Cologne in Germany recently received the President's Award of the World Council on Isotopes (WCI) in recognition of his sustained pioneering work on nuclear data

related to development of accelerator-based radionuclides for medical applications. The award was presented to him during the 11th International Conference on Isotopes, organized by the Canadian colleagues under the umbrella of WCI, in July 2023, in Saskatoon, Saskatchewan, Canada.

Syed Qaim has been in contact with several sections of the IAEA for the last 40 years. He taught at several training courses, undertook expert missions, and trained 14 IAEA-Fellows at FZJ. With the NDS he maintained a special relationship. He was the German Member in the International Nuclear Data Committee (INDC) for 14 years, therefrom for about 5 years as its Chairman. During this period, he advised the NDS in its efforts to diversify its nuclear data programme by including non-energy related applications as well. In particular, he provided strong guidance and support with nuclear data for medical applications. He also co-directed three Workshops on this topic held at the ICTP Trieste.

Prof. Qaim officially retired many years ago, but he is still active both in teaching and research. In recent years he received many honours. The present award is implicitly a recognition of his lifetime work. The NDS congratulates him and wishes him all the best for the future.

Computer Codes, Data Libraries and Web News

Off-line distribution of whole EXFOR

1. X4Pro - universal, fully relational EXFOR database SQLite; includes data points in original and computational forms, data for automatic renormalization by new monitor cross sections and decay data. The package includes examples in Python and Fortran. Now issued for whole EXFOR data library: <u>https://nds.iaea.org/cdroms/#x4pro1</u>.

2. X5 - comprehensive EXFOR in JSON. X5 presents EXFOR meta-data (codes and free text), information from EXFOR dictionaries, data in original and computational forms, data for automatic renormalization, reaction definition in ENDF MF.MT terms. X5 files are stored in sub-directory structure: one JSON file per EXFOR Entry, and do not require any database support. The package includes examples of Python codes to build data indices, plot using the Plotly package, and a JS-interpreter presenting JSON files as interactive tree in the user's Webbrowser.

Download: https://nds.iaea.org/cdroms/#x5json.

3. C5 - full EXFOR translated to C5. Computational format C5 extends C4 format which was designed for comparison of experimental data with evaluations and therefore uses ENDF coding (MF-MT-ZA). C5 is generated by a code "x4toc5.java", based on universal EXFOR-Java parser using EXFOR Dictionaries, EXFOR-ENDF translation Dictionaries, Archive of Monitors, Decay-Data from ENSDF and other supplementary data. C5 extensions include statistical and systematic uncertainties, and optionally may include monitor data, renormalized data, and results of some operations. Five versions of data are available:

- EXFOR-C5v0: (using the default from C4)
 - converted incident energy from C.M. to Lab
 - converted Rutherford-Ratio to B/SR
- EXFOR-C5v1: options from EXFOR-C5v0 + - datasets with unknown MT are included (MT=0)
- EXFOR-C5v2: options from EXFOR-C5v0 +
 - angle and data: C.M. to Lab. (for MT4)
 - replaced Q-Value by E-Level
 - reset MT51, 601, 651, etc. by MT+iLevel
 - sorted data
- EXFOR-C5v3: options from EXFOR-C5v2 + - auto-renormalized by modern monitor CS data
- EXFOR-C5v4: options from EXFOR-C5v3 + - auto-renormalized using modern Decay-data.

The package includes a script for creating single C5 file to provide backward compatibility with XC4 data distributions for WPEC-SG30 members, Empire and TALYS codes, examples in Python creating data index and cross section plotting with Plotly. Download: https://nds.iaea.org/cdroms/#c5.

IBANDL-Archive

Since beginning of 2023, the full content of Ion Beam Analysis Data Library (IBANDL) is available for download. The distribution includes original R33 files in sub-directory structure, an index of datasets as a CSV file, history of updates. Versions of the data library are stored with timestamps. Available on:

https://nds.iaea.org/public/IBANDL-Archive/.

The data are issued under the license: Creative Commons - Attribution 4.0 International (CC BY 4.0)

NDS Meeting Reports

(TM = Technical Meeting, RCM = Research Coordination Meeting, CM = Consultants' Meeting, WS = Workshop, CRP = Coordinated Research Project)

Consultancy Meeting on Nuclear Level Densities

26-28 June 2023, Vienna, Austria Scientific Secretary: P. Dimitriou 9 participants and IAEA staff



Participants of the CM

At this Consultancy Meeting participants discussed the scope, methods, outputs, and work program of a new planned CRP on Improving Nuclear Level Densities for Applications. The status of derived experimental nuclear level density data and global models was reviewed, and potential improvements to the RIPL level density module were recommended. A summary of the meeting will be available in INDC(NDS)-0883.

Consultancy Meeting on GNDS/FUDGE/TAGNDS

22-25 May 2023, Vienna, Austria Scientific Secretary: J.-Ch. Sublet 9 participants and IAEA staff



Participants of the CM

The main aim of this Consultants' Meeting was to assess the actual capabilities, successfully deployed methods, tools and protocols, and future needs in terms of nuclear model code outputs in the General Nuclear Data Structure (GNDS) and their processing into useful application forms. It also focused on building a modern durable partnership between fundamental sciences and application needs, in support of high-fidelity multi-physics simulation efforts.

The meeting brought together different experts able to determine and support the necessary enhancements, processes and schemas foreseen for the multiple applications in energy, non-energy, earth and life sciences to be served by GNDS and in support of high-fidelity Multiphysics simulation efforts. Eight experts attended (physically) the meeting.

21st Atomic Processes in Plasmas (APiP) Conference

15-19 May 2023, Vienna, Austria Scientific Secretary: C. Hill127 participants and IAEA staff



Participants of the APIP Conference

This biennial meeting was first held in 1977 as an American Physical Society Topical Conference but is now an international event, albeit one heavily attended by participants of the US National Laboratories. The COVID-19 pandemic led to its postponement from 2021. The APiP conference focuses on atomic processes that are involved in the study of plasmas over a wide range of densities and temperatures (eV to a few keVs). The event consisted of 57 invited and contributed oral presentations and 47 posters. The prize for the best poster was awarded to Roshani Silwal from Appalachian State University by the DDG-NA at a short presentation.

More details, including the Book of Abstracts are available at <u>https://amdis.iaea.org/meetings/apip21/</u>.

27th Technical Meeting of the Atomic and Molecular Data Centres Network

15-19 May 2023, Vienna, Austria Scientific Secretary: K. Heinola 19 participants and IAEA staff



Participants of the DCN Meeting

The 27th Meeting of the Data Centres Network (DCN) was attended by 16 participants (3 virtual) representing Member States Argentina, Australia, China, France, Italy, Japan, Korea, Lithuania, Russia, United Kingdom and USA. The DCN meeting was organized in conjunction with the APiP Conference (see information on 21st APiP) held at IAEA Headquarters and allowing DCN and APiP participants to attend both events. The DCN meeting reviewed current activities of the national data centres and discussed acute data requirements and activity needs raised within the nuclear fusion community. The importance of data related to tungsten was stressed. Its excited ground states, electron ionization and charge states have an increasing importance as the application of tungsten as fusion reactor first-wall material is expected to increase in the near future. Moreover, impurity species puffed into the edge plasma and separatrix region play an important role in energy mitigation at the wall and the corresponding atomic and molecular data needs were reviewed. The topic of organizing an uncertainty workshop was reviewed and next steps outlined: a code comparison and error propagation for N as a test case was planned due to its ITER relevance and suitable complexity.

Technical Meeting of the International Network of Nuclear Reaction Data Centres

9-12 May 2023, Vienna, Austria Scientific Secretary: N. Otsuka 30 participants and IAEA staff



In-person and virtual participants of the NRDC

24 participants representing 12 cooperative Centres from seven Member States (China, Hungary, Japan, Korea, Russia, Ukraine and USA) and two International Organizations (NEA, IAEA) as well as a participant from Kazakhstan were represented at the meeting. Main topics of the present meeting were the EXFOR transmission statistics, EXFOR coverage and quality control, revision of coding rules and manuals, EXFOR/CINDA dictionaries as well as improved tools for compilation and dissemination.

The JAEA Nuclear Data Centre started compilation of neutron-induced reaction data measured at J-PARC and measured with their participation, on a trial basis, for the articles published in 2019 and later. As JAEA stabilized the compilation activity, the meeting agreed to transfer compilation responsibility of the relevant data to JAEA officially.

NDS presented development of a new Python script producing the EXFOR/CINDA dictionary via a dictionary in JSON. This dictionary is currently just an intermediate file, but it could be useful for software engineers and end users.

To resolve the issue of differences in the same EXFOR entry obtained from two difference centres, NDS prepared the "EXFOR Master File" in 2005. This file was continuously updated by NDS and shared among the centres as a "backup" maintained by each centre locally. The participants supported releasing EXFOR Master File to the public with version control by DOI (document object identifiers). NDS is currently working on it.

A summary report of the meeting, including the list of the 32 conclusions and 95 actions is available as INDC(NDS)-0879. All progress reports, working papers and slides are available on the meeting web page (http://nds.iaea.org/nrdc/nrdc 2023/).

Consultancy Meeting on the Needs for a Comprehensive European Plan to Acquire and Curate Nuclear Data

25-27 April 2023, Vienna, Austria Scientific Secretary: P. Dimitriou 8 participants and IAEA staff



Participants of the CM

This Consultants' Meeting was held at the IAEA to discuss the needs for a comprehensive European plan to acquire and curate nuclear data. Participants representing nuclear data groups, the nuclear physics community (NuPECC), and the existing funding agency (EURATOM), reviewed the current status of nuclear data curation in Europe, including coordination, funding, and capacity building. A summary of the discussions as well as the list of recommendations and actions will be included in the report of the meeting as INDC(NDS)-0875.

Consultancy Meeting to Plan the Molecules in Edge Plasmas Coordinated Research Project

20-21 April 2023, Vienna, Austria Scientific Secretary: C. Hill 13 participants and IAEA staff

A two-day Consultancy Meeting was held, in hybrid format, to set out the scope and planned outputs of the newly approved Molecules in Edge Plasmas CRP, which is to hold its first Research Coordination Meeting later this year. Amongst other objectives, it will establish a trusted repository of evaluated data concerning the molecular species, particularly metal and nitrogen hydrides, relevant to the diagnostics and safety assessment of fusion energy reactors.

More details are available at

https://amdis.iaea.org/meetings/molecules-cm/.

First Research Coordination Meeting on Atomic Data for Injected Impurities

27-29 March 2023, virtual eventScientific Secretary: C. Hill13 participants and IAEA staff

The first Research Coordination Meeting of the AMD Unit's new CRP on Atomic Data for Injected Impurities in Fusion Plasmas was held in virtual format. Participants met online and reviewed Workplans for the calculation and evaluation of new data sets essential to the modelling of such impurity species, which are important for redistributing the power load on plasma-facing components, mitigating plasma disruptions and for diagnostic purposes in magneticconfinement fusion devices.

Second Research Coordination Meeting on Hydrogen Permeation

22-24 February 2023, Vienna, Austria Scientific Secretary: K. Heinola 33 participants and IAEA staff



In-person and virtual participants of the RCM

The 2nd Research Coordination Meeting of the CRP on Hydrogen Permeation in Fusion Materials was attended by 29 participants (11 online) representing 15 Member States. Participants presented progress reports of each project and the status of the ongoing round-robin activities were reviewed. Scientific discussions focused on analyses of experimental hydrogen permeation and retention findings on various fusion materials (EUROFER97, irradiated and nonirradiated tungsten, etc.) as well as on computational findings and data needs, such as the potential barriers and energy landscapes at material interfaces and joints. The latter concerns especially the fusion reactor tungsten-based armour components' W-Cu interfaces, which have been scrutinized within this CRP by utilizing quantum mechanical tools, such as the Electron Density Functional Theories (DFT). Samples resulting from the experimental round-robin activity of neutron-irradiated fusion materials (collaboration with SCK-CEN BR2 reactor at Mol. Belgium) are under irradiation and sample distribution for hydrogen permeation experiments is expected to take place in the second half of 2023.

Consultancy Meeting on Reaction Modelling and Nuclear Data Evaluation using EMPIRE

6-10 February 2023, Sao Jose dos Campos, Brazil Scientific Secretary: R. Capote Noy 6 participants and IAEA staff

The EMPIRE system is widely used in nuclear data evaluations, in particular with many evaluations performed within the International Nuclear Data Evaluation Network (INDEN). The latest major release happened ten years ago. The EMPIRE code plays a critical role in evaluations of neutron induced reaction on heavy nuclides, particularly on actinides. The participants of this Consultants' Meeting met to coordinate a new release of the EMPIRE system including the latest developments in theory and data processing capabilities. The summary of the discussions and outcomes of the meeting will be published as INDC(NDS)-0874.

Technical Meeting on Nuclear Data Needs for Antineutrino Spectra Applications

16-20 January 2023, Vienna, Austria Scientific Secretary: P. Dimitriou 50 participants and IAEA staff



In-person and virtual participants of the TM

This was the 2nd Technical Meeting on nuclear data for antineutrino spectra applications and was attended by 50 participants in person and virtually.

The participants reviewed the status of reactor antineutrino facilities and experiments, antineutrino flux and spectra modelling, nuclear data and their associated uncertainties, with relevance to both basic research - Standard Model physics and beyond the Standard Model searches- and applications in areas such as nuclear non-proliferation.

The progress that has been made since the first meeting held in 2019 was assessed, and areas for improvement and priority actions to reach the recommended objectives were identified. Special reference was made to the Snowmass 2021 White Paper, as well as to requirements for open research data and data preservation.

Selected Charts, Reports and Documents

INDC(NDS)-0747 Long-term International Collaboration to Improve Nuclear Data Evaluation and Evaluated Data Files, Summary Report of the Technical Meeting, 18-21 December 2017, prepared by D. Brown, D. Rochman and R. Capote Noy, March 2023.

INDC(NDS)-0858 Generating an ACE-formatted Photonuclear Data Library from IAEA/PD-2019 using ACEMAKER, prepared by D. Lopez Aldama and R. Capote Noy, May 2023.

INDC(NDS)-0863 Compilation of Nuclear Data Experiments for Radiation Characterization, Summary Report of the Technical Meeting, 10-14 October 2022, prepared by L. Giot, O. Buss, M. Gilbert, A. Kahler and J.-Ch. Sublet, March 2023.

INDC(NDS)-0865 Neutron Data Standards, Summary Report of the 24th Technical Meeting, 18-22 October 2022, prepared by D. Neudecker and G. Schnabel, August 2023.

INDC(NDS)-0867 International Network of Nuclear Structure and Decay Data (NSDD) Evaluators, Summary Report of the 24th Technical Meeting, 24-28 October 2022, prepared by J. Chen, A. Negret and P. Dimitriou, May 2023.

INDC(NDS)-0869 Evaluation and Recommendation of Photon Strength Function Data, Summary Report of the Consultants' Meeting, 28 November – 1 December 2022, prepared by S. Goriely, M. Wiedeking and P. Dimitriou, July 2023.

INDC(NDS)-0875 Needs for Comprehensive European Plan to Acquire and Curate Nuclear Data, Summary report of the Consultants Meeting, 25-27 April 2023, prepared by G.-E. Koerner, P. Dimitriou, et al., August 2023.

INDC(NDS)-0876 Summary Report from the Consultants' Meeting on GNDS/FUDGE/TAGNDS, 22-25 May 2023, prepared by C. Mattoon and J.-Ch. Sublet, July 2023.

INDC(NDS)-0879 International Network of Nuclear Reaction Data Centres, Summary Report of the Technical Meeting, 9-12 May 2023, prepared by N. Otuka and D. Brown, June 2023.

INDC(NDS)-0881 21st Atomic Processes in Plasmas Conference, Summary Report of a Technical Meeting, 15-19 May 2023, prepared by C. Hill, July 2023.

INDC(NDS)-0882 Verification of the Energy Dependence of the GEF Code Fission Product Yields Using Delayed Neutron Temporary Data, prepared by

D.E. Gremyachkin, A.S. Egorov, K.V. Mitrofanov,

V.F. Mitrofanov and V.M. Piksaikin, July 2023.

INDC(SPN)-4 Comparison of Isomeric Ratios in TENDL-2019, JEFF-3.3, ENDF/B-VIII.0 and EXFOR, prepared by A. Rodrigo, O. Cabellos and N. Otuka, June 2023.

Available cost-free on request only for teachers and scientists from developing countries:

Chart of the Nuclides 2022 Japanese Nuclear Data Committee and Nuclear Data Center, Japan Atomic Energy Agency.

Karlsruher Nuklidkarte *Wall chart of the nuclides and folding chart with booklet, 10th edition (2018).*

In Memoriam

Dieter Seeliger



We regret to inform you that Prof. Dr. Dieter Seeliger passed away on 28 July 2023.

Prof. Dr. Seeliger was nuclear physicist who studied physics at the University of Moscow and in Dubna. In 1972 he was appointed a professor for nuclear physics at the Technical University Dresden and Director thereof. Shortly after his connection with Nuclear Data Section was established when he was appointed a Liaison Officer to the NDS. The core data determined at the TU Dresden were made available for worldwide exchange via NDS and included in CINDA index. For this purpose, all data libraries available at the NDS could be made available to the developers and users of nuclear facilities in the GDR by setting up and operating a computer-aided database at the TU Dresden.

He served as member of the International Nuclear Data Committee (INDC) from 1980 until 1991 and chaired the Committee for one term of 4 years. He also actively participated in the coordinated research projects (CRPs) of the IAEA, published country specific progress reports and organized Symposia and training courses at TU Dresden.

He will be greatly missed.

Nuclear Data Services – Contact Points

 For services to customers in USA and Canada:

 US National Nuclear Data Center, Bldg. 197D, Brookhaven National Laboratory, P.O. Box 5000, Upton, NY 11973-5000, USA.

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For services to customers in OECD/NEA Data Bank member countries: NEA Data Bank, OECD Nuclear Energy Agency, 46, quai Alphonse Le Gallo F-92100 Boulogne-Billancourt, France. Tel. +33 1 7321 (plus extension); Website: <u>http://www.oecd-nea.org/databank/</u> Contact: M. Fleming, Tel.: +33 1 73 21 28 22, Email: <u>michael.fleming@oecd-nea.org</u>;.

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Website: <u>http://cdfe.sinp.msu.ru/</u> Contact: V.V. Varlamov, Email: <u>varlamov@depni.sinp.msu.ru</u>;.

<u>For services to customers in China</u>: China Nuclear Data Center, China Institute of Atomic Energy, P.O. Box 275(41), Beijing 102413, China. Tel. +86 10-6935-7275; Fax +86 10-6935-8119 Contact: Ge Zhigang, Email: <u>gezg@ciae.ac.cn</u>;

Computer codes of US origin to all countries (there are charges and release restrictions): Radiation Safety Information Computational Center (RSICC), Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6003, USA. Tel. +1 865-574-6176; Fax +1 865-241-4046; Email: pdc@ornl.gov

<u>Computer codes of non-US origin to all countries</u> (there may be release restrictions): NEA Data Bank (see above) Contact: A. Dufresne, Email: <u>Alice.DUFRESNE@oecd.org</u>, Tel.: +33 1 73 21 28 30

IAEA-NDS on-line services at Website <u>https://nds.iaea.org/</u> Users in India, China, Russia and neighbouring countries may use IAEA-NDS mirror websites:

http://www-nds.org.in (India); http://www-nds.ciae.ac.cn/ (China); http://www-nds.atomstandard.ru/ (Russia).

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