Nuclear Data Newsletter

https://nds.iaea.org/
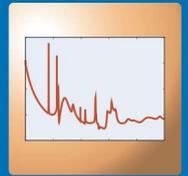
ISSN 0257-6376

No. 70, January 2021

Contents

From the Section Head

A very happy and healthy 2021 to all of you!

In my last addressing in the previous Newsletter I wrote: "I do not exactly know what the second half of the year brings for the Nuclear Data Section, and obviously we all would want to go back to 'really normal'. "
Well, as you know that didn't happen, although there was some temporary relief during the summer months in Europe at least, and we can now state that almost the entire year 2020, for both our private and professional lives, was strongly affected by the COVID-19 pandemic.

At the moment of writing, the Nuclear Data Section is mostly working from home, although we are allowed to enter the office for a few time blocks per week.
Visitors and regular "in-person" international IAEA meetings are however still not allowed.
We adapted to the new "virtual" circumstances, managed to hold many meetings, attracted more participants than we had in the "in person" meetings and we published many reports.
So even though in home office, our administration is in "business as usual" mode.
We started off a new Coordinated Research Project (CRP) on data evaluation of Fission Yields, which aims to produce high quality evaluated data for many actinide targets including the major actinides at different neutron incident energies. There were 51 participants in the meeting, which shows a rather large interest in this very specialized field.

Detailed nuclear reaction evaluation methodology and on-going evaluations were discussed in the yearly INDEN meetings on actinides and structural materials. In addition, we hosted meetings on neutron standards and nuclear data for the back end of the fuel cycle.

Our Atomic and Molecular Data Unit held two virtual Research Coordination Meetings for their Coordinated Research Projects on atomic data for fusion design.

Artificial Intelligence and Machine Learning are now rapidly invading all branches of science, and nuclear data is no exception to that. In this Newsletter you will find a short summary on a Consultancy Meeting we held recently. As always, all presentations can be found on our website.

As for my personal technical work, I am trying to use the COVID lockdown to clean up my to-do list with finalization of the software that has been lying on the shelf for too long, and you can read about it on the next page.

Computer Codes, Data Libraries and Web News

TALYS

A new webpage with software for nuclear data evaluation has been launched nds.iaea.org/talys.

It contains various tools and data libraries which may be helpful for nuclear data evaluation, **not only** for use in combination with TALYS, but in general. This software has been recently discussed at video meetings such as WPEC-SG49, WPEC-SG50 and JEFF.

Tar packages and tutorials for the following software are available:

EXFORTABLES: A code and database for EXFOR in tabular directory-structured format, including statistics of comparison with the world's major nuclear data libraries.

RESONANCETABLES: A code and database for average resonance parameters such as thermal cross sections, resonance integrals and Maxwellian-averaged cross sections, from a variety of original sources.

ENDFTABLES: A code to run an ENDF library into individual tables per reaction channel.

LIBRARIES-2020: The world's major nuclear data libraries and EXFOR into a directory-structured and tabular format, including plots for all reaction channels.

In the near future, the codes TASMAN (for uncertainty quantification with TALYS) and TEFAL (for ENDF formatting) will also be uploaded. The page will contain TALYS itself as well, but that release awaits an updated TALYS version and tutorial.

CONDERC

The IAEA NDS has recently launched a project "Compilation of Nuclear Data Experiments for Radiation Characterization (CoNDERC)" with the aim of transferring the experimental integral radiation information into technology. Experimental database can then be used as a part of the Validation and Verification (V&V) processes of nuclear model and code systems.

This was made possible thanks to the participation of multiple individuals and institutions that are assembling several databases and code infrastructures mainly associated with inventory, activation-transmutation, source term and radiation shielding R&D.

https://nds.iaea.org/conderc/
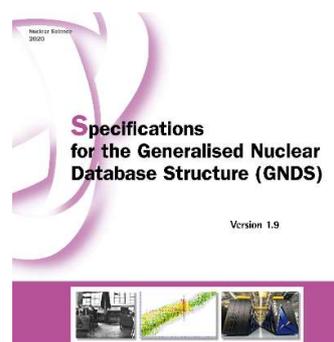
GNDS

Following the official publication of the Specifications for the Generalised Nuclear Database Structure (GNDS) version 1.9 under the auspices of the OECD/NEA databank, nuclear scientists all over the world can now rely on an increasing set of particle transport libraries ported in this enhanced multi-physics nuclear database structure:

TENDL-2019 @
https://tendl.web.psi.ch/tendl_2019/tar.html
ENDF/VIII.O @
https://www.nndc.bnl.gov/endf/b8.0/gndsfiles.html
JEFF-4.0 @   https://nds1.gitlab.io/nds/jeff4t0.html
https://www.oecd-nea.org/jcms/pl_39689/specifications-for-the-generalised-nuclear-database-structure-gnds.

NDS Staff Items

Paraskevi (Vivian) Dimitriou

Prior to joining the Nuclear Data Section in January 2021, Vivian worked at the Institute of Nuclear and Particle Physics of the National Center for Scientific Research "Demokritos" developing global models for nuclear reactions relevant to nuclear astrophysics and evaluating nuclear data for basic sciences and applications. Vivian studied physics at the National Kapodistrian University of Athens and completed her DPhil on pre-equilibrium nuclear reaction theory at the University of Oxford. She held an INFN Post-doctoral Fellowship at the INFN Sezione di Pavia and a European Marie Curie Fellowship at the Université Libre de Bruxelles before joining the National Center for Scientific Research "Demokritos".

In the period from 2012 to 2019, she worked at the Nuclear Data Section where she was responsible for a wide range of projects on nuclear structure and decay data, as well as nuclear reaction data.

From her new position as Nuclear Data Physicist in the Nuclear Data Development Unit, she will coordinate and participate in activities aiming at developing, improving and disseminating nuclear data for various applications.

NDS Meeting Reports

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

Consultants' Meeting of the International Nuclear Data Evaluation Network (INDEN) on the Evaluated Data of the Structural Materials

14 – 17 December 2020, Vienna, Austria
Virtual event
Scientific Secretary: G. Schnabel
25 participants and IAEA staff

The International Nuclear Data Evaluation Network (INDEN) aims to enhance and broaden multi-lateral collaborations on nuclear data evaluations, taking advantage of available expertise in Member States. The INDEN webpage is available at www-nds.iaea.org/INDEN. A working group on "Evaluations of Structural materials" held its third (virtual) meeting to discuss evaluation and validation methodologies for structural materials, and to review the status and problems of the evaluations for mid-

mass and some heavy structural materials. Extensive discussions were held on on-going evaluations of iron and chromium isotopes, which as components of stainless steel, are extremely important for many applications. Discussion included issues of evaluation methodology, required input experimental data, calculations and impact of direct neutron capture, inelastic scattering experiments, and reaction modelling both in the resonance (R-matrix) and fast neutron regions. New preliminary evaluations of Cr and Fe isotopes produced within the collaboration and an updated evaluation of Mn-55 are available from the INDEN webpage. Additional discussions covered on-going evaluations efforts on lead, copper, and tantalum targets. Validation and benchmarking of several evaluations were discussed including some new benchmarks for iron and copper data.

Presentations made at the meeting reflecting the work in progress are available at www-nds.iaea.org/index-meeting-crp/CM-INDEN-strucmat-2020-12/. The summary report of the meeting is in preparation and will be published as INDC(NDS)-0824.

Consultants' Meeting on Machine Learning for Nuclear Data

8 – 11 December 2020, Vienna, Austria
Virtual event
Scientific Secretary: G. Schnabel
18 participants and IAEA staff

In view of the fast advancing adoption of machine learning in various domains, a virtual Consultants' Meeting was held to bring together researchers from nuclear physics and machine learning to present their on-going work and achievements and discuss directions of development. The background of the participants was very diverse which was reflected in a colorful program including talks such as prediction of parameters in nuclear models and the detection and localization of anomalies in nuclear power plants. Talks on machine learning methodology hinted at the large potential of modern data analysis techniques to improve nuclear data evaluations. The meeting sparked broad interest and demonstrated that the application of machine learning gains attraction in the field of nuclear data. This is also encouraging news for an envisaged cross-cutting technical meeting on machine learning involving several departments of the IAEA, which is currently in the planning stage.

First Research Coordination Meeting on Hydrogen Permeation in Fusion Relevant Materials

23- 27 November 2020, Vienna, Austria
Virtual event
Scientific Secretary: K. Heinola
43 participants and IAEA staff

43 participants representing 15 Member States joined with IAEA staff for the First Coordination Meeting on hydrogen fuel permeation and retention in nuclear fusion reactor materials. Talks and reports covered following topics: fundamental atomistic modelling of hydrogen interactions with reactor wall materials; experimental hydrogen permeation research studying the effect of hydrogen gas loading and ion implantation as well as hydrogen plasma exposure; mechanisms for permanent retention of hydrogen; effect of neutron irradiation to hydrogen retention and permeation in fusion materials; multi-scale simulations of hydrogen permeation through fusion reactor components. Plans for the next steps were outlined and requirements for experimental round-robin exercises as well as simulation code comparisons were agreed. An in-person meeting for the CRP participants is planned for second half of 2021 to review progress of the ongoing research and the round-robin and code comparison activities. Meeting details can be found at https://amdis.iaea.org/meetings/hydrogen-permeation-rcm1/.

Consultants' Meeting of the International Nuclear Data Evaluation Network (INDEN) on Actinide Evaluation in the Resonance Region

17 - 19 November 2020, Vienna, Austria
Virtual event
Scientific Secretary: R. Capote Noy
22 participants and IAEA staff

The International Nuclear Data Evaluation Network (INDEN) aims to enhance and broaden multi-lateral collaborations on nuclear data evaluations, taking advantage of available expertise in Member States. The INDEN webpage is available at https://www-nds.iaea.org/INDEN. A working group on "Actinide Evaluations in the Resonance Region" held its third meeting to study methods of evaluation in the Unresolved Resonance Region (URR) and development of new evaluated files in the resonance region with focus on major fissile isotopes – ^{235}U, ^{239}Pu and ^{233}U. The meeting was held virtually with more than 20 participants per day, and extensive time allocated for presentations and associated discussions. The current status and future plans of on-going evaluation efforts of neutron induced reactions on fissile targets were reviewed.

Both experimentalists, evaluators and data testers fruitfully interacted. New updated (beta) evaluations were presented, and results discussed for all three fissile isotopes. A comprehensive comparison with newly available data as well as with existing evaluations was shown. Promising convergence was observed between fission and capture cross sections of new evaluated files of U-235. More work is needed for U-233 and Pu-239 targets.

Further information is available on the web: https://nds.iaea.org/index_nds_meetings.htm.
The Meeting summary report is in preparation.

Consultants' Meeting on Nuclear Data Form and Observable for the Safe Monitoring, Characterization, Handling and Disposal of Nuclear Fuel and Irradiated Material from Nuclear Power Plant, Pile, Experiment and Facility

2 - 4 November 2020, Vienna, Austria
Virtual event
Scientific Secretary: J.-Ch. Sublet
28 participants and IAEA staff

The purpose of the meeting was to assess members needs in terms of research, compilation and assembling of the specific nuclear data forms and observables databases needed for robust nominal and conceptual simulations of time-dependent nuclear inventory, radiological

characterization and source terms for the fission, fusion, accelerator, life, earth, research sciences applications.

The summary report that resumes the debate is already available:indc-nds-0822.pdf (iaea.org).

More details can be found on the webpage of the meeting: https://www-nds.iaea.org/index-meeting-crp/CM-McDDD/.

Consultants' Meeting on Neutron Data Standards

12 - 16 October 2020, Vienna, Austria
Virtual event
Scientific Secretary: G. Schnabel
45 participants and IAEA staff

This meeting was organized to review the status of ongoing work for the development of the next version of the Neutron Cross Section Standards which will be released within a few years. The IAEA standards and reference data webpage was updated, the latest data are available at www-nds.iaea.org/standards/.

Twenty-three talks were presented and addressed ongoing experimental and evaluation work for most of the Standard Cross Sections and Reference Cross Sections, as well as the development of updated evaluation methodologies, procedures, and codes. Efforts are directed firstly, to update and complete the experimental input database for the fit. Secondly, we aimed toward resolving existing discrepancies, establishing realistic uncertainties and correlations, and exploring the possibility of extending the applicable energy ranges of several important reactions in the suite of Standards and Reference Cross Sections through acquisition of new and or improved data.

The presentations are available on the meeting website at www-nds.iaea.org/index-meeting-crp/CM-NDS-2020-10/ and the INDC(NDS)-0820 summary report is in preparation.

## Second Research Coordination Meeting on Atomic Data for Vapour Shielding

7 – 9 October 2020, Vienna, Austria
Virtual event
Scientific Secretary: K. Heinola
10 participants and IAEA staff

Eight participants representing seven Member States (Australia, China, India, Netherlands, Spain, Syria, USA) joined this second Coordination Meeting to report and discuss progress of research related to vapour shielding phenomena of nuclear fusion devices. Reports on theoretical research comprised of fundamental calculations of atomic and molecular processes in the fusion plasma as well as simulations of interaction processes of the plasma and the liquid metals used as fusion reactor wall material.

Experimental research focused on fundamental experiments of atomic structure of liquid fusion materials and of fusion plasma-liquid metal experiments utilizing linear plasma devices and stellarator-type fusion device. A review and plans for next steps were outlined and new collaboration activities were launched.

Meeting information is available at https://amdis.iaea.org/meetings/vapour-shielding-rcm2/.
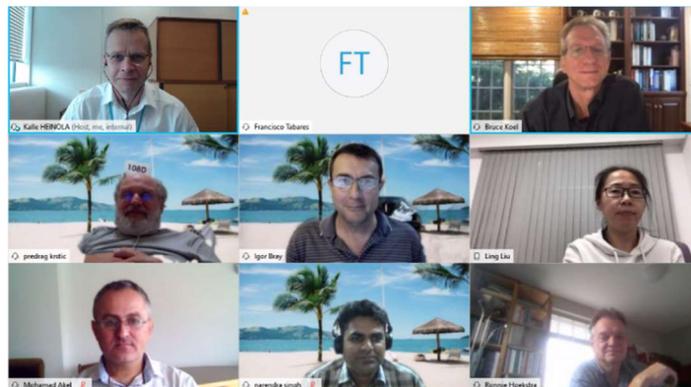
Consultants' Meeting on Development of CascadesDB Database for Irradiation

2 October 2020, Vienna, Austria
Virtual event
Scientific Secretary: C. Hill
4 participants and IAEA staff

This meeting, with the Chair of the Advisory Board for the CascadesDB database project, Andrea Sand (now at Aalto University) assessed the prospects for further calculations, data input and database development within this project which collects Molecular Dynamics simulations of the initial damage caused by energetic neutron impact on materials of relevance to fusion energy research. CascadesDB is available at https://cascadesdb.iaea.org.

Consultants' Meeting on the Development and Population of DefectDB

28 September – 2 October 2020, Vienna, Austria
Virtual event
Scientific Secretary: C. Hill
4 participants and IAEA staff

This meeting brought together staff from the Atomic and Molecular Data (AMD) Unit and experts from CEA/Paris Saclay on the computational technique of Density Functional Theory for the calculation of the properties of radiation-induced defects in materials of interest in nuclear science and engineering. Their advice has helped further the development, by the AMD Unit, of DefectDB, an online database of such calculations, available at https://db-amdis.org/defectdb.

First Research Coordination Meeting on Updating Fission Yields
31 August – 4 September 2020, Vienna, Austria
Virtual event
Scientific Secretary: R. Capote Noy
51 participants and IAEA staff

More than 50 international experts from 16 countries attended the meeting, making it one of the largest Research Coordination Meeting ever held. Such large participation reflects the high interest in the project of scientists dealing with fission product yields (FPY) from around the world.

FPY evaluations require both experimental data and theoretical efforts to produce successful evaluations. The presentations by the participants were followed by some brief discussions. The discussion time was constrained by the limited time for the online meeting due to the wide range of time zones involved.

The 24 meeting presentations are available at nds.iaea.org/index-meeting-crp/FissionYields2020/.

The meeting participants recognized that many activities related to the new FPY evaluations will be incorporated into this CRP, as shown in all the presentations, including experimental measurements, modelling, evaluation, and validation. The scope and goals of the CRP were reviewed. Four working groups were defined, group coordinators are listed below in parentheses:

(a) Availability of experimental FPY data for evaluations (B. Pritychenko – BNL).
(b) New FPY experimental data (O. Serot, CEA/DEN).
(c) FPY evaluations (R. Capote – IAEA and R. Mills –UK)
  -FPY modelling subgroup: (F. Minato – JAEA)
(d) FPY validation (O. Cabellos – UPM).

The meeting report will be published as INDC(NDS)-0817 and is in preparation.

Selected Charts, Reports and Documents

IAEA-NDS-0223 Rev. 1 ACEMAKER-2017: A code package to produce ACE-formatted files for MCNP calculations, prepared by D. Lopez Aldama, September 2020.

IAEA-NDS-0232 Processing of the Evaluated Photonuclear Data Library (IAEA/PD-2019), prepared by H. Kawada, J.-C. Sublet, S. Okumura and T. Kawano, August 2020.

IAEA-NDS-0234 RESONANCETABLES-1.0: Database for thermal cross sections, MACS and average resonance parameters, prepared by A. Koning and D. Rochman, December 2020.

IAEA-NDS-0235 EXFORTABLES-1.0: An experimental nuclear reaction database based on EXFOR, prepared by A. Koning, December 2020.

IAEA-NDS-0236 Tools for TALYS: Autotalys, T6, TENDL, libraries and more, prepared by A. Koning, December 2020.

INDC(CZR)-0004 Peak Neutron Production from the ^{7}Li(p,n) Reaction in the 20-35 MeV Range, prepared by M. Majerle, et al., September 2020.

INDC(EUR)-0037 Results of time-of-flight transmission measurements for ^{155,157}Gd at a 10m station of GELINA, prepared by M. Majerle, et al., September 2020.

INDC(NDS)-0800 Summary report from the Consultants' Meeting on Evaluation of Fundamental Data on Beryllium-containing Species for Edge Plasma Modelling, prepared by C. Hill, September 2020.

INDC(NDS)-0804 Summary report of the Technical Meeting on Actinide Evaluations in the Resonance Region, prepared by M. Fleming and R. Capote Noy, December 2020.

INDC(NDS)-0806 Summary report of the Consultants' Meeting of the International Nuclear Data Evaluation Network (INDEN) on the Evaluated Data of Structural Materials, prepared by A. Trkov, S. Kopecky and R. Capote Noy, December 2020.

INDC(NDS)-0814 The Importance of Resonance Self-Shielding Part 2, prepared by D.E. Cullen, D. Lopez Aldama and A. Trkov, August 2020.

INDC(NDS)-0815 Photon Strength Functions in Thermal Neutron Capture II, prepared by J. Kopecky, August 2020.

INDC(NDS)-0816 Table of Recommended Nuclear Magnetic Dipole Moments: Part II, Short-lived States, prepared by N.J. Stone, September 2020.

INDC(NDS)-0819 A Survey of ENDF/B-VIII Resonance Parameters (MF=2), prepared by D.E. Cullen, November 2020.

INDC(NDS)-0821 Addendum to IAEA(NDS) reports on the Neutron Capture Photon Strength Functions, prepared by J. Kopecky and S. Goriely, November 2020.

INDC(NDS)-0825 Processing La-139 in the Unresolved Resonance Region for the FENDL Library, prepared by D. Lopez Aldama and R. Capote Noy, January 2021.

INDC(SLO)-0004 On the Analysis of Benchmarks with ^{233}U fuel and Be or Polyethylene reflectors, prepared by A. Trkov and R. Capote Noy, January 2021.

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

Chart of the Nuclides 2014 JAEA Nuclear Data Centre.

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

In Memoriam

Kevin McLaughlin

We regret to inform you that Kevin McLaughlin passed away in October 2020. Kevin was staff member of the Nuclear Data Section from 1982 to 2003, having previously worked at AERE Harwell. Kevin was the Section's expert for the formats, handling and updating of all data files and authored several INDC reports on nuclear data library format and processing. With this experience he was an excellent teacher to the participants of the IAEA-NDS workshops at the International Centre for Theoretical Physics (ICTP) in Trieste. He was a hard and reliable worker, always in a good spirit, most helpful to the other staff when they encountered a problem and the one who contributed much to the enjoyable working climate of the Section.

Anyone who met Kevin knows he was always willing to walk the extra mile to help, he will be greatly missed.

Konstantin Ivanovich Zolotarev

Konstantin Zolotarev passed away on 22 August 2020.

After graduating from the Moscow Physical Engineering Institute in Obninsk in 1969, he worked 51 year in the Institute of Physics and Power Engineering at first in the neutron dosimetry laboratory and since 1988 in the Nuclear Data Center (Centr po Yadernym Dannym). Some results of his reactor experiments carried out at Leningrad NPP (RBMK reactor), Aktau (BN-350 fast reactor), Dimitrovgrad (research reactors) are of special value for the standardization of neutron spectra. Later he became the leading specialist in the evaluation of neutron dosimetry reaction.

His works were characterized by special care in the analysis of the evaluation. The experimental data sets from EXFOR, corrected by him and renormalized to the latest standards were the driving force for new international project of storing in the EXFOR not only the original data, provided by the authors, but also data verified (and corrected, if it is needed) from our present knowledge of methods and data used in the measurements and data reduction.

His contributions to numerous IAEA coordinated research projects over decades as well as separate data development projects for the Nuclear Data Section will remain extremely valuable. The release of the IRDFF-II neutron dosimetry library in 2020 which includes a large share of Konstantin's evaluations will remain one of his most enduring results.

His in-depth knowledge, and his quiet but very helpful and friendly nature will be greatly missed.

Maurice Green
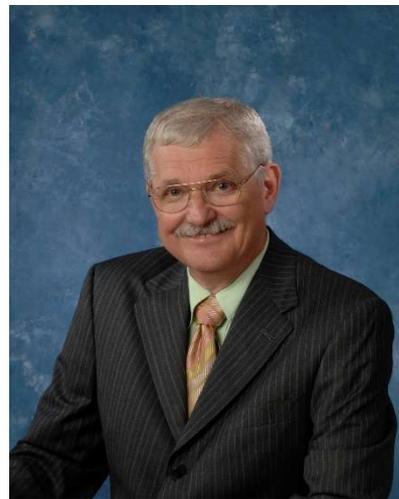
Only recently were we informed that Maurice Greene passed away on 13 June 2020. He worked at the Oak Ridge National Laboratory (ORNL) as a nuclear engineer for 43 years (1963-2006). With regard to one of his most noteworthy accomplishments and contributions to the Nuclear Data Community, Maurice was the original author and developer of the AMPX cross-section processing code package: a modular system of FORTRAN computer programs that relate to nuclear analysis with a primary emphasis on tasks associated with the production and use of multigroup and continuous energy cross-sections. AMPX has been and continues to be used to produce nuclear data libraries for the SCALE code package that is developed at ORNL. In addition, Maurice served as Chair of the CSEWG Formats and Processing committee from 1999 until 2006. His extensive knowledge and contributions to the ENDF/B Formats were instrumental to the development and maintenance of the modern ENDF Formats that are used by all of the international nuclear data library projects. Maurice was very creative, and he had a keen sense of humor. Maurice will be greatly missed by all those who knew him and worked with him.

Nuclear Data Services – Contact Points

<u>For services to customers in USA and Canada</u>:
US National Nuclear Data Center, Bldg. 197D, Brookhaven National Laboratory, P.O. Box 5000,
Upton, NY 11973-5000, USA.
Tel. +1 631-344-2902; Fax +1 631-344-2806;
Website: http://www.nndc.bnl.gov/
Email: nndc@bnl.gov
For information regarding on-line services, contact: B. Pritychenko: pritychenko@bnl.gov
For information regarding general NNDC services, contact: Letty Krejci: lkrejci@bnl.gov

<u>For services to customers in OECD/NEA Data Bank member countries</u>:
NEA Data Bank, OECD Nuclear Energy Agency, 46, quai Alphonse Le Gallo
F-92100 Boulogne-Billancourt, France.
Tel. +33 1 7321 (plus extension);
Website: http://www.oecd-nea.org/databank/
Contact: F. Michel-Sendis, Tel.: +33 1 73 21 28 23, Email: franco.michel-sendis@oecd-nea.org;.

<u>For services to the customers from the former USSR</u>:
<u>Neutron data</u>: Russia Nuclear Data Center, Centr Jadernykh Dannykh (CJD), Fiziko-Energeticheskij Institut, Ploschad Bondarenko,1,
249033 Obninsk, Kaluga Region, Russian Federation.
Tel. +7 08439-9-5803; Fax +7 08439-68235;
<u>Photonuclear data</u>: Centre for Photonuclear Experiments Data, Centr Dannykh Fotoyadernykh Eksperimentov (CDFE),
Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie Gory, 119 922 Moscow, Russian Federation.
Tel. +7 495-939-3483; Fax +7 495-939-0896;
Website: http://cdfe.sinp.msu.ru/
Contact: V.V. Varlamov, Email: varlamov@depni.sinp.msu.ru;.

<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: gezg@ciae.ac.cn;

<u>Computer codes of US origin to all countries</u> (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: Alice.DUFRESNE@oecd.org, Tel.: +33 1 73 21 28 30

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