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Nuclear Data Newsletter

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Contents

From the Section Head

Greetings from Vienna, which seems to have skipped winter this year.

In the Atomic and Molecular Data Unit, we organized meetings on both the Data Centre Network and the Code Centre Network. A particular objective of the latter is to create a database of collisional cascade molecular dynamics (MD) simulations on the effect of neutron radiation on materials relevant to nuclear fusion applications. The resulting CascadesDB resource is the basis of many computational studies for fusion design.

A rather special meeting was the Consultants' Meeting of the International Nuclear Data Evaluation Network (INDEN) on Evaluated Data for Structural Materials, not only because of the importance of the INDEN series for the future of evaluated data libraries, but also because it was the last meeting coordinated by Andrej Trkov, who has just retired as you are reading this.

Quite some progress was made on the identification and compilation of available and missing Experimental Nuclear Reaction (EXFOR) data for fission yields. The Nuclear Data Section is going to put more effort into fission yields in the coming years, among others with the start of a new Coordinated Research Project (CRP) on Updated Fission Yield Data for Applications coming June.

Perhaps the most challenging part of nuclear reaction data evaluation is the ability to describe or predict cross sections and other data for actinides. For that, the second meeting of the CRP on Recommended Input Parameter Library for Fission Cross Section Calculations (RIPL) has been held, to enable nuclear model codes to converge on their description of fission observables.

Finally, I have tried to keep my own scientific developments alive as well. On the next pages you will see that there are new releases of TALYS and TENDL, as well as a new web tool to predict the production of medical isotopes, which Marco Verpelli and I developed.

As for the Nuclear Data Section and you as readers, I hope for a productive new nuclear data decade!

Danas Ridikas-Section Head, Physics Section, Melissa Denecke-Director, Division of Physical and Chemical Sciences (NAPC), Arjan Koning-Section Head, Nuclear Data Section wearing NAPC-Division branded T-shirts.

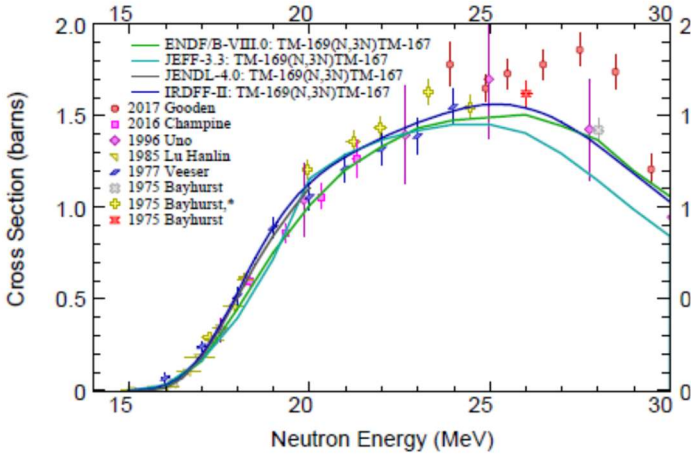
Computer Codes, Data Libraries and Web News

IRDFF-II: A New Neutron Metrology Library

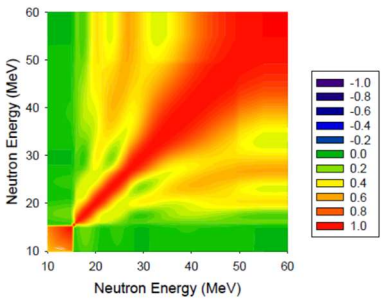
https://www-nds.iaea.org/IRDFF/

A new International Reactor Dosimetry and Fusion File (IRDFF-II) was released in December 2019 and is documented in A. Trkov, *et al*,. Nuclear Data Sheets **163** (2020) 1-108. The library addresses incident neutron energies from 0 up to 60 MeV and includes 119 metrology reactions with full covariance information (*e.g.*, see the plots of evaluated cross sections vs selected experimental data from EXFOR and corresponding correlation and uncertainties for the reaction ^{169}Tm(n,3n) below). The library also includes tables of recommended decay data, isotopic abundances, 4 cover cross sections for self-shielding corrections and 7 cumulative fission yields recommended for the dosimetry using fission reactions. Several reference neutron fields are also provided with recommended sets of activation measurements in those fields that can be used for validation. The library has been thoroughly validated using spectrum averaged cross section (SACS) measurements.

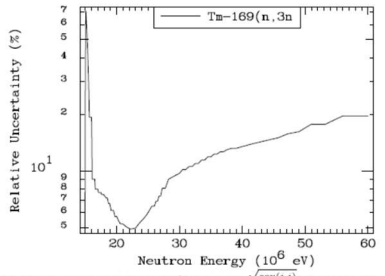
The library can be used in a broad range of applications from lifetime management and assessments of nuclear power reactors to other neutron metrology applications such as BNCT, therapeutic use of medical isotopes, nuclear physics measurements, and reactor safety applications. Library evaluations are based on a least-square analysis of mainly experimental data, and so the reaction library also represents an ideal benchmark collection for validation and improvement of theoretical nuclear reaction models.



(a) Comparison to selected experimental data from EXFOR [7



(a) Cross-section correlation matrix.

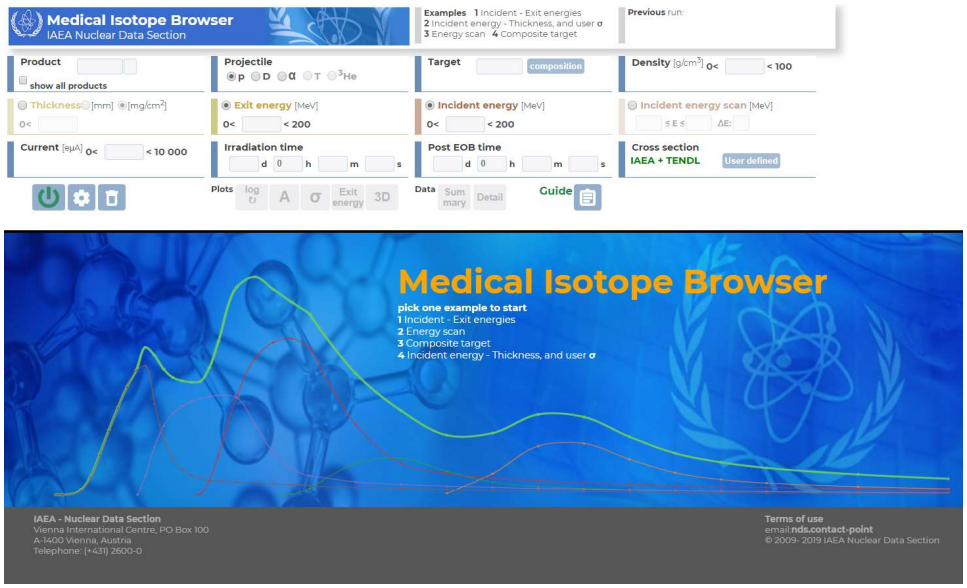


(b) One-sigma uncertainties in % ($\equiv 100 \times \frac{\sqrt{cov(i,i)}}{\mu_i}$), being μ_i the corresponding cross-section mean value.

Medical Isotope Browser – a tool for novel radioisotope production

A new web tool has been developed which allows direct prediction of the production yield of a medical isotope from the user's input. The Medical Isotope Browser can be used by medical scientists and the radiopharmaceutical industry to discover radioisotope production routes not yet explored. The production of a medical isotope for therapy or diagnosis depends on very complex nuclear reaction processes, which are only available to nuclear physicists via measurements and nuclear reaction theories. The Medical Isotope Browser makes this fundamental information accessible to many non-specialized users through a Graphical User Interface for isotope production. The nuclear data behind the tool comes from 2 sources: Cross section data for about 150 reaction channels which have been evaluated by experts over the past 20 years, and the TALYS-based TENDL library which provides an estimate for all the other channels.

The Medical Isotope Browser is available at https://nds.iaea.org/mib. The first version is restricted to isotopes produced by charged-particle accelerators. The user can specify the characteristics of the accelerator, such as the projectile (proton, deuteron, triton, Helium-3 or alpha particle), current in mA, the incident and exit energy, and specify the target material and the desired produced radioisotope. After a simple mouse click, the required isotopic yield as a function of irradiation and cooling time, as well as a complete description of all the produced impurities is obtained, virtually instantaneously. The next version will include medical isotope production with research reactors and via electron beams (through photonuclear reactions).



CascadesDB database

The Atomic and Molecular Data Unit released the official interface to the CascadesDB database (https://cascadesdb.iaea.org/) - a searchable repository of over 1500 Molecular Dynamics simulations of collisional cascades: the radiation damage in materials due to energetic neutrons which is of importance to nuclear fusion energy research. The project is overseen by an advisory board of representatives from Member States who attended a Technical Meeting at IAEA Headquarters in October 2019.

TALYS-1.95

A new release of the TALYS nuclear model code, TALYS-1.95 is available at www.talys.eu.
As usual, the Introduction of the manual contains a section called "From TALYS-1.9 to TALYS-1.95" summarizing the new features and keywords.
Improved photon strength function models and a model for partial damping for fission are among the notable extensions.

TENDL-2019

A new release of the TALYS Evaluated Nuclear Data Library, TENDL-2019, is now available at https://tendl.web.psi.ch/tendl_2019/tendl2019.html and succeeds the TENDL-2017 library.
The collection contains complete ENDF-6 formatted data files, including covariance data and up to 200 MeV, for 2813 isotopes (all stable or with half-life >1sec) for incident neutrons, photons, protons, deuterons, tritons, Helium-3, and alpha particles.
Among the new features are:

- Use of the latest collections of neutron resonance parameters and further improved description of experimental thermal cross section values, including correct isomeric branching.
- Covariance matrices for all nuclides for all incident particles (TENDL-2017 only had this for neutrons, photons and protons).
- General improvement of implemented ENDF-6 procedures, resulting from users' feedback in the last 2 years.

Web addresses

The Nuclear Data Section web site can be now accessed using a simpler address:

nds.iaea.org

which is easier to type on mobile devices. The traditional web address **www-nds.iaea.org** is of course still valid, and any bookmark or link already existent will continue to work.

NDS Staff Items

More details about the Nuclear Data Section Staff can be found at: http://www-naweb.iaea.org/napc/nd/aboutus.asp.

We welcome **Georg Schnabel** who joined the Nuclear Data Section on 6 January 2020 as Nuclear Physicist (Codes development).
Prior to this position, Georg worked in the Division of Applied Nuclear Physics at Uppsala University in Sweden and in the Laboratory for Studies and Applications of Nuclear Reactions at CEA Saclay in France developing mathematical methods and computational procedures for the uncertainty quantification of high-energy spallation models and the model-based evaluation of nuclear data.
He studied physics at the Vienna University of Technology with specializations in theoretical physics, statistics, and computer science, and subsequently completed a PhD in the field of nuclear data evaluation at the Atominstitut and Vienna University of Technology.
As a member of the Nuclear Data Development Unit, Georg will organize and take part in activities to extend and improve nuclear data and their utility 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 Evaluated Data for Structural Materials

2-5 December 2019, Vienna, Austria
Scientific Secretary: A. Trkov
9 participants and IAEA staff

Participants of the CM

The International Nuclear Data Evaluation Network (INDEN) is an activity aimed at streamlining evaluation activities and enhancing multi-lateral collaboration, taking advantage of expertise in different laboratories in Member States. A working group on "Evaluated data of Structural Materials" held its second meeting to review the on-going evaluations of Ni isotopes (TENDL), Cu isotopes (ORNL), Cr isotopes (BNL and IAEA), and Fe-56 (CEA/DEN, IAEA, CENDL). The problems of Fe-56 were discussed in depth. Results presented show potential problems in the measured inelastic cross section as well as the need to use transmission data with thick (2 inches) samples to constraint the fit of R-matrix parameters. Further information is available on the web: https://www-nds.iaea.org/index-meeting-crp/CM-INDEN-IV-2019/. The Meeting summary report is in preparation.

Technical Meeting on the Development of Software Programs and Database tools for Modelling Edge Plasma Processes in Fusion Devices

27 – 29 November 2019, Vienna, Austria
Scientific Secretary: C. Hill
12 participants and IAEA staff

This meeting brought together experts in collisional processes and spectroscopy to write and release a new version of the "Classification of Plasma Processes" document that can be used by database tools in the standardized description of their data sets. An online version is available at https://www-amdis.org/databases/processes. The meeting also recommended flexible and comprehensive standards for software programs and databases to use in the description and specification of atomic and molecular species and states. Further details are available at https://www-amdis.org/meetings/software-tools/.

Participants of the TM on the Development of Software Programs

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

21-24 October 2019, Vienna, Austria
Scientific Secretary: R. Capote
9 participants and IAEA staff

The International Nuclear Data Evaluation Network (INDEN) is an activity aimed at streamlining evaluation activities and enhancing multi-lateral collaboration, taking advantage of expertise in different laboratories in Member States. A working group on "Actinide Evaluations in the Resonance Region" held its second meeting to study methods of evaluation in the Unresolved Resonance Region (URR). A new method to validate existing URR evaluations was presented by researchers from RPI, USA. The current status of on-going evaluation efforts of neutron induced reactions on Pu-239 and U-235 was reviewed and differences between existing evaluations in the resonance region were discussed. The overall objective is to co-ordinate the activities in different laboratories with the final goal of obtaining consistent evaluated data files that respect the differential data. Further information is available on the web: https://www-nds.iaea.org/index-meeting-crp/TM-INDEN-2019/. The Meeting summary report is in preparation.

Participants of the INDEN TM

Technical Meeting of the Code Centres Network

16-19 October 2019, Vienna, Austria
Scientific Secretary: C. Hill
19 participants and IAEA staff

Participants of the TM of CCN

This meeting discussed the ongoing development of the CascadesDB database (https://cascadesdb.iaea.org/) of collisional cascades simulations in materials of relevance to

fusion applications and its inclusion in a planned, broad-ranging suite of databases for fusion and fission material science. The participants particularly focused on the development of a database of DFT calculations for the prediction of the behaviour and evolution of radiation-induced defects in reactor materials. Further details are available at https://www-amdis.org/meetings/ccn-6/.

Second Research Coordination Meeting on Recommended Input Parameter Library for Fission Cross Section Calculations

7-11 October 2019, Vienna, Austria
Scientific Secretary: R. Capote
10 participants and IAEA staff

Nowadays advanced modelling codes play a significant role in nuclear data evaluation to meet the needs of updated and more reliable data for applications. Modelling codes require substantial numerical input, therefore the IAEA produced the Reference Input Parameter Library (RIPL) released in January 2009, which is available on the Web through http://www-nds.iaea.org/RIPL-3/. Due to the increasing importance of modelling in nuclear data evaluation, the improvement of fission input parameters is considered a high priority. To meet these needs, a new IAEA CRP was started in 2017. Review of the on-going work and coordination of this work for the next two years was undertaken at the meeting. Good progress in updating many of the RIPL data was achieved. It was agreed that the final meeting of the CRP will be held in summer 2021.
A technical document describing both the nuclear reaction formalism and model parameters included in the updated database will be produced and the updated database will be made available for online distribution.

Technical Meeting of the Atomic and Molecular Data Centres Network

30 September-2 October 2019, Vienna, Austria
Scientific Secretary: K. Heinola
12 participants and IAEA staff

The 25th Technical Meeting of the Atomic, Molecular and Plasma-Material Interaction Data Centres Network was represented by eleven participants (Argentina, China, Germany, Italy, Japan, Korea, Russia, United Kingdom, USA) and one observer (USA). Main purpose of the meeting was to monitor the global data centre activities for nuclear fusion, to discuss the objectives and recent developments, and the current and future requirements for fusion-relevant data. Discussions about coordinated activities on data and uncertainty evaluations resulted in a data centre activity focusing on uncertainty evaluation studied with various computational methodologies. This activity would be launched early 2020, and the results would be collected and evaluated at the next GNAMPP meeting, or at the 26th Data Centres Network meeting. More information and the meeting presentations are available at the AMD Unit's new prototype website https://www-amdis.org/meetings/dcn-25/ .

Participants of the TM of A&M DCN

Consultants' Meeting of the planned Coordinated Research Project (CRP) on Hydrogen Permeation

26-27 September 2019, Vienna, Austria
Scientific Secretary: K. Heinola
7 participants and IAEA staff

Participants of the CM

The main purpose of this meeting was to discuss the objectives and outcomes of a new CRP focusing on the important topic of permeation of hydrogen plasma fuel particles through fusion reactor's wall materials and components. Information on hydrogen diffusivity, trapping/detrapping/retrapping, solubility, effect of impurities and interfaces, effect of intrinsic defects as well as neutron irradiation-induced defects, must be understood and evaluated for assessing the real permeation values. These will be used in modelling the in-vessel source term,

and the ex-vessel release term used in the fusion reactor safety assessments for licensing future fusion facilities. More information including meeting presentations are available at the AMD Unit's new prototype website https://www-amdis.org/CRP/hydrogen-permeation.

Technical Meeting on Processing Codes

23-26 September 2019, Vienna, Austria
Scientific Secretary: A. Trkov
24 participants and IAEA staff

Participants of the TM on Nuclear Data Processing

This meeting was a follow-up of previous meetings held on this subject (latest one in September 2018). A number of codes that can process evaluated nuclear data files have become available. The meeting assessed current status and availability of nuclear data processing systems, putting emphasis on their capability/capacity to support Monte Carlo calculations, including the treatment of self-shielding in the unresolved resonance region. The focus of this meeting was on (but not limited to) the ability to prepare data in ACE format for Monte Carlo calculations. More details, including the presentations, are available from: https://www-nds.iaea.org/index-meeting-crp/TM-Nuclear%20Data%20Processing/.

Technical Meeting on Nuclear Data for Fusion Neutronics

2-5 September 2019, Vienna, Austria
Scientific Secretary: A. Trkov
18 participants and IAEA staff

Participants of the FENDL TM

The status of the FENDL-3.1 library was reviewed in view of the recommendations from the previous meeting in 2018. It was decided to adopt the IAEA INDEN evaluation for ^{56}Fe and a modified ^{16}O evaluation provided by QST and JAEA, Japan. The Activation library will be adopted from TENDL-2017, except for evaluations that are included in the IRDFF-II library; for incident charged particles, preference will be given to the evaluations in the medical isotope cross section library. With the proposed changes the library FENDL-3.2 for fusion neutronics calculations will be released from the IAEA. The meeting presentations and the meeting report are available from https://www-nds.iaea.org/index-meeting-crp/TM%20FENDL/.

Selected Charts, Reports and Documents

Atomic and Plasma-Material Interaction Data for Fusion, Volume 18, 2019.

The articles collected in this volume address the effect that such damage to one proposed material, tungsten, has on its relevant properties – in particular, its resistance to erosion in proximity to a fusion plasma and its propensity to absorb and retain the tritium fuel. It is crucial for the commercial viability of a fusion reaction based on the deuterium-tritium process that any material that is exposed to the plasma does not exist naturally and must be "bred" from the interaction of neutrons with lithium in the reactor blanket in a process working at a nearly 100% conversion efficiency for sustainable, long term operation of the reactor.
This edition of APID contains contributions from participants in the coordinated research project entitled Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices (2013-2018). Nineteen research groups from ten different Member States participated and attended three research coordination meetings over the five years of the project. The IAEA officer responsible for this volume was C. Hil of the Division of Physical and Chemical Sciences.

INDC(CCP)-0461 Russian Nuclear Data Center: History of Creation and Achievements, prepared by V.N. Manokhin, A.I. Blokhin and A.V. Ignatyuk., December 2019.

INDC(EUR)-0034 Results of Time-of-Flight Transmission Measurements for ^{103}Rh at a 50m Station of GELINA, prepared by Y.K. Kim, et al., January 2020.

INDC(JPN)-0205 Proceedings of the 2018 Symposium on Nuclear Data, 29-30 November 2018, Tokyo, Japan, edited by S. Chiba, C. Ishizuka, K. Tsubakihara and and O. Iwamoto, November 2019.

INDC(KAS)-0002 Proceedings of the Tenth AASPP Workshop on Asian Nuclear Reaction Database Development, 24-27 June 2019, Almaty, Kazakhstan, edited by T. Zholdybayev and N. Otuka, September 2019.

INDC(NDS)-0694 Summary Report of the Consultants' Meeting on Compensating Effects due to Nuclear Reactions and Material Cross Correlations in Integral Benchmarks, 28 September-1 October 2015, Vienna, prepared by A.C. (Skip) Kahler, V. Pronyaev and A. Trkov, January 2020.

INDC(NDS)-0779 Summary Report of the Technical Meeting on Atomic, Molecular and Plasma-Material Interaction Data Evaluation and Development, 19-21 November 2018, Vienna, prepared by C. Hill, January 2020.

INDC(NDS)-0780 Summary Report of the Second Research Coordination Meeting on Data for Atomic Processes of Neutral Beams in Fusion Plasmas, 18-20 February 2019, Vienna, prepared by C. Hill, February 2019.

INDC(NDS)-0791 A Global Fitting Method with the R-Matrix Code RAC, prepared by Zhenpeng Chen, Yeying Sun, and P. Dimitriou, December 2019.

INDC(NDS)-0794 Table of Recommended Nuclear Magnetic Dipole Moments, prepared by N.J. Stone, November 2019.

INDC(NDS)-0795 Summary Report of the Technical Meeting on Nuclear Data for Neutron Activation Analysis and Dosimetry, 15-18 July 2019, Vienna, Austria, prepared by A. Trkov, August 2019.

INDC(NDS)-0796 Evaluation of ^{50}Cr(n,γ)^{51}Cr, ^{56}Fe(n,x)^{54}Mn, ^{57}Fe(n,x)^{56}Mn, and ^{68}Zn(n,x)^{67}Cu Reaction Cross Sections for the IRDFF library, prepared by K.I. Zolotarev, August 2019.

INDC(NDS)-0797 Summary Report of the Technical Meeting on FENDL Library for Fusion Neutronics Calculations, 2-5 September 2019, Vienna, Austria, prepared by D. Leichtle and A. Trkov, October 2019.

INDC(NDS)-0798 Summary Report of the Technical Meeting on Processing Codes, 23-26 September 2019, Vienna, Austria, prepared by A.C. (Skip) Kahler and A. Trkov, October 2019.

INDC(NDS)-0799 Photon Strength Functions in Thermal Neutron Capture, prepared by J. Kopecky, January 2020.

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).*

Chart of the Nuclides *(Wall chart) prepared by Knolls Atomic Power Laboratory (KAPL) and distributed by Lockheed Martin (17th edition, revised 2009).*

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In Memoriam

Ratko Janev

Ratko Janev died in Belgrade on 31 December 2019. He was the head of the Atomic and Molecular Data Unit from 1986 and subsequently served as a member of the IFRC Sub-Committee for atomic and molecular data. He was a prolific and extremely knowledgeable atomic physicist, proponent and evaluator of fundamental data for fusion, he continued to contribute his expertise to the Unit's activities after leaving the Agency, most recently as a participant in a CRP devoted to vapour shielding launched in 2019. The depth of his scholarship will be greatly missed by the entire plasma physics community.

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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.
Tel. +1 631-344-2902; Fax +1 631-344-2806; Email: nndc@bnl.gov; Worldwide Web: http://www.nndc.bnl.gov/
For information regarding on-line services, contact: B. Pritychenko: pritychenko@bnl.gov
For information regarding general NNDC services, contact: M. Blennau: blennau@bnl.gov

For services to customers in OECD/NEA Data Bank member countries:
NEA Data Bank, OECD Nuclear Energy Agency, Le Seine Saint-Germain, 12 blvd. des Iles,
F-92130 Issy-les-Moulineaux, France.
Tel. +33 1 4524 (plus extension); Fax +33 1 45241110;
Email: michael.fleming@oecd.org; data@oecd-nea.org; Worldwide Web: http://www.oecd-nea.org/databank/ contact: M. Fleming, ext. 1072.

For services to the customers from the former USSR:
Neutron data: 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;
Photonuclear data: 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;
Email: varlamov@depni.sinp.msu.ru; Worldwide Web: http://cdfe.sinp.msu.ru/; contact: V.V. Varlamov.

For services to customers in China:
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Tel. +86 10-6935-7275; Fax +86 10-6935-8119; Email: gezg@ciae.ac.cn; contact: Ge Zhigang.

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

Computer codes of non-US origin to all countries (there may be release restrictions):
NEA Data Bank (see above)
Email: is Alice.DUFRESNE@oecd.org; contact: A. Dufresne, ext. 1008.

IAEA Nuclear Data Section offers data centre services primarily to non-OECD countries
(except Russian Federation and China, see above). However, most products advertised in this Newsletter, specifically INDC reports, IAEANDS documents, etc., are provided upon request to customers in all countries.
IAEA-NDS on-line services at Worldwide Web: http://www-nds.iaea.org/ and https://nds.iaea.org/
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http://www-nds.indcentre.org.in (India); http://www-nds.ciae.ac.cn/ (China); http://www-nds.atomstandard.ru/ (Russia).

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