

**A newsletter of the Nuclear Data Section (NDS)  
No. 53, May 2012**

ISSN 0257-6376

<http://www-nds.iaea.org/>

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*Nuclear Data Section Library*

## From the Section Head

The name 'Nuclear Data Section' overlooks the fact that a part of the NDS programme covers atomic and molecular data work, which is focused on fusion applications and so is particularly important for ITER and the planning of future DEMO devices. In addition to reactions of atoms and molecules, the interaction of plasma with materials is considered as crucial; unless the issues of dust and the design of diverters can be solved, fusion will not be able to mature into an energy generating technology. See p. 3 for further details and visit the Atomic and Molecular (A+M) link <http://www-amdis.iaea.org/>.

Unfortunately potential security risks, outside NDS control, occurred during February and March this year resulting in the NDS web page being unavailable for several days. Even after its reinstatement, problems continued in some services for a longer period of time. NDS regrets this break in services and apologises to its users for any inconvenience caused. All necessary steps are being taken to ensure no such outage occurs again.

Two programmatic developments in 2011 are of note: the publication of the technical document 'Nuclear Data for the Production of Therapeutic Radionuclides' (STI/DOC/010/473) (see p. 14), brings to a conclusion a very successful medical CRP; and a test version of the enlarged and energy extended dosimetry file (IRDF) is now available, designed for a wider range of applications, including fusion - there are also plans to validate it in a future CRP.

All services provided to users are free of charge. Please contact us at the following addresses:

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# Computer Codes and Data Libraries - News

Databases and libraries are available for download or on CD-ROM/DVD cost-free on request

Please find a complete list of all computer codes and data libraries available from NDS on:

<http://www-nds.iaea.org/cd-catalog.html>

**EMPIRE-3.1** - A new version EMPIRE-3.1 (codename Rivoli) was released in February 2012 and is available from the IAEA (<http://www-nds.iaea.org/empire>) and US National Nuclear Data Center, BNL, USA (<http://www.nndc.bnl.gov/empire>). Platform independent retrieval of EXFOR (C4) data has been implemented and the whole system, including the Graphical User Interface, is fully operational both on Mac OS X and Linux. EMPIRE is intended to be a general, flexible, and easy to use tool for basic research and evaluation of nuclear data. It offers the possibility of combining several theoretical approaches, choosing between alternative input parameters and calculating an extended set of observables in a single run. Nuclear data evaluation is facilitated by the ENDF-6 formatting, file verification and graphical comparison with experimental data. Major new features include exclusive spectra and DDXs in the HMS pre-equilibrium emission model, fully integrated with RIPL-3 library of input parameters, ability to use soft-rotor potentials implemented in the OPTMAN optical model solver database, and a new parametrization of EGSM level densities.

**EXFOR** - Experimental nuclear reaction cross section data - update 30 March 2012 contains 144 322 data tables from 19 394 experimental works. The NDS retrieval system for EXFOR data now has additional new features – automatic renormalization of original data according to new standards and searching for the relevant publications in the NSR and CINDA bibliographical databases if they are missing in EXFOR. Released March 2012, <http://www-nds.iaea.org/exfor/exfor.htm>

**JEFF-3.1.2** – the Joint Evaluated Fission and Fusion File, version 3.1.2 - is an evaluated library produced via an international collaboration of Data Bank member countries coordinated under the auspices of the NEA Data Bank. The latest update concerns 115 materials and presently contains incident neutron data for 381 isotopes or elements from  $^1\text{H}$  to  $^{255}\text{Fm}$ . Released February 2012, <http://www-nds.iaea.org/exfor/endlf.htm> and [http://www.oecd-nea.org/dbforms/data/eva/evatapes/jeff\\_31/JEFF312/](http://www.oecd-nea.org/dbforms/data/eva/evatapes/jeff_31/JEFF312/)

**ENDF/B-VII.1** - Evaluated Nuclear Data Library, version VII.1 - released by the Cross Section Evaluation Working Group (CSEWG) as the latest recom-

mended evaluated nuclear data file for use in nuclear science and technology applications. It incorporates advances made in the five years since the release of ENDF/B-VII.0, including many new evaluations in the neutron sublibrary (423 in all) with covariances (over 190), new fission product yields and a greatly expanded decay data sublibrary. Released December 2011,

<http://www-nds.iaea.org/exfor/endlf.htm> and <http://www.nndc.bnl.gov/exfor/endlf7.1.jsp>

**POINT2011 beta4** - is ENDF/B-VII.1 (beta4) data processed by D. Cullen into pointwise format at a set of temperatures relevant for nuclear reactor and astrophysical applications. Released November 2011, <http://www-nds.iaea.org/point2011b/>

**POINT2012** - is ENDF/B-VII.1 official release data (December 2011) processed by D. Cullen into pointwise format at a set of temperatures relevant for nuclear reactor and astrophysical applications. Released February 2012, <http://www-nds.iaea.org/point2012/>

**DXS** - Damage and gas production cross-sections – the latest upgrade includes the atom displacement cross-sections by neutrons and protons for eight pure metals and gas production cross-sections for four materials up to incident energy 3 GeV. Released November 2011, <http://www-nds.iaea.org/ndspub/download-endlf/DXS/>

**NSR** – Nuclear Science References (NSR) database is the world's only comprehensive source of low and intermediate energy nuclear physics bibliographical information containing more than 200 000 articles going back to the inception of nuclear science. Recently new improvements were implemented for the NSR web application: diverse search options, recent NSR references, direct access to EXFOR data from the NSR database, Google Scholar connection and other features. Released database version 28 March 2012, includes 355 new entries and 32 corrected entries. <http://www-nds.iaea.org/nsr>.

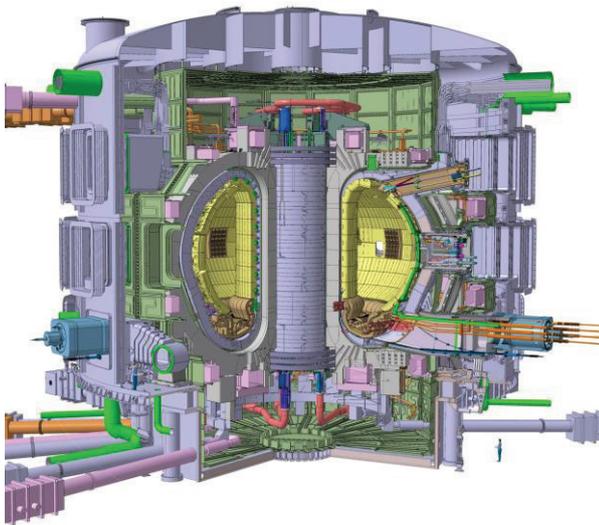
**IBANDL-2012** – A further new CD version of IBANDL has been developed to include new data sets, previously only available in the web version, and improvements to the internal structure of the database to accommodate particle induced gamma ray emission (PIGE) data.

*According to SciVerse Scopus, the largest bibliographic database of abstracts and citations for academic journal articles, EMPIRE: Nuclear Reaction Model Code System for Data Evaluation, and RIPL – Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations, published in the Special Issues of Nuclear Data Sheets, vol. 108, no. 12, Dec. 2007 and vol. 110, no. 12, Dec. 2009 respectively, have reached the milestone number of 110 and 70 cited publications respectively. Compared to Google Scholar which includes reports as well as journal articles, EMPIRE has 138 and RIPL 82 citations. However, the Handbook for calculations of nuclear reaction data, RIPL-2 (IAEA-TECDOC-1506) has received the most citations with 172.*

# Data for Fusion Energy

The IAEA has long supported the international effort to develop fusion energy. The biennial IAEA Fusion Energy Conference is the top meeting in the field and the Nuclear Fusion journal founded by IAEA is one of the leading journals. The IAEA coordinated the INTOR International Tokamak Reactor design effort in the 1980s and cooperated with the ITER Project throughout its design. ITER (Latin for 'the way') is now under construction near Cadarache, France.

The Nuclear Data Section contributes to the development of fusion energy by providing libraries of atomic, molecular, plasma-material interaction and neutron and charged particle irradiation data. In this article we focus on the work of the Atomic and Molecular Data Unit (AMDU). The primary objective of the Unit is to provide internationally recommended databases on atomic, molecular and plasma-material interaction (A+M+PMI) processes relevant to fusion energy research. These databases are accessible at <http://www-amdis.iaea.org/>.



*The ITER machine is based on the tokamak concept of magnetic plasma confinement, in which the fusion fuel is contained in a doughnut-shaped vessel. The height of the entire device is 29 m while the vacuum vessel has a major radius of 6.2 m and a height of 10.2 m. The plasma-facing materials are beryllium for the main wall (indicated in yellow) and tungsten for the divertor region (indicated in brown).*

## A+M Databases

**ALADDIN** (<http://www-amdis.iaea.org/ALADDIN/>) is the principal numerical database maintained by the Unit. It contains data on atomic and molecular collisions, which includes photon and electron impact processes and heavy particle collisions, and data on particle-surface interaction, which includes reflection, penetration, physical sputtering, chemical sputtering and radiation-enhanced sublimation. The data come largely from CRPs, consultancies and other activities of the A+M Data Unit and are recommended data at the time of their compilation.

Deuterium-tritium fusion takes place at very high temperatures. In the centre of the confined plasma the temperature must be above 100 million degrees K (thermal energy above 10 keV). At such high temperature not only the primary plasma constituents D and T but also impurities such as C, O and even Fe are fully stripped of electrons. In the outer regions of the confined plasma the typical thermal energy is much less, down to about 10 eV, and in the divertor region, where most of the plasma-wall interaction takes place, the thermal energy can drop below 1 eV. Under those conditions molecules are formed and can survive.

See <http://www-amdis.iaea.org/w/> for explanation of some of the concepts of plasma confinement and for more information about atomic, molecular and plasma-material interaction data in fusion energy research.

The Unit maintains a numerical database (ALADDIN) and other numerical datasets, a search engine (GENIE) to find and access numerical data hosted elsewhere, a bibliographical database (AMBDAS) and since 2010 a wiki-style Knowledge Base on A+M+PMI data for fusion. Coordinated Research Projects (CRPs) are organized to encourage worldwide collaboration in the production and validation of new data. Technical and Consultants Meetings are held to support the activities of the Unit and coordinate database work throughout Member States. Among the recurring meetings of this kind are the coordination meetings of the international Atomic and Molecular Data Centres Network (DCN), those of the Code Centres Network (CCN) and meetings devoted to the development of XML standards for exchange of A+M and PMI data. Once every two to three years the Unit organizes a training workshop in the area of plasma modelling with use of A+M+PMI data, and at times the Unit cooperates in more advanced workshops. The AMDU is advised by the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC). Priorities for data evaluation are also assessed by the DCN. The IFRC Subcommittee on Atomic and Molecular Data and the Data Centres Network each meet biennially, in alternate years.

Several further numerical datasets are accessible through the A+M Data Unit home page. These are data for specific atomic or molecular systems that do not fit well into the ALADDIN framework. There are links to external databases including Open-ADAS: the core atomic data developed in the ADAS project. For each atomic and ionic system up to  $Z=79$  (Au) rate coefficients calculated by FLYCHK are provided as a function of temperature in the coronal (low density) limit for processes of direct collisional ionization, excitation autoionization, radiative recombination and dielectronic recombination. The

FLYCHK radiative cooling rate coefficients for line radiation and recombination radiation are also given. Another recent dataset provides the results of detailed structure calculations using the LANL atomic physics codes for atoms and ions of argon, chlorine and silicon.

**GENIE** (<http://www-amdis.iaea.org/GENIE/>), the ‘General Internet Search Engine for Atomic Data’, provides a common query interface to multiple databases for atomic structure and spectroscopy and for electron-atom collisions. Currently nine structure and spectroscopy databases and six collisional databases may be accessed by GENIE. Like our bibliographical and numerical databases GENIE is accessible without log-in or password.

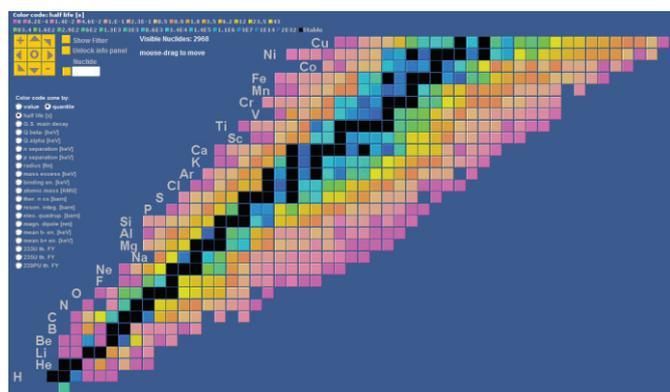
**AMBDAS** the Atomic and Molecular Bibliographic Data System, (<http://www-amdis.iaea.org/AMBDAS/>), contains about 50 000 entries going back to 1950 of articles and reports on atomic, molecular and plasma-surface interaction data relevant to fusion energy research. The broad categories in AMBDAS are structure and spectra, atomic and molecular collisions and surface interactions.

Entries are classified by process and reactants and classified as experimental or theoretical. Relevant energy values or energy ranges are also provided. The entries in AMBDAS are linked to the on-line version of the paper via its digital object identifier (doi) where it is available.

**Knowledge Base Wiki:** <http://www-amdis.iaea.org/w/>, the success and impact of Wikipedia has inspired us to start a wiki-style knowledge base on data sources, data production, data needs, and related information about atomic, molecular and plasma-material interaction in fusion energy research and related fields. This knowledge base quickly became one of the most visited areas of the A+M web pages, which attests to the attractive format and easy access that is offered by this mode of presentation. The information on the wiki is addressed to fusion plasma researchers and atomic, molecular and materials physicists in a way that complements our traditional databases with the aim to encourage collaboration and relevant new research. The knowledge base is public on the web, but editing is restricted to those that have obtained a password.

## LiveChart of the Nuclides

Devised within the Nuclear Data Section, the **LiveChart of the Nuclides** is an application to browse nuclear structure and decay data in an interactive way. **LiveChart** takes most



of its structure and decay data from ENSDF. It has been available online since 2009, and has evolved in such a manner as to help the user to show or discover patterns in nuclear data. As an on-going project **LiveChart** is continuously being developed and updated (see ND Newsletter Nos. 47 p. 4, 50 p. 3 and 51 p. 5). Recent new additions comprise data on:

- thermal neutron cross-section, resonance integrals and Westcott g factors from S.F. Mughabghab, INDC-NDS-440,
- fission yields from JEFF 3.1.1,
- Q-values and masses from the Atomic Mass Data Centre.

The user interface has also been enriched and now has more than 30 colour codes as well as new filtering criteria.

The application is available online at <http://www-nds.iaea.org/livechart>. Your feedback on these features is welcomed, email: [services@iaeaand.iaea.org](mailto:services@iaeaand.iaea.org).

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Since 1962, NDS has been storing and distributing documents that originated under the auspices of the INDC (see photo of the NDS Library on front page). In 2004 the viability of converting these documents, as well as IAEA-NDS and other NDS technical reports, to electronic format was investigated. By the end of 2011 the project related to the INDC documents had been completed - there are currently more than 2500 documents available. Work is on-going with other documents. At the same time, the NDS publications website has been significantly improved and all available documents and reports in the INDC- and IAEA-NDS series, IAEA-TECDOCs, conference proceedings and NDS staff publications can be accessed at <http://www-nds.iaea.org/publications/>.

I have been in post here at the IAEA for almost three years now. This period has seen many technological changes within the IAEA including the change to a one-house enterprise system (AIPS), as well as changes in NDS staff brought about by rotation policy - at the end of February we said goodbye to Mark Kellett (see p. 15). I look forward to continued challenges during the coming years as well as continued interaction with all of you in the nuclear data world.

*Robin Forrest*

# NDS Meeting Reports

Meeting reports, when finalised, available at <http://www-nds.iaea.org/publications/>

## Consultants Meeting (CM) on XML Schema for Atoms, Molecules and Solids (XSAMS) NIST, Gaithersburg, USA, October 3 – 5, 2011

Scientific Secretary: Bas Braams, Local organizer: Yuri Ralchenko, 8 participants

The XML Schema for Atoms, Molecules and Solids (XSAMS) is designed for transmission of numerical data concerning structure, spectra, collision cross-sections and rate coefficients for atomic, molecular and plasma-material interaction processes. The original development of XSAMS grew out of discussions between people from the National Institute of Standards and Technology (NIST) in the USA, the Paris Observatory and the IAEA about data exchange. XSAMS has been adopted by the European Virtual Atomic and Molecular Data Centre (VAMDC) and a pilot implementation has also been made on the main NIST atomic spectra database. The A+M Data Unit coordinates the development of the XSAMS standard. The CM at NIST was held in order to review the experience with implementations of XSAMS and the developments made by VAMDC to the preliminary standard XSAMS version 0.1.1. The meeting also offered an opportunity to advertise the Schema outside the community of developers. Following recent additions to describe spectral line shapes and molecular spectra the Schema now appears mature and stable for the description of atomic and molecular processes. More work is most needed in the area of interactions with surfaces and solids.

## Consultants Meeting (CM) on Beta-Delayed Neutron Emission Evaluation Vienna, Austria, October 10 – 12, 2011

Scientific Secretary: Daniel Abriola, 6 participants



*Participants of the CM on  
Beta-Delayed Neutron Emission Evaluation*

The main objective of this meeting was to consider the usefulness of initiating a Coordinated Research Project (CRP) on beta-delayed neutron emission. An accurate knowledge of the amount of beta-delayed neutrons released by neutron-rich fission products is indispensable for the control and kinetic behaviour of fission reactors. These data are also important for decay-heat calculations, astrophysics and nuclear theory. A review of the current state of affairs regarding the available compilations and new data from recent measurements was discussed, as well as possible ways to set up a dedicated database of evaluated data and how to update existing databases. The outcome of the meeting was that a proposal for a CRP on beta-delayed neutron emission should be made.

## IAEA Workshop on Monte Carlo Radiation Transport and Associated Data Needs for Medical Applications

Hosted by ICTP Trieste, Italy, October 17 – 28, 2011

Director: Roberto Capote, Workshop Assistant: Kira Nathani, 7 Lecturers, 55 participants from 30 countries

Monte Carlo (MC) techniques have been used extensively in medical physics applications, and offer the most powerful tool for modelling radiation transport in different media. The availability of general purpose MC codes (e.g. EGSnrc, Penelope and Geant4) combined with ever increasing computer speed and decreasing costs have led to a boom in MC studies in recent years.

The workshop constituted a unique opportunity for participants to gain extensive and up-to-date training on the use and understanding of cutting edge techniques for medical physics applications. The course was based on the EGSnrc system, a package developed by the National Research Council (NRC) of Canada for the coupled transport of electrons, photons and pos-



*Lecturers and Assistant of Workshop*

itrons. The BEAMnrc code was also covered allowing participants to learn how to model specific linear accelerators and other radiation sources employed in both diagnosis and radiotherapy.

With over 110 applications, this workshop ranges among the most sought after IAEA/NDS workshops, which resulted in one of the largest ever held. The selected participants—approximately fifty-five in total—hailed from a wide variety



*Participants of the IAEA Workshop on Monte Carlo Radiation Transport and Associated Data Needs for Medical Applications*

of both developed and developing countries. A total of seven external lecturers made presentations at the workshop and tutored the students at the laboratory sessions. The workshop was judged to be extremely successful from both the students' and lecturers' point of view.

Further detail on this workshop can be found on <http://www-naweb.iaea.org/na/news-na/na-medical-physics.html>

### **Technical Meeting (TM) on Long-Term Needs for Nuclear Data Development Vienna, Austria, November 2 – 4, 2011**

Scientific Secretary: Robin Forrest, 21 participants and IAEA staff



*Participants of the TM on Long-Term Needs for Nuclear Data Development*

The TM was convened to provide guidance on developing the programme of work over the next decade. This long term view complements advice given to NDS by the International Nuclear Data Committee (INDC). A similar meeting was last held in 2000 when useful guidance was provided, in particular on expanding the NDS programme to include charged particle data. Following presentations by each of the participants on particular topics covering the broad areas of medical and analytical applications, energy production, data libraries, basic science and tools/visualisation, subsequent extensive discussion led to a set of recommendations for the directions of future work. Report of meeting at: <http://www-nds.iaea.org/publications/indc/indc-nds-0601/>.

## Workshop on Development of Nuclear Data Libraries Vienna, Austria, November 28 – December 2, 2011

Scientific Secretary: Roberto Capote, 4 lecturers, 9 participants and IAEA staff



*Participants of the Workshop on Development of Nuclear Data Libraries*

The GANDR system for the global assessment of nuclear data (<http://www-nds.aiea.org/gandr>) has been developed over several years with major support from the IAEA. The system has been effectively used to produce nuclear-reaction evaluations of tungsten and manganese isotopes. A small workshop was organized to teach the theoretical foundations of nuclear data evaluation starting from selection and corrections of relevant experimental data to the calculation of uncertainties of the nuclear reaction model. Practical exercises on the use of the GANDR system to combine model and experimental uncertainties aiming at producing a nuclear data evaluated file were also undertaken. A workshop on a similar topic is scheduled for the winter of 2013.

## 3<sup>rd</sup> Research Coordination Meeting (RCM) on Characterisation of Size, Composition and Origins of Dust in Fusion Devices Vienna, Austria, November 30 – December 2, 2011

Scientific Secretary: Bas Braams, 12 participants and IAEA staff

Plasma-wall interaction creates dust and in a long-pulse machine such as ITER or a fusion reactor the potential for tritium accumulation in dust and the combustion hazard is a concern. Total amount of dust, amount of mobilizable dust, amount of dust on hot surfaces, and amount of tritium accumulated in dust are all subject to strict safety limits that must be verified throughout the operation of the device. The CRP on ‘Characterization of size, composition and origin of dust in fusion devices’ was formed to improve our knowledge of properties, production mechanisms and dynamics of dust in



fusion devices. This CRP held its final RCM in December 2011. A welcome output of the CRP will be a dust database, based on automated analysis of tens of thousands of images of dust particles taken from fusion and laboratory plasma experiments. The effort is centred at IPP Garching, but NDS staff are involved in the discussions and NDS expects to host the database in due time. Participants also agreed to produce a review article intended for Fusion Science and Technology and to produce individual contributions for APID Vol. 18.

*Participants of the 3<sup>rd</sup> RCM on  
Characterisation of Size, Composition and Origins of Dust in Fusion Devices*

## 7<sup>th</sup> Non Local Thermodynamic Equilibrium (NLTE) Code Comparison Workshop Vienna, Austria, December 5 – 9, 2011

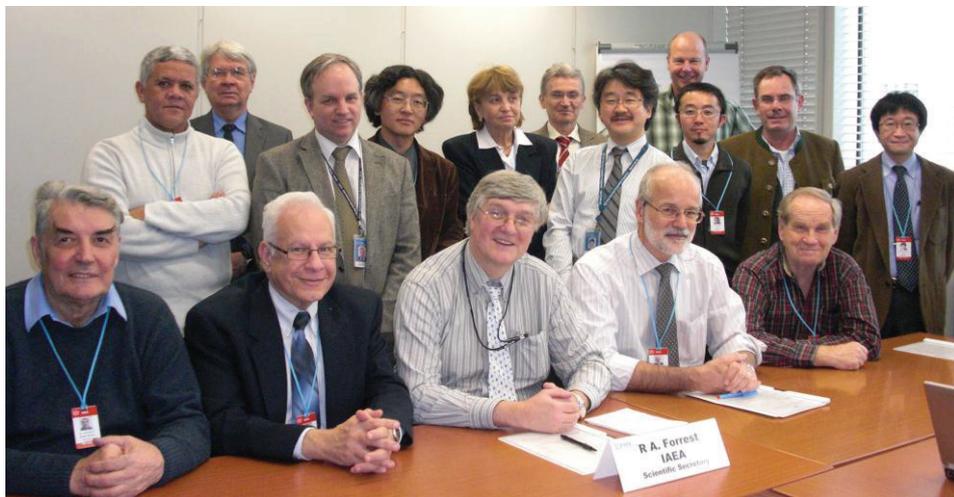
Scientific Secretary: Hyun-Kyung Chung, 23 participants and IAEA staff

The purpose of the NLTE code comparison workshops is to bring together developers of codes for atomic kinetics in finite density plasmas and to perform detailed comparison of calculations on well-defined test cases. The seventh in the series of NLTE code comparison workshops was organized in Vienna in cooperation with IAEA. Participants submitted results from 19 codes for more than 50 test cases in the workshop and these were discussed in detail. A meeting report will be prepared for journal publication and the publication of detailed comparisons of specific cases will be considered by participating code developers and case coordinators.

## 3<sup>rd</sup> Research Coordination Meeting (RCM) on Nuclear Data Libraries for Advanced Systems: Fusion Devices (FENDL-3) Vienna, Austria, December 6 – 9, 2011

Scientific Secretary: Robin Forrest, 13 participants and IAEA staff

The FENDL-3 library is a set of data to satisfy the needs of fusion technology. It will update FENDL-2.1 by increasing the number of materials, extending the energy range above 20 MeV and providing reaction data for incident protons and



*Participants of the 3<sup>rd</sup> RCM on  
Nuclear Data Libraries for Advanced Systems: Fusion Devices*

deuterons in addition to neutrons. For neutron-induced reactions covariance data will be as complete as possible. Such a library will be able to address the needs of the fusion community by providing input data for calculations on ITER, IFMIF and DEMO. During the meeting, a series of presentations describing the work done in the preparation of the latest test version and its processing and testing were discussed. As this was the final RCM, the various actions needed to complete the library and the composition of the report and documentation were agreed.

## 2<sup>nd</sup> Research Coordination Meeting (RCM) on Prompt Fission Neutron Spectra of Actinides Vienna, Austria, December 13 – 16, 2011

Scientific Secretary: Roberto Capote, 15 participants

The RCM was convened to review the status of the project. In-depth technical discussions on theoretical modelling of prompt fission spectra took place covering both deterministic and Monte Carlo methods. Review of the status of available

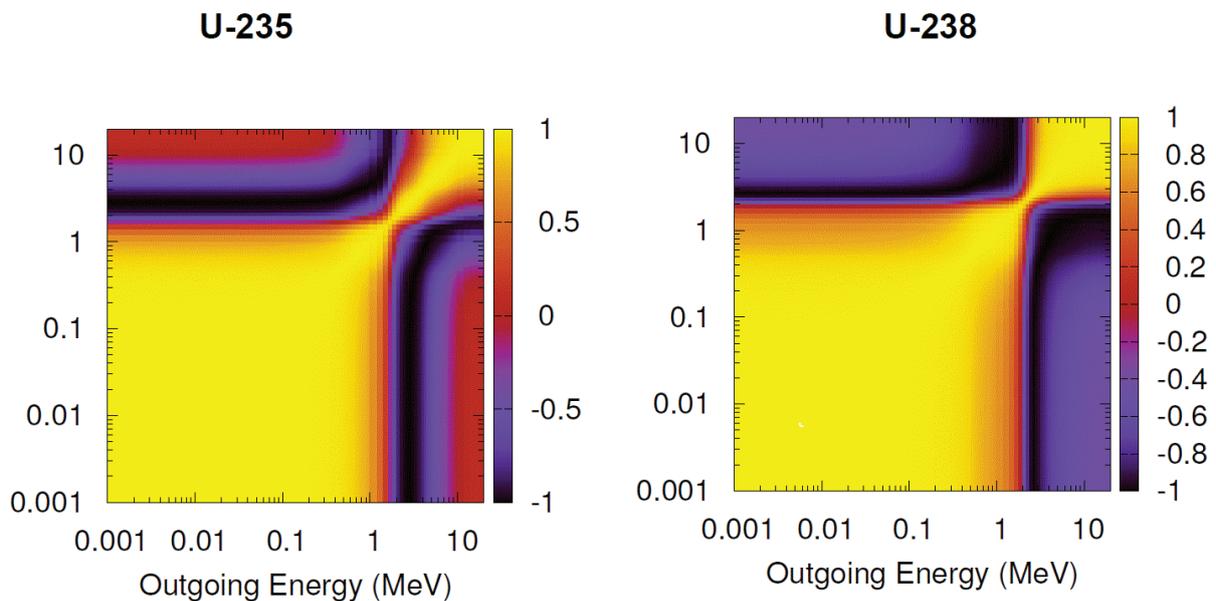
experimental data to be used in evaluation work was also undertaken. A series of conclusions, recommendations and actions were approved with the goal for these to be achieved by the end of 2013, before the next



*Participants of the 2<sup>nd</sup> RCM on Prompt Fission Neutron Spectra of Actinides*

meeting. The structure of the technical report will cover Experiments; Modeling (Los Alamos Model, Monte Carlo methods, etc.); Evaluations (spectrum + covariances), and Benchmarks.

Additional information will be available in the Summary Report to be published as INDC(NDS)-0608 in 2012. Presentations at the meeting are available at <http://www-nds.iaea.org/pfns/rcm2>



*Evaluated covariance matrices of prompt fission neutron spectra (PFNS) for 0.5 MeV neutrons incident on U-235 (left) and U-238 (right) nuclei (from P. Talou presentation at the 2<sup>nd</sup> RCM, Vienna, December 2011)*

### Technical Meeting (TM) on Improving the Database for Physical and Chemical Sputtering Vienna, Austria, December 12 – 13, 2011

Scientific Secretary: Bas Braams, 7 participants and IAEA staff

This TM brought together a group of people that have contributed in the past and continue to contribute to the database of sputtering, reflection and erosion properties for plasma-facing materials. The key objective was to assess the quality of the existing database and identify areas where the database could be improved with relatively modest effort. The



*Participants of the TM on Improving the Database for Physical and Chemical Sputtering*

most important area appears to be that of mixed materials, especially various Be-W alloys. In the near term several datasets that are already available need to be incorporated into the ALADDIN database. Parameters were specified for some new calculations that should be done with use of the binary collision approximation (i.e. the SDTrimSP family of codes) for interaction of H and He with mixed materials.

## Technical Meeting (TM) on Ab-Initio-based Methods for Plasma-material Interaction in Fusion Devices

Vienna, Austria, December 14 – 15, 2011

Scientific Secretary: Bas Braams, 11 participants and IAEA staff



*Participants of the TM on Ab-Initio-based Methods for Plasma-material Interaction in Fusion Devices*

This TM was held back-to-back with the TM on improving the database for physical and chemical sputtering in order to raise awareness of computational tools and needs for the study of plasma-material interaction and encourage new work and new collaborations among the PMI community and other computational materials scientists. The meeting brought together computational scientists active in the field of plasma-material interactions for fusion applications with experts from materials science that use the best available computational methods in their work but that may apply these methods to other problems in materials science.

## ICTP-IAEA Workshop on Atomic, Molecular and Plasma-Material Interaction Data and Codes for Fusion Plasma Modelling ICTP, Trieste, Italy, January 23 - 27, 2012

Director: Bas Braams, IAEA-Staff: Hyun-Kyung Chung, Local Organizer: J. Niemela,  
10 Lecturers: 21 participants from 14 countries



*Participants of the ICTP-IAEA Workshop on Atomic, Molecular and Plasma Material Interaction Data and Codes for Fusion Plasma Modelling*

Following similar joint workshops in 2003, 2006 and 2009, the aim of the workshop was to bring together plasma modellers that use atomic, molecular and plasma-material interaction (A+M+PMI) data in their work with researchers in the field of atomic, molecular or plasma-material interaction physics that produce relevant data. The following countries and international organizations were represented (in brackets the total number if more than one): Algeria, Burundi, Cameroon, China (2), Finland, France (2), Germany (6), India (6), Italy (2), Japan, Kazakhstan, Pakistan, Tunisia (3), USA (2); IAEA (2), ICTP.

The workshop was addressed to early-career researchers, generally beyond the level of a Ph.D., who wanted to broaden their outlook with respect to plasma modelling and relevant A+M+PMI processes. Lecturers D. Reiter, K. Ohya and B. Ziaja-Motyka presented plasma modelling, Yu. Ralchenko and H.-K. Chung presented computational procedures for atomic processes and spectroscopy, Yaming Zou, R. Hutton and J. Clementson described EBIT atomic data experiments, M. Telmini spoke on electron-molecule collisions and K. Nordlund, A. Allouche and P. Giannozzi presented plasma-material interaction processes. All participants presented a poster and a short talk to introduce their poster.

The ICTP offers an excellent environment and the workshop was much appreciated by lecturers and participants alike both for the training role and for the opportunity to meet colleagues and make new contacts (for further details see <http://www-amdis.iaea.org/Workshops/ICTP2012/>).

**Consultants Meeting (CM) on Procedures for Evaluation of  
Atomic, Molecular and Plasma-material Interaction Data for Fusion  
National Institute for Fusion Science (NIFS), Toki City, Japan, February 7 – 9, 2012**

Scientific Secretary: Hyun-Kyung Chung, Local organizer: Izumi Murakami, 13 participants

The CM at NIFS is part of a long term effort by NDS to reinvigorate data evaluation work and establish a standard library of atomic, molecular and plasma-material interaction data for fusion. In order to allow more participants actively engaged in data evaluation to attend, it was agreed to hold the meeting at NIFS in Japan. Participants reviewed current data evaluation activities in their data centres, data evaluation methods especially for theoretical data, and definition of concepts for standard data and uncertainties. Participants value the coordinating role of the IAEA for data evaluation and establishment of a standard library. Preparations were made for a larger technical meeting on data evaluation for fusion to be held in September 2012 in Daejeon, Korea.

**Consultants Meeting (CM) on XML Schema for Atoms, Molecules and Solids (XSAMS)  
in conjunction with the annual meeting of the Virtual Atomic and Molecular Data Centre (VAMDC)  
Vienna, Austria, February 20 – 22, 2012**

Scientific Secretary: Bas Braams, 9 participants and IAEA staff

About twenty implementations of XSAMS are currently in progress, largely due to the adoption of XSAMS by the Virtual Atomic and Molecular Data Centre (VAMDC), a European Framework-7 project. The 2012 annual meeting of VAMDC was held at the University of Vienna, 21 - 24 February, and a CM on XSAMS was organized overlapping that meeting. The first day of the CM was devoted to a comprehensive review of modifications that were made to XSAMS in connection with the VAMDC implementations. The second and third day of the CM was largely combined with the VAMDC annual meeting. At the conclusion of the CM the XSAMS steering committee met to evaluate the implementation experience. It was decided to adopt the present VAMDC XSAMS as the international standard. It was also agreed that for the next year or two XSAMS work should be focused on broader implementation and on the development of tools to work with XSAMS output.

**Consultants Meeting (CM) on Further Development of EXFOR  
Vienna, Austria, March 6 – 9, 2012**

Scientific Secretary: Stanislav Simakov, 9 participants and IAEA staff

Organized in accordance with a recommendation of the NRDC Technical Meeting held 23 - 24 May 2011 (<http://www-nds.iaea.org/publications/indc/indc-nds-0593/>), the main goal of the meeting was to assess needs and ways for development of the EXFOR formats to meet future requirements. Participants reported the difficulties of coding complex reaction and supplemental experimental information in the present EXFOR exchange format, their dissatisfaction regarding complex EXFOR dictionaries for encoding reaction string and shared their experiences from working with other databases and formats (NRDF, ROOT, ENDF/GND, XSAMS). It was decided to:

- explore options for further extensions of the exchange format for facilitating the coding of experimental results,
- continue development of editors and other software for compilers,
- continue development of EXFOR/XML output for easier access by both computer programs and people.



*Participants of the CM on Further Development of EXFOR*

A summary report of the meeting will be available as INDC(NDS)-0614.

## External Event

### Theme Meeting on Nuclear Reaction Data Evaluation, Bhaba Atomic Research Centre (BARC), Mumbai, India, February 13 - 17, 2012

IAEA-NDS staff member Roberto Capote, together with Andrej Trkov, a former staff member now at the Institut Jožef Stefan, Slovenia, lectured at a workshop hosted at BARC. Over thirty participants attended the workshop where the emphasis was hands-on training using EMPIRE-3.1 (Rivoli) and GANDR 4.6 systems for nuclear data evaluation. Participants held extensive discussions on the latest releases of both EMPIRE and GANDR packages. Codes were distributed to participants.



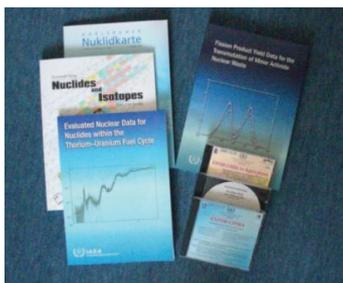
*Participants of the Theme Meeting on Nuclear Reaction Data Evaluation*

## In Memoriam



Alan Bowen Smith, an eminent physicist in the field of nuclear data, died on 5 January 2012 at age 87. Alan was employed at Argonne National Laboratory for his entire active career from 1953 to 1992. Thereafter, he served in an emeritus status until his death. His field of research was applied nuclear physics, with a focus on measurement and nuclear model analyses of fast-neutron total, elastic-scattering, and inelastic-scattering cross-sections in support of the development of the neutron optical model. Alan was universally respected and admired by those who knew him. In recognition of his body of scientific work and many other contributions to his field, Alan was honored with fellowship appointments in both the American Physical Society and the American Nuclear Society. He was also a recipient of the University of Chicago Distinguished Service Award. Above all, he was a friend, colleague, and valued mentor to three generations of nuclear scientists.

# Selected Charts, Reports and Documents



All INDC series reports are available online:

[http://www-nds.iaea.org/publications/indc\\_groups.php](http://www-nds.iaea.org/publications/indc_groups.php)

## Recent Releases:

**INDC(NDS)-0595** Summary Report of an IAEA Technical Meeting on Nuclear Structure and Decay Data (NSDD) Network, Vienna, 4-8 April 2011, prepared by D. Abriola, A.L. Nichols, J.K. Tuli, October 2011.

**INDC(NDS)-0596** Summary Report of an IAEA Technical Meeting on Intermediate-term Nuclear Data Needs for Medical Applications: Cross Sections and Decay Data, Vienna, 22-26 August 2011, prepared by A.L. Nichols, S.M. Qaim, R. Capote Noy, September 2011.

**INDC(NDS)-0598** Missing Levels with Two Superimposed Sequences, prepared by J.F. Shrinier, Jr., G.E. Mitchell, October 2011.

**INDC(NDS)-0599** Summary Report of an IAEA Consultants Meeting on Beta-delayed Neutron Evaluation, Vienna, 10-12 October 2011, prepared by D. Abriola, B. Singh and I. Dillmann, December 2011.

**INDC(NDS)-0600** Summary Report of an IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange, Summary Report from the 21st Meeting of the A+M Data Centres Network, Vienna, 7-9 September 2011, prepared by H.-K. Chung, November 2011.

**INDC(NDS)-0601** Summary Report of an IAEA Technical Meeting on Long-term Nuclear Data Needs, Vienna, 2-4 November 2011, prepared A. Plompen, R.A. Forrest, January 2012.

**INDC(NDS)-0602** Summary Report of the Third Research Coordination Meeting on Nuclear Data Libraries for Advanced Systems - Fusion Devices (FENDL 3), Vienna, 6-9 December 2011, prepared by M. Sawan, R.A. Forrest, March 2012.

**INDC(NDS)-0606** Summary Report of an IAEA Consultants Meeting on XML Schema for Atoms, Molecules and Solids (XSAMS), Vienna, 3-5 October 2011, prepared by B.J. Braams, December 2011.

**INDC(NDS)-0611** FENDL-3.0: Processing the Evaluated Nuclear Data Library for Fusion Applications, prepared by D. Lopez Aldama, R. Capote Noy, December 2011.

**INDC(NDS)-0612** New Evaluated Neutron Cross Section Libraries for the GEANT4 Code, prepared by E. Mendoza, D. Cano-Ott, C. Guerrero, R. Capote Noy, February 2012.

**INDC(NDS)-0613** Summary Report of a Joint ICTP-IAEA Workshop on Fusion Plasma Modelling Using Atomic and Molecular Data, prepared by B.J. Braams, March 2012.

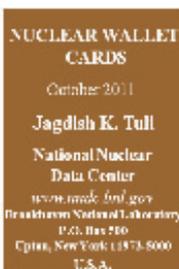
**INDC(CCP)-0454** Neutron-induced Fission Cross Sections of Am and Cm Isotopes (Final Report of RC-14485) Resonance and Fast Neutron Induced Fission Cross Sections of Americium and Curium Nuclides, prepared by A.A. Alekseev, A.A. Bergman, A.I. Berlev, E.A. Koptelov, A.S. Egorov, B.F. Samylin, A.M. Trufanov, B.I. Fursov, V.S. Shorin, January 2012.

**INDC(HUN)-0037** Measurement of  $^{241}\text{Am}$  Ground State Radiative Neutron Capture Cross Section with Cold Neutron Beam, prepared by T. Belgya, L. Szentmiklósi, Z. Kis, N.M. Nagy, J. Kónya, January 2012.

**Nuclear Data Sheets Special Issue on Nuclear Reaction Data**, Vol. 112, No. 12 (2011). Special Issue on *ENDF/B-VII.1 Library*, Editor: P. Obložinský. Containing eight papers on various aspects of the new ENDF/B-VII.1 library. Limited hard copies available on request.

**Nuclear Wallet Cards 2011** 8th Edition, by Jagdish K. Tuli, National Nuclear Data Center.

<http://www.nndc.bnl.gov/wallet/wc8.html>



This booklet presents selected properties of all known nuclides and their known isomeric states. Properties given are:

- Spin and parity assignments
- Nuclear mass excesses
- Half-life, isotopic abundances
- Decay modes

Appendices contain properties of elements, fundamental constants and other useful information. These pocket size wallet cards are available as hard copy on request.

## Also Available:

**Chart of the Nuclides 2010** IAEA Nuclear Data Centre.

**Chart of the Nuclides** (Wall chart) prepared by Knolls Atomic Power Laboratory (KAPL) and distributed by Lockheed Martin (17<sup>th</sup> edition, revised 2009). Available cost-free on request only for **teachers and scientists from developing countries**.

**Chart of the Nuclides** (Book) prepared by Knolls Atomic Power Laboratory (KAPL) and distributed by Lockheed Martin (17<sup>th</sup> edition, revised 2009). Available cost-free on request only for **teachers and scientists from developing countries**.

**Karlsruher Nuklidkarte** Wall chart of the nuclides from Karlsruhe, 7<sup>th</sup> edition (2006). Available cost-free on request only for **teachers and scientists from developing countries**.

**Karlsruher Nuklidkarte** Desk chart of the Nuclides from Karlsruhe, 7<sup>th</sup> edition (2006). Available cost-free on request only for **teachers and scientists from developing countries**.

**NOTE to Universities:** earlier editions of KAPL and Karlsruhe Nuclides Charts, in book form, are available cost free for student use (as long as supplies last).

# Coordinated Research Projects

IAEA Coordinated Research Projects (CRPs) are a valuable mechanism for stimulating research in IAEA Member States of relevance to the IAEA programmes. Details of the CRPs of the Nuclear Data Section, both active and recently completed, can be found at: <http://www-naweb.iaea.org/napc/nd/crps.asp>.

Two new CRPs are:

**Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials:** There is very active interest at present in the properties of beryllium as a wall material exposed to plasma in a fusion reactor environment. The new CRP on Data for erosion and tritium retention in beryllium plasma-facing materials is intended to enhance the knowledge base on relevant particle-material interaction processes. The key processes to be studied in the CRP are physical and chemical sputtering by H, He and Be, which release beryllium impurities into the plasma, trapping and reflection of hydrogen on beryllium surfaces, the transport of hydrogen in beryllium and means to extract trapped tritium. The CRP will bring together experimentalists and computational theorists that are engaged in studies of plasma-material interaction with beryllium and related mixed materials and of hydrogen migration in solid beryllium. The first research coordination meeting of the new CRP is planned for September 2012.

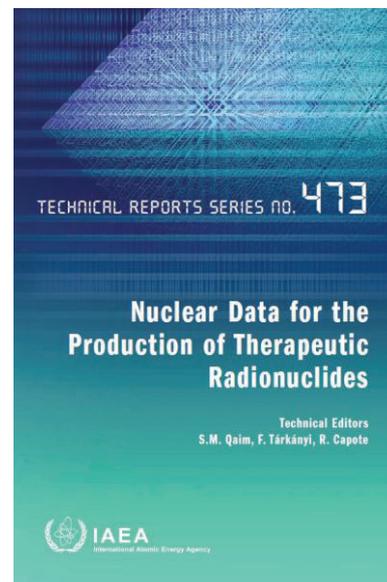
**Charged-particle nuclear data for medical isotope production:** A new CRP on Nuclear data for charged-particle monitor reactions and medical isotope production is planned to start at the end of 2012 as discussed in a Summary Report of the recently held Consultants Meeting published as INDC(NDS)-0591. The main planned outputs of the project will be new measurements and recommended evaluations of decay and cross-section data for reactions used to monitor charged-particle beams, and for production of novel positron and alpha emitters used in both diagnostic and therapeutic studies. Nuclear reaction modelling of studied charged-particle induced reactions is also within the scope of the project. Specific goals of the CRP are defined in the above mentioned report. Interested parties may contact the project officer Roberto Capote ([Roberto.CapoteNoy@iaea.org](mailto:Roberto.CapoteNoy@iaea.org)).

Technical reports detailing the outcome of IAEA-CRPs can be accessed electronically on:

<http://www-pub.iaea.org/MTCD/publications/>

The final technical report of the corresponding CRP **Nuclear Data for the Production of Therapeutic Radionuclides** is available at:

[http://www-nds.iaea.org/radionuclides/TECDOC/IAEA\\_TRS473\\_Therapeutic\\_Radionuclides.pdf](http://www-nds.iaea.org/radionuclides/TECDOC/IAEA_TRS473_Therapeutic_Radionuclides.pdf)



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## Staff Items

for all NDS staff details: <http://www-naweb.iaea.org/naweb/nd/aboutus.asp>



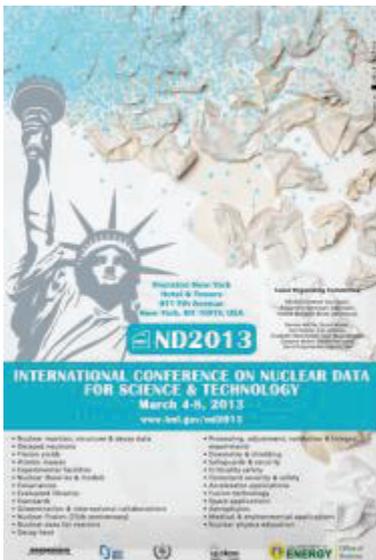
After seven years in NDS Mark Kellett has left the IAEA. During his stay in the Nuclear Data Section, he dedicated his technical efforts mainly to decay data, by providing keywords for the NSR database (<http://www-nds.iaea.org/nsr/>), and also continuing the development of evaluated decay data files in support of the JEFF library project. Mark was the project officer for two CRP initiatives – the updated decay data library for actinides ([http://www-nds.iaea.org/act\\_ddl/public.html](http://www-nds.iaea.org/act_ddl/public.html)) and the reference database for neutron activation analysis (<http://www-nds.iaea.org/naa/public.html>). Mark also took an active part in the decay heat related activities within the Section, and contributed to the related work of WPEC sub-group 25. We wish him every success in the next phase of his career and expect our strong technical links to be maintained.

It is anticipated that an announcement regarding a successor for Mark Kellett in the position of Nuclear Physicist will be made in the next issue of the ND Newsletter.

The position of **Nuclear Data Physicist, Head Nuclear Data Development Unit**, will become vacant as of April 2013 due to the retirement of the present incumbent Daniel Abriola. The person appointed will be specifically responsible for the planning and implementation of the data development, data validation and technology transfer activities of the Nuclear Data Development Unit, and will assist in administrative tasks for the Section, including programme and budget issues. Interested applicants please monitor the IAEA website as it is expected that a vacancy notice will be posted in the next few months at [https://recruitment.iaea.org/phf/p\\_vacancies.asp](https://recruitment.iaea.org/phf/p_vacancies.asp).

## Forthcoming Event

### ND-2013



**Objective:** to bring together scientists and engineers involved in the production and use of nuclear data for various applications.

**History:** held every three years, this conference is part of a series; the location alternates between the USA, Europe and Asia.

**Topics:** nuclear reaction data, nuclear structure and decay data, delayed neutrons, fission yields, atomic masses, experimental facilities and detection techniques, nuclear data measurements and analysis, nuclear theories, models and data evaluation, uncertainty quantification and covariances, evaluated nuclear data libraries, nuclear data processing, nuclear data adjustment, validation of evaluated data, integral experiments.

**IAEA-NDS:** has limited funds at its disposal to help meet the costs of attendance by selected specialists from developing countries with low economic resources. In summer 2012, a Note Verbale will be sent to Ministries of Foreign Affairs of IAEA Member States with the request that they draw the attention of the appropriate governmental authorities to this fact. **Requests can only be considered if they are submitted by a government on behalf of one of its specialists.**

This newsletter, as well as previous issues, can be accessed electronically at:  
[http://www-pub.iaea.org/books/IAEABooks/View\\_Newsletters/60/Nuclear-Data-Newsletter](http://www-pub.iaea.org/books/IAEABooks/View_Newsletters/60/Nuclear-Data-Newsletter)

To ensure continued receipt of your Nuclear Data Newsletter, please keep us informed of any change in address:  
 email: [services@iaeaand.iaea.org](mailto:services@iaeaand.iaea.org)

## 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](mailto:nndc@bnl.gov); Worldwide Web: <http://www.nndc.bnl.gov/>

For information regarding on-line services, contact: B. Pritychenko: [pritychenko@bnl.gov](mailto:pritychenko@bnl.gov)

For information regarding general NNDC services, contact: M. Blennau: [blennau@bnl.gov](mailto: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: [Emmeric.Dupont@oecd.org](mailto:Emmeric.Dupont@oecd.org) or [db@nea.fr](mailto:db@nea.fr); Worldwide Web: <http://www.oecd-nea.fr/databank/>; contact: E. Dupont, ext. 1084.

### For services to the customers from the former USSR:

Neutron data: Russia Nuclear Data Center, Centr Jadernykh Dannykh (CJD), Fiziko-Energeticheskij Institut, Ploschad Bondarenko,  
249020 Obninsk, Kaluga Region, Russian Federation.

Tel. +7 08439-9-8982; Fax +7 095-230-2326;

Email: [blokhin@ippe.ru](mailto:blokhin@ippe.ru); Worldwide Web: [www.ippe.ru/podr/cjd/](http://www.ippe.ru/podr/cjd/); contact: A.I. Blokhin.

Charged-particle data: Russia Nuclear Structure and Reaction Data Center (CAJAD), Kurchatov Institute,  
Kurchatov Square 1, 123 182 Moscow, Russian Federation.

Tel. +7 095-196-9968; Fax +7 095-882-5804;

Email: [sbabykina@polyn.kiae.su](mailto:sbabykina@polyn.kiae.su); contact: S. Babykina.

Photonuclear data: Centre for Photonuclear Experiments Data, Centr Dannykh Fotoyadernykh Eksperimentov (CDFE),  
Skobel'syn 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](mailto:varlamov@depni.sinp.msu.ru) or [varlamov@depni.npi.msu.su](mailto:varlamov@depni.npi.msu.su); Worldwide Web: <http://cdfe.sinp.msu.ru/>; contact: V.V. Varlamov.

### For services to customers in China:

China Nuclear Data Center, China Institute of Atomic Energy, P.O. Box 275(41), Beijing 102413, China.

Tel. +86 10-6935-7275; Fax +86 10-6935-7008; Email: [gezg@ciae.ac.cn](mailto: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 37831-6362, USA.

Tel. +1 865-574-6176; Fax +1 865-574-6182;

Email: [pdc@ornl.gov](mailto:pdc@ornl.gov) Worldwide Web: <http://rsicc.ornl.gov/CustomService.aspx>

### Computer codes of non-US origin to all countries (there may be release restrictions):

NEA Data Bank (see above)

Email: [Juan.Galan@oecd.org](mailto:Juan.Galan@oecd.org); contact: J. Galan, 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/>

Users in India and neighbouring countries may use

IAEA-NDS mirror at Worldwide Web: <http://www.nds.indcentre.org.in>

## Impressum

Nuclear Data Newsletter, No. 53, May 2012

The Nuclear Data Newsletter is prepared by the  
Division of Physical and Chemical Sciences, Department of Nuclear Sciences and Applications

International Atomic Energy Agency  
Vienna International Centre, PO Box 100, 1400 Vienna, Austria  
Printed by the IAEA in Austria, May 2012