

IAEA Nuclear Data Section: Progress Report, 2009/10
Summary of Nuclear Data Studies by Staff of the IAEA Nuclear Data Section
11 May 2009 – 1 April 2010

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1. Staff

The authorized staff level of the Nuclear Data Section (NDS) consists of a total of 17 professionals and support staff.

- Alan Nichols retired as ND Section Head end-April 2009; Robin Forrest started as Section Head in July 2009.

There were several other changes in NDS staff during the period covered by this report:

in Nuclear Data Services Unit (NDSU):

- Alberto Mengoni, (Unit Head) terminated his contract in June 2009, position still vacant; Vladimir Pronyaev was given a consultancy contract for six months (June – December 2009) in order to ensure the provision of technical support in NDSU during the period of recruitment for a new NDSU Head;
- Georgina Bush retired in December 2009, succeeded by Janet Roberts as of January 2010);
- Lidija Vrapcenjak succeeded Janet Roberts as Section Secretary;
- Alexander Oechs, Clerk, succeeded Lidija Vrapcenjak as Clerk.

in Atomic and Molecular Data Unit:

- Bob Clark (Unit Head) retired July 2009; succeeded by Bas Braams September 2009;
- Denis Humbert succeeded by Hyun Chung as of October 2009;
- Marco Verpelli terminated his contract December 2009, position still vacant.

2. Data Compilations

2.1 EXFOR and Dictionaries

Over the previous year, NDS staff have distributed 6 CPND TRANS files (D067 - D072) containing 127 new entries (42 compiled at NDS, 17 at ATOMKI, 7 at UkrNDC, 59 in India and 2 in KAERI) and 64 revised entries, 10 neutron TRANS files (3135 - 3144) containing 40 new entries (21 compiled at NDS, 5 at UkrNDC, 3 entries in KAERI, 7 in India and 3 in China) and 645 revised entries, 2 PhND TRANS files (G019,G020), containing 9 new entries (1 compiled at NDS, 1 in UkrNDC and 7 in KAERI) and 13 revised entries. The compilations

consist of new literature as well as important old references for Coordinated Research Projects.

KAERI Nuclear Data Evaluation Group (KAERI-NDEL) continues EXFOR compilation for neutron, charged-particle and photon induced reaction data measured in Korea on a trial basis. So far three neutron entries (31666, 31668, 31675), two CPND entries (D0569, D0570) and one PhND entry (G0015) have been finalized.

As of 15 May 2009, 59 TRANS files were received, checked (with feedback to the originating centres) and processed, of which 57 were final versions that were added to the master file. These final transmissions contained 582 neutron entries (89 new, 493 revised), 501 CPND entries (329 new, 172 revised) and 33 photonuclear entries (13 new, 20 revised).

NDS staff have produced and distributed two regular transmissions of the EXFOR/CINDA dictionaries (TRANS.9098-9099) in EXFOR, DANIEL (backup) and archive format.

Two lists of compilation mistakes have been updated:

- Feedback from general users/compilers: http://www-nds.iaea.org/nrdc/exfor_err1.html ;
- Feedback from WPEC SG-30: http://www-nds.iaea.org/nrdc/exfor_err3.html .

Three new lists of EXFOR outliers submitted by E. Dupont (CEA Saclay, NEA Data Bank) and A. Koning (NRG, Petten) were checked and the results were distributed to other centres. The correction process of the mistakes is being monitored by NDS staff.

2.2 Coverage control

Under the EXFOR compilation control system, NDS staff scans over 80 journal titles (mainly through the Internet) for the purpose of compilation coverage control. The current status of these compilation activities has been made available to EXFOR compilers on the NDS Web site during the course of this year.

Over 650 journal issues from 1990 to 2010 were added to the database for EXFOR compilation control system in late 2009/2010. Journal references that should be compiled elsewhere were also dispatched to the relevant centres (Japan, Russia, Hungary and NEADB).

All references missing from EXFOR were sent to the responsible centres for compilation, together with pdf. copies of the papers, where necessary.

Other EXFOR database statistics available from the NDS Web site:

- contributions to EXFOR according to individual centres,
- history (Preliminary, TRANS files, database updates),
- general statistics (contents by Quantities, Targets, Reactions, etc.).

NDS continues to save articles in pdf. format. Articles stored previously on the shelf at NDS are now held in electronic form. All articles compiled during this year in other centres have been scanned and stored in pdf. format by NDS. More than 900 files were saved in pdf. format during the year.

2.3 CINDA

CINDA Master file

The up-to-date CINDA Master File is available via the NDS compilers' Web site. An automatic update using the EXFOR database has been carried out three times (April 2009, December 2009, March 2010). A Sybase/MySQL-dump of the complete CINDA database was sent to NNDC. A few new CINDA lines (one exchange file from NDS) have been prepared manually where some coding errors were corrected.

2.4 Evaluated data libraries, files and programs

Various new or revised evaluated data libraries, files and programs for data checking, processing and graphical presentation were added to the NDS Web site and distributed on CD-ROM (see below).

3. Services

Web Services

Further improvements have been implemented in the Web EXFOR-CINDA-ENDF retrieval systems since the last NRDC meeting:

- ENDF (Evaluated Nuclear Data Files):
 - Processing ENDF-MF33 with following visualization of covariance matrices were added to the ENDF Web interface (includes 3D animation, cross-reaction and cross-material correlations, relative and absolute cross section uncertainties)
 - ENDF-Archive: collection of evaluated data libraries for FTP downloading (37 libraries): <http://www-nds.iaea.org/ndspub/download-endf/>
 - new evaluated libraries included in the ENDF database:
 - TENDL-2009 TALYS-based Evaluated Nuclear Data Library
 - ROSFOND-2010: neutron library, 686 materials, Obninsk, Russia
 - CENDL-3.1 Chinese evaluated neutron data library, issued in 2009
 - ROSFOND-2008: neutron library, 683 materials, Obninsk, Russia
- EXFOR:
 - Production of isotopes coded as ELEM/MASS: filtering and quick plot, sorting T4
 - Users' definition of ENDF:MF/MT for conversion EXFOR data to format C4 and advanced plotting
 - Search by compiling Center-ID
 - Search by outgoing particle coded in SF3,4,7
 - Correction of experimental data in computational formats (and following plotting)
 - Full EXFOR in C4 computational format was regularly produced (quarterly) and delivered to WPEC group SG-30
- Web-ZVView was developed and released allowing remote plotting via Web on server side without downloading actual program

The Web EXFOR-CINDA-ENDF retrieval system is functioning at NNDC, BARC (India) and IPEN (Brazil). Statistics for usage of the Web retrieval system are presented on figures below.

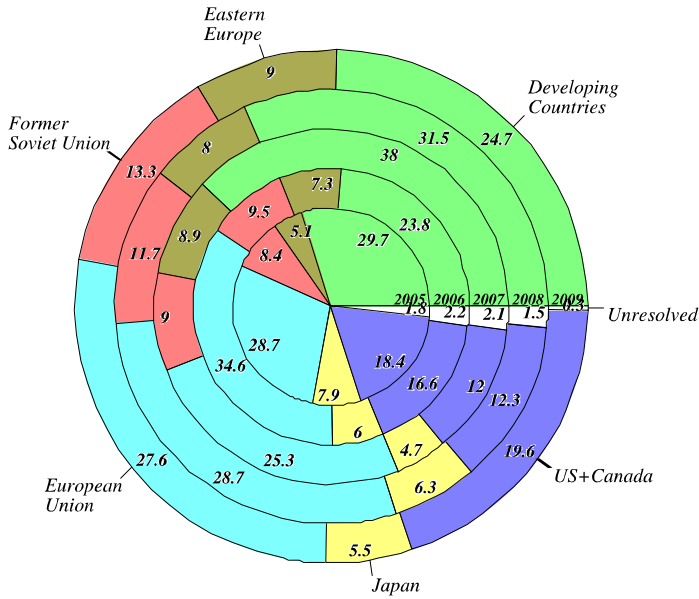
CD-ROMs

- “EXFOR/CINDA for Windows” CD: one official issue;
- “EXFOR/CINDA for Applications” for Linux, Windows and Macintosh issued twice; also distributed together as part of EndVer/GUI-CD and Empire-package.

NDS+IPEN+BARC

Nuclear Data Services: Web Statistics

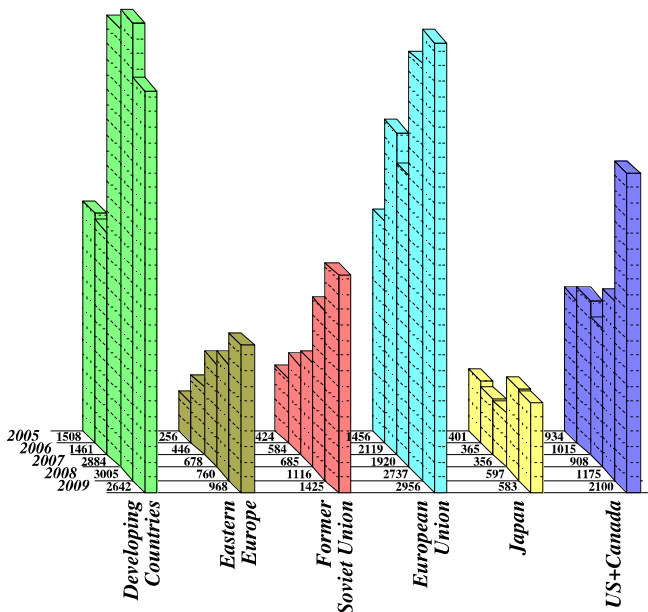
Geographical Distribution (%)



Total per Year (Number of accesses + retrievals)



Average per Month (Number of accesses + retrievals)



- | Service | Comment |
|------------------------|--------------|
| Computer Codes | |
| Documents | |
| OtherData | |
| IBANDL | |
| PGAA | |
| PhotoNuclear | |
| RIPL | Theory |
| FENDL | Fusion |
| Masses | |
| IRDF | Dosimetry |
| Thermal Capture | |
| Wallet Cards | |
| Med.Radioisotope.Prod. | |
| NGAtlas | Activation |
| RNAL | |
| ENSDF | Structure |
| MIRD | Medical |
| LiveChartNucl | Structure |
| CINDA+NSR Bibliography | |
| EXFOR | Experimental |
| ENDF | Energy |

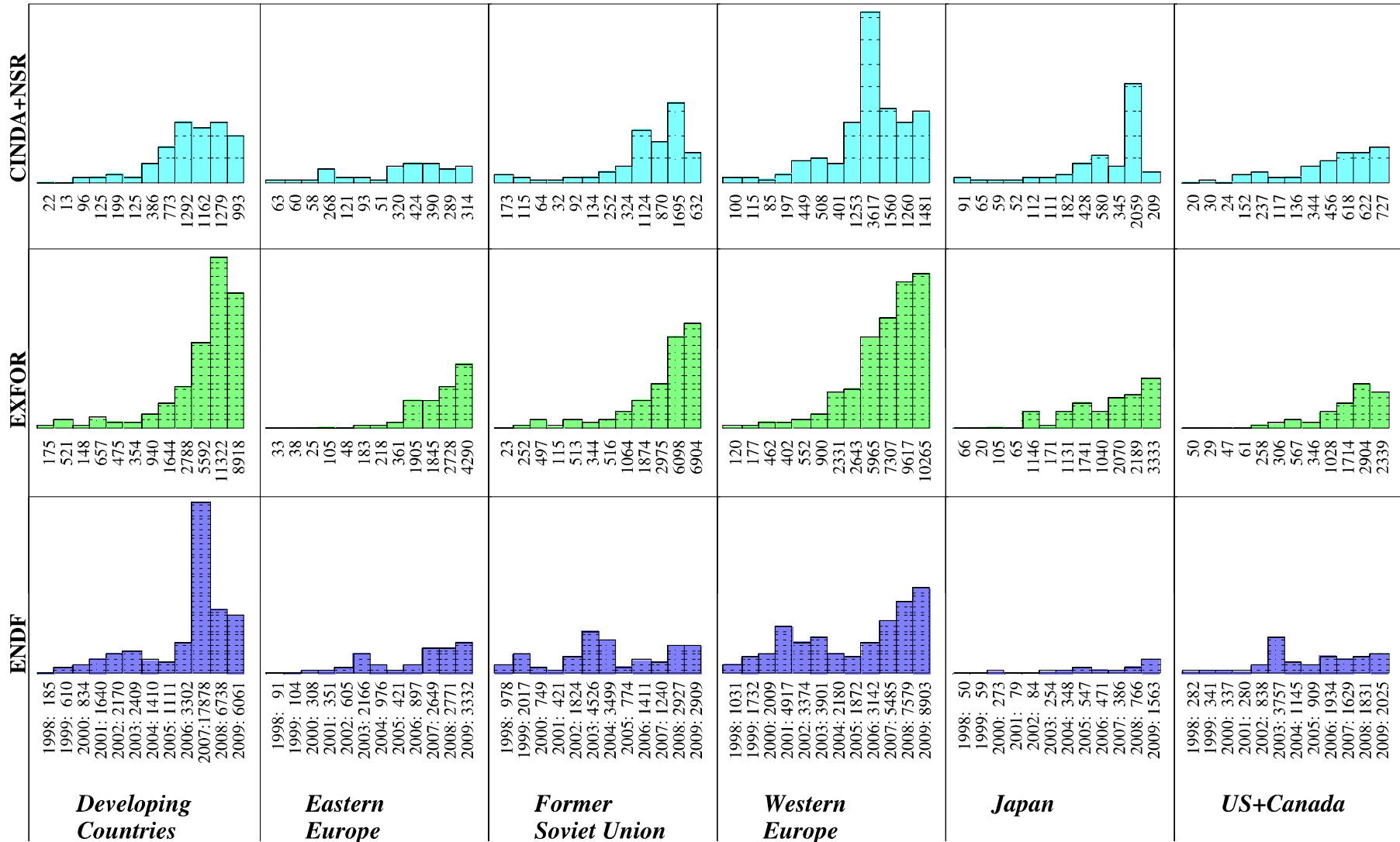


Fig. 2. IAEA Web statistics: geographical distribution of databases' retrievals

5. Nuclear Data Developments

Although direct nuclear data developments are outside the immediate operations of the NRDC, a brief summary of their activities is given below.

Co-ordinated Research Projects (CRPs):

- *Development of a Reference Database for Ion Beam Analysis*: finished, awaiting report.
- *Updated Decay Data Library for Actinides*: finished, awaiting report.
- *Reference Database for Neutron Activation Analysis*: finished, awaiting report.
- *Heavy Charged-Particle Interaction Data for Radiotherapy*: on-going.
- *Minor Actinide Neutron Reaction Data (MANREAD)*: on-going.
- *Nuclear Data Library for Advanced Systems – Fusion Devices (FENDL-3)*: on-going.

6. Publications (2009-2010)

6.1 Journals

Low and medium energy deuteron-induced reactions on ^{27}Al

by R. Bém, E. Šimečková, M. Honusek, U. Fischer, S.P. Simakov, R.A. Forrest, M. Avrigeanu, A.C. Obreja, F.L. Roman and V. Avrigeanu, *Phys. Rev.* **C79** (2009) 044610.

JENDL Actinoid file 2008

by O.Iwamoto, T.Nakagawa, N.Otuka, S.Chiba, K.Okumura, G.Chiba, T.Ohsawa and K.Furutaka, *J. Nucl. Sci. Technol.* **46** (2009) p. 510, also published in Proc. 2008 Annual Symposium on Nuclear Data (NDS2008), 20-21 November 2008, Ricotti, Tokai, Japan, JAEA-Conf. 2009-004 (2009).

The JEFF-3.1/-3.1.1 radioactive decay data and fission yields sub-libraries

by M.A. Kellett, O. Bersillon and R.W. Mills, OECD Data Bank 2009 – JEFF Report 20, ISBN 978-92-64-99087-6, NEA no. 6287.

Nuclear Data Sheets for A = 84

by D. Abriola, *et. al.*, *Nucl. Data Sheets*, **110** (2009) pp. 2815-2944.

RIPL – Reference input parameter library for calculation of nuclear reactions and nuclear data evaluations

by R. Capote Noy, *et. al.*, *Nucl. Data Sheets*, **110** (2009) pp. 3107-3214.

Cross sections of the reaction $^{231}\text{Pa}(d,3n)^{230}\text{U}$ for the production of $^{230}\text{U}/^{226}\text{Th}$ for targeted alpha therapy

by A. Morgenstern, O. Lebeda, J. Stursa, R. Capote, M. Sin, F. Bruchertseifer, B. Zielinska and C. Apostolidis, *Phys. Rev.* **C80** (2009) 054612.

The determination of beam quality correction factors: Monte Carlo simulations and measurements

by D.M. Gonzalez-Castano, G.H. Hartmann, F. Sanchez-Doblado, F. Gomez, R.P. Kapsch, J. Pena and R. Capote, *Physics in Medicine and Biology*, **54** (2009) pp. 4723-4741.

Evaluation and use of the prompt fission neutron spectrum and spectra covariance matrices in criticality and shielding

by I. Kodeli, A. Trkov, R. Capote, Y. Nagaya and V. Maslov, *J. Nucl. Instr. Meth. Physics Research, Section A: Accelerators, spectrometers, detectors and associated equipment*, **610** (2009) pp. 540-552.

High-accuracy $^{233}\text{U}(n,f)$ cross-section measurement at the white-neutron source n_TOF from near-thermal to 1 MeV neutron energy

by M. Calviani, R. Capote, *et. al.*, *Phys. Rev.* **C80** (2009) 044604.

The n_TOF total absorption calorimeter for neutron capture measurements at CERN
by C. Guerrero, R. Capote, *et al.*, (the n_TOF Collaboration), *J. Nucl. Instr. Meth. Physics Research, Section A: Accelerators, spectrometers, detectors and associated equipment*, **608** (2009) pp. 424-433.

Radiative recombination and photoionization cross sections for heavy element impurities in plasmas: II. Ions of Si, Cl, Ar, Ti, Cr, Kr, and Xe
by M.B. Trzhaskovskayaa, V.K. Nikulin and R.E.H. Clark, *Atomic Data and Nuclear Data Tables* **95** (2009) pp. 987-1050.

X-ray spectroscopy of buried layer foils irradiated at laser intensities in excess of 10^{20} W/cm²
by S.N. Chen, P.K. Patel, H.-K. Chung, A.J. Kemp, S. Le Pape, B.R. Maddox, S.C. Wilks, R.B. Stephens and F.N. Beg, *J. Phys. Plasmas* **16** (2009) 062701.

Applications of NLTE population kinetics
by H.-K. Chung, R.W. Lee, *J. High Energy Density Physics* **5** (2009) pp. 1-14.

Ab initio calculation of the photoelectron spectra of the hydroxycarbene diradicals
by L. Koziol, V.A. Mozhayskiy, B.J. Braams, J.M. Bowman, A.I. Krylov, *J. Phys. Chem. A* **113** (2009) pp. 7802-7809.

Full-dimensional ab initio potential energy surface and vibrational configuration interaction calculations for vinyl
by A.R. Sharma, B.J. Braams, S. Carter, B.C. Shepler and J.M. Bowman, *J. Chem. Phys.* **130** (2009) 174301.

Ab initio modeling of molecular IR spectra of astrophysical interest: application to CH₄
by R. Warmbier, R. Schneider, A.R. Sharma, B.J. Braams, J.M. Bowman and P.H. Hauschildt, *J. Astronomy and Astrophysics*, **495** (2009) pp. 655-661.

Permutationally invariant potential energy surfaces in high dimensionality
by B.J. Braams and J.M. Bowman, *Int. Reviews in Physical Chemistry* **28** (2009) pp. 577-606.

6.2 Conference Presentations and Proceedings

Measurements of the ^{90,91,92,93,94,96}Zr(n,γ) cross-sections at n_TOF
by P.M. Milazzo, R. Capote, A. Mengoni, *et al.*, (the n_TOF collaboration), Proc. 2nd Int. Conf., Current Problems in Nuclear Physics and Atomic Energy (NPAE-Kyiv2008), 9-15 June 2009, Kiev, Ukraine, pp.500-503.

A dispersive, lane-consistent optical potential, coupled-channel optical model code OPTMAN and its application
by E.Sh. Soukhovitski, S. Chiba, R. Capote J.M. Quesada, Proc. 2008 Annual Symposium on Nuclear Data, 20-21 November 2008, Ricotti, Tokai, Japan, (JAEA-Conf 2009-004) pp. 51-57.

Current status of nuclear reaction data file for astrophysics (NRDF/A)
by T. Yoshida, N. Furutachi, M. Kimura, M. Asano, T. Togashi, H. Murakami, K. Kato and N Otuka, Proc. 2008 Annual Symposium on Nuclear Data, 20-21 November 2008, Ricotti, Tokai, Japan, (JAEA-Conf 2009-004) pp. 79-81.

Nuclear Reaction Data Center Network: International and Asia
by K. Kato and N. Otuka, AIP Conf. Proc. – Nuclear Physics and Applications: 1st Ulaanbaatar Conf. on Nuclear Physics and Applications, Editors: D. Dashdorj, U. Agvaanluvsan and G.E. Mitchell, 1109 (2009) pp. 157-164, American Institute of Physics, Melville, New York, ISBN: 978-0-7354-0646-9.

n_TOF experiment: Past, present and future

by S. Marrone, R. Capote, A. Mengoni, (the n_TOF Collaboration), AIP Conf. Proc. – Nuclear Physics and Applications: 1st Ulaanbaatar Conf. on Nuclear Physics and Applications, Editors: D. Dashdorj, U. Agvaanluvsan and G.E. Mitchell, 1109 (2009) pp. 78-83, American Institute of Physics, Melville, New York, ISBN: 978-0-7354-0646-9.

Atomic, molecular and plasma-surface interaction data for fusion energy research

by R.E.H. Clark and D. Humbert, AIP Conf. Proc. – ICAMDATA-2008: 6th Int. Conf. on Molecular Data and Their Applications, Editors: Shaoping Zhu, Jun Yan, 1125 (2009) pp. 197–206, American Institute of Physics, Melville, New York, ISBN: 978-0-7354-0661-2.

Development of new standards for exchange of atomic and molecular data

by Yu. Ralchenko, R.E.H. Clark, M.-L. Dubernet, S. Gagarin, D. Humbert, P.A. Loboda, N. Moreau, E. Roueff and D.R. Schultz, AIP Conf. Proc. – ICAMDATA-2008: 6th Int. Conf. on Molecular Data and Their Applications, Eds. Shaoping Zhu, Jun Yan, 1125 (2009) pp. 207-216, American Institute of Physics, Melville, New York, ISBN: 978-0-7354-0661-2.

Multi-code *ab initio* calculation of ionization distributions and radiation losses for tungsten in tokamak plasmas

by Yu. Ralchenko, J. Abdallah, Jr., A. Bar-Shalom, J. Bauche, C. Bauche-Arnoult, C. Bowen, H.-K. Chung, J. Colgan, G. Faussurier, C.J. Fontes, M. Foster, F. de Gaufridy de Dortar, I. Golovkin, S.B. Hansen, R.W. Lee, V. Novikov, J. Oreg, O. Peyrusse, M. Poirier, A. Sasaki, H. Scott and H.L. Zhang, AIP Conf. Proc. – Atomic Processes in Plasmas: Proc. 16th Int. Conf. on Atomic Processes in Plasmas, Editor: K.B. Fournier, 1161 (2009) pp. 242-250, American Institute of Physics, Melville, New York, ISBN: 978-0-7354-0661-2.

7. Workshops 2009/2010

- The 3rd DAE-BRNS Theme Meeting on EXFOR Compilation of Nuclear Data: Department of Physics, University of Rajasthan, Jaipur, 3 - 7, November, 2009.

8. Visits and Inter-centre Cooperation

- V. Zerkin and N. Otsuka (NDS) to JCPRG, Hokkaido University, Japan: utilization of EXFOR. 14 - 30 March 2009.
- V. Zerkin (NDS) to NNDC/BNL: software development for management and Web-retrieval of ENDF, CINDA and EXFOR Relational Databases. 13 July – 7 August 2009.
- V. McLane, (ex-NNDC) to NDS: correction of old EXFOR entries according to new Exchange Format rules; preliminary processing and discussions on new REACTION code format. 28 September – 9 October 2009.
- H. Noto (JCPRG) to NDS: charged-particle nuclear data compiled in NRDF but not EXFOR, translate NRDF data files missing in EXFOR into EXFOR format. 1 - 30 August 2009.
- N. Otsuka (NDS) to KAERI: technical assistance for compilation and utilization of future EXFOR compilations. 8 – 10 December 2009.