

## **NDS/IAEA Activities and available Services related to the Nuclear Data**

S.P. Simakov

Nuclear Data Section  
International Atomic Energy Agency, Vienna, Austria

This mini-workshop gives an introduction to the Nuclear Data Section (NDS, <https://www-nds.iaea.org>) of IAEA, overviews the main databases, collection of computing codes and information resources, which are developed, maintained and distributed by NDS.

The practical exercises comprise the on-line demonstration of the available nuclear databases and information resources, typical requests/queries for various nuclear reaction and structure quantities.

The last part of min-workshop presents the USB with the evaluated and experimental reaction cross sections databases and retrieval software (EXFOR/CINDA/Endver/Prepro/ZVView) as well as nuclear reaction code (Empire) and shows how to start to work with them.

The content of this mini-workshop:

- I. Introduction: Nuclear Data Section of IAEA
- II. Nuclei Structure Databases
  - LiveChart, NuDat, ENSDF, DDEP – Retrieving Interfaces to the Nuclei Structure Data
- III. Nuclear Reaction Databases of General Use
  - EXFOR – repository of Experimental Reaction Data and retrieving interface
  - ENDF – collection of Evaluated Reaction Cross Sections and retrieving interface
  - RIPL – Reference Input Parameters for Nuclear Reaction Model Calculations
- IV. Nuclear Reaction Databases for the specific Applications
  - Standards - Nuclear Reaction data used as Standards
  - IRDFF – cross sections for Dosimetry at Fission, Fusion and Accelerator facilities
  - IBANDL – experimental and evaluated data for Ion Beam Analysis of materials
  - FENDL – nuclear reaction cross sections for neutronics analysis of Fusion facilities
  - PGAA – neutron reaction data for Prompt Neutron Activation Analysis
  - NAA – neutron reaction data for Delayed Neutron Activation Analysis
  - Medical Portal – reaction cross section data for Medical applications
  - High Energies – Cross Section Libraries and Benchmarks for Spallation
  - Data for Safeguards – summary of Neutron Reaction and Decay data for Safeguards
- V. Stopping Power for Electrons, Light and Heavy Ions
  - Stopping Power for Light and Heavier Ions at NDS
  - Links to other Reference stopping power Databases
- VI. Scientific Bibliography Resources
  - CINDA – Bibliographical References for published Nuclear Reaction Data
  - NSR – Bibliographical References for published Articles on Nuclear Physics
  - INIS – the IAEA International Nuclear Information System for non-conventional publications on the peaceful uses of nuclear Science and Technology
- VII. Collections of Codes at NDS
  - those used for Nuclear Reaction modelling, Applications, Data processing and plotting.
- VIII. On- and off-line Dissemination
  - of the Nuclear Data, Software and Documentation
- IX. Databases and Codes on the USB “Mini-workshops”

## I. Introduction: Nuclear Data Section of IAEA

NDS belongs to the Division of Physical and Chemical Sciences which is a part of the Department of Science and Applications (<http://www.iaea.org/OurWork/>). NDS employs 12 professionals and consists of 3 Units: (i) Atomic and Molecular Data, (ii) Nuclear Data Development and (iii) Nuclear Data Services.

The mission and the work' style of NDS is defined as: (i) development, collection and maintenance of the Nuclear and Atomic Data and documentation for the peaceful nuclear applications such as fundamental science, nuclear energy, analytical techniques, medicine, environment etc.; (ii) dissemination of this information to the 162 IAEA Member States for their capacity developments; (iii) transfer the basic Nuclear Knowledge from the developed to developing countries.

The specific of the NDS' work and outcomes is characterised by: (i) many NDS databases (e.g., EXFOR, Standards, IRDFF, FENDL, ...) are considered as internationally accepted reference sources of numerical data and documentation; (ii) unrestricted access to the information and (iii) political neutrality. This explains a difference between NDS of IAEA and other Nuclear Data Centres. For example: OECD Nuclear Energy Agency serves to OECD Stakeholders (31 countries), the National Nuclear Data Centres - to own countries, as e.g. NNDC/BNL – to USA.

NDS performs a technically work through the implementation of: (i) Coordinated Research Projects (CRP) which have to solve particular tasks, last 4 - 5 years and involve experts from 10 - 20 countries; (ii) Data Development Projects (DDP), which resolve long standing issue during a longer period with a help of external Experts. The NDS staff is involved in all these activities as managers and technical experts.

NDS transfers the basic Nuclear Knowledge through: (i) coordination of two Networks: Nuclear Reaction Data Centres (NRDC) and Nuclear Structure and Decay Data (NSDD); (ii) organisation of trainings: IAEA workshops, ICTP-Trieste schools etc.; (iii) mirroring of the NDS web-page and databases to China (<http://www-nds.ciae.ac.cn/>) and India (<http://www-nds.indcentre.org.in/>); (iv) responds to the technical requests from organisations and individuals, dispatch documentations as hard copies and databases on CD-ROM/DVD.

## II. Nuclear Structure and Decay Data

To provide access, search and display of the nuclear structure and radioactive decay data, NDS develops the interactive interface **LiveChart of Nuclides** accessible through internet <https://www-nds.iaea.org/> or as App "Isotope Browser" on Google Play <http://play.google.com/store/apps> for mobile devices. An example of nuclear structure data the use can receive is displayed in Fig. 1.

LiveChart provides essential nuclear structure data (most of them together with uncertainties) for:

- ground states: Isotope Abundance;  $J^\pi$ ; half-life  $T_{1/2}$  or width  $\Gamma$ ;  $Q$ -values for  $\beta$ ,  $\alpha$ ,  $EC$ ,  $\beta^-n$   
Nucleon Separation Energies  $S_n$ ,  $S_p$   
Isotope Atomic Mass  $M$ ; Mass Excess  $\Delta$ ; Binding Energy; Isospin  
thermal capture cross section  $\sigma(n_{th}, \gamma)$ ; Resonance Integral  $RI$ ; Fission Yields  
Electr. & Magnetic Moments  $\mu$ ; Nuclei Radius  $R$ ; Dipole or Quadrupole Moments  
Decay info (Modes, Emission radiation Energy and Probabilities, Mixing  $\delta$  ...) ...;
- excited states:  $U$ ,  $J^\pi$ ,  $T_{1/2}$ , de-excitation  $\gamma$  ( $E_\gamma$ ,  $E_i \rightarrow E_f$ , Multipolarities, Branching, Bands ...).

LiveChart also provides atomic masses and some nuclear reaction data:

- Masses,  $Q$ ,  $S_n$  - from the Atomic Mass Data Centre (AMDC), <https://www-nds.iaea.org/amdc/>, latest version – 2012;
- Thermal cross capture sections  $\sigma(n_{th}, \gamma)$ , Resonance Integrals, Resonance Fission Integrals from evaluation of S. Mughabghab, Atlas of Neutron Resonances, 2006
- Independent and Cumulative Fission Yields - from the JEFF project evaluations [http://www.oecd-neo.org/dbforms/data/eva/evatapex/jeff\\_32/](http://www.oecd-neo.org/dbforms/data/eva/evatapex/jeff_32/)

LiveChart derives this information from the following resources: (i) ENSDF evaluation ( $\approx 3000$  nuclides) produced by the NSDD network which is coordinated by NDS <https://www-nds.iaea.org/nsdd/>; (ii) TUNL evaluation (light nuclei  $A = 3 - 20$ ), <http://www.tunl.duke.edu/nucldata/index.shtml>.

It is worthwhile to note that other nuclear Decay Data Evaluation Project (DDEP) coordinated by CEA/LNHB <http://www.nucleide.org/DDEP.htm> also recommends the evaluated decay data for 215 nuclides.

The existence of several "independent" evaluation projects and databases explains the differences one may observe for nuclear structure quantities.

The Nuclear Ground states properties are also available from NDS as a compact Pocket Booklet "Nuclear Wallet Cards" by J.K. Tuli, 2011, BNL. It includes isotope abundance, mass excesses,  $J^\pi$ ,  $T_{1/2}$  and decay modes.

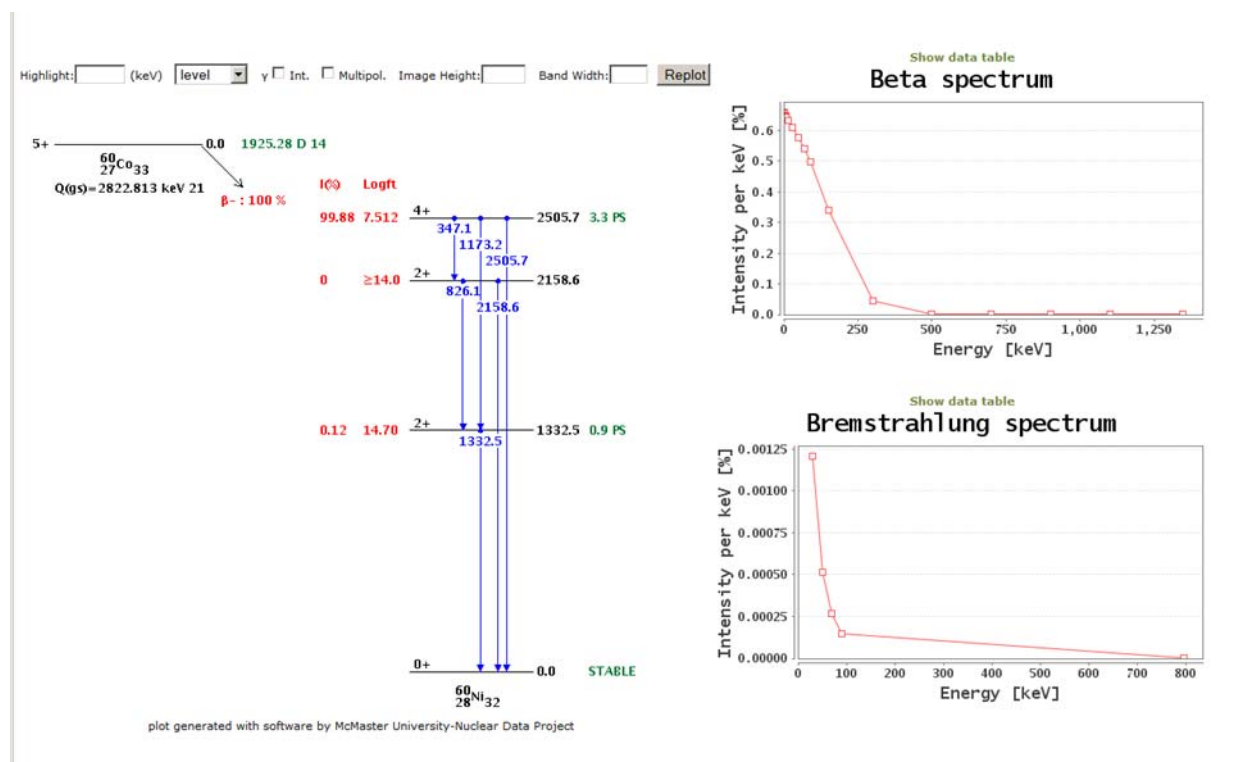


Fig. 1. Retrieve of the  $^{60}\text{Co}$  decay information by LiveChart: discrete  $\gamma$ -rays,  $\beta^-$  and X-ray energy spectra.

### III. Nuclear Reaction Databases of General Use

#### EXFOR - a unique repository of Experimental Reaction Data

The regular collection of experimental cross section data has started as the Cross-Section Information Storage and Retrieval System (CSISRS) in the USA in 1960th. In 1970 CSISRS was transformed in the EXchange FORmat (EXFOR) and was maintained by four Nuclear Data Centres (NEA, NDS, USA, USSR). Since 1976 the NDS of IAEA manages a network of 14 national Nuclear Reaction Data Centres (NRDC, <https://www-nds.iaea.org/nrdc/>): assign compilation, receives newly compiled or updated Entries, stores the master EXFOR file and provide internet access to the database <https://www-nds.iaea.org/exfor/exfor.htm>.

NDS regularly scans approximately 60 journals to search for publications relevant for EXFOR. NRDC compiles measured data and generates about 500 new Entries per year. The compilation time of new publications lasts 6 months. EXFOR is updated practically every month and contains now data from 20,600 experiments or 12 million experimental points.

The scope or dominant nuclear quantities (*EXFOR coding*) are demonstrated by their “abundances” in EXFOR (relative number of Entries):

- Cross Sections (*CS*) for (*N,TOT*), (*G,ABS*), (*N,EL*), (*N,G*), (*P,INL*), (*D,A*), (*A,3N*) ... - 51%
- Differential Angular (Partial) distributions,  $d\sigma/d\Omega$  (*DA*, *DAP*) for (*P,EL*), (*N,INL*) ... - 39%
- Resonance Parameters (*RP*): Energy (*EN*), Spin/Parity ( $\pm J$ ), width (*WID*) for (*N,0*), (*N,EL*) - 9%
- Cross Sections Partial (*CSP*) for (*N,INL*), (*P,D*), ... - 8%
- Fission Yields (*FY*) for (*N,F*), (*0,F*) - 5%
- Polarization (*POL*) Parameters - 5%
- Double differential Angular-Energy distributions or  $d^2\sigma/d\Omega/dE$  (*DAE*) - 5%
- Thick/Thin Targets, Partial, Differential, Saturated ... Yields (*TTY*) - 2%
- outgoing Particles Multiplicity (*MLT*) for induced (*N,F*), and spontaneous (*0,F*) fission - 2%
- Cross sections Averaged over incident energy or SPectrum (*SPA*) - 1%

The data for 336 incident and outgoing nuclear reaction particles or ions are compiled in EXFOR:

- Neutrons (*N* or *0-NN-I*) - 49% (decreasing)
- Protons (*P*), Deuterons (*D*), Alphas (*A*),  $^3\text{He}$  (*HE3*),  $^3\text{H}$  (*T*) - 40% (increasing)
- Gammas (*G* or *0-G-0*, and even *DG* – decay *G*) - 6%
- Spontaneous Fissions (*0*) - 2%
- Electrons (*E*) - 0.1%
- “Exotic”: Pion (*PIP*, *PIN*), Kaon (*Kn*),  $\eta$  (*ETA*),  $\pi$  (*AP*),  $\pi$  (*AN*),  $\Lambda$  (*LM*) ~ 0.1%
- Heavy Ions from Li-6 to U-238 - rest ( $\approx 3\%$ ).

The data for 105 reaction targets are compiled in EXFOR:

- Elements/Isotopes - from H (7%) via U (12%) to still unnamed 118\*-294 (1 experiment)
- Compounds (\*-CMP), Oxides (\*-OXI), Alloys (ALY), Hydrides (HYD), Water (H-WTR), Air (N-AIR), Benzene (H-BNZ) ...

EXFOR covers 22 orders of the incident particles energy range from ultra-cold neutrons with energy  $1.10^{-7}$  eV to  $4 \cdot 10^{15}$  eV protons.

The EXFOR retrieval systems developed by NDS allows users to search, plot, convert ratio of cross sections to absolute one, automatically renormalize them to the new standards, modify the original data by experts' corrections stored in EXFOR (Fig. 2), construct covariance matrices and perform many other operations with experimental and evaluated data.

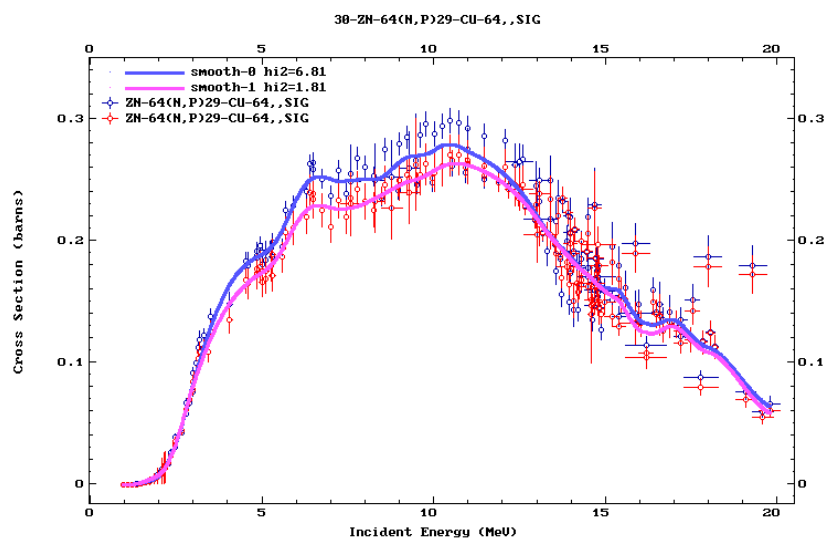


Fig. 2. Example of original (blue) EXFOR and corrected by expert (red) data for the  $^{64}\text{Zn}(n,p)^{64}\text{Cu}$  reaction. The two fitted curves act as eye-guides.

Many Request Examples and Video-Guides are given on the EXFOR web-page <https://www-nds.iaea.org/exfor/exfor.htm>.

The actual challenges for EXFOR are: (i) covariance matrices, which are now available only for  $\approx 70$  Entries of total 20,000!, see Fig. 3; (ii) specification of the components of uncertainties for many Entries; (ii) new EXFOR quantities, such as  $\beta^-$  ( $B^-$ ) decay probabilities ( $P_n$ ) and energy spectra ( $DE$ ) for the individual precursors, (iii) collection and compilation of the neutron sources spectra used by experimentalists for the measurements of the energy averaged quantities.

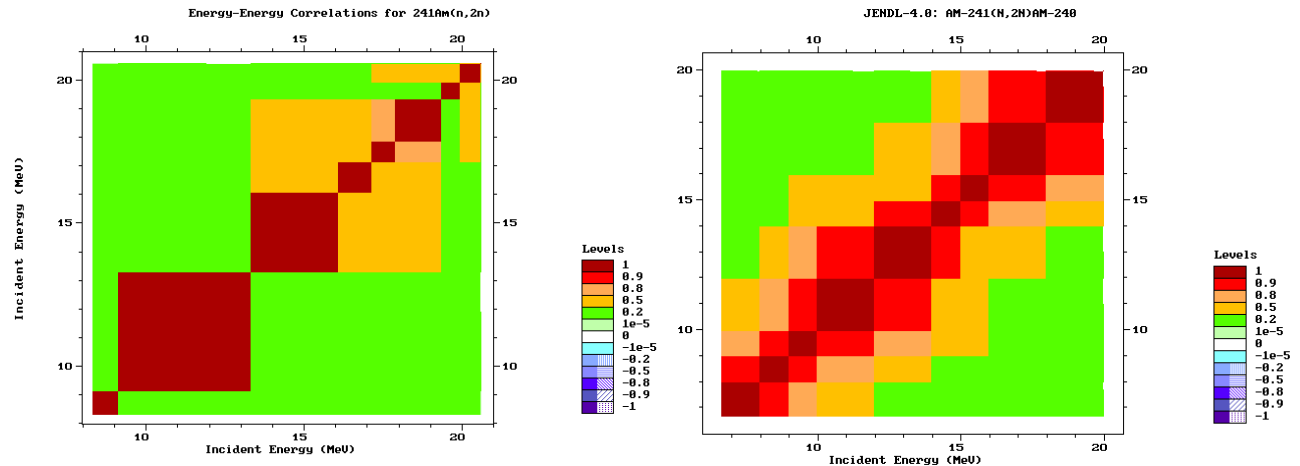


Fig. 3. Retrieve and plotting of the experimental (left, Entry 23114) and evaluated (right, TENDL-2010) energy-energy correlation matrices for the  $^{241}\text{Am}(n,2n)$  reaction cross section.

### ENDF – collection of Evaluated Nuclear reaction Data Files

The ENDF database (<https://www-nds.iaea.org/exfor/endl.htm>) contains the evaluated files for the n,  $\gamma$ , p, d, t,  $^3\text{He}$ ,  $^4\text{He}$  induced reactions, thermal scattering, spontaneous fission, photo-nuclear, photo- and electro-atomic, radioactive decay:

- 27 for the general use or for application oriented
- 16 archival, i.e. the previous versions, some even in the previous format ENDF-5
- 3 derived, i.e. converted in point-wise (ENDF/B-VI.8 and JENDL-3.3 at 300<sup>0</sup>K) or group-wise (IRDF-2002) ENDF-6 formatted presentation.

ENDF has the major (inter)national libraries and actual versions: ENDF/B-VII.1 - US Evaluated Nuclear Data Library coordinated by BNNL, JEFF-3.2 - European Evaluated Fission and Fusion File coordinated by NEA Bank, JENDL-4.0u - Japanese Evaluated Nuclear Data Library, CENDL-3.1 - Chinese Evaluated Nuclear Data Library, ROSFOND-2010 - Russian Evaluated Nuclear Data Library and others. The data are stored in the ENDF-6 format.

POINT-2012 is the ENDF/B-VII.1 neutron reaction library converted in the point-wise format for easier use at the set of ambient temperatures from 0 to 2100<sup>0</sup>K and from 0.1eV to 10keV ( $\approx M^\circ\text{K}$ ).

NDS uses following processing codes to work with ENDF-6 formatted files: PREPRO-2012 and PLOTTAB-2013 - to process and plot cross section data (free available), NJOY-99 and 2012 – to process, plot and generation ACE files for MCNP (used internally).

### RIPL - Reference Input Parameter Library

The Reference Input Parameter Library (<https://www-nds.iaea.org/RIPL-3/>) for the nuclear reaction cross sections calculations was developed as an outcome of the several Coordinated Research Projects: RIPL-1 was released in 1998, RIPL-2 - 2006, RIPL-3 - 2009. NDS plans new CRP to extent RIPL for the prompt fission neutron spectra from fissile nuclei.

RIPL-3 recommends the main parameters needed for modelling of nuclear reactions:

- Masses: experimental or evaluated mass excesses ,  
ground state properties (deformation parameters, radii, diffuseness ...),  
natural Abundances, Nuclear Matter Densities,
- Levels: discrete and decay data,
- Resonances: average spacings of neutron resonances,
- Optical Model Parameters (OMP): phenomenological OMP, Deformation Parameters,
- Densities: Level Density Parameters (phenomenological and microscopic),
- Gamma: Experimental and Theoretical Giant Dipole Resonance (GDR) Parameters ,
- Fission: Empirical and Theoretical Fission Barriers.

RIPL web page also hosts several freely distributed nuclear reaction model codes with sources, input parameters, test cases and documentation:

- SCAT2000 (O. Bersilon) – optical model code
- ECIS (J. Raynal) – optical coupled-channel model code
- OPTMAN (E. Soukhovitskii) – optical model with coupling deformed rotary states
- PFNS (P. Talou) – Los Alamos Model Prompt Fission Neutron Spectra model.

#### IV. Nuclear Reaction Databases for the specific Applications

##### Neutron Cross Section Standards

The neutron cross section standards service as the mostly precise known cross sections and are often used as a reference in the measurements of other cross sections. This database is developed under auspices of NDS as a long term Data Development Project: <https://www-nds.iaea.org/standards/>.

The latest version, issued in 2006, has 11 reactions and 1 spontaneous fission spectrum, which are listed in the Table 1 with indication of the energy range and established accuracy. As an example, the  $^{235}\text{U}(\text{n},\text{f})$  cross section is shown in Fig .4.

Table 1. Nuclear Reaction Cross Sections and  $^{252}\text{Cf}(\text{s.f.})$  spectrum Standards.

Reaction	Previous Version: 1987	Actual Version: 2002-2005/06	
	Neutron Energy Range	Neutron Energy Range	Uncertainty
H(n,n)	1 keV to 20 MeV	1 keV to 20 MeV	0.2 – 0.3 %
$^3\text{He}(\text{n},\text{p})$	0.0253 eV to 50 keV	0.0253 eV to 50 keV	0.30 – 5.0 %
$^6\text{Li}(\text{n},\text{t})$	0.0253 eV to 1 MeV	0.0253 eV to 2.8 MeV	0.15 – 3.0 %
$^{10}\text{B}(\text{n},\alpha_0+\alpha_1)$	0.0253 eV to 250 keV	0.0253 eV to 1 MeV	0.24 – 3.0 %
$^{10}\text{B}(\text{n},\alpha_1\gamma)$	0.0253 eV to 250 keV	0.0253 eV to 1 MeV	0.08 – 1.5 %
C(n,n)	up to 1.8 MeV	up to 1.8 MeV	0.2 – 0.8 %
$^{197}\text{Au}(\text{n},\gamma)$	0.0253 eV, 0.2 to 2.5 MeV	0.0253 eV, 0.2 to 2.5 MeV	0.14 – 2.2 %
$^{235}\text{U}(\text{n},\text{f})$	0.0253 eV and 0.15 - 20 MeV	0.0253 eV, 0.15 to 200 MeV	0.15 – 4.5 %
$^{238}\text{U}(\text{n},\text{f})$	threshold to 20 MeV	2 to 200 MeV	1.2 – 4.5 %
$^{238}\text{U}(\text{n},\gamma)$		0.0253 eV to 2.2 MeV	0.50 – 3.0 %
$^{239}\text{Pu}(\text{n},\text{f})$		0.0253 eV to 200 MeV	0.24 – 4.5 %
$^{252}\text{Cf}(\text{s.f.})$	Spontaneous Fission Neutron Spectrum from 0.1 to 20 MeV		0.2 - 8.5 MeV < 2%



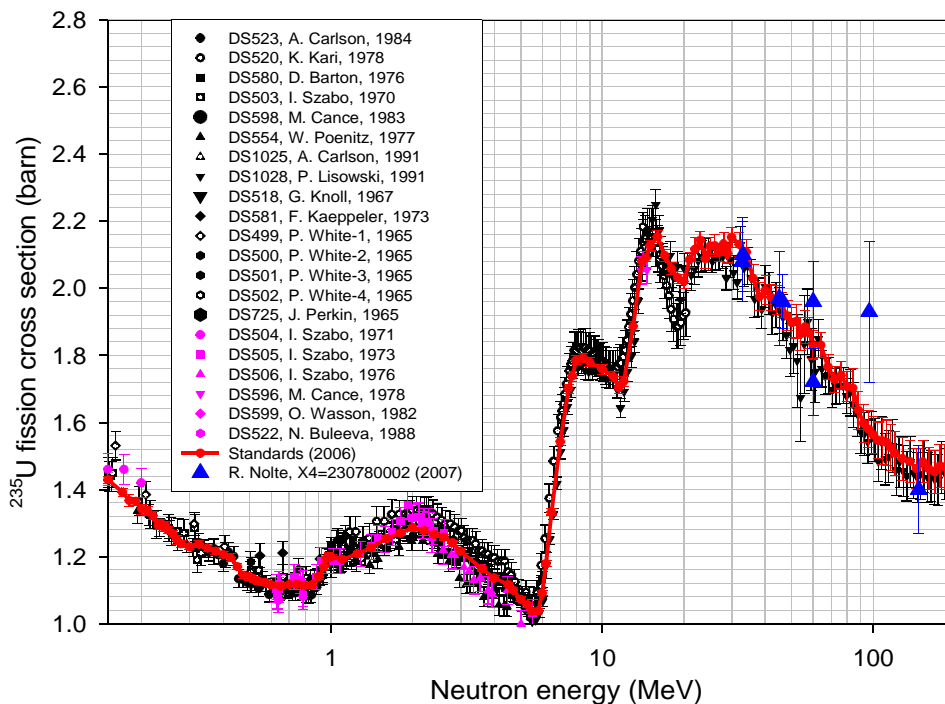


Fig. 4. All available experimental data and standard cross sections for  $^{235}\text{U}(n,f)$  reaction in the energy range 0.2 - 200 MeV.

External experts and NDS currently work on evaluation and inclusion in Standards of the new reactions (see *Report INDC(NDS)-0583*): Prompt Fission Neutron Spectrum (PFNS) from  $^{235}\text{U}(n_{th},f)$ ; discrete  $\gamma$ -ray production from  $^7\text{Li}(n,n'\gamma)$  and  $^{48}\text{Ti}(n,n'\gamma)$ ; fission cross sections  $^{209}\text{Bi}(n,f)$  and  $^{nat}\text{Pb}(n,f)$ .

### International Reactor Dosimetry and Fusion File (IRDFF)

The IRDFF library (<https://www-nds.iaea.org/IRDFF/>) serves as internationally accepted reference cross sections for dosimetry at the power and research fission, fusion and accelerator nuclear facilities. These cross sections are used to monitor or measure the neutron fluence and to determine the energy spectra of facilities.

IRDFF was being developed under the NDS coordination since 1982. The IRDF(F) database history with number of included reactions and main references are summarised here:

1982: <a href="#">IRDF-82</a>	35 reactions, IAEA-NDS-41
1993: <a href="#">IRDF-90 v. 2</a>	37 reactions, IAEA-NDS-141
2006: <a href="#">IRDF-2002</a>	69 reactions, Tech. Rep. 452
2012: <a href="#">IRDFF, v. 1.00</a>	69 reactions, INDC(NDS)-0616.

Actual version IRDFF-1.05 (released in Nov 2014) contains 76 dosimetry reactions, plus 3 cover materials (B, Cd, Gd) and covers energy range from  $10^{-4}$  eV up to 60 - 200 MeV.

Currently NDS runs CRP on “Testing and Improving of IRDFF” (<https://www-nds.iaea.org/IRDFFtest/>) with goals to extend IRDFF (new reactions, higher energies), experimentally validate, remove discrepancies and reduce uncertainty.

### Fusion Evaluated Nuclear Data Library (FENDL-3)

FENDL Library (<https://www-nds.iaea.org/fendl30/>) serves for neutronics characterization of the operated or projected Fusion Facilities (JET, ITER, IFMIF, DEMO). It was developed in frames of several CRPs: FENDL-2.0 was released in 1997, FENDL-2.1 - in 2004, the latest version FENDL-3.0 - in 2013.

FENDL-3 is an essential extension of FENDL-2.1: (i) incident particle energies exceed now 20 MeV, at least up to 60 MeV to cover IFMIF, (ii) has more materials, now 180 targets, (iii) additionally to the neutrons, the charged particles (p, d) and photons were included, (iv) cross sections have uncertainties.

FENDL-3.0 library contains:

- evaluated nuclear reaction ENDF-6 formatted data as a general purpose file FENDL-3 (E < 150 MeV) and an activation file FENDL-3/A (E < 60 MeV),
- covariances as a 'shadow library' based on TENDL-2010 for 180 targets,
- processed files in the PENDF, GENDF, ACE and MATXS formats.

### Prompt Gamma-ray Neutron Activation Analysis (PGAA)

PGAA (<https://www-nds.iaea.org/pgaa/>) serves for the non-destructive Elemental Analysis of materials by using characteristic prompt discrete  $\gamma$ -rays from neutron capture reactions which however usually do not form products with delayed  $\gamma$ -rays. PGAA has been released by the IAEA CRP (1999 – 2003) and covers materials from H to U.

PGAA database contains following recommended data at thermal neutron energy:

- prompt (in some cases also delayed) discrete gamma energies  $E_{\gamma i}$ ;
- partial & total isotopic capture cross sections  $\sigma_{\gamma}^{ZA}(n_{th}, \gamma_i)$ ,  $\sigma_{\gamma}^{ZA}(n_{th}, \gamma)$ ;
- Westcott  $g$ -factors to account for *non-1/v* absorber;
- parameters to account for the *epithermal* n-spectrum component:  
 $\sigma = \sigma_0 (g_w + r \cdot s)$ ,  $\sigma_0$  – value at neutron speed 2200 m/s  
where  $r$  – index for epithermal fraction,  $s$  – reduced resonance integral;
- prompt  $k_0$  factor  $k_0 = \frac{P_a(E_{\gamma,a}) \sigma_{0,a} \theta_a/M_a}{P_c(E_{\gamma,c}) \sigma_{0,c} \theta_c/M_c}$

where

$a$  - stands for *Analyte (isotope of interest)* co-irradiated with *comparator c*,

$P(E_{\gamma})$  - absolute  $\gamma$ -ray emission Probability with energy  $E$ ,

$\sigma$  – capture cross section,  $\square$  - abundance,  $M$  – molar mass.

Standard comparator by convention is a cross section  $\sigma = 0.3326(7)b$  for  $E_{\gamma} = 2223 \text{ keV}$  from the  $^1\text{H}(n, \gamma)$  reaction.

### Neutron Activation Analysis: $k_0$ -NAA standardization

The NAA database (<https://www-nds.iaea.org/naa/portal.htmlx>) serves for the non-destructive nuclear Elemental Analysis of materials by detection of the delayed  $\gamma$ -rays from the neutron capture reaction products. The sensitivity of the method is on the level  $\approx \mu\text{g}$  for 60 elements.

It relies on the comparator method, i.e. on finding the concentration of Analyte ( $a$ ) to be co-irradiated with Au sample (by convention, the yield of  $E_{\gamma} = 411.8 \text{ keV}$  from  $^{197}\text{Au}(n, \gamma)$  is adopted as standard).

The basic relation:

$$\rho_a = \frac{(N_p/Wt_mSDC)_a}{(N_p/Wt_mSDC)_{Au}} \frac{\varepsilon_{p,Au}}{\varepsilon_{p,a}} \frac{1}{k_{0,Au}(a)} \frac{f+Q_{0,Au}(a)}{f+Q_{0,a}(a)}.$$

The irradiation facility specific parameters are: number of the detector counts ( $N$ ) and efficiency ( $\varepsilon$ ), sample mass ( $W$ ), and set of corrections ( $S D C$ ), thermalized n-spectrum temperature  $T$ , thermal-to-



epithermal ratio  $f$ , deviation parameter  $\alpha$  from the perfect  $1/E$  epithermal spectrum, fast spectrum parameters.

The composite parameters which comprised the nuclear data constants are available in the  $k_0$ -NAA database:

$$k_{0,Au}(a) \quad - \quad k_0 \text{ factor for Analyte,}$$

$$Q_0 = I_0/\sigma_0 \quad - \quad Q_0 \text{ factor (resonance integral ratio to 2200 m/s cross section).}$$

These parameters could be found in the experimental [k<sub>0</sub>-NAA database](http://www.iupac.org/) maintained by the International Union of Pure and Applied Chemistry (<http://www.iupac.org/>) or based on it “classic” [k<sub>0</sub>-NAA database](http://www.kayzero.com/), maintained by the k<sub>0</sub>-International Scientific Committee (<http://www.kayzero.com/>).

NDS/IAEA run CRP (2005-2010) to improve the status of reference  $k_0$ -NAA. The final report and data base is not available yet, see [NAA portal](http://www.naweb.iaea.org/napc/iachem/K0-IAEA.html).

The complimentary IAEA project run by the Industrial Application and Chemistry Section of IAEA develops the  $k_0$ -IAEA software (<http://www-naweb.iaea.org/napc/iachem/K0-IAEA.html>).

## Ion Beam Analysis Nuclear Data Library – IBANDL

IBANDL (<https://www-nds.iaea.org/exfor/ibandl.htm>) contains experimental ( $\approx 2,800$  datasets) and evaluated cross sections (based on the SigmaCalc code by A.F. Gurbich, NIM B136(1998)60) and serves as a base for the Analytical Ion Beam Analysis (IBA) which includes several techniques:

- EBS - Elastic proton Backscattering Spectroscopy: detection of protons from (p,p<sub>el</sub>)
- NRA - Nuclear Reaction Analysis: reaction ejectiles from (p, $\alpha_{0,1}$ ), (d,p<sub>0,1</sub>), (<sup>3</sup>He, $\alpha_{0,1}$ ), ( $\alpha$ ,p<sub>0,1</sub>) ...
- PIGE - Particle Induced Gamma-ray Emission: gammas from (p,p' $\gamma_i$ ), (p,x $\gamma_i$ ), (d,p' $\gamma_i$ ) ...

IBA techniques use interaction of fast ( $\sim 1 - 10$  MeV) charged particles with materials to determine the elemental composition and profile up to 500  $\mu$ m surface depth by measuring the back scattered protons, light ions or characteristic prompt  $\gamma$ -rays.

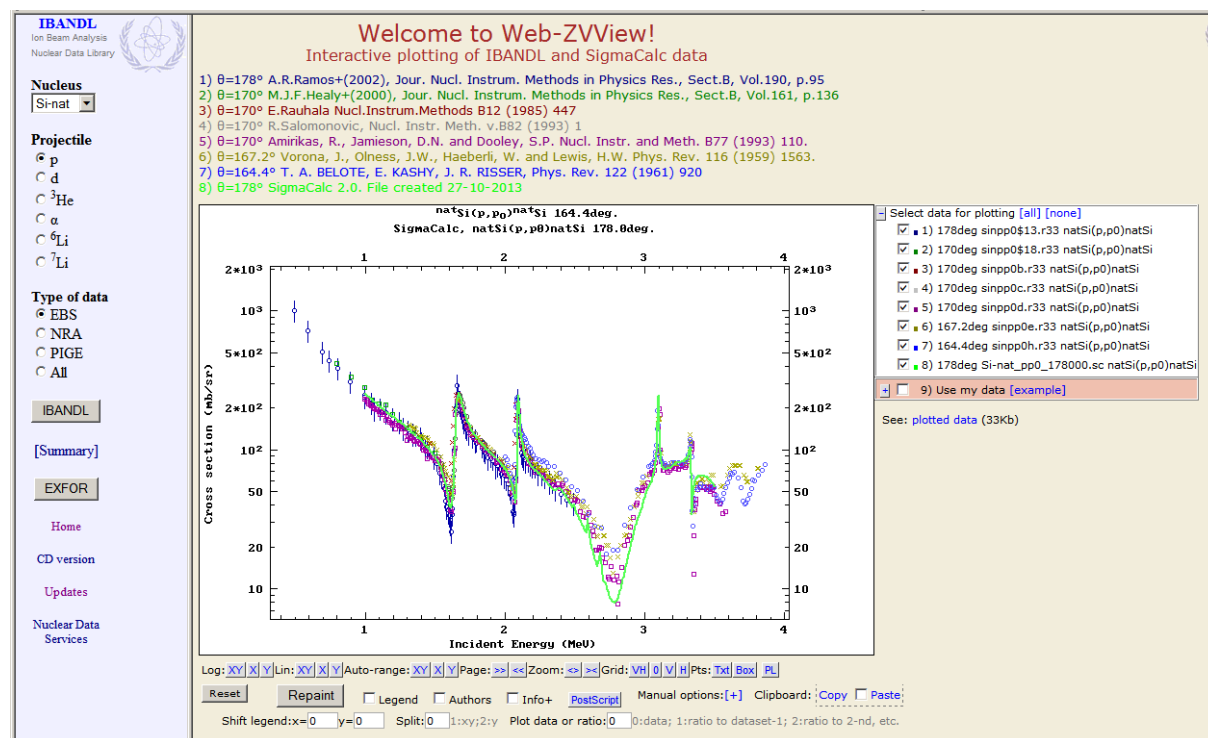


Fig. 5. The web page of the IBANDL database with capabilities to extract and plot the IBA angular differential cross sections versus incident proton energy.

The software used for the IBA practical application is the code SIMNRA, version 6 <http://home.rzg.mpg.de/~mam/> or 7 by M. Mayer et al., NIM B332(2014)176.

NDS maintains the IBANDL library which contains the experimental and evaluated reaction data, Fig. 5. NDS also runs CRP since 2010 to extend the scope of IBANDL by inclusion of the new PIGE data.

### Medical Portal – Nuclear Data for Medical Applications

This dedicated medical data portal (<https://www-nds.iaea.org/medportal/>) contains experimental, evaluated and recommended cross sections for:

- (p,x), (d,x) reactions producing Diagnostic Radioisotopes, i.e.  $\gamma$  or  $e^+$  emitters for diagnosis,
- (p,x), (d,x), ( $\alpha$ ,x) reactions producing Therapeutic Radionuclides, i.e. clinically established or emerging emitters for treatment,
- Beam Monitor activation reactions (p,x), (d,x), ( $^3\text{He}$ ,x), ( $\alpha$ ,x) to monitor ion beam dose,
- Phase-Space Database for External Radiotherapy with a help of  $^{60}\text{Co}$  source, Photon or Electron Linacs,
- Heavy Charged Particle Interaction data with materials relevant to radiotherapy, i.e. the data needed to model beam collimation and collision with patient tissue and detectors (*CRP on "Heavy charged-particle interaction data for radiotherapy", 2007-2011*),
- MIRD - Medical Internal Radiation Dose = energy absorbed in the infinite material due to uniformly distributed source (calculated by Radlist code using ENSDF data).

The example of the available experimental, theoretical and evaluated data for the production of the emerging therapeutic radioisotope by reaction  $^{169}\text{Tm}(p,n)^{169}\text{Yb}$  is shown in Fig. 6.

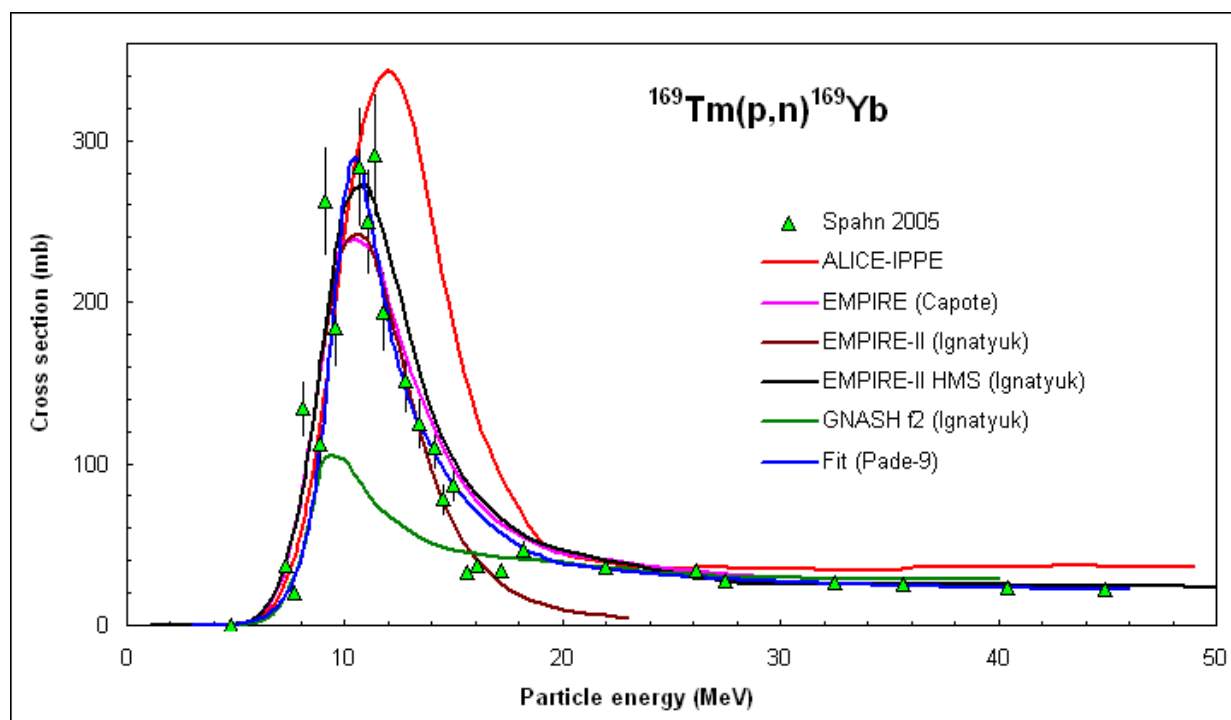


Fig. 6. The cross sections for production of the emerging therapeutic radioisotope  $^{169}\text{Yb}$  by reaction  $^{169}\text{Tm}(p,n)$ .

### High Energies: Cross Section Libraries and Benchmarks

The set of the evaluated nuclear reaction data libraries dedicated to the high energy applications (up to 150 MeV or 1 GeV) are collected on the web-pages <https://www-nds.iaea.org/ads/> and <https://www-nds.iaea.org/ads/adshe.html>.

**ADS-2.0** library for Accelerator Driven Systems exists since 2006 and contains:

- 155 isotopes from H-1 to Cm-247,
- compound materials: H<sub>2</sub>O, D<sub>2</sub>O and Graphite (thermal scattering law),
- neutron energy range from 10<sup>-5</sup> eV up to 150 MeV,
- data in the formats: ENDF, ACE for MCNP, 421 groups GENDF at set of T = 300 – 2000 °K.

**ADS-HE** library is an extension to the Higher Energies 1 GeV released in 2012:

- 10 isotopes: Hg-202, Pb-208, Bi-209, Th-232, U-235,238, Np-237, Pu-239, Am-242, Cm-245,
- source of information: a new HE evaluations by *S. Yavshits et al.*, *INDC(NDS)-0615, 2012*,
- data are available in different formats (ENDF, ACE), as plots, plus NJOY inputs ...

A dedicated web page "**IAEA Benchmark of Spallation models**",

(<https://www-nds.iaea.org/spallations/>, Fig. 7) contains:

- results and docs of series of the dedicated IAEA Meetings held 2008 to 2010,
- data for Targets A > 12, Incident Particles p and n, Energies from 20 MeV to 3 GeV,
- reaction models verified: those used in the MCNPX, PHITS and GEANT codes,
- collection of the relevant experimental data (references to publications, links to EXFOR, plots):  
 $d^2\sigma/dE/d\Omega$  for production of n, p, d, t, <sup>3</sup>He, <sup>4</sup>He,  $\pi^+$ ,  $\pi^-$ , mass/charge/isotope distributions, neutron multiplicities ...,
- results of calculations and intercomparison with measurements: plots, tables, figure-of-merits .

**Nuclear Data Services**  
Section Données Nucléaires, AIEA

Databases » EXFOR | ENDF | CINDA | IBANDL | Medical | PGAA | NGAtlas | RIPL | FENDL | IRDF-2002 | IRDFF

**IAEA Benchmark of Spallation Models**

**Introduction**

Spallation reactions are nuclear reactions playing an important role in a wide domain of applications ranging from neutron sources for condensed matter and material studies, transmutation of nuclear waste and rare isotope production to astrophysics, simulation of detector set-ups in nuclear and particle physics experiments, and radiation protection near accelerators or in space.

The simulation tools developed for these domains use nuclear model codes to compute the production yields and characteristics of all the particles and nuclei generated in these reactions. The codes are generally Monte-Carlo implementations of Intra-Nuclear Cascade (INC) or Quantum Molecular Dynamics (QMD) models followed by de-excitation (principally evaporation/fission) models.

The International Atomic Energy Agency (IAEA) and the Abdus Salam International Centre for Theoretical Physics (ICTP) have recently organised an expert meeting on model codes for spallation reactions. The experts have discussed in depth the physics bases and ingredients of the different models in order to understand their strengths and weaknesses. Since it is of great importance to validate on selected experimental data the abilities of the various codes to predict reliably the different quantities relevant for applications, it has been agreed to organise an international benchmark of the different models developed by different groups in the world. The specifications of the benchmark, including the set of selected experimental data to be compared to models, have been fixed during the workshop.

The benchmark is organised under the auspices of IAEA in 2008 and the analysis of the results will be done with the help of an International Advisory Board. The first results discussed at the next Accelerator Applications conference (AccApp'09) to be held in Vienna in May 2009.

**Objectives**

- To assess the prediction capabilities of the spallation models used or that could be used in the future in high-energy transport codes.
- To understand the reason for the success or deficiency of the models in the different mass and energy regions or for the different exit channels
- To reach a consensus, if possible, on some of the physics ingredients that should be used in the models.

Fig. 7. Front web-page of the IAEA Benchmark of Spallation Models.

## Data for Safeguards - summary of Neutron Reaction and Decay data for Safeguards

The IAEA Handbook of Nuclear Data for Safeguards *INDC(NDS)-0534, Aug 2008* and dedicated web-page <http://www-nds.iaea.org/sgnucdat/> contain the recommended data (including uncertainties) for:

- section A: decay data,  $\sigma(n_{\text{thermal}}, \gamma)$ , resonance integrals,  $v_{\text{total}}$  and  $v_{\text{delayed}}$  (8 groups) for actinides and their natural decay products;
- section B: decay data and  $\sigma(n_{\text{thermal}}, \gamma)$  for some important fission products;

- section C: chain, independent and cumulative fission product yields for selected actinides caused by thermal, fast and 14 MeV neutrons;
- section D: decay data for specific activation products.

The decay data includes  $T_{1/2}$ , decay modes, Energies & Probabilities of  $\alpha$ ,  $\gamma$ - and X-rays.

The preference for the source of data was given to evaluated data recommended by international working groups. If not, the data were adopted from evaluations ENSDF, ENDF/B-VII or JEFF-3.1. If uncertainties were not quantified in the evaluated data sources, they were either adopted from the original documentations or estimated from the experimental data.

As an example of data, Fig. 8 shows the cumulative yields of fission fragments caused by fast neutrons in the main fuel isotopes  $^{235}\text{U}$ ,  $^{238}\text{U}$  and  $^{239}\text{Pu}$ . The uncertainties of evaluated data at the level of 2-10% which is lower than the difference for the specific fission fragments yields can allow to measure concentration of fissile elements.

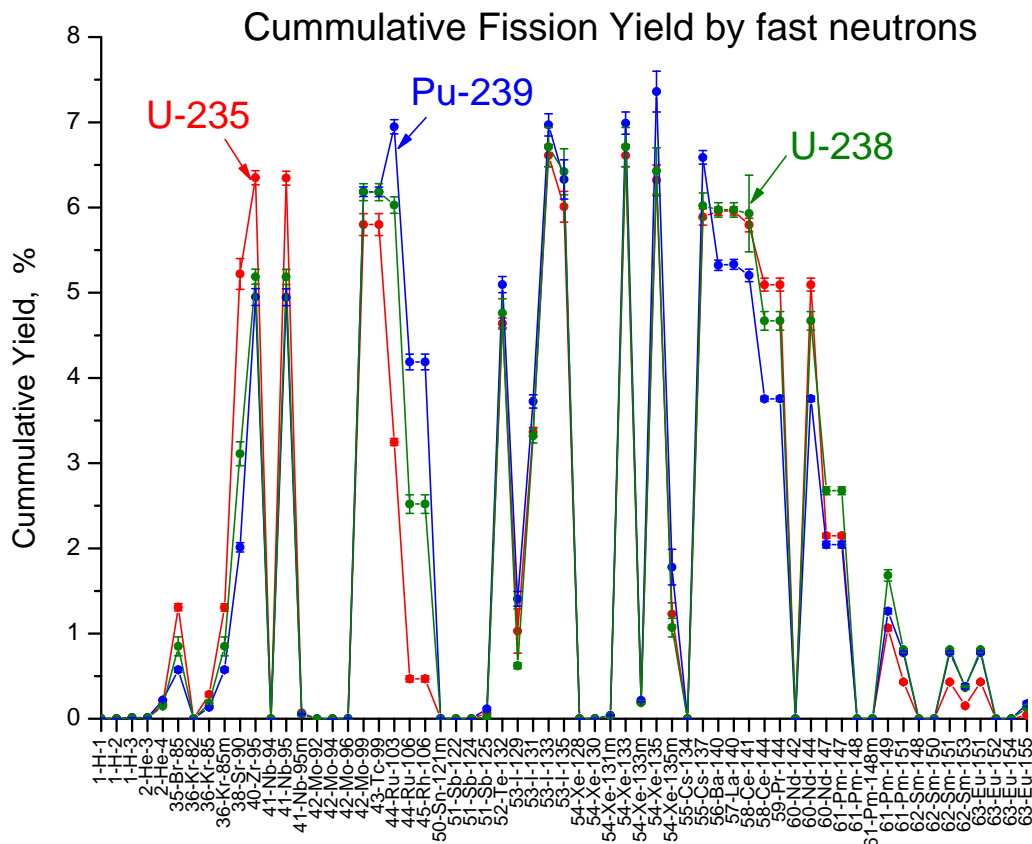


Fig. 8. Cumulative fission fragments yields and uncertainties.

## V. Stopping Power for Electrons, Light and Heavy Ions

Stopping Power for Light Ions is an electronic and nuclear stopping power database maintained by Prof. Helmut Paul (University of Linz, Austria), which is also regular mirrored on the NDS web page <https://www-nds.iaea.org/stopping/> (last version – Sep 2014).

The database contains:

- Hydrogen-, He- an heavier Ions in many pure and compound materials,
- numerical data, graphs, computer programs, statistical analysis and comments.

NDS provides the hyperlinks to the other well established reference databases or software:

- SRIM - Stopping and Range of Ions in Matter by J. Ziegler (USA), <http://www.srim.org/>.

- Stopping-Power and Range Tables by NIST, USA, <http://www.nist.gov/pml/data/star/index.cfm>:
  - ESTAR for electrons in 72 materials and energy range 10 keV to 1000 MeV,
  - PSTAR for protons in 74 materials and energy range 1 keV to 10 GeV,
  - ASTAR for alphas in 74 materials and energy range 1 keV to 1 GeV.

## VI. Scientific Bibliography Resources

CINDA (<https://www-nds.iaea.org/exfor/cinda.htm>, maintained by NDS) is a Computer Index of Nuclear Reaction Data. It has short information about  $\approx 60,000$  publications relevant to the measurement, calculation and evaluation of nuclear reactions (updated 2 times per year by automatic import from EXFOR and NSR).

NSR (<http://www.nndc.bnl.gov/nsr/>, maintained by BNL) is a Nuclear Science Reference database of indexes to more than 200,000 articles on Nuclear Physics (compiled manually).

EXFOR collection of papers, lab reports, thesis etc. has  $\approx 36,000$  pdf files (used internally for the compilation purposes).

It is worthwhile to note that the CINDA, NSR and EXFOR databases are hyper-linked each other that allows the quick inter-database on-line search for documentation and numerical data.

NDS Publication Portal (<https://www-nds.iaea.org/publications/>) has  $\approx 3,000$  documents. It includes: national labs and NDS reports (free); IAEA TecDocs since 1962 (free); Conference proceedings organised by IAEA (free); publications of the NDS staff as a collection of Titles, Abstracts and *doi*: links.

NDS collaborates with the main IAEA Library which provides access to scientific journals and helps to find the rare or historical documents; as well as with the Department of Energy of IAEA, which indexes the non-conventional literature publications on peaceful uses of nuclear Science and Technology in the International Nuclear Information System (INIS, <http://www.iaea.org/inis/>,  $\approx 3.6$  millions of records).

## VII. Collection of the computing codes at NDS

Although NDS of IAEA was not meant to be a repository of computer codes (as NEA Data Bank in Paris or RSICC in Oak Ridge), however we have several open source software from authors, labs or data development networks.

(i) Physical Quantities Simulation/Calculation Codes:

DROSG-2000 - accelerator based neutron source reactions Li(p,n), T(d,n), D(d,n) etc., (*M. Drosg*), <https://www-nds.iaea.org/drosg2000.html>

Larelkin - two-body Relativistic Kinematics (*M. Drosg*), <https://www-nds.iaea.org/public/libraries/larelkin/>

EMPIRE-3.2.2 - nuclear reaction model code (*M. Herman et al.*) <http://www.nndc.bnl.gov/empire/>, portable (plug & play) version for Windows (*V. Zerkov*) <https://www-nds.iaea.org/cdroms/>

RIPL-3 - collection of nuclear reaction modelling codes <https://www-nds.iaea.org/RIPL-3/>

GMA – least-squares method for simultaneous evaluation of reaction cross sections (*W.P. Poenitz et al.*), <https://www-nds.iaea.org/standards/codes.html>

STAYSL PNNL – determination of neutron spectrum at fission and accelerator-based neutron sources from activation measurements (*L. Greenwood*)

SPECTER, SPECOMP – radiation damage parameter calculation and determination displacement cross sections for compound materials (*L. Greenwood*): <https://www-nds.iaea.org/irdf2002/codes/index.htmlx>



(ii) Nuclear Data Processing, Checking and Plotting Codes

MF, MF-2 -missing level corrections using neutron-resonance spacings,  
(Gary E. Mitchell, John F. Shriner) <https://www-nds.iaea.org/missing-levels/>  
RR\_UNC and COVEIG – calculate spectrum averaged cross sections from the ENDF-6 formatted data with covariance and eigenvalues, (A. Trkov) <https://www-nds.iaea.org/IRDFF/>  
PREPRO-2012 and PLOTTAB - the ENDF/B-6 pre-processing code and plotting utility (D. Cullen) <https://www-nds.iaea.org/public/endl/prepro/>  
ENDF-6 utilities and checking codes, <https://www-nds.iaea.org/public/endl/utility/>  
ENSDF utilities and checking codes, [https://www-nds.iaea.org/public/ensdf\\_pgm/index.htm](https://www-nds.iaea.org/public/ensdf_pgm/index.htm)  
ENDVER - the ENDF-6 files VERification support package (A.Trkov), <https://www-nds.iaea.org/public/endl/endver/>  
ZVView - interactive plotting of nuclear data (V. Zerkin): <https://www-nds.iaea.org/public/zvview/>  
myEXFOR, myENDF, myENSDF, myPlot - tools for processing the EXFOR, ENDF and ENSDF data: under testing, for access - contact V. Zerkin, NDS.

Several other codes are available on the NDS pages.

## VIII. On- and off-line Dissemination

Following a Greening policy, NDS prefers to distribute the information on-line. Most of nuclear databases are available for downloading from the site <https://www-nds.iaea.org/cdroms/>.

On wish they could also be ordered as CD or DVD. In this case the individual selection of desirable databases can be done on this site (only fragment is shown):

### Nuclear Data on CD/DVD-ROMs

Select products from the list below

#	Product	Issued	Title [Link] Comment [Download]
1 <input type="checkbox"/>	ADS v-2.0	Dec-2008	Application Library for Accelerator Driven Systems [page]
2 <input type="checkbox"/>	EMPIRE-3.2.2 Portable for Windows	Jan-2014	System of codes for nuclear reaction calculations and nuclear data evaluation [screen-shots] <a href="#">Download</a> (zip, 753Mb)
3 <input type="checkbox"/>	ENDF libraries	Aug-2013	30 Evaluated Data Libraries including ENDF/B-VII.1, JEFF-3.2, JENDL-4.0u2, CENDL-3.1, ROSFOND-2010
4 <input type="checkbox"/>	EPDL97	Mar-2002	Photon and Electron interactions <a href="#">Download</a> (zip, 58Mb)
5 <input type="checkbox"/>	EXFOR-CINDA for Windows	Apr-2013	Database (MS-Access) and retrieval system (Java-2). Portable. [screen-shots] <a href="#">Download</a> (zip, 247Mb)
6 <input type="checkbox"/>	EXFOR-CINDA for Applications + Endver/GUI	Feb-2014	Database retrieval systems for Linux, Windows and Mac. Includes Endver/GUI package integrated with Prepro-2012 and full EXFOR database. Portable: does not need neither installation nor configuration. [screen-shots] <a href="#">Download</a> (tar.gz, 386Mb)
7 <input type="checkbox"/>	FOND2.2	Mar-2002	Evaluated Neutron Data Library <a href="#">Download</a> (zip, 21Mb)
8 <input type="checkbox"/>	IBANDL	Mar-2014	Ion Beam Analysis Data Library [web] <a href="#">Download</a> (zip, 45Mb, data + Web interface for Windows)

On the user specific request sent to the e-mail address [nds.contact-point@iaea.org](mailto:nds.contact-point@iaea.org), NDS will send out:

- hardcopies of INDC Reports, Charts of Nuclides, Nuclear Wallet Cards etc.
- NDS Newsletters (issued two times per year) which describes the current NDS activities, convened and planned Meetings, latest publications etc.

## IX. Databases/Codes on USB “Miniworkshops”

The USB stick distributed among School participants has three directories.

### 1. Directory "ENDF\_Libraries", volume ~ 3,000 Mb (most of the files are zipped).

It is a collection of the ENDF-6 formatted Evaluated Nuclear Reaction Libraries for General Use and for specific Applications.

Click on readme.htm to see content, to navigate and retrieve needed data files.



2. Directory "**x4app-2014-02-04**", volume ~ 950 Mb.

It is EXFOR and CINDA databases with PREPRO, Endver, ZVView processing and plotting codes as well as the proper documentation.

To start run scripts: *run\_x4cd.bat* (Windows), *run\_x4cd.sh* (Linux), *run\_x4cd-mac.sh* (MacOSX).

3. Directory "**Empire322zv2win**", volume ~ 3,000 Mb.

It is a nuclear reaction modeling code Empire. The package contains platform independent version of Empire, the databases RIPL, EXFOR in computer readable format C4 and documentation.

N.B. It is a beta version of the package. NOT intended to be RE-DISTRIBED. Not all menu options are active.

To start run the script *run\_empire.bat* which will invokes the start sample case "neutron + Pd-105" (more info in the file *readme.txt*).

To get more knowledge on how to use Empire package see materials of the IAEA Empire workshops,

e.g. recently held <https://www-nds.iaea.org/index-meeting-crp/EmpireWorkshop2013/index.htm>) or apply for announced ones.