

# International efforts to improve atomic and nuclear databases for energy and non-energy applications

Alan L. Nichols

*The Nuclear Data Section of the International Atomic Energy Agency has been involved in the formulation and maintenance of a wide range of atomic and nuclear databases for over 40 years. Much of the development work and the assembly of these dedicated databases require the involvement of external consultants and expertise from around the world, brought together to work in unison through well-defined IAEA coordinated research projects (CRPs) and more modest data development programmes (DDPs). A summary is given of the most recent CRPs and DDPs, and selected studies are described in detail to provide some indication of specific achievements that have been and are being made with respect to both energy and non-energy related applications.*

**Keywords:** Atomic and nuclear databases, coordinated research projects, cross-sections, decay data.

BOTH the development and maintenance of various types of atomic and nuclear databases are major features of the work undertaken by the consultants and staff of the Nuclear Data Section (NDS) at the International Atomic Energy Agency (IAEA). Efforts are always being made to identify the intermediate- and long-term data needs of a wide range of user communities that includes design engineers and operators of power reactors, and fuel handling/reprocessing facilities, medical physicists, analytical scientists and nuclear physicists undertaking basic research studies.

Multinational meetings are organized by NDS staff to debate atomic and nuclear data issues, and formulate appropriate work programmes that will adequately respond to the needs of various scientific communities<sup>1-4</sup>. IAEA coordinated research projects (CRPs) are reasonably substantial, and are initiated to maintain links between those laboratories with the necessary expertise to measure and evaluate the desired data for subsequent assembly as an appropriate database for worldwide adoption. Particularly well-focused and highly-specialized pieces of work can frequently be undertaken by means of more modest initiatives (referred to as data development projects (DDPs)). As shown in Table 1, the technical debate and databases produced through the good efforts of the IAEA NDS over the last 10 years are extensive.

A number of recently completed and on-going projects are described below that highlight the important function of the IAEA NDS in catalysing and organizing in a

timely manner the evolution of specific nuclear databases of importance to users worldwide. Consideration is given below to the following recently completed and on-going activities: Reference Input Parameter Library-phases 2 and 3 (RIPL-2 and 3); prompt gamma-ray neutron activation analysis (PGAA); A + M data for fusion plasma diagnostics; Th-U fuel cycle; cross-sections for the production of therapeutic radionuclides.

## Reference input parameter library

An important trend in the evaluation of neutron and charged-particle nuclear data is the increased use of nuclear reaction theory to compute cross-sections, spectra and angular distributions for a variety of applications. This use of model codes offers many advantages such as the preservation of the energy balance and coherence of partial cross-sections with total and/or reaction cross-sections. Such theoretical approaches also allow the prediction of nuclear data for unstable nuclei and fill gaps in the existing experimental data. Nuclear reaction theory is believed to be in a position to meet many requirements for various practical applications. Major sources of uncertainty are the input parameters required to undertake the theoretical calculations.

The practical use of nuclear model codes requires considerable numerical input data that describes the properties of nuclei under consideration and the interactions involved. Therefore, the IAEA has organized extensive coordinated efforts to develop, and assemble a library of evaluated and tested input parameters for nuclear model calculations. Considering such a task is so immense, the decision was

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**Table 1.** Recent coordinated research projects and data development studies dedicated to the recommendation of atomic and nuclear data

Title	Duration	No. of participants	Status, November 2006
Charged-particle cross-section database for medical radioisotope production: Diagnostic radioisotopes and monitor reactions	1995–2000	11	Completed and documented
Compilation and evaluation of photonuclear data for applications	1996–1999	11	Completed and documented
Fission product yield data for the transmutation of minor actinide nuclear waste	1997–2002	12	Completed*
Atomic and plasma-wall interaction data for fusion reactor divertor modelling	1998–2000	13	Completed and documented
Charge exchange cross-section data for fusion plasma studies	1998–2000	12	Completed and documented
Nuclear model parameter library for nuclear model calculations of nuclear data (Reference Input Parameter Library-phase 2 (RIPL-2))	1998–2001	13	Completed and documented
Update of X-ray and gamma-ray decay data standards for detector calibration and other applications	1998–2003	13	Completed*
Development of a database for prompt gamma-ray neutron activation analysis (PGAA)	1999–2003	10	Completed and documented
WIMS-D library update	1999–2003	13	Completed*
International Reactor Dosimetry File-2002 (IRDF-2002)	2001–2004	8	Completed and documented
Atomic and molecular data for fusion plasma diagnostics	2001–2005	12	Completed*
Molecular processes in edge plasmas	2001–2005	11	Completed*
Tritium inventory in fusion machines	2002–2007	12	On-going
Improvement of neutron cross-section standards	2002–2006	14	Completed – document in preparation
Evaluation of nuclear data for the Th–U fuel cycle	2002–2007	10	Completed – database/document in preparation
Parameters for the calculation of nuclear reactions of relevance to non-energy nuclear applications (Reference Input Parameter Library-phase 3 (RIPL-3))	2003–2007	12	On-going
Nuclear data for the production of therapeutic radionuclides	2003–2007	9	On-going
Atomic and molecular data for plasma modelling	2004–2007	14	On-going
Atomic data for heavy element impurities in fusion reactors	2005–2008	12	On-going
Development of a reference nuclear database for ion beam analysis	2005–2008	9	On-going
Reference database for neutron activation analysis	2005–2008	6	On-going
Updated decay data library for actinides	2005–2008	6	On-going
Data for surface composition dynamics relevant to erosion processes	2006–2010	12	On-going
Phase-space database for external beam radiotherapy	2006–2008	8	On-going

\*Status: Document submitted for publication – data available on the web.

taken to produce these data in a series of well-defined steps. An electronic starter file was developed and made available to users worldwide in 1998 as RIPL-1<sup>5</sup>. A second step followed immediately afterwards with the initiation of a CRP entitled ‘Nuclear model parameter library for nuclear model calculations of nuclear data (Reference Input Parameter Library-phase 2 (RIPL-2))’. These studies resulted in the revision and extension of the starter file to produce a consistent library containing recommended input parameters, large amounts of theoretical data suitable for nuclear reaction calculations, and a number of computer codes for parameter retrieval, determination and other uses. The primary objectives of RIPL-2 were as follows:

- Test and improve nuclear model parameters for theoretical calculations of nuclear reaction cross-sections at incident energies below 10 MeV;
- Produce a well-tested input data library for calculations of nuclear reactions by means of nuclear reaction codes;
- Develop user-oriented retrieval tools and interfaces to established codes for nuclear reaction calculations;
- Publish a technical report<sup>6</sup> and ensure that the library and tools are available on-line (<http://www-nds.iaea.org/RIPL-2/>) and on CD-ROM.

RIPL-2 is targeted at users of nuclear reaction codes interested in low-energy nuclear applications. Incident and outgoing particles include neutrons, protons, deuterons, tritons, <sup>3</sup>He, <sup>4</sup>He and  $\gamma$ , with energies up to ~100 MeV. The numerical data and computer codes included in the library are arranged in seven directories:

Directory	Contents
Masses	Atomic masses
Levels	Discrete level schemes
Resonances	Average neutron resonance parameters
Optical	Optical model parameters
Densities	Level densities (total and partial)
Gamma	Gamma-ray strength functions
Fission	Fission barriers and level densities

A website allows the downloading of entire RIPL-2 segments, individual files and selected data. Furthermore,

some basic calculations and graphical comparisons of parameters are also available.

While RIPL-2 constitutes a consistent set of nuclear reaction input parameters, the database is limited to neutron-induced reactions up to 20 MeV (i.e. typical for conventional power reactors). Extensions to the RIPL-2 database are required in order to address the needs of other emerging nuclear-based technologies, such as accelerator driven waste incineration, radioisotope production for diagnostics and therapy, charged-particle beam therapy and materials analysis. There is also a worldwide interest in nuclear astrophysics, which is constrained to relying upon theoretical calculations of nuclear reaction cross-sections when modelling the distribution of isotopes throughout the universe. Therefore, a third and final phase of the RIPL project was conceived during 2002–03 to address ‘Parameters for the calculation of nuclear reactions of relevance to non-energy nuclear applications’. Specific initiatives within RIPL-3 have included the following:

- Update of the level scheme database starting from the latest ENSDF library (October 2005) – these newly-derived discrete level files have also been tested and validated;
- Extension of the format of the optical model segment;
- Development and compilation of new potentials to describe the interaction of charged particles with nuclei, and nucleon scattering on deformed targets.

General structure of RIPL-3 will be based on RIPL-2, with minor format changes to accommodate the additional information required for non-energy applications. Emphasis has been placed on the determination of data uncertainties and validation using large-scale calculations of nuclear reactions across the Periodic Table. Complementary programming on interface development has also been recommended to ensure that those observables predicted by means of the RIPL-3 library have well-defined and unique values. On completion, RIPL-3 should be a reliable tool for the guidance of theoretical calculations at incident energies up to 200 MeV.

### Database for prompt gamma-ray neutron activation analysis

Neutron-capture prompt gamma-ray activation analysis (PGAA) is a non-destructive radioanalytical method of rapid or simultaneous *in situ* multi-element analyses across the Periodic Table from hydrogen to uranium. Analyses for hydrogen and boron are especially important because of the lack of other reliable analytical techniques for trace levels of these elements. PGAA is extremely sensitive for the quantitative determination of boron compared with destructive chemical techniques<sup>7,8</sup>. Over the last 15 years, the adoption of PGAA has increased because of the avail-

ability of high-flux thermal and cold beams from neutron guides<sup>9</sup>. Guided beams can be free of fast neutrons and superfluous gamma rays to give improved signal-to-background ratios. Thermal guide studies have also shown that spectral quality is an important factor in performing high-sensitivity analyses<sup>8</sup>. Thus, prompt gamma-ray neutron activation analysis has become a well-established analytical method with applications in many areas of study<sup>10–13</sup>. Nevertheless, inaccurate and incomplete data have been a significant problem in the quantitative analysis of complicated capture-gamma spectra by means of PGAA. Therefore, the IAEA initiated a CRP in 1999 to improve the quality and quantity of data required to apply PGAA reliably in such fields as materials science, chemistry, geology, mining, archeology, environmental monitoring, food analysis and medicine.

**Table 2.** Example data – adopted prompt and decay gamma rays from thermal neutron capture

<sup>A</sup> Z	<i>E<sub>γ</sub></i> (keV)	$\sigma$ ( <i>E<sub>γ</sub></i> ) (barns)	<i>k<sub>0</sub></i>
Hydrogen ( <i>Z</i> = 1), At. wt. = 1.00794(7), $\sigma_{\gamma}$ = 0.3326(7)			
<sup>1</sup> H	<b>2223.24835(9)</b>	<b>0.3326(7)</b>	<b>1.0000(21)</b>
<sup>2</sup> H	6250.243(3)	0.000519(7) <sup>a</sup>	0.001560(21)
Helium ( <i>Z</i> = 2), At. wt. = 4.002602(2), $\sigma_{\gamma}$ = 4.2E–11(12)			
<sup>3</sup> He	<b>20520.46</b>	<b>4.2(12)E–11</b>	<b>3.2(9)E–11</b>
Lithium ( <i>Z</i> = 3), At. wt. = 6.941(2), $\sigma_{\gamma}$ = 0.045(3), $\sigma_{\alpha}$ ( <sup>6</sup> Li) = 71.3(5)			
<sup>6</sup> Li	477.595(3)	0.00153(8)	0.00067(4)
<sup>7</sup> Li	<b>980.53(7)</b>	<b>0.00415(13)</b>	<b>0.00181(6)</b>
<sup>7</sup> Li	<b>1051.90(7)</b>	<b>0.00414(12)</b>	<b>0.00181(5)</b>
<sup>7</sup> Li	<b>2032.30(4)</b>	<b>0.0381(8)</b>	<b>0.0166(4)</b>
<sup>6</sup> Li	6768.81(4)	0.00151(9)	0.00066(4)
<sup>6</sup> Li	7245.91(4)	0.00247(14)	0.00108(6)
Beryllium ( <i>Z</i> = 4), At. wt. = 9.012182(3), $\sigma_{\gamma}$ = 0.0088(4)			
<sup>9</sup> Be	<b>853.630(12)</b>	<b>0.00208(24)</b>	<b>0.00070(8)</b>
<sup>9</sup> Be	<b>2590.014(19)</b>	<b>0.00191(15)</b>	<b>0.00064(5)</b>
<sup>9</sup> Be	<b>3367.448(25)</b>	<b>0.00285(22)</b>	<b>0.00096(7)</b>
<sup>9</sup> Be	<b>3443.406(20)</b>	<b>0.00098(7)</b>	<b>0.000330(24)</b>
<sup>9</sup> Be	5956.53(3)	1.46(12)E–4	4.9(4)E–5
<sup>9</sup> Be	<b>6809.61(3)</b>	<b>0.0058(5)</b>	<b>0.00195(17)</b>
Boron ( <i>Z</i> = 5), At. wt. = 10.811(7), $\sigma_{\gamma}$ = 0.104(20), $\sigma_{\alpha}$ ( <sup>10</sup> B) = 764(25)			
<sup>10</sup> B(n, $\alpha$ )	<b>477.595(3)</b>	<b>716(25)</b>	<b>201(7)</b>
<sup>10</sup> B	6739.67(17)	0.0113(10)	0.0032(3)
Carbon ( <i>Z</i> = 6), At. wt. = 12.0107(8), $\sigma_{\gamma}$ = 0.00351(5)			
<sup>12</sup> C	<b>1261.765(9)</b>	<b>0.00124(3)</b>	<b>0.000313(8)</b>
<sup>12</sup> C	<b>3683.920(9)</b>	<b>0.00122(3)</b>	<b>0.000308(8)</b>
<sup>12</sup> C	<b>4945.301(3)</b>	<b>0.00261(5)</b>	<b>0.000659(13)</b>
<sup>13</sup> C	8174.04(18)	1.09(6)E–5	2.75(15)E–6
Oxygen ( <i>Z</i> = 8), At. wt. = 15.9994(3), $\sigma_{\gamma}$ = 1.90E–4(19)			
<sup>18</sup> O	197.142(4)d	3.15(22)E–7	6.0E–8[99%]
<sup>16</sup> O	<b>870.68(6)</b>	<b>1.77(11)E–4</b>	<b>3.35(21)E–5</b>
<sup>16</sup> O	<b>1087.75(6)</b>	<b>1.58(7)E–4</b>	<b>2.99(13)E–5</b>
<sup>17</sup> O	1981.95(9)	2.0(4)E–7	3.8(8)E–8
<sup>16</sup> O	<b>2184.42(7)</b>	<b>1.64(7)E–4</b>	<b>3.11(13)E–5</b>
<sup>16</sup> O	<b>3272.02(8)</b>	<b>3.53(23)E–5</b>	<b>6.7(4)E–6</b>

<sup>a</sup>Total deuterium isotopic cross-section.

**Table 3.** Example listing of the most intense thermal neutron-capture gamma rays ordered by energy

$^A_Z$	$E_\gamma$ (keV)	$\sigma_\gamma^Z(E_\gamma)$ (barns)	$k_0$	$E_\gamma, \sigma_\gamma^Z(E_\gamma)$ for associated intense gamma rays
$^{127}\text{I}$	124.2810(20)	0.180(13)	0.0043(3)	133.6110(1.42), 442.901(0.600), 27.3620(0.43)
$^{51}\text{V}$	124.453(4)	0.23(5)	0.014(3)	1434.10(4.81), 125.082(1.61), 6517.282(0.78)
$^{51}\text{V}$	125.082(3)	1.61(4)	0.0958(24)	1434.10(4.81), 6517.282(0.78), 645.703(0.769)
$^{115}\text{In}$	126.3720(20)	4.0(3)	0.106(8)	1293.54(131), 1097.30(87.3), 416.86(43.0)
$^{141}\text{Pr}$	126.8460(20)	0.307(15)	0.0066(3)	176.8630(1.06), 140.9050(0.479), 1575.6(0.426)
$^{191}\text{Ir}$	126.958(3)	1.86(10)	0.0293(16)	351.689(10.9), 328.448(9.1), 84.2740(7.7)
$^{103}\text{Rh}$	127.20(3)	5.27(21)	0.155(6)	180.87(22.6), 97.14(19.5), 51.50(16.0)
$^{186}\text{W}$	127.43(4)	0.129(5)	0.00213(8)	685.73(3.24), 479.550(2.59), 72.002(1.32)
$^{133}\text{Cs}$	127.5000(20) <i>d</i>	0.310(11)	7.1E-03[11%]	176.4040(2.47), 205.615(1.560), 510.795(1.54)
$^{169}\text{Tm}$	130.027	0.940(25)	0.0169(5)	200(8.72), 149.7180(7.11), 140(5.96)
$^{133}\text{Cs}$	130.2320(20)	1.410(21)	0.0322(5)	176.4040(2.47), 205.615(1.560), 510.795(1.54)
$^{127}\text{I}$	133.6110(10)	1.42(10)	0.0339(24)	442.901(0.600), 27.3620(0.43), 58.1100(0.28)

The resulting evaluated gamma-ray activation file (EGAF) is a database of ~32,000 adopted prompt gamma rays and ~3000 gamma rays emitted by radioactive decay, covering all stable isotopes of the elements from hydrogen to uranium. The  $k_0$  formulation is commonly used in activation analysis because this product of the yield and cross-section can usually be measured with greater accuracy than either parameter alone. A value of  $k_0$  for a gamma ray emitted from isotope  $i$  is defined relative to the hydrogen standard on a mass scale:

$$\begin{aligned}
 k_0(E_\gamma) &= k_Z(E_\gamma)/k_{\text{H}}(2223) \\
 &= [\sigma_\gamma^Z(E_\gamma)/A_r(Z)]/[\sigma_\gamma^{\text{H}}(2223)/A_r(\text{H})] \\
 &= 3.03 \times [\sigma_\gamma^Z(E_\gamma)/A_r(Z)],
 \end{aligned}$$

where  $\sigma_\gamma^Z(E_\gamma)$  is the partial elemental cross-section in barns for the production of gamma ray  $E_\gamma$  from element  $Z$ , assuming natural abundance, and  $A_r(Z)$  is the relative atomic weight of the element  $Z$ . Selected gamma rays with  $k_0$  values >1% of the most intense transitions are listed in Table 2, while those that are >10% are shown in bold type. Although omitted from this summary table, gamma rays with  $k_0 < 1\%$  of the largest value are included in the full database. Gamma rays from radioactive decay are denoted by *d* immediately after the energy and uncertainty. Energy-ordered gamma rays are also included in the final database for each element with isotopic identification, energy and uncertainty in keV, and the partial cross-section  $k_0$  and their uncertainties (Table 3).

Uncertainties defined in Tables 2 and 3 are contained within parentheses, and are expressed in terms of the last digit or digits of the recommended value. These uncertainties are the standard deviation corresponding to the 1 $\sigma$  confidence level, for example:

$$125.082(3) \equiv 125.082 \pm 0.003,$$

$$1234.5(12) \equiv 1234.5 \pm 1.2,$$

$$4.5(3)\text{E-}5 \equiv (4.5 \pm 0.3) \times 10^{-5}.$$

### Atomic and molecular data for fusion plasma diagnostics

Plasmas generated in fusion energy research cover a wide range of conditions involving the plasma constituents, electron temperature and density, as well as the electric and magnetic fields. These plasmas possess edge/divertor and core regions, and their physical conditions differ considerably. Under such circumstances, plasma diagnosis is a complex problem requiring many different types of atomic and molecular data for sound quantitative interpretation:

- Soft X-ray spectroscopy and optical spectroscopy can be used in the core region, requiring information on the emission properties of the plasma. Some data can be measured directly in experimental devices such as the electron beam ion trap.
- Temperatures are significantly lower in the edge/divertor region, and there is a relatively high concentration of neutral species. Molecules will form in this region, requiring extensive data on a variety of molecular processes for diagnostic procedures, while processes such as charge exchange will also be important (radiative, and electron and heavy-particle collisional processes).

A CRP was established in 2001 with the objective of identifying the A + M data needs in order to diagnose and characterize the core and edge plasmas, and the velocity distribution of fusion alpha particles. This project has focused on various types of diagnostic techniques used in large fusion machines, including plasma impurity emissions, charge exchange and neutral-beam-based emission diagnostics, and the plasma neutrals analysis method for alpha-particle diagnostics. The main aims were to identify the specific processes for which data are most urgently needed, and to generate these data for addition to the cross-section database on collisional processes and for beam spectroscopy.

New data were generated for a variety of processes that impact on a number of diagnostic procedures for fusion plasmas:

- Cross-section data were measured and calculated to analyse spectral observations near the strike zone and divertor where alpha particles interact with molecules<sup>14</sup>;
- Both thermal and fast cross-section data for electron and proton impact were generated for helium-beam diagnostics<sup>15,16</sup>;
- Data were produced for use in the determination of ion species from light elements such as helium, boron and hydrocarbons, as well as the heavy elements such as tungsten<sup>17–20</sup>;
- Large amounts of data on spectral properties were generated for use in the spectral analysis of plasma emissions;
- Determination of X-ray emission data from impact on surfaces;
- Data were generated for use in hydrogen charge exchange spectroscopy to determine the flow and temperature of impurities in the divertor region.

As well as being published in refereed journals during the course of the CRP, these data have been added to various electronic databases, including the ALADDIN system of the IAEA. All participants have also summarized their results for publication in an issue of *Atomic and Plasma-Material Interaction Data for Fusion*<sup>21</sup>.

### Th–U fuel cycle

Past developments in nuclear technology have mainly been based on uranium–plutonium thermal and fast reactors in order to improve the utilization of sources of natural uranium. However, new concepts for nuclear power production have been investigated in recent years in order to explore other means of satisfying the need for increased inherent safety, reducing the risk of fissile material proliferation, and addressing the problem of long-term radioactive waste disposal. These studies have included the thorium-based nuclear fuel cycle which offers a number of advantages:

- <sup>232</sup>Th neutron capture yields <sup>233</sup>U – highly efficient fuel that can be adopted to create the concept of a thermal-breeder reactor based on thorium;
- Long-lived higher actinides are the main source of long-term radioactive waste, and their build-up is much more modest in thorium than uranium fuel;
- Thorium fuel is more proliferation-resistant due to the resulting highly-radioactive constituents that cannot be easily separated from the fuel by chemical means;
- World reserves of thorium are much larger than uranium reserves.

As a consequence of the factors listed above, there is a rising interest in innovative fuel cycle concepts based on thorium. Unfortunately, due to the previous lack of interest in the thorium fuel cycle, the quality of nuclear data for

the relevant materials is significantly lower than for comparable materials in the uranium and mixed-oxide fuel cycles<sup>22,23</sup>.

Important experimental measurements of the cross-sections of materials relevant to the Th–U fuel cycle have been reported recently – these data require evaluation, verification and validation on the basis of integral benchmarks. There has also long been a need to improve the recommended nuclear data for the Th–U fuel cycle, and an IAEA CRP was initiated in 2002 to undertake the necessary work<sup>24</sup>:

- Neutron cross-section data for <sup>232</sup>Th, <sup>231,233</sup>Pa and <sup>232,233,234,236</sup>U;
- Critical assessment of available experimental information, and renormalization to standard cross-sections, if necessary;
- Evaluation of experimental data, derivation of resonance parameters (when relevant), and completion of data by means of nuclear-model calculations to produce a suitably comprehensive database in ENDF-6 format;
- Verification of the formatted data;
- Processing of the data into application libraries for validation against benchmark test cases<sup>25</sup>.

Examples of the measured and evaluated neutron-induced fission cross-section data for <sup>232</sup>Th and <sup>231</sup>Pa are shown in Figures 1 and 2 respectively. Considerable effort has been expended to assess with some accuracy, the important and complex resonance regions near the first-chance fission thresholds of <sup>232</sup>Th and <sup>231</sup>Pa, as highlighted by the detail within the insets of Figures 1 and 2.

This programme was extended to include the production of covariance data for some of the nuclides to cover both the resonance and fast regions (<sup>232</sup>Th and <sup>231,233</sup>Pa). Covariance information for the resonance region of <sup>232</sup>Th was derived by Leal *et al.*<sup>26</sup>, while covariances for the fast neutron region of <sup>232</sup>Th were independently calculated by three different groups for subsequent study and assessment. Covariance data are also available for the <sup>231,233</sup>Pa cross-sections. This work is outlined on the IAEA NDS website: <http://www-nds.iaea.org/Th-U/>

### Cross-sections for the production of therapeutic radionuclides

Radiopharmaceuticals play an important role in nuclear medicine in terms of both diagnostic investigations and therapeutic treatment. The role of nuclear data is mainly with respect to ensuring the quality assurance of the radioactive materials and methods adopted in such work<sup>27,28</sup>. Generally, the radionuclides used in nuclear medicine possess particular decay characteristics – low-energy  $\alpha$ ,  $\beta^-$  and Auger electron emitters. While effective in diagnostic and therapeutic treatments, these somewhat elusive decay characteristics can create difficulties when using such properties to determine their production cross-

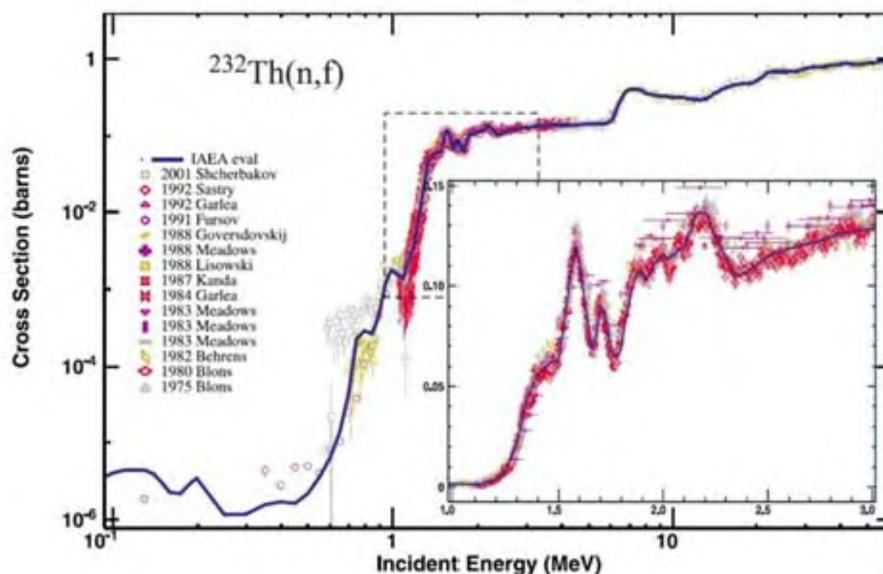


Figure 1. Measured and evaluated cross-section data for  $^{232}\text{Th}(n, f)$ .

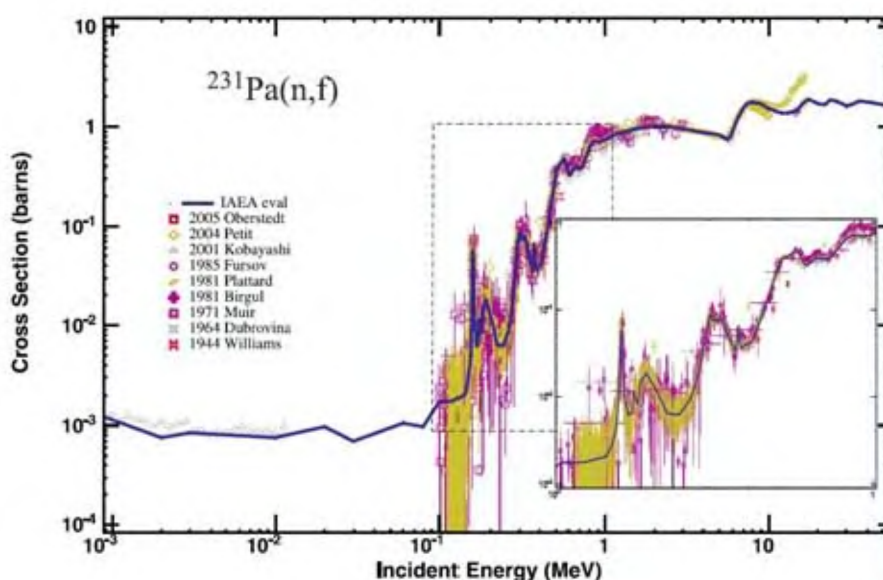


Figure 2. Measured and evaluated cross-section data for  $^{231}\text{Pa}(n, f)$ .

sections to ensure a pure radionuclidic product. While the diagnostic and therapeutic properties of specific radionuclides have been demonstrated in various medical trials and they can be produced in sufficient quantities, knowledge of their production reaction cross-sections is poorly defined.

Two IAEA CRPs have been successfully organized with the primary aim of improving the production cross-section data for both diagnostic and therapeutic radionuclides:

- (a) Charged-particle cross-section database for medical radioisotope production: diagnostic radioisotopes and monitor reactions;

- (b) Nuclear data for the production of therapeutic radionuclides.

The reaction cross-section studies for diagnostic radionuclides<sup>29</sup> were completed in 2001 and their data are available through an IAEA website (<http://www-nds.iaea.org/medical/>), while the equivalent therapeutic work is close to completion<sup>30</sup>. Lists of the therapeutic radionuclides and the production reactions under study are given in Tables 4 and 5, based on two categories:

- Therapeutic radionuclides that have proven clinical use (Table 4) – Established radionuclide;



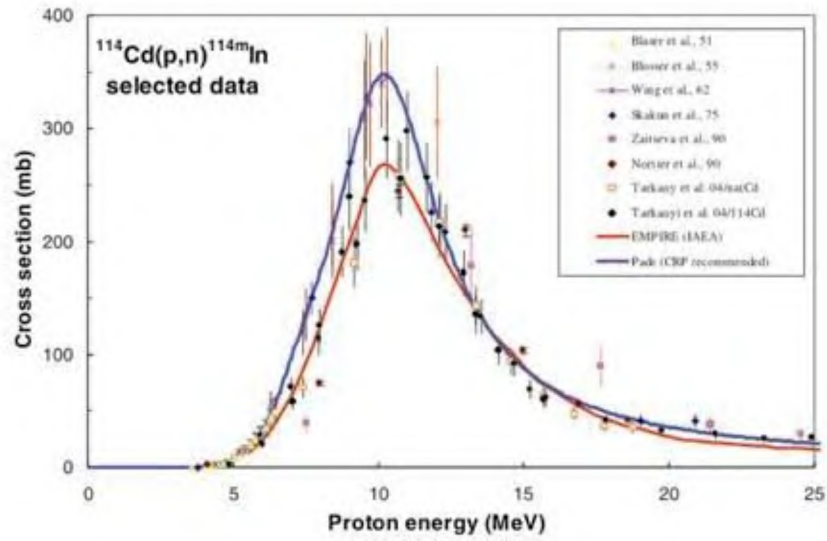


Figure 3. Measurements and calculations of the  $^{114}\text{Cd}(p, n)^{114\text{m}}\text{In}$  cross-section.

Table 4. Established therapeutic radionuclides

Established radionuclide	Production route	R/A*
$^{32}\text{P}$	$^{31}\text{P}(\text{n}, \gamma)$	R
	$^{32}\text{S}(\text{n}, \text{p})$	R, A
$^{89}\text{Sr}$	$^{88}\text{Sr}(\text{n}, \gamma)$	R
	$^{89}\text{Y}(\text{n}, \text{p})$	R, A
$^{90}\text{Y}$	$^{235}\text{U}(\text{n}, \text{f})^{90}\text{Sr} \rightarrow ^{90}\text{Y}$ generator	R
	$^{89}\text{Y}(\text{n}, \gamma)$	R
	$^{90}\text{Zr}(\text{n}, \text{p})$	R
$^{103}\text{Pd}$	$^{102}\text{Pd}(\text{n}, \gamma)$	R
	$^{103}\text{Rh}(\text{p}, \text{n})$	A
	$^{103}\text{Rh}(\text{d}, 2\text{n})$	A
$^{125}\text{I}$	$^{124}\text{Xe}(\text{n}, \gamma)^{125}\text{Xe} \rightarrow ^{125}\text{I}$	R
	$^{124}\text{Te}(\text{d}, \text{n})$ – also impurity in $^{124}\text{I}$ production	A
	$^{125}\text{Te}(\text{p}, \text{n})$ – also impurity in $^{124}\text{I}$ production	A
$^{131}\text{I}$	$^{130}\text{Te}(\text{n}, \gamma)^{131}\text{Te} \rightarrow ^{131}\text{I}$	R
	$^{235}\text{U}(\text{n}, \text{f})$	R
$^{137}\text{Cs}$	$^{235}\text{U}(\text{n}, \text{f})$	R
$^{153}\text{Sm}$	$^{152}\text{Sm}(\text{n}, \gamma)$	R
	$^{153}\text{Eu}(\text{n}, \text{p})$	R, A
$^{186}\text{Re}$	$^{185}\text{Re}(\text{n}, \gamma)$	R
	$^{186}\text{W}(\text{p}, \text{n})$	A
	$^{186}\text{W}(\text{d}, 2\text{n})$	A
$^{188}\text{Re}$	$^{186}\text{W}(\text{n}, \gamma)^{187}\text{W}(\text{n}, \gamma)^{188}\text{W} \rightarrow ^{188}\text{Re}$ generator	R
	$^{187}\text{Re}(\text{n}, \gamma)$	R
$^{192}\text{Ir}$	$^{191}\text{Ir}(\text{n}, \gamma)$	R
	$^{192}\text{Os}(\text{p}, \text{n})$	A
	$^{192}\text{Os}(\text{d}, 2\text{n})$	A

\*R, Reactor; A, Accelerator.

- Less-commonly used but potentially important radionuclides for which medical applications have been demonstrated (Table 5) – Emerging radionuclide.

Experimental data compilations and data selection, theoretical calculations and the final evaluations for each of the reactions producing therapeutic radionuclides will become available within a few months. For example, two of

Table 5. Emerging therapeutic radionuclides

Emerging radionuclide	Production route	R/A/D*
$^{64}\text{Cu}$	$^{63}\text{Cu}(\text{n}, \gamma)$	R
	$^{64}\text{Ni}(\text{p}, \text{n})$	A
	$^{64}\text{Ni}(\text{d}, 2\text{n})$	A
	$^{68}\text{Zn}(\text{p}, \text{x})$	A
	$\text{Zn}(\text{d}, \text{x})$	A
	$^{64}\text{Zn}(\text{n}, \text{p})$	R
$^{67}\text{Cu}$	$^{67}\text{Zn}(\text{n}, \text{p})$	R
	$^{68}\text{Zn}(\text{p}, 2\text{p})$	A
	$^{70}\text{Zn}(\text{p}, \alpha)$	A
$^{67}\text{Ga}$	$^{68}\text{Zn}(\text{p}, 2\text{n}), ^{67}\text{Zn}(\text{p}, \text{n})$	A
$^{86}\text{Y}$	$^{86}\text{Sr}(\text{p}, \text{n})$	A
$^{105}\text{Rh}$	$^{104}\text{Ru}(\text{n}, \gamma)^{105}\text{Ru} \rightarrow ^{105}\text{Rh}$	R
$^{111}\text{In}$	$^{111}\text{Cd}(\text{p}, \text{n}), ^{112}\text{Cd}(\text{p}, 2\text{n})$	A
$^{114\text{m}}\text{In}$	$^{113}\text{In}(\text{n}, \gamma)$	R
	$^{114}\text{Cd}(\text{p}, \text{n})$	A
	$^{116}\text{Cd}(\text{p}, 3\text{n})$	A
	$^{114}\text{Cd}(\text{d}, 2\text{n})$	A
$^{124}\text{I}$	$^{124}\text{Te}(\text{p}, \text{n})$	A
	$^{124}\text{Te}(\text{d}, 2\text{n})$	A
	$^{125}\text{Te}(\text{p}, 2\text{n})$	A
$^{149}\text{Pm}$	$^{148}\text{Nd}(\text{n}, \gamma)^{149}\text{Nd} \rightarrow ^{149}\text{Pm}$	R
$^{166}\text{Ho}$	$^{165}\text{Ho}(\text{n}, \gamma)$	R
	$^{164}\text{Dy}(\text{n}, \gamma)^{165}\text{Dy}(\text{n}, \gamma)^{166}\text{Dy} \rightarrow ^{166}\text{Ho}$	R
$^{169}\text{Yb}$	$^{168}\text{Yb}(\text{n}, \gamma)$	R
	$^{169}\text{Tm}(\text{p}, \text{n})$	A
	$^{169}\text{Tm}(\text{d}, 2\text{n})$	A
$^{177}\text{Lu}$	$^{176}\text{Yb}(\text{n}, \gamma)^{177}\text{Yb} \rightarrow ^{177}\text{Lu}$	R
	$^{176}\text{Lu}(\text{n}, \gamma)$	R
	$^{176}\text{Yb}(\text{d}, \text{x})$	A
$^{211}\text{At}$	$^{209}\text{Bi}(\alpha, 2\text{n})$	A
$^{213}\text{Bi}$	Decay of $^{225}\text{Ac}$	D
$^{225}\text{Ac}$	$^{226}\text{Ra}(\text{p}, 2\text{n})$	A
	Decay of $^{233}\text{U} \rightarrow ^{229}\text{Th}$	R, D

\*R, Reactor; A, Accelerator; D, Natural decay.

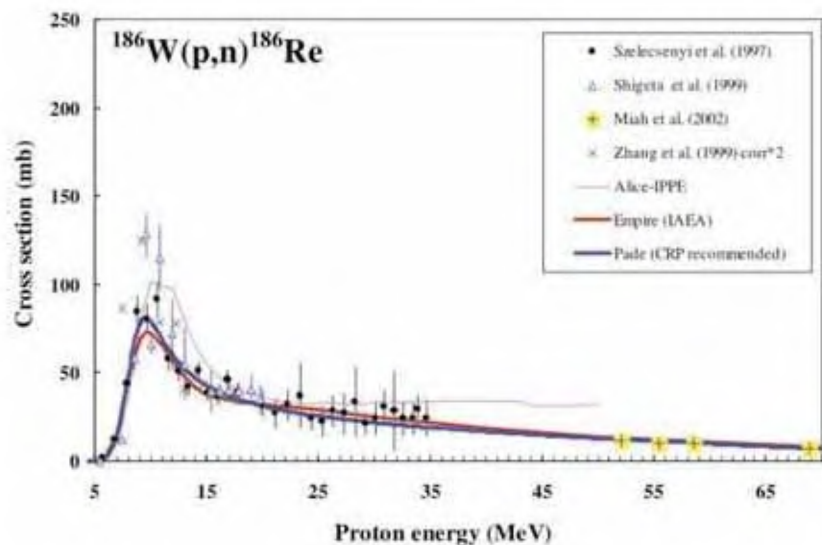


Figure 4. Measurements and calculations of the  $^{186}\text{W}(p, n)^{186}\text{Re}$  cross-section.

the reactions under study for the production of  $^{114\text{m}}\text{In}$  and  $^{186}\text{Re}$  are shown in Figures 3 and 4 respectively. The recommendations for both established and emerging therapeutic radionuclides, and validation/testing of the cross-section library should be available by the end of 2007. As a consequence of the work undertaken during the course of the two CRPs noted above, the resulting completeness and accuracy of the cross-section data for the production of these nuclides, along with a re-definition of their decay data, should be extremely beneficial in ensuring their safe and efficient application in nuclear medicine<sup>31–33</sup>.

## Conclusions

Various well-defined initiatives are supported by the IAEA NDS and their staff to produce and improve specific atomic and nuclear data. The most recent data development projects have been noted, and a select number have been described in reasonable detail. One extremely important feature of all of these studies is the participation of experts from around the world, as identified and organized through the efforts of the IAEA. Each package of work has definite goals, with the primary aim of producing accessible data files for users in member states of the IAEA. For further information see <http://www-nds.iaea.org> and <http://www-amdis.iaea.org>.

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