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INTERMEDIATE ENERGY DATA

A report by the Working Party
on International Evaluation Co-operation
of the NEA Nuclear Science Committee

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NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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The OECD Nuclear Energy Agency (NEA) was established on 1st February 1958 under the name of OEEC European Nuclear Energy Agency. It received its present designation on 20th April 1972, when Japan became its first non-European full Member. NEA membership today consist of all OECD Member countries, except New Zealand and Poland. The Commission of the European Communities takes part in the work of the Agency.

The primary objective of the NEA is to promote co-operation among the governments of its participating countries in furthering the development of nuclear power as a safe, environmentally acceptable and economic energy source.

This is achieved by:

- *encouraging harmonization of national regulatory policies and practices, with particular reference to the safety of nuclear installations, protection of man against ionising radiation and preservation of the environment, radioactive waste management, and nuclear third party liability and insurance;*
- *assessing the contribution of nuclear power to the overall energy supply by keeping under review the technical and economic aspects of nuclear power growth and forecasting demand and supply for the different phases of the nuclear fuel cycle;*
- *developing exchanges of scientific and technical information particularly through participation in common services;*
- *setting up international research and development programmes and joint undertakings.*

In these and related tasks, the NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has concluded a Co-operation Agreement, as well as with other international organisations in the nuclear field.

FOREWORD

A Working Party on International Evaluation Co-operation was established under the sponsorship of the OECD/NEA Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation, and related topics. Its aim is also to provide a framework for co-operative activities between members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The working party determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

The parties to the project are: ENDF (United States), JEF/EFF (NEA Data Bank Member countries) and JENDL (Japan). Co-operation with evaluation projects of non-OECD countries, specifically the Russian BROND and Chinese CENDL projects, are organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

Subgroup 13 of the working party was initiated with the objective to assess nuclear data needs in the intermediate energy range. The major tasks of the subgroup were to identify the needs for experimental and evaluated data, the suitable data formats to be used, and the methodology to be used in data calculations. The assembly of a pilot evaluation was also being scheduled in a second phase of the project.

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TABLE OF CONTENTS

INTERMEDIATE ENERGY DATA

1. Introduction

Subgroup 13 (SG13) on Intermediate Energy Nuclear Data was formed by the NEA Nuclear Science Committee in 1994 to solve common problems of intermediate energy nuclear data for nuclear applications. The first meeting was chaired by the monitor, the late Dr. Kikuchi of JAERI, during the Gatlinburg conference on Nuclear Data for Science and Technology in 1994. The enormous interest in accelerator-driven systems that has emerged in the past decade has resulted in the associated interest, and importance, of intermediate energy nuclear data. Of course, this topic itself covers many aspects, from basic nuclear model calculations and microscopic experiments to applied transport calculations. The main scope of SG13 has always been to focus the present expertise in the various branches of research, thereby primarily using transmutation of waste as the objective.

The general nature of SG13, combined with the aforementioned boost in accelerator-driven system research, has entailed that the range of SG13 has become very wide. With various national and international activities on intermediate energy nuclear data now well underway, it may be the right moment to finalise this subgroup and to discuss possible new subgroups that handle the most crucial subtopics of intermediate energy nuclear data, i.e. subgroups that are entirely devoted to more strictly defined tasks.

In this final report, we give an overview of the present status of the various activities of SG13. First, we go in some detail. At the end we give a summarised list. We also provide a list of recommendations for follow-up actions.

We mention that most reports related to SG13 can be obtained electronically from the NEA Data Bank. In particular the following WWW-pages contain relevant documents:

- http://www.nea.fr/html/science/pt/iend.html
- http://www.nea.fr/html/trw/nucdat/high.html
- http://www.nea.fr/html/trw/nucdat/iend/iend.html

2. General scope

Many applications, such as accelerator-based transmutation of waste, energy amplification, medical research, astrophysical applications and also fusion research, require nuclear data that go beyond the traditional evaluation limit of 20 MeV. Whereas low-energy neutron-induced reactions already have been extensively evaluated, mainly for conventional reactor purposes, the situation for protons and neutrons above 20 MeV is less clear. The purpose of SG13 was to investigate the nuclear data needs for applications and to provide the link with nuclear reaction physics. Important topics that have been, and are still, considered are:

- Investigation of nuclear data needs from the point of view of applications. Which nuclear data have the highest priority?

- Recommendations for experiments.

- Compilation of existing experimental data into computational format (EXFOR; NEA Data Bank).

- Assessment of the current status of nuclear models and associated codes (and comparison of such codes in a benchmark).

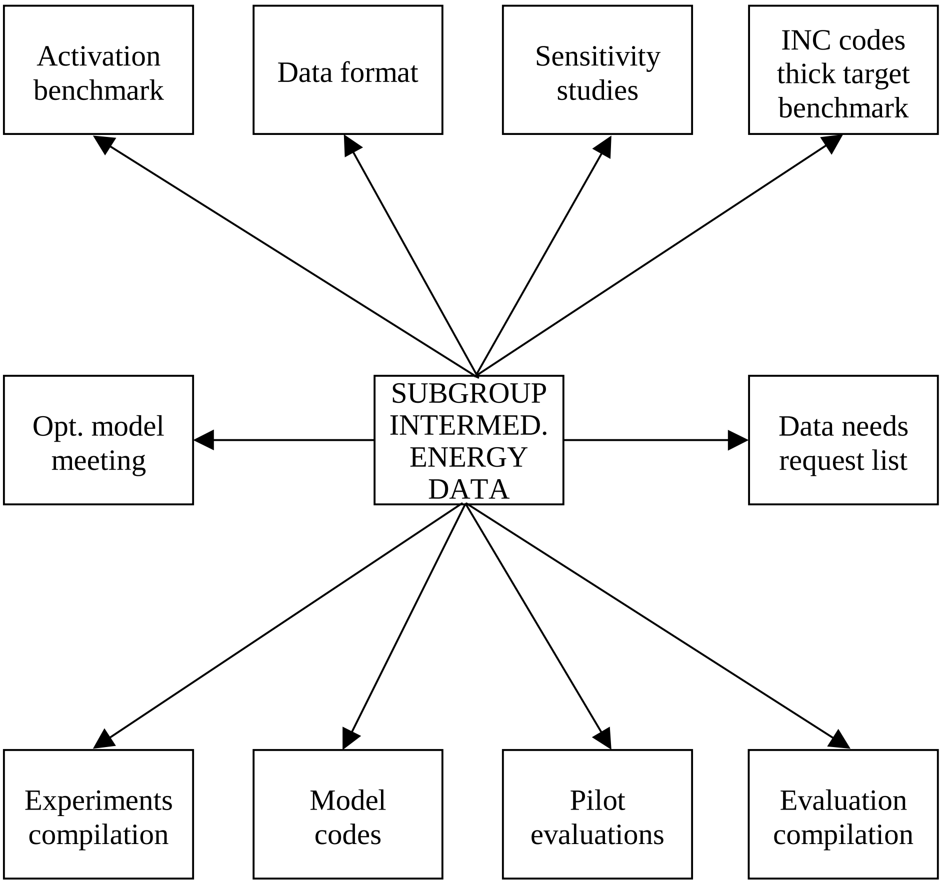
- Recommendation and organisation of specialists meetings on topics that are crucial for improving the quality of intermediate energy nuclear data.

- Discussion of ENDF-format aspects for evaluated nuclear files (i.e. Can we create nuclear data libraries in analogy with low-energy applications?) and organisation of pilot evaluations.

- Application of basic nuclear data in transport calculations.

A more schematic outline is presented in Figure 1 which at one point defined all the task forces of SG13. Some of the task forces have received more attention than others and we will use this scheme as a guideline to enumerate the accomplishments of SG13.

Figure 1. Task forces of SG13



3. Activities and their status

3.1 Data needs

An important task was to investigate the nuclear data requirements from the point of view of applications. As follow-up of the study made in Ref. [1], Kikuchi and Fukahori [2] have made a systematic inquiry on the type of incident particle, target nuclei and physical quantities. This study is not only aimed at nuclear energy applications, but also serves medical and astrophysical purposes. For accelerator-driven systems, the requested data comprise transport libraries, activation and damage cross-sections of accelerator components, double-differential light-particle cross-sections and spallation product yields for a whole spectrum of nuclides and recoils. To meet these requests, the subgroup has defined a high priority request list which may serve as a guideline for necessary measurements for accelerator-driven system research. This is a separate activity which is presented in the next subsection.

3.2 High-Priority Nuclear Data Request List for Intermediate Energies

The present High-Priority Request List (HPRL) for Intermediate Energy Nuclear Data (IEND) deviates considerably from the first, preliminary versions. The initiative for maintaining this HPRL was taken in 1994, as a guideline for necessary measurements for accelerator-based transmutation research.

As expected, the most difficult aspect of maintaining a HPRL turned out to be keeping it within bounds; several suggestions from both the applied and fundamental community were added to the list until at some point the list provided enough experimental work for the next millennium. Clearly, the adjective “high-priority” was no longer appropriate. On the other hand, several conferences in the field and personal communications between scientists have arguably led to more consensus on the required data. Accordingly, a new HPRL has been created by means of a threefold reduction:

- fewer nuclides;
- a smaller energy region (for evaluated data files only: $E < 200$ MeV);
- fewer types of cross-sections to be measured.

As usual, scientists are still invited to criticise this choice and to argue that other nuclides or reactions are more, or at least equally, important. Keep in mind however that this should remain a HIGH-PRIORITY list. If it gets too big by new additions, other nuclides/cross-sections should be left out to keep this project focused.

3.2.1 Nuclides

The proposal is to include 10 nuclides in this list, which cover both the periodic table and various applications. They are the most abundant (apart from ^{100}Mo) isotopes of:

- one material for medical purposes: O;
- three structural materials: Al, Fe and Ni;
- one fission product: Mo;
- one "nuclear model" material: Zr;
- two target materials: W and Pb;
- two actinides: Th and U.

Table 1 may be referred to for a more detailed list.

3.2.2 Energies

The highest energy in the HPRL is now 200 MeV. Not only does this coincide with the new upper limit of intermediate energy evaluated data files (Los Alamos has chosen 150 MeV), it is also near the maximum energy of some of the remaining experimental facilities (AGOR-KVI, Groningen, Holland; Svedberg Lab., Uppsala, Sweden; Louvain-la-Neuve, Belgium and NAC, Faure, South Africa are examples of such laboratories). The proposed energy grid for neutron and proton production cross-sections has been chosen so that it may overlap with existing measured cross-sections for other nuclides or incident particles.

3.2.3 Cross-sections

Another reason to keep the number of isotopes limited is that we may eventually obtain "complete" sets of experimental nuclear data. This is of critical importance to nuclear model calculations. If elastic and total (reaction)

Table 1. High-Priority Nuclear Data Request List for Intermediate Energies

Nuclide	Cross-section	Energy (MeV)	Purpose
^{16}O	(p,reac)	10,15,20,30,40,60,80,100,150,200	O,M,A
	(n,xn)	27,41,61,70	M,A,N
^{27}Al	$(p,p),(p,p')A_y,(p,\mathrm{reac})$	20,30,40,50,60,80,100,150,200	O,A,F
	$(n,n),(n,n')A_y,(n,\mathrm{reac})$	40,50,60,70,80,100	O,A,F
	(n,xn)	25,45,80	A,F,N
^{56}Fe	(p,reac)	10,15,20,30,40,60,80,100,150,200	O,A,F
	$(n,xn),(n,xp)$	25((n,xp)only),45,80	A,F,N
^{58}Ni	(p,xn)	80,160	A,F,N
	(p,xp)	25,45	A,F,N
	$(n,xn),(n,xp)$	25,45((n,xn) only),80	A,F,N
^{90}Zr	$(n,xn),(n,xp)$	25,45,80	N,A,F
	(p,xp)	25,45	N,A,F
^{100}Mo	$(p,p),(p,p')A_y,(p,\mathrm{reac})$	20,30,40,50,60,80,100,150,200	O,M,A
	$(n,n),(n,n')A_y,(n,\mathrm{reac})$	20,30,40,50,60,70,80,100	O,M,A
	$(n,xn),(n,xp)$	25,45,80	M,A,N
	(p,xn)	25,45,60,80,160	M,A,N
^{184}W	$(p,p),(p,p')A_y,(p,\mathrm{reac})$	20,30,40,50,60,80,100,150,200	O,A
	$(n,n),(n,n')A_y,(n,\mathrm{reac})$	15,20,30,40,50,60,70,80,100	O,A
	$(n,xn),(n,xp)$	25((n,xp) only),45,80	N,A
	(p,xn)	25,45,80,113,160	N,A
	(p,xp)	25,45,80,160	N,A
	$(p,f),(n,f)$	50,100,150,200	A,N
^{208}Pb	(p,reac)	40,60,80,100,150,200	O,A,M
	$(n,n),A_y$	60,70,80,100	O,A,M
	$(n,xn),(n,xp)$	25,45,80	A,M,N
	(p,xp)	25,45,160	A,M,N
	$(p,f),(n,f)$	50,100,150,200	A,M,N
^{232}Th	$(p,p),(p,p')A_y,(p,\mathrm{reac})$	20,30,40,50,60,80,100,150,200	O,A
	$(n,n),(n,n')A_y,(n,\mathrm{reac})$	6,8,10,15,20,30,40,50,60,70,80,100	O,A
	$(n,xn),(n,xp)$	25,45,80	A,N
	$(p,f),(n,f)$	50,100,150,200	A,N
^{238}U	$(p,p),(p,p')A_y,(p,\mathrm{reac})$	20,30,40,50,60,80,100,150,200	O,A,M
	$(n,n),(n,n'),A_y,(n,\mathrm{reac})$	6,8,10,15,20,30,40,50,60,70,80,100	O,A,M
	$(n,xn),(n,xp)$	25,45,80	A,N,M
	$(p,f),(n,f)$	50,100,150,200	A,N,M

A: Accelerator-Driven Systems, F: Fusion (E_n < 50 MeV), M: Medical,
N: Nuclear reaction models, O: Optical models, A_y: Analysing power

cross-sections for both neutrons and protons (to construct a 0-200 MeV optical model) as well as a complete set of (*p*,*xn*),(*p*,*xp*),(*n*,*xn*) and (*n*,*xp*) cross-sections are available, code developers can narrow down the uncertainties in their calculations, which has an immediate, positive impact on predictions for other nuclides where no experimental data exist. Of the whole periodic table, ^{90}Zr is the closest to this ideal situation. Therefore, the remaining measurements for this nuclide are included in the list.

There are two important quantities not on the list, which are however equally important. They are not yet included in the main table since the database of these cross-sections has not yet been investigated to designate the top-priority nuclei and energies.

- Residual production cross-sections. A lot of these requirements have been or will be met by the experimental group of Dr. Michel, Hannover. Since the total collection of measured data is so large, it is difficult to see on short notice where particular shortcomings exist for the ten selected nuclei.

- Deuteron up to alpha production cross-sections. Although these cross-sections are much smaller than the neutron and proton production cross-sections (for heavier targets at least), they are still important for e.g. damage, heating and gas production. Since the measurements are very scarce, both for incident neutrons and protons, the requirements for these quantities apply to almost every nuclide.

The last column of Table 1 gives the possible applications of the measured cross-sections, thereby attempting to give a priority order as well. Optical model and nuclear reaction model requirements have an indirect character: the quality of these data determines the quality of the whole evaluated data file.

3.2.4 Future

This is a request list for experiments and indirectly for evaluations. At present, there is a 100% overlap between experiment and evaluated data requirements. High-energy evaluations completely consist of results from nuclear model calculations that have been tuned to experimental data. An exception to this may be residual production cross-sections. These are so difficult to predict (see the NEA benchmark by Michel and Nagel – a factor of two on average is considered good!) that it may be more appropriate to directly include experimental data in activation data files. This however, needs further discussion. In sum, the HPRL for IEND is now much shorter than it was before, though still quite substantial. Therefore, results of sensitivity calculations are needed to narrow down the HPRL.

Finally, we mention that some experimental groups are already taking items of this list into account in their programme, e.g. IPN in Louvain-la-Neuve where (n,xp) cross-sections for various isotopes in the 25-65 MeV region are being measured. Accordingly, a revised request list is expected before long.

3.3 Compilation of experimental data

Computational documentation of experimental nuclear reaction data is extremely important. It will assist nuclear scientists in choosing new experiments and benchmarking model codes. At the NEA Data Bank, the collection of intermediate-energy experimental data has been significantly extended in the past years. At the moment, the total charged-particle EXFOR database contains about 20 Mb of relevant data. Updating EXFOR with charged-particle induced data is a relatively new activity and consequently there is still a considerable gap between the data measured in the past and the data actually stored in EXFOR [1]. As a probably redundant statement, *we strongly recommend continuation of updating the EXFOR database*[1]. Accelerator-driven system research requires a charged-particle database that is as comprehensive as the neutron database that has been maintained by the National Nuclear Data Centres over the years.

3.4 Nuclear models

It is obvious that the evaluation of high-energy data is mainly provided by nuclear model codes, which are benchmarked against crucial experiments. Initially, nuclear model codes with application above 20 MeV were part of SG13 too. This has however been transferred to SG12 (nuclear model validation). Nuclear models and codes do however come into play in the various benchmarks that were initiated by SG13. They are discussed in the next subsection.

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[1] The cost of a single update in EXFOR is negligible compared to the total cost of the associated experiment, while general availability and easy retrieval of the data is, next to the actual scientific publication, the most important manifestation of any experiment!

3.5 Specialist meetings and benchmarks

With the increasing interest in intermediate-energy applications, various low-energy directed model codes have been extended to higher energies to meet the data requirements. These codes, together with intranuclear cascade programs that were already suitable for high energies, have been compared with each other and with experimental neutron and proton reaction cross-sections and spectra in the NEA Code Comparison Meeting [3]. Rather large predicted differences were observed which, not surprisingly, have led to further research recommendations. To discuss and solve these problems, SG13 has initiated the following activities:

3.5.1 NEA Specialist Meeting on the Nucleon-Nucleus Optical Model up to 200 MeV

This [4] was held in November 1996, at CEA Bruyères-le-Chatel, France. Perhaps the most conspicuous problem that was revealed in the NEA Code Comparison Meeting was an unacceptable spreading (up to 50%) of the predicted proton reaction cross-sections. One of the conclusions of the Optical Model Meeting was that old, global optical models were no longer suitable to satisfy intermediate energy nuclear data needs. Improved parametrisations are required.

3.5.2 International codes and model comparison for intermediate energy activation yields

A benchmark of codes for residual production cross-sections [5] was organised by the NEA, co-ordinated by R. Michel (University of Hannover) and P. Nagel (NEA, Paris). These quantities turned out to be among the most difficult to predict in nuclear reaction physics. Codes that predict the data, on average, within a factor of two of the experimental data *are considered good*. The precise reason for this large discrepancy is not yet known, although it is clear that the effects of different optical models, level densities and mechanisms like high-energy fission and multiple pre-equilibrium emission have a drastic influence on the predictions. It seems that a sensitivity study on this topic would be very useful. Another SG13 report that addresses these problems is written by Mashnik *et al*. [6].

3.5.3 *Thick target benchmark*

A thick target benchmark [7] was organised at the NEA. Participants were asked to predict the neutron yields per proton and the mass distribution of spallation products for a cylindrical tungsten target bombarded by 800 MeV protons. Conclusions are given by Sobolevsky [8]. The general conclusion is that the neutron yield and leakage are well predicted but that product yields prediction gives problems (up to an order of magnitude difference).

3.6 Data formats and evaluated data libraries

3.6.1 *ENDF format for high energies*

Several format proposals for high-energy evaluated data files have been considered [9,10], all based on ENDF6 rules [11], and there is now reasonably good agreement on the format from the evaluators' point of view. For the construction of a high energy data file, procedures different from those used in the low energy files have to be employed, since it is no longer possible to store all reactions that describe different sequential particle emissions in separate MT-numbers. On the other hand, detailed low energy neutron data remain as important as in normal reactor calculations. Therefore, as a general rule, the detailed representation of cross-sections below 20 MeV should be left untouched as much as possible. For energies above 20 MeV, the detailed information concerning each individual excited state of the target nucleus and each particular sequential reaction chain are somewhat less important. Therefore, almost all reaction information should be lumped in MT5, which comprises all non-elastic processes that are not explicitly considered in other MT-numbers (such as fission). The particle and product yields and the outgoing energy-angle distributions can then be stored in MF6/MT5.

Besides consisting of reliable cross-sections, the quality criterion for a nuclear data file is a successful check by the standard ENDF-utility codes CHECKR, FIZCON and PSYCHE [12] and successful processing by the code NJOY [13] into both multi-group format for deterministic codes and a continuous-energy MCNP-library. In another recent SG13 document [14], a set of special rules and recommendations for an evaluated nuclear data file are given, such that the NJOY-processing conditions are obeyed. In general, the procedure follows the method that is used in Los Alamos to create 150 MeV libraries.

3.6.2 High-energy transport files: Status in May 1998

The collection of transport data files that exceed 20 MeV and have proven to be applicable in transport calculations is [15,16,17,18,19]:

- Los Alamos National Laboratory: Neutrons and protons 0-150 MeV
  - ^{1,2}H, ^{12}C, ^{14}N, ^{16}O, ^{27}Al, ^{28,29,30}Si, ^{31}P, ^{40}Ca, ^{50,52,53,54}Cr, ^{54,56,57,58}Fe, ^{58,60,61,62,64}Ni, ^{63,65}Cu, ^{93}Nb, ^{182,183,184,186}W, ^{204,206,207,208}Pb
- ECN Petten/CEA Bruyères-le-Chatel: Neutrons and protons 0-150 MeV
  - ^{54,56}Fe, ^{58,60}Ni
- ECN Petten/EC (IABAT project): Neutrons and protons 0-150 MeV
  - ^{204,206,207,208}Pb (under development)
- FZK Karlsruhe/INPE Obninsk: Neutrons: 0-50 MeV
  - ^{12}C, ^{16}O, ^{23}Na, ^{28}Si, ^{39}K, ^{51}V, ^{52}Cr, ^{56}Fe, ^{208}Pb, ^{232}Th, ^{233}Pa, ^{233,238}U, ^{239}Pu
- JAERI: JENDL high-energy file up to 50 MeV

3.6.3 MENDL and WIND activation/transmutation libraries

The Medium Energy Nuclear Data Library, MENDL [20], contains residual production cross-sections for neutrons with energies up to 100 MeV incident on stable and unstable nuclei. In total, 57,000 threshold reactions are included for elements ranging from Aluminium to Polonium. MENDL has been created by Shubin, Lunev, Konobeyev and Dityuk. The Waste Incineration Nuclear Data Library, WIND [21], contains fission and residual production cross-sections for neutrons up to 100 MeV for uranium, neptunium and plutonium isotopes. WIND is made by Konobeyev, Korovin, Preslavtsev, Plyaskin and Stankovsky. A drawback of the original form of these libraries was that they were not processable due to an alternative method to store the residual production cross-sections. It was a SG13 task to transform MENDL and WIND to the ENDF6-format [22]. The same methods are now used to extend well tested low-energy activation libraries, such as EAF-97, to higher energies.

4. Final status: Summary

We summarise some of the important accomplishments of SG13:

- The data needs as required by the applied community are categorised (see however, the next section on recommendations).
- The most significant deficits of our nuclear modelling capability have been diagnosed. Accordingly, relevant meetings and benchmarks have been suggested, organised and reviewed:
  - International code comparison for intermediate energy nuclear data: the thick target benchmark.
  - International codes and model comparison for intermediate energy activation yields.
  - NEA Specialists Meeting on the Nucleon-Nucleus Optical Model up to 200 MeV.
- A high-priority request list for experiments has been set up and maintained.
- The experimental database EXFOR has been extended with charged-particle induced data. SG13 has initiated both the recommendations for data to be included and the actual compilation of the data.
- The procedures for high-energy files in ENDF6-format have been defined in a unique way that guarantees NJOY-processibility.
- The MENDL and WIND activation/transmutation libraries have been documented, stored and transformed into ENDF6-format.
- A book-keeping of all available $E > 20$ MeV data files is maintained at the NEA.

5. Recommendations

As stated in the introduction, in the four years of existence of SG13 it became clear how many different aspects come into play when considering intermediate energy data. To do a serious job, one should treat nuclear reaction theories and models, experiments, data needs from the applications, data formats and application of data libraries in macroscopic transport analyses at about the same level of intensity. Now that the initial stages have been handled by SG13, we would like to recommend somewhat more specialised activities.

Some of the SG13 activities could be continued under different platforms, e.g. the high-priority request list should be part of the Working Party on International Nuclear Data Measurement Activities (WPMA). Nuclear models have already been transferred to Subgroup 12.

Subgroup 1: Intermediate energy data needs and experiments

The tasks of this subgroup would be:

- The study on data needs of Ref. [2] was the first serious set-up of its kind. In the past few years, research on accelerator-driven systems has really advanced. It is appropriate to set up an up-to-date data needs request list from the people that use the data that our community delivers. Ideally, priorities are given, which can then be reflected on the aforementioned high-priority request list.

- Further compilation of EXFOR-entries and input from users considering appropriate storage of data relevant for model calculations.

- To keep track of ongoing relevant experiments.

Subgroup 2: Intermediate energy data libraries

The tasks of this subgroup would be:

- Review, maintenance and testing of high-energy libraries. The first subject is the whole LA150 transport library from Los Alamos National Laboratory. Initial reviewing of that library is already underway.

- Application of high-energy data files in transport codes (MCNP)

Other alternatives for subdivision are of course open for discussion at the WPEC and NSC meeting.

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