International Atomic Energy Agency

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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

Summary Report of the
1st Research Coordination Meeting on

"Nuclear Model Parameter Testing for Nuclear Data Evaluation" (Reference Input Parameter Library: Phase II)

IAEA Headquarters
Vienna, Austria
25 - 27 November 1998

Prepared by
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February 1999

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Abstract

The report describes findings and conclusions of the 1st Research Coordination Meeting on Nuclear Model Parameter Testing for Nuclear Data Evaluation (Reference Input Parameter Library: Phase II). In particular, a critical review of the RIPL Starter File was performed, and a detailed scope and workplan of the RIPL-II project were prepared.

February 1999

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1. Summary of the Meeting

Objectives and Participation

The 1st Research Co-ordination Meeting (RCM) on "Nuclear Model Parameter Testing for Nuclear Data Evaluation (Reference Input Parameter Library: Phase II)" was held at the IAEA Headquarters in Vienna, Austria, from 25 to 27 November 1998.

The purpose of the meeting was to work out a detailed scope and working plan of the Coordinated Research Project (CRP), including tasks and responsibilities of participating laboratories, and agree on future coordination procedures. Phillip G. Young of the Los Alamos National Laboratory, U.S.A., was elected as the chairman of the CRP and served as the chairman of the meeting. The detailed Agenda is attached (see Appendix 1).

The meeting was attended by chief scientific investigators of six out of seven laboratories participating in the project, and by two cost-free observers. The participating laboratories were represented by T. Belgya (Budapest, Hungary), O. Bersillon (Bruyères-le-Châtel, France), R. Capote Noy (Habana, Cuba), T. Fukahori (Ibaraki-ken, Japan), A.V. Ignatyuk (Obninsk, Russia), P.G. Young (Los Alamos, U.S.A.). Furthermore, S. Goriely (Brussels, Belgium) and V. Maslov (Minsk, Belarus) attended as observers. For the full list including affiliations see Appendix 2.

Main Conclusions and Recommendations

It was concluded that the Phase I of the development of the Reference Input Parameter Library, conducted during 1994-1997, produced valuable results. In particular, timely completion and release of the RIPL Starter File (Web and CD-ROM) in May 1998, followed by publishing the RIPL Handbook (TECDOC-1034) in August 1998 were appreciated.

The meeting recommended to proceed with the Phase II of the RIPL project as originally planned. To this end, a detailed scope and workplan of the CRP were prepared. The CRP should be completed by the end of 2001, with the official release of the library in spring 2002.

The 2nd RCM is scheduled for spring 2000. T. Fukahori indicated that JAERI might be willing to host the meeting.

2. Objectives of the CRP

Objectives of the CRP as defined by the IAEA were explained by the Scientific Secretary of the project. In particular, the purpose of this new CRP is:

- to produce an internationally recognized library of input parameters for nuclear model calculations of nuclear reaction data for applications,
- to test thoroughly all segments of the Starter File of the Reference Input Parameter Library, focusing on optical model parameters and nuclear level density parameters,

- to improve critical segments (discrete level schemes, optical model parameters, level densities),
- to extend several segments,
- to develop standard interface software for selected nuclear reaction codes, and
- to develop library management and retrieval tools.

  Full explanation can be found in the Information Sheet on the CRP (see Appendix 3).

3. Presentations

Several technical papers on topics related to the Reference Input Parameter Library were presented orally or distributed in written form. Of specific interest was the presentation by S. Goriely on needs and use of RIPL for astrophysics applications. It appears that the astrophysics community may represent an important user group of RIPL.

More details on some of the papers can be found in Appendix 4.

4. Critical Review of the RIPL Starter File

In general, the Starter File of the Reference Input Parameter Library was found to be a valuable product. Individual segments were critically reviewed with the findings explained below.

4.1 Segment 1: Atomic masses and deformations

No fundamental criticism of this segment was formulated. However a specific shortcoming was mentioned in relation to segment 5 on nuclear level density. It concerns the definition of the shell correction energy. Namely, the “shell correction energy”, that differs from the “microscopic energy” defined in the FRDM model, should be estimated and tabulated in order to provide nuclear level density users with a consistent set of data and to avoid misinterpretation of the data recommended by RIPL.

Experimental ground-state masses given in the moller.dat file do not correspond to the latest recommended experimental compilation of Audi and Wapstra (1995). An update of the file would be preferable.

At present, only one mass model (including masses, deformations and microscopic energies) is included in RIPL. Other models could be added in other_files, and in particular extra nuclear structure properties required by other segments (optical potential, nuclear level density) could be provided in segment 1. It concerns mainly mass density distribution parameters or pairing properties. Isotopic abundances of relevance in given calculations could also be added. Furthermore, fission barriers based on theoretical calculations could be added.

4.2 Segment 2: Discrete level schemes

It was noted that for the RIPL Starter File an entirely new discrete levels library has been created by the Budapest group according to the recommended principles, using the Evaluated

Nuclear Structure Data File, ENSDF as a source. The following deficiencies were identified:

- Formats of numbers in fields are not in FORTRAN format.
- Number of levels in the final state is limited to 100. This is a problem of the present Bologna format.
- Gamma branching ratios are omitted for some nuclei.
- Number of significant digits for branching ratios should be increased.
- Spins are not always given if they are ambiguous.
- Number of branching ratios is limited to 18.
- Temperature of some nuclei in budapest_cumulative.dat falls below the acceptable values.

4.3 Segment 3: Average neutron resonance parameters

For several nuclei new experimental data on the average resonance parameters were published. These data should be analyzed and included in the recommended file. It is reasonable to extend the file to include the available data for the p-wave neutron resonances.

It was noted that an extensive work on neutron resonances has been published in October 1998 by Springer Verlag under the Landolt-Börnstein series, Group I, Volume 16, Low Energy Neutron Physics,

"Tables of Neutron Resonance Parameters"

by S.I. Sukhoruchkin et al. from Gatchina, Russia. It should be the most complete, fully up-to-date work. It consists of 500 pages of text including tables plus a CD-ROM, for a price of DM 4,800.

4.4 Segment 4: Optical model parameters

The RIPL Starter File is comprised of formatted optical model parameters for approximately 300 cases. Major areas for improvement, that were discussed, include the following:

- The existing file includes many single-energy parameterizations that are not directly useful for model calculations which require data at many energies.
- The collection of global and local phenomenological potentials should be expanded at Bruyères-le-Châtel and Petten.
- More extensive testing of the parameterizations in the library is needed.
- Inclusion of a more general microscopic model approach should be considered for unmeasured target nuclei.
- A user subroutine should be developed that provides automatic selection of recommended parameters for a wide variety of target nuclei.

4.5 Segment 5: Level densities

New results of Thielemann *et al.* have appeared on the systematics of nuclear level densities in the framework of the back-shifted Fermi gas model. A more clear description of the recommended global parameters for the Gilbert-Cameron approach and GSM is needed.

The codes for microscopical calculations with the Moeller-Nix schemes were tested by the Habana group. An extensive table of the microscopic calculations of the level densities for astrophysical applications was prepared by the Brussels group. More detailed description of the codes and input parameters is required. Furthermore, the extensive file moller_levels.dat should be split into subfiles according to Z.

The test of the Avrigeanu code for the partial level densities is in progress. It would be useful to produce a recommended approach from the many approaches presently included in the avrigeanu.for file.

It was noted that a useful paper describing the Avrigeanu code has been published recently, see M. Avrigeanu and V. Avrigeanu: Partial level densities for nuclear data calculations, Comp. Phys. Communic. 112 (1998) 191-226.

The fission barrier parameters for 45 actinide nuclides presently included in the RIPL Starter File represents a limited set for many practical requests. The recommended parameters should be extended by inclusion of heavier transplutonium nuclei, i.e. Bk and Cf as well as pre-actinide nuclei. For the latter nuclei charged-particle fission probability data should be analyzed within the accepted approach for the level density.

4.6 Segment 6: Gamma-ray strength functions

The following deficiencies were observed:

- The file kopecky.dat containing experimental strength functions is in a text format which is not suitable for reading by a FORTRAN code.
- Fig. 6.1 in the TECDOC contains enhancement factors k_0 to be applied to the calculated strength functions in order to bring them into agreement with the experimental results. These factors are not consistent with the level densities recommended in RIPL.
- Shell effects are not included in E1 GDR widths.

4.7 Segment 7: Continuum angular distributions

No deficiencies were identified.

5. Scope and Workplan of the CRP

The scope and workplan of the CRP were discussed in detail. The conclusions are explained below.

5.1 Detailed scope

The RIPL-II project will include the following major activities: testing, improvements and extensions, development of interfaces to selected nuclear reaction codes, and development of retrieval tools/Web.

Testing

Testing of the parameter files for RIPL-II will generally be divided into three parts that include:

1) testing of the files for accuracy, completeness, etc., with the aim of removing all typographical errors or errors in transmission of data to the files;

2) testing of retrieval capabilities of interfacing computer codes; and

3) physics tests based on comparison of model code or other calculations using the RIPL data base with experimental data, systematics, or other criteria such as smoothness of results.

The initial testing under the CRP will emphasize items 1) and 2) above. Physics tests under item 3) will be performed as soon as the various segments are completed.

Improvements and extensions

Segment 1:

- A precise definition of shell correction energy required in the nuclear density segment will be given with the accompanying data.

- An updated moller.dat file will be provided including the recommended Audi-Wapstra (1995) experimental data.

- The ETFSI model calculations related to atomic masses, shell corrections, density distribution parameters and pairing properties will be added to other_files of the segment, including a complete readme file.

- "Experimental" deformations derived from B(E2) transition probabilities will be added to the other_files according to the published compilation of Raman *et al* (1987).

- Isotopic abundances will be provided in a separate file and added to the segment.

- Calculated fission barrriers will be included into other_files.

Segment 2:

- Upgrading, improvement and reformatting of the segment will be done:
  a. Revision will include updating of the data based on ENSDF2.
  b. Improvement will include changing the format of the file in such a way that information loss would be minimised and that problems listed in 4.2 are removed. The extension and the change of the format will proceed in an iterative discussion with other RIPL participants. To this end, a sample of the new budapest_levels.dat will be provided by 1st of May 1999.

- Reanalysis of cumulative plots will be done in order to derive new values of the N_{max} and E_c and T parameters compatible with the constant temperature model for the low energy nuclear level densities. The fit to the cumulative number of levels will be limited with some constraints obtained from previous works and done in cooperation with segment 4.5. A reusable code will be provided that works on the budapest_levels.dat. A separate file of the fit results will be maintained.

- For testing, a FORTRAN program will be provided that reads the whole file, and also makes some self-tests. This will also provide a sample for reading the file.

Segment 3:

- The general checking of the Starter File data will be done.
- The p-wave resonance parameters will be included.

Segment 4:

- New Optical Model parameterizations with smooth energy dependence and covering broad energy ranges should be added in some individual cases where sufficient data exist and thorough analyses have been performed.

- This segment should be extended by adding new global phenomenological Optical Model parameterizations for nucleon-nucleus interaction, at least for spherical nuclei.

- As the phenomenological approach is of limited applicability for nuclei far from stability, one also has to consider a microscopic approach to construct the optical potentials, e.g. the approach of Jenkenne, Lejeune, and Mahaux as modified and extended by E. Bauge *et al.*

Segment 5:

- The general checking of the Starter File data will be done.

- The recommended global and local systematics of the GSM parameters will be described.

- The table of the ULB calculations for the total level densities will be added to the RIPL-II working file as other_files.

- The recommended fission parameters will be extended to heavier transplutonium and lighter pre-actinide nuclei.

Segment 6:

- Additional systematics will be supplied for M1 and E2 transitions by Fukahori.

- Shell-dependent formula for the GDR width (Thielemann and Arnould 1983) should be included.

- Consistency between GDR parameters of the RIPL Starter File and the Varlamov experimental compilation (see file varlamov.dat) should be checked.

- Hybrid formula for the E1 strength function by Goriely 1998, which improved agreement with the experimental data at energies below neutron binding, should be included.

- An attempt should be undertaken to fit the most recent compilation of GDR parameters by Varlamov to obtain improved global systematics using shell dependent GDR width and recommended shell corrections.

- kopecky.dat file should be reformatted into the computer readable format.

Segment 7:

Improvements should be introduced in the light of recent developments as necessary (e.g. Alice HMS code of Chadwick and Blann).

Interfaces to nuclear reaction codes

Interfaces to the following codes will be developed:

ECIS (Koning)
SCAT2 (Capote)
GNASH (Young, Ignatyuk)
ALICE95 (Fukahori), ALICE-F (Fukahori), ALICE-IPPE (Ignatyuk)
SINCROS (Fukahori)
EMPIRE (Herman)
STAPRE (Capote)

It is understood that the latest versions of the codes available from the NEA Data Bank, Paris, should be used. If new versions of the codes will be developed and interfaced under the RIPL-II project, the authors will submit them into the NEA Data Bank for distribution before the end of the project.

Retrieval tools, Web

HTML documents and associated programs (cgi-bin) for the Web site operated by the IAEA Nuclear Data Section will be prepared by Fukahori in cooperation with NDS. Prepared will be retrieval tools at least for supplying actual values stored in the RIPL Final File for all segments, except the optical potential segment and those segments in which only computer codes are given. Additional functions will be included, to the extent possible. For instance, capability to retrieve/calculate Q-values and threshold energies of certain reactions and particle binding energies for individual isotopes will be included in the mass segment.

Retrieval tools for UNIX platforms will be prepared in a way similar to the Web. For this purpose, NDS should prepare basic tools such as FORTRAN, C and Perl.

Extensive data files of some segments will be split according to Z or A. In particular, this applies to moller_levels.gz and to budapest_levels.dat.

For FTP, suitable compressing and archiving software will be selected, for example, GZIP which can be freely distributed to all users.

5.2 Expected products

The outputs from the CRP will include the following five items:

1) Tested and validated Reference Input Parameter Library for nuclear model calculations of nuclear reaction data for applications.

2) User oriented interfaces for selected nuclear reaction codes (ECIS, SCAT2, GNASH, SINCROS, ALICE, STAPRE and EMPIRE).

3) Retrieval tools in the Web electronic format and also in the standalone CD-ROM format.

4) Handbook of the Reference Input Parameter Library which will also serve as the CRP final report and will be published as a TECDOC.

5) The Library, interfaces, retrieval tools and Handbook will be produced both in the Web and CD-ROM electronic formats. The Web version will be available via the Internet on the IAEA Nuclear Data Services Web server. The CD-ROM version will be produced primarily for PC users and for the users with limited access to the Internet. The CD-ROM will also serve an important function of a referenceable source for the RIPL data.

5.3 RIPL Final File

In terms of overall structure, the RIPL Final File will not differ substantially from the present RIPL Starter File. In terms of format, the Final File will have a well defined format rather than a free format adopted for the Starter File. More details are given below.

Structure

Segment 1:

The title "Atomic masses and deformations" will be kept for the segment though extra data will be added. As a matter of fact, most of the added data are derived from mass models. The present structure of the segment will be kept. Only corrections and new files will be added.

Segment 2:

The present structure of the segment will be kept.

Segment 3:

The present structure of the segment will be kept.

Segment 4:

The Final File of optical model parameters will distinguish individual and global parameterisation. In particular, the Final File should be comprised of the following:

a) Individual Optical Model parameterization coming from
   - a selection among the potentials given in the RIPL Starter File compilation, and
   - recent analysis covering broad energy ranges.

b) Global Optical Model parameterization
   - deduced from experimental data, and
   - based on a microscopic approach (after solving possible formal problems in their release).

Segment 5:

The present structure of the segment will be kept.

Segment 6:

The present structure of the segment will be kept.

Segment 7:

The present structure of the segment will be kept.

Format

Two general rules were accepted:

- The format of each segment must be fixed as soon as possible. This new format should never be changed in order to avoid the need to rewrite retrieval tools and HTML (cgi-bin) documents.

- The format of each segment must be homogenized. This means that all files, in particular those included into other_files, must be given in the same format as the recommended file.

Segment 1:

Homogenous format is required.

Segment 2:

The segment must be completely reformatted. Belgya will prepare a new format and distribute it to CRP participants for comments.

Segment 3:

All files in other_files will be transformed to the format accepted for the recommended file.

Segment 4:

The present format approved for the RIPL Starter File will be continued, but the possible alternate format will be developed by Fukahori for consideration.

Segment 5:

All files in other_files will be transformed to the format accepted for the recommended one. Single-particle level file by Goriely will be provided in the same format as adopted in the RIPL Starter File.

Segment 6:

An appropriate format to represent experimental strength functions should be developed.

Segment 7:

No change.

5.4 Detailed working plan

A detailed working plan for the RIPL-II activities, including coordination procedures were discussed and agreed upon.

Distribution of responsibilities

Following the practice established in development of the RIPL Starter File, a coordinator was identified for each segment of the RIPL Final File. The role of a segment coordinator is to oversee and coordinate the relevant work done by the CRP participants and other contributors, with an overall responsibility for the whole segment.

Segment 1 - Goriely
Segment 2 - Belgya
Segment 3 - Ignatyuk
Segment 4 - Bersillon
Segment 5 - Ignatyuk (total)
Capote (partial)
Ignatyuk with assistance of Maslov (fission)
Segment 6 - Obložinský with assistance of Plujko
Segment 7 - Obložinský

Individual tasks

The CRP at the moment includes seven regular participants with Research Agreements and Research Contracts. In addition, one Technical Contract was awarded to perform less critical tasks in support of the CRP. As in the past, contributions are expected also from scientists formally not associated with the RIPL-II project. Individual tasks, termed as program (Agreements) or workplan (Contracts), are listed below.

1) P. Young (Los Alamos), Research Agreement (RA) 10309

Scope: Implementation and testing of RIPL input parameters in the GNASH reaction code.

Program:
1. Develop link between RIPL and GNASH for 3 input parameter segments: atomic masses, discrete levels and level densities.
2. Perform calculations of selected reactions induced by neutrons, gamma and protons and test related input parameters.
3. Assist in improvements of the optical model parameter segment.

2) O. Bersillon (Bruyères-le-Châtel), RA 10304

Scope: Testing and improvement of optical model potentials for RIPL.

Program:
1. Assess the quality of the RIPL optical model segment.
2. Provide new parameterization of phenomenological optical model that is smoothly varying in broad energy ranges.
3. Extend optical model parameterization by applying microscopic optical model approach to nuclei where experimental data are lacking.
4. Contribute to nuclear level densities by improved parameterization of its energy dependence using microscopical approach.

3) T. Fukahori (JAERI), RA 10305

Scope: Development of retrieval tools and nuclear model parameter testing.

Program:
1. Coordinate development of standardized format for the Reference Input Parameter Library and conversion of all files into this standardized format.
2. Develop user-oriented retrieval tools for Web and for Unix. Specifications will be prepared for this purpose for each segment.
3. Develop interface to reaction codes SINCROS-II and ALICE-F and ALICE95.
4. Perform reaction cross section calculations and testing of input parameters.

4) A. Koning (Petten), RA 10306

Scope: Nuclear model parameter testing and retrieval tools.

Program:
1. Extend the optical potential segment of the RIPL by adding new phenomenological optical model parameterizations.
2. Design an interface between the optical potential segment and the coupled-channel code ECIS.
3. Perform testing of optical model parameterizations.

5) A.V. Ignatyuk (Obninsk), RA 10307

Scope: Validation of nuclear level density parameters in calculations with ALICE and GNASH.

Work plan for the 1st year:
1. Develop interface between RIPL and reaction codes ALICE and GNASH.
2. Perform calculations of particle emission spectra and threshold.
3. Analyse performance of the RIPL nuclear level density and resonance parameter segments.
4. Transform the resonance parameter and nuclear level density segments into one format.
5. Add parameters of p-wave resonances into the recommended file.
6. Perform the general test of the level density segment and prepare more clear description of the recommended global parameters.

6) T. Belgya (Budapest), Research Contract (RC) 10367

Detailed research objective:
- Testing, updating and improvement of the RIPL Starter File, segment Discrete Level Schemes. This includes both the file with discrete levels (energies, spins, parities, branchings, completeness) and with the cumulative plots.
- Testing, extension and improvement of the RIPL Starter File from the point of view of nuclear structure expertise, particularly related to level densities (reanalysis of cumulative plots, shell corrections and ground state deformations).

Scope: Testing and improvement of the RIPL segment Discrete Level Scheme and related parameterization of nuclear level densities.

Work plan for the 1st year:
1. Perform basic testing of the RIPL segment Discrete Level Schemes.
2. Prepare upgrading, improvement and reformatting of the segment.
3. Reanalyze cumulative plots from the point of view of constant temperature level densities.
4. Prepare preliminary file with shell corrections for level densities.

7) R. Capote (Habana), RC 10366

Detailed research objective:
- Testing of the RIPL Starter File, particularly parameterization of total nuclear level densities and optical model potentials.
- Developing of interfaces between RIPL and the optical model code SCAT2, and between RIPL and the nuclear reaction code STAPRE.
- Testing of tools and parameterization for microscopic nuclear level densities.

Scope: Testing of the RIPL Starter File, particularly level densities and optical model potentials.

Work plan for 1st year:
1. Develop interface RIPL/SCAT2.
2. Perform initial testing of RIPL optical model potentials.

3. Develop interface RIPL/STAPRE, and prepare testing of total level densities.
4. Perform initial testing of microscopic total nuclear level densities.
5. Perform initial testing of p-h microscopic nuclear level densities, including comparison with avrigeanu.for.

8) V. Plujko (Kiev), Technical Contract (TC) 10308

Scope: Testing and improvements of gamma-ray strength functions for nuclear model calculations of nuclear data.

Work plan for the 1st year:
1. Perform critical analysis of gamma-ray strength functions of the RIPL Starter File.
2. Recommend immediate modifications and improvements of the segment, including new format and consistency with Varlamov GDR parameters.
3. Develop formalism to calculate E1 strength functions within the framework of the dissipative Fermi-dynamical approach with shell effects.
4. Develop computer code to calculate E1 strength functions for cold and heated nuclei in the middle and heavy mass region.

RIPL-II site

The RIPL-II file will be created at the DEC Alpha computer of the IAEA Nuclear Data Section. This working site will contain the RIPL Starter File plus all new/modified files submitted for inclusion into the RIPL-II project.

The access will be restricted to participants of the RIPL-II project. Details will be announced by the Scientific Secretary.

<u>**Appendix 1**</u>

International Atomic Energy Agency
First Research Co-ordination Meeting on
Nuclear Model Parameter Testing for Nuclear Data Evaluation
(Reference Input Parameter Library: Phase II)

IAEA Headquarters, Vienna, Austria
25 - 27 November 1998
Meeting Room A-12-46

AGENDA

Wednesday, 25 November

09:00 - 09:20 Registration (Registration desk, C-tower, ground floor)

09:30 - 10:00 Opening Session

- Opening (D.W. Muir, Head, IAEA Nuclear Data Section)
- Election of chairman (Obložinský)
- Adoption of Agenda (Chairman)
- Goals of the CRP (Obložinský)

10:00 - 12:00 Presentations

- Nuclear data for nuclear astrophysics (Goriely, 15')
- Other papers and reports (Meeting participants, 15' maximum each)

14:00 - 18:00 Critical Review of the RIPL Starter File

- Discrete level schemes (Belgya)
- Optical model parameters (Young, Bersillon)
- Level densities (Ignatyuk)
- Other segments

Thursday, 26 November

09:00 - 12:00 Proposed RIPL-II Activities

- Improvements and extensions
- Testing
- Interfaces to nuclear reaction codes
- Retrieval tools, Web

14:00 - 18:00 Scope and Workplan of the CRP

- Detailed scope
  * Goals and priorities
  * Expected products
- RIPL Final File
  * Structure and contents
  * Format
- Detailed working plan
  * Distribution of responsibilities
  * Individual tasks
  * CRP participation

9:00 - 21:00 Meeting Dinner

Friday, 27 November

09:00 - 12:00 Drafting the Meeting Report

- Scope of the CRP
- RIPL Final File
- Workplan of the CRP

14:00 - 17:00 Concluding Session

- Adoption the Meeting Report
- Final discussion, adjournment

Notes

1. Participants may bring extended abstracts (two pages) of their papers, reports and other contributions for inclusion into the Meeting Report.

2. Coffee breaks will be introduced at both morning and afternoon sessions as appropriate. Lunches will be served at the IAEA Cafeteria between 12:00 - 14:00.

Appendix 2

International Atomic Energy Agency

First Research Co-ordination Meeting on
Nuclear Model Parameter Testing for Nuclear Data Evaluation
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IAEA Headquarters, Vienna, Austria
25 - 27 November 1998

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*) Unable to attend

Appendix 3

INTERNATIONAL ATOMIC ENERGY AGENCY

Information Sheet on a Coordinated Research Project (CRP)

1. *Title of CRP*: Nuclear Model Parameter Testing for Nuclear Data Evaluation (Reference Input Parameter Library: Phase II)

2. ***Background Situation Analysis (Rationale/Problem Definition)***

A long standing problem - how to meet future nuclear data needs with limited experimental resources - puts considerable emphasis on nuclear model computation capabilities. Originally, almost all nuclear data was provided by measurement programs. Over time, theoretical understanding of nuclear reaction phenomena has reached a considerable degree of maturity, and nuclear modeling has become an integral part of the production of evaluated nuclear data. Due to widespread use of nuclear models in generating evaluated data, there is a substantial demand for well established input parameters needed to perform such calculations.

When considering low-energy nuclear reactions induced with light particles, such as neutrons, protons, deuterons, alphas and photons, one addresses a broad range of applications, from nuclear power reactors and shielding design, through cyclotron production of medical radioisotopes and radiotherapy, to transmutation of nuclear waste. In these and many other applications one needs a detailed knowledge of cross sections, spectra of emitted particles and their angular distributions, and of isotope production. For low incident energies, in particular, nuclear theorists have established nuclear reaction models that cover almost all aspects of nuclear physics involved and, thus, also all data of practical interest. These nuclear reaction models are optical (including direct interactions), statistical compound nuclear decay (including fission), and preequilibrium/multistep.

The practical use of nuclear model codes requires a considerable quantity of numerical input that describes various properties of the nuclei involved such as nuclear masses, discrete levels, neutron resonances, optical model parameters, nuclear level densities including fission barriers, and gamma-ray strength functions. Leading nuclear data laboratories, groups and experts have used a variety of different input sets, often developed over years in their own laboratories. Many of these input databases were poorly documented (or not documented at all) and not always made available to other users. With the overall aging of the Nuclear Data evaluation community, there is a real threat that the accumulated immense knowledge of input parameters and the related state-of-the-art may be lost for future applications.

Given this situation, a project was proposed, with the aim to develop an internationally recognized input parameter library, with contributions from all major evaluation groups around the world. The idea was discussed in the nuclear data community in the beginning of 1990s and it was enthusiastically supported by the International Nuclear Data Committee as a top priority nuclear data project for the IAEA.

An ultimate objective of any international effort along these lines is to develop a library of evaluated input model parameters. Considering that such a task indeed is immense, it was decided to proceed in two major steps. First, to summarize the present knowledge on input parameters, whenever possible critically analyzing these parameters, and to develop a single Starter File of input model parameters. This data base will be of immediate practical value for a number of users and should represent a firm basis for future improvements and developments. The second step should focus on the testing and validation of the Starter File, its improvement and extension, and on development of standard interface software for selected nuclear reaction codes and library management tools.

With this objective in mind the IAEA initiated, in 1994, the Coordinated Research Project under the title *"Development of Reference Input Parameter Library for Nuclear Model Calculations of Nuclear Data (Phase I: Starter File)"*. The project was conducted in 1994-1997 and it actually produced the Starter File. The Starter File contains numerical data organized into seven segments:

1. Atomic Masses and Deformations
2. Discrete Level Schemes
3. Average Neutron Resonance Parameters
4. Optical Model Parameters
5. Level Densities (Total, Fission, Partial)
6. Gamma-Ray Strength Functions
7. Continuum Angular Distributions.

The Starter File has been released both in the Web format (see http://www-nds.iaea.or.at/ripl/) and on CD-ROM (see IAEA-NDS-CD-02) with the release date 15 May 1998. The Starter File is targeted at users of nuclear reaction codes interested in low energy nuclear applications, such as fission and fusion energy, radioisotope production, neutron/proton cancer therapy shielding and transmutation of nuclear waste. Incident and outgoing particles can be n, p, d, t, ^{3}He, ^{4}He and γ, with the energies up to 100 MeV. A TECDOC was published with a full description of the Starter File (see IAEA-TECDOC-1034, August 1998).

These favourable results of Phase I make it possible to proceed along the original plan and complete the development of the Reference Input Parameter Library by performing Phase II of the project. Phase II constitutes a new CRP with two important basic tasks:

- testing of Starter File to guarantee requested quality of data, and
- development of utility tools to facilitate the use of the Starter File in practical applications.

3. *Overall Objective*

The overall objective of the new CRP is to produce a well tested and validated Reference Input Parameter Library for nuclear model calculations of nuclear reaction data with user-oriented interfaces to nuclear reaction codes.

4. *Specific Research Objective (Purpose)*

The purpose of the new CRP is to produce an internationally recognized library of input parameters for nuclear model calculations of nuclear reaction data for applications, to test thoroughly all segments of the Starter File of the Reference Input Parameter Library, focusing on optical model parameters and nuclear level density parameters, to improve critical segments (discrete levels by reanalyzing cumulative plots, optical model parameters by including phenomenological parameterization in broad energy ranges, level densities by including shell corrections for total level densities), to extend several segments (include deformation of collective states and extend the compilation of giant dipole resonances), to develop standard interface software for selected nuclear reaction codes, and to develop library management and retrieval tools.

5. *Expected Research Outputs (Results)*

The outputs from the CRP will be:

a) A tested and validated Reference Input Parameter Library for nuclear model calculations of nuclear reaction data for applications.

b) User oriented interfaces for selected nuclear reaction codes (ECIS, SCAT2, GNASH, SINCROS, ALICE, STAPRE and EMPIRE).

c) Retrieval tools in the Web electronic format and also in the stand alone CD-ROM format for different computer platforms (VMS, Windows, Unix).

d) A handbook of the Reference Input Parameter Library which will also serve as the CRP final report and will be published as a TECDOC.

e) The Library, interfaces, retrieval tools and Handbook will be produced both in the Web and CD-ROM electronic formats. The Web version will be available via the Internet on the IAEA Nuclear Data Services Web server. The CD-ROM version will be produced primarily for PC users and for the users with limited access to the Internet.

6. *Participants*

In order to participate in the CRP each participant must enter into a Research Agreement or a Research Contract with the IAEA. Participants from developed countries (as defined by the IAEA) enter into Research Agreements. The only financial support received from the IAEA under a Research Agreement is transportation and per diem of the chief scientific investigator or his representative to attend periodic CRP meetings. Participants from developing countries (as defined by the IAEA) can enter into Research Contracts. Under a Research Contract, in addition to financial support to attend CRP meetings, the participant receives limited financial support for research (typically US$ 5,000 per contract year). Research Contracts are reviewed (based on annual reports) and, subject to approval by the Director General, renewed each year for the duration of the CRP.

7. *Duration*

The CRP will run for three years (1998 - 2001).

8. *Additional Information*

Additional information can be obtained from:

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Appendix 4

Extended abstracts of technical papers

Page

Nuclear inputs for astrophysics applications

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1 Introduction

Nuclear reaction rates are obviously quantities of fundamental importance in nuclear astrophysics (for a review see for example [1]). The thermonuclear reactions of astrophysical interest mainly concern the capture of nucleons or α-particles[1]. Although important effort has been devoted in the last decades to measure reaction cross sections, most of the nuclear astrophysics applications still require the use of theoretical predictions to estimate experimentally unknown rates. Most of the nuclear ingredients in reactions rate calculations need to be extrapolated in an energy and mass domain out of reach of laboratory simulations. In addition, astrophysical applications (e.g the r- or p-process of nucleosynthesis) often involve a large number (thousands) of unstable nuclei, so that only global approaches can be used. For these reasons, among the different approaches available to predict the nuclear inputs, the most physically sound global approaches are preferred, while phenomenological highly-parametrized models fitted on scarce experimental data are usually avoided. Quite often, such demanding requirements forced nuclear astrophysicists to develop their own tools and built their own Reference Input Parameter Library (RIPL). However, it should be stressed that numerous astrophysical applications also deal with experimentally known nuclei. In that case, though the energy domain might differ from the one of interest in other traditional nuclear applications, astrophysicists make use of the same recommended (local or global) ingredients as in other fields of nuclear physics. The major theories used in nuclear reaction calculations for astrophysical application are rapidly reviewed in the coming section.

2 The nuclear astrophysics RIPL

Regular updates as well as improvements are brought to the Hauser-Feshbach codes dedicated to astrophysical applications. Such codes (for example MOST for Modèle

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[1]Spallation reactions induced by the interaction of primary particles with relative energies in excess of some tens of MeV per nucleon are not considered in the present paper

Statistique [2]) include all experimental data available on nuclear masses, deformations, spectra of low lying states, giant dipole energies and widths. Information on neutron resonance spacings at the neutron separation energies is also introduced to normalize the nuclear level densities (NLD). When the nuclear ingredients to the Hauser-Feshbach model cannot be determined from experimental data, use is made preferentially of microscopic or semi-microscopic global predictions based on sound and reliable nuclear models which, in turn, can compete with more phenomenological highly-parametrized models in the reproduction of experimental data. The major global theoretical inputs used in present nuclear reaction calculations for astrophysics applications are described below.

2.1 Atomic masses and deformations

Atomic masses enter all chapters of nuclear astrophysics. Their knowledge in indispensable to estimate the rate and energetics of any transformation. The so-called macroscopic–microscopic models are known to be able to reproduce the measured masses with a root mean square deviation of about 700 keV at the expense of a relatively large number of free parameters which makes the extrapolation far away from experimental regions sometime hazardous. The most popular version is the FRDM model [3]. More reliable and sophisticated microscopic models in the HFB or RMF approaches are available, but give rise to rms deviations of about 2 MeV which remains too high for most of the astrophysical applications. A compromise between the accuracy of the phenomenological microscopic–macroscopic models and the reliability of the microscopic theories is found in the newly-developed Extended Thomas-Fermi plus Strutinsky Integral (ETFSI) method. The ETFSI model is a high-speed approximation to the Hartree-Fock method with pairing correlations treated in the usual BCS approach [4]. Based on a Skyrme-type interaction and a δ-function pairing force the parameters of which are fitted on known nuclear masses, the ETFSI model predicts nuclear masses with an rms deviation of about 700 keV as the phenomenological models. Moreover, the ETFSI method is expected to be more reliable in its extrapolation far away from the experimentally known region thanks to its high degree of coherence between the macroscopic and microscopic parts of the binding energy. Another advantage of the ETFSI method concerns the Strutinsky Integral method used to derive the shell correction part and which avoids the ambiguities of the traditional Strutinsky-averaging procedure related to the continuum single-particle states and the plateau condition. The ETFSI approach also predicts deformations and nuclear charged radii in close agreement with experimental data. For these major reasons, the ETFSI model is now widely used for astrophysical applications, in particular in r-process nucleosynthesis calculations.

2.2 Nuclear level densities

Most of nuclear applications still make use of the popular back-shifted Fermi gas model (BSFG)–or some variant of it– to estimate the spin-dependent NLD, particularly in view of its ability to provide simple analytical formulae [5]. It should be reminded that the BSFG model essentially introduces phenomenological improvements to the original analytical formulation of Bethe, and consequently none of the important shell, pairing, deformation or collective effects are properly accounted for in such a description. Drastic approximations are usually made in deriving analytical formulae and often their shortcomings in matching experimental data are overcome by empirical parameter adjustments. In particular, it is well accepted that the shell correction to the NLD cannot be introduced by neither an energy shift, nor a simple energy-dependent level density parameter, and that the complex BCS pairing effect cannot be reduced at low energies to an odd-even energy back-shift (e.g [6]). A much more sophisticated formulation of NLD than the one used in BSFG approach is required if one pretends to describe the excitation spectrum of a nucleus analytically, especially because of the very high sensitivity of the NLD to the different empirical parameters. Because of the phenomenological character of all NLD formulae proposed so far, their application is far from being reliable especially when experimentally unknown nuclei are considered. Even for known nuclei, the requirement of fitting experimental data, mainly the s-neutron resonance spacings at an excitation energy equal to the neutron separation energy, does not at all ensure the correct energy dependence of the predicted level density.

To improve the reliability of NLD calculation, more sophisticated models (based on the statistical approach, as well as the exact combinatorial method and making use of a discrete single-particle level distribution) have been proposed. These approaches have the advantage of treating in a natural way shell, pairing and deformation effects on all the thermodynamic quantities. In particular, the computation of the NLD by the microscopic statistical technique corresponds to the exact result that the analytical approximation tries to reproduce, and remains by far the most reliable method for estimating NLD. However, such models are still not free from uncertainties, and in particular, lead to relatively poor fits to experimental data because of their strong dependence on the choice of the single-particle potential and pairing strength. A compromise between the reliability of the model and its ability to reproduce experimental data can be found in the microscopic model based on the partition function method and making a consistent use of all nuclear structure ingredients predicted by the ETFSI model, i.e the single-particle level scheme, pairing strength and deformation [2, 6]. Such a global model is parameter free and has been shown to reproduce experimental neutron spacings within a factor of about 3. The fact that microscopic approaches do not provide an easy-to-compute prescription can be solved by providing level densities in a table format, as already proposed on the Brussels web-site http://astro.ulb.ac.be/iaa.htm.

2.3 Optical potential

Most of the astrophysical applications take nowadays the optical potential for neutrons and protons for the work of Jeukenne et al. [7] derived from "next-to-first" principles with a Reid's hard core nucleon–nucleon interaction by applying the Brückner–Hartree–Fock approximation. An updated version was recently proposed by Bauge et al. [8].

Regarding the α-nucleus optical potential, the situation is much less optimistic. The very-low energies of relevance in astrophysical environments (far below the Coulomb barrier) make the extrapolation of global potentials quite hazardous as shown by the new results in the ^{144}Sm$(\alpha,\gamma)^{148}$Gd experiment [9]. In addition to the global potentials proposed by [10, 11], a new global α-optical potential was recently proposed in order to take into account the strong energy dependence and nuclear structure effects affecting the imaginary part of the potential [12].

2.4 γ-ray strength function

The total photon transmission coefficient from a compound nucleus excited state is one of the key ingredients for statistical cross section evaluation. In particular, the Maxwellian-averaged radiative capture rates at temperatures of relevance in astrophysical environments strongly depends on the low-energy tail of the electric giant dipole resonance (GDR). In addition to the generalized Lorentzian model [13], a new expression of the γ-ray strength function was proposed recently [15]. It corresponds to a hybrid model describing exactly the high-energy Lorentzian shape observed in photoabsorption data and the improved expression of the $E1$ strength function at energies below the neutron separation energy as given by [14].

To evaluate the GDR energy and width, macroscopic models describing the relative motions of protons against neutrons are traditionally considered (e.g [16]). Use is also made of the GDR energies predicted by [17] with a renormalized np interaction of strength $K = 1360A^{-1/6}$ MeV fm^3 derived from a least-square fit to the experimental GDR energies [15]. The expression for the GDR widths is taken from [18] where a damping width describing the coupling between the dipole oscillations and the surface vibration is introduced to explain the shell effects observed in the GDR widths.

2.5 Fission barriers

Fission barriers are quantities of importance in the r-process of stellar nucleosynthesis. Until recently, fission barriers used in astrophysical calculations were calculated exclusively on the basis of one form or another of the liquid-drop model. In an attempt to provide better extrapolation far away from the experimentally known region, the ETFSI model as now been extended to the calculation of the fission barriers. The ETFSI model is able to predict the experimentally known barriers within 1.5 MeV [19].

3 Conclusions

As shown in the previous sections, nuclear astrophysicists usually call for the same ingredients as nuclear physicists to estimate the nuclear reaction cross-sections, though many astrophysics applications involving a large number of unstable nuclei require the use of global approaches. The extrapolation to exotic nuclei or energy ranges far below the Coulomb barrier also constrains the use of nuclear models to the most reliable ones, even if more empirical approaches sometime present a better ability to reproduce experimental data. A subtle compromise between the reliability, accuracy and applicability of the different available theories has to be found according to the specific application considered.

References

[1] Arnould M., Takahashi K., 1998, Rep. Prog. Phys. 99, 1.

[2] Goriely S., 1997, In: G. Reffo et al. (eds) Nuclear Data for Science and Technology, Italian Physical Society, p. S11.

[3] Möller P., Nix J.R., Myers W.D., Swiatecki W.J., 1995, At. Data Nucl. Data Tables 59, 185.

[4] Aboussir Y., Pearson J.M., Dutta A.K., Tondeur F., 1995 At. Data Nucl. Data Tables 61, 127.

[5] Thielemann F.K., Arnould M., Truran J.W., 1986, In: Vangioni-Flam et al. (eds.) Advances in Nuclear Astrophysics, Editions Frontières, Gif-sur-Yvette, p. 525

[6] Goriely S., 1996, Nuc. Phys. A605, 28.

[7] Jeukenne J.P. , Lejeune A., Mahaux C., 1977, Phys. Rev C16, 80.

[8] Bauge E., Delaroche J.P., Girod M., 1998, Phys. Rev. C58, 1118.

[9] Somorjai E., Fülöp Zs. et al., 1998, Astr. Astrophys. 333, 1112.

[10] Avrigeanu V., Hodgson P.E., Avrigeanu M., 1994, Phys. Rev. C49, 2136.

[11] Atzrott U., Mohr P., Abele H., Hillenmayer C., Staudt G., 1996, Phys. Rev. C53, 1336.

[12] Grama C., Goriely S., 1998 in Proc. Intern. Conference on Nuclei in the Cosmos (Volos, Greece).

[13] Kopecky J., Chrien R.E., Nucl. Phys. A468 (1987) 285.

[14] Kadmenskii S.G., Markushev V.P., Furmann V.I., Sov. J. Nucl. Phys. 37 (1983) 165.

[15] Goriely S., 1998, Phys. Lett. B 436, 10.

[16] Myers W.D., Swiatecki W.J. et al., 1977, Phys. Rev. C15, 2032.

[17] Van Isacker P., Nagarajan M.A., Warner D.D., 1992, Phys. Rev. C45, R13.

[18] Thielemann F.-K., Arnould M., in: Proceedings of Conference on Nuclear Data for Science and Technology, (eds. K. Böckhoff, Reidel, Dordrecht, 1983) 762.

[19] Mamdouh A., Pearson J.M. Rayet M., Tondeur F., 1998, Nucl. Phys. in press.

RIPL Starter File Parameter Validation for Actinide Nuclei

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Nuclear reaction theory calculations are of particular importance for actinide nuclei data evaluation. Pending and future requests on actinide nuclear data hardly ever would be meet with measured data base. Current measured cross section data base for actinide nuclei in most cases is restricted to fission data, in some cases they are supplemented with inelastic scattering or capture data. Our evaluation approach is based on nuclear reaction theory application for data analyses. Recently it was employed for evaluation of nuclear data files for 243-Cm, 245-Cm, 246-Cm, 241-Am, 242m-Am, 242g-Am, 243-Am, 238-Pu, 242-Pu, 238-Np, fission data fit within Hauser-Feshbach-Moldauer theory serves as a major constraint for capture, (n,n') and (n,xn) data prediction. Available neutron-induced fission cross section data could be described with a statistical theory approach from 1 keV up to 40 MeV incident neutron energy [1,2]. On this basis fission level density and fission barrier parameters were obtained for 49 Th - Cf nuclei.

Measured data base for 238-U nuclide provides a unique possibility to compare calculated data with measured total, elastic, inelastic, fission, capture, (n,2n), (n,3n) and (n,4n) data up to 40 MeV [2,3]. A coupled channels optical model is adopted for n+238-U interaction data analysis. A consistent description of total and inelastic scattering data below 1 MeV incident neutron energy might be used to refine the recommended in Starter File optical potential parameter set. The direct excitation of ground state rotational band levels 0+-2+-4+-6+-8+ was estimated within rigid rotator model, as compared with 0+-2+-4+ coupling basis recommended either by Haouat et al. (1982) and Young (1995). Present potential parameters were obtained by fitting neutron total cross section data, angular distribution data up to 30 MeV incident neutron energy and neutron strength functions. In the optical potential, proposed by Young (1995) there is a relatively small volume absorption term. It influences total cross section data fit, but changes drastically the reaction cross section shape above 10 MeV. We argue that adding volume absorption term one faces severe problems with consistent description of fission and (n,xn) reaction cross section data in 10-40 MeV incident neutron energy range [2]. To follow the fission data trend above 20 MeV, we should introduce instead additional decrease of imaginary potential term W_D. Proton- induced reaction data for 238-U also were described [2].

Constant temperature level density parameters U_c, U_0 and T, another important ingredient of statistical theory calculation, are defined by fitting cumulative number of low-lying levels. Current values of constant temperature model parameters U_c, U_0 and T [4] generally are discrepant with Starter File estimates made based solely on cumulative plot fits. Producing fits of cumulative plots, latter parameters might lead to incorrect estimates of the cut-off energy, above which appreciable missing of levels starts. Another obvious consequence is incorrect extrapolation of level density shape even in a few-MeV excitation energy range. In present approach constant temperature model parameter T has a meaning of nuclear temperature, in other words it is correlated with level density shape, extrapolated from the excitation energy equal to the binding energy of the neutron to the matching point U_c. Another constant temperature model parameter U_0 is not much different from the odd-even correction to the excitation energy, used in the level density model. Smooth trends revealed in this parameter values make them particularly suitable for extrapolations to lower and higher mass actinide nuclei.

The statistical Hauser-Feshbach-Moldauer theory calculation of neutron-induced reactions for 238-U shows fair description of available data base. Our experience of using nuclear reaction theory with relevant input parameters, which are consistent or coincide with RIPL Starter File recommendations provides a clear evidence of rather high potential of RIPL Starter File for data prediction.

References:

1. V.M. Maslov, Fission Level Density and Barrier Parameters for Actinide Neutron-Induced Cross Section Calculations, INDC(BLR)-013, 1998, IAEA, Vienna.

2. V.M. Maslov and A. Hasegawa, Neutron-Induced Fission Cross Sections of Uraniums up to 40 MeV, Proc. 3d Specialists Meeting on High Energy Nuclear Data, March 30-31, 1998, JAERI, Tokai, Japan.

3. V.M. Maslov, Yu.V. Porodzinskij, A. Hasegawa and K. Shibata, Neutron Data Evaluation of 238-U, JAERI-Research, 98-040, 1998.

4. V.M. Maslov and Yu.V. Porodzinskij, Actinide Level Density Parameter Systematics, JAERI-Research, 98-038, 1998.

Japanese Proposal and Contribution for IAEA/CRP on RIPL-II

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1. Introduction

As starting of RIPL-II project, it is important to consider the potential activities and possible contributions in Japan. Japanese Nuclear Data Committee (JNDC) organizes an Evaluating Calculation Support System Working Group (ECSS-WG) to investigate the subjects related to the RIPL-II project. In this report, the activities of this working group are introduced as potential studies for validating model parameter and the development of the integrated nuclear data evaluation system (INDES) and its parameter database (EVLDF). The Japanese possible contributions for RIPL-II project are also reported as well as user requirements and proposals.

2. Japanese Activities Related to RIPL-II Project

2.1 Potential Studies for Validating Model Parameters

In the ECSS-WG, following potential studies are being carried out. For the optical model potential parameters, studied are the folding model and dispersion relation, microscopic approach (JLM model), and global potential parameter for intermediate energy region with the parameter determination for Dirac equation and Chiba's global description. For the level density parameters, formula based on Fermi Gas Model with unified shell and pairing effect and parameter systematics are considered. Some systematics for gamma-ray strength function are also studied.

2.2 Integrated Nuclear Data Evaluation System and its Parameter Library

Nuclear data evaluation is required to obtain the most reliable data sets for the evaluated nuclear data files. The evaluation must be done by using experimental data and by many complicated theoretical calculations with various basic data such as optical potential parameters, level density parameters, and level scheme. Japanese Evaluated Nuclear Data Library, version 3 (JENDL-3)[1)] released in 1989 was accomplished by great efforts of many evaluators with many intricate works. Integrated Nuclear Data Evaluation System (INDES) was developed to keep their experiences and basic data of nuclear physics used for the evaluation of JENDL-3, and to support new evaluations. Roughly classified, the INDES functions are of three categories, which are to retrieve basic data described above, to set up input data of theoretical calculation codes automatically, and to select the most suitable set of theoretical calculation codes applying knowledge engineering technology.

The model parameter databases is called '*Evaluation Data Files* (EVLDF)'[2)]. Parameters to be used in theoretical calculations of nuclear data are stored in EVLDF which consists of several parameter files and an index file. The parameters provided in EVLDF are optical potential parameters, level density parameters, level scheme, deformation parameters, and basic information of nuclei. The current format of EVLDF is capable of storing parameters used for the evaluation work of JENDL-3. Basic rules of EVLDF format are described as following:

1) Each line of EVLDF consists of 80 columns. The columns from 73 to 80 are used for sequential number of lines or other purposes.
2) Characters from A to Z should be capital letters.
3) The smallest group of lines is a "record".
4) A record name is given in the columns from 1 to 10.
5) Each record can be continued to the next line.
6) In the case where a record is repeated, "+" is given in the first column of the following records.
7) Data in the columns from 11 to 72 depend on the record name. Usually, data in the columns from 11 to 72 are given in a free format.
8) In any lines, any comment can be given after a semi-colon (";").
9) Some records have corresponding END records. A group of lines from a line with record name to its END record is a "section". A section can include other sections inside.
10) In many cases, nuclide is represented with an integer calculated from atomic number, mass number and meta-stable number as (atomic number)×10000 + (mass number)×10 + (meta-stable state number). The mass number and meta-stable state number are 0 for natural elements. This integer is called as a "nuclide name".

3. Proposals and Requests to RIPL-II Project

From Japanese user side, followings are requested and proposed.

1) To validate parameters systematically with the points of physical and application-oriented (testing by some of popular model codes using evaluation) ways.
2) To adopt standard and unified format to make interface program production easier as much as possible. For example, the format of level scheme database in the RIPL Starter File should be changed, since the sum of gamma-ray branching ratios often violate to be unity and so on.
3) To summarize and integrate retrieval and interface programs to make their usage easier for users with considering the operation systems like UNIX, Windows, WWW, etc.

4. Possible Japanese Contributions to RIPL-II Project

The possible Japanese contributions to the RIPL-II project are being considered as following.

1) To validate parameters with calculating cross section by some of model codes used to nuclear data evaluation.
2) To develop retrieval and interface tools based on INDES for UNIX plat form. For this purpose, it is possible to consider standard format of RIPL-II and to convert the format to create the libraries used in the tools, if necessary.
3) To develop retrieval tools for WWW. The example tools for mass and level scheme data are available already.

References

1) K. Shibata, et al., *JAERI*-**1319** (1990).
2) T. Nakagawa, *JAERI-Data/Code* **97-053** (1998).

RECENT ACTIVITIES AT LOS ALAMOS IN NUCLEAR DATA EVALUATION AND NUCLEAR MODEL CODE DEVELOPMENT

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ABSTRACT

An update is given of activities at Los Alamos National Laboratory directed at improvement of nuclear data libraries and nuclear model codes. Relationship of this work to the Reference Input Parameter Library (RIPL) is discussed.

I. INTRODUCTION

This report summarizes recent activities of the Nuclear Theory and Applications Group (T-2) at Los Alamos National Laboratory in the areas of nuclear data evaluation and nuclear model code development. The discussion addresses recent improvements and extensions of the Los Alamos 150-MeV library, benchmark testing results for the library, and interactions with the Cross Section Evaluation Working Group (CSEWG) to incorporate the library into the ENDF/B system. Ongoing activities aimed at improving the ENDF/B-VI data base over the conventional energy region up to 30 MeV are described, including collaborative efforts with the X-division Code Integration Group (X-CI) to improve photon production data in evaluations of thermal neutron-induced reactions. Efforts in T-2 to modernize and improve our nuclear reaction theory calculations, centered around development of a new GNASH-type code, are summarized.

II. NUCLEAR DATA EVALUATION

A. Intermediate Energy Data Evaluation Activities

1. The Los Alamos 150-MeV Library

The Los Alamos 150-MeV library is a assemblage of neutron-, proton-, and photon-induced nuclear data libraries spanning the incident projectile energy region from subthermal (or threshold) to 150 MeV. The library has been developed at Los Alamos (Chadwick, Young) but includes collaborative activities with scientists from ECN Petten (Koning), JAERI (Chiba, Fukahori), and Bologna (Herman). The approach followed in producing the library has been to utilize the GNASH (and FKK-GNASH) code system[1] to calculate the data at all energies for incident protons and photons, and above 20 MeV for neutrons, joined with ENDF/B-VI evaluations at lower energies. The models used include Hauser-Feshbach theory for equilibrium decay; preequilibrium theory with either semiclassical exciton theory or quantum mechanical Feshbach, Kerman, Koonin theory; level densities from the 1975 Ignatyuk formulation; transmission coefficients from spherical or deformed optical models; and direct reactions calculated with the ECIS code. Extensive use is made of experimental data in benchmarking and improving the calculations for heavier target nuclei, and are used directly in evaluating the data for the lightest targets. Several existing or pending publications describe the libraries.[2-7] Examples of particle and photon emission spectra from neutron reactions on ^{12}C are given in Fig. 1, and recoil nuclei emission spectra from n + ^{28}Si reactions are illustrated in Fig. 2.

For incident neutrons and protons, the library presently consists of evaluations for targets of $^{1,2}H$, ^{12}C, ^{14}N, ^{16}O, ^{27}Al, ^{31}P, $^{28,29,30}Si$, ^{40}Ca, $^{50,52,53,54}Cr$, $^{54,56,57,58}Fe$, $^{58,60,61,62,64}Ni$, $^{63,65}Cu$, ^{93}Nb, $^{182,183,184,186}W$, $^{196,198,199,200,201,202,204}Hg$, and $^{206,207,208}Pb$. The library for incident photons is currently limited to targets of ^{56}Fe, ^{184}W, and ^{208}Pb. Over the coming year we expect to complete evaluated files for photon-induced reactions on ^{2}H, ^{12}C, ^{16}O, ^{27}Al, ^{28}Si, ^{40}Ca, ^{58}Ni, and ^{63}Cu. Additionally, improvements are planned for several of the neutron-induced evaluations, based on new measurements of neutron total cross sections completed at the WNR facility at LANSCE.

The entire 150-MeV library for incident neutrons and protons was submitted for inclusion the ENDF/B-VI evaluated nuclear data base. As a condition for acceptance of the library by CSEWG, a formal review of the files was performed by the Nuclear Energy Agency Subgroup 13 of the Working Party on Evaluation Cooperation (specifically by A. Koning at ECN Petten and T. Fukahori at JAERI). On the basis of these and other reviews, a number of corrections were incorporated into the file, especially concerning data treatment near reaction thresholds. The final library was approved by Subgroup 13 and subsequently accepted by CSEWG for Release 6 of ENDF/B-VI. The library has been supplied to the National Nuclear Data Center at Brookhaven and is available from the Group T-2 web site (http://t2.lanl.gov).

Extensive benchmark testing of the libraries against microscopic experimental data was carried out during development of the library. For example, angle-integrated neutron, proton, deuteron, and alpha emission spectra from the p + ^{58}Ni evaluation are compared to measurements at 90 MeV in Fig. 3. Similarly, measurements of production cross sections for various residual nuclei from p + ^{16}O reactions are compared to the library in Fig.4.

Several integral benchmark experiments have been calculated with the newly developed MCNPX Monte Carlo particle transport code by R. Little of Group X-CI at Los Alamos. A comparison of his calculations of lethargy fluence on the beam axis for 68-MeV protons incident on a 40 cm-thick iron slab is given in Fig. 5. The calculation with the 150-MeV library (labeled MCNPX calculation) is compared in the figure with results from various versions of the LAHET internuclear cascade/evaporation code. Additionally, measurements of neutron transmission through 60 cm of water are compared to MCNPX calculations with the 150-MeV library in Fig. 6, and a calculation of neutron transmission through 30 cm of lead versus neutron energy is compared to experimental data in Fig. 7.

2. Activation data library

A new transmutation/activation library for neutrons and protons up to 150 MeV has been created (Koning, Chadwick). The nuclear data in these libraries stems from two sources: for neutrons below 20 MeV, we use data from the ECN/EAF96.0 transmutation file (as corrected by M. Herman); for neutrons above 20 MeV and for protons at all energies, we have calculated reaction cross sections from systematics and residual production cross sections with the nuclear model code HMS-ALICE. The extension to 150 MeV is made for over 600 target nuclei and covers all targets in the EAF library except actinides. The resulting two libraries, AF150N and AF150P, are represented in the ENDF-6 format. The libraries have been checked with ENDF-6 preprocessing tools and have been processed with NJOY into libraries for the transmutation code CINDER-90.

B. Lower Energy Data Evaluation Activities

1. n + ^{16}O R-matrix analysis and evaluation update

The R-matrix analysis used for ENDF/B-VI is being revisited (Hale), with significant updating of the experimental data base used in the analysis. The motivation for this activity is persistent questions from analysis of integral critical experiments where ^{16}O is a reflector, which appear to require more forward peaking of neutrons at lower energies. In addition, the evaluated data in the MeV region is being reevaluated (Young) to accommodate new measurements from LANSCE and from Japan.

2. Neutron Data Evaluations for ^{35,37}Cl

New evaluations have been completed of thermal neutron capture gamma-ray spectra (Frankle, Adams, Reedy) and of all neutron-induced reactions above the resonance region (Young) for neutron reactions on ^{35}Cl and ^{37}Cl . The target application for this work is oil well logging technology, which required that as much detailed information as possible be included for discrete gamma rays. Accordingly, extensive detail is included in the evaluation of (n,γ), (n,n'γ), (n,2nγ), (n,pγ), etc., reactions. The thermal neutron capture gamma-ray spectra are entirely determined from an assessment of experimental data. The GNASH code was utilized for much of the evaluation in the MeV region, making appropriate use of the experimental data base. The resonance parameter analysis from the JENDL evaluation was adopted.

3. Discrete gamma-ray data for thermal neutrons

Similar to ^{35,37}Cl, thermal neutron capture gamma-ray spectra have been evaluated for the following series of target nuclei: ^{9}Be, ^{14}N, ^{19}F, ^{23}Na, ^{24,25,26}Mg, ^{27}Al, ^{32,33,34}Si, ^{32,33,34,36}S, ^{39,40,41}K, ^{40,42,43,44,46,48}Ca, ^{45}Sc, ^{46,47,48,49,50}Ti, ^{51}V, ^{55}Mn, ^{50,52,53,54}Cr, ^{54,56,57,58}Fe, ^{58,60,61,62,64}Ni, ^{63,65}Cu, and ^{182,183,184,186}W. These results, which are based on the most recent experimental data, are being systematically incorporated into ENDF/B-VI evaluations (Frankle, Young).

4. n + ^{169}Tm evaluation update

New measurements of neutron-induced radiative capture cross sections for Tm are being carried out at LANSCE. In support of this activity, we have updated the GNASH analysis used for ENDF/B-VI. When the experiments and supporting calculations are complete, we expect to update the ENDF/B-VI evaluation of ^{169}Tm.

5. Uranium isotope evaluations

We are systematically analyzing neutron reactions on several uranium isotopes in an attempt to produce better evaluated data files for the minor isotopes whose data base is poor. Additionally, we are investigating updates to the evaluations for ^{233}U, ^{235}U, and ^{238}U based on improved experimental data as well as better analyses. In particular, we hope to improve these latter evaluations to address persistent (mainly minor) deficiencies in calculating integral experiments. To date, we have produced a new evaluation for ^{235}U that mainly updates the cross sections for new experimental data. The updated n + ^{235}U evaluation is compared to new measurements from LANSCE/WNR of the fission cross section in Fig. 8 and to new neutron total cross section measurements (Lisowski, 1990) in Fig. 9.

III. NUCLEAR MODEL CODE DEVELOPMENT

In T-2 we are developing a new version of the GNASH code for modeling nuclear reactions up to a few hundred MeV. The code is based on many of the existing concepts within GNASH, but will introduce some new capabilities. At low energies, width fluctuation corrections will be calculated directly (rather than being obtained from other codes). A variety of state-of-the-art level density, optical model, and fission models will be included. Additionally, a Monte Carlo Hauser-Feshbach capability will be included that will facilitate full preservation of ejectile correlation information, as well as exact kinematics for nuclear recoil and light particle ejectiles. A preequilibrium module that uses Monte Carlo methods, described below, will be linked to the new code.

We are close to completing a new Hybrid Monte Carlo Simulation (HMS) preequilibrium code that can be applied to model preequilibrium reactions up to 300-400 MeV. The Monte Carlo feature allows a straightforward treatment of multi-particle emission, which becomes important at the higher energies (and is not limited to two fast particles). The preequilibrium cascade is treated by following the successive creation of *2p1h* states in the scattering, along with the decay of *2p1h*, *1p1h*, and *1h* states. Angular effects are treated with the theory of Chadwick-Oblozinsky that considers the momentum-structure of particle-hole states to determine the accessible phase space for preequilibrium emission at various angles. The code produces a history file that summarizes the ejectile information for each event, preserving all correlation information. This information can then be used in one of two ways: as input to a subsequent Monte Carlo equilibrium decay code; or, after collapsing the information into inclusive emission spectra, as input to a conventional equilibrium decay code. Aspects of the physics of this approach are described in Chapter 7 of the RIPL handbook; this new code will be made available to RIPL-II.

IV. OTHER ACTIVITIES

Work is proceeding toward development of an improved global optical model (Madland) for used in nuclear data evaluations at intermediate energies. Improvements to the spallation physics used in internuclear cascade codes such as LAHET are being investigated (Mashnik, Sierk), and the finite-range liquid drop model by Möller, Nix, Myers, and Swiatecki is being utilized to calculate fission barrier parameters for use in establishing systematics of such parameters (Möller) for reaction theory calculations. Development of the CINDER'90 nuclide buildup and depletion code continues, and an improved evaluation of delayed neutron spectra from fission in the usual 6 time-group blocks is being carried out for ENDF/B-VI (Wilson). Finally, new formats are being developed and the NJOY code is being modified for processing the 150-MeV libraries for use in the new MCNPX Monte Carlo particle transport code.

REFERENCES

1. P.G.Young, E.D.Arthur, and M.B.Chadwick, "Comprehensive Nuclear Model Calculations: Theory and Use of the GNASH Code," Proc. Workshop NUCLEAR REACTION DATA AND NUCLEAR REACTORS, ICTP, Trieste, Italy, 15 April - 17 May 1996 [Ed: A. Gandini and G. Reffo, World Scientific Publ. Co., Singapore (1998)] p. 227-404.

2. M. B. Chadwick, H. B. Blann, L. J. Cox, P. G. Young, and A. Meigooni, "Calculation and Evaluation of Cross Sections and Kerma Factors for Neutrons up to 100 MeV on Carbon," *Nucl. Sci. Engr.* **123**, 17 (1996).

3. M. B. Chadwick and P. G. Young, "Calculation and Evaluation of Cross Sections and Kerma Factors for Neutrons up to 100 MeV on ^{16}O and ^{14}N," *Nucl. Sci. Eng.* **123**, 1 (1996).

4. M. B. Chadwick, P. G. Young, S. Chiba, S. C. Frankle, G. M. Hale, H. G. Hughes, A. J. Koning, R. C. Little, R. E. MacFarlane, R. E. Prael, and L. S. Waters, "Cross Section Evaluations to 150 MeV for Accelerator-Driven Systems and Implementation in MCNPX," Nucl. Sci. Eng. (to be published in 1999) [LA-UR-98-1825 (1998)].

5. P. G. Young and M. B. Chadwick, "Nuclear Data Libraries for Incident Neutrons and Protons to 150 MeV in ENDF-6 Format," Proc. American Nuclear Society Topical Meeting on *Nuclear Applications of Accelerator Technology,* Albuquerque, New Mexico, 16-20 November 1997, to be issued.

6. P. G. Young and M. B. Chadwick, "Neutron- and Proton-Induced Nuclear Data Libraries to 150 MeV for Accelerator-Driven Applications," Proc. *Int. Conf. on Nuclear Data for Science and Technology,* Trieste, Italy, 19-24 May 1997 [Eds: G. Reffo, A. Ventura, and C. Grandi, Società Italiana di Fisica, Editrice Compositori, Bologna (1997)] p. 1440 (LA-UR 97-2449).

7. M. B. Chadwick, "Nuclear Data for Neutron and Proton Radiotherapy and for Radiation Protection," in preparation (International Commission on Radiation Units and Measurements, Bethesda, MD, 1998).

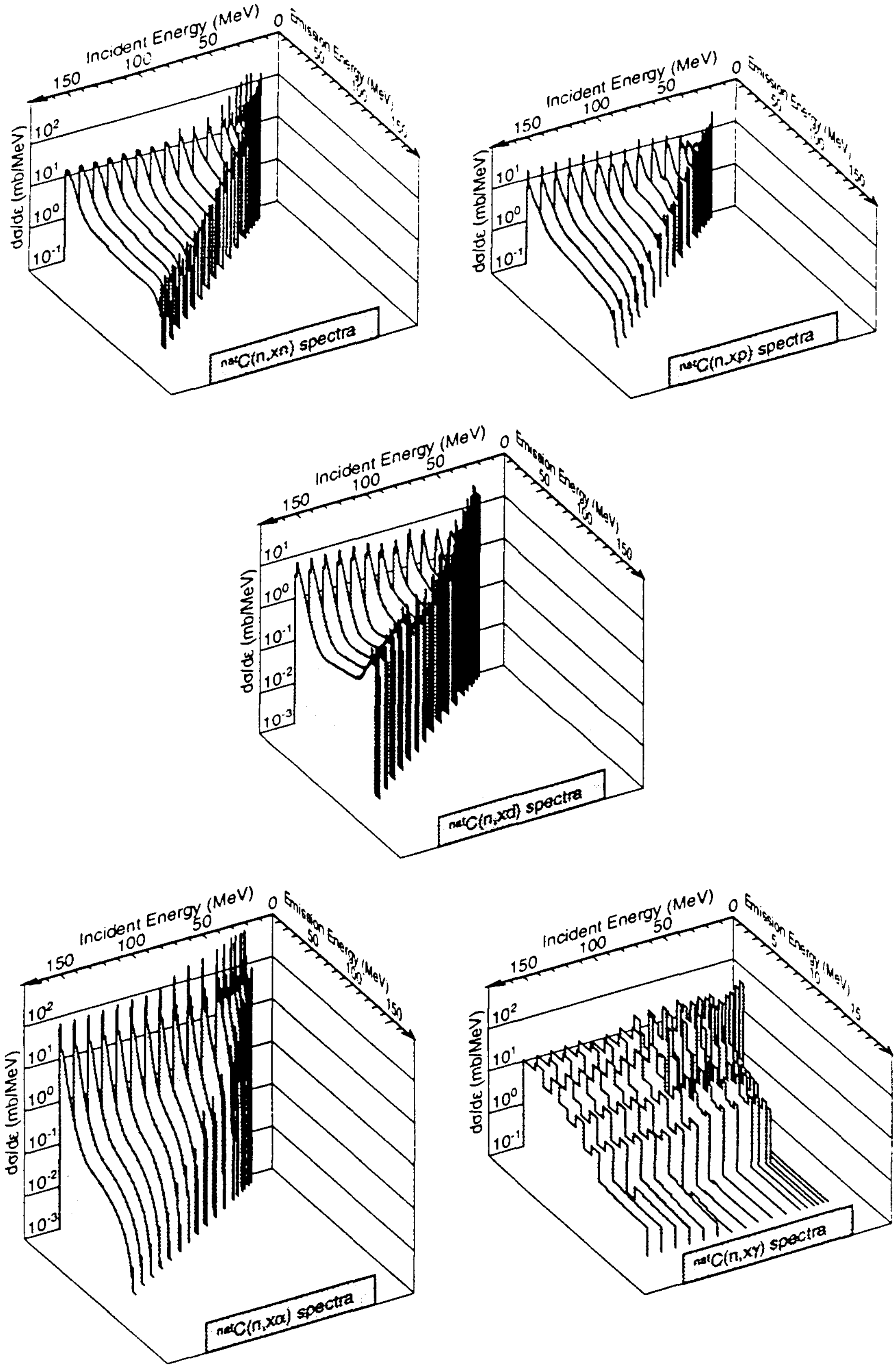

Fig. 1. Angle-integrated light-particle and photon emission spectra from n + ^{nat}C reactions from the 150-MeV library.

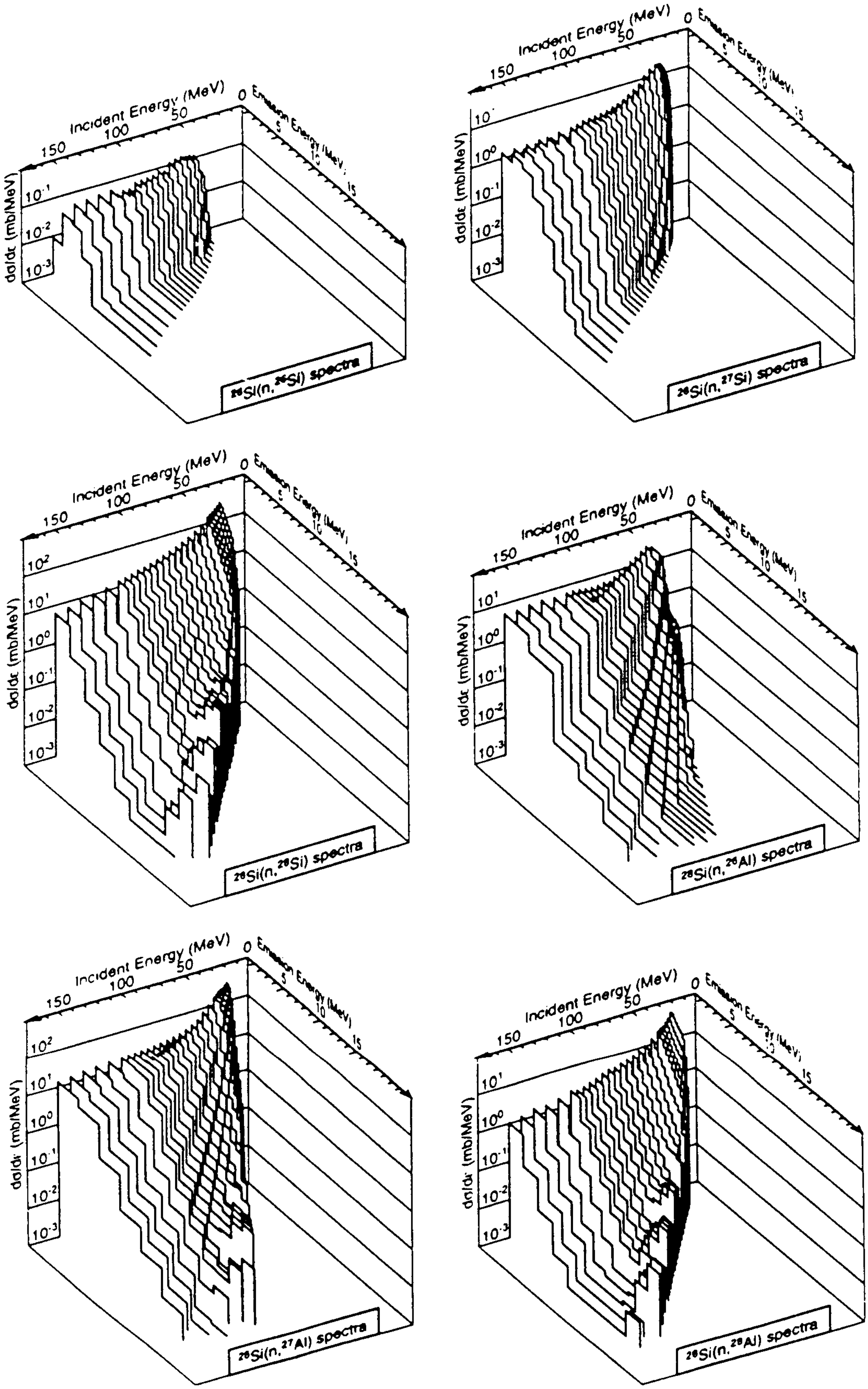

Fig. 2. Angle-integrated recoil spectra from n + ^{28}Si reactions from the 150-MeV library.

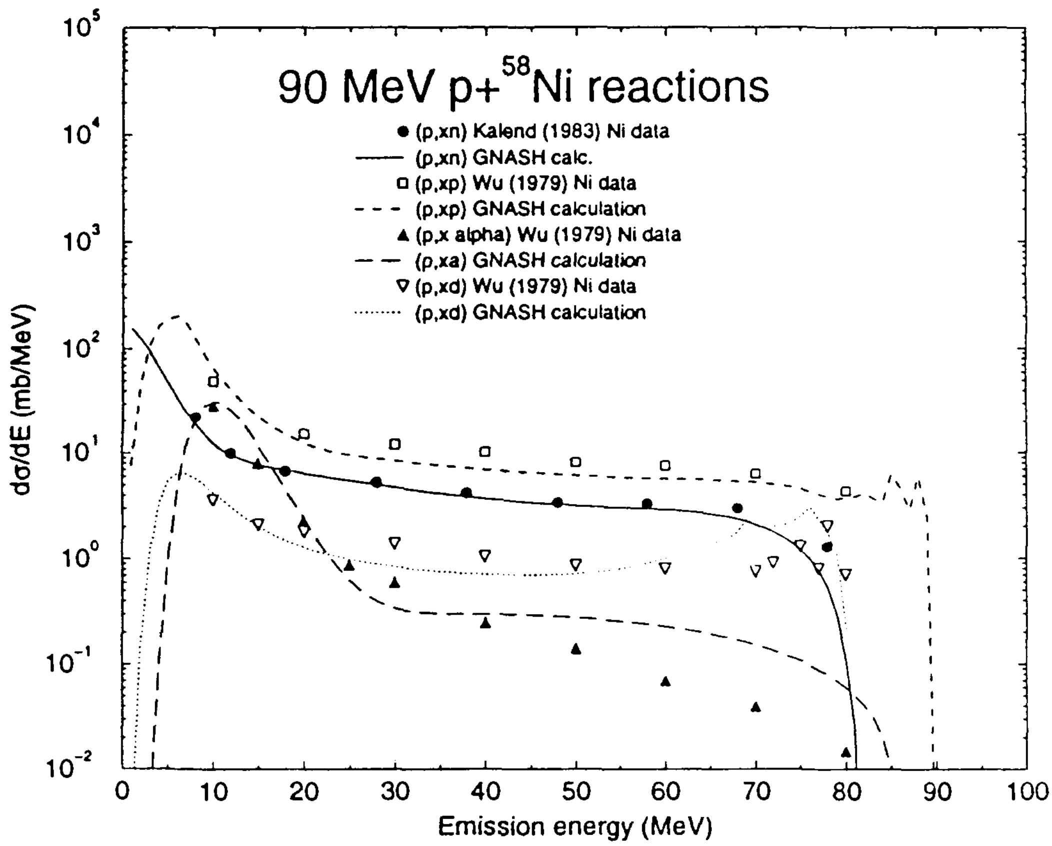

Fig. 3. Calculated neutron, proton, deuteron, and alpha emission spectra from p + ^{58}Ni reactions compared to experimental data at 90 MeV.

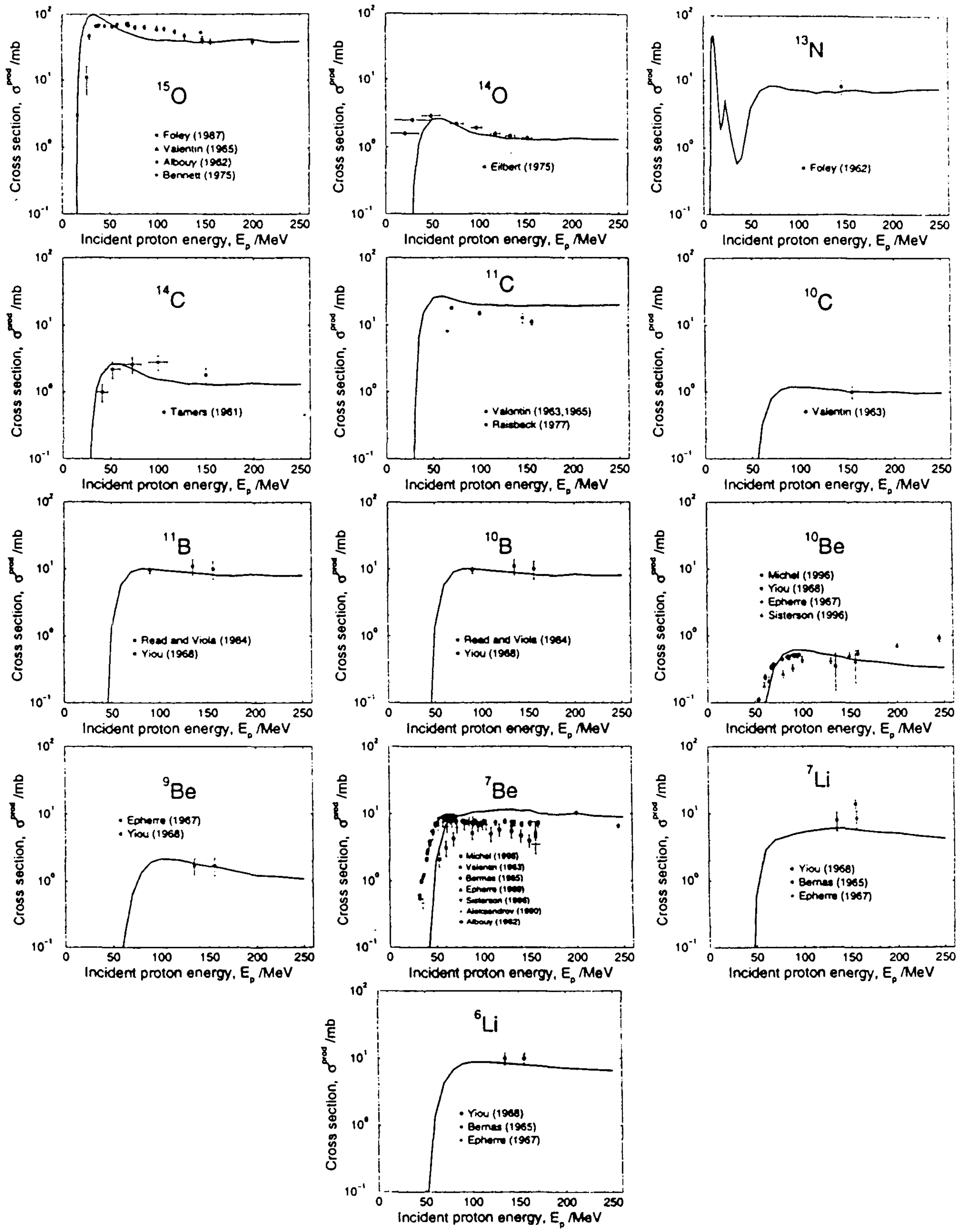

Fig. 4. Calculated recoil nuclei cross sections from the p + ^{16}O library compared to experimental data.

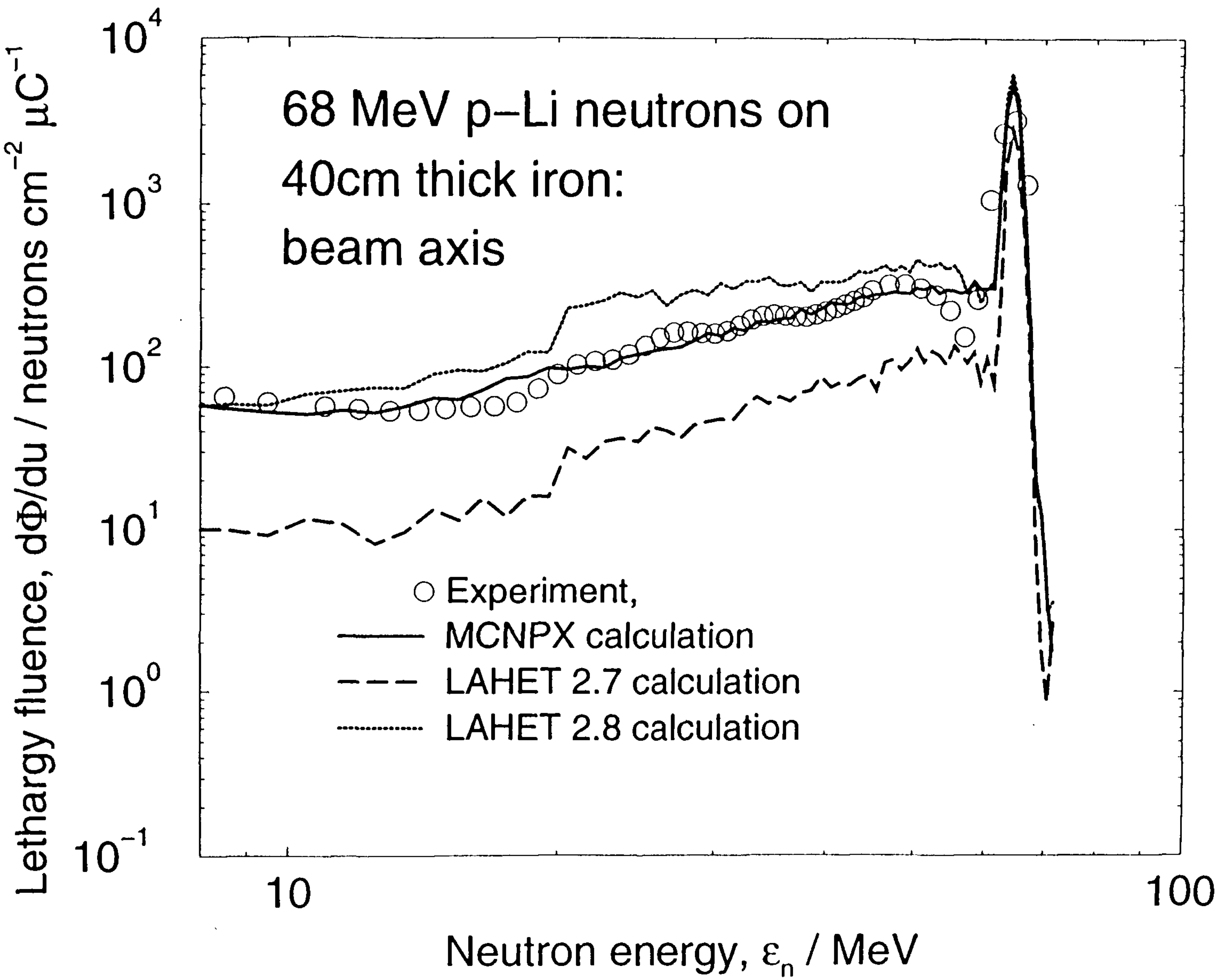

Fig. 5. Calculations and measurements of lethargy fluence from 68-MeV p+Li neutrons incident on a 40-cm thick slab of Fe.

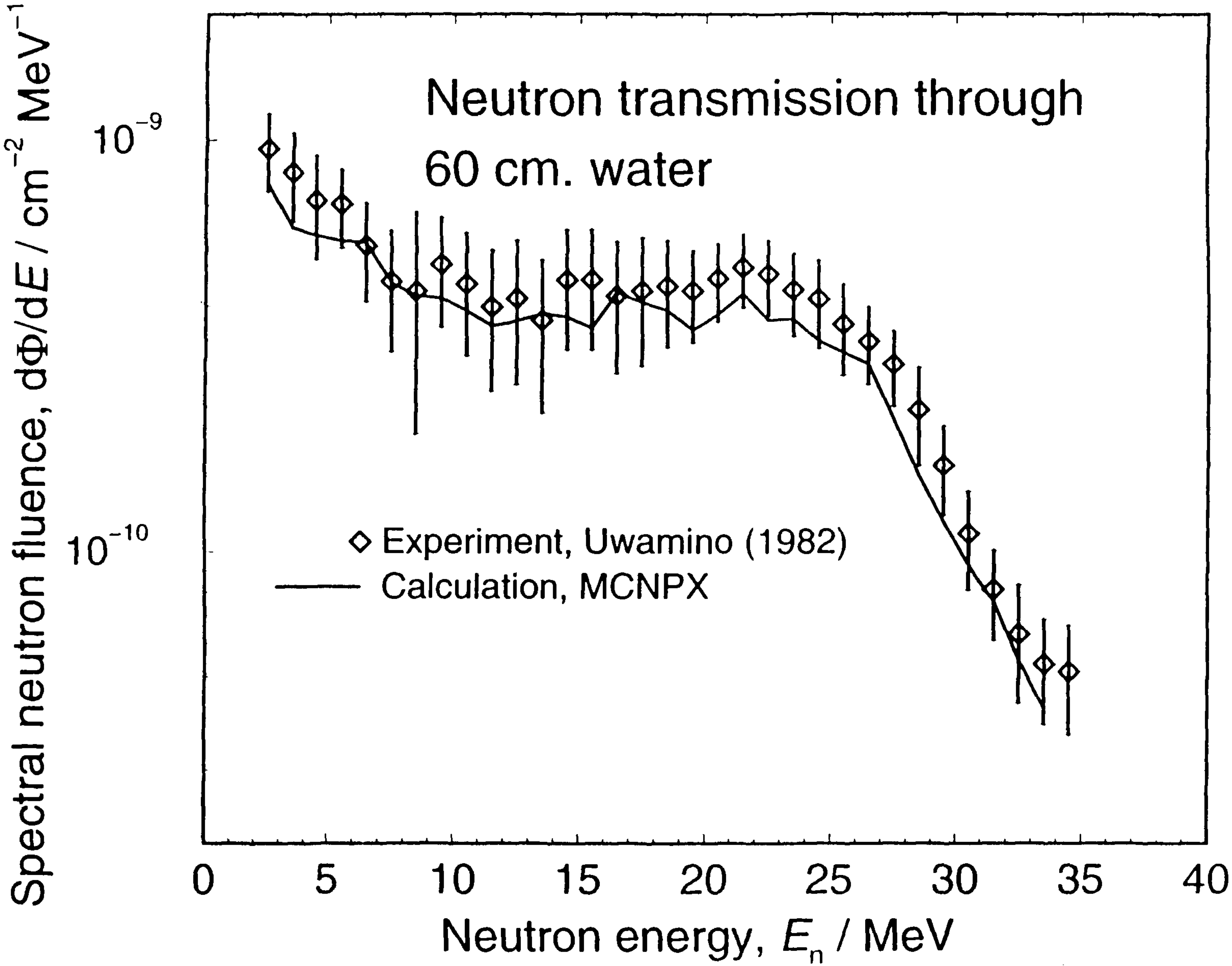

Fig. 6. MCNPX calculations using the 150-MeV library of neutron transmission through 60 cm of water compared to experimental data.

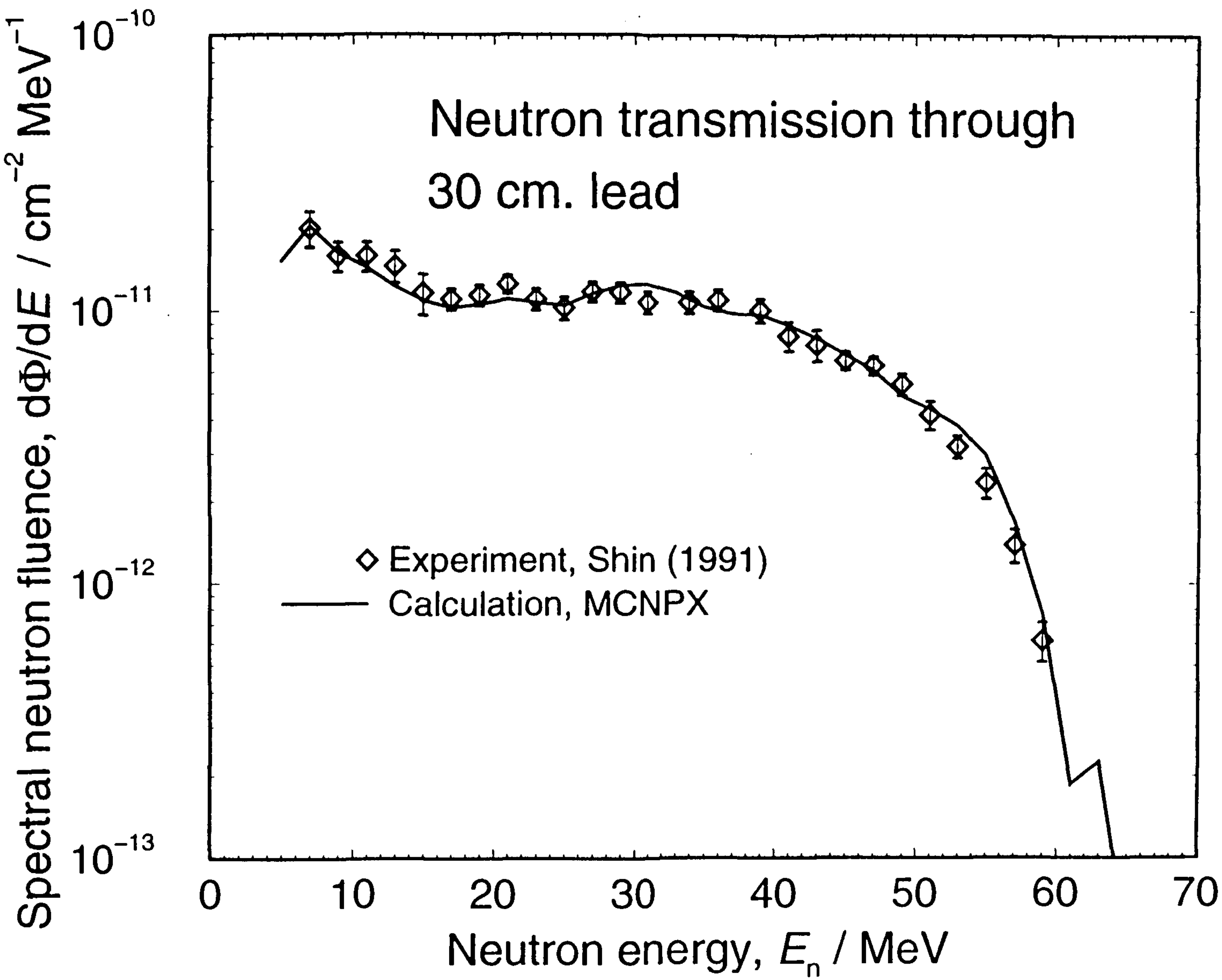

Fig. 7. MCNPX calculations using the 150-MeV library of neutron transmission through 30 cm of lead compared to experimental data.

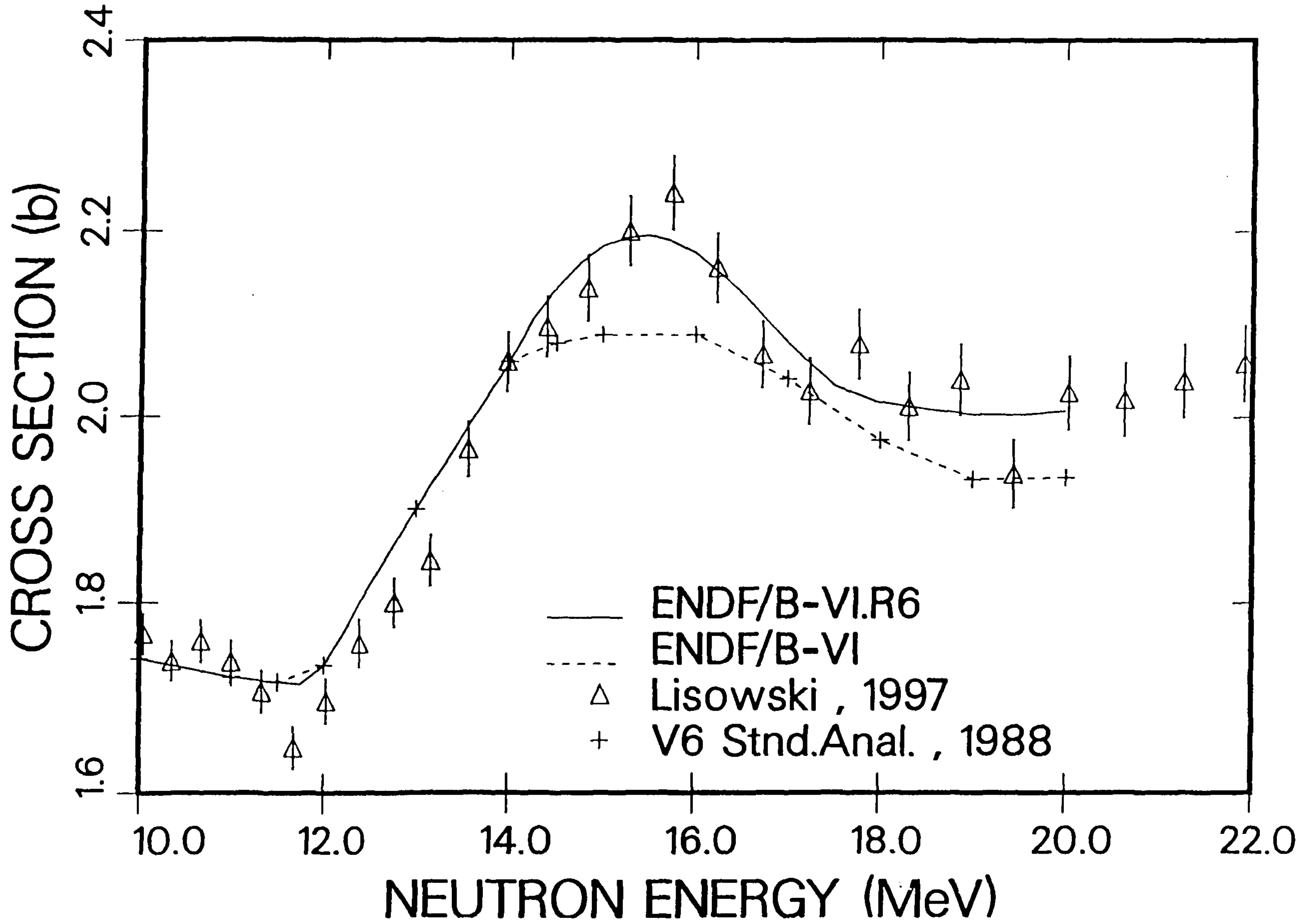

Fig. 8. Comparison of the new $^{235}U(n,f)$ evaluated cross section with the measurements of Lisowski et al. and with the existing ENDF/B-VI evaluation.

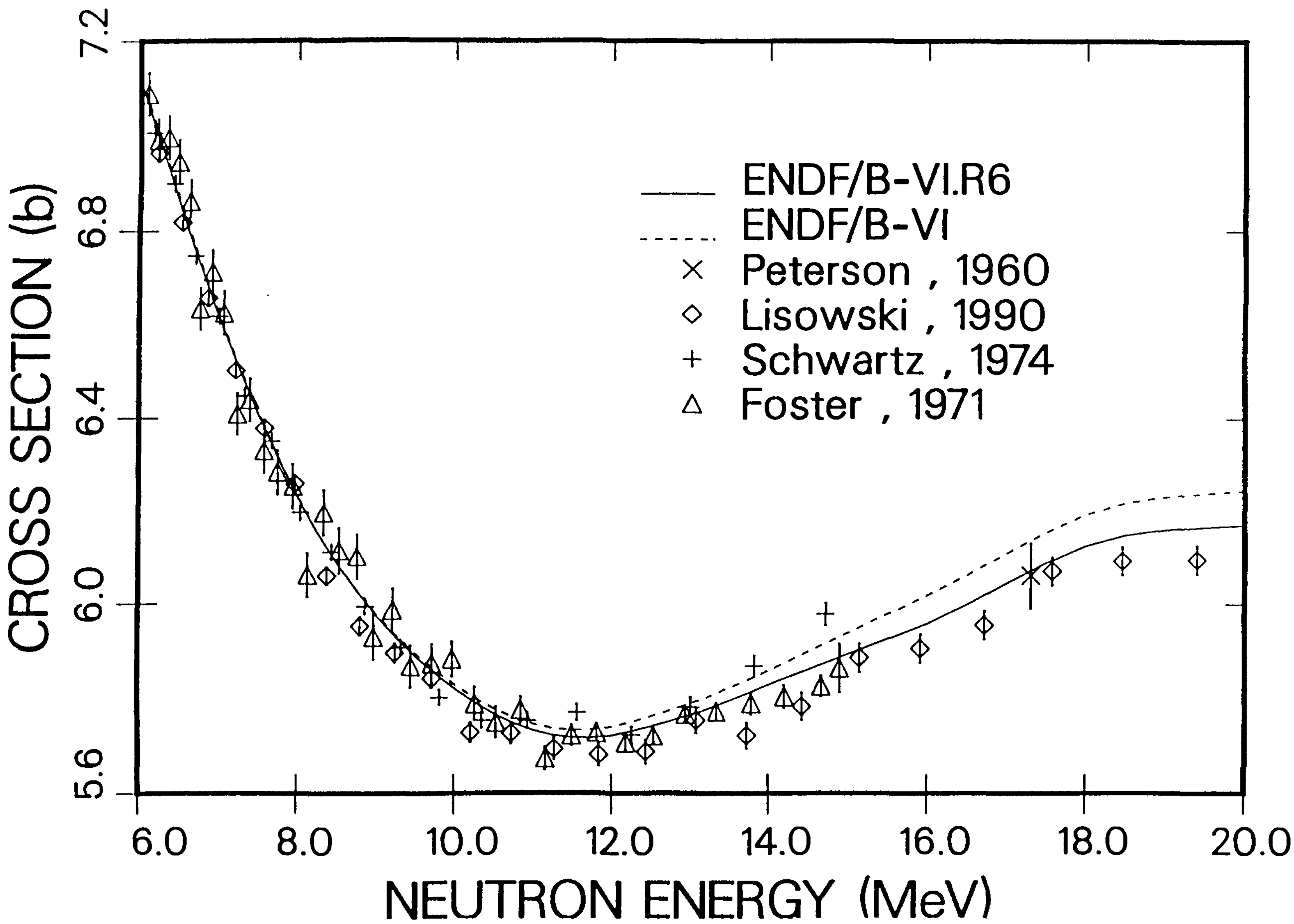

Fig. 9. Comparison of the revised ^{235}U evaluated neutron total cross section with new measurements by Lisowski et al. and with the existing ENDF/B-VI evaluation.

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