International Atomic Energy Agency

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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

STANDARD INPUT DATA SETS FOR NUCLEAR MODEL COMPUTATIONS OF NUCLEAR DATA

Summary Report of the IAEA Consultants' Meeting hosted by the Centro di Calcolo del E.N.E.A. Bologna, Italy and held at Sirolo (Ancona), Italy, from 21 to 25 June 1993

G. Reffo, M.B. Chadwick, A.V. Ignatyuk,
J. Kopecky, D.W. Muir and A.B. Pashchenko

September 1993

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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ABSTRACT

The present report contains the Summary of the IAEA Consultants' Meeting (CM) on "Standard Input Data Sets for Nuclear Model Computations of Nuclear Data", held at Sirolo near Ancona, Italy, from 21 to 25 July 1993. This CM was organized by the IAEA Nuclear Data Section (NDS) with the co-operation and assistance of local organizers of the Centro di Calcolo del ENEA, Bologna.

The purpose of the meeting was to provide the IAEA with technical advice on the Agency's plan to assemble a reference library of numerical data for input to nuclear reaction theory computer programs. Five experts from four countries attended the meeting.

The main objectives of the Consultants' Meeting were achieved to a large extent and, as a result of discussions, the next steps in the work programme were worked out.

The detailed conclusions and recommendations of the CM prepared by the IAEA consultants are included in this Summary Report.

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IAEA Consultants' Meeting on

"Standard Input Data Sets for Nuclear Model Computations of Nuclear Data"

Ancona, Italy
21 to 25 June 1993

(1) Introduction

Following the recommendation of the International Nuclear Data Committee (INDC), an advisory body for the nuclear data programme of the IAEA, the Nuclear Data Section has initiated a new project for the development of the Reference Nuclear Parameter Library for Nuclear Model Computation. This project was rated by the INDC at its March 1993 meeting to be of high priority in the Agency's future nuclear data programme.

(2) Objectives of the Meeting

The purpose of the present meeting was to provide the IAEA with technical advice on the Agency's plan to assemble a reference library of numerical data for input to nuclear reaction theory computer programs; in particular, to advise on the scope, format and work schedule for assembling input data files of atomic masses, shell corrections and deformations, discrete level properties, average neutron resonance parameters, level density parameters, fission barrier and gamma-ray strength function parameters and optical model parameters.

(3) Organization of the Meeting

The meeting was organized by the IAEA Nuclear Data Section (NDS) with the co-operation and assistance of local organizers of the Centro di Calcolo del ENEA, Bologna, and held at Sirolo near Ancona from 21 to 25 June 1993.

Dr. G. Reffo of the Centro Ricerche Energia "E. Clementel" del ENEA, Bologna, was selected as Meeting Chairman and Dr. A. Pashchenko served as Scientific Secretary. The meeting agenda is given below as Attachment 1. The meeting was attended by five experts from four Member States. A list of meeting participants is given in Attachment 2.

The meeting had a full and excellent support from local organizers.

(4) Conclusions and Recommendations

The main objectives of the Consultants' Meeting were achieved to a large extent and, as result of discussions, the next steps in the work programme were worked out.

The meeting participants recommended that the IAEA and interested participants pursue all possible means for providing financial support for this work. However, with respect to central service aspects of the work, especially format conversion codes, online storage and retrieval and related documentation, up to now it has not been able to identify any likely funding source. Therefore it was recommended that the IAEA Nuclear Data Section assume the responsibility for providing these needed central services as part of its future programme of activity. Approximately one-quarter of the time of a programmer-physicist appears sufficient to meet current needs.

It was noted that the above mentioned level of effort will be adequate only if, at the same time, a standing technical committee is formed to assist in the coordination and planning of the project. Such a committee should have 8 - 10 members, drawn from various disciplines that correspond to sublibraries that constitute the parameter library (atomic masses and related data, discrete-level parameters, average resonance parameters, optical model parameters, level density and fission barrier parameters, gamma-ray strength functions), as well as advisors on methods for the evaluation of parameters and their uncertainties.

Actions to increase co-operation were discussed. The meeting participants pointed out that they need to seek an appropriate framework in which scientists can find support, not only for periodic advisory group meetings in which indications are given on how to address and solve the problems, but also for spending time together to work on solving important open problems. More common work is needed to discuss and repeat the necessary analysis calculations.

It was recommended that the Agency investigate possible solutions for finding adequate funding for this joint work.

It was pointed out that the most effective mechanism for the organization of complex activities performed in support of the Reference Nuclear Parameter Library would be to organize the work as a series of the related IAEA Coordinated Research Programmes (CRPs). This meeting concluded that the highest priority for the next CRP would be one to address the evaluation of average neutron resonance parameters and their relation to the level density description. It was stressed that the accuracy of calculated cross sections depends directly on our knowledge of level density and this, in turn, depends sensitively on average neutron resonance parameters such as D_{obs}, average radiative widths, and neutron strength functions. The cumulative number of low lying levels is another type of experimental information that is very important for

any total or partial level-density model, and hence for calculations of cross-sections by statistical methods. In recent years different nuclear data groups have produced different recommended sets of average parameters and there exist large discrepancies among these recommendations. To achieve the accuracy required, for example, for reactor safety analysis or radiation therapy treatment planning, it is therefore urgent to obtain a consensus on more accurate values of these average neutron resonance parameters.

It was pointed out that at the level density meeting in 1989 in Bologna, ENEA Bologna was asked to act as a permanent center for level density research because of the extensive experience of its staff and because of the ideal computer infrastructure available in Bologna. It was recommended that ENEA Bologna include as a part of this activity also the updating of the average resonance parameter file. This center should provide office facilities and travel support for those experts which cannot receive IAEA fellowships, especially those from developed countries which do not have the resources to support international travel for such purposes.

The IAEA consultants noted that it is very important to coordinate this project with related projects in other data centers. For example, both the JAERI Nuclear Data Center and the Chinese Nuclear Data Center have ongoing efforts on parameter library development. It was recommended that these centers be invited to more actively participate in the Agency project.

The detailed conclusions and recommendations of the meeting prepared by the IAEA consultants are presented in Attachment 3 of this report.

(5) Future Meetings

The meeting participants recommended that further development of coordinated efforts be considered at a consultants' meeting on "Reference Nuclear Parameter Libraries for Nuclear Data Computation" which should be organized in Bologna, Italy, in September 1994.

(6) Acknowledgements

The participants very much hope that the recommendations of this meeting may be acted upon by the Agency for the mutual benefit of its Member States.

The participants wish to thank the Agency for focussing much needed attention on the important problems discussed here and wish to thank Dr. Reffo of ENEA Bologna for the efficient organization of the meeting and for the warm hospitality extended to its participants.

Attachment 1

International Atomic Energy Agency

IAEA Consultants' Meeting

on

"Standard Input Data Sets for Nuclear Model Computations of Nuclear Data"

Sirolo (Ancona), Italy

21 to 25 June 1993

PROPOSED AGENDA

Monday, 21 June

08:00 a.m.	Opening of the Meeting Host (G. Reffo) IAEA (A.B. Pashchenko) Election of the Chairman Adoption of the Agenda
08:30 a.m.	Session 1: Model Independent Parameters. 1. Atomic Masses. 2. Shell Corrections and Ground State Deformation Parameters.
12:00 p.m. to 02:00 p.m.	Lunch
02:00 p.m.	Session 1: (continued) 3. Evaluated Discrete Level Schemes.

Tuesday, 22 June

	Session 2: Model Dependent Parameters.
08:00 a.m.	1. Resonance Parameter File.
10:00 a.m.	2. Discussion on Average Resonance Parameters and Tentative Organization of a Starter File.
12:00 p.m. to 02:00 p.m.	Lunch
02:00 p.m.	Session 2: (continued) 2. Discussion on Average Resonance Parameters and Tentative Organization of a Starter File (continued).

Wednesday, 23 June	Session 2: (continued).
08:00 a.m.	3. Optical Model Parametrization: Discussion about the Definition of Universal Formalism/s and Inherent Format/s. Tentative Organization of a Starter File.
12:00 p.m. to 02:00 p.m.	Lunch
02:00 p.m.	Session 2: (continued). 4. Total Level Density Problems: General Discussion on available Approaches and on possible Recommendations. Tentative Discussion on possible Recommendations for Parameter Systematics.
Thursday, 24 June	Session 2: (continued).
08:00 a.m.	5. Level Density for Fission and Fission Barrier Parameters.
09:30 a.m.	6. Partial Level Density: General Discussion on available Approaches and Discussion on possible Recommendations.
12:00 p.m. to 02:00 p.m.	Lunch
02:00 p.m.	Session 2: (continued). 7. Gamma-ray Strength Functions, Recommendations.
04:00 p.m.	Session 3: Conclusions and Recommendations. 1. General Discussion on the Future Scope of the Input Parameter Data Project. 2. Discussion on how to involve more Manpower. 3. Organization of Working Groups to draft the Report of the Meeting. 4. Drafting of Meeting Conclusions.
Friday, 25 June	
08:00 a.m.	Session 3: (continued). 5. Completion of the CM Working Group Reports.
12:00 p.m. to 02:00 p.m.	Lunch

02:00 p.m. Session 4: FINAL CONSIDERATIONS

1. Discussion of Conclusions and Recommendations.
   Drafting of the CM Conclusions and Recommendations.

2. Corrections and Adoption of the Final Report.
   Adoption of Schedule for Work and Future Meetings.

3. Closing of the CM.

Attachment 2

Consultants' Meeting on

"Standard Input Data Sets for Nuclear Model Computations of Nuclear Data"

Ancona, Italy

21 to 25 June 1993

LIST OF ATTENDEES

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Attachment 3

CONCLUSIONS AND RECOMMENDATIONS

of the

IAEA Consultants' Meeting on

"Standard Input Data Sets for Nuclear Model Computations of Nuclear Data"

Ancona, Italy
21 to 25 June 1993

1. LIBRARIES OF MODEL PARAMETERS

1.1. Model Independent Parameters

1.1.1. Atomic Masses, Shell Corrections and Deformation Paramters

A report has been distributed describing a starter file on atomic masses [1]. The file has been delivered to the Agency for distribution. This consists of experimental atomic masses of A. Wapstra et al. [2] and of model calculations by P. Möller [3], with shell and pairing corrections. We are aware of updating efforts by P. Möller and by G. Audi and we look forward to their future contributions to this project.

Recommendations

The ground state deformation parameters from the Los Alamos group have not yet been obtained. D. Muir has been asked to contact P. Möller in order to obtain his deformation parameter file [4], as well his latest updated mass compilation.

1.1.2. Evaluated Discrete Level Scheme

Starter files are available from Obninsk [5], Bruyères-le-Châtel [6] and Bologna [7], for details see the summary report of the previous meeting, section 1.1.3, ref. 8.

Recommendations

There is a clear necessity to develop a single recommended file which must be continuously updated to take into account recent additions to ENSDF. To this end format translation codes are needed.

1.2. Model Dependent Parameters

1.2.1. Average Resonance Parameters

Since the last meeting, in addition to the Mughabghab compilation [9], now we have available for comparison 3 newer files that can be distributed as starter files. These have been delivered by Obninsk [5], Bologna [7] and by the Chinese Nuclear Data Center [10].

A comparison has been made between the recommendations of Bologna and Obninsk which indicated that for approximately 20% of the nuclei there exist differences exceeding 30%.

Recommendation

Discrepancies found among the different files should be resolved by a meeting of principal investigators, with the aim of arriving at a single recommended file. As an initial step all available files should be merged in tabular form by the Nuclear Data Section. This will allow a direct comparison of the parameters in various libraries and could also be used by the users as preliminary values in applied calculations.

We would appreciate it if the Chinese average resonance file that has been made available to the Agency could be supplemented with the full documentation of their analysis. We should very much welcome a member of the CNDC in this Agency project both to illustrate the detail of the work produced and to have the benefit of suggestions from the CNDC.

We also would appreciate it if JAERI Nuclear Data Center would supply the Agency their file of recommended parameters.

There are new experimental data sets of neutron resonance parameters that should be incorporated into future analyses.

The Bologna table for total radiative widths of neutron resonances was discussed, and we recommend that, in addition to the standard deviation of the Chi-squared distributions, the measurements errors be included.

1.2.2. Optical Model Parameter Sets

The essence of the problem was already outlined in the previous meeting [8]. Acting on a recommendation of that meeting, during the 1992 Trieste courses of Nuclear Theory for Applications, J.J. Schmidt initiated an activity aimed at the compilation of computer-accessible Optical Model Parameters published after the 1976 Perey's [11] compilation.

This meeting appreciates this prompt response to this need, and we very much hope that the activity will continue to be supported by the Agency.

Recommendations

The optical model compilation of Bruyères-le-Châtel, Obninsk and Bologna should be transmitted by the Nuclear Data Section to M. Avrigeanu. The Bologna file provides an example in which a general comprehensive potential form has been adopted together with a format that make the parameter sets easily computer-retrievable. We believe it essential that the compilation being made by J.J. Schmidt and M. Avrigeanu exhibit this same features.

We think that compilations are not a complete solution to the problem and believe that some selections of recommended potentials by optical model experts is necessary. Such a selection of local and global potentials might be analogous to (and influenced by) the reviews of P.G. Young and by P.E. Hodgson in Paris [12] and by Takaaki Ohsawa [13].

The expertise gained in various laboratories like Bologna, Obninsk, Los Alamos, Livermore and Bruyères-le-Châtel, for example, must be taken as a starting point for discussions of recommendations and we suggest that an ad hoc meeting should take place at the occasion of the Gatlinburg International Conference on Nuclear Data for Science and Technology to document and preserve this expert knowledge.

We imagine, then, that this parameter project would eventually produce two results, namely,

(1) a large compilation of all optical-model parameter sets without any specific recommendations,

(2) a document drawn upon the experience and guidance of experts, recommending optical-model parameter sets for local and global optical models, for different projectiles, and for nuclei covering the periodic table.

These two activities should be mutually supportive and continued in parallel.

1.2.3. Total Level Density

Our recommended model for level density description, as disucssed in our previous report [8] is that of A. Ignatyuk et. al. [14].

The Agency has received level density parameter systematics on diskettes based upon Obninsk and Bologna neutron resonance parameter analyses.

Recommendations

We have new sets of evaluation of D_{obs}, low lying levels, and shell corrections which provide the possibility of a re-evaluation of previous level density parameter systematics. These would considerably improve the reliability of level density calculations and consequently of cross section calculations.

The main problem which needs to be solved is the provision of financial support for the travel of experts to enable them to carry out this joint work.

Recently a subgroup on level density has been approved in the frame of the IEC (International Evaluation Cooperation) Working Party of the NEANSC. Even though this new subgroup is limited to the major isotopes of Fe, Cr, and Ni, we recommend that the Agency's activities takes the results of this subgroup into account.

1.2.4. Partial Level Density

In addition to microscopic approaches available from Bologna, a calculational effort of partial level density for nuclei in the s-d region using the SU3 symmetry group method has started, in order to investigate the effect of configuration mixing on partial level density. This effort is being carried out in a cooperation between the Ohio University and Obninsk.

There exists some progress by Anzaldo on an improved formula for an equispaced Fermi gas model which should appear shortly in Z. Phys.

Another recent development in the theory of partial level density is the work of M. Chadwick and P. Obložinský [15] in which the linear momentum structure of the level density is considered. This allows a new and straightforward determination of angular distributions in preequilibrium reactions.

Recommendations

In addition to the use of the particle-hole systematics from Bologna, we recommend that M. Chadwick and M. Herman produce a document which reviews the status of partial level density approaches with special emphasis on applications.

1.2.5. Level Density for Fission

Fission barrier values from the G. Smirenkin and A. Ignatyuk groups for actinides have been delivered on diskettes. These parameters can be taken as a starter file for the parameter library purpose.

Recommendation

The parameters obtained by A. Ignatyuk correspond to level density parameters for the fission channel obtained in a way consistent with the level density obtained from neutron resonance analysis of actinides. After the re-analysis of the experimental data for neutron resonances in conjunction with Bologna and other groups, we recommend that the corresponding necessary revision of the parameter for fission channels be performed.

The planned cooperation between Obninsk and Los Alamos will be welcomed in this context.

1.2.6. Gamma-ray Strength Functions Parametrization

The approach of Kopecky-Uhl for gamma-ray strength functions, as described in ref. [8], was shown to work well for almost the entire periodic table, except highly deformed nuclei [16,17]. It is important to study the physics behind this problem.

Well documented, model independent evaluations of experimental strength functions for E1 and M1 transitions are available [18].

The application of recent D_{obs} (see section 1.2.1.) will improve the understanding of strength function fluctuations beyond the expected width fluctuation effect.

Recommendations

We recommend that J. Kopecky update the strength functions using the newly evaluated D_{obs}.

In addition to the parametrization of giant resonance parameters by Dietrich and Berman, see ref. [8], there are several semiphenomenological systematics available. We recommend that J. Kopecky provide a collection of these systematics to the NDS.

We consider the contribution of M. Uhl very beneficial to the further development of the gamma-ray strength function model parametrization and recommend his continued involvement.

2. GENERAL RECOMMENDATIONS AND CONCLUSIONS

(1) The meeting participants recommended that the IAEA and interested participants pursue all possible means for providing financial support for this project. However, with respect to central service aspects of the work, especially format conversion codes, online storage and retrieval and related documentation, up to now we have not been able to identify any likely funding source. Therefore we recommend that the IAEA Nuclear Data Section assume the responsibility for providing these needed central services as part of its future programme of activity. Approximately one-quarter of the time of a programmer-physicist appears sufficient to meet current needs.

The above mentioned level of effort will be adequate only if, at the same time, a standing technical committee is formed to assist in the coordination and planning of the project. Such a committee should have 8-10 members, drawn from various disciplines that correspond to sublibraries that constitute the parameter library (atomic masses and related data, discrete-level parameters, average resonance parameters, optical model parameters, level density and fission barrier parameters, gamma-ray strength functions), as well as advisors on methods for the evaluation of parameters and their uncertainties.

(2) The most effective mechanism for the organization of complex activities performed in support of the Reference Nuclear Parameter Library would be to organize the work as a series of related IAEA Coordinated Research Programmes (CRPs). This meeting concluded that the highest priority for the next CRP would be one to address the evaluation of average neutron resonance parameters and their relation to the level density descriptions.

The accuracy of calculated cross sections depends directly on our knowledge of level density and this, in turn, depends sensitively on average neutron resonance parameters such as D_{obs}, average radiative widths, and neutron strength functions. The cumulative number of low lying levels is another type of experimental information that is very important for any total or partial level-density model, and hence for calculations of cross sections by statistical methods. In recent years different nuclear data groups have produced different recommended sets of average parameters and there exist large discrepancies among these recommendations.

To achieve the accuracy required, for example, for reactor safety analysis and radiation therapy treatment planning, it is therefore urgent to obtain a consensus on more accurate values of these average neutron resonance parameters.

(3) At the level density meeting in 1989 in Bologna, ENEA Bologna was asked to act as permanent center for level density research. It was recommended that ENEA Bologna include as a part of this activity also the updating of the average resonance parameter file.

We need to seek an appropriate framework in which scientists can find support, not only for periodic advisory groups in which indications are given on how to address and solve the problems, but also for spending time together to work on solving important open problems. More common work is needed to discuss and repeat the necessary analysis calculations.

We recommend that the Agency investigate possible solutions for finding adequate funding for this work.

(4) It is very important to coordinate this project with related projects in other data centers. For example, both the JAERI Nuclear Data Center and the Chinese Nuclear Data Center have an ongoing efforts on parameter library development. We recommend that these centers more actively participate in the Agency project.

3. FUTURE MEETINGS

The meeting participants recommended that further development of coordinated efforts be considered at a Consultants' Meeting on "Reference Nuclear Parameter Libraries for Nuclear Data Computation" which should be convened in Bologna, Italy, in September 1994.

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