International Atomic Energy Agency

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INTERNATIONAL NUCLEAR DATA COMMITTEE

REFERENCE NUCLEAR PARAMETER LIBRARY FOR NUCLEAR DATA COMPUTATION

Summary Report of a Consultants' Meeting
organized by the International Atomic Energy Agency
and held in Vienna, Austria, 13-15 November 1991

Prepared
by

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and

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IAEA Nuclear Data Section
Vienna, Austria

January 1993

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

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IAEA Nuclear Data Section
Vienna, Austria

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Abstract

The present Report contains the Summary of the IAEA Consultants' Meeting on the "Reference Nuclear Parameter Library for Nuclear Data Computation". The Meeting Conclusions and Recommendations and practical steps and actions to be taken under guidance and/or under the sponsorship of the Agency for assembling a reference library of nuclear model input parameters are included in this Summary Report.

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Summary of the Meeting

An important trend in the evaluation of neutron and charged-particle nuclear reaction data at low energies (0-30 MeV) is the increased use of nuclear reaction theory codes to compute the required cross sections and spectra. As a method of evaluation, such "model" codes offer many advantages over simple, unphysical curve fitting.

A barrier to the wider use of the more complete physical models is that they require a large volume of numerical input data. The most important input data types are

(a) atomic masses;
(b) shell corrections;
(c) deformations;
(d) discrete-level properties (energy, spin, parity, decay branching ratios);
(e) average neutron resonance parameters [D_0, S_0, S_1, $\Gamma_\gamma(J,\pi)$];
(f) optical model parameters;
(g) fission barrier parameters;
(h) level density parameters;
(i) γ-ray strength function parameters.

To this end a Consultants' Meeting was convened by the International Atomic Energy Agency in order to provide the Agency with technical advice on its plan to assemble a reference library of nuclear-model input parameters.

Since the project to create a reference library of parameters is still at a very early stage, it was necessary to review in broad terms the needs of the data modelling and evaluation community, the opportunities provided by recent advances in both physics and computers, and the difficulties that may impede future progress.

The scope of the meeting included both

* solutions that are practical immediately or in a short time and that are based on selected methodologies, codes and parameterizations currently in use;

* proposals for solutions, to be pursued over a longer time period, aimed at providing better physical understanding of nuclear-reaction phenomena;

Accordingly a number of practical steps and actions have been proposed, to be taken under the guidance and/or under the sponsorship of the Agency.

#6015N

1. Libraries of Model Parameters

1.1 Model Independent Data

1.1.1 Atomic Masses

Atomic masses are needed in a number of investigations and calculations, including nuclear-model cross-section calculations. In some applications (such as cross sections for the r-process in nuclear astrophysics), it is important also to have nuclear masses even for exotic nuclei quite far from the valley of stability.

Recommendations:

- We recommend the use of the latest issue of the Wapstra, et al., data tables (Ref. 1). For missing nuclei it is recommended to use the Möller et al. mass formula (Ref. 2).

- The Agency should make the merged data tables available on file (Ref. 3).

1.1.2 Shell Corrections and Ground State Deformation Parameters

The necessity was felt to have available a file of shell corrections and ground state deformations.

- It is recommended that the Agency contact the Los Alamos Nuclear Theory Group in order to get from them a file containing both types of information.

1.1.3 Evaluated Discrete Level Schemes

One of the most time-consuming activities in nuclear model code input preparation is the creation of evaluated data files describing the discrete-level structure for all the residual nuclei involved in a complex nuclear reaction.

This activity generally begins with retrievals from the Evaluated Nuclear Structure Data File (ENSDF), which is maintained by the U.S.A. National Nuclear Data Center based on contributions from a data-evaluation network co-ordinated by the IAEA. It is important to recognize that the ENSDF contains adopted data for levels observed in experiments, which in many cases must be supplemented by additional data (J, π, branching ratios) in order to be used for practical cross section calculations. It was noted that some institutes or laboratories have already generated local libraries of evaluated discrete level schemes, derived from the basic information in ENSDF in this way. It was also noted that each group has its own format and corresponding code system for manipulating the data.

There are available the following two files:

- Bologna-Livermore file
  (directly usable as it is for nuclear data evaluation; contains about 1500 level schemes, with gamma branching ratios and decay schemes available for about 30% of them);

- Bruyères-le-Châtel file
  (essentially a compacted form from ENSDF; contains all nuclei);

- Obninsk file
  (compacted form from ENSDF; contains level schemes, with gamma branching ratios and decay schemes).

Recommendations:

- We recommend that the discrete level files not be burdened with extraneous information beyond what is necessary for the computation of nuclear reaction data, so the file will be limited to level energy, spin and parity, complete γ-decay schemes and conversion coefficients.

- The file format of Bologna should be used, with the introduction of conversion coefficients.

- It is agreed to have a starter file consisting of the semievaluated Bologna - Livermore file, supplemented where necessary by the Bruyères-le-Châtel file, after convertion into the Bologna format.

- The Agency should provide one person (for example, from IEAV - Sao José dos Campos, SP, BRAZIL) for a suitable length of time to be spent in Bologna and in Bruyères-le-Châtel (BRC) with the task of caring for the implementation into the Bologna file of the missing nuclei. This effort should lead to the creation of a code that converts ENSDF data to the Bologna format, taking advantage of the existing BRC code that already performs part of the required translation.

- It should be the task of the Agency to encourage evaluators to arrive at a file of complete evaluated level schemes, based on both experimental and evaluated data, with complete information in the energy region where no level loss is suspected.

- It should be the responsibility of the Agency to store and distribute the library and associated computer programs. It is expected that updates will be sent to the Agency by the responsible specialists whenever major updates are finalized.

2. Model Dependent Data

2.1 Average Resonance Parameters

Four sets of average resonance data (D_o, S_1 and $\Gamma_\gamma(J,\pi)$) are available. They originate from BNL (Mughabghab et. al., Ref. 4), Bologna (to be submitted to Atomic and Nuclear Data Tables), Obninsk (Ref. 5) and CNDC (Ref. 6).

Bologna and Obninsk offered to provide a critical comparison of the available parameter tabulations, provided an exchange of visitors can take place.

Recommendations:

- Bologna and Obninsk should perform the critical intercomparison of the four available files and produce a set of recommended values.

- An update activity of the BNL compilation of resonance parameters (Ref. 4) should be performed.

2.2 Optical Model Parameter Sets (OMP)

One of the concerns of evaluators is the tremendous amount of information on optical model parameterization buried in the literature.

The only large-scale attempt to make such information available to scientists as a single unified data set was published by Perey in 1976 (Ref. 7).

During this meeting it was pointed out how useful it would be to have such a compilation updated and available also as a data file directly accessible from cross section codes.

In order to make available all the work appearing in the literature after the compilation by Perey, it is necessary to consider how to organize a new compilation of optical model parameters.

The Consultants' Meeting is aware of the problems arising from the different types of parameter sets (such as global, regional, local, non-local) and many different types of potentials existing in the literature.

In order to create such a file, it is necessary first to categorize the different optical models and formulations and hence to define the format.

Such a complicated process obviously needs careful specialized consideration, so we considered that the establishment of such a group for this purpose might be considered by the Agency in the future.

Also it was pointed out that generally the optical model potential for statistical model calculations at lower energies for neutrons are relatively well defined. The situation with respect to the charged particle OMP is not relatively well defined. For example the OMP data for charged particles are obtained from high energy data and therefore are expected to give poor results for calculations near threshold (≈ 5 MeV).

After considering the present complex status of OMP data, the committee orientation is to address efforts towards <u>compilation</u> and not <u>recommendation</u> which should be made at a later stage. The survey of recent literature on OMP can be aided by INIS retrievals at the IAEA. The compilation effort should involve interaction with the authors to ascertain the correct applicability of the published OMP data.

Recommendations:

- To limit the compilation to incident particles: neutrons, protons and alpha particles, up to 30 MeV.

- Efforts should be made to obtain information in Perey's data in electronic format.

- To take into account the information in the NEA specialists' Meeting held in Paris in 1985 (Ref. 8), as well as in recent IAEA Co-ordinated Research Programmes (Ref. 9).

- To consider the possibility that an effort like that of Perey could be undertaken as an activity of the faculty members of interested universities.

- Each OMP set should have a specification about which experimental data have been used (total, elastic, polarization, angular distribution, etc.), energy range where the set was found, mass range, particle type, optical model approximation used.

- As an interim near-term step, it would be useful if the ORNL, BRC and Obninsk groups would submit to the Agency a set of sources of recommended global and regional OMP sets.

2.3 Fission Barrier Parameters

The Consultants' Meeting suggested including in the parameter library the necessary information for fission-barrier parameterization.

In addition to the parameterization of J.E. Lynn at AERE there is the work of J.W. Behrens, H.C. Britt, A.V. Ignatyuk and G.N. Smirenkin (Ref. 10-14).

Recommendations:

- The fission-barrier data from the Obninsk work should be complemented by the regional sets of level density parameters for actinides as discussed in the following section 2.4.3.

2.4 Level Density Parameters

2.4.1 Total Level Density Parameters

From a review of recent work aimed at gaining a better understanding of the problem, we can now foresee the possibility of soon having new approaches ready for parameter systematics studies.

In particular the efforts in Obninsk, in India and in Bologna appear to offer excellent prospects for a useful cooperative effort under the auspices of the Agency.

It was pointed out that the approach adopted in Obninsk apparently is the only one that takes into account the energy dependence of the level density parameter as well as collective effects. The special features included in this approach make it useable also for fission level density needs.

Recommendations:

- It was recommended to use the level density approach suggested by Ignatyuk (Ref. 15). This has to be coupled with results of the parameter systematics work done in Obninsk (Ref. 16).

- The above mentioned systematics were based on the compilation by Mughabghab (Ref. 4) and other data available at that time. It was recommended to update them by use of the more recent D-values from the forthcoming intercomparison to be performed within the collaboration Bologna-Obninsk, mentioned in section 2.1.

- It was strongly recommended that the Agency take action to encourage the collaboration between the Obninsk, Bologna and Indian groups.

2.4.2 Partial Level Density Parameters

There is no large selection of approaches in this case. The group in Bologna has recently published an attempt to compute partial level density in the frame of BCS theory. This work makes use of combinatorial calculations, applied to a basis of shell model Hamiltonian eigenvalues. They have shown that the Williams formula is not always reliable.

Recommendations:

- For practical applications the Williams formulae (Ref. 17) can be used as a rough approximation (but not close to magic numbers and not for high exciton numbers).

- For more realistic calculations the users are referred to the methods published in (Ref. 18-21).

2.4.3 Level Density Parameters for Fission

It was concluded that the approach proposed by Ignatyuk for treating collective enhancements also applies to the fission level density, which supports the need for the level density collaboration recommended in the above 2.4.1.

Recommendation:

- An action has been given to Obninsk to make these parameters available in a table including the fission barriers.

2.5 Gamma-ray Strength Function Parameterization

There has been a long dispute about the reliability of the Brink-Axel approximation, used for the determination of the outgoing gamma channel parameters. Criticism has centered on certain simplifying assumptions that are normally made. This concern is quite justified in view of the impact that such assumptions have in certain calculations, such as isomeric ratios.

At the meeting it was noted that recent progress has been achieved on this subject by Kopecky and Uhl (Ref. 22) for spherical nuclei. The improvements can be summarized as follows:

- the excitation-energy dependence of the target absorbing gamma rays has been accounted for by introduction of an energy dependence of the Lorentzian half-width.

- a physically plausible finite limit for the gamma-ray strength function at zero gamma-ray energy has been assumed.

With these improvements a better comparison with experiment has been obtained, while the entire treatment appears much more realistic.

Recommendations:

- For E1 transitions in spherical nuclei to use the Kopecky-Uhl approach (Ref. 23), and for rare earth nuclei to use the standard split Lorentzian. (It should be kept in mind that the predictive accuracy of this approach is ~ 30%. The normalization to the total average radiative width of neutron resonances improves the accuracy of capture calculations which are important for the purpose of evaluation.)

- For M1 and E2 transitions to use the Brink-Axel approach with Kopecky systematics (Ref. 23).

- The Agency should distribute in electronic format the compilation of the giant resonance parameters by Dietrich and Berman (Ref. 24), which is being prepared at the CNDC-IAE in Beijing (Ref. 25).

- Concerning giant resonance parameter systematics, the existence of two semiphenomenological systematics has been pointed out, one by Bergère (Ref. 26) and one by G. Reffo (Ref. 27).

2.6 Future Meetings

The meeting participants recommended that further development of co-ordinated efforts be considered at a Consultants' Meeting on "Reference Nuclear Parameter Library for Nuclear Data Computation" which should be organized in Bologna, Italy, in June 1993.

Conclusions

We feel that the recommendations formulated at this meeting, are in tune with and enforce the traditional role of the Agency in the organization of joint efforts and in the dissemination of scientific information and know-how for peaceful applications of nuclear science.

We hope very much that the modest contribution from this meeting may be pursued further by the Agency in the mutual benefit of its Member States, especially those which need more help, understanding and solidarity.

We wish to thank the Agency for the warm hospitality and, most of all, for focussing much needed attention on the important problems discussed here.

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Appendix 1

IAEA Consultants' Meeting on a Reference Nuclear Parameter Library for Nuclear Data Computation
IAEA Headquarters, Vienna
13-15 November 1991

Main Meeting Room = A-1972
Working Group Room "A" = A-2413 (INIS Conference Room)
Working Group Room "B" = A-2340 (NDS Library)

AGENDA

Wednesday, 13 November 1991
9:30

I. Organization Matters, CRP Final Report, Adoption of Agenda for CM
II. Informal Presentations (A. Ignatyuk, chairman)

13:00-14:30
Lunch

14:30-17:30
III. Working Group/Plenary (G. Reffo, chairman)

(a) ground-state masses, Q-values, thresholds;
(b) discrete-level properties (energy, spin, parity, deformation parameters, decay branching ratios)
(c) average resonance parameters (D-sub-0, S-sub-0, Gamma-sub-gamma(spin,parity))
(d) optical model parameters (global, regional, individual)
(e) fission barrier parameters
(f) gamma-ray strength functions.

17:30
Agency Hosted Recception, Working Group Room "B"

Thursday, 14 November 1991
9:30

III. Working Group/Plenary (continued)

13:00-14:30
Lunch

14:30-18:00
III. Working Group/Plenary (continued)

Friday, 15 November 1991
9:30
IV. Drafting of Meeting Conclusions

13:00-14:30
Lunch

14:30-18:00
V. Wrap-up Session/Plenary

(a) Discussion/correction of Draft Meeting Conclusions
(b) Adoption of schedule for work and future meetings

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Appendix 2

IAEA Consultants' Meeting on

"Reference Nuclear Parameter Library for Nuclear Data Computation"

13-15 November 1991, IAEA Headquarters, Vienna
Meeting Room A1972, ext. 1381

LIST OF PARTICIPANTS

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November 1, 1991

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Dear Doug,

I am enclosing Tom Burrows' thoughts on the kinds of data required for nuclear model calculations. I hope you will find them useful during your upcoming meeting, "Reference Nuclear Parameter Library for Nuclear Data Computation".

As you know, it has been nearly 20 years since I worked actively in the nuclear model field. I would not have had much to add to the discussions on the types of data which should be included in such a library. However, I have some general ideas about what will be required in the future and how the work might be organized. Since, I will not be able to attend, I am writing this letter to give you a flavor of what I might have said.

Nuclear data libraries are essential to the development and maintenance of nuclear based technologies. Originally almost all nuclear data was provided by measurement programs. Over time, nuclear theory has developed and become an important source of evaluated nuclear data. The nuclear measurement program could never supply all of the needed data, so results of theoretical programs have been assimilated in order to supplement the measurement results. It has become alarmingly clear recently that the measurement programs in the US and in Western Europe are declining with the shut down of facilities and the retirement without replacement of many of the experimentalists. It would be a disaster if either Western Europe or the US should lose all its experimental capacity. If we assume that enlightened minds will not allow that to occur, then how will we meet the nuclear needs of the future with extremely limited experimental capability.

The answer must be to devote increased resources to the development and application of nuclear theory to meet new data requirements. If this is to be successful, the current activity in the theory area needs increased coordination. This coordination should have as one crucial component, the production of a single reference-parameter data base. The data base should have an agreed processing-oriented format and a package of associated codes which everyone can use. The data entered into this file should be "evaluated" and "benchmarked" against experimental data measurements. The file should contain all the parameters which are required as input data for the important nuclear models and the programs which do calculations based on these models. The format cannot be tied exclusively to any one or several existing programs. It must be general and expandable. Output modules will have to be developed to prepare input data for any given nuclear model code.

It is very possible that the role of experimental measurement programs will change from being basic data providers to the role of making the "benchmark" measurements which will be required to validate models and calculational results. I believe that we should start now to prepare for this developing scenario. Collection and distribution of existing parameter libraries can only be a temporary measure. I hope that your meeting will have time to address these more general issues and recommend a program for solving them.

I am sorry that I will not be able to present these ideas in person. Good luck and I hope you have a successful meeting.

Sincerely,

Charlie

Charles Dunford

DATE: November 1, 1991

TO: C.L. Dunford

FROM: T.W. Burrows

SUBJECT: Nuclear Structure Data for the Nuclear Model Data Base

The nuclear structure portion of the proposed nuclear model data base should probably consist of the bound state properties and their deexcitation patterns. The basic organization would be by nuclide and then level. All information should be given in standard units (*e.g.*, eV or keV for level energies and seconds for half-lives). This file should be either people readable or have associated with it a simple translator to put it into a easily read format. There would also have to be a code to translate from ENSDF to this format and an interactive code or module to select information from the nuclear structure file.

The contents and structure of this portion of the proposed nuclear model data base should be complete and versatile enough to meet the current requirements and possible new requirements. A possible basic structure of the file would be:

Nuclide This would consist of at least a unique identifier and the creation or revision date of the nuclide.

Level The following information would be stored:

1. Level energy and uncertainty (center of mass)
2. Spin and Parity. An unresolved question is how to handle multiple spin and parity assignments. Should we give just the first one listed in ENSDF or give up to a maximum of perhaps four and allow the user *via* to select one.
3. Half-life and uncertainty. Need for this quantity will probably be application dependent. For example, if one were interested in prompt photon production, the half-life could be used to end the calculation of the cascade γ intensities. This quantity would also be of interest in the calculation of isomer production ratios.
4. Number of decay modes. With the exception of some ground states and isomeric levels this will be one since we are dealing only with bound states. The need for this information may again be application dependent; for example, the 0^+ ground state of ^{212}Po has a $0.298\mu s$ half-live and, thus, its α radiation might reasonably be

considered prompt.

Decay Modes For each decay mode, the following information would be stored:

1. Decay mode identifier
2. Fractional decay and uncertainty
3. Nuclide fed
4. Number of radiations for this decay mode

Radiations For each type of radiation, sufficient information would be stored so that the production cross section of the radiation could be calculated and its cascade followed. In the case of γ's which will dominate the file this would consist of the following:

1. Gamma energy and uncertainty (laboratory system)
2. Total ($I_{\gamma+ce}$) fractional branching ratio and uncertainty
3. Level fed
4. Photon fractional branching ratio and uncertainty
5. Conversion electron fractional branching ratios and uncertainties.
6. Pair production fractional branching ratio and uncertainty

Data for other radiations would be stored similarly

Most of the data would be obtained from the Adopted Levels, Gamma data sets. When I originally worked on a code to do this, gammas were not included in the adopted data sets. Now with the exception of $A = 21 - 44$ and a few other cases all nuclei have these data where relevant (Before the next *Table of Isotopes* is produced all nuclides will have these data). The ENSDF decay data sets would be used to obtain the remaining radiation information.

COMMENTS ON REFERENCE NUCLEAR PARAMETER LIBRARY FOR NUCLEAR DATA COMPUTATION

C.Y. Fu

At the request of D.C. Larson, I report a few observations I have made from an ongoing project that may be of interest to the participants of the upcoming meeting on Reference Nuclear Parameter Library for Nuclear Data Computation. The observations are the results of my involvement in the NEACRP/NEANDC Intercomparison of ^{52}Cr, ^{56}Fe, and ^{58}Ni cross sections in the ENDF/B-VI, JEF-2/EFF-2, and JENDL-3 evaluations. As ecpected, most of the discrepancies found among the evaluations are in areas where there are little or no experimental data and the evaluations were based on model calculations. The members of this NEACRP/NEANDC subgroup are now trying to resolve these discrepancies by studying the differences in the models used and the differences in their input parameters.

The work is far from complete but some useful information has already emerged. The following comments are precise only for ^{58}Ni but the implications are quite general.

Optical Model Parameters

In trying to compare the effects of the optical model parameters used for ENDF/B-VI and EFF-2 in the TNG code, I found that I had to modify TNG to accept the neutron parameters used for EFF-2 developed by Mario Uhl. Uhl started with the Rapaport set but had to introduce energy-dependent radii and diffusenesses in order to fit the total cross sections down to 1 MeV. The input of TNG does not at present accommodate energy-dependent radii and diffusenesses.

This raises the question of how general the format of the parameter library should be for the phenomenological optical model. Similar questions could be raised for deformed, microscopic, or dispersive optical models.

Level Densities

ENDF/B-VI (TNG code) and JENDL-3 (PEGASUS code) used the Gilbert-Cameron formulas while EFF-2 (MAURINA code) had the backshifted model. The two types of level density formulas, when fitted to the same discrete levels and the same s-wave level spacing, give different energy shapes, particularly above the neutron separation energy. An exact conversion does not exist.

At high excitation energy, perhaps above 15 MeV, the Ignatyuk correction for the disappearance of shell effects is needed. This is now used in several codes, including the widely used code GNASH.

Whether one uses the backshifted or the Gilbert-Cameron, with or without the Ignatyuk correction, the meaning of the Fermi-gas parameter 'a' is different because of the different manner the pairing and shell corrections enters the formula.

The number of discrete levels used can influence the determination of the level density parameters. The calculations for the three evaluations used different number of discrete levels for ^{58}Ni. The cutoff energy for discrete levels used varied between 3.5 MeV and 4.6 MeV. Because there is a large concentration of levels between 3.5 and 4.6 MeV in ^{58}Ni, level densities fitted to the discrete levels are also different.

Therefore before one compiles the level density parameters, one must define the formulas and the way the level densities are matched to the discrete region. I have heard comments that the backshifted model has little theoretical justification at high excitation energy but cannot recall who made the comments.

Differences in Precompound Models

The precompound models used for ENDF/B-VI (TNG), Eff-2 (MAURINA), and JENDL-3 (PEGASUS) are different. In particular, the α-preformation factors used in the various models have completely different definitions. These definitions were given by: Kalbach for ENDF/B-VI, Milazzo-Colli for EFF-2, and Iwamoto-Harada for JENDL-3. Therefore, input parameters for the precompound part of one code have absolutely no meaning for another.

The precompound models are at present very diverse. Fifteen years ago we already heard of three: the exciton model of Griffin, the hybrid model, and the master-equation approach. Then there emerged several options for the complex-particle preformation factors, several approximations to conserve angular momentum, many attempts at computing angular distributions, photon emission models, and several quantum-mechanical models.

I would recommend that parameter compilation for the precompound models be put off for the moment.

Concluding Remark

At present if I were to do a evaluation, I would be happy if someone could tell me what level density parameters to use, at least what to start with. Suppose the valuation were for a medium mass nuclide below 20 MeV, I would need at least seven sets of level density parameters corresponding to the residual nuclei of the (n,γ), (n,n'), (n,2n), (n,np), (n,nα), (n,p), and (n,α) reactions. Some of the residual nuclei have no neutron resonance data, hence no directly measured level spacings. A model to interpolate between and to extrapolate from measured level density data seems a good and important area for research.