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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

Summary Report of the IAEA Consultants' Meeting on "CHARGED-PARTICLE AND PHOTONUCLEAR DATA LIBRARIES FOR FENDL"

hosted by the U.S. National Nuclear Data Center
at the Brookhaven National Laboratory, Upton, New York 11973, U.S.A.
8-9 October 1992

Prepared
by

A.B. Pashchenko
IAEA Nuclear Data Section
Vienna, Austria

January 1993

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Abstract

The present Report contains the Summary of the IAEA Consultants' Meeting on the Charged-Particle and Photonuclear Data Libraries for FENDL, which was hosted by the U.S. National Nuclear Data Center (NNDC) at the Brookhaven National Laboratory, Upton, NY, U.S.A. and held from 8-9 October 1992. This CM was organized by the IAEA Nuclear Data Section (NDS), with the co-operation and assistance of local organizers from the Lawrence Livermore National Laboratory and the U.S. National Nuclear Data Center.

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IAEA Consultants' Meeting on

"Charged-Particle and Photonuclear Data Libraries for FENDL"

8-9 October 1992
Brookhaven National Laboratory, Upton, New York, U.S.A.

(1) Introduction

This meeting was organized in response to a recommendation of the IAEA Advisory Group Meeting on "FENDL-2 and Associated Benchmark Calculations", held in Vienna from 18 to 22 November 1991. The basic objective of the recommended meeting was to assess the requirements, present status and availability of evaluated charged-particle and photonuclear data files for the IAEA Fusion Evaluated Nuclear Data Library (FENDL) Project. Therefore, special emphasis was placed on the discussion of discrepancies revealed in the thermonuclear reaction cross sections for the hydrogen and helium isotopes from the most important charged-particle nuclear data libraries (CPNDL files): ECPL-92 (Lawrence Livermore National Laboratory) and ECPNDL (Institute of Experimental Physics, Arzamas) with the purpose to come to an agreement on what to use for FENDL.

(2) Organization of the Meeting

The meeting was organized by the IAEA Nuclear Data Section (NDS) with co-operation and assistance of local organizers from the Lawrence Livermore National Laboratory and the US National Nuclear Data Center. The meeting occurred immediately proceeding the BNL-92 Symposium on Nuclear Data Evaluation Methodology in order to maximize the interactions between the data developers and users. The meeting agenda is given below as Attachment 1. The meeting was attended by 16 scientists from 6 Member States. Scientists working in the field from Brookhaven National Laboratory and from the National Nuclear Data Center were also invited to participate in the meeting. A list of these participants is given in Attachment 2. Dr. Roger M. White of Lawrence Livermore National Laboratory, Livermore, California, U.S.A., was selected as meeting Chairman. During the meeting the participants formed two working groups to address thermonuclear and photonuclear matters separately. These groups were chaired by R.M. White and S.I. Warshaw respectively.

(3) Summary of Conclusions and Recommendations

A major overall conclusion of the meeting is that the ENDF/B-VI charged-particle sublibrary for the important energy-producing charged-particle reactions for fusion energy applications, i.e., $D(d,n)^3He$, $D(d,p)T$, $T(d,n)^4He$, $T(t,2n)^4He$ and $^3He(d,p)^4He$, be adopted for the FENDL project. In this sense, the previously worrisome "discrepancies" between thermonuclear reaction cross-sections for helium and hydrogen isotopes from different data files have been resolved. However, a difference of ~4% still exists in the low-energy cross section for the $T(d,n)^4He$ reaction, which is larger than the uncertainty placed on this cross section by the evaluators. The participants recommended that the evaluations of the $T(d,n)^4He$ reaction be investigated at low energy by evaluators from three laboratories (Arzamas, Russia; Los Alamos and Livermore, U.S.A.) so that this difference can be resolved. Also, participants recommended that the FENDL library be expanded to include angular distribution data for the reactions listed above and integrated cross sections and angular distributions of the reactions between the isotopes of hydrogen and lithium, beryllium and boron. In addition, it was recommended that an ENDF/B-VI format extension for charged-particle representations be adopted.

The participants noted that the analysis of nuclear processes for the International Thermonuclear Experimental Reactor (ITER) Project show the necessity to take into account photonuclear reactions produced by high-energy photons. The principal sources of these photons are reactions of radiative capture of charged particles in the plasma ($E\gamma<24$ MeV), direct radiative capture of fast neutrons ($E\gamma<21$ MeV), and inelastic scattering of neutrons from the DT reaction ($E\gamma<14$ MeV). Therefore, another important recommendation was that an evaluated library of photonuclear data for energies up to 25 MeV should be prepared for incorporation into FENDL for the structural, superconducting and shielding materials for ITER. This library would be designated EPNDL-1 and initially contain evaluations already prepared by CDFE and JNDC.

Considerable progress has been achieved in understanding the role of sequential (z,n) reactions for inventory calculations. The participants recommended that this work be continued at Karlsruhe, Germany, and Arzamas, Russia, and to make corresponding libraries available to the IAEA, including the supporting computer codes.

The Consultants' Meeting recognizes that cross sections of high-energy charged-particle induced reactions which are required for other applications such as medical therapy and space vehicle shielding are related by physics to the specific concerns of the FENDL project. The participants encourage the National Nuclear Data Center at Brookhaven to continue its evaluation effort in the area of high-energy charged-particle reaction evaluations.

Finally, the participants noted that new experimental, evaluational and theoretical efforts have been started or are planned in several countries in the area of Evaluation of Charged-particle and Photonuclear Data for Fission and Fusion Application, and the co-ordination of these efforts by the Agency appears to be very timely and desirable. So the Consultants' Meeting recommend that the IAEA should set up a new Co-ordinated Research Programme on this topic to support the Agency's FENDL Project.

The detailed conclusions and recommendations of the two working groups that were formed during the Consultants' Meeting are presented in Attachment 3 and 4.

(4) Acknowledgements

The meeting participants hope very much that the modest contribution from this meeting may be pursued further by the Agency at 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 the staff of the US National Nuclear Data Center for the warm hospitality.

PROPOSED AGENDA

ATTACHMENT 1

IAEA Consultants' Meeting on
Charged-Particle and Photonuclear Data Libraries for FENDL
8-9 October 1992
National Nuclear Data Center
Brookhaven National Laboratory
Upton, New York, USA

Main Meeting Room: NNDC Conference Room, Bldg. 197D
Working Group A: NNDC Conf. Room A, Bldg. 197D
Working Group B: NNDC Conf. Room B, Bldg. 197D

Thursday, 8 October 1992, NNDC Conference Room (all)

9:00 I. Opening of Consultants' Meeting: Dr. A. Pashchenko, Nuclear Data Section, IAEA, Vienna.

1. Announcement of Organization Matters, Election of Chairman for Consultants' Meeting, and Adoption of Agenda.

9.20 2. Outline of some problems unique to charged-particle data evaluations: R.M. White, LLNL.

9.30 3. Outline of problems unique to developing a photonuclear evaluated data file: V. V. Varlamov, Moscow State University/S. I. Warshaw, LLNL.

9.40 II. Formation of Working Groups (all)

1. Working Group A: Charged Particle Data Evaluations
Election of Chairman for Working Group A
NNDC Conf. Room A, Bldg. 197D

[See Page 3 for detailed agenda of Working Group A]

2. Working Group B: Photonuclear Data Evaluations
Election of Chairman for Working Group B
NNDC Conf. Room B, Bldg. 197D

[See Page 4 for detailed agenda of Working Group B]

9.45 III. Informal Presentations in Working Groups A and B (see pages 3 and 4)

10 45 Coffee Break

11·00 Continuation of Informal Presentations in Working Groups A and B

PROPOSED AGENDA

12:30 Lunch Break, BNL Cafeteria

13:45 Informal Presentations in Working Groups A and B (see pages 3 and 4)

15:30 Coffee Break

16:00 Continuation of Informal Presentations in Working Groups A and B and Development of Outline of Technical Reports for both Working Groups.

18:00 Adjourn for the evening

Friday, 9 October 1992, NNDC Conference Rooms A and B

9:00 Technical Discussion and Writing of Working Group Reports

10:30 Coffee Break

11:00 Completion of Working Group Reports

12:30 Lunch Break, BNL Cafeteria

14:00 IV. NNDC Main Conference Room (all)
Plenary Session, Consultants' Meeting Chairman

1. Reports from Chairmen of two Working Groups

2. Drafting of Meeting Conclusions (all)

16:00 Coffee Break

16:15 3. Adoption of schedule for work and future meetings

4 Corrections and Adoption of the Final Report

18:00 Adjourn

PROPOSED AGENDA

Detailed Agenda for Working Group A—Charged Particle Data Evaluations

Thursday, 8 October 1992, NNDC Conference Room A

10:00 Informal Presentations on Charged Particle Data Evaluation (~15 minutes each)

Data Evaluations and Comparisons

1. Status and Future of Evaluated Thermonuclear Data Library for Charged Particles, B. Ya. Guzhovskij, Arzamas, Russia
2. The Compilation, Calculation and Evaluation of Charged Particle Nuclear Data at CNDC, ZHUANG Youxiang, CNDC
3. Use of R-matrix Theory in Charged Particle Evaluations, Gerry Hale, LANL
4. Intercomparison of Charged Particle Evaluations, Roger White, LLNL

Coffee Break

Data Processing for Applications

1. Description of Cross Section Energy Dependences by Spline Functions in ENDF/B-6 Format, A. G. Zvenigorodskij, Arzamas, Russia
2. Constants and Software Provision for Calculation of Integral Values of <sigmaV> for Maxwellian and Other Equilibrium Spectra, A. G. Zvenigorodskij, Arzamas, Russia
3. The Thermonuclear Data File TDF and TDFLIB Routines for Fusion Applications, S. I. Warshaw, LLNL

Charged Particles and Activation

1. Nuclear Data Libraries for Sequential (x,n) Reactions in Fusion Materials Activation Calculations, P. Oblozinsky, Bratislava
2. Status and Future of Evaluated Activation Data Library for Charged Particles, B. Ya. Guzhovskij, Arzamas, Russia

Related Topics

1. High Energy Proton Evaluations, S. Pearlstein, BNL
2. High Energy Gamma Sources in Thermonuclear Reactors, B Ya. Guzhovskij, Arzamas, Russia
3. Evaluated Data on Nuclear Structure in FENDL Compilation, A. G Zvenigorodskij, Arzamas, Russia

12.30 Lunch Break, BNL Cafeteria

13.45-15:30 Complete Informal Presentations and Working Group discussions
16 00-18 00 Begin outline of Technical Report of Working Group on Charged Particles

Friday, 9 October 1992, NNDC Conference Room A

9 00-12.30 Complete Working Group Report on Charged Particle Evaluations

PROPOSED AGENDA

Detailed Agenda for Working Group B—Photonuclear Data Evaluation

Thursday, 8 October 1992, NNDC Conference Room B

10:00 Informal Presentations on Photonuclear Data Evaluation

1. Present Status of Evaluation Work on Photonuclear Data at JNDC, N. Kishida, CRC Research Institute, Japan
2. Status of Photonuclear Reaction Data Library, V. V. Varlamov, Moscow State University
3. Absorption Cross Sections of Hard Photons, P. Oblozinsky, Bratislava
4. Photonuclear Reaction Cross Section Evaluation, V. V. Varlamov, Moscow State University

12:30 Lunch Break, BNL Cafeteria

13:45-
15:30 Complete Informal Presentations and Working Group Discussions

16:00-
18:00 Begin outline of Technical Report of Working Group on Photonuclear Reactions

Friday, 9 October 1992, NNDC Conference Room B

9:00-
12:30 Complete Working Group Report on Photonuclear Data Evaluations

ATTACHMENT 2

IAEA Consultants' Meeting on

"Charged-Particle and Photonuclear Data Libraries for FENDL"

8-9 October 1992,
Brookhaven National Laboratory, Upton, New York, U.S.A.

LIST OF PARTICIPANTS

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Anatoly B. PASHCHENKO

The end-users of these charged-particle reaction evaluations are most often in need of processed information, i.e., Maxwellian-averaged reaction rates, and related quantities. It is recognized that much of this processed information currently being used in fusion applications is extremely outdated and some previously recommended files are derived from incorrect data. There are three new independent sources for this information which the Working Group has intercompared. The analytic expressions provided by Arzamas (Ref. 2) and Los Alamos (Ref. 3) and the processed library and routines from Livermore (Ref. 4) are in substantial agreement and represent a significant improvement over what has been previously available. The Working Group strongly recommends that the fusion applications community avail themselves of this improved information.

For fusion reactor designs employing beams of neutral atoms of ^{2}H and $^{6,7}Li$ with energy of ~1 MeV injected into the plasma, in-flight reaction cross sections are required. For this application both integrated cross sections and angular distribution information are required in a processed form. The Working Group recommends that a processed data file, based upon the ENDF/B-VI charged-particle sublibrary and other evaluations available from Arzamas, Los Alamos and Livermore, be developed in a manner similar to the TDF file and TDFLIB routines currently available from Livermore.

Analysis of nuclear processes for ITER show the necessity to take into account photonuclear reactions produced by high-energy photons. The principal sources of these photons are reactions of radiative capture of charged particles in the plasma ($E\gamma<24$ MeV), direct radiative capture of fast neurons ($E\gamma<21$ MeV), and inelastic scattering of neutrons from the DT reaction ($E\gamma<14$ MeV). Therefore, a library of photonuclear data for energies up to 25 MeV should be prepared for the structural and shielding materials for ITER.

The Working Group note that in the field of charged-particle activation a considerable progress has been achieved in understanding of the role of sequential (z,n) reactions for inventory calculations. Libraries KFKSPEC and KFKXN have been created in their starting version. The Working Group recommends to make these libraries available to the IAEA including the corresponding supporting computer codes. The participants recommend to continue in the above effort in Karlsruhe, Germany, particularly

a) to improve starting libraries by better modelling of d,t and ^{3}He emission as well as by considering special important cases such as $^{7}Li(t,\gamma)^{10}Be$,

b) to identify important reacton chains via inventory calculations and validate the corresponding parts of the libraries by comparing with existing experimental data,

c) to perform activation benchmark experiments.

The Working Group recognizes that high-energy charged-particle induced cross sections are required for other applications such as medical therapy and space vehicle shielding are related by physics to the specific concerns of the FENDL project. We encourage the Data Center at Brookhaven to continue its evaluation effort in the area of high-energy charged-particle reaction evaluations.

The Working Group recognizes that new experimental, evaluational and theoretical efforts have been started or are planned in several countries in the area of Evaluation of Charged-particle and Photonuclear Data for Fission and Fusion Application, and the co-ordination of these efforts by the Agency appears to be very timely and desirable. The IAEA should arrange a Co-ordinated Research Programme on this topic to support the IAEA FENDL Project.

Finally, the Working Group recommended that continued checks and further development of co-ordinated efforts be considered at the IAEA Specialists' Meeting on "Evaluation of Charged-particle and Photonuclear Data for the IAEA FENDL Project", which should be organized in Moscow, Russia, or Smolenice, the Czech and Slovak Federal Republic, in September 1993. Drs. V. Varlamov and P. Oblozinsky are asked to investigate possibilities to host the planned meeting in Russia or in the Czech and Slovak Federal Republic and to inform the Nuclear Data Section in time.

References

1. Report INDC(NDS)-260/L+F, 1992. Summary report of the IAEA Advisory Group Meeting on "FENDL-2 and Associated Benchmark Calculations", Vienna, 18-22 November 1991, A.B. Pashchenko and D.W. Muir, Eds.

2. S. Abramovich et. al., Nuclear Physics Constants for Thermonuclear Fusion. Report INDC(CCP)-326, March 1991.

3. H.-S. Bosch, G.M. Hale. Improved Formulas for Fusion Cross Sections and Thermal Reactivities. Nuclear Fusion 1992, Vol. 32, No. 4, p. 611.

4. R.M. White, D.A. Resler and S.I. Warshaw. Evaluation of Charged-Particle Reactions for Fusion Applications. In.: Nuclear Data for Science and Technology, Springer-Verlag, 1992. Proceedings of an International Conference, held at Jülich, Germany, 13-17 May 1991, p. 834, S.M. Qaim, Ed.

Working Group B
Photonuclear Data Evaluation

Participants: Y. Kikuchi, N. Kishida, P. Oblozinsky, G. Reffo, V. Varlamov, S. Warshaw

Chair: S. Warshaw

Scientific Secretary: V. McLane

Observers: C. L. Dunford, H. Takahashi

Introduction: Unique Aspects of Experimental Photonuclear Data (wp7), S. Warshaw

a) There is a great variation in the spectral content of the photon sources that were used. This variation may be responsible for the discrepancies observed.

b) There are many different data methods used to reduce the spectrally-broadened data to their monochromatic (or monoenergetic) equivalent. These differences may also be responsible for observed discrepancies.

c) Much data has been obtained without identifying the specific reactions responsible

The major problem in photonuclear evaluation is to find the best way to make use of these kinds of information and still arrive at a meaningful evaluation.

Introduction by V. Varlamov of paper by B. Guzhovskii

High Energy Gamma source in Thermonuclear Reactor (wp1)

This important paper shows how hard photons arise in a thermonuclear plasma, and shows a connection between photonuclear information and the properties of the plasma. It establishes the importance of photonuclear reactions for thermonuclear reactors. These (γ,x) reactions have implications for personnel safety, structural integrity of thermonuclear reactors, and plasma diagnostics.

Recommendations:

1. Concentrate on evaluating photonuclear neutron production and particle capture cross sections important for incorporation into FENDL..

   Priority 1: light nuclei in fusion fuel

   Priority 2: structural, superconducting, and shielding materials

2. Set highest priority for evaluating photonuclear data corresponding to photons produced by DT (16.4 MeV), DD (23.8 MeV), and TT (12.3 MeV) for diagnostics of heating in plasma. (This focuses on GDR cross sections).

3. Determine what the gamma spectrum looks like in the plasma in order to assess the effects of thermal broadening on photonuclear reactions.

Present Status of Evaluation Work on Photonuclear data at JNDC (wp2), N. Kishida

The Japanese Nuclear Data Committee (JNDC) plans to evaluate natural isotopes, transuranic nuclei, and fission products.

1. **JNDC is systematically and comprehensively evaluating photoabsorption and photoneutron data based on experiments taken with positron annihilation photon sources. The evaluated data will be presented in the ENDF-6 format and will include data from GDR to meson threshold ($E_\gamma \leq 140$ MeV).**

2. They are calculating branching ratios of (γ,n), (γ,p), *etc.*, reactions using the MCPHOTO and ALICE-F codes.

3. They are evaluating isotope production cross sections by using the absorption cross sections and the branching ratios.

JNDC is developing a photonuclear reaction data index, based on CINDA, and taken in part from the NBS Photonuclear Data Index and the CDFE Photonuclear Data publication. It will be completed by the end of 1992.

Photonuclear Data Evaluation at CDFE (wp4, wp5), V. Varlamov

1. CDFE is evaluating data for isotopes from all types of photon sources.

2. CDFE is obtaining systematics & using these systematics to do evaluation, normalization and calibration of the data taken with different kinds of photon sources

3. CDFE's evaluation procedure is nuclear model independent.

Conclusions

1. A systematic analysis of total photoneutron reaction cross sections obtained in experiments with different kinds of photon sources has been carried out for different nuclei

2 The discrepancies in the data are presumed to be due to the differences in the effective apparatus functions (photon spectra) used, calibration, and normalization

3 These three types of systematic errors are energy dependent That, essentially, complicates the use of traditional methods of data evaluation.

4 CDFE is proposing a technique of photonuclear reaction cross section evaluation that is based on the method of reduction, which makes it possible to take into account all these systematic errors.

5. The method of reduction does not claim to be an unfolding, extraction or restoration of the cross section, but only a reduction of the data to an apparatus function of the desired quality. The method opens up the possibility of finding the most reasonably achievable monoenergetic representation of the cross section.

6. The evaluation technique was used to obtain evaluated total photoneutron cross sections and covariance matrices for several nuclei.

Absorption Cross Sections of Hard Photons (wp4), P. Oblozinsky

A systematic method of modeling data from GDR to meson threshold for medium and heavy nuclei (employed successfully by JNDC) was described. The treatment is based on Levinger's Quasi-Deuteron Model as extended by Chadwick, Oblozinsky, Hodgson, and Reffo.

Summary

1. Photonuclear reactions can occur in thermonuclear reactors because of hard γ production. These reactions and the hard photon spectrum need to be investigated.

2. CDFE is providing methods of reconciling cross section data taken with different kinds of photon sources and processed with different spectral methods.

3. JNDC is successfully utilizing the GDR model and the Quasi-Deuteron Model of Chadwick, Oblozinski, Hodgson & Reffo to represent photonuclear cross sections.

4. CDFE and JNDC have started photonuclear data evaluations.

Recommendations

0. The IAEA should set up a CRP for photonuclear data evaluation for FENDL. The CRP should include evaluators, theorists, and experimentalists as participants.

1. Studies should be initiated on the following questions.

   - Can the Quasi-Deuteron Model be applied to (γ,f)?
   - Can the Quasi-Deuteron Model be applied to light nuclei?
   - Can the single-channel components of $\sigma(\gamma,xn)$ be identified in neutron multiplicity measurements? Is it important?

2. A comparison should be done between evaluations and true monochromatic data.

3. New measurements should be done with monochromatic sources.

4. Studies should be done on the gamma spectrum in the plasma of a thermonuclear reactor.

5. It is necessary to establish which photonuclear activation reactions are important in reactor inventory calculations.

6. JNDC should send a photonuclear data representative to the next Nuclear Reaction data Centers Meeting.

Actions

1. NDS — Initiate EPNDL-1 with CDFE and JNDC results (using the usual logistics of data transfer).

2. JNDC,CDFE — Cooperate to continue CINDA-like index of photonuclear data and to include index to EXFOR data.

3. CDFE,JNDC — Exchange current evaluation results, with copies to NNDC and LLNL.

Working Papers

1. HIGH-ENERGY GAMMA SOURCE IN THERMONUCLEAR REACTOR
   B. Ya. Guzhovkii

2. EVALUATION OF PHOTONUCLEAR REACTION CROSS SECTION (I)
   N. Kishida

3. PRESENT STATUS OF EVALUATION WORK ON PHOTONUCLEAR DATA AT JNDC.
   N. Kishida

4. STATUS OF PHOTONUCLEAR REACTION DATA LIBRARY.
   V. Varlamov, et al.

5. PHOTONUCLEAR REACTION CROSS SECTION EVALUATION.
   V. Varlamov, et al.

6. ABSORPTION CROSS SECTIONS OF HARD PHOTONS
   P. Oblozinsky

7. UNIQUE ASPECTS OF PHOTONUCLEAR DATA
   S. Warshaw