INTERNATIONAL ATOMIC ENERGY AGENCY

INDC(NDS)-425
Distr.: RS

I N D C INTERNATIONAL NUCLEAR DATA COMMITTEE

Summary Report of the Consultants' Meeting on

Improvement of the Standard Cross Sections for Light Elements

IAEA Headquarters

Vienna, Austria

2 - 4 April 2001

Prepared by
A.D. Carlson, D.W. Muir and V.G. Pronyaev

June 2001

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

Produced by the IAEA in Austria
June 2001

INDC(NDS)-425
Distr.: RS

Summary Report of the Consultants' Meeting on

Improvement of the Standard Cross Sections for Light Elements

IAEA Headquarters

Vienna, Austria

2 - 4 April 2001

Prepared by
A.D. Carlson, D.W. Muir and V.G. Pronyaev

Abstract

This report summarizes the results of the Consultants' Meeting on Improvement of the Standard Cross Sections for Light Elements. The approaches and computer programs used for evaluation of neutron standard cross sections and their uncertainties were presented by the participants. Special attention was paid to the reasons for strong uncertainty reduction observed in the model fits. The meeting participants discussed the plan of the INDC recommended Co-ordinated Research Project (CRP) on "Improvement of the Standard Cross Sections for Light Elements". This CRP will address the problem of uncertainty reduction along with other methodological improvements needed in order to produce a new, and internationally accepted, evaluation of neutron standard cross sections for light elements.

June 2001

CONTENTS

1. SUMMARY OF THE MEETING

Objectives of the meeting

The objectives of the meeting were the following:

- to discuss the requirements for the Standard Cross Sections;
- to review the results of new measurements;
- to review the codes used for resonance cross section evaluation, paying special attention to the methods of the error propagation and any approximations used;
- to outline the program of the work to be done which should lead to a better understanding of the origin of the strong uncertainty reduction in model fitting;
- to prepare the tasks to be addressed under the planned CRP on Improved Standard Cross Sections for Light Elements and the list of potential contributors.

Participants' presentations and discussions

The meeting was opened by D.W. Muir, who summarized the objectives of the meeting. The major objective was to prepare the tasks to be addressed under the IAEA CRP, the beginning of which is planned in 2002. D.W. Muir gave an explanation of the general framework and procedures under which the CRPs develop and showed how the CRP mechanism could be important for the completion of the present tasks. After brief self-introductions of the participants (see list of participants in Appendix 2), A.D. Carlson was elected chairman.

After discussion, the participants adopted the proposed Agenda and Schedule (see Appendix 1).

The requirements of the neutron cross section standards were discussed by A.D. Carlson. The combined ENDF and NEANDC/INDC standards list includes at present the following reactions covering the energy ranges: H(n,n) from 1 keV to 20 MeV, ^{3}He(n,p) from thermal to 50 keV, ^{6}Li(n,t) from thermal to 1 MeV, ^{10}B(n,α) from thermal to 250 keV, ^{10}B(n,$\alpha_1\gamma$) from thermal to 250 keV, C(n,n) from thermal to 1.8 MeV, Au(n,γ) for thermal and from 0.2 to 2.5 MeV, ^{235}U(n,f) for thermal and from 0.15 to 20 MeV and ^{238}U(n,f) from threshold to 20 MeV. The uncertainties obtained for the ENDF/B-VI evaluation of the standards have been considered by the most experts as too small. Of particular concern are the cases where the ENDF/B-V and ENDF/B-VI evaluations do not agree within their uncertainties. This led to the CSEWG Standards Subcommittee supplying expanded uncertainties. The ENDF/B-VI standards evaluation involved a generalized least squares analysis, R-matrix analyses and a procedure for combining these analyses. The experimental database for the least square analysis can include a very large number of data types. The experimental database for the R-matrix evaluation of the light element standards includes other cross section data involving the same compound nucleus (charged-particle data) as well as differential cross section and polarization data. The small uncertainties obtained for the light element standards were largely a result of the R-matrix analyses.

The present status of the experimental database for standard cross sections and methods used for generation of covariance matrices of uncertainties of experimental data was presented by A.D. Carlson. New experimental data are available for angular distributions for the H(n,n) reaction for the neutron energies of 10, 14, 28-75, 96, and 162 MeV. The work at 185-195 MeV is in progress. Evaluated cross sections, which take these data into account, can be changed by more than 1% near energies of 10 and 14 MeV. Back angle scattering data at some energies have the largest changes. For reactions induced by neutrons on ^{10}B, a significant amount of work has been done. Some of the most recent measurements indicate an internal inconsistency, which may be resolved with branching ratio work which is now underway. Based on analyses with some of the new data for the $^{235}U(n,f)$ cross section, changes of more than 1% will occur for this cross section. Significant changes should also be seen for the $^{238}U(n,f)$ cross section. Standards for neutron energies above 20 MeV can also be substantially improved due to the appearance of new experimental data. The covariance matrix of uncertainties of experimental data is generated from short-energy range (statistical), medium-energy range and long-energy range correlation components of the total uncertainties. At present the database contains discrepant data and attention should be paid to any statistical treatment of these data.

G.M. Hale presented the R-matrix code EDA. The code is based on an exact R-matrix formulation of multichannel nuclear reaction theory. For parameter search, the minimum chi-square fit to the experimental data for all channels leading to the same compound nucleus is used. The covariance matrix of the uncertainties of the experimental data includes only statistical and normalization uncertainty components for evaluation of the uncertainty of the parameters. Some parameters predicted by microscopic nuclear models can be used as prior values for a search. The use of the physical model introduces important constraints on the cross sections, their relations and functional dependencies. The accuracy of the evaluation of the standard cross sections is substantially increased due to the inclusion of the reactions leading to the same compound nucleus. The inclusion of experimental differential cross section and polarization data reduces ambiguities in the parameters. Preliminary results of a new evaluation for the $^{1}H(n,n)$ reaction were shown. The uncertainty of data obtained in this evaluation for the neutron total cross section is, as in all model fits, extremely low. The reduction of the central uncertainties in the cross section is on the order of $N^{-1/2}$, where N is a total number of experimental points used in the fit. The reason for this pure “statistical” behavior of the uncertainty of evaluated data is not so clear because the points belonging to one experimental data set are not independent and usually have noticeable cross-energy correlations.

Ms. N.M. Larson presented the code SAMMY, which is based on the Reich-Moore approximation to the multilevel multichannel R-matrix theory. This code was initially developed for neutron induced reactions taking into account channels and levels contributing in the resonance energy range for medium and heavy nuclei. At the present time, it can be used for R-matrix fits of integral cross sections and elastic scattering angular distributions for nucleons or light particle induced reactions. Unlike EDA, it can not treat in one run reactions going through the same compound nucleus but induced with particles different from the entrance channel particle. The code also can not process polarization data. It has extended options for introducing the corrections for experimental effects (Doppler and resolution broadening, sample finite-size corrections, background separation) and uses Bayes' method for parameter searching. It allows full implementation of the error propagation law for data covariance matrices constructed from statistical and systematic components of uncertainty (no medium range correlations) and uses an iterative method of solution for strong non-linear (cross section versus parameters) problems.

T. Kawano presented the code KALMAN, a code which can not be used for automated complex parameter searching by itself, but is used for reconstruction of point-wise cross sections and covariance matrices of their uncertainties from evaluated Reich-Moore resonance parameters and their uncertainties. The KALMAN code is basically a least squares shell which can be used to obtain solutions of the generalized least square equations and, if provided sensitivity coefficients, it can be used for tests of the error propagation law in more complex fitting codes.

Chen Zhenpeng presented the reduced R-matrix code RAC. The formalism used includes the width of reduced channels and other channels which are not considered explicitly (due to the absence of data or their contribution being minor), or have contributions from the direct reaction mechanism. This treatment should restore the consistency between total and partial cross sections for the conditions when experimental data for some partial channels are incomplete, absent or can not be interpreted in the framework of the compound nucleus reaction mechanism. This is often the case when the incident particle energy is above a few MeV. The RAC code also treats all other reactions leading to the same compound nucleus in the fitting procedure. Integral and differential cross sections and polarization data can be used in the parameter search. The inter-comparison between RAC and EDA codes done for reactions going through the compound systems ^{7}Li, ^{11}B and ^{17}O have shown good agreement in the searched parameters. At present, only diagonal covariance matrices of uncertainties of the experimental data can be used in the fitting procedure.

H.M. Hofmann presented the resonating group method and code package used for microscopic calculations of nuclear structure and nuclear reaction parameters in the light nuclear systems. It was shown that for A=3 and 4, the microscopic model can predict the parameters and cross sections with "data quality", and for heavier systems the bound and resonance state parameters can be used as initial parameters for further R-matrix adjusting. This is especially important for introducing in the R-matrix fits prior information about distant and wide resonances.

S. Tagesen presented the GLUCS code implementing Bayes' method for least-squares fitting. GLUCS uses a non-model approach and processes the cross sections in the continuous energy (usually group-structured) presentation. The modified version of GLUCS can take into account the relationship existing between total and partial cross sections and use data on "redundant" cross sections in the processing. A non-informative data set (a set with realistic data values but extremely large uncertainties) covering the whole energy range, where experimental data are given, is used as a prior. If there is one experimental data set having no correlations with other sets and covering the whole energy range of interest, it can be taken as a prior. In this case Bayes' approach is fully equivalent to the generalized least square method when no correlations exist between prior and experimental data. Significant attention was paid to the construction of realistic covariance matrices of uncertainties of the experimental data. Contributions of short energy, medium energy and long energy range correlation components are evaluated based on the information given by experimenters.

D.W. Muir presented the code ZOTT99, which uses a partitioned form of the generalized least square method. The partitioned form is completely equivalent to the generalized form of the least square solution. However it allows avoiding inversion of the large covariance matrix of all the data that is done in the generalized form, requiring instead only the inversion of matrices of differences between the data, which have smaller size in many cases. Contrary to GLUCS using the Bayes' method, the treatment of data correlations is completely general. The code works with the covariance matrix of uncertainties of the data in its most general form and, if provided with sensitivity coefficients, it can be used for testing the error propagation law in R-matrix codes.

The round-table discussions began with the analysis of different factors influencing the reduction of the uncertainty in the model fits. The influence of the physical model can be easily seen in a simple case where a set of non-correlated data points (diagonal covariance matrix of the uncertainty of the data) is fitted with some model by adjusting the parameters. In this adjustment the evaluated parameters and covariance matrix of the uncertainties of the parameters can be obtained. If chi-square per degree of freedom of this fit is on the order of one, the covariance matrix of the uncertainty of the evaluated data calculated from the covariance matrix of the uncertainty of the parameters and the sensitivity coefficients can be compared with the initial covariance matrix of the data. This matrix calculated from the uncertainty of the parameters will have reduced variances compared with the variances of the initial non-correlated data set but now will also contain some correlations between the data points. New evaluated data will have a functional form characteristic of this model with adjusted parameters. Specific functional form, reduction of the variances and appearance of the correlations between data points are clearly the result of application of the physical model to the data fit. If the experimental database used for the model fit includes different data sets with more complex covariance matrices (non-diagonal for each data set with correlations present between different data sets) the analysis of error propagation to the covariance matrix of the evaluated data can also be more complex. This analysis will be an important topic for the study.

The true R-matrix model should not only include the true functional relations between parameters and cross sections but also a complete set of the parameters determining the cross sections for a given energy range. However this is difficult to obtain when resonances have rather large widths and the contribution from non-compound reaction mechanisms is substantial. This is just the case for the interaction of high-energy incident particles with light nuclei. As a result, there is no guarantee that the shape or magnitude of the cross section predicted by the model is the most realistic. It also means that the error propagation from the covariance matrix of the uncertainty of the experimental data to the covariance matrix of the uncertainty of the parameters in the model fit can not be fully justified as is the case for a true model function.

The influence of the constraints and relations introduced by the R-matrix model on the different observables and between them was discussed in detail. Some constraints bring in strong limitations on the possible values of the observables. The inclusion of the channel which is the inverse to the channel of the standard reaction and inclusion of other reaction channels going through the same compound nucleus in the simultaneous parametric fit have the most important consequences. The reduction of the uncertainty of the standard reaction cross section due to these aspects of the physical model can be studied through the inclusion and exclusion of these channels.

Other reasons for having uncertainty reductions that are not always justified are rather well known and common for parametric model and general least square fits. An important consideration is the treatment of discrepant data. If chi-square per degree of freedom obtained in the fit is substantially higher than one, the treated data should be considered as discrepant and the uncertainties assigned to the evaluated data should be treated as too (on the order of the square root of chi-square) low. The evaluator should return to the analysis of the experimental data and revise the experimental database in such a way that it will not be discrepant. Most often this leads to the revision (increasing) of the uncertainties for the work which may contain some unaccounted for errors or corrections. This procedure leads to the increasing of the uncertainty of the evaluated data. Another source of non-justified uncertainty reduction is neglecting the correlations which exist between different experimental data sets. These are correlations due to use in the measurements of common standards, or detectors, or made at the same installation, etc. Neglecting these correlations leads to the treatment of the uncertainty as being more statistical (uncorrelated) than it really is and to extreme reduction of the uncertainty in cases where there are a lot of measurements, as there are for the standard reaction cross sections.

Test cases designed to provide a better understanding of the uncertainty reduction in the complex model fits were discussed. H.K. Vonach presented work done on a comparison of the Bayes' approach to the non-model continuous (group-structured) energy evaluation of the ^{52}Cr(n,p) reaction with a Pade-approximation (model) fit. Both evaluations used the same experimental data sets. When the central values and the covariance matrix of the uncertainty of the evaluated cross sections were calculated from the values and the uncertainty of the evaluated Pade parameters for the same energy group structure as for the Bayes' approach, the two approaches are very similar. The variances evaluated in the model fit are only slightly lower than those evaluated in the Bayes approach. Although the Pade-approximation technique is not based on any particular physical model, the uncertainty reduction due to error propagation from the experimental data to the parameters and back to the evaluated cross section should be the same as for a single channel R-matrix physical model fit.

T. Kawano presented a test case for studying uncertainty reduction in an R-matrix fit for resonances in the cross section. The code used was GFR. The energy range from 0 to 50 keV in ^{56}Fe, containing 1 strong s-wave resonance near 27 keV and 5 other distant s-wave resonances was used for investigation of R-matrix model error propagation. The 18 parameters in this fit included positions of the resonances, elastic scattering neutron widths and negligibly small gamma-ray widths. Fictitious experimental data for the total cross section were generated then from realistic parameters of these resonances using R-matrix formulae and Monte Carlo simulation for the statistical spreading of the data. The total uncertainty of the data was fixed at the level of 5% and 3 pseudo-experimental data sets with covariance matrices of the uncertainties were prepared: a) with total uncertainty given as a statistical uncertainty, b) with 50% correlations between the energy points (3.5% statistical and 3.5% systematical error) and c) with 99% correlations between the points. The number of these pseudo-experimental points was distributed equidistantly in the energy range from 0 to 50 keV and for the R-matrix parameter search they had the values of 5, 10, 25, 50, 100, 250 and 500. In each case the R-matrix fit was done with a search for the parameters and their covariance matrix of uncertainty and then the evaluated curve and its covariance matrix of uncertainty was reconstructed. Although the results obtained for the case of 99% correlations had shown some numerical instability, a general conclusion is the following: The model fit reduces the statistical component of the uncertainty of the data but introduces additional medium and long-range correlations between data points due to the model predicting the curve shape. This means that experts can not analyze the strong reduction of uncertainty (variances) in the model fits without analysis of the whole covariance (correlation) matrix of the uncertainty. The same conclusion can be drawn from the example shown by Chen Zhenpeng: the initially uncorrelated set of “experimental” data after linear-model least square fitting converts in an evaluated data set with reduced variances (central uncertainties) but substantial correlations (non-diagonal covariances) between evaluated data points.

The guidance suggested by the participants, related to the preparation of the test cases for the study of error propagation and uncertainty reduction in the model least-square fits and in different R-matrix codes were the following in general:

- To begin the study with simple cases and then move in the direction of more complex ones.
- To study each factor which influences the uncertainty reduction separately, if possible.

In particular it is proposed:

- To prepare a simple one-channel test case for a light element standard cross section (probably ^{6}Li(n,t) reaction is the best candidate) with computer simulated pseudo-experimental (but realistic) data sets having covariance matrices of uncertainty reflecting different levels of correlations between data points (similar to the test case prepared by T. Kawano for ^{56}Fe, see above). To use this test case for study of the error propagation in different R-matrix fitting codes and their inter-comparisons. The purpose of this test is to demonstrate how the error propagation in the R-matrix codes treats the short-energy range and long-energy range correlation components of the experimental data uncertainties.

- To prepare a test case similar to that described above but with a few pseudo-experimental data sets (with no correlations between data belonging to the different data sets) but having realistic (short- and long-energy range) correlations between data belonging to the same data set. To use this test case for inter-comparison between R-matrix model fits and non-model general least square and Bayesian descriptions. The purpose of this test is to show how the long-energy range correlation components of the covariance matrix are reduced in the data treatment with model and non-model descriptions.

- Using experimental data available for reactions induced by neutrons on ^{6}Li (total, elastic and (n,t)) show how the constraints from the physical model lead to changes in the covariance matrix of uncertainty and to compare it with the use of “redundant” data in the generalized least-square or Bayesian descriptions. The purpose of this test is to demonstrate the influence of the unitarity relations and other constraints on the evaluated central values and covariances.

- Using experimental data available for all reaction channels leading to the same compound nucleus (e.g. ^{7}Li) show how the inclusion and exclusion in the R-matrix model fit of the inverse reaction $^4He(t,n)^6Li$ will influence the central values and covariance matrix of uncertainty of the evaluated standard reaction cross section.

- Use the uncertainty in the energy calibration of the experimental data and the energy bias which may be caused by neglecting the influence of the resolution function of the experiment, for strongly changing cross sections (threshold or *1/V* dependence) to show how it can (or cannot) lead to uncertainty underestimation.

- Using a discrepant sub-set of data together with consistent experimental data sets in one least-square fit, show that with generally low chi-square per degree of freedom, the uncertainty assigned to the evaluated data in the region where the data are discrepant can be too small. The general case of uncertainty underestimation in fits with high chi-square per degree of freedom is well known. But low chi-square does not guarantee that uncertainties are not underestimated for some local energy ranges.

- Using the most comprehensive analysis of a set of experimental data, which takes into account correlations between different experimental data, treat them as non-correlated. Then perform similar but simple test cases to evaluate the uncertainty reduction due to neglecting these correlations.

Studies of all these test cases, checking of codes and the inter-comparisons are crucial for answering the question: What is the realistic level of uncertainty, which can be obtained in the fits?

All CM participants expressed their wish to take part in the project. The tasks, which can be addressed and solved first by the CM participants, as they are seen now, are the following:

1. For the combined description of data in the microscopic Resonanting Group Method (RGM) and the R-matrix approach (EDA code):
   a) Continue to develop the capability to obtain complex-energy poles and residues of the S-matrix in the RGM (conversion from k-plane to E-plane pole presentation);
   b) Compare these quantities for the A=4 system obtained in the R-matrix fit and in the RGM;
   c) Compare S-matrix poles, phase shifts, etc. for the ^7Li system (n+^6Li reactions) with an analysis in which resonances occur at high energies;
   d) Do RGM calculations for the ^{11}B system and compare the result with the R-matrix data fit;
   e) Make an estimation of possible hidden model uncertainties in R-matrix analyses.
2. For R-matrix codes (RAC, SAMMY, EDA, GFR, RESCAL) and least-square codes (GMA, GLUCS, ZOTT, KALMAN) make inter-comparisons, tests and evaluations:
   a) Document what was done already in the RAC-EDA comparisons for n+^6Li, n+^{10}B and n+^{16}O;
   b) Include SAMMY and RESCAL in the RAC-EDA inter-comparison for n+^6Li, n+^{10}B and n+ ^{16}O;

c) Document predictions of n+^{3}He -> p+t reaction verified by experimental data;

d) In the case of ^{16}O demonstrate with SAMMY the role of Doppler and resolution broadening on the cross section and parameter evaluation;

e) To prepare, with the modified RAC code, an evaluation of the ^{6}Li(n,t), ^{10}B(n,a) and ^{12}C(n,n) standard reaction cross sections and inter-compare with the results obtained with other R-matrix codes;

f) Inter-comparisons with various R-matrix codes for a simple parameter set, e.g. n+^{6}Li, α+t mock-up with only few resonances, observables to be calculated: σ_{tot}, $\sigma_{n,n}(\theta)$, $A_y(n)$, $\sigma_{n,t}$, $\sigma_{n,t}(\theta)$, $\sigma_{t,n}$, $\sigma_{t,n}(\theta)$, $A_y(t)$;

g) Demonstrate influence of other channels leading to the same compound nucleus by including and excluding these data in R-matrix fits;

h) Inter-comparisons for R-matrix fitting of synthesized data (generated from the test parameters by Monte Carlo, as proposed by T. Kawano, see above): search for parameters and covariance matrix of their uncertainties and calculation of evaluated cross section curves from parameters and their covariance matrix of uncertainty;

i) Demonstrate the influence of the number of data points included in the analysis on the reduction of the uncertainty in the model fit. Show how the "normalization" (long-energy range correlation) uncertainty in the experimental data is reduced (if it will be reduced) in the model fit;

j) Use the same synthesized data and covariance matrix of uncertainties in GMA, GLUCS, KALMAN and ZOTT. Compare the output cross sections, and covariances with those of the R-matrix codes. Try changing the normalizations of some of the data sets to see the response of the codes to this change;

k) Always make sure that numerical instability and loss of precision in the calculations does not influence the result;

l) Check all covariance matrices at each step for positive definiteness.

3. For code modifications:

a) Modify SAMMY to allow the inclusion of other channels leading to the same compound nucleus in the simultaneous fit, inclusion of reaction angular distributions in the fit, inclusion of data on cross section ratios, and inclusion of polarization data;

b) Modify RAC to allow inclusion of the full treatment of covariance matrices of general type;

c) Extend the GFR code to be a more general R-matrix code.

4. For study of the uncertainty reduction due to underestimation of correlations between data, and methods of preparation of the covariance matrices of uncertainty of experimental data:

a) Study methods to estimate medium-energy range correlations for components of the uncertainty having these properties or when some data sets are discrepant compared with the rest of the database in some local energy regions;

b) Study of the approximations used in some R-matrix codes where the covariance matrix of uncertainty of experimental data consists only of short-energy and long-energy range components. The medium-energy range component is ignored;

c) Study approaches which might allow the identification of systematic errors related with the method of measurement;

d) Update the experimental database for standards evaluations, paying special attention to the discrepant data.

5. For the study of procedures for combination of evaluations prepared with R-matrix and generalized least-square methods:

a) Get sensitivities from R-matrix fits and use them in least square programs;

b) Consider the R-matrix fit as a prior for further least-square evaluation.

The participants discussed the means by which the program of improvement of the light element standard evaluations can be implemented. It was recognized that the IAEA Co-ordinated Research Project (CRP) provides the best mechanism for the participation of all groups from developing and developed countries that actively are working in this field to contribute in the program. The success of the final stage of the project, producing the light element standards evaluations with realistic matrices of the uncertainties, depends to a large extent on the implementation of the initial stages of the project. The participants approved the title of the proposed CRP as CRP on “Improved Standard Cross Sections for Light Elements”.

A few groups have been considered as the potential contributors to this CRP:

- G. Hale, LANL, USA
- Ms. N. Larson, ORNL, USA
- A. Carlson, NIST, USA
- T. Kawano, Kyushu University, Japan
- H. Vonach and S. Tagesen, IIK, Austria
- H. Hofmann, University of Erlangen-Nuremberg, Germany
- Chen Zhenpeng, Tsinghua University, China
- S. Badikov and E. Gaj, IPPE, Russia
- Soo Youl Oh, KAERI, Republic of Korea

The work can be done with at least 5 research agreements and 3 research contracts. Unfortunately, due to the specificity of the problem, it is difficult to expect much more participation of scientists from developing countries in this project. If additional groups show interest to the project, they can be invited to participate in the CRP at any stage of the project. The holding of the CRP was strongly endorsed by the participants.

Meeting conclusions and recommendations

Needs in new nuclear reaction standards

Nuclear reaction standards are the basic quantities needed in nuclear reaction cross section measurements and evaluations. Standards include the evaluated cross sections as well as the covariance matrices of their uncertainties. The last evaluation of the standards was completed in 1987. The uncertainties obtained in that evaluation were so low that experts considered them as unrealistic. This led to a scaling up of those uncertainties keeping the correlation matrices unchanged. After the expenditure of such a large effort on the evaluation of covariance matrices of uncertainties for the standards, the final procedure used was not internally consistent. The smallest uncertainties were observed in the R-matrix model fits used for the light element standards evaluations.

The preparation of new versions of national and international evaluated data libraries should begin with a re-evaluation of the standards. Realistic uncertainties in the R-matrix model fits for light element standards should be obtained. Re-evaluation of the standards should be done with the inclusion of new experimental data. This total effort will produce new internationally recognized standards, which may be rather different from the standards used now.

Tasks to be solved

The following tasks should be completed in the new standards evaluation:

- To improve, to test and to inter-compare R-matrix model codes used for light element standards evaluations;
- To study the error propagation in the R-matrix fits of the experimental data and to justify the uncertainties obtained in these fits;
- To study the uncertainty reduction due to treatment of partially discrepant data and due to neglecting important correlations in and between different experimental data sets;
- To update the database of experimental data for standards evaluations resolving the discrepancies between different experimental data sets;
- To prepare new evaluations for the light element standards;
- To study and prepare a procedure for combining the evaluations of the light and heavy elements.

IAEA CRP on Improvement of Light Element Standards Evaluations

The CRP should concentrate on improving and documenting the methodology (primarily R-matrix analyses) used in the evaluation of light element neutron cross section standards and the "combination procedures" used to perform a simultaneous evaluation of all neutron standards data at the final stages of the standards evaluation process. A particular goal is to better understand the origins of the reduction of uncertainties often seen in the R-matrix analyses of the cross sections of the H(n,n), ^{3}He(n,p), ^{6}Li(n,t), ^{10}B(n,α) and ^{10}B(n,$\alpha_1\gamma$) reactions. More generally, the project should attempt to examine all sources of bias or uncertainty associated with the use of practical R-matrix codes for data evaluation. The CRP should develop improved evaluation methodology, which will be applied to the analysis of the critically reviewed database of experimental information being prepared by the complementary WPEC (NEA) activity on neutron standards. This methodology and improvements in various codes and procedures will also have the value in making improvements to the evaluation of cross sections other than the standards.

2. APPENDICES

Appendix 1: Agenda and time schedule

Monday, 2 April 2001

Morning: 09:30 - 12:30

1. Opening of the meeting and election of the chairperson (10’).

2. Adoption of the agenda (10’).

3. Requirements of the Standard Neutron Cross Sections (15’).

4. Experimental database for improvement of Standard Cross Sections and methods used for generation of covariance matrices of experimental data (25’).

5. Review of the R-matrix model codes (EDA, SAMMY, ORMAP, KALMAN) used for resonance cross section evaluations (20’ to 40’ for each presentation):

   – basic approximations (physical approximations, limits on the types of reactions and number of channels);
   – computational limitations (experimental data uncertainties to be taken into account by the codes, implementation of error propagation, evaluated data uncertainties obtained by the codes).

Afternoon: 14:00 - 18:00

6. Theoretical model calculations for the light nucleus systems and their influence on determination of the R-matrix parameters (parameters of distant levels, resonances with large widths, etc.) (40’).

7. Review of stand-alone least-square analysis codes (GMA, GLUCS, KALMAN, ZOTT) and their basic limitations (20’ to 40’ for each presentation).

Tuesday, 3 April 2001

Morning: 09:00 - 12:00

8. Analysis of error propagation in the R-matrix least square fits and uncertainty reduction, taking into account:
   – physical model and physical constraints (unitarity, causality, partial-wave expansion, etc.);
   – data for many open reaction channels;
   – effect of correlations among the experimental data and treatment of data normalization uncertainties;
   – inclusion of contributions from non-statistical reaction mechanisms.

9. Preparation of test cases for better understanding of the origin of the strong uncertainty reduction observed in recent R-matrix fits of the data:
   - study of interactions between correlations in the input data and non-linearity of the models;
   - relationship between parameter sensitivities and output covariances;
   - realistic cases for resonance reactions based on comparison of R-matrix model fits with model-free fits.

12:00 - 14:00 ***Lunch***

Afternoon: 14:00 - 18:00

Item 9 will be continued.

10. Preparation of the program for re-evaluation of the standard cross sections for light elements:

   - improvement of R-matrix codes;
   - improvement in the procedure for combining the R-matrix and generalized least-square results (R-matrix fit as a shape fit, use this fit as a prior for the following generalized least-square procedure);
   - preparation of the covariance matrices of the uncertainties for experimental data (mainly from the NEA Subgroup on Standards);
   - combining of the results of the R-matrix model fits for light elements with the results of model-free least square fits of smooth cross sections for heavy elements.

<u>Wednesday, 4 April 2001</u>

Morning: 09:00 - 14:00

11. Preparation of the Co-ordinated Research Project proposal, including:

- title of the CRP;
- background situation analysis;
- overall objective;
- specific research objectives (purpose);
- expected research output (results);
- general action plan;
- list of potential participants and their contribution;
- detailed plan of work for participants for the first year.

Appendix 2: List of participants

AUSTRIA

Mr. Siegfried TAGESEN
Institut für Isotopenforschung und Kernphysik der Universität Wien
Boltzmanngasse 3
A-1090 Vienna

Phone: +43 1 4277 51755
Fax: +43 1 4277 51752
E-mail: Tagesen@ap.univie.ac.at

Mr. Herbert K. VONACH
Institut für Isotopenforschung und Kernphysik der Universität Wien
Boltzmanngasse 3
A-1090 Vienna

Phone: +43 1 3177205
Fax: +43 1 4277 51752
E-mail: Herbert.Vonach@utanet.at
E-mail: Vonach@ap.univie.ac.at

CHINA

Mr. CHEN Zhenpeng
Physics Department
Tsinghua University
Beijing, 100084

Phone: +86 10 62782163
Fax: +86 10 62781604
E-mail: wbzhu@chinaren.com

GERMANY

Mr. Hartmut M. HOFMANN
Room No. 02.534, Building B2
Institut für Theoretische Physik III
Universität Erlangen-Nürnberg
Staudtstrasse 7
D-91058 Erlangen

Phone: +49 9131 852 8470
Fax: +49 9131 852 7704
E-mail: hmn@theorie3.physik.uni-erlangen.de

JAPAN

Mr. Toshihiko KAWANO
Department of Advanced Energy Engineering Science
Kyushu University
6-1 Kasuga-kouen, Kasuga-shi
Fukuoka-ken 816-8580

Phone: +81 92 583 7587
Fax: +81 2 583 7586
E-mail: Kawano@aees.kyushu-u.ac.jp

UNITED STATES OF AMERICA

Mr. Allan D. CARLSON
National Institute
of Standards and Technology (NIST)
100 Bureau Drive Stop 8463
Gaithersburg, MD 20899-8463
Phone: +1 301 975 5570
Fax: +1 301 975 4766
Fax: +1 301 869 7682 (for larger jobs)
E-mail: Carlson@nist.gov
E-mail: Allan.Carlson@nist.gov

Mr. Gerald M. HALE
Group T-16, MS B-243
Los Alamos National Laboratory
Los Alamos, NM 87545
Phone: +1 505 667 7738
Fax: +1 505 667 9671
E-mail: GHale@lanl.gov

Ms. Nancy M. LARSON
Bldg 6011, Rm 118, MS 6370
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831-6370
Phone: +1 865 574 4659
Fax: +1 865 574 3527
E-mail: LarsonNM@ornl.gov

IAEA, Vienna, AUSTRIA

Mr. Vladimir G. PRONYAEV (Scientific Secretary)
IAEA Nuclear Data Section
Wagramer Strasse 5
P.O. Box 100
A-1400 Vienna
Phone: +43 1 2600 21717
Fax: +43 1 26007
E-mail: V.Pronyaev@iaea.org

Mr. Douglas W. MUIR
IAEA Nuclear Data Section
Wagramer Str. 5
P.O. Box 100
A-1400 Vienna
Phone: +43 1 2600 21709
Fax: +43 1 26007
E-mail: D.Muir@iaea.org

Appendix 3: List of papers/viewgraphs presented by participants and discussed during the meeting

1. A.D. Carlson, “Requirements of the Neutron Cross Section Standards”, transparencies of the report presented at this meeting, 2-4 April 2001.

2. A.D. Carlson, “Experimental Database for the Improvement of the Neutron Cross Section Standards”, transparencies of the report presented at this meeting, 2-4 April 2001.

3. G.M. Hale, “R-matrix Theory for Standards Evaluation of Light Elements”, transparencies of the report presented at this meeting, 2-4 April 2001.

4. N.M. Larson, “The R-matrix Code SAMMY”, transparencies of the report presented at this meeting, 2-4 April 2001.

5. H.M. Hofmann, “Standard Cross-Sections and Microscopic Theoretical Calculations”, transparencies of the report presented at this meeting, 2-4 April 2001.

6. T. Kawano, “Investigation on the Relation between R-Matrix Analysis and Experimental Errors by means of a Numerical Simulation”, transparencies of the report presented at this meeting, 2-4 April 2001.

7. S. Tagesen, “Application of Bayes’ Equations to Cross Section Evaluations”, transparencies of the report presented at this meeting, 2-4 April 2001.

8. Chen Zhenpeng, “Introduction of R-Matrix code RAC”, transparencies of the report presented at this meeting, 2-4 April 2001.

9. Chen Zhenpeng, “Covariance Matrix and Error Propagation”, transparencies of the report presented at this meeting, 2-4 April 2001.

10. D.W. Muir, “Evaluation of Correlated Data using Partitioned Least Squares: A Minimum-Variance Derivation”, transparencies of the report presented at this meeting, 2-4 April 2001.

Appendix 4: Some viewgraphs presented at the meeting

Requirements of the Neutron Cross Section Standards

Allan D. Carlson

Ionizing Radiation Division
National Institute of Standards and Technology

For a thin sample, the neutron cross section is given by

$$\sigma = \frac{R}{N\phi}$$

R is the reaction rate

N is the total number of nuclei in the sample

ϕ is the neutron fluence

With the use of a standard cross section

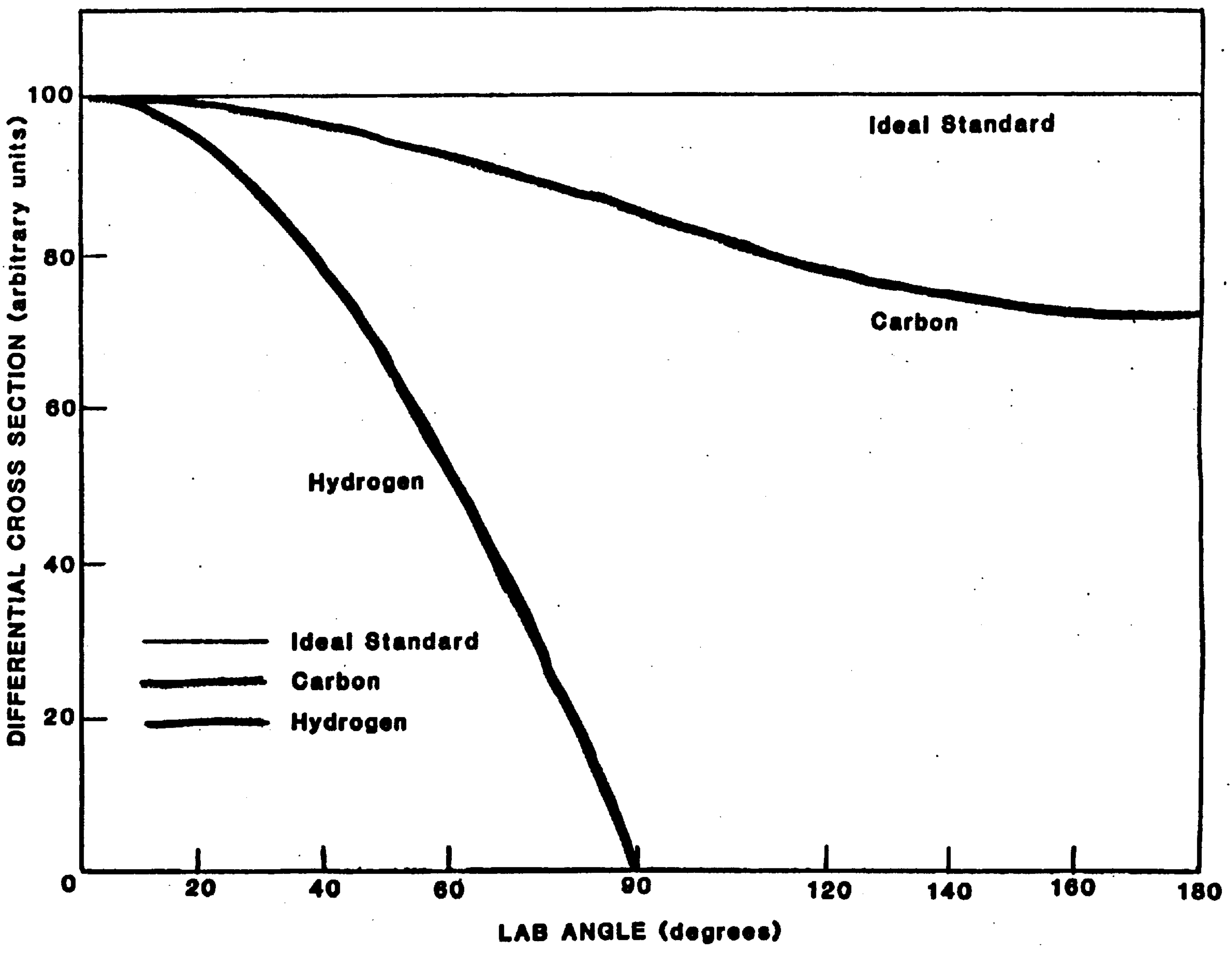
$$\sigma = \sigma_s \frac{R\,N_s}{R_s N}$$

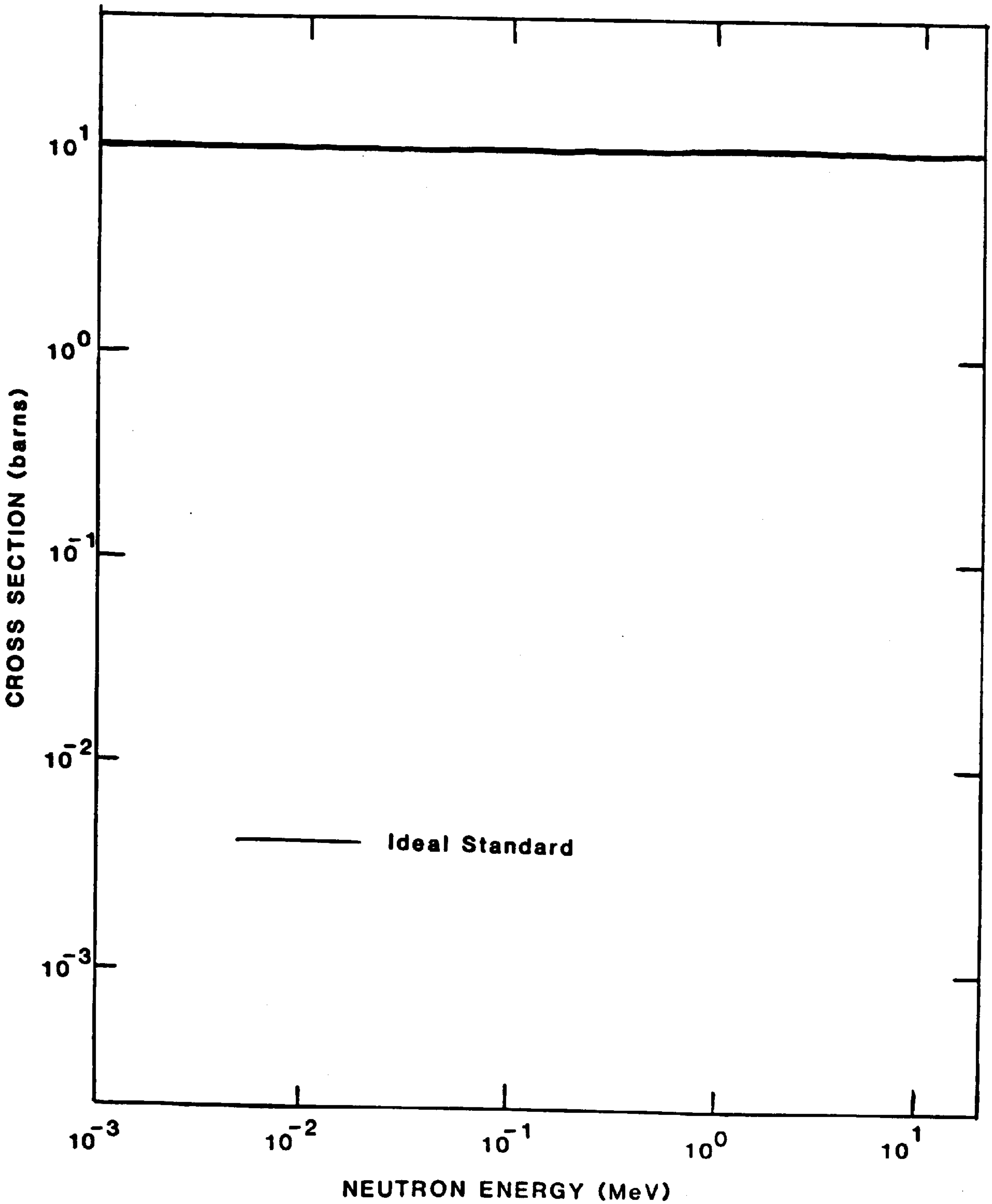
Desired Properties of Standard Cross Sections

- Accurately known
- Large magnitude
- Smooth and relatively constant (vs E and θ)
- Usable for prompt and activation measurements
- Can be used with samples having favorable physical and chemical properties

Must be able to use in an appropriate detector which:

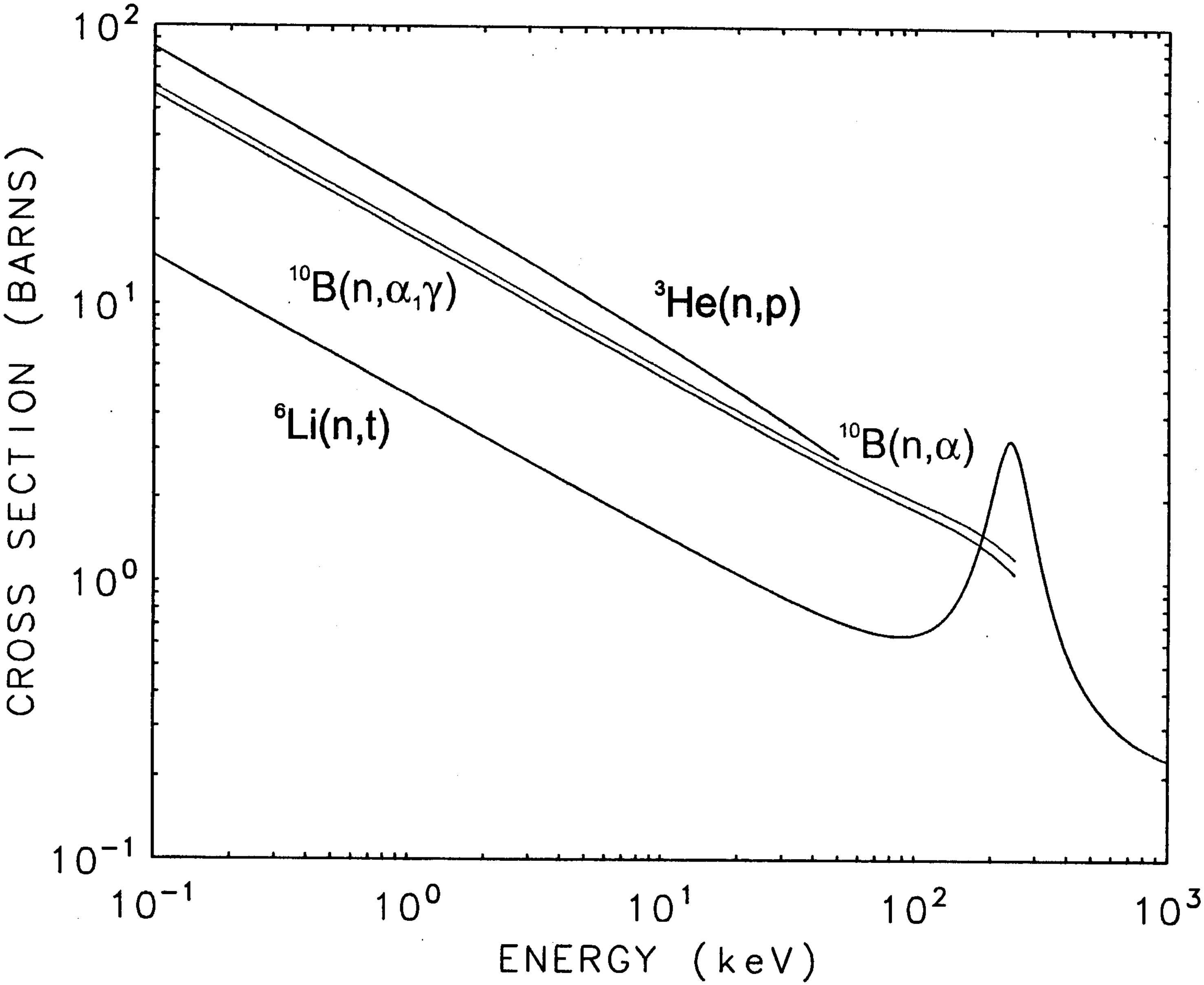
- Is easy to use
- Preferably works for both white source and monoenergetic neutrons
- Has good timing
- Has good separation between foreground and background events
- Has small experimental or calculated corrections
- Is useful over a large energy region
    - Is inexpensive/easy to build


DIFFERENTIAL CROSS SECTION (arbitrary units)
100
80
60
40
20
0
20
40
60
90
120
140
160
180
LAB ANGLE (degrees)
Ideal Standard
Carbon
Hydrogen
Ideal Standard
Carbon
Hydrogen

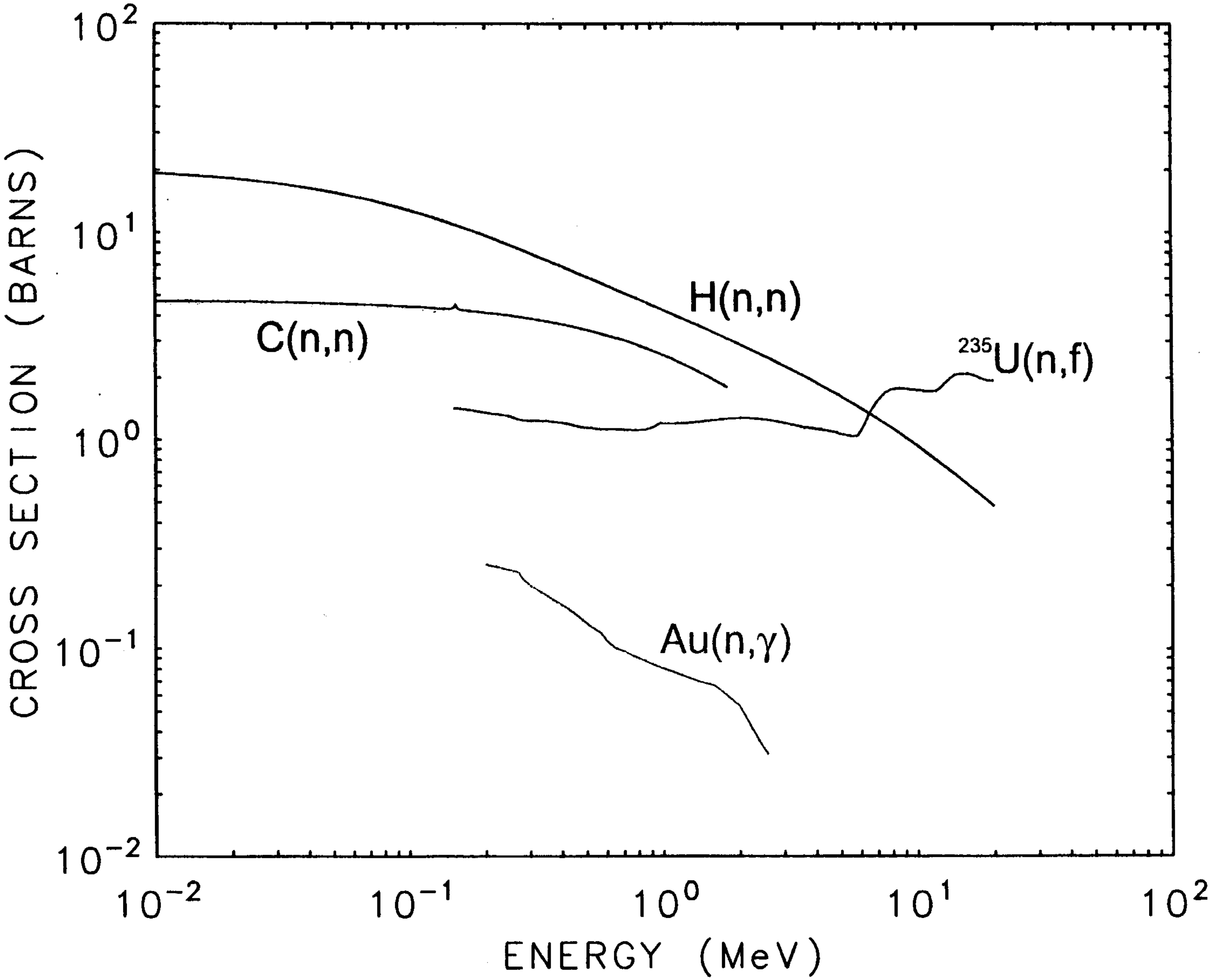


CROSS SECTION (barns)
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
Ideal Standard
10^{-3}
10^{-2}
10^{-1}
10^0
10^1
NEUTRON ENERGY (MeV)

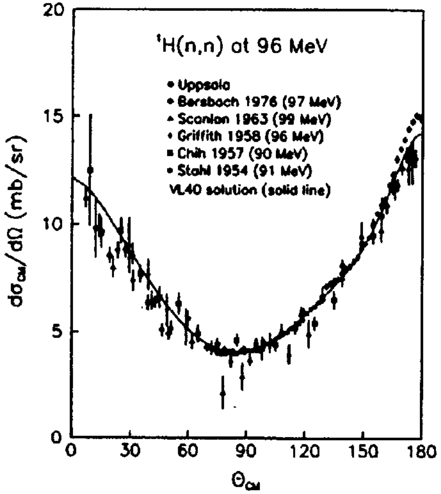
The Lower Energy Neutron Cross Section Standards



The Higher Energy Neutron Cross Section Standards



International Evaluation of The High Energy Neutron Cross Section Standards



International Atomic Energy Agency

INDC(NDS)-368
Distr.: G+J

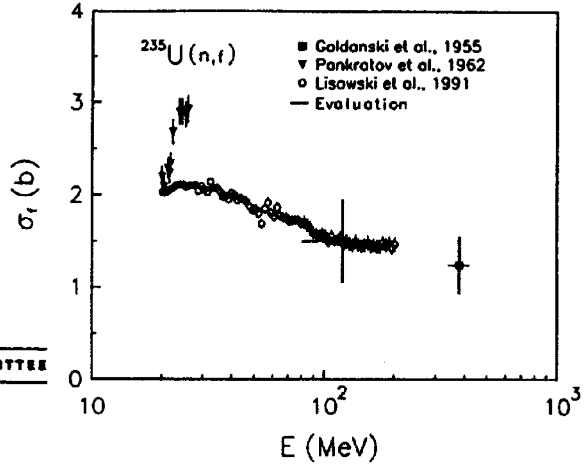
INDC

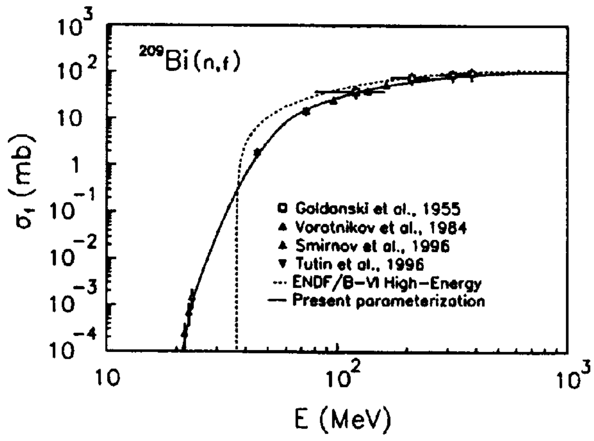
INTERNATIONAL NUCLEAR DATA COMMITTEE

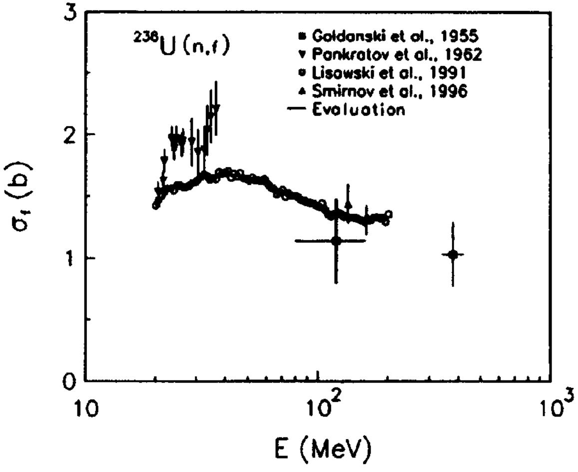
UPDATE TO NUCLEAR DATA STANDARDS FOR NUCLEAR MEASUREMENTS

A.D. Carlson (National Institute of Standards and Technology, Gaithersburg, MD USA),
S. Chiba (Japan Atomic Energy Research Institute, Tokai-mura, Japan),
F.-J. Hambsch (Institute for Reference Materials and Measurements, Geel, Belgium)
N. Olsson (Department of Neutron Research, Uppsala University, Uppsala, Sweden),
A.N. Smirnov (V.G. Khlopin Radium Institute, Saint-Petersburg, Russia)

Summary Report of a Consultants' Meeting held in Vienna, Austria







THE NEUTRON CROSS SECTION STANDARDS

Reaction	Energy Range
H(n,n)	1 keV to 20 MeV
^{3}He(n,p) *	thermal to 50 keV
^{6}Li(n,t)	thermal to 1 MeV
^{10}B(n,α)	thermal to 250 keV
^{10}B(n,$\alpha_1\gamma$)	thermal to 250 keV
C(n,n)	thermal to 1.8 MeV
^{197}Au(n,γ)	thermal, 0.2 to 2.5 MeV
^{235}U(n,f)	thermal, 0.15 to 20 MeV
^{238}U(n,f) **	threshold to 20 MeV

* ENDF standard, not in NEANDC/INDC Standards File
** not an ENDF standard, in NEANDC/INDC Standards File

SIMULTANEOUS EVALUATION DATABASE

$^{6}Li(n,t)$ — ^{6}Li total cross section

$^{6}Li(n,n)$ — ^{6}Li total cross section

$^{10}B(n,\alpha_0)$ — ^{10}B total cross section

$^{10}B(n,\alpha_1)$ — ^{10}B total cross section

$^{10}B(n,n)$ — ^{10}B total cross section

$Au(n,\gamma)$

$^{235}U(n,f)$

$^{238}U(n,f)$

$^{238}U(n,\gamma)$

$^{239}Pu(n,f)$

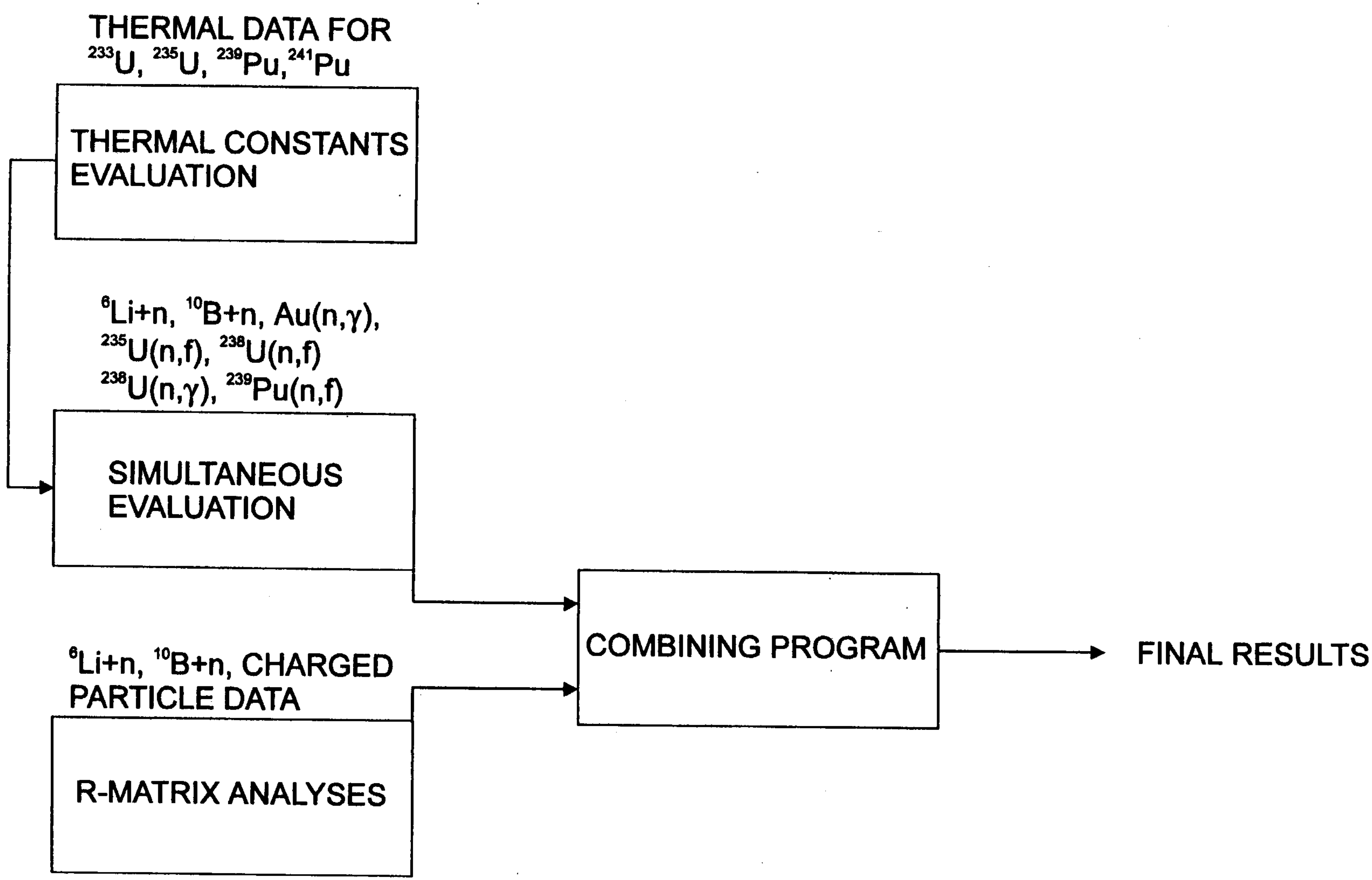
DATA TYPES USED IN THE ENDF/B-VI SIMULTANEOUS EVALUATION

Type	Data Type	Example
1	Absolute cross section	$\sigma_{nf}(^{235}U)$
2	Cross section shape	$c*\sigma_{n\alpha}(^{6}Li)$, c unknown
3	Absolute cross section ratio	$\sigma_{nf}(^{238}U)/\ \sigma_{nf}(^{235}U)$
4	Ratio shape	$c*\sigma_{nf}(^{235}U)/\sigma_{n\alpha}(^{6}Li)$ c unknown
5	Sum of cross sections	$\sigma_{tot}(^{6}Li)=\sigma_{nn}(^{6}Li)+\sigma_{n\alpha}(^{6}Li)$
6	Spectrum averaged cross section	$\sigma_{nf}(^{235}U)$ averaged over ^{252}Cf spont. fission spect
7	Absolute ratio of cross section/ sum of cross sections	$\sigma_{nf}(^{235}U)/\ \sigma_{n\alpha}(^{10}B)$, where $\sigma_{n\alpha}(^{10}B)=\sigma_{n\alpha_0}(^{10}B)+\sigma_{n\alpha_1}(^{10}B)$
8	Shape of Type 5 data	
9	Shape of Type 7 data	

R-MATRIX EVALUATION DATABASE FOR ENDF/B-VI EVALUATION

^{6}Li Total		^{10}B Total	
^{6}Li(n,n)	Integral Data	^{10}B(n,n)	Integral Data
^{6}Li(n,n)	Differential Data	^{10}B(n,n)	Differential Data
^{6}Li(n,n)	Polarization Data	^{10}B(n,n)	Polarization Data
^{6}Li(n,t)	Integral Data	^{10}B(n,α_0)	Integral Data
^{6}Li(n,t)	Differential Data	^{10}B(n,α_0)	Differential Data
^{6}Li(n,t)	Polarization Data	^{10}B(n,α_1)	Integral Data
^{4}He(t,n)	Differential Data	^{10}B(n,α_1)	Differential Data
^{4}He(t,t)	Differential Data	^{7}Li(α_0,α_0)	Differential Data
^{4}He(t,t)	Polarization Data	^{7}Li(α,α_1)	Differential Data
		^{7}Li(α,n)	Differential Data

Standards EvaluationProcedure



1. The first topic of discussion was the uncertainties for the ENDF/B-VI standards. At the last CSEWG meeting there **was much concern expressed about the seemingly small uncertainties** obtained from the combination of the R-matrix and simultaneous evaluations. These uncertainties had been considered too small by the phase I reviewers. At that meeting comments were made by some individuals that they felt that users would not use these uncertainties but instead would arbitrarily increase them to what they considered a more acceptable level. **A strong statement was made that the standards subcommittee should provide such expanded uncertainties since they have had the closest contact with the data base and could make better estimates of more 'acceptable' values.** The standards subcommittee did supply these expanded uncertainties at the present meeting. These uncertainties are estimates such that if a modern day experiment were performed today on a given standard using the best techniques, those results should fall within these expanded uncertainties (2/3 of the time). They take into account data inconsistencies and concerns about R-matrix parameters. These uncertainties are attached to these minutes along with a sampling of the combination output uncertainties for comparison. Note that it is not assumed that the uncertainties are totally correlated within the energy ranges given. It is recommended that these expanded uncertainties be put in file 1 and in the documentation for the standards. (Minutes of the May 1990 CSEWG Meeting)

Estimated (Expanded) Uncertainties Compared with those Obtained from the Evaluation Process

(Note the two types of uncertainties are defined differently)

^{6}Li(n,t) Cross Section

Energy Range (keV)	Estimated Uncertainty (%)	Comb. Result (%)
(1.E-08) - 0.1	0.3	(0.14)
0.1 - 1	0.5	(0.14)
1 - 10	0.7	(0.14)
10 - 50	0.9	(0.16)
50 - 90	1.1	(0.25)
90 - 150	1.5	(0.33)
150 - 450	2.0	(0.29)
450 - 650	5.0	(0.32)
650 - 800	2.0	(0.36)
800 - 1000	5.0	(0.39)

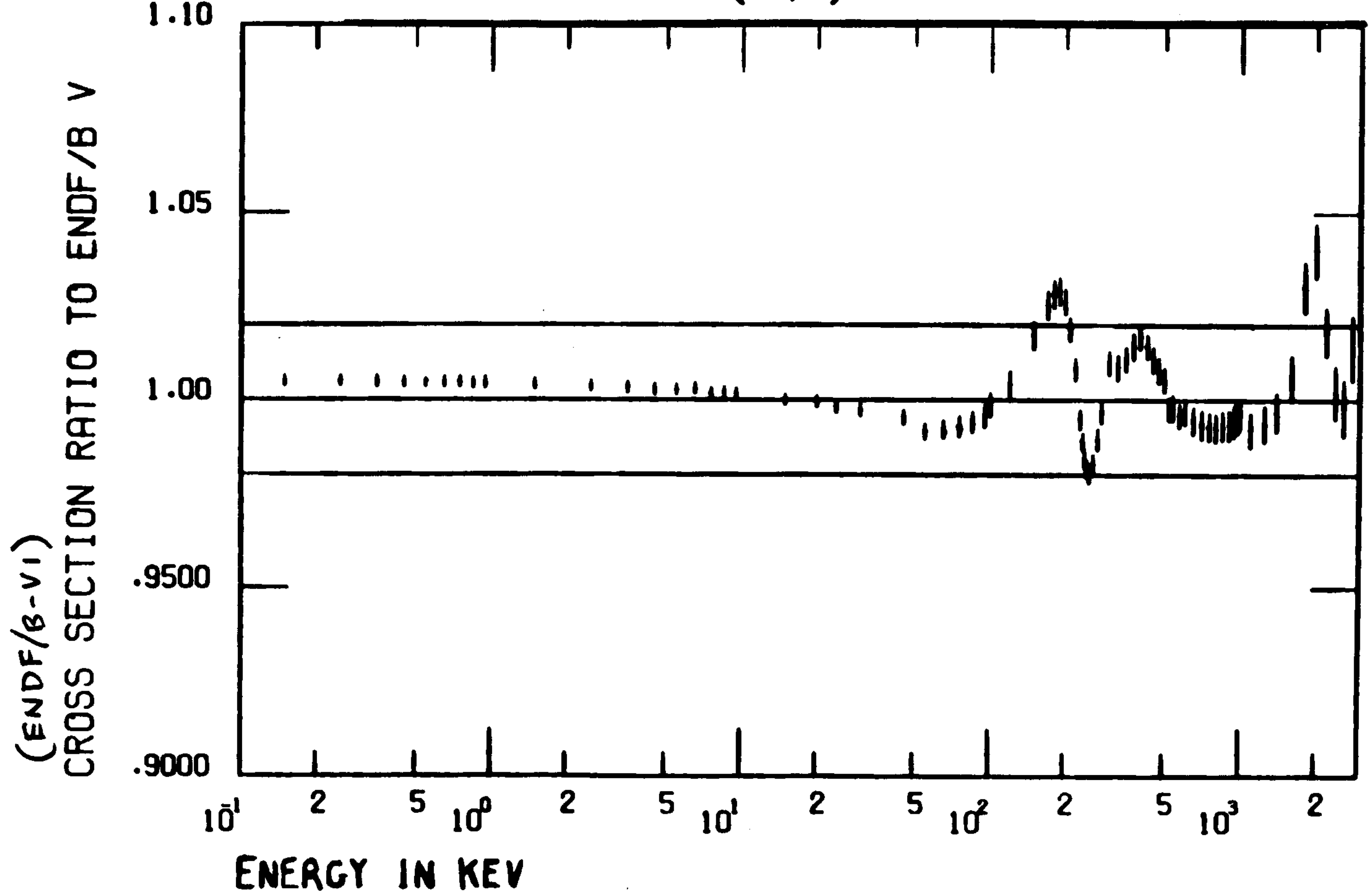
$^{10}B(n,\alpha)$ Cross Section

Energy Range(keV)	Estimated Uncertainty (%)	Comb. Result (%)
(1.E-08) - 0.1	0.2	(0.16)
0.1 - 5	0.4	(0.17)
5 - 30	0.6	(0.20)
30 - 90	1.0	(0.34)
90 - 150	1.6	(0.46)
150 - 200	2.1	(0.57)
200 - 250	2.7	(0.60)

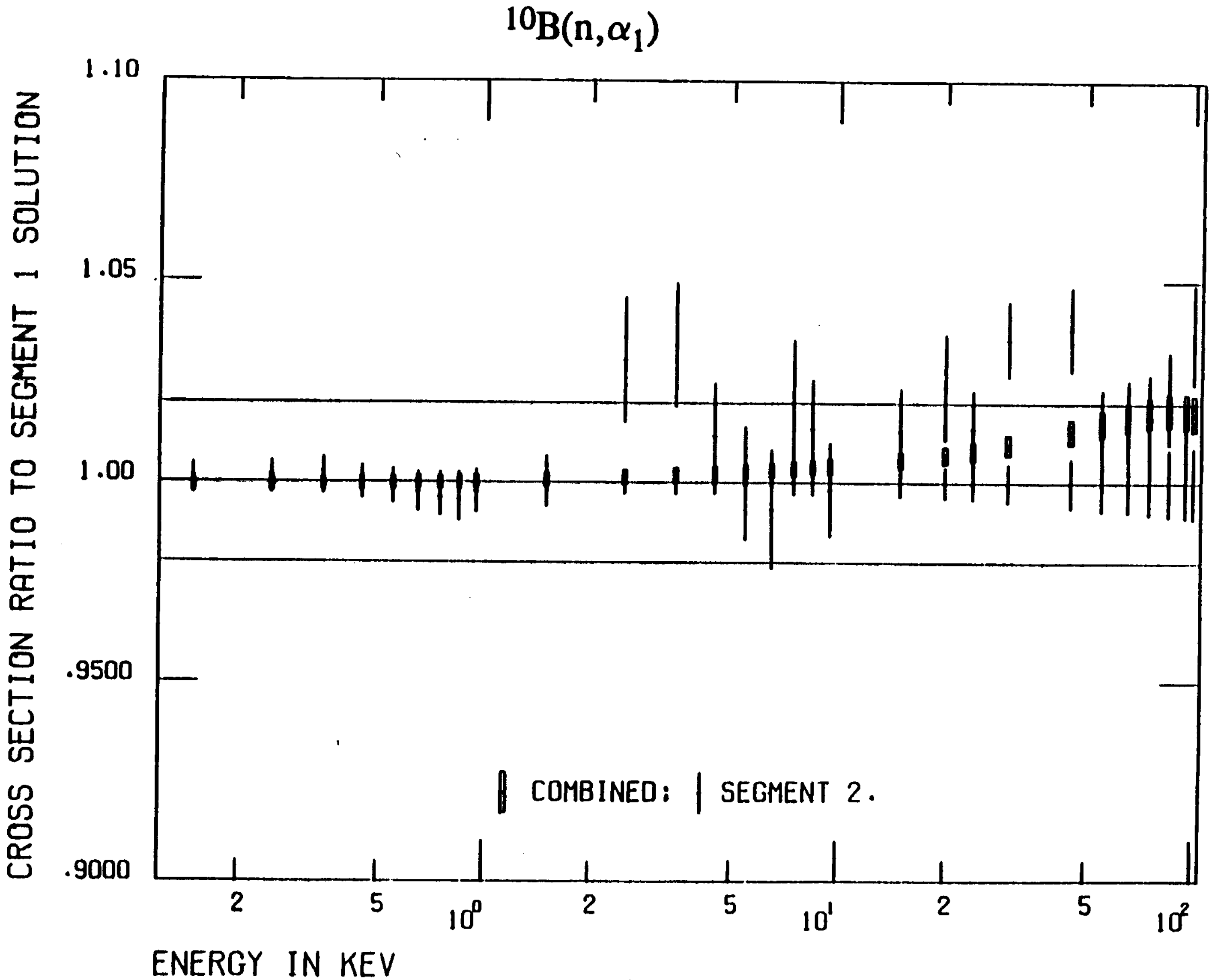
$^{10}B(n,\alpha_1)$ Cross Section

Energy Range(keV)	Estimated Uncertainty (%)	Comb. Result (%)
(1.E-08) - 0.1	0.2	(0.16)
0.1 - 5	0.4	(0.17)
5 - 30	0.6	(0.20)
30 - 90	1.0	(0.34)
90 - 150	1.5	(0.48)
150 - 200	2.0	(0.58)
200 - 250	2.5	(0.62)

$^{6}Li(n,t)$

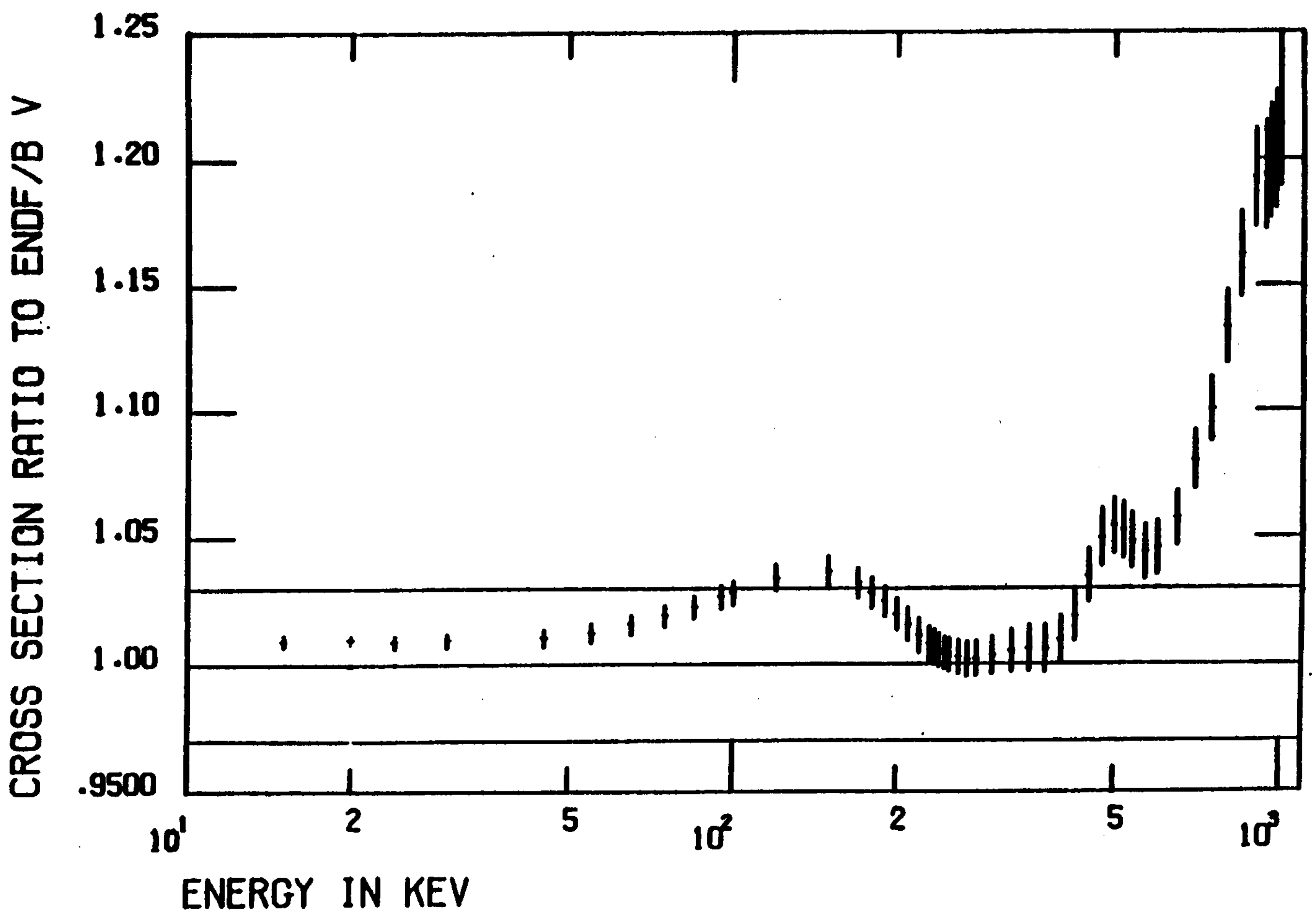


1.10
1.05
1.00
.9500
.9000
CROSS SECTION RATIO TO ENDF/B V
(ENDF/B-VI)
10⁻¹
2
5
10⁰
2
5
10¹
2
5
10²
2
5
10³
2
ENERGY IN KEV



Cross section ratios to the segment 1 solution for the $^{10}B(n,\alpha_1)$ reaction from about 0.2 keV to 100 keV. The rectangles refer to the ratio of the combination output to the R-matrix fit of the segment 1 data. The ┼'s refer to the ratio of the simultaneous evaluation of the segment 2 data to the R-matrix fit of the segment 1 data. The error bars indicate the uncertainties for the fits. The error bars on the unit ratio line are the uncertainties in the R-matrix fit of the segment 1 data. The lines at ratios of 0.98 and 1.02 are guides to the eye.

$^{10}B(n,\alpha_1)$



Ratio of the result of this evaluation process to that of ENDF/B-V for the $^{10}B(n,\alpha_1)$ reaction from about 10 keV to 1 MeV. The lines at ratios of 0.97 and 1.03 are guides to the eye.

Experimental Database for the Improvement of the Neutron Cross Section Standards

Allan D. Carlson

Ionizing Radiation Division
National Institute of Standards and Technology

New Experiments for the Standards Database
$^{++}$means the data have been reviewed and are in the library
$^{+}$means the data are available and the review process is underway
no superscript means that final data are not available (possibly final data not taken yet)

H(n,n)
$^{+}$Nakamura, J. Phys. Soc. Japan 15 (1960) 1359, 14.1 MeV; error in transformation from laboratory to CMS angles; needs correction for proton scattering, an estimate of error associated with neglecting these corrections was made; tail problems; note Table II uncertainty is statistical only (mb/sr).

$^{+}$Shirato, J. Phys. Soc. Japan 36 (1974) 331, 14.1 MeV, needs correction for proton scattering; tail problems

$^{+}$Ryves, 14.5 MeV, σ(180°)/σ(90°), Ann. Nucl. Energy 17, 657 (1990)

$^{+}$Bateman, 10 MeV, angular distribution from 60° to 180°, Fusion Eng. & Design 37, 49 (1997); additional work was done on this experiment. Data is now finalized and submitted for publication (Boukharouba et al.)

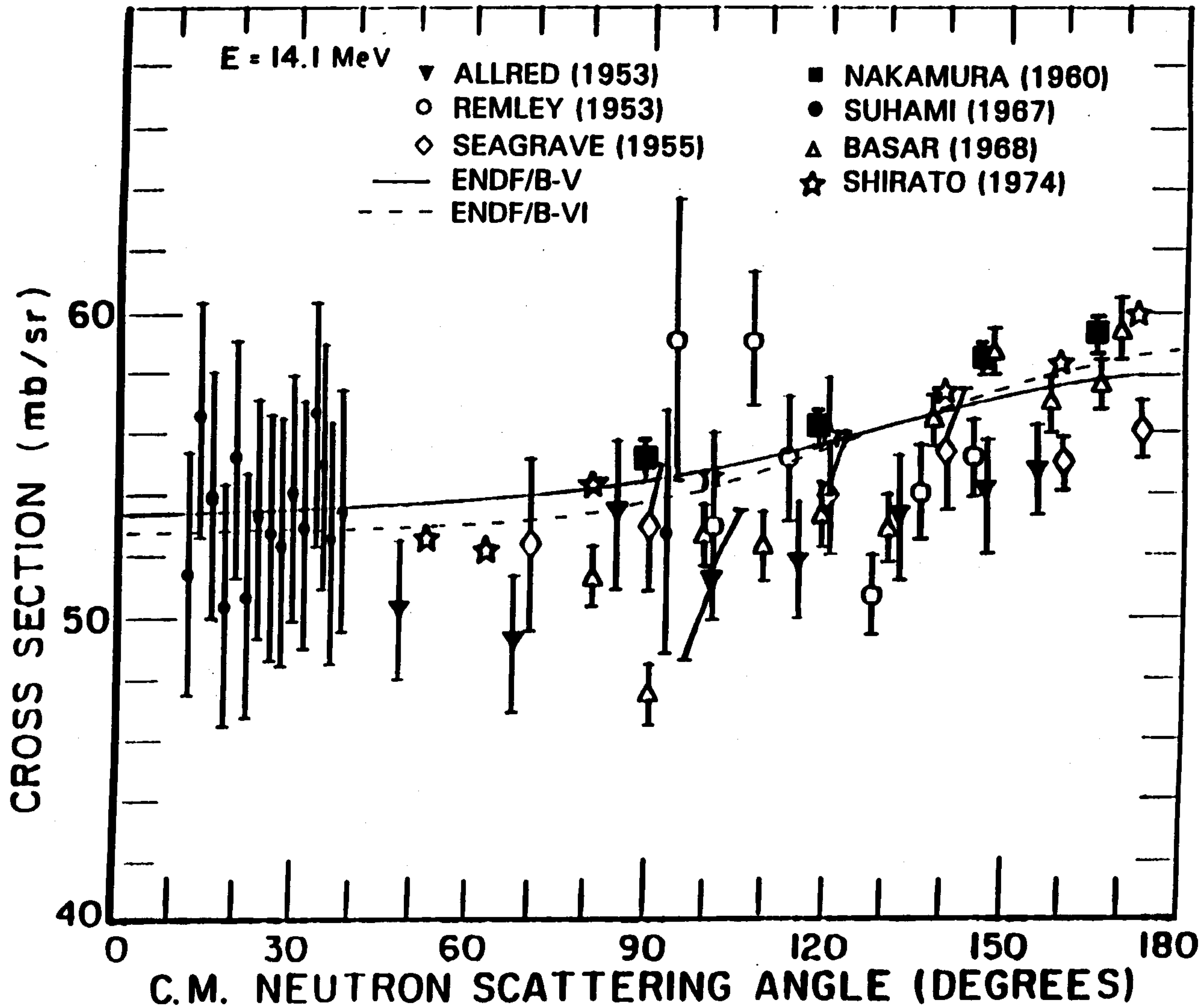
$^{+}$Buerkle, 14.1 MeV, angular distribution from 89.7° to 155.7°, Few-Body Systems 22, 11 (1997)

Olsson (Uppsala group), 96 & 162 MeV, angular distribution from 70° to 180°

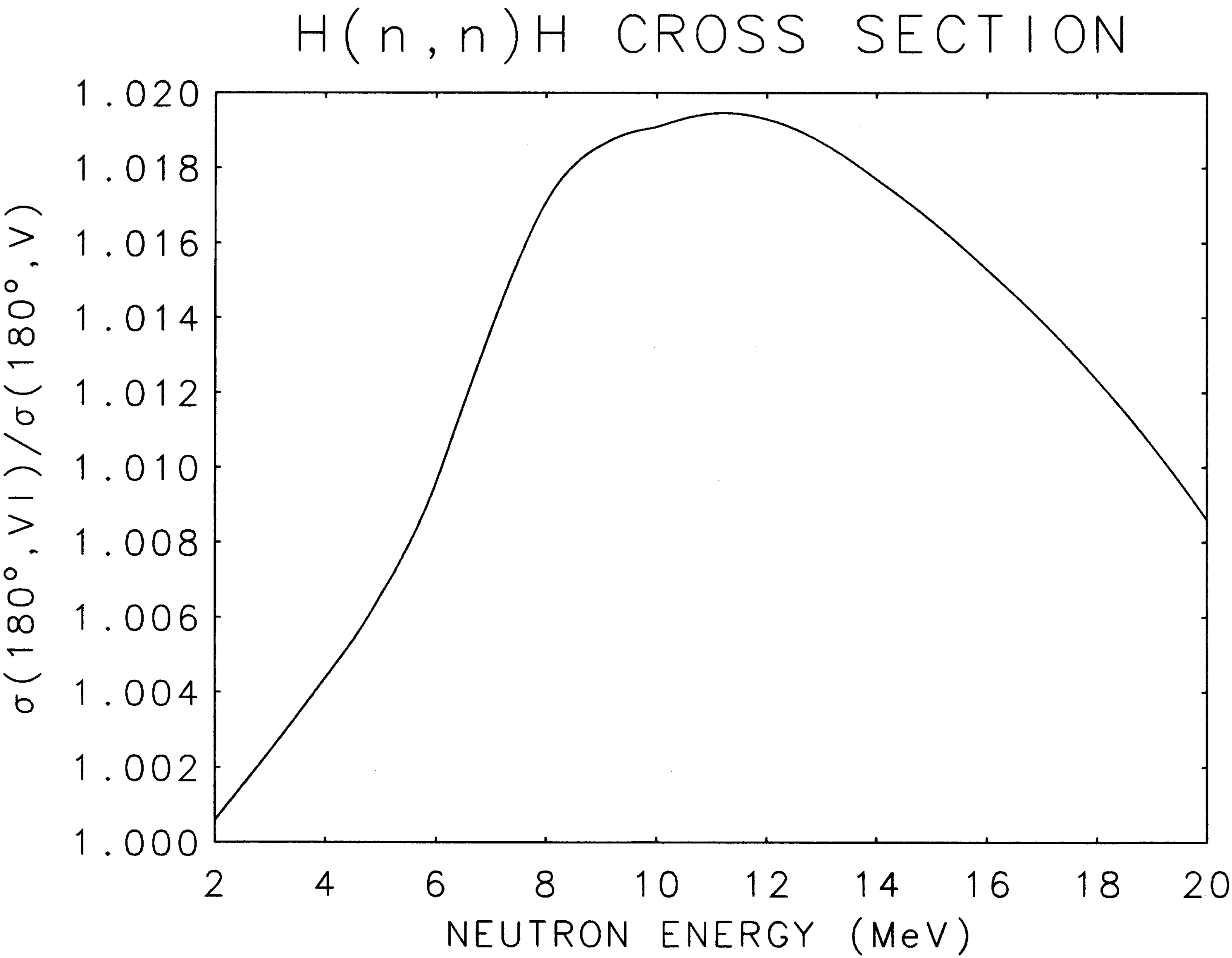
Benck, (Louvain la Neuve) 28-75 MeV, angular distribution from 40° to 140°

Peterson (IUCF) 185-195 MeV, angular distribution from 90° to 180°. In progress but new leadership on the experiment and analysis (Yuezheng Zhou)

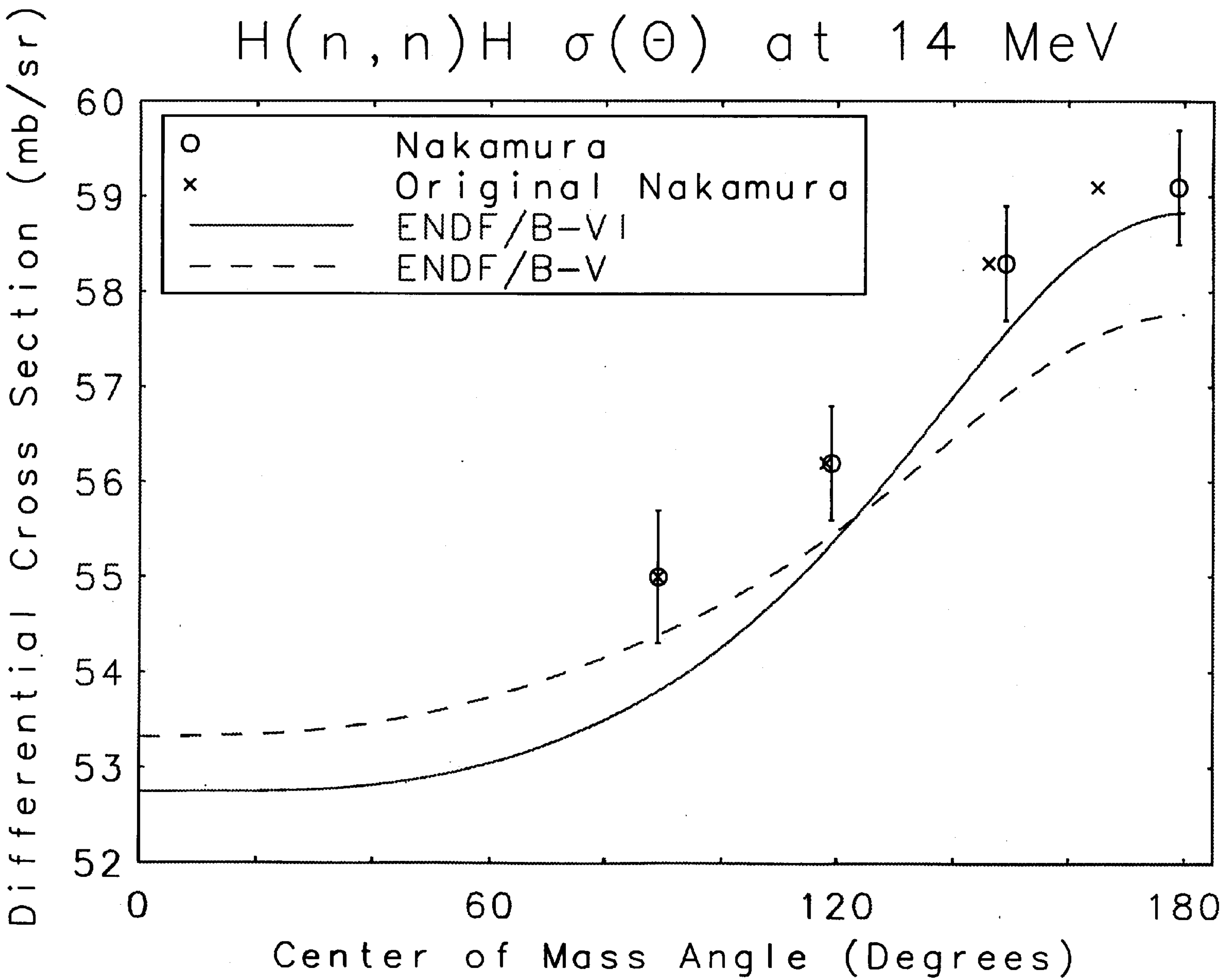
H(n,n)



Measurements of the hydrogen scattering cross section at 14.1 MeV compared with the ENDF/B-V and ENDF/B-VI evaluations. The references for the experimental data are given in reference [41].



H(n,n)H CROSS SECTION
σ(180°,VI)/σ(180°,V)
1.020
1.018
1.016
1.014
1.012
1.010
1.008
1.006
1.004
1.002
1.000
2
4
6
8
10
12
14
16
18
20
NEUTRON ENERGY (MeV)


H(n,n)H σ(Θ) at 14 MeV
Nakamura
Original Nakamura
ENDF/B-VI
ENDF/B-V
Differential Cross Section (mb/sr)
Center of Mass Angle (Degrees)
60
59
58
57
56
55
54
53
52
0
60
120
180

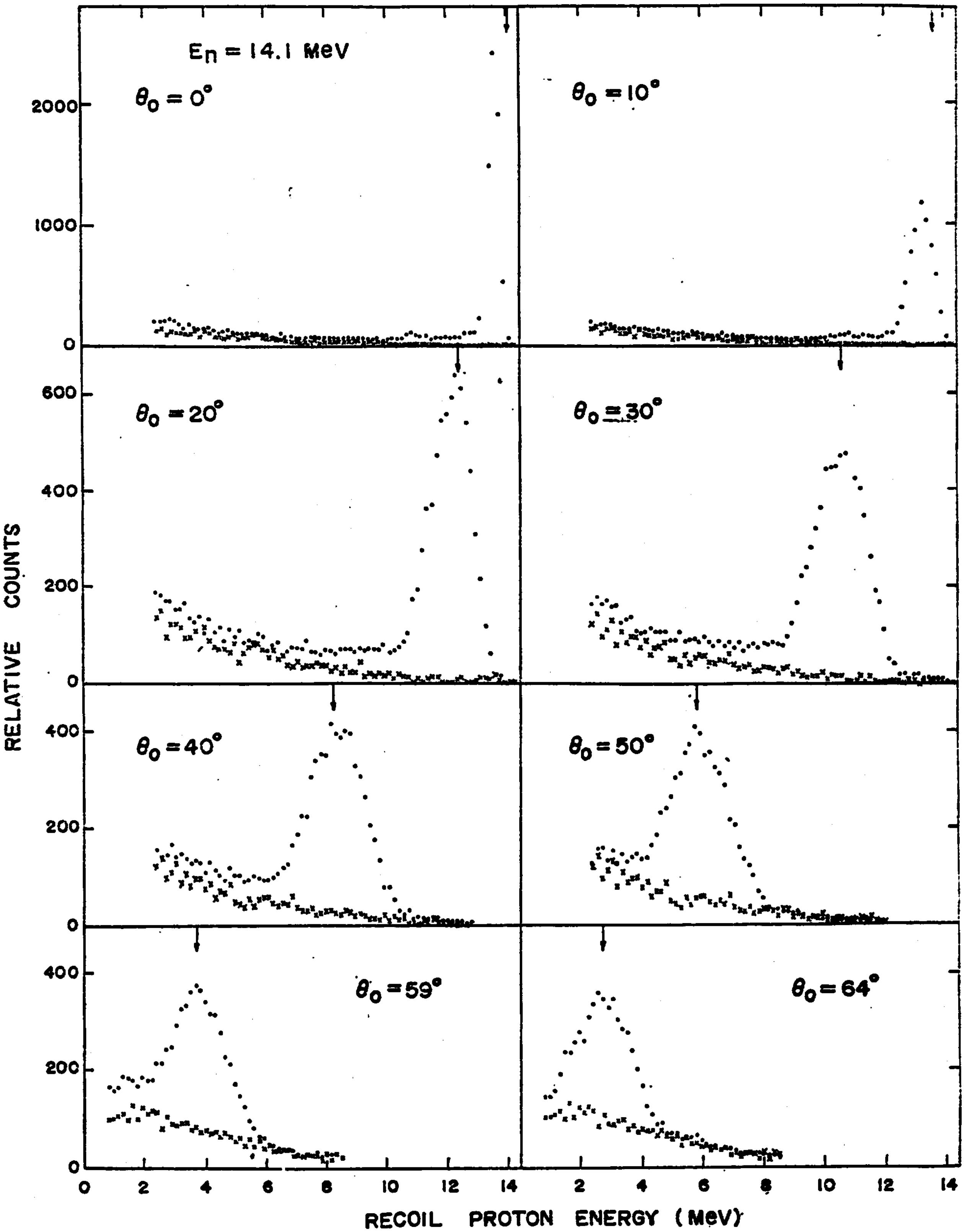
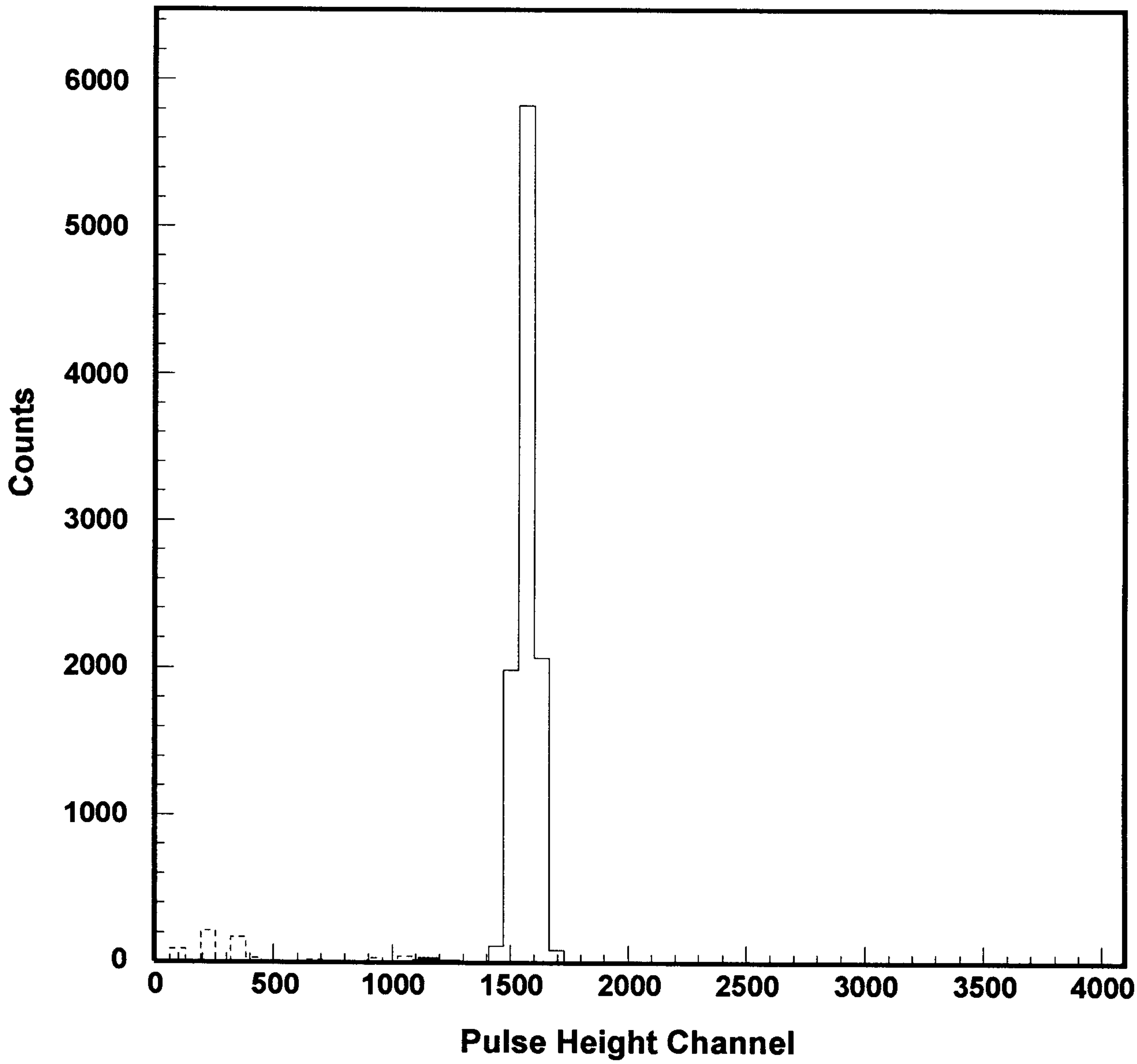
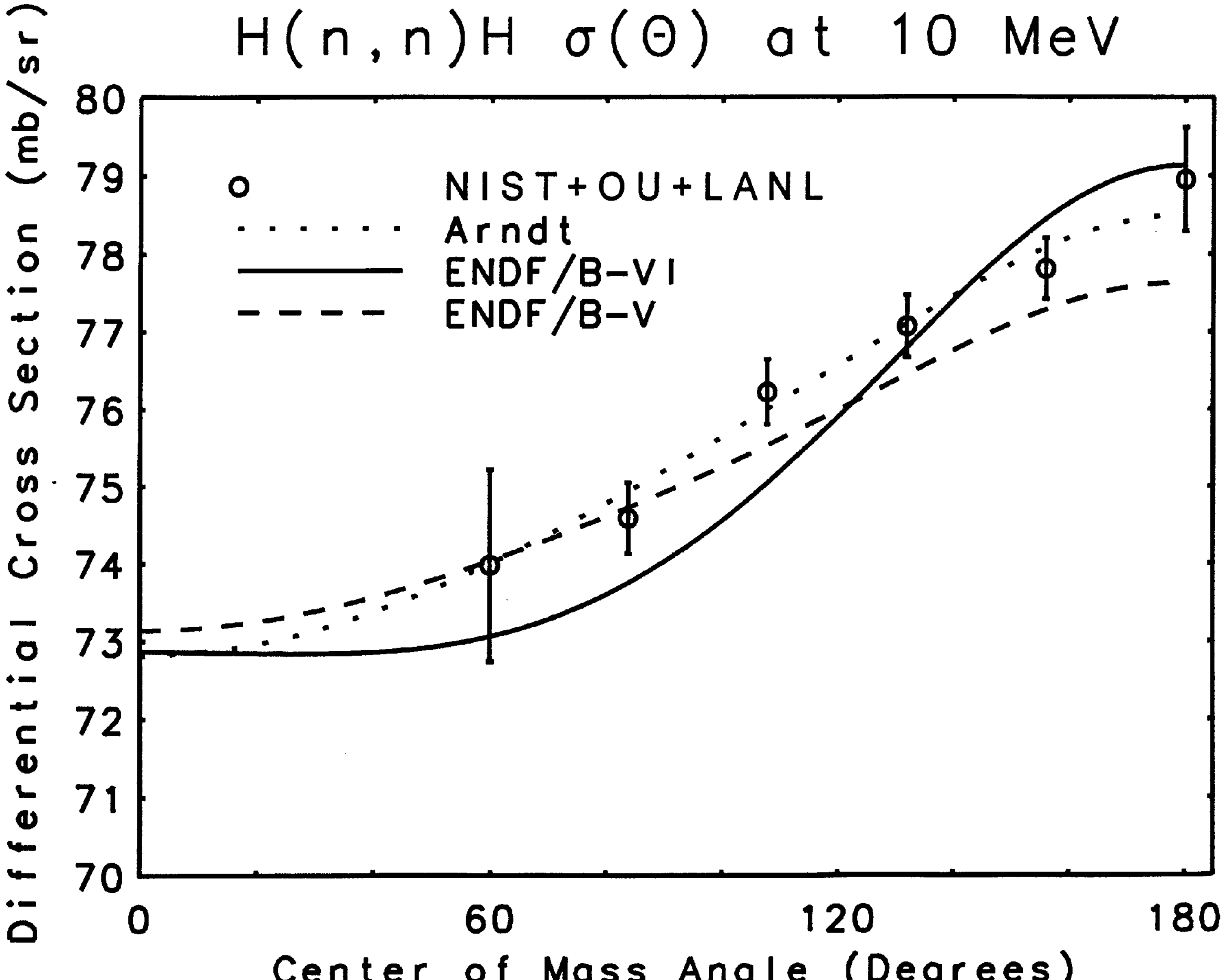
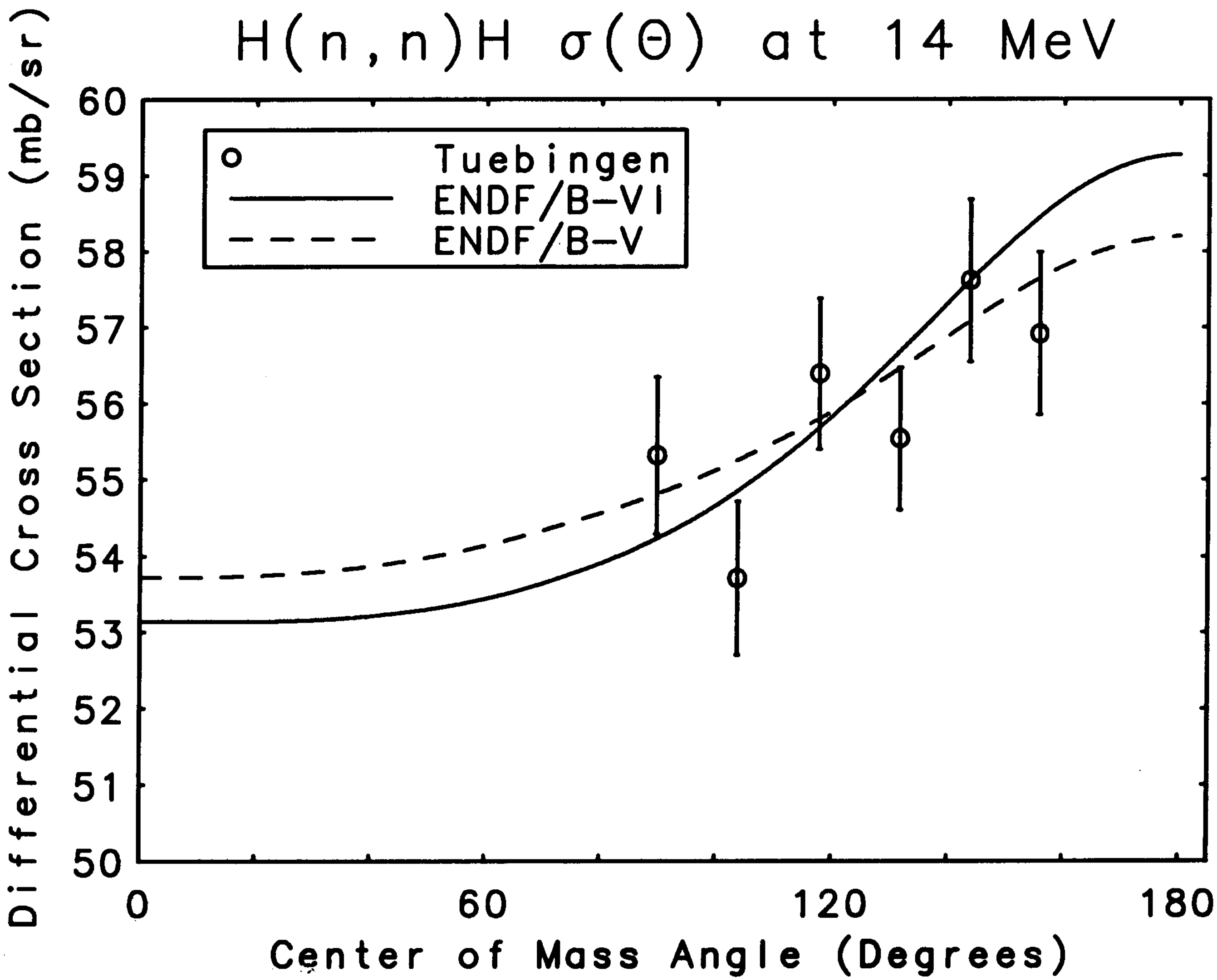


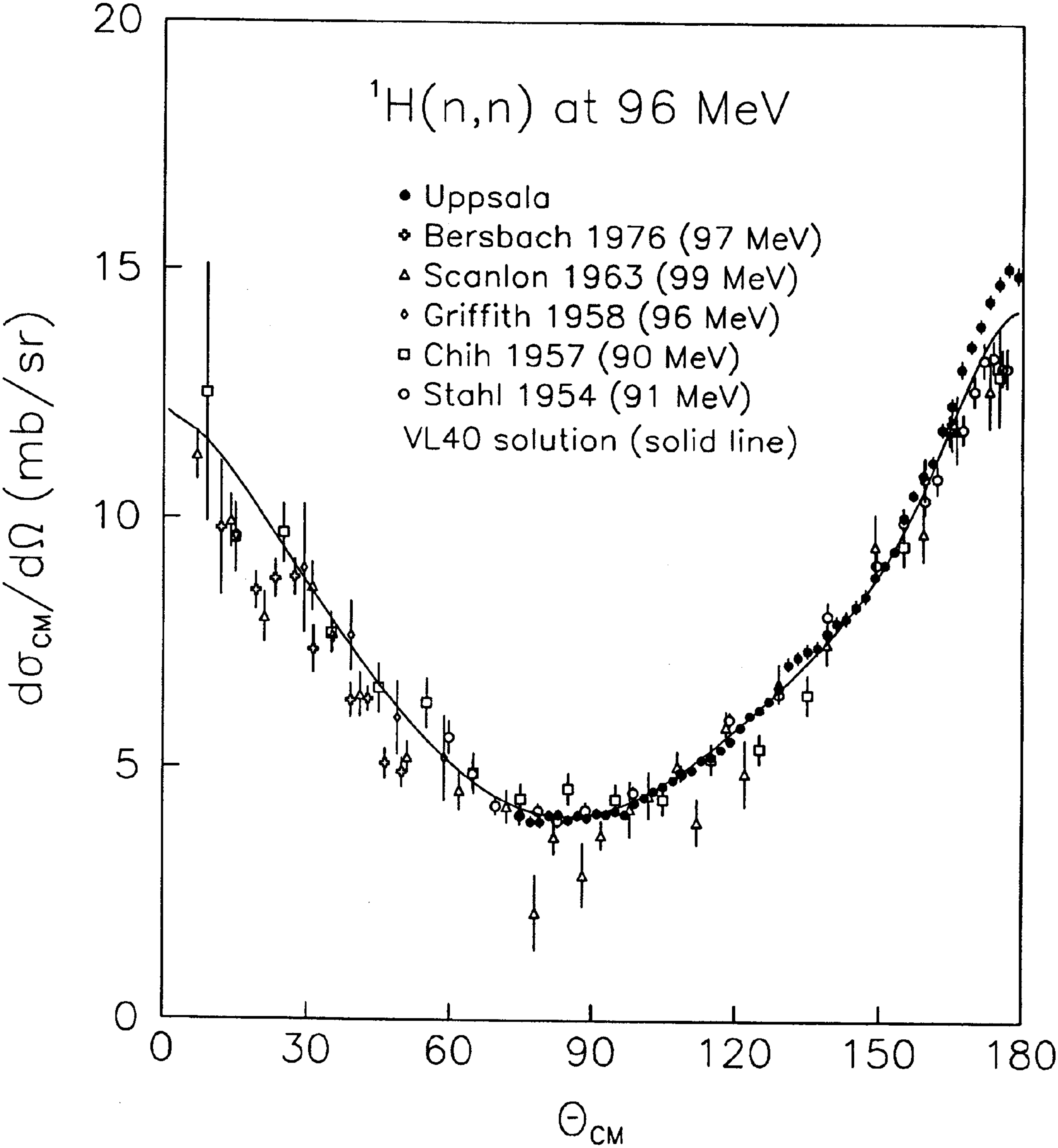
Fig. 1. Recoil proton energy spectra measured at various setting angles θ_0 of the counter telescope axis with respect to the incident neutron direction. The cross marks represent radiator-out backgrounds measured under the same condition for incident neutron flux as the case of radiator-in counts indicated with the solid circles. The spectra are uncorrected for energy losses of protons in radiator and for the energy spread (300 keV) of incident neutrons. The arrows indicate recoil proton energies (E_p) calculated from $E_p = E_n \cos^2\theta_0$, where $E_n = 14.1$ MeV.



Pulse height distribution obtained for a 12° telescope in the NIST-OU-LANL hydrogen angular distribution measurement at 10 MeV neutron energy. The solid line is the foreground. The dashed line is the background.


H(n,n)H σ(Θ) at 10 MeV
NIST+OU+LANL
Arndt
ENDF/B-VI
ENDF/B-V
Differential Cross Section (mb/sr)
80
79
78
77
76
75
74
73
72
71
70
0
60
120
180
Center of Mass Angle (Degrees)


H(n,n)H σ(Θ) at 14 MeV
Tuebingen
ENDF/B-VI
ENDF/B-V
Differential Cross Section (mb/sr)
Center of Mass Angle (Degrees)
60
59
58
57
56
55
54
53
52
51
50
0
60
120
180



$^1H(n,n)$ at 96 MeV
Uppsala
Bersbach 1976 (97 MeV)
Scanlon 1963 (99 MeV)
Griffith 1958 (96 MeV)
Chih 1957 (90 MeV)
Stahl 1954 (91 MeV)
VL40 solution (solid line)
$d\sigma_{CM}/d\Omega$ (mb/sr)
Θ_{CM}
0
5
10
15
20
0
30
60
90
120
150
180

^{3}He(n,p)
$^{++}$Borzakov, 0.26 keV to 142 keV, relative to ^{6}Li(n,t), Sov. J. Nucl. Phys. 35, 307 (1982)

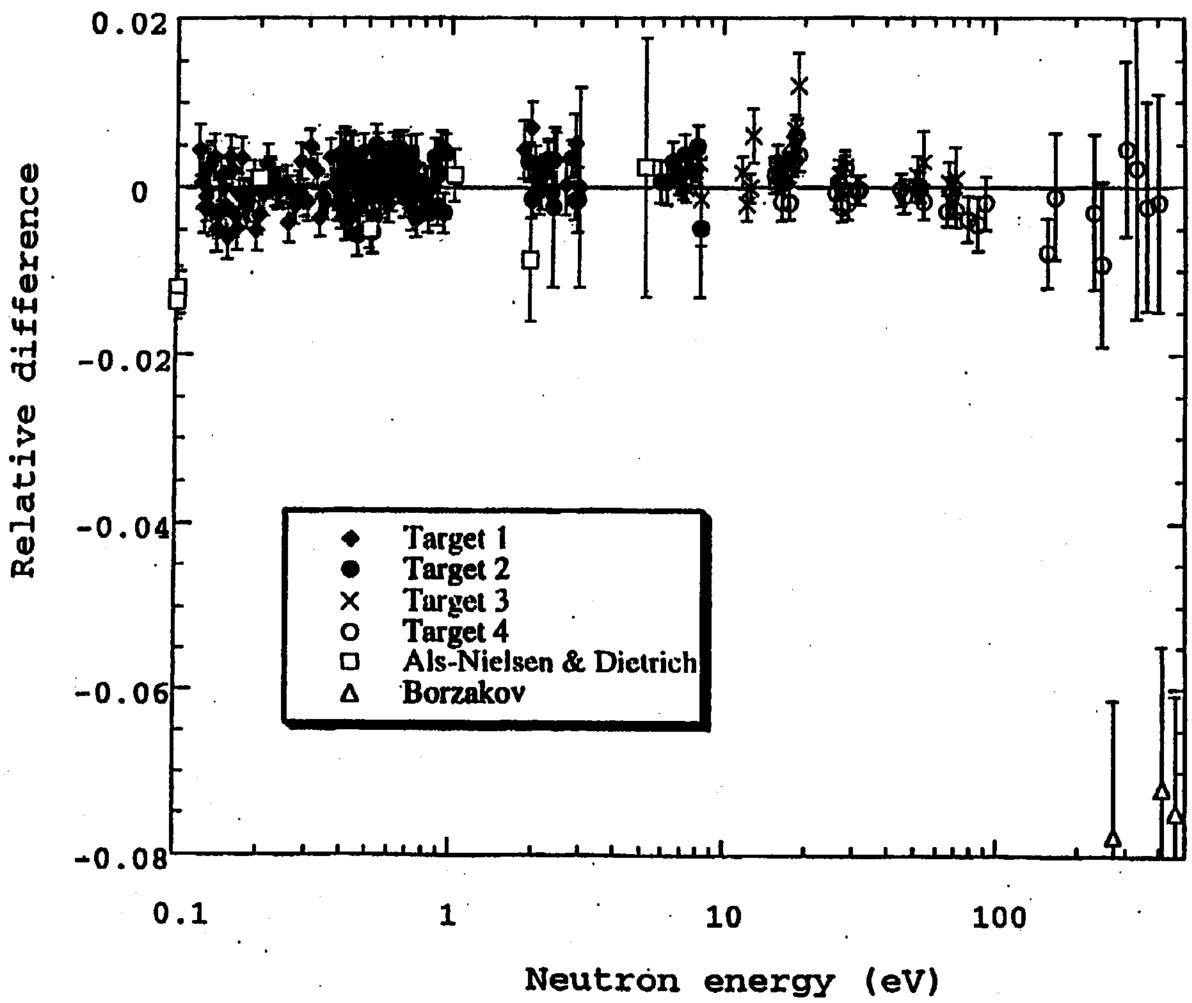
^{3}He total cross section
+Keith, 0.1 to 500 eV, BAPS DNP Oct 1997 paper IG.03 and thesis of D. Rich

^{6}Li(n,t)
Bartle, 2 to 14 MeV, angular distribution, Proc. Conf on Nuclear Data for Basic and Applied Science, Sante Fe (1985), p. 1337

Koehler, 1 keV to 2.5 MeV, angular distribution data (ratio of forward and backward hemispheres responses), private comm.

Gledenov, .025 eV, ??, 87KIEV 2 237

Zhang Guohui, 3.67 and 4.42 MeV, angular distribution, Comm. Of Nuclear Data Progress No.21 (1999) China Nuclear Data Center, also NSE 134, 312 (2000)



Relative difference between the data of Keith et al., using 4 different sample thicknesses, and a 1/v fit to the cross section. Also shown is a sampling of the data of Als-Nielsen & Dietrich, and Borzakov.

ZHANG et. al.

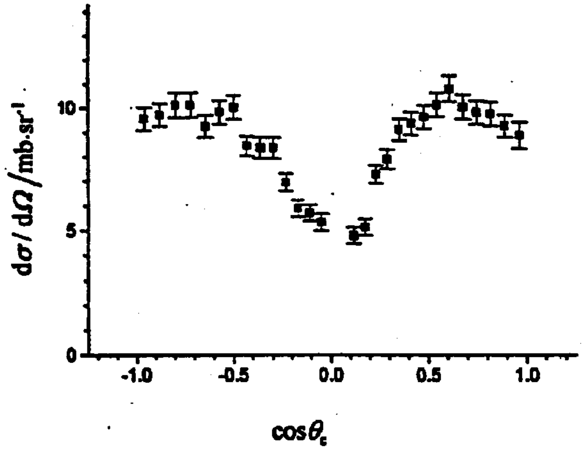


Fig. 3 Differential cross section for ^{6}Li(n,t)^{4}He reaction at E_n=3.67±0.20 MeV

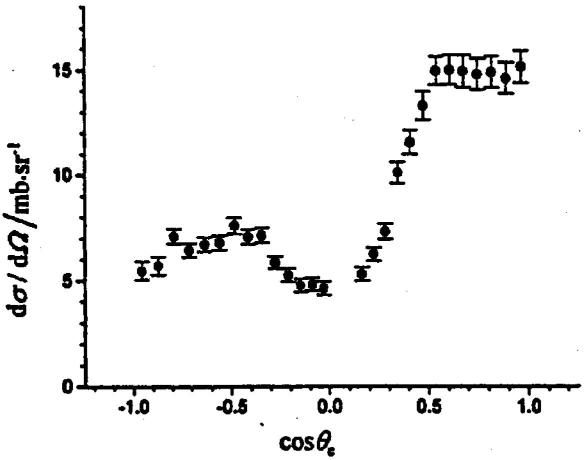


Fig. 4 Differential cross section for ^{6}Li(n,t)^{4}He reaction at E_n=4.42±0.20 MeV

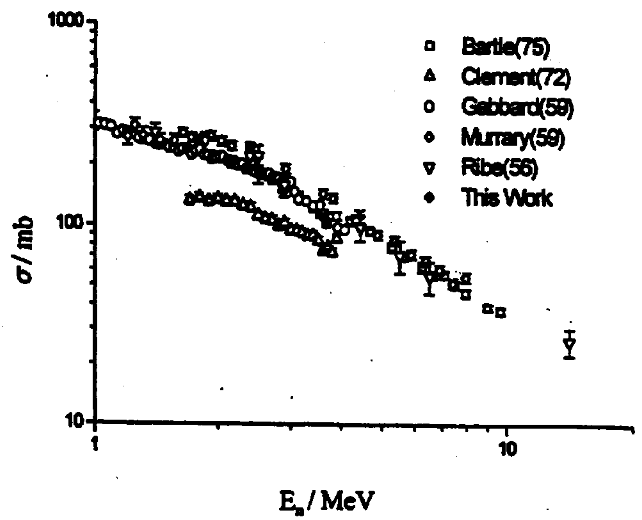


Fig. 5 The result of ^{6}Li(n,t) ^{4}He cross section compared with other measurements

^{10}B(n,$\alpha_1\gamma$)
$^{++}$Schrack, 0.2 MeV to 4 MeV, relative to Black Detector (at ORNL), NSE 114, 352 (1993)

$^{+}$Schrack, 10 keV to 1 MeV, relative to H(n,n) prop ctr (at ORNL), Proc. Conf. on NDST, Gatlinburg (1994)p. 43

$^{+}$Schrack, .3 MeV to 10 MeV, relative to ^{235}U(n,f) ion chamber (at LANL), Private comm.

^{10}B(n,α) Branching Ratio
$^{++}$Weston, 0.02 MeV to 1 MeV, Solid State detectors, NSE 109, 113 (1991)

Hambsch and Bax, keV to MeV, Frisch gridded ion chamber, Van de Graaff and linac data, in progress.

^{10}B(n,α)
Haight, 1 MeV to 6 MeV, angular distribution at 300, 600, 900 and 1350, private comm.

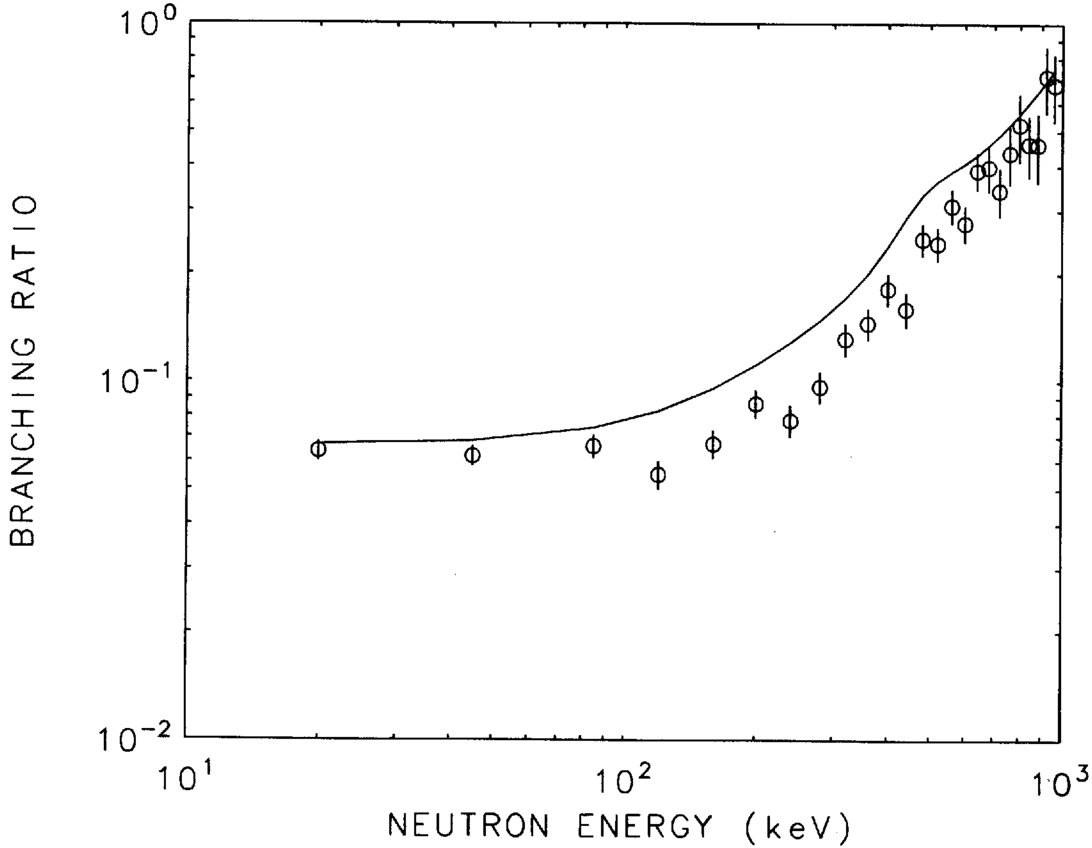
^{10}B total cross section
Wasson, 0.02 MeV to 20 MeV, NE-110 detector, Proc. Conf. on NDST, Gatlinburg (1994), p. 50

Plompen, 0.3 MeV to 18 MeV, scintillator, LiI and Li-glass detectors, Proc. Conf. on NDST, Gatlinburg (1994), p. 47 and Proc. Conf. on NDST, Trieste (1997), p. 1283

Brusegan, 80 eV to 730 keV, Li-glass detector, Proc. Conf. on NDST, Gatlinburg (1994)p. 47 and Proc. Conf. on NDST, Trieste (1997)p. 1283

^{10}Be(p,n) ^{10}B
Massey, E_p from 1.5 MeV to 4 MeV, data at 0°, private comm. New measurements to be made at lower energies (~.5 MeV). Also possibly ^{10}Be (p,α)

Measurements of The $^{10}B(n,\alpha)$ Branching Ratio by Weston compared with ENDF/B-VI



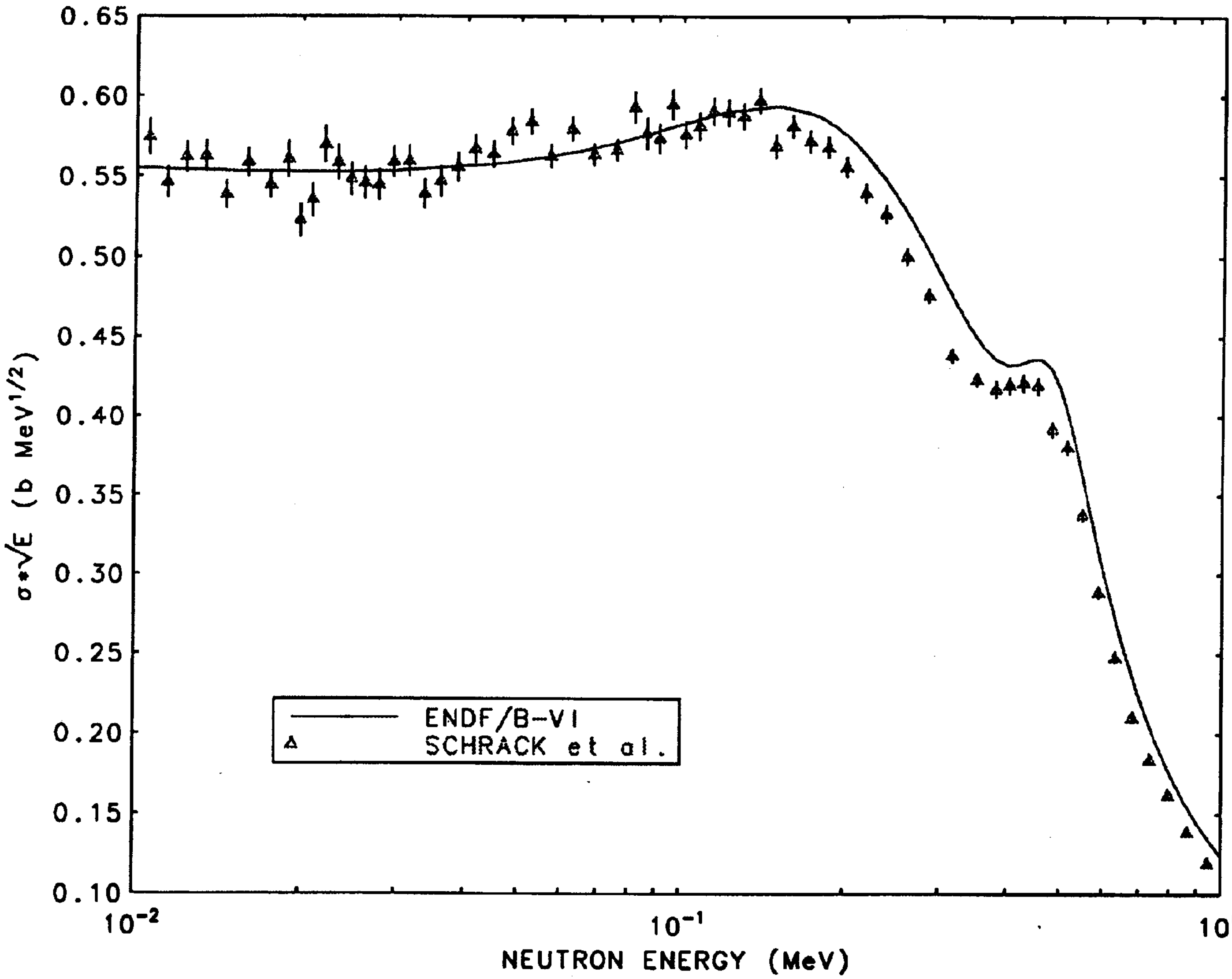


Fig. 14 $^{10}B(n,\alpha_1\gamma)$ cross section measurements by Schrack et al at ORELA (PC mon)

NOTE!!!

Weston data => $\sigma(n,\alpha_0)/\sigma(n,\alpha_1)$ is low compared with ENDF/B-VI in the hundred keV energy region

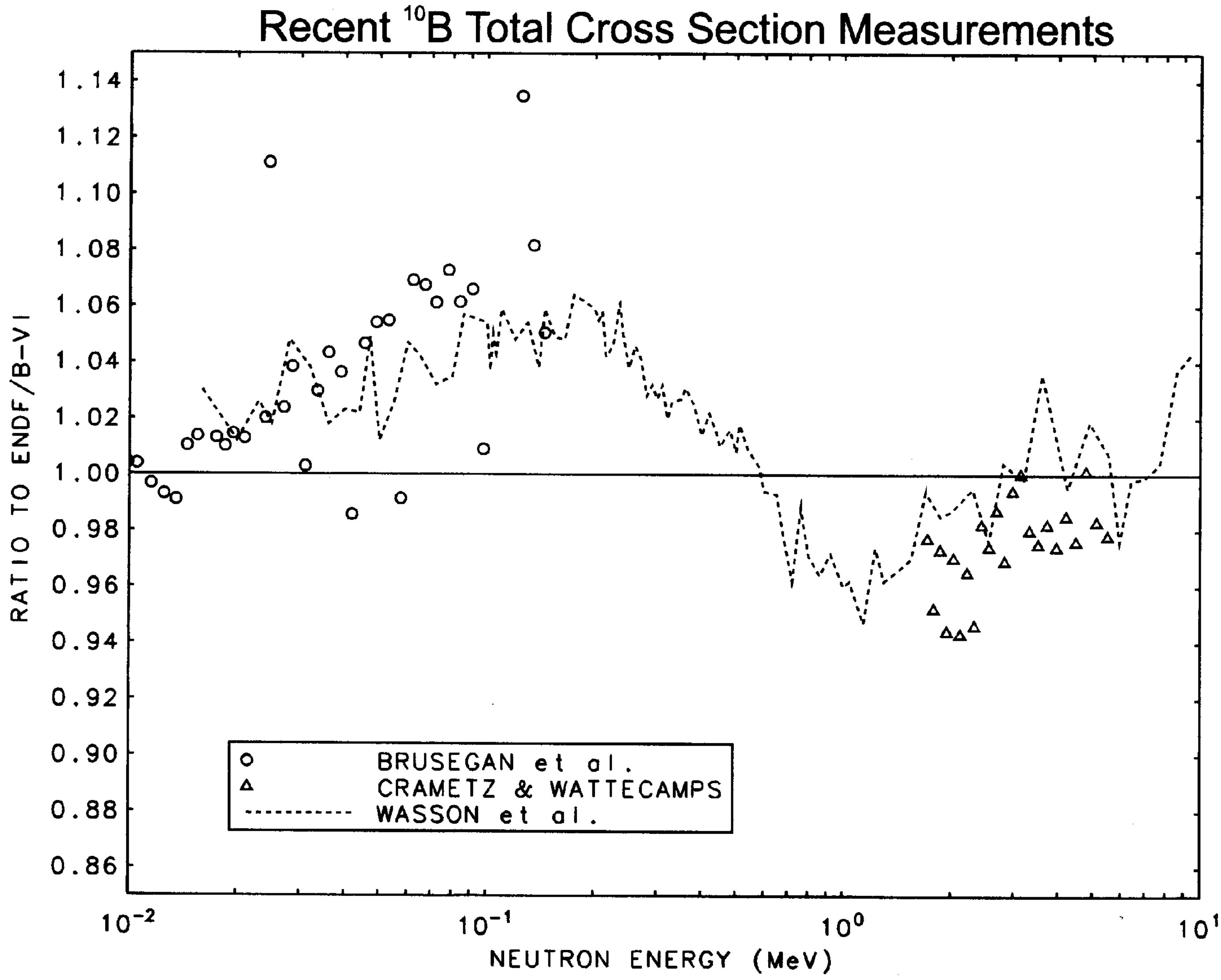
Schrack data => $\sigma(n,\alpha_1)$ is low compared with ENDF/B-VI in the hundred keV energy region

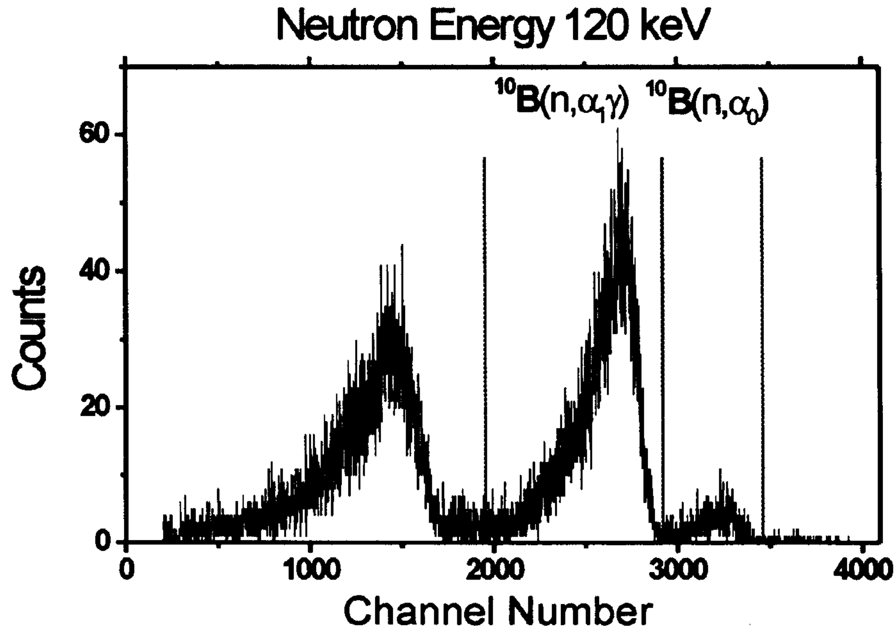
Therefore $\sigma(n,\alpha_0)$ must be low compared with ENDF/B-VI in the hundred keV energy region

And $\sigma(n,\alpha_0) + \sigma(n,\alpha_1)$ must be low compared with ENDF/B-VI in the hundred keV energy region

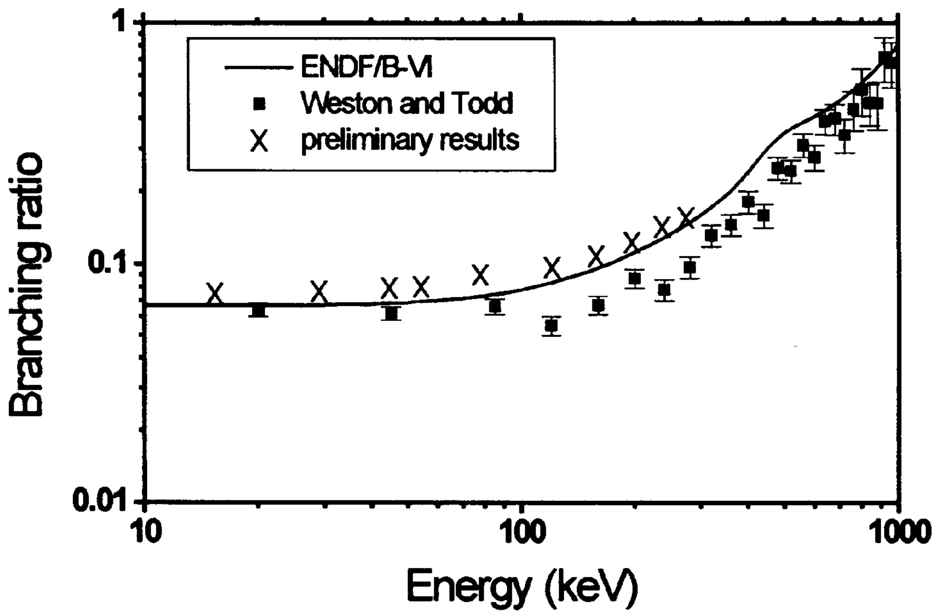
And $\sigma_T = \sigma(n,\alpha_0) + \sigma(n,\alpha_1) + \sigma(n,n)$ should be low compared with ENDF/B-VI in the hundred keV energy region

But the recent measurements of σ_T are higher than ENDF/B-VI !!!

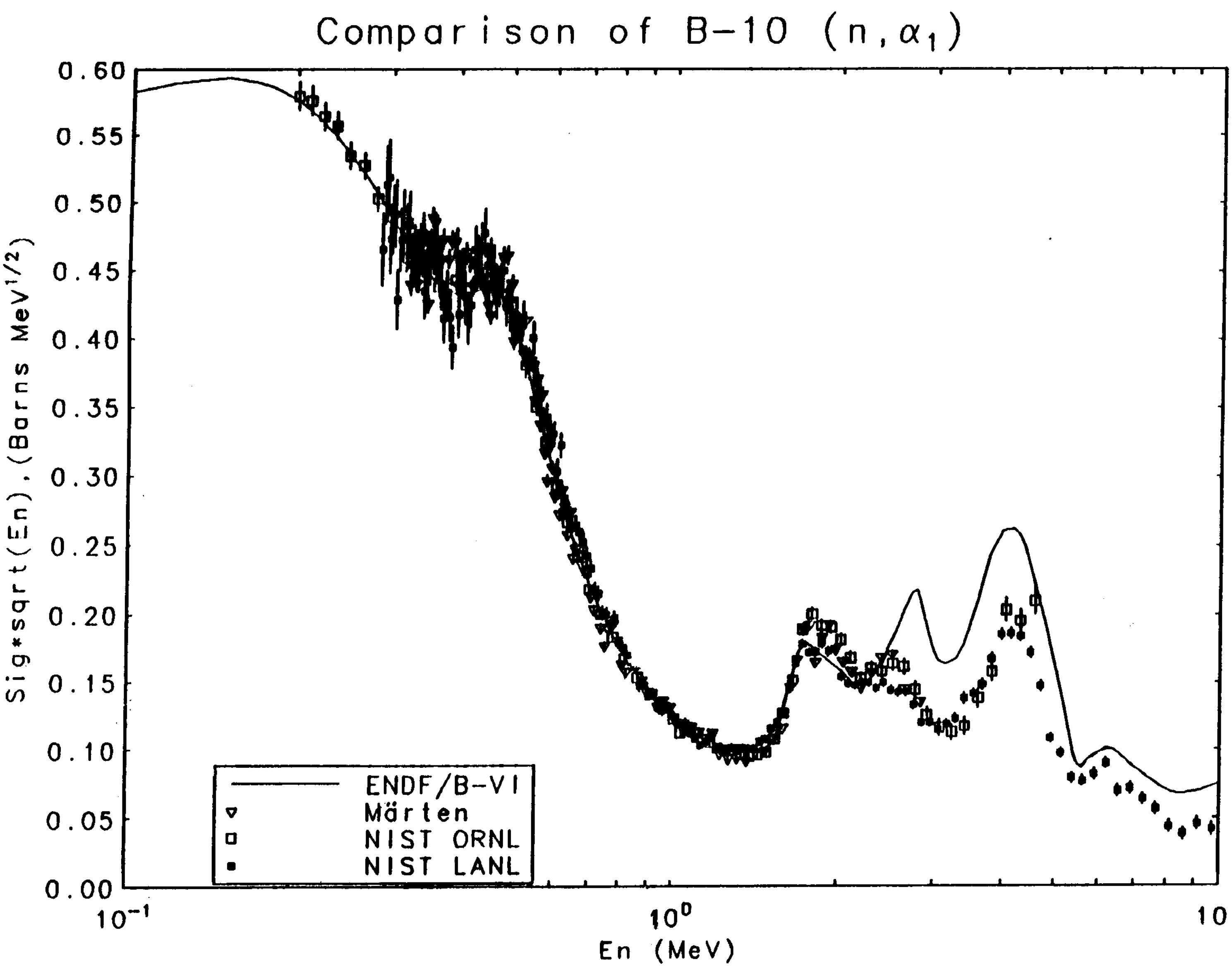

Recent ^{10}B Total Cross Section Measurements
RATIO TO ENDF/B-VI
1.14
1.12
1.10
1.08
1.06
1.04
1.02
1.00
0.98
0.96
0.94
0.92
0.90
0.88
0.86
10^{-2}
10^{-1}
10^{0}
10^{1}
NEUTRON ENERGY (MeV)
BRUSEGAN et al.
CRAMETZ & WATTECAMPS
WASSON et al.



Pulse height distribution with the FGIC for 120 keV neutrons and a 30 $\mu g/cm^2$ ^{10}B deposit.



Preliminary Hambsch results of the $^{10}B(n,\alpha)$ branching ratio compared with the ENDF/B-VI evaluation and the results of Weston et al.



Comparison of the $^{10}B(n,\alpha_1\gamma)$ cross section measurements of Märten with the NIST ORNL and NIST LANL data of Schrack et al. Also shown is the ENDF/B-VI evaluation.

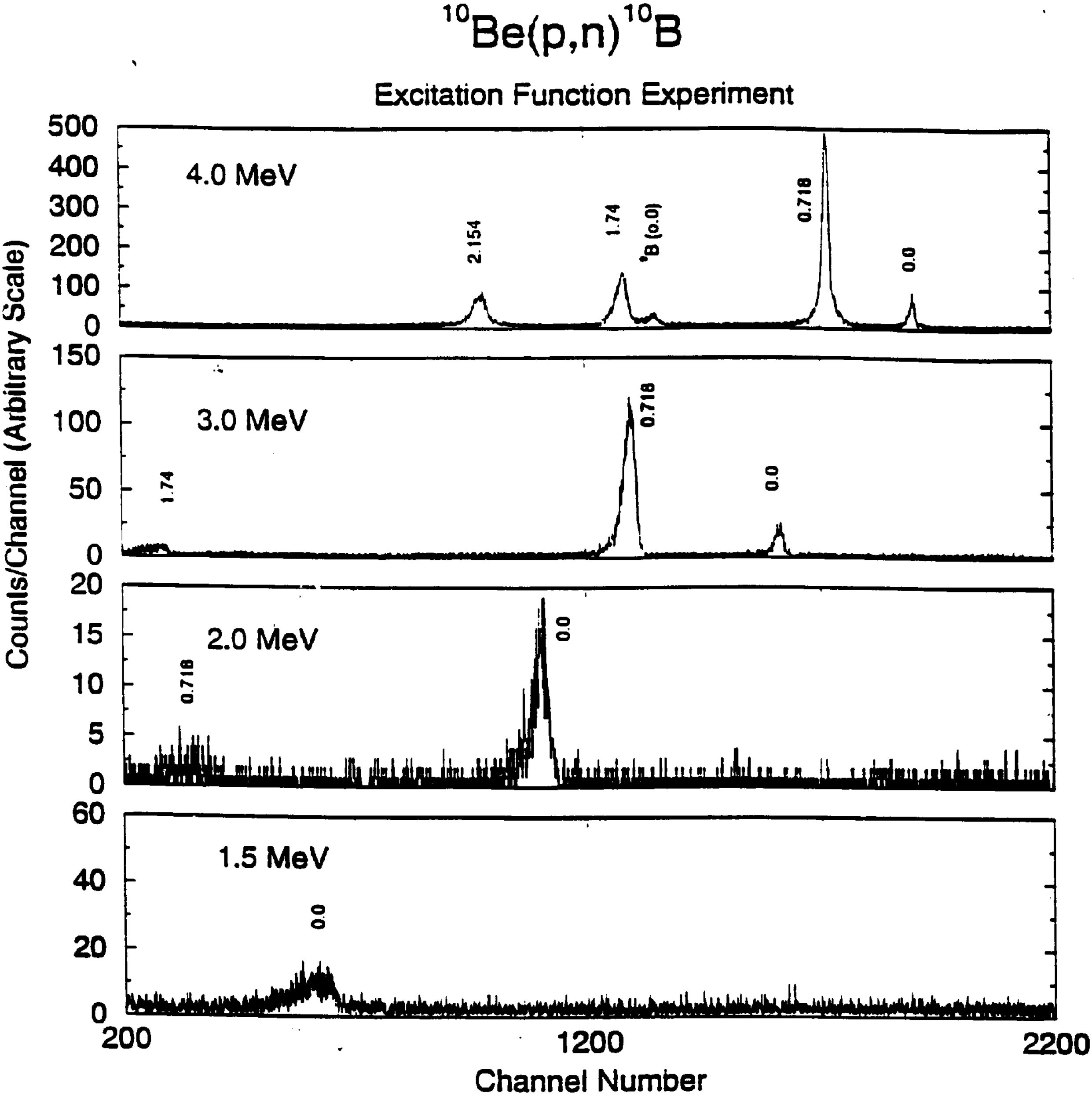


Fig. 11. Neutron spectra from the $^{10}Be(p,n)^{10}B$ reaction at 0° for neutron energies from 1.5 to 4.0 MeV.

Au(n,γ)
++Sakamoto, 23 keV and 967 keV, photoneutron source, activation experiment, NSE 109,215 (1991)

++Davletshin, .16 MeV to 1.1 MeV, relative to H(n,n), Sov. J. At. Energy 65, 91 (1988),
(Corrected data from Sov. J. At. Energ. 58, 183 (1985))

++Davletshin, .16 MeV to 1.1 MeV, relative to H(n,n), Sov. J. At. Energy 65, 91 (1988),

++Davletshin, .62 MeV to .78 MeV, relative to ^{235}U(n,f), Sov. J. At. Energy 65, 91 (1988),

Kazakov, Yad Konstanty, 44, 85 (1990)

Demekhin, 2.7 MeV, Proc. 36th All Union Conf. on Nuclear Data, p. 94 (1986)

Voignier, ~.5 MeV to ~3 MeV, private comm.

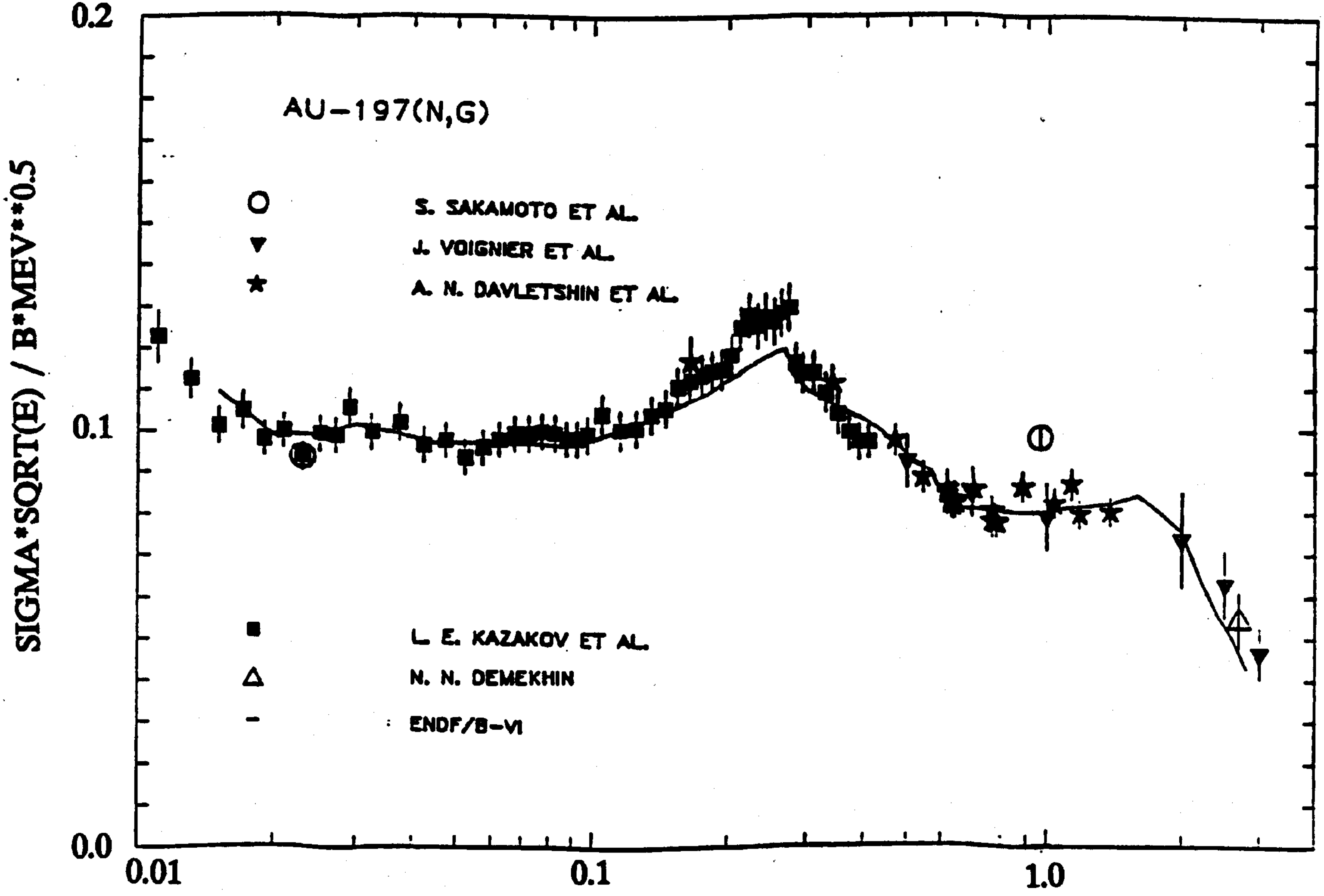


Fig. 10 Comparison of the Global Evaluation Result (ENDF/B-VI) for $^{197}Au(n,\gamma)$ with New Experimental Data

$^{235}U(n,f)$
Newhauser, 34, 46, and 61 MeV MeV, absolute, needs additional analysis.

+Carlson, 0.3 MeV to 3 MeV, relative to black detector, Proc. IAEA Advisory Group Meeting on Nuclear Standard Reference Data, Geel Belgium, p.163, IAEA-TECDOC-335 (1985)

+Carlson, 2 MeV to 30 MeV, relative to H(n,n), Proc. Spec. Meeting on Neutron Cross Section Standards for the Energy Region above 20 MeV, Uppsala, Sweden, 1991, Report NEANDC-305, "U", p. 165

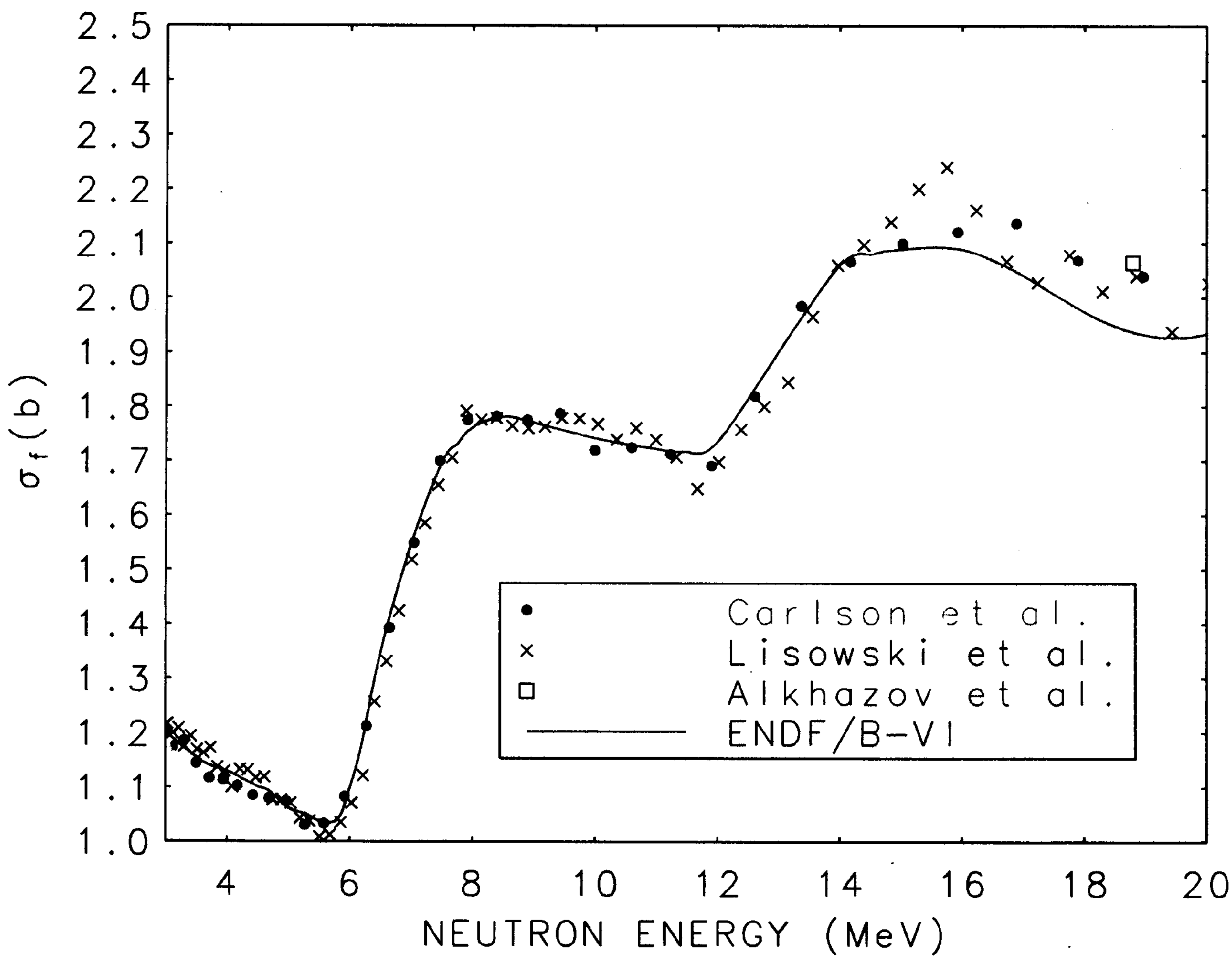
+Johnson, 1 MeV to 6 MeV, relative to a dual thin scintillator, Proc. Conf. on NDST Mito (1988) p.1037

+Iwasaki, 14 MeV, relative to H(n,n) and associated particle, Proc. Conf. on NDST Mito (1988) p. 87

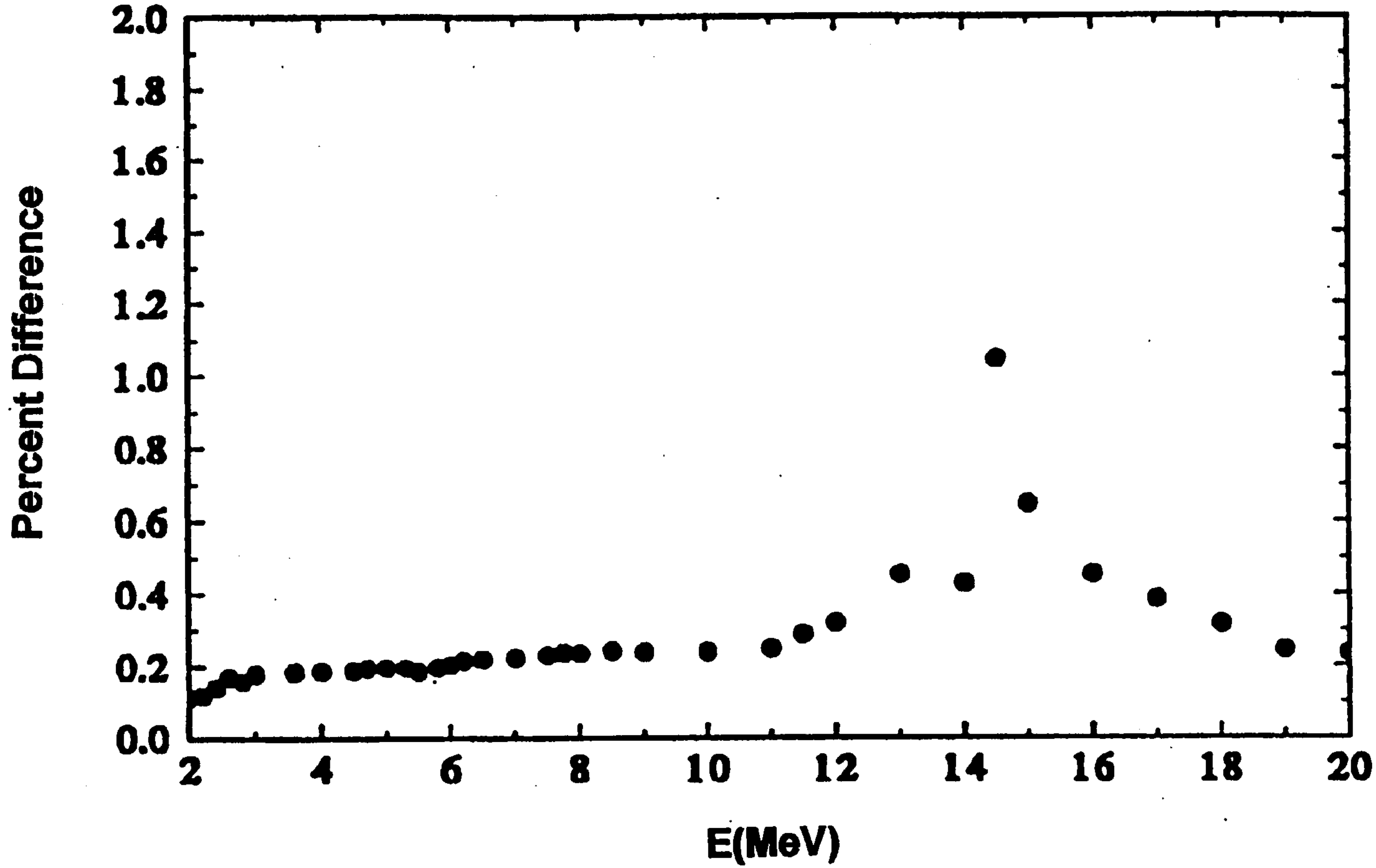
+Lisowski, 3 MeV to 200 MeV, relative to H(n,n), Proc. Spec. Meeting on Neutron Cross Section Standards for the Energy Region above 20 MeV, Uppsala, Sweden, 1991, Report NEANDC-305, "U", p. 177, and private communication.

Merla, ++2.56, +4.45, ++8.46, +14.7, +18.8 MeV ?, associated particle, Proc. Conf. on NDST Juelich (1991) p.145

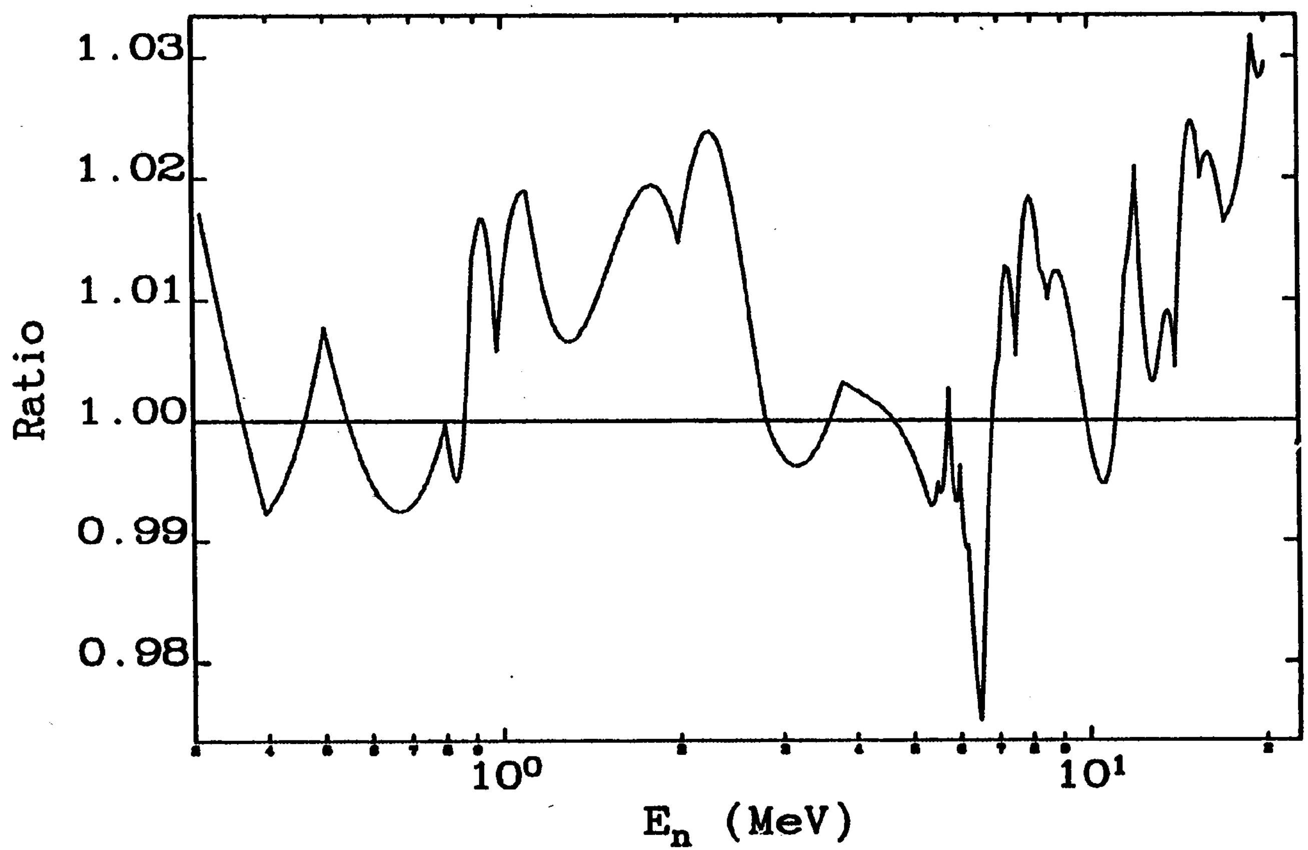
Recent Measurements of The $^{235}U(n,f)$ Cross Section



Estmated Change in The Evaluated $^{235}U(n,f)$ Cross Section From Data Obtained Since The ENDF/B-VI Evaluation and Before 1992



Ratio of The $^{235}U(n,f)$ Cross Section Evaluation of White to The ENDF/B-VI Evaluation



$^{238}U(n,f)$

Newhauser, 34, 46, and 61 MeV MeV, absolute

Baba, 0.5 MeV to 7 MeV and 14 MeV, relative to $^{235}U(n,f)$, J. Nucl. Sci. & Techn.,26,11 (1989)

$^{+}$Lisowski, 0.8 MeV to 350 MeV, relative to H(n,n), Proc. Spec. Meeting on Neutron Cross Section Standards for the Energy Region above 20 MeV, Uppsala, Sweden, 1991, Report NEANDC-305, “U”, p. 177, and private communication.

$^{+}$Merla, 5 MeV +?, associated particle, Proc. Conf. on NDST Juelich (1991) p.145

Shcherbakov, 1-200 MeV, relative to $^{235}U(n.f)$, ISTC 609-97, see also Fomichev, 0.7 MeV to 200 MeV, relative to $^{235}U(n.f)$, Proc. Conf. on NDST, Trieste (1997), p.1283

$^{++}$Winkler, 14.5 MeV, relative to $Al(n,\alpha)$ & $^{56}Fe(n,p)$, Proc. Conf. on NDST Juelich (1991), p.514

$^{238}U(n,\gamma)$

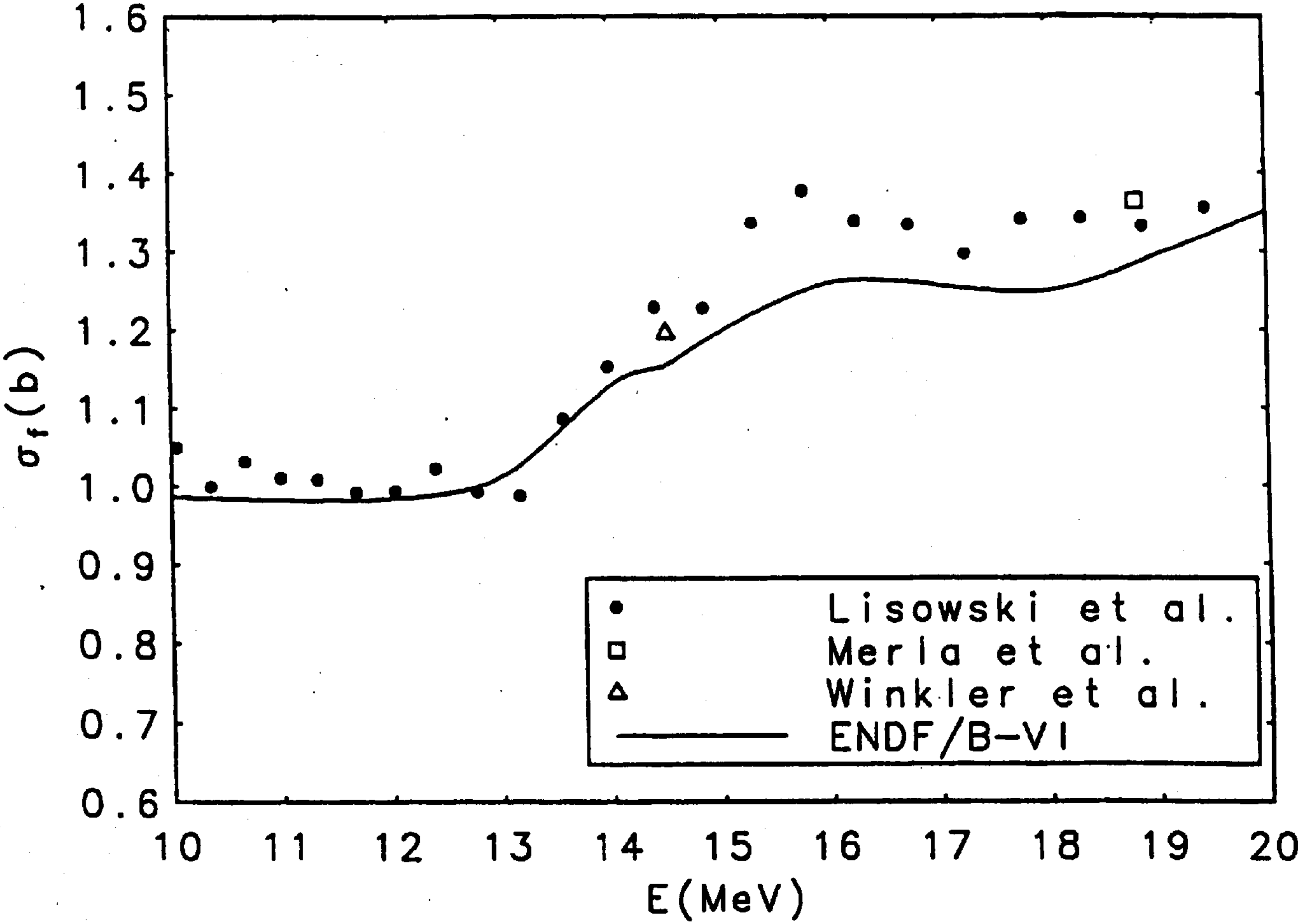
$^{++}$Kobayashi, 0.024 MeV, 0.055 MeV, 0.146 MeV, relative to $^{10}B(n,\alpha_1\gamma)$, Proc. Conf. on NDST Juelich (1991), p. 65

$^{+}$Quang, 23 keV and 964 keV, photoneutron source, activation experiment, NSE 110, 282 (1992)

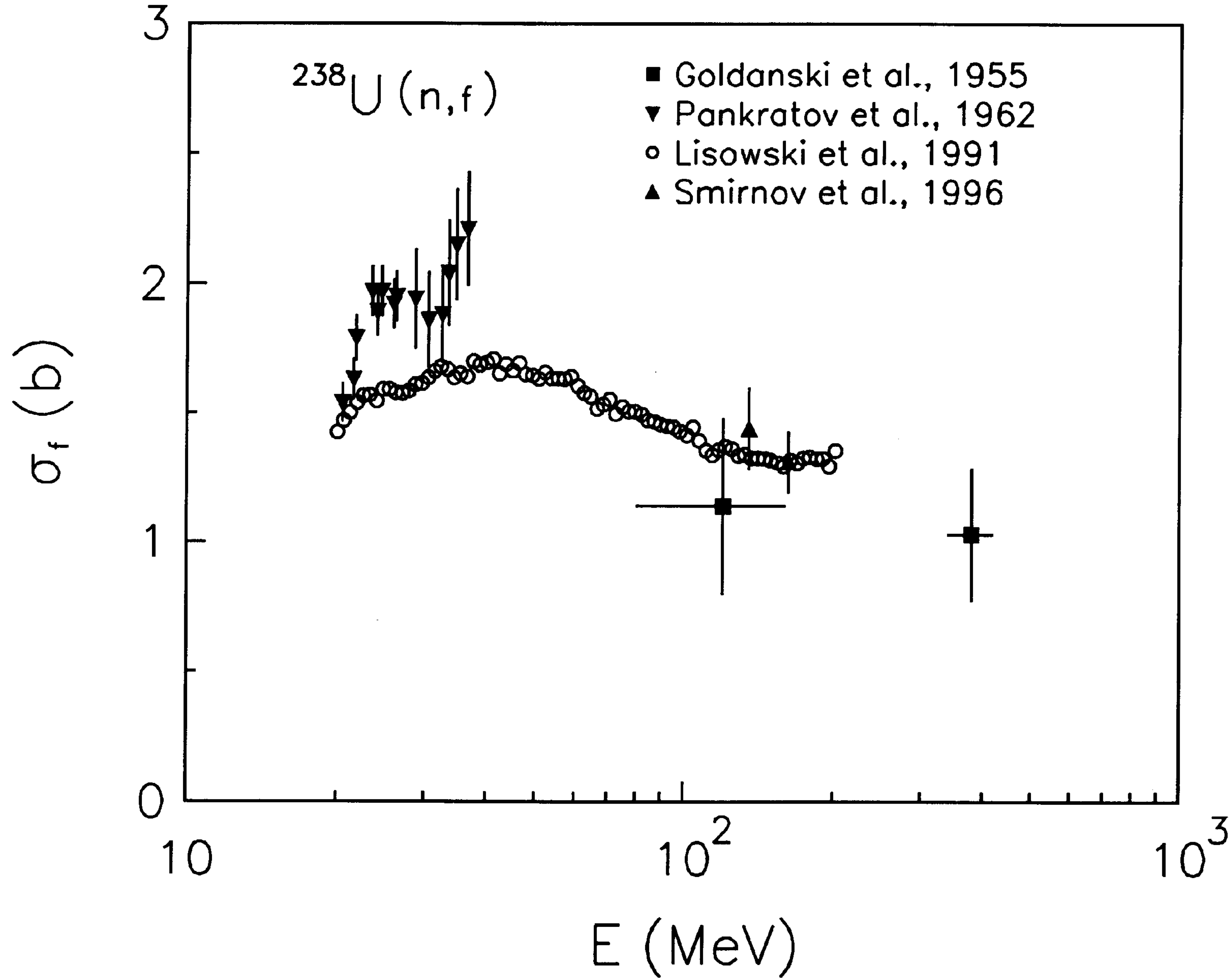
$^{++}$Adamchuck, 10 eV to 50 keV, relative to $^{10}B(n,\alpha_1\gamma)$, J. Atomic Energy, 65, 920 (1989)

$^{++}$Buleeva, 0.34 MeV to 1.39 MeV, relative to H(n,n) and $^{235}U(n,f)$, Sov. J. Atomic Energy, 65, 930 (1989)

Voignier, ~0.5 to 1 MeV, private comm.



Recent measurements of the $^{238}U(n,f)$ cross section compared with the ENDF/B-VI evaluation.



$^{238}U(n,f)$
Goldanski et al., 1955
Pankratov et al., 1962
Lisowski et al., 1991
Smirnov et al., 1996
σ_f (b)
E (MeV)
0
1
2
3
10
10^2
10^3

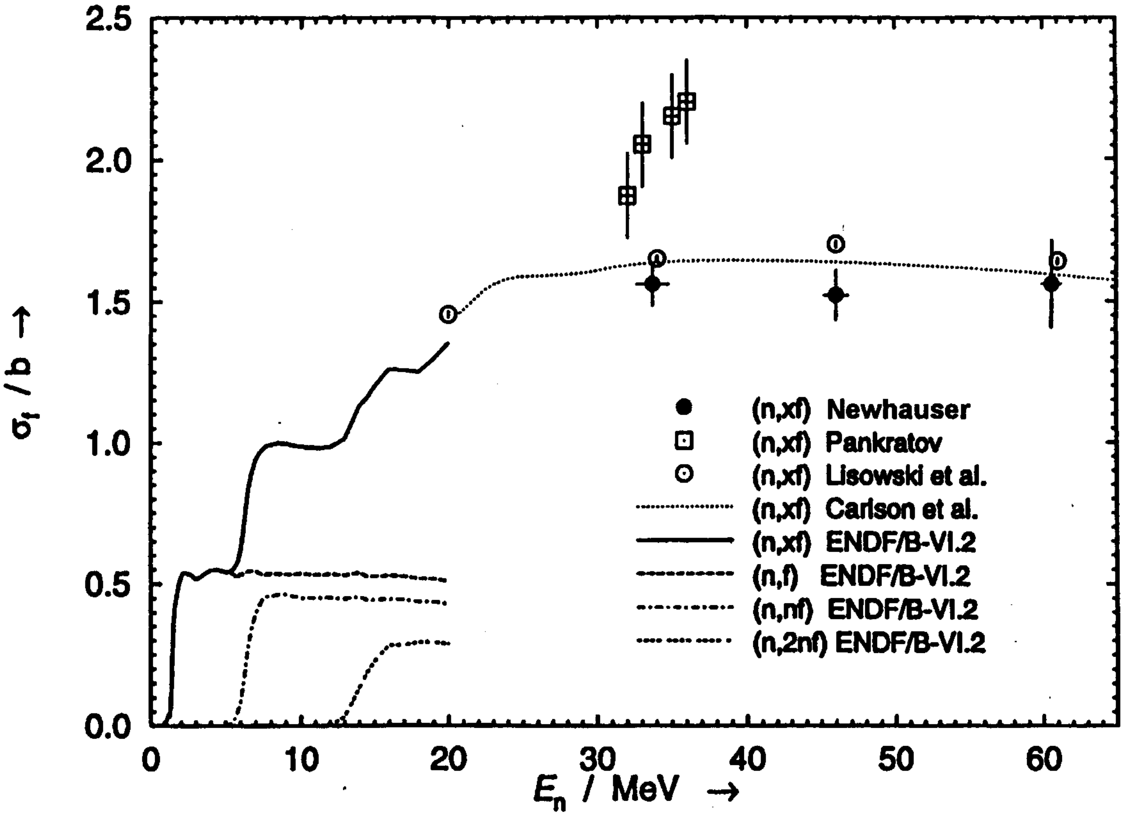
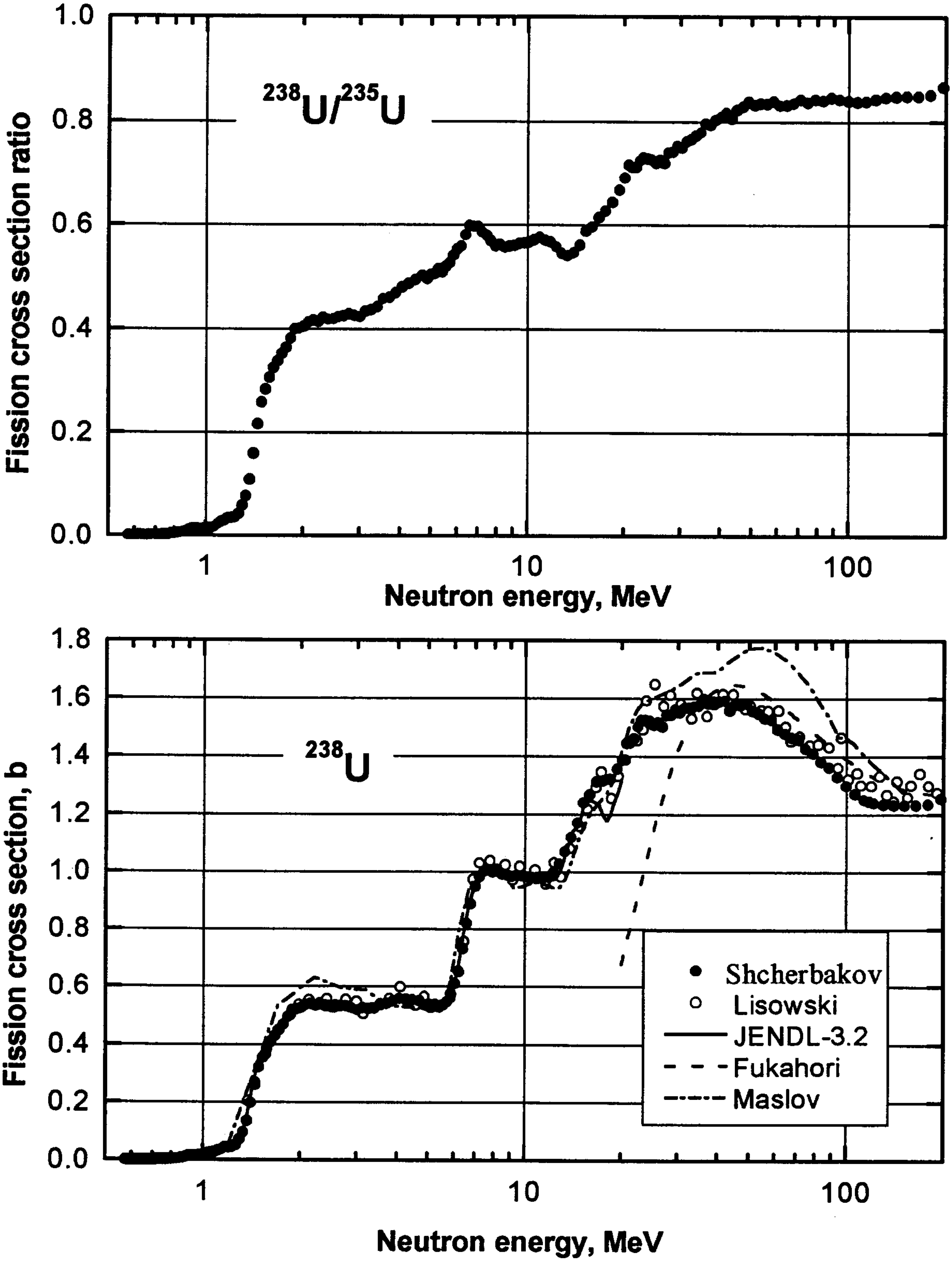


Figure 1. Fission cross section values σ_f from the present work (solid points) were measured in pseudo-monoenergetic neutron fields with nominal peak neutron energies of 33.7 MeV, 46.0 MeV, and 60.6 MeV, respectively. Also shown are *selected* experimental values from Pankratov [5], Lisowski *et al.* [6], Carlson *et al.* [12], and values from the evaluated nuclear data files [13] for the total fission cross section, denoted by (n,xf); simple fission, denoted by (n,f); second chance fissions, denoted by (n,nf); and third chance fissions, denoted by (n,2nf). The multiplicity of fission mechanisms and their corresponding thresholds lead to the pronounced stair-step structure in σ_f up to about 20 MeV, above which σ_f remains nearly constant.



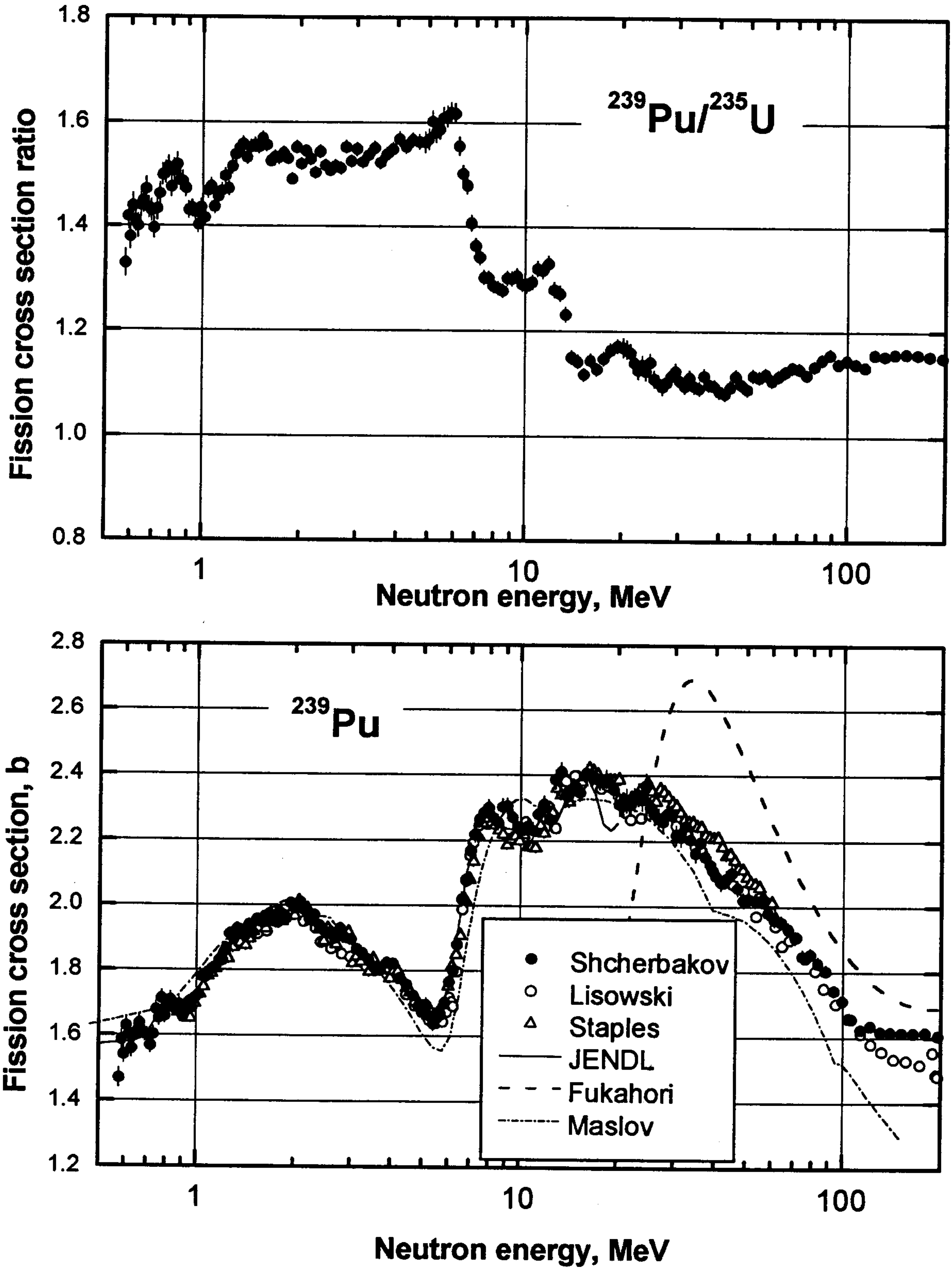
Fission cross-section ratio U238/U235 (upper part) and fission cross-section of U238 (lower part) in the neutron energy range 0.5-200 MeV.

^{239}Pu(n,f)

Shcherbakov, 1-200 MeV, relative to ^{235}U(n.f), ISTC 609-97

$^{+}$Staples, 0.5 MeV to 400 MeV, relative to ^{235}U(n,f), NSE 129, 149 (1998)

Lisowski, 0.8 MeV to 350 MeV, relative to H(n,n), Proc. Spec. Meeting on Neutron Cross Section Standards for the Energy Region above 20 MeV, Uppsala, Sweden, 1991, Report NEANDC-305, "U",



Fission cross-section ratio Pu239/U235 (upper part) and fission cross-section of Pu239 (lower part) in the neutron energy range 0.5-200 MeV.

The Correlation Matrix

- Constructed from
  - the normalization uncertainty.
  - energy dependent uncertainty components.

The correlation matrix element C_{ik} is given by:

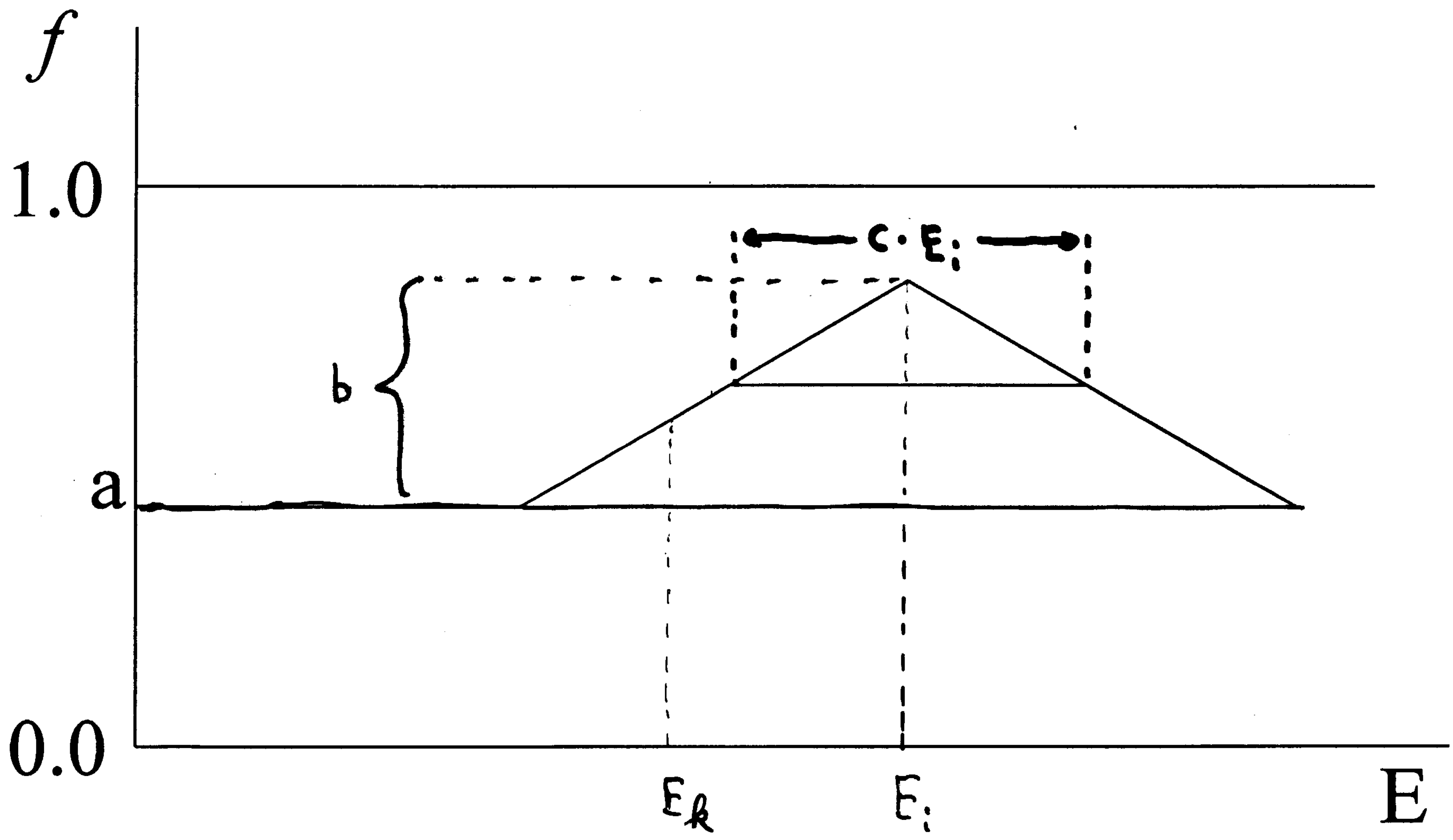
$$C_{ik} = \frac{e_n^2 + \sum_m e_{mi} e_{mk} f_{ik}}{E_i^2 E_k^2}$$

Where, $e_n^2 = \sum_i e_{ni}^2$ for the normalization uncertainties.

E_i and E_k are the total uncertainties.

m is the error component index with the sum going over all the systematic energy dependent uncertainty components.

f_{ik} is a correlation factor.



$0. \leq a, b, c \leq 1.0$

Introduction of R-Matrix code RAC

Chen zhenpeng
Physics Department, Tsinghua University, Beijing, PRC.

Our R-matrix code RAC is designed with Reduced R-Matrix Theory of A.M. Lane and R.G. Thomas.

Formula for R-Matrix

$$R_{cc'} = \sum_{\lambda\mu}^{N_1} \gamma_{\lambda c} \times \gamma_{\mu c'} A_{\lambda\mu} + \sum_{\lambda}^{N_2} \frac{\gamma_{\lambda c'} \times \gamma_{\lambda c}}{E_\lambda - E} + R_{cc'}^{\infty} \qquad (1)$$

$$\left[A^{-1}\right]_{\lambda\mu} = \left[E_\lambda^{res} - E + \sum_c (S_c(E) - b_c)\gamma_{\lambda c}\gamma_{\mu c} - \frac{i}{2}\Gamma_{\lambda\mu}^{e}\right]\delta_{\lambda\mu} \qquad (2)$$

In equation (1), the second and third terms represent distance levels.

In equation (2), the $\Gamma_{\lambda\mu}^{e}$ represents total width of all reduced channels.

If $\Gamma_{\lambda\mu}^{e}$=0, they become the General R-Matrix Formula.

The Width of Reduced Channels $\Gamma_{\lambda\mu}^{e}$

The reduced channels may include:

The uninterested channels; The channels without data;

The open channels which belong to direct reaction.

So that there is a possibility **to improve the unitarity** by including the contribution of reduced channels.

The reduced R-Matrix code can be used to analyze the data in higher energies; For example, the data of ^{17}O system for $E_n = 6.0 \sim 10.5$ MeV has been analyzed by using RAC. In this energy range, the inelastic scattering cross sections are relative large, but it is hard to determine those values; some other channels maybe open. Anyway, their contributions can be represented by **one parameter** $\Gamma_{\lambda\mu}^{e}$ --the Reduced channels width. The fitting for total cross sections and integrated cross sections of ^{16}O(n,α)^{13}C are pretty good. (Show old transparencies).

Types of experiment data

The types of experiment data can be analyzed by RAC include all data exist in one nuclear system, which include the data in **normal reaction channels** and the data in **inverse reaction channels**. The types of data are the same as those analyzed by EDA. For example:

Total cross section of neutron; Integrated cross sections;
Elastic scattering cross sections; Inelastic scattering cross sections;
Reaction cross sections; Polarization;

Limits

In RAC all data and parameters are put in two huge adjustable arrays. So **there are not any limit exist in this code**, which include:

Number of the open channels, Number of levels, Number of data,
Number of orbital angular momentum ………………

Comparison

The comparison between RAC and EDA has been done; For ^{7}LI system□^{11}B system and ^{17}O, the agreement of calculated results are very well. (Show old transparencies).

Covariance Matrix and Error Propagation

The Covariance Matrixes of data are supposed as diagonal. The improvement about taking into account of Covariance Matrixes of data has not finished. Some ideas will be shown as follow.

Covariance Matrix and Error Propagation

Chen zhenpeng
Physics Department, Tsinghua University, Beijing, PRC.

1. **Basic formula**

For any fitting model:

$$\bar{y} - \bar{y}_0 = D(\bar{c} - \bar{c}_0)$$
$$D_{ki} = (\partial y_k / \partial c_i)_0 \qquad (3)$$

Y -- observable, D --sensitive matrices, C –parameters.

k=1, 2, …, n. n---number of data.

i=1, 2, …, m. m---number of parameters.

The covariance matrix of $\bar{C}$ is,

$$V_{\bar{c}} = (D^{+} V^{-1} D)^{-1} \qquad (4)$$

V is the covariance matrix of data sets.

$$V^{-1} = \begin{bmatrix} V_1^{-1} & & & 0 \\ & V_2^{-1} & & \\ & & \ddots & \\ 0 & & & V_k^{-1} \end{bmatrix} \qquad (5)$$

So that, the covariance matrix of calculated results is:

$$V_{\bar{y}} = D V_{\bar{c}} D^{+} \qquad (6)$$

D_{ki} is calculated by finite difference method in code.

2. **Error of neglecting correlation**

The formula about covariance matrices are perfect; but where and how to construct the exact ***V*** of data is a big problem. Usually, V is supposed as diagonal, but D and then $V_{\bar{c}}$ is not diagonal, so the $V_{\bar{y}} = D V_{\bar{c}} D^{+}$ is not diagonal too.

Due to supposing ***V*** as diagonal, some errors of $V_{\bar{c}}$ will be brought, and subsequently uncertainty of $V_{\bar{y}} = D V_{\bar{c}} D^{+}$ will be reduced inevitably. It's not clear that for general situation what's the percentage of the errors occupied in total uncertainty. **It's necessary to do a test about the errors caused by neglecting of correlations existing between the experimental data.**

3. Including Covariance matrix of data in curve fitting by least-square method has a possibility to produce standards cross sections with higher precision.

An example (given by D.L. Smith) shows that, if the correlated error is included in calculation, the final relative errors become smaller.

Data table

Para.	Uncorrelated error	correlated error	total error
σ_1	$0.01\sigma_1$	$0.02\sigma_1$	$E_1 = (0.01\sigma_1)^2 + (0.02\sigma_1)^2$
σ_2	$0.01\sigma_2$	$0.02\sigma_2$	$E_2 = (0.01\sigma_2)^2 + (0.02\sigma_2)^2$

Let r = σ_1 / σ_2, what is the error of the ratio r (E_r)□

The covariance matrix for the set (σ_1, σ_2) is:

$V_{11} = (0.01\sigma_1)^2 + (0.02\sigma_1)^2$ $V_{12} = (0.02\sigma_1)(0.02\sigma_2)$

$V_{21} = (0.02\sigma_1)(0.02\sigma_2)$ $V_{22} = (0.01\sigma_2)^2 + (0.02\sigma_2)^2$

$E_1/\sigma_1 = E_2/\sigma_2 = 2.236\%$

The correlation coefficient between σ_1 and σ_2 is:

$C_{12} = C_{21} = V_{12}/(E_1 \times E_2) = 0.8$

By using the law of error propagation, we got:

$(E_r/r)^2 = (E_1/\sigma_1)^2 + (E_1/\sigma_1)^2 - 2\times0.8\times(E_1/\sigma_1)(E_1/\sigma_1)$

$= 1.414\%$ (with correlation).

$(E_r/r)^2 = (E_1/\sigma_1)^2 + (E_1/\sigma_1)^2 = 3.162\%$ (neglect correlations).

4. R-matrix model curve fitting by least-square method has a possibility to produce standards cross-sections with higher precision.

An example (taken from my textbook) shows that, the estimator of observable given by least-square method has higher precision than correspond original experimental data.

Experimental data: (the track of meson)

i	1	2	3	4
X(i)	0.0	0.5	1.0	1.5
Y(i)	1.61	1.32	0.80	0.70
σ(i)	0.14	0.14	0.14	0.14

Fitting model: $y = c_1 + c_2 x = 1.595 \square 0.65x$

Covariance matrix of C□ $V_c = $ 0.014 -0.012
-0.012 0.016

Covariance matrix of y: $V_y =$
0.014 0.008 0.002 -0.004
0.008 0.006 0.004 0.002
0.002 0.004 0.006 0.008
-0.004 0.002 0.008 0.014

Standard variance $\sigma(y_1) = \sigma(y_4) = 0.12 < 0.14$

Standard variance $\sigma(y_2) = \sigma(y_3) = 0.08 < 0.14$

Error sources of Data

1. The uncertainties of energy calibration of experimental data.
2. The uncertainties of normalization factor for data.
3. The uncertainties of the uncertainties of data given by experimenters.
4. The un-consistent of data among multi- open reaction channels.
   Especially, the un-consistent of among data of reactions and inverse reactions.
5. Usually there are no correlation information given by experimenters.
   Supplemental provision of covariance matrices by experimenters should be quite helpful.
6. The errors exist in V used in fitting.

So, The first step is to select good data sets for fitting.

The second step is to construct a good covariance matrix V of data.

Maybe, the final uncertainty mainly comes from the uncertainty of data.

Error Sources of Model

The multi-channels and multi-levels R-matrix theory can be used to describe a light nucleus system, but **it is approximative inherently.**

If the parameters of distant levels and width of reduced channels are taken into account appropriately, it should be said that no serous approximations exist.

The main approximations exist in taking into account data for many open reaction channels.

Due to the discrepancy of data for many open reaction channels existing, it is very hard or impossible to get very good fits for each type of data. The main goal should be to get:

1. The best fits for the standard cross sections, which will be recommended (with relative heavy weights).
2. A very good fits for total cross sections of neutron (with relative heavy weights).
3. A good fits for polarization.

The data of other channels should be assigned with relative lightweights.

So the uncertainty of standard cross sections recommended will be minimized as small as possible.

Summary

1. Recommend : The neutron source of En=17.0MeV to 40.0MeV is available in China Institute of Atomic Energy; some experiments about neutron scattering have been done for the research on Dispersive Optical Model. The standard cross section of H(n,n)H has been used in dealing with the data. The experimenters find and suggest that **the standard cross section of H(n,n)H from 14.0MeV to 50.0MeV need to be improved.**

2. Including the contribution of **reduced channels** in R-matrix analyses has a possibility **to improve the unitarity**.

3. Supplemental provision of covariance matrices by experimenters should be quite helpful.

4. R-matrix Model-fitting by least-square method has a possibility to produce standards cross-sections with higher precision.

5. Including Covariance matrix of data in R-matrix Model-fitting by least-square method has a possibility to produce standards cross sections with higher precision.

6. It's necessary to do a test about the errors caused by neglecting of correlations existing between the experimental data.

Standard X-Sections and Microscopic Theoretical Calculations

Hartmut M. Hofmann
Institut für Theoretische Physik III
Universität Erlangen-Nürnberg

April 2nd 2001

Theoretical results never reach the precision of data analysis

$\Rightarrow$ Forget theory altogether ! ? NO !

All data have errors !

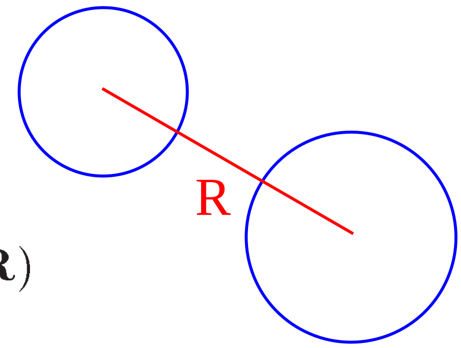
small $\Leftrightarrow$ big
statistical $\Leftrightarrow$ systematic

angular or energy mismatch

What to do with inconsistent data ?

Resonating Group Model Ideas

Composite system



RGM Ansatz $\Psi_l = \sum_{k=1}^{chan} \psi_{chan}^{k} \cdot \chi_{rel}^{lk}(\mathbf{R})$

Variation $\langle \delta \Psi_l \mathcal{A} | \mathrm{H} - \mathrm{E} | \; \Psi_l \rangle = 0$

Channel function $\psi_{chan} = [Y_L(\hat{\mathbf{R}}) \otimes [\phi_1^{j_1} \otimes \phi_2^{j_2}]^{S_c}]^J$

Ansatz $\psi = \psi_{chan}(\sum_i b_i \cdot \mathrm{Gaussian})$ (bound state)

or $\chi_{rel}^{lk}(R) = \delta_{lk} \cdot F_k(R) + a_{lk} \cdot \tilde{G}_k(R) + \sum_i b_{lki} \cdot$ Gaussian (scattering state)

Variational parameters a_{lk} and $b_{(lk)i}$

Decompose Hamiltonian

$$H - E = H_1 - E_1 + H_2 - E_2 +$$
$$\sum_{\substack{i \in 1 \\ j \in 2}} V_{ij} - V_{Coul} +$$
$$T_R + V_{Coul} - (E - E_1 - E_2) =$$
$$H_1 - E_1 + H_2 - E_2 + V_{short} + H_R - \tilde{E}$$

with $\mathcal{A} \cdot (H_i - E_i)\phi_i = 0$ and $(H_R - \tilde{E})F/G = 0$

$\Rightarrow$ All integrals shortranged

Note: Relative thresholds fixed by $\tilde{E}$

Resonating Group Model Technicalities

⇒ Expand all Functions including F and G

- in terms of Gaussians
- times solid spherical harmonics
- times monomials in R^2

⇒ All individual integrals analytically calculable,
provided potential is of Gaussian form including differential operators
All Operators allowed which occur in Argonne and Bonn (r-space) potentials

- Correct center of mass motion
- No limit on number of channels
- No limit on number of nucleons
- Up to 6 clusters, i.e. up to 6 orbital angular momenta

⇒ Allow for distortion of fragments via different ϕ and/or different decompositions of the system

Three- and more-body channels approximately treated via two-body channels

Fragment wave functions ϕ_1 and ϕ_2 must be strongest bound in given model-space
⇒ Relative thresholds can only be changed by increasing dimension of model-space or other potential

Realistic NN-interactions

versus
effective ones

Examples: Bonn, Argonne-14, Argonne-18

Start from deuteron p - n
S,D-wave 2 configurations

binding due to tensor force

proceed via $^3\mathrm{H}/^3\mathrm{He}$ N - N - N
S,P,D,F-waves S,P,D,F 37 configurations

to $^4\mathrm{He}$
Some hundred configurations

present limit $^6\mathrm{Li}$
Some thousand configurations

All nuclei $\mathrm{A} \geq 3$ underbound due to missing three-nucleon force

Larger systems: Use effective NN-forces with reduced repulsive core

$\Rightarrow$ nuclei $\mathrm{A} \leq 4$ bound via central force alone, just one configuration
$\Rightarrow$ higher orbital symmetry
$\Rightarrow$ much simpler wave functions, nuclei up to $\mathrm{A} = 12$ accessible

Effective Interactions versus Realistic ones

Effective interactions

- simple wave functions
- comparatively fast calculations, e. g. $^{10}\mathrm{B}$ - neutron scattering
- parameter studies possible
- model space dependence unclear
- severe overbinding possible
- limited energy range, $\mathrm{E}_{\mathrm{threshold}} + \approx$ 25 MeV

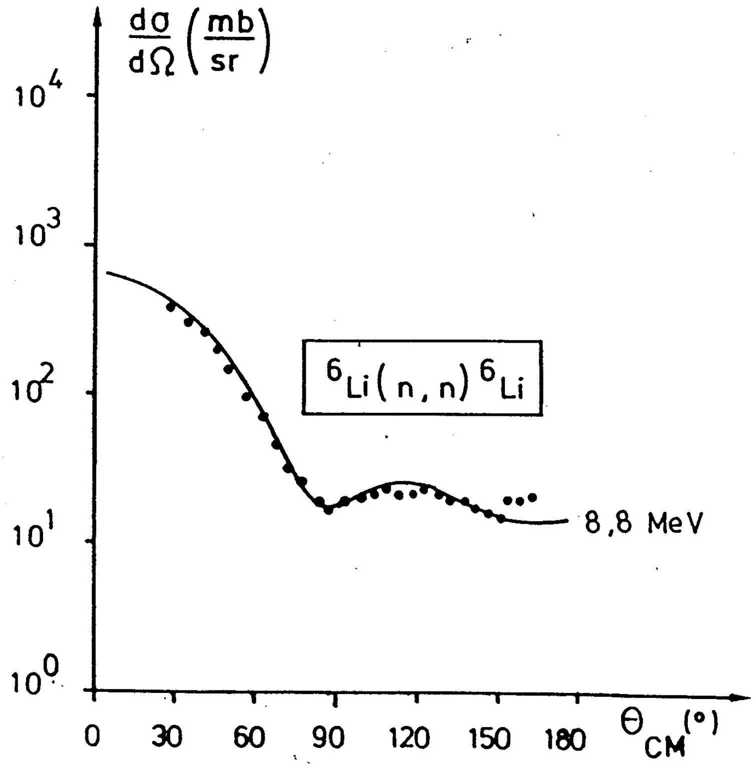
Realistic interactions

- complicated wave functions
- tedious long lasting calculations
- model spaces increase rapidly with A, limit around A = 6
- parameterfree calculation
- calculation improves with increasing model space
- no overbinding possible
- large energy range, up to pion threshold

Strategy

Study small system A
Reduce model space till qualitative change
Use this model space as input for A + 1 system

Typical Resonating Group Result



M. Herman 1985 unpublished
see also 'Use of the Optical Model for ... Neutron Cross-Sections ...', NEADC-222 'U' page 77, OECD Paris 1986

What Can Microscopic Theoretical Calculations do for Standard X-Sections ?

Data analysis might yield several solutions

⇒ Theory can help to pick one
Example: neutron-triton scattering
Scattering length (Rauch 1985):
$a_s = 4.98 \pm 0.29$ fm and $a_t = 3.13 \pm 0.09$ fm
$a_s = 2.20 \pm 0.31$ fm and $a_t = 4.05 \pm 0.09$ fm
G. M. Hale 'EDA'-analysis 1989, using p-$^{3}\mathrm{He}$ data : $a_s > a_t$
microscopic calculations 1999-2001 : $a_s > a_t$

Comparison of data analysis versus theory can indicate systematic deviations

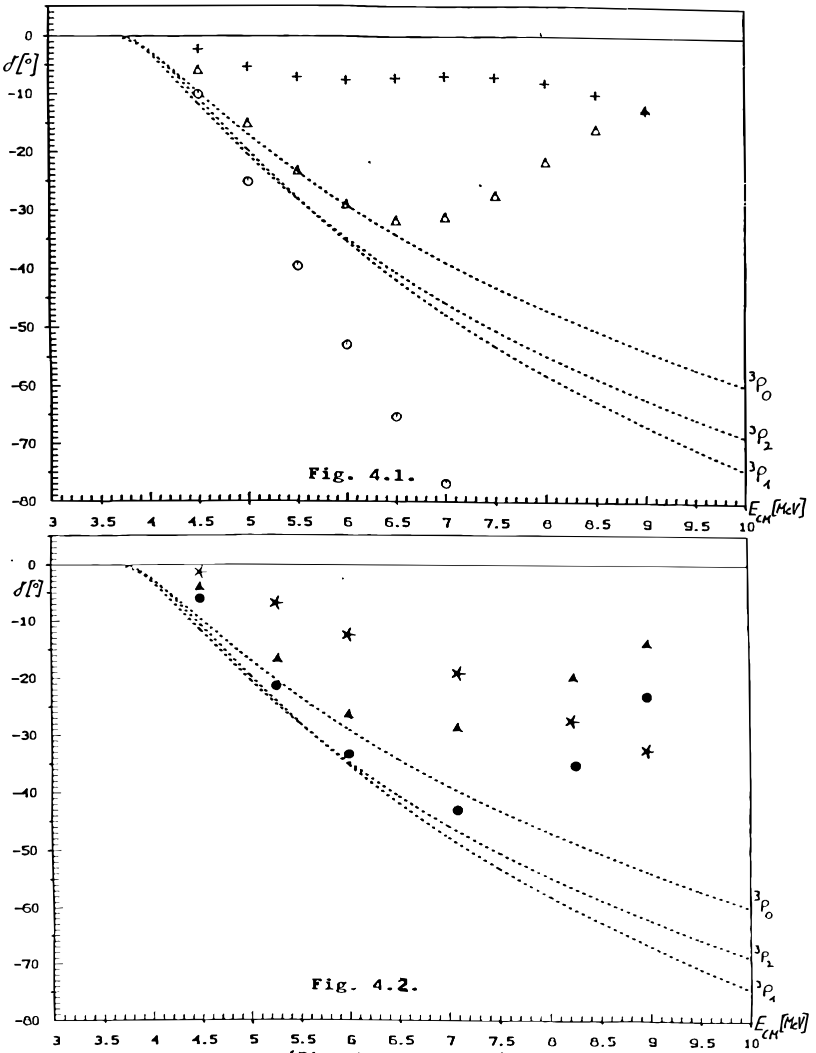
⇒ Theory can hint which additional data to include
Example: deuteron-deuteron scattering

Results from charge conjugate channels can reveal underlying structure, even despite obvious differencies
Example: $^{7}\mathrm{Li}$ / $^{7}\mathrm{Be}$

Deuteron-Deuteron Scattering

P-wave phase shifts strongly splitted in R-matrix analysis
tiny splitting in RGM calculation (Fig. 4.1)

Adding polarization data of Gruebler et al. Nucl.Phys. A193(1973)149 reduces splitting appreciably (Fig. 4.2)



(Fig. 4.1. und 4.2.)

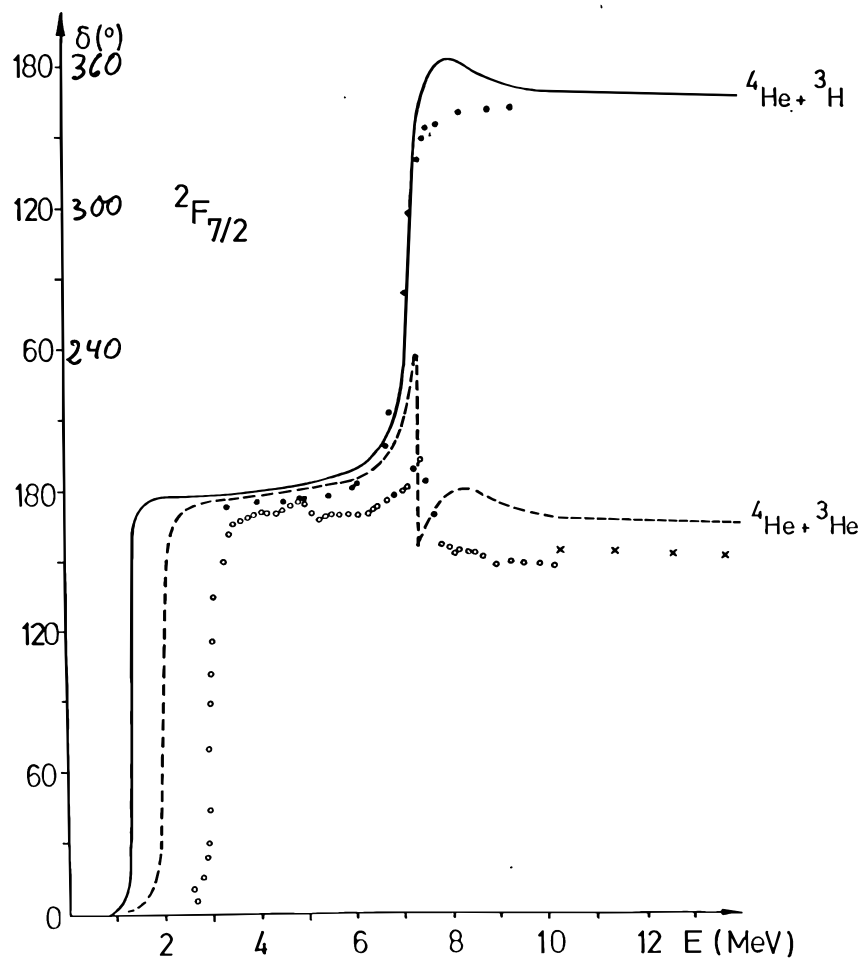
Diagonalstreuphasen für die Partialwellen negativer Parität der (^2H + ^2H) - Zerlegung im Vergleich mit R - Matrixergebnissen. Fig. 4.1. zeigt die Resultate einer R - Matrix - Analyse ohne, Fig. 4.2. mit Berücksichtigung von Analysierstärkemessungen bei der $^2H(d,d)^2H$ - Streuung ([Gr72]).

+,✶: $^3P_2$; △,▲ : $^3P_1$; ○,● : $^3P_0$

Resonant Structures in $^{7}\mathrm{Li}$ / $^{7}\mathrm{Be}$

F-wave scattering phase shifts display pronounced differencies in $\alpha -^{3}$ H and $\alpha -^{3}$ He scattering in experiment and calculation

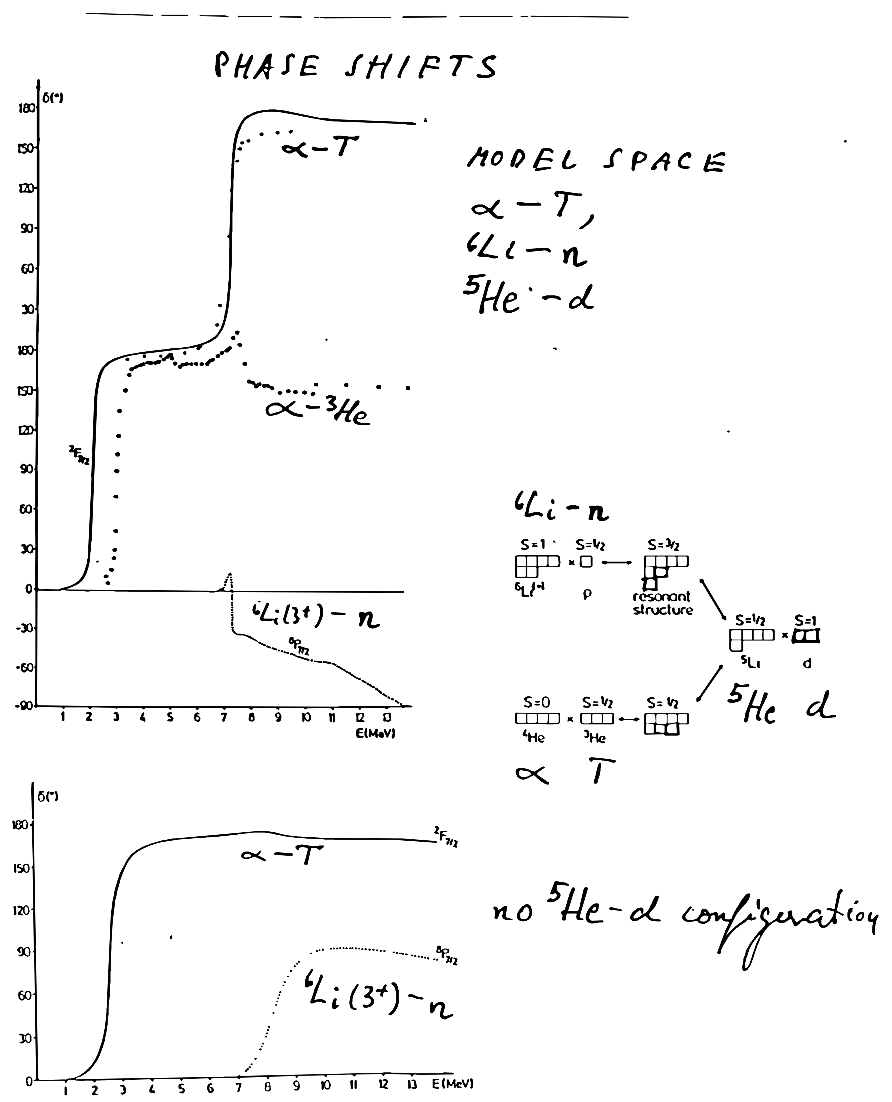
Differencies are caused by the $^{6}\mathrm{Li}(3^{+})$ - nucleon thresholds of 0.23 MeV and 1.48 MeV resp. relative to second $\frac{7}{2}^{-}$ -resonance



Only Multi-Channel Calculation Reproduces Data

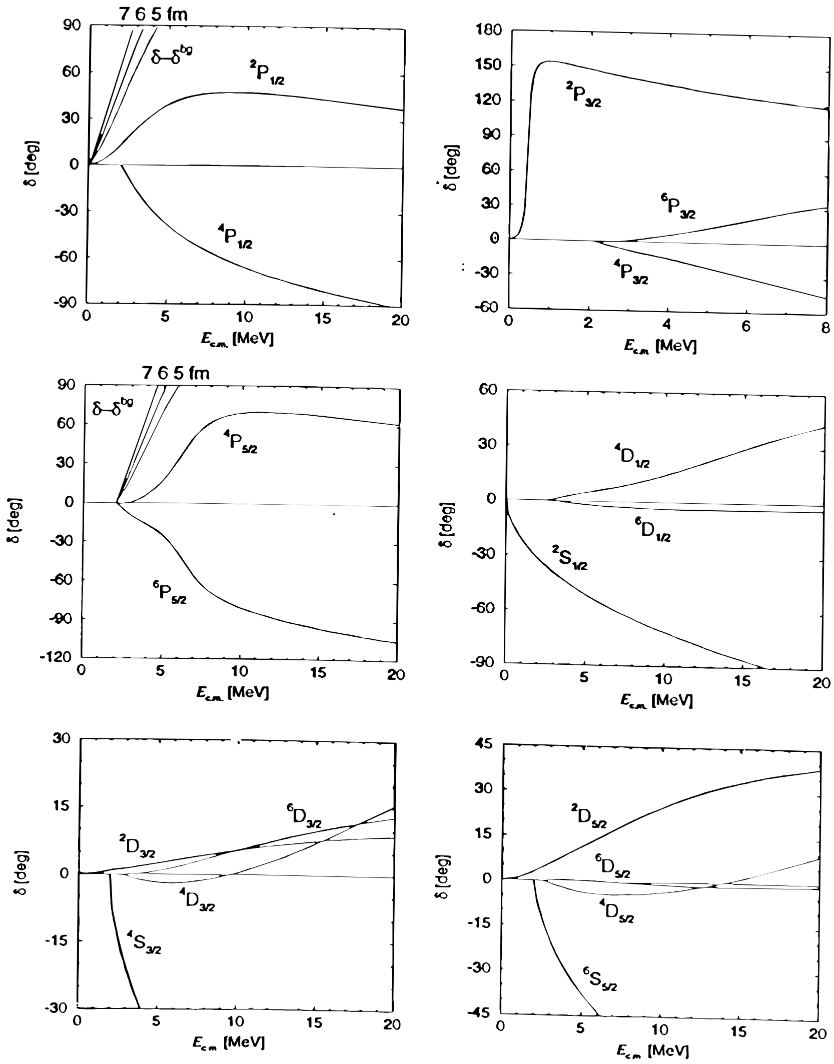
^{5}He - d configuration couples genuine ^{6}Li(3^+) -neutron resonance into α- triton channels due to different orbital symmetries
Nucl.Phys. A410(1983)208

7/2$^-$ States in ^{7}Li



^{6}He - n Scattering Phase Shifts

Phase shift do not reach 90 degrees
⇒ Resonance parameters ambiguos
⇒ Aim: Compare complex energy S-matrix poles
Phys.Rev. C55(1997)688



Direct Comparison of Phase Shifts TOO Sensitive

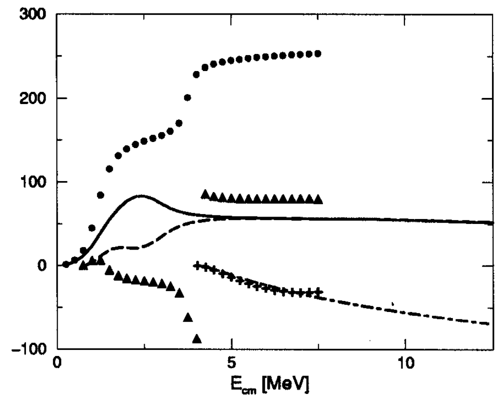


Figure 1: Elastic 0^- phase shifts for all physical two-fragment channels. The data from the R-matrix are denoted by full dots ($t-p$ channels), full triangles ($^3\mathrm{He}-n$ channels), and crosses ($d-d$ channels). The calculated phase shifts are denoted by full lines, dashed lines, and dashed-dotted lines, respectively.

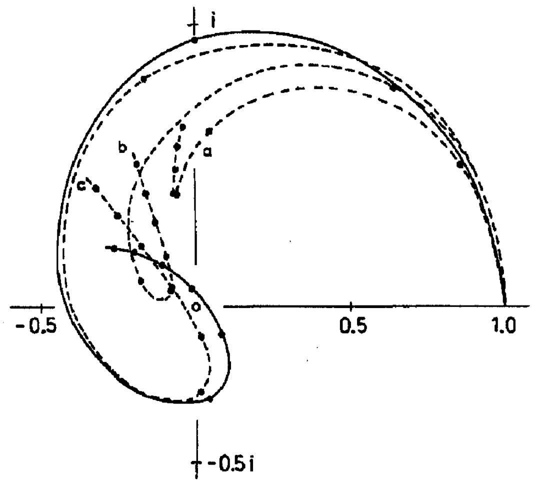


Figure 2: Argand plot of the $^3P_0$ elastic $t-p$ S-matrix elements extracted from the R-matrix (full) and calculations for various model spaces (dashed lines). The full calculation (dashed line c) passes the origin, marked as a small circle in the middle of the figure, on the other side. The dots on the curves denote steps of one MeV in the center-of-mass energy.

see Nucl.Phys. A613(1997)69

Theory can predict X-section

- at higher energies
- on unstable targets

Example: neutron - $^{6}\mathrm{He}$ scattering
$\Rightarrow$ Extraction of resonance parameters ambigous

Search for common parametrisation

Direct comparison of phase shifts TOO sensitive
S-matrix pole positions ?

Microscopic theory codes utilize massively parallel computers

$\Rightarrow$ CPU-time no essential problem

However, for multi-channel systems model consistency problematic

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1) 26007
cable: INATOM VIENNA
telex: 1-12645
telephone: (43-1) 2600-21710

Online: TELNET or FTP: iaeand.iaea.org
username: IAEANDS for interactive Nuclear Data Information System
usernames: ANONYMOUS for FTP file transfer;
FENDL2 for FTP file transfer of FENDL-2.0;
RIPL for FTP file transfer of RIPL;
NDSONL for FTP access to files saved in “NDIS” Telnet session.
Web: http://www-nds.iaea.org