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NUCLEAR DATA STANDARDS

A report by the Working Party
on International Evaluation Co-operation
of the NEA Nuclear Science Committee

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In these and related tasks, the NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has a Co-operation Agreement, as well as with other international organisations in the nuclear field.

FOREWORD

A Working Party on International Evaluation Co-operation was established under the sponsorship of the OECD/NEA Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation and related topics. Its aim is also to provide a framework for co-operative activities between members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The working party determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

The parties to the project are: ENDF (United States), JEF/EFF (NEA Data Bank member countries) and JENDL (Japan). Co-operation with evaluation projects of non-OECD countries is organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

This report was issued by Subgroup 7, which was in charge of producing new evaluated neutron cross-section standards. When starting the project, there was a general consensus on the need to update these standards, as significant improvements had been made to the experimental database since 1991 when the last evaluation of these standards was performed. The present work was accomplished through efficient collaboration between a task force of the US Cross-section Evaluation Working Group (CSEWG), a Co-ordinated Research Project (CRP) of the International Atomic Energy Agency (IAEA) and Subgroup 7 of the Working Party on International Evaluation Co-operation (WPEC) of the NEA Nuclear Science Committee.

The opinions expressed in this report are those of the authors only and do not represent the position of any member country or international organisation. This report is published on the responsibility of the Secretary-General of the OECD.

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SUMMARY

Work is reported on the results of an international effort to evaluate the neutron cross-section standards. The evaluations include the H(n,n), ^{6}Li(n,t), ^{10}B(n,α), ^{10}B(n,α1γ), ^{197}Au(n,γ), ^{235}U(n,f) and ^{238}U(n,f) standard reactions. Evaluations were also produced for the non-standard ^{238}U(n,γ) and ^{239}Pu(n,f) reactions. This effort was performed so as to include new experiments in the standards that have been established since the ENDF/B-VI standard evaluation was completed, and to improve the evaluation process. Evaluations were not undertaken for the ^{3}He(n,p) and C(n,n) standards. These standards are carried over from ENDF/B-VI. The interest in standards above 20 MeV led to the extension of the ^{235}U(n,f) and ^{238}U(n,f) cross-sections to 200 MeV. The ^{239}Pu(n,f) cross-section was also extended to 200 MeV. The general trend observed for the evaluations is an increase in the cross-sections for most of the reactions from fractions of a per cent to several per cent compared with the ENDF/B-VI results.

NUCLEAR DATA STANDARDS

Introduction

Standards are the basis for the neutron reaction cross-section libraries. Significant improvements have been made in the standard cross-section database since the last complete evaluation of neutron cross-section standards, almost 20 years ago. It is important to re-evaluate these cross-sections taking into account new experimental data and improved evaluation techniques. In response to requests for improvements in the standards, the Cross-section Evaluation Working Group (CSEWG) formed a task force, the Working Party on International Evaluation Co-operation of the Nuclear Energy Agency Nuclear Science Committee formed a subgroup and the International Atomic Energy Agency (IAEA) formed a Co-ordinated Research Project (CRP). These groups have worked co-operatively to improve the evaluation process. The emphasis has been on the H(n,n), $^{10}B(n,\alpha)$ and fission standards. Table 1 shows the standards and the energies where they are considered standards. Extended energy ranges compared with the ENDF/B-VI results were obtained for the cross-sections of $^{235}U(n,f)$ and $^{238}U(n,f)$ from 20 MeV to 200 MeV, and for $^{10}B(n,\alpha)$ and $^{10}B(n,\alpha_1\gamma)$ from 250 keV to 1 MeV. Work is continuing on the extension of the H(n,n) standard to 200 MeV.

Table 1. The neutron cross-section standards

Reaction	Standard energy range
H(n,n)	1 keV to 20 MeV
$^{3}He(n,p)$	0.0253 eV to 50 keV
$^{6}Li(n,t)$	0.0253 eV to 1 MeV
$^{10}B(n,\alpha)$	0.0253 eV to 1 MeV
$^{10}B(n,\alpha_1\gamma)$	0.0253 eV to 1 MeV
C(n,n)	0.0253 eV to 1.8 MeV
$Au(n,\gamma)$	0.0253 eV, 0.2 MeV to 2.5 MeV
$^{235}U(n,f)$	0.0253 eV, 0.15 to 200 MeV
$^{238}U(n,f)$	2 MeV to 200 MeV

The $^{238}U(n,f)$ cross-section, which is an NEANDC/INDC standard, was accepted as an ENDF standard at the fall 2004 CSEWG meeting. However 2 MeV was recommended as the lower bound for use of this cross-section as a standard. The use of this cross-section from threshold to 2 MeV is discouraged as a standard due to the very rapid change of this cross-section in that energy range and the very small cross-section in the threshold energy region. The present evaluation of this cross-section does extend down to 1 MeV so it can be used at the lower energies that are needed for applications.

Evaluation objectives

The largest contribution to the evaluation process has been made by the IAEA CRP. The CRP has included membership from Austria, Belgium, China, Germany, Japan, the Republic of Korea, Russia and the USA. The main objectives of the evaluation are the following:

- to improve the methodology for determination of the covariance matrix used in cross-section evaluations;
- to upgrade the computer codes using this methodology;
- to study the reasons for uncertainty reduction in R-matrix and model independent fits;
- to evaluate cross-sections and covariance matrices for the light elements, H(n,n), $^{3}He(n,p)$, $^{6}Li(n,t)$, $^{10}B(n,\alpha 1\gamma)$ and $^{10}B(n,\alpha)$;
- to establish the methodology and computer codes for combining the light element with the heavy element evaluations leading to a final evaluation of the neutron cross-section standards.

The evaluation work includes:

- improvements to the experimental data in the standards database and methods for handling discrepant data;
- R-matrix evaluation of the hydrogen scattering cross-section and conversion of measurements relative to the hydrogen cross-section to the new standard;
- studies of the effect of Peelle’s Pertinent Puzzle (PPP) and its effect on the standards;

- evaluation work on microscopic calculations leading to independent determinations of R-matrix poles;
- studies of the small uncertainties resulting from evaluations;
- smoothing procedures;
- providing results for use in the cross-section libraries of evaluation projects.

The evaluation efforts [1] have led to a large quantity of results. Extensive documentation [2] of the work done on the evaluation is being prepared. The present report is a summary of that document.

Database studies

The status of the standards database [3] was reported on recently. For each experiment in the database, the documentation was investigated for possible corrections that may need to be made and for errors or missing information. This investigative procedure in many cases led to estimates of the uncertainties and correlations within an experiment and correlations with other experiments. This information was used to obtain covariance matrices for the measurements that were used in the evaluation process. The database included both shape and absolute cross-section measurements and their ratios. It also included data involving the ^{238}U(n,γ) and ^{239}Pu(n,f) cross-sections. There are many very accurate measurements of these cross-sections. The use of these additional data improves the database as a result of ratio measurements of those cross-sections to the traditional standards. Measurements of the ^{235}U and ^{239}Pu fission cross-sections in the ^{252}Cf spontaneous fission neutron spectrum were also included in the database. These data can be obtained with high accuracy and are only weakly dependent on the uncertainties in the ^{252}Cf spontaneous neutron fission spectrum. These data can have an important effect on the normalisation of the evaluated cross-sections. Scattering and total cross-section data have also been included for ^{6}Li and ^{10}B, since they provide information on the standard cross-sections. Charged-particle data were included as well, since they can be used in R-matrix analyses to provide improved cross-sections for the light element standards. No evaluation of the C(n,n) cross-section was made because very little new data have been obtained subsequent to the ENDF/B-VI evaluation; what was obtained is in good agreement with that evaluation.

Significant improvements were obtained for the thermal constants used in the evaluation. This was largely due to the very accurate coherent scattering measurements for ^{235}U obtained by Arif [4] that were used to provide a more accurate scattering cross-section, and an improved analysis of the Gwin [5] ν-bar uncertainties.

A large database of measurements, a significant portion of which were assembled by Poenitz [6] for the ENDF/B-VI standards evaluation, was used for the evaluation. In addition to the data sets introduced after the ENDF/B-VI evaluation and before the initiation of this evaluation, more than 30 data sets had been added to the standards database. Work has been done to understand the experiments and possible problems with them that may cause discrepancies to exist. During the ENDF/B-VI evaluation process, unusual results [7] were observed with the code GMA [8] when correlated discrepant data were used. To remove problems associated with these discrepancies, data greater than three standard deviations away from the output results were down-weighted in the ENDF/B-VI GMA evaluation. This had the effect of making χ^2 per degree of freedom essentially one. For the R-matrix code EDA [9] that was also used in the ENDF/B-VI standards evaluation, its output covariances were modified by the χ^2 per degree of freedom value of the fit. This procedure is equivalent to increasing the uncertainty of all the experimental data in the fit, not just the outliers. This procedure was also used for the present evaluation. It would be better if the sources of the discrepancies could be found, as the evaluation could then be performed with consistent data sets. This is a very difficult task since there are thousands of data points. To reduce the effect of discrepant data on the GMA analysis and the RAC [10] R-matrix evaluation for the database of neutron experiments used in the present international evaluation, deviations of experimental measurements from the output of the evaluation were compared with the uncertainties on the data. The outliers were defined as those for which the difference from the evaluated output value was above two standard deviations for a single point or above one standard deviation for a few sequential points. The uncertainty of outliers was increased by adding an additional component to the covariance matrix of the uncertainty of each outlying data set. The length of correlation for this additional medium energy range correlation component was evaluated from an analysis of the energy dependence of the discrepancy. This results in a much better χ^2 per degree of freedom and larger uncertainty in the evaluated results. The change in the cross-section from this procedure is small.

Hydrogen evaluation

The hydrogen scattering cross-section below 20 MeV neutron energy was evaluated at LANL using the R-matrix code EDA. Calculations of the angular distribution using these R-matrix parameters are in much better agreement with recent measurements [11] than the ENDF/B-VI evaluation. Comparisons of the new hydrogen evaluation with other evaluations are shown in Figure 1. With the availability of the new hydrogen standard, all data in the database relative to hydrogen cross-sections were converted so they are relative to the new standard. After this conversion process was completed, a hydrogen re-evaluation was recommended as a result of preliminary data testing due to concerns about the thermal capture cross-section. The re-evaluation resulted in small changes in the hydrogen standard cross-section. The conversion process was not re-done, but uncertainties on the converted data were increased to account for the changes in the hydrogen cross-section.

The database contained measurements relative to several different versions of total cross-sections. Further, a number of experiments were in the database that used different laboratory angles, and different versions of the differential cross-section. The effect of the change in the hydrogen standard cross-section causes, for example, a change as large as 0.5% for the evaluated ^{235}U(n,f) cross-section. There are plans to extend the hydrogen evaluation to 200 MeV neutron energy.

Peelle's Pertinent Puzzle (PPP)

Problems associated with PPP were observed early in the evaluation process [12]. A test run using a model-independent least-squares code fitting the logarithm of the cross-section produced higher cross-sections than a run fitting the cross-section. There were discrepant data in the test run. The problem appears to be largely a result of using discrepant data but it is also is caused by the existence of data correlations. This is the maxi-PPP verses mini-PPP effect. The EDA R-matrix analysis uses only statistical uncertainties for the cross-sections, but also includes a procedure for fitting normalisations that takes into account the normalisation uncertainties; this procedure does not suffer the PPP problem, as it is equivalent to the Propagated Uncertainty Method [13]. Analyses using the RAC R-matrix code (Tsinghua Univ.) that include medium-range correlations do suffer this problem to some degree. A number of methods for reducing PPP have been employed, such as using per cent uncertainties, using a logarithmic transformation or the Box-Cox transformation. The GMA code was modified by adding the Chiba-Smith [14] option to handle PPP problems. This option, called GMAP, re-normalises the experimental absolute errors on the assumption that it is the fractional error that actually reflects the accuracy the experimenter has provided. This approach appears to have significantly reduced the PPP effect. Comparisons using the Chiba-Smith, Box-Cox and logarithmic transformation are in good agreement for a number of test cases. An important outcome of this work is the observation that special care should be exercised to reduce the effect of discrepant data and PPP to improve the quality of any nuclear data evaluation.

Theoretical model calculations

Theoretical calculations have been made to help describe some of the light-nuclei standard cross-sections. As there are relatively few nucleons involved for the ^{4}He compound nucleus, it was possible to use the Refined Resonating Group Model (RRGM) to obtain information about the ^{3}He(n,p) cross-section. This model allows realistic nuclear interactions to be used; however it requires very large computer resources. Using effective NN potentials allowed heavier nuclei to be studied, such as the A=7 case which provided information on the ^{6}Li(n,t) standard. Using effective potentials allowed the calculations to be done with a standard personal computer. The work on these two standards progressed well. The calculations produced results that are rather close to those given by R-matrix analyses. Transforming the RRGM results to R-matrix poles provided guidance for initial values in the R-matrix analyses. This work led to improved values of the parameters and more realistic uncertainties in the cross-sections. There were cases where the information on the poles allowed limitations in experimental data sets to be recognised.

The small uncertainty problem

The small uncertainties obtained in the ENDF/B-VI evaluation process [7] were of great concern. An important task for the present effort was to try to understand in detail how standard error propagation in model-independent or R-matrix analyses could result in such small uncertainties, and whether there were more reasonable corrections or algorithms to employ. Work was undertaken on the small uncertainty problem through comparisons of several tests of model-independent and R-matrix codes using a common database.

The R-matrix codes used in this study were EDA (LANL), SAMMY [15] (ORNL) and RAC (Tsinghua University). The generalised least-squares codes used were GLUCS [16] (University of Vienna), GMAP (IAEA and IPPE) and SOK [17] (LANL). A code based on an analytical approximation model, PADE2 [18] (IPPE), was also used. It was necessary to select a database containing measurements that could be properly used in the comparison. For example some of the codes could not handle certain types of input data correlations. For the comparison tests, it was assumed that no correlations exist between the data sets. The only correlations within the data sets were assumed to be short energy range (statistical) and long energy range (normalisation).

The generalised least-squares codes were easily found to be in good agreement. Comparisons of the R-matrix codes proved to be more difficult since the input and analysis conditions were difficult to standardise. Studies employing

SAMMY were particularly useful in understanding differences obtained with different codes, as it was possible to do SAMMY fitting that corresponded essentially to that done by RAC, and in a different scheme it was possible to do fitting that corresponded essentially to that by EDA. Good agreement was eventually obtained for the cross-sections obtained from the R-matrix analyses. The small differences obtained with the codes could be explained as a result of different procedures, different chi-square expressions and some PPP effects that may be present in the RAC results. The variances and covariances also agreed well with some local differences. A measure of that agreement was given by a comparison of the sum of all elements of the covariance matrix of the evaluated data, which agreed within 1% for EDA and RAC. These differences were probably mainly due to numerical precisions of the solutions.

The large amount of data for charged-particle-induced reaction channels may be an important factor in the large reduction in the calculated uncertainty. A large amount of charged-particle data, especially differential elastic scattering cross-sections, are claimed to have very small uncertainties. It is possible that systematic errors may not have been fully estimated. The option of increasing the uncertainties of outlying data for charged-particle data was used in RAC. These changes and the changes in the neutron database uncertainties noted previously for discrepant data led to somewhat larger uncertainties for the results.

An important result of the present work is that it is essential to consider the covariances, not just the variances, in applications of cross-sections to practical systems.

Evaluation procedure

It was decided that a combination procedure similar to that used for the ENDF/B-VI standards evaluation would be used to obtain the standards. All the standards except the H(n,n), ^{3}He(n,p) and C(n,n) cross-sections were evaluated using the GMAP code, with a combining procedure using input from the RAC and EDA R-matrix analyses, and a thermal constants evaluation. The Axton evaluation [19] of the thermal constants with the associated variance-covariance data for ^{233}U, ^{235}U, ^{239}Pu and ^{241}Pu was used as input to the GMAP code since it includes accurate cross-sections which have been measured relative to the neutron cross-section standards. Thus this evaluation would have an impact on the determination of the standards.

The R-matrix analyses used charged-particle data and the lithium and boron neutron databases, including total and scattering cross-section data for these nuclides. The only lithium and boron data for direct use in the GMAP code were the ratio measurements. The R-matrix and GMAP data are totally independent of each other. There are no common data sets and no data sets that have correlations between the R-matrix and GMAP data. For the ^{6}Li(n,t), ^{10}B(n,α) and ^{10}B(n,α1γ) R-matrix work, the cross-sections obtained from the RAC and EDA analyses were not identical. The cross-sections from the RAC and EDA analyses were averaged (un-weighted) and used as the R-matrix input to GMAP. The covariance matrix used with these central values was that from the RAC code, as its results appeared more physically reasonable. The R-matrix input and thermal constants data were treated like the additions of other data sets to the GMAP code. At each energy point, half the difference between the RAC and GMAP results was treated as a model uncertainty that was added to the RAC covariance of uncertainties. This then takes into account the differences obtained between the RAC and EDA analyses. The results of these analyses are shown in Figures 2-4.

Smoothing of the evaluation

The results of the combination procedure were not smooth. For the ^{6}Li(n,t), ^{10}B(n,α1γ) and ^{10}B(n,α) cross-sections smoothing was not required since the highest weight went to the cross-sections used in the R-matrix analyses. For the heavy element standards, there were some models that could provide insight on how to define the curves. It was determined that a simple smoothing algorithm would be satisfactory for most cases. It was used sparingly for the heavy element cross-sections. A patch using the shape of the Maslov [20] evaluated curve was applied in the 50-60 MeV region for the ^{235}U(n,f) cross-section where a rather large fluctuation, assumed to be statistical, occurred.

Results of the evaluation

The cross-sections obtained for the ^{6}Li(n,t), ^{10}B(n,α), ^{10}B(n,α1γ), Au(n,γ), ^{235}U(n,f) and ^{238}U(n,f) standard cross-sections, as well as the ^{238}U(n,γ) and ^{239}Pu(n,f) cross-sections, are shown in Figures 5-14. In Figures 5-7, the data are the combined results shown in Figures 2-4, respectively. They are re-plotted without the additional data for clarity. All uncertainties shown are one standard deviation value. The standards obtained from this work were given to the CSEWG in November 2005 as the proposed standards for the ENDF/B-VII library.

Some benchmark data testing has been done using these data. The quantity K1 calculated from the evaluation is 721.6 b. This should be compared with the "preferred" value of 722.7 b determined by Hardy [21]. The agreement is quite good when one considers that the uncertainty in the Hardy value is 3.9 b. Preliminary criticality calculations using these data [22] are generally in better agreement than those obtained with the ENDF/B-VI standards.

It is anticipated that additional work will be done on the hydrogen standard cross-section to extend it to 200 MeV. Evaluations for the $^{3}He(n,p)$ and C(n,n) standards were not made. Those standards will be carried over from the ENDF/B-VI files.

Conclusions

Neutron cross-section standards have been re-evaluated for use by international nuclear data evaluation projects. Their first use has been in the new ENDF/B-VII library. This has been a successful international effort. It is important to continue to maintain the database and improve the analysis procedure used in determining the standards. A new IAEA Data Development Project has been approved that is focused on the maintenance of the neutron cross-section standards. This project could provide a method for obtaining standards evaluations that will be up-to-date when they are needed by the various nuclear data evaluation projects.

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[23] Carlson, A.D., S. Chiba, F-J. Hambsch, N. Olsson, A.N. Smirnov, "Update to Nuclear Data Standards for Nuclear Measurements", *Summary Report of an International Atomic Energy Agency Consultants' Meeting on Nuclear Data Standards*, 2-6 Dec. 1996, Vienna, Austria, INDC(NDS)-368 (1997).

FIGURES

Figure 1. Comparison of the present hydrogen evaluation to other evaluations

The ENDF/B-VI and ENDF/B-V total cross-sections are compared with the present results. Also the laboratory zero degree differential cross-sections for the ENDF/B-VI and ENDF/B-V evaluations are compared with the results of this evaluation.

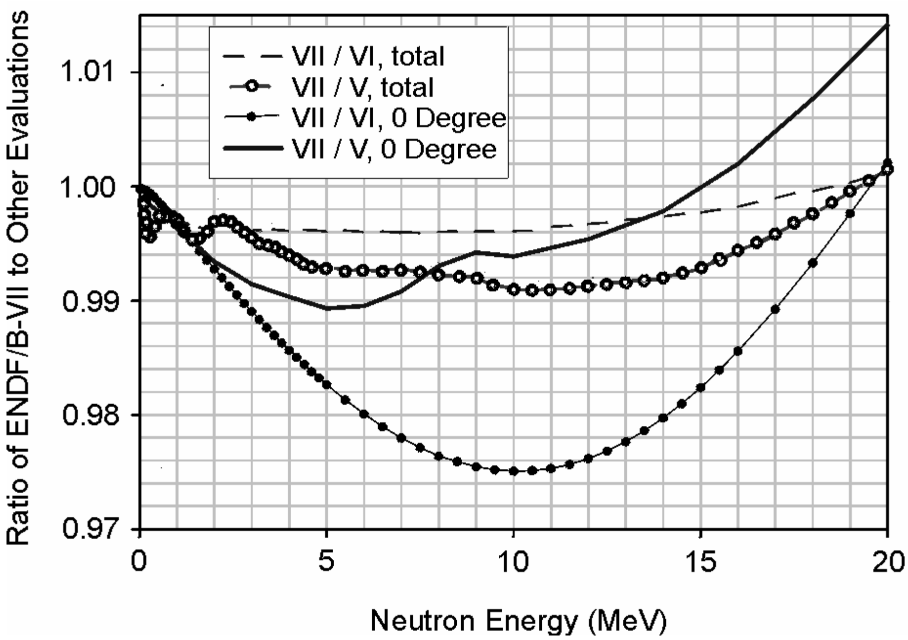


Figure 2. Comparison for the $^{6}Li(n,t)$ cross-section of the ENDF/B-VI evaluation with the EDA R-matrix analysis, the RAC R-matrix analysis and the combined result. The combined result is the final result from this evaluation.

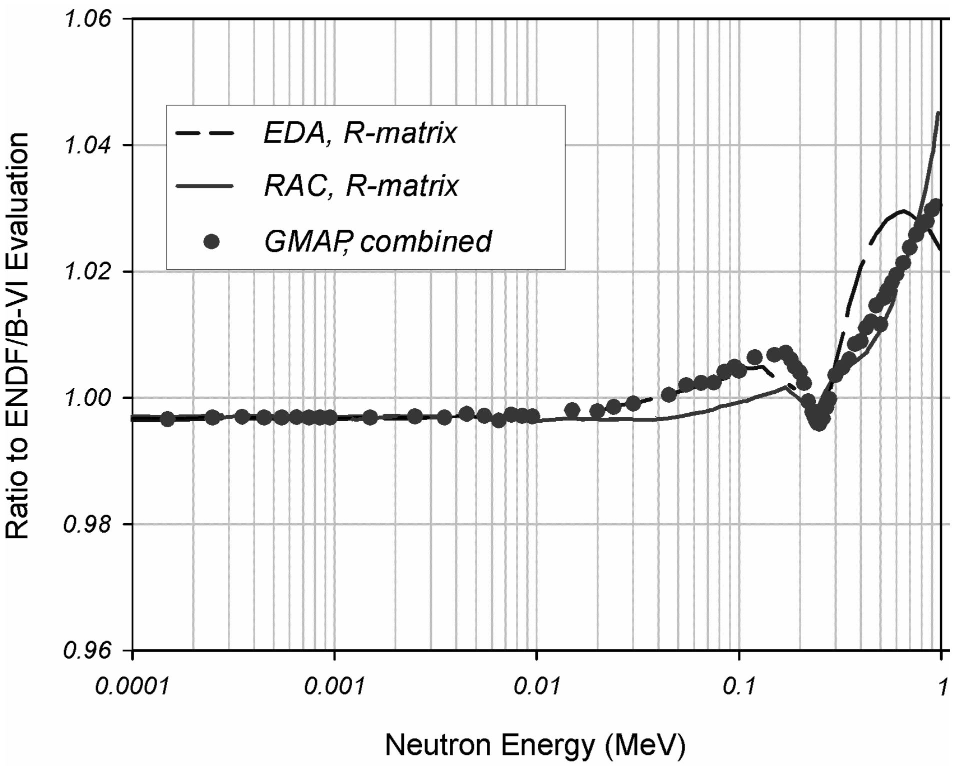


Figure 3. Comparison for the $^{10}B(n,\alpha)$ cross-section of the ENDF/B-VI evaluation with the EDA R-matrix analysis, the RAC R-matrix analysis and the combined result. The combined result is the final result from this evaluation.

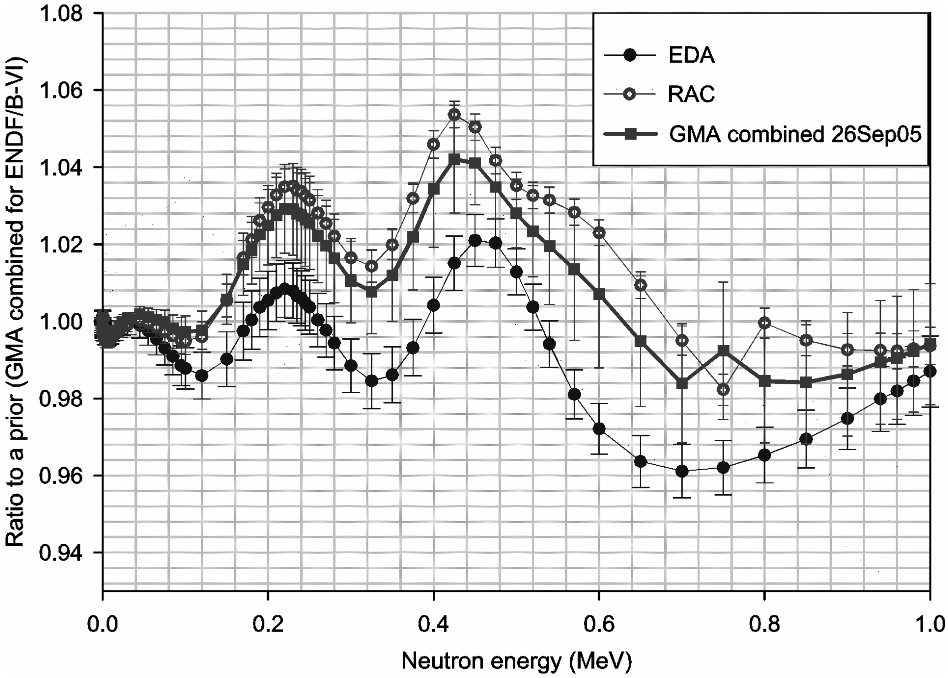


Figure 4. Comparison for the $^{10}B(n,\alpha 1\gamma)$ cross-section of the ENDF/B-VI evaluation with the EDA R-matrix analysis, the RAC R-matrix analysis and the combined result. The combined result is the final result from this evaluation.

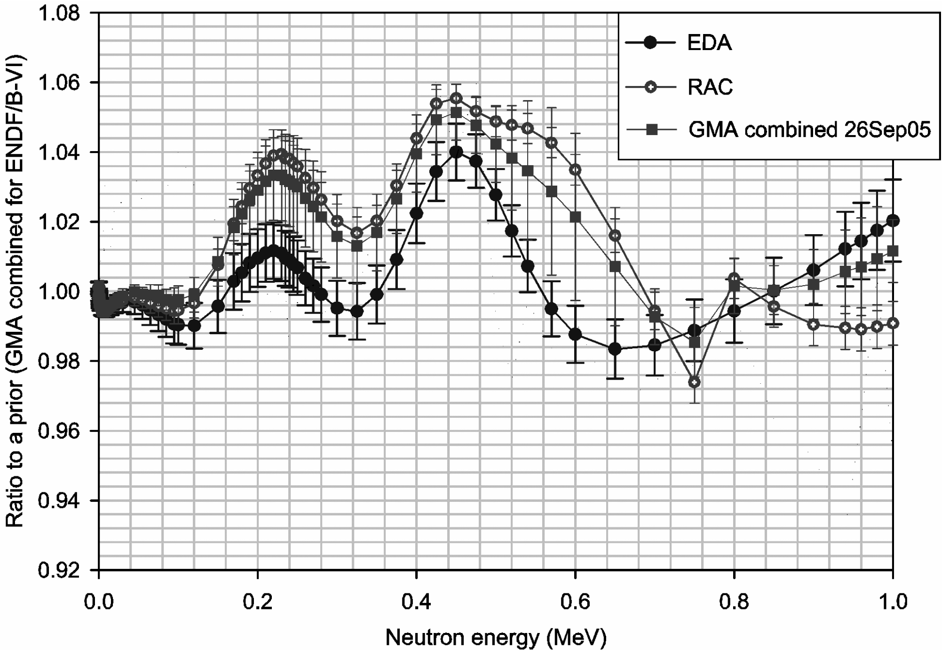


Figure 5. Comparison of the $^{6}Li(n,t)$ cross-section from this evaluation with the ENDF/B-VI evaluation

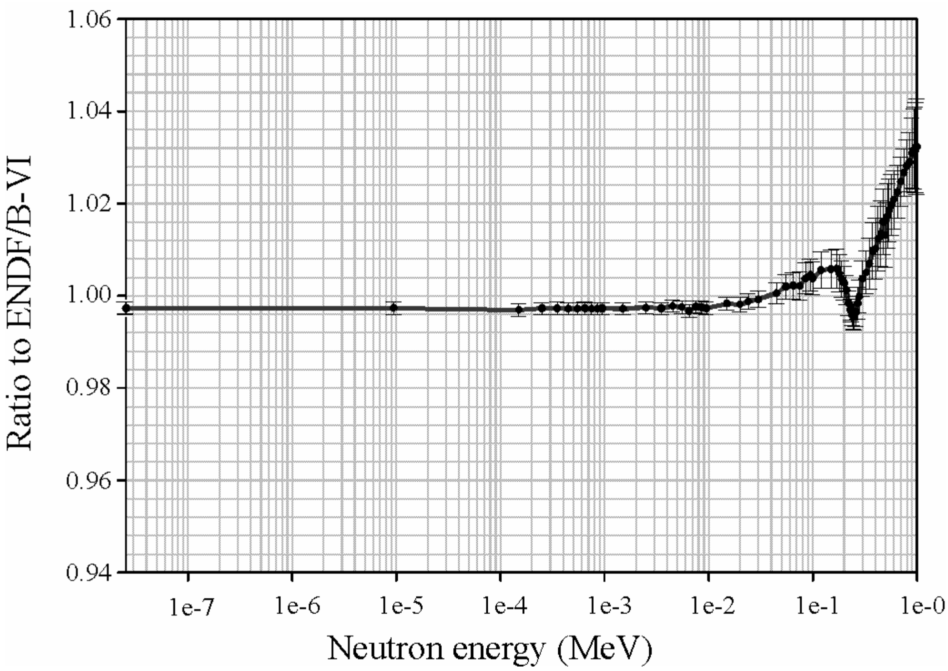


Figure 6. Comparison of the $^{10}B(n,\alpha)$ cross-section from this evaluation with the ENDF/B-VI evaluation

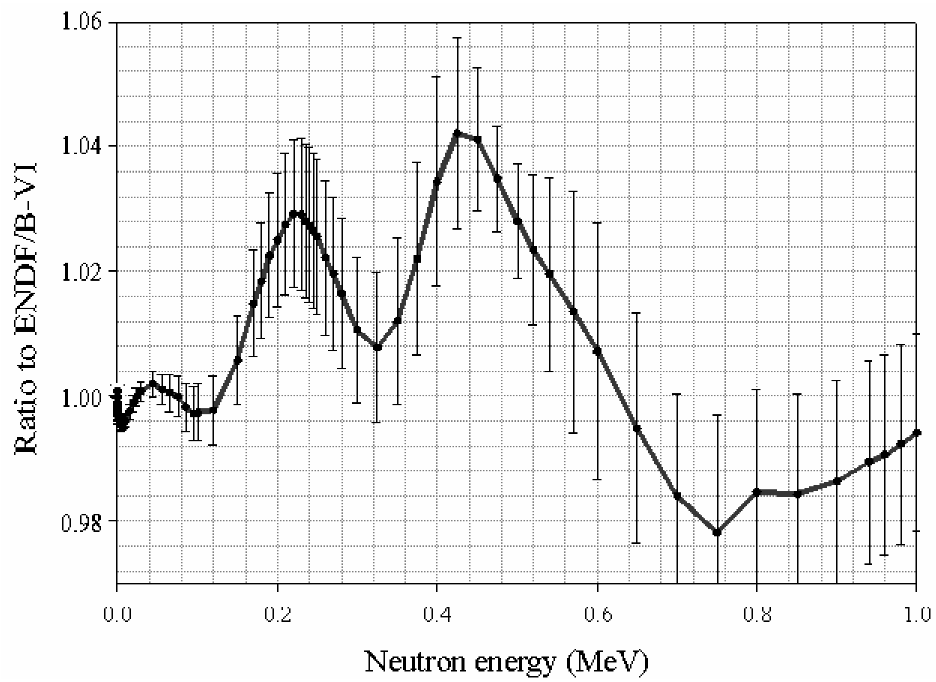


Figure 7. Comparison of the $^{10}B(n,\alpha 1\gamma)$ cross-section from this evaluation with the ENDF/B-VI evaluation

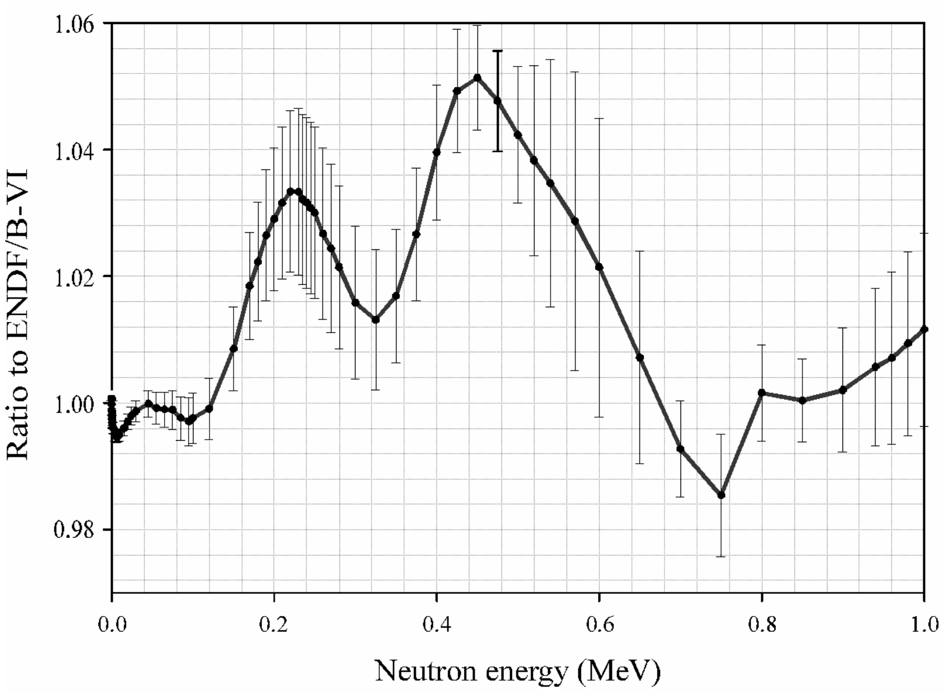


Figure 8. Comparison of the Au(n,γ) cross-section from this evaluation with the ENDF/B-VI evaluation

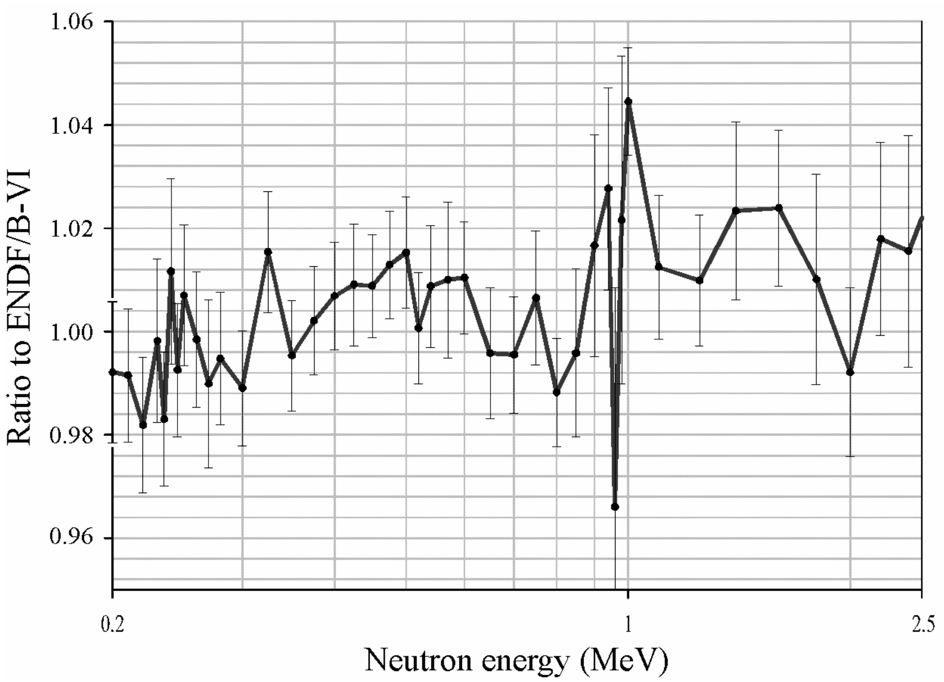


Figure 9. Comparison of the ^{235}U(n,f) cross-section up to 20 MeV from this evaluation with the ENDF/B-VI evaluation

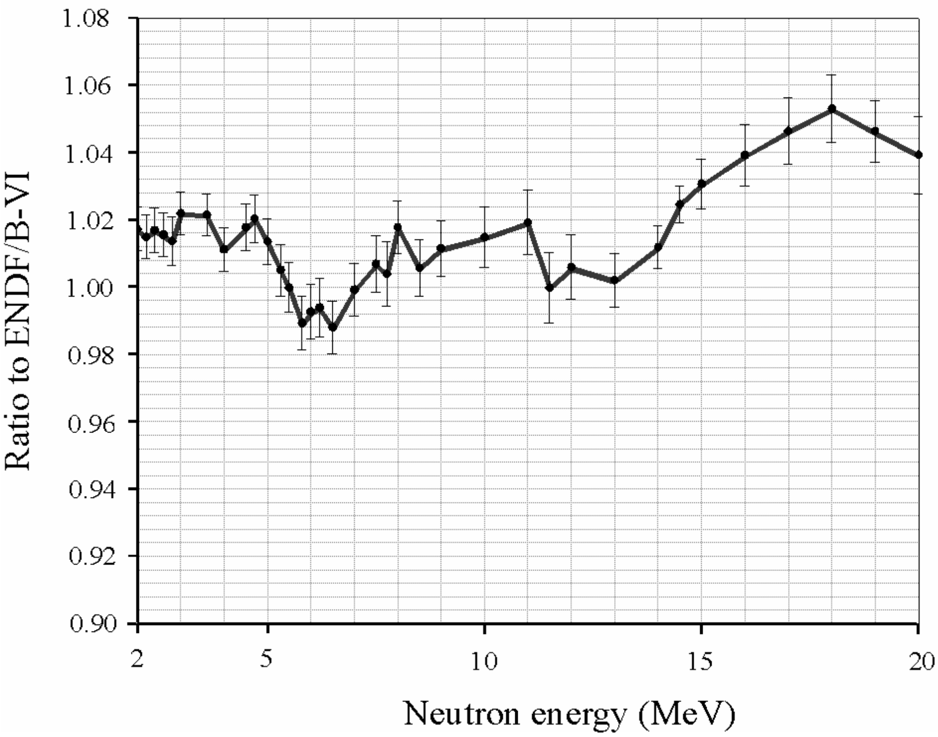


Figure 10. Comparison of the $^{235}U(n,f)$ cross-section from this evaluation with the ENDF/B-VI evaluation up to 20 MeV and with updated values [23] above 20 MeV

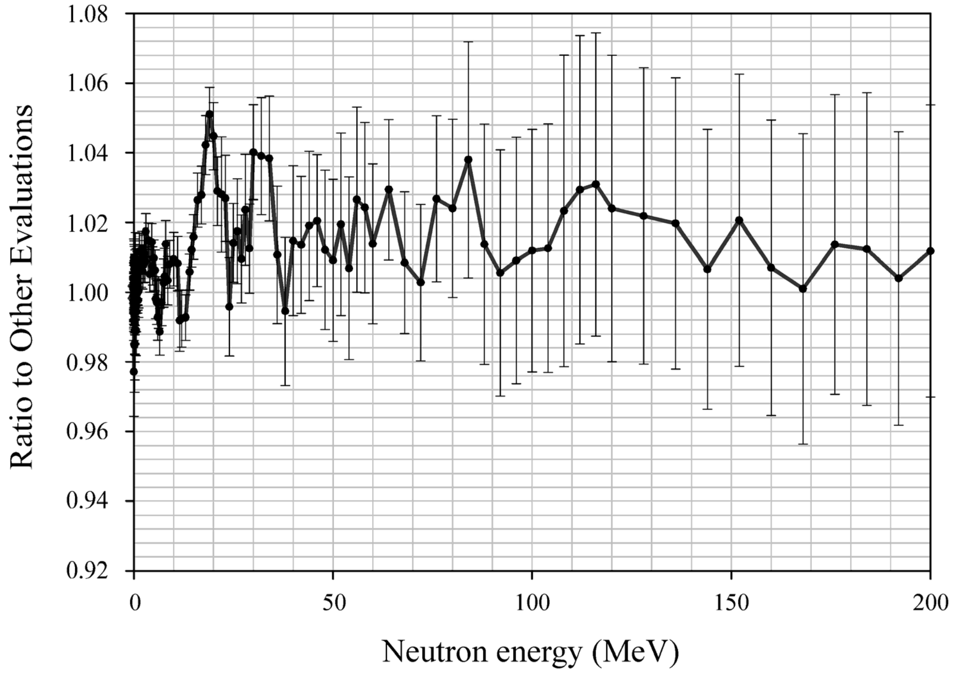


Figure 11. Comparison of the ^{238}U(n,f) cross-section from this evaluation with the ENDF/B-VI evaluation

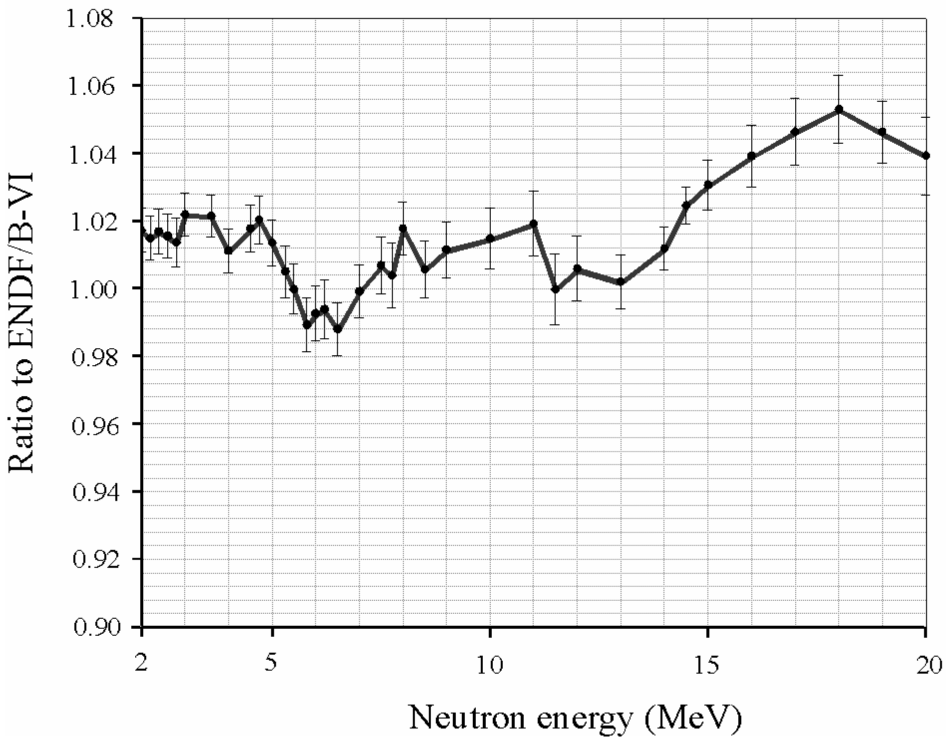


Figure 12. Comparison of the ^{238}U(n,f) cross-section from this evaluation with ENDF/B-VI evaluation up to 20 MeV and with updated values [23] above 20 MeV

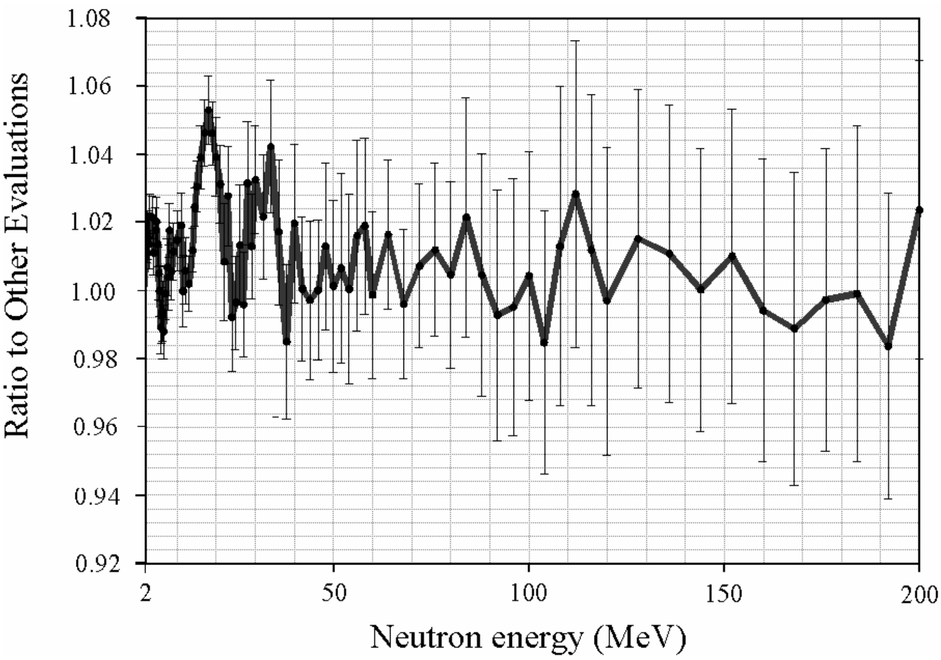


Figure 13. Comparison of the $^{238}U(n,\gamma)$ cross-section from this evaluation with the ENDF/B-VI evaluation

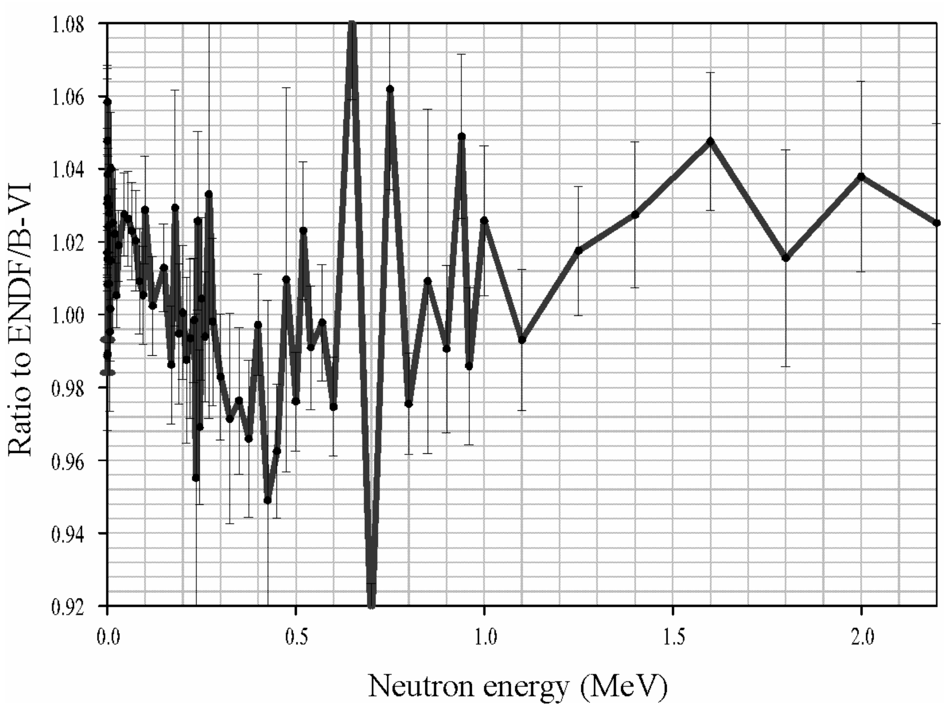
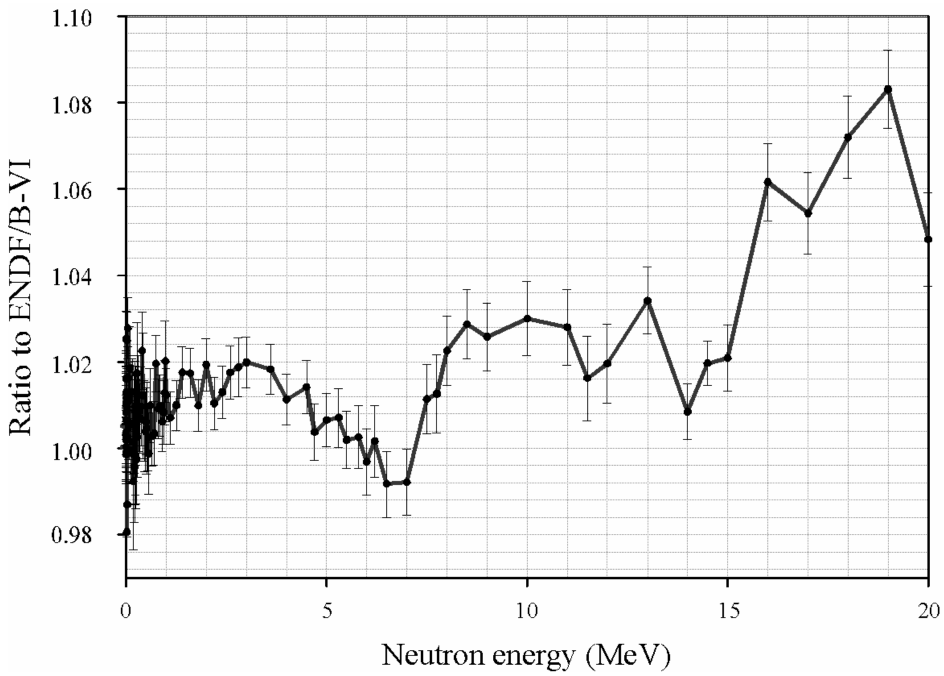


Figure. 14 Comparison of the ^{239}Pu(n,f) cross-section from this evaluation with the ENDF/B-VI evaluation

There are results from this evaluation up to 200 MeV, however comparisons can not be made with the ENDF/B-VI evaluation as it only extends to 20 MeV



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