International Atomic Energy Agency

INDC(NDS)-311
Distrib.: G

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

On the Development of the Fusion Evaluated Nuclear Data Library (FENDL)

Three Papers (1992 - 1993)

by

S. Ganesan, D.W. Muir and A.B. Pashchenko

December 1994

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

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On the Development of the Fusion Evaluated Nuclear Data Library (FENDL)

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Abstract

This report presents a compilation of the three papers presented by the IAEA Nuclear Data Section in 1992-1993 period. This documentation is of interest from both historical point of view and as a document of the technical and co-ordination activities carried out at the Agency. The three papers are:

1. "IAEA Activities in Nuclear Data Processing for Thermal, Fast and Fusion Reactor Applications Using the NJOY System", *Seminar on NJOY-91 and THEMIS, OECD/NEA Data Bank, Saclay, France, 7-9 April 1992*, by S. Ganesan and D.W. Muir.

2. "Current Status of Production of Coupled Neutron-photon Multigroup Cross Section Libraries of FENDL for Use in Fusion Neutronics Calculations", *International Workshop on Nuclear Data for Fusion Reactor Technology, Del Mar, California, U.S.A., 3-6 May 1993*, by S. Ganesan.

3. "Status of FENDL Activation File and Plans for Future Development", *International Workshop on Nuclear Data for Fusion Reactor Technology, Del Mar, California, U.S.A., 3-6 May 1993*, by A.B. Pashchenko.

December 1994

Reproduced by the IAEA in Austria
December 1994

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IAEA ACTIVITIES IN NUCLEAR DATA PROCESSING FOR THERMAL, FAST AND FUSION REACTOR APPLICATIONS USING THE NJOY SYSTEM.

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ABSTRACT

The International Atomic Energy Agency has recently initiated a number of activities in the area of nuclear data processing towards satisfying urgent needs of applied calculations. This paper briefly summarizes the on-going IAEA activities in nuclear data processing for thermal, fast and fusion research and power reactor applications using the NJOY code system. The activities that are described are (1) Processing of selected basic data libraries for elements of interest to Agency's program on Fusion Evaluated Nuclear data Library (FENDL); (2) Co-ordination and participation in the WIMS Library Update Project (WLU Project) which aims towards updating and improving the multigroup nuclear data input to the thermal reactor lattice cell code WIMS; (3) Training activities in the use and applications of the NJOY system at the IAEA Headquarters, Vienna, mainly for the IAEA fellowship applicants from IAEA Member States; and (4) Verification of the accuracy of data processing using NJOY and other processing codes that are available, i.e., the continuation of the IAEA nuclear data processing code verification project. These four activities, all of which heavily use the NJOY system, are briefly discussed in this paper.

IAEA ACTIVITIES IN NUCLEAR DATA PROCESSING FOR THERMAL, FAST AND FUSION REACTOR APPLICATIONS USING THE NJOY SYSTEM.

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1.INTRODUCTION

After a development period of 10-15 years, improved basic evaluated nuclear data libraries such as ENDF/B-VI, JENDL-3.1, BROND and JEF-2 have become available [1]. There are many reactor physicists around the world who are interested in updating and improving the multigroup nuclear data input to neutronic codes and point-data input to Monte-Carlo codes. The International Atomic Energy Agency has recently initiated a number of activities in the area of nuclear data processing toward satisfying the urgent needs of such calculations. This paper briefly summarizes the on-going IAEA activities in nuclear data processing for thermal, fast and fusion research and power reactors applications using the NJOY system. The IAEA activities on nuclear data processing consist of four different tasks which cover applied calculations for thermal, fast and fusion research and power reactors using NJOY [2-7] which is well known as the most general purpose and versatile nuclear data processing code system. These are as follows:

a. Using the NJOY to process selected basic data libraries for elements of interest to Agency's program to develop a Fusion Evaluated Nuclear data Library (FENDL). The intermediate results can also be post-processed by the interested users for fast reactor applications.

b. Co-ordination and participation in the WIMS Library Update Project (WLU Project) which aims toward updating and improving the multigroup nuclear data input to the thermal reactor lattice cell code WIMS.

c. Training activities in the use and applications of NJOY at the IAEA Headquarters, Vienna, mainly for IAEA fellowship applicants from the IAEA Member States.

d. Verification of the accuracy of data processing using NJOY code system and other processing code systems that are available, i.e., the continuation of the IAEA nuclear data processing code verification project.

These four activities, all of which heavily use the NJOY system, are briefly discussed in this paper.

2. AGENCY'S PROGRAM ON FUSION EVALUATED NUCLEAR DATA LIBRARY (FENDL).

2.1 Introduction

The IAEA Nuclear data Section, in co-operation with several national nuclear data centres and research groups, is creating an internationally available Fusion Evaluated Nuclear Data Library (FENDL), which will serve as a comprehensive source of processed and tested nuclear data tailored to the requirements of the Engineering and Development Activities (EDA) of the International Thermonuclear Experimental Reactor (ITER) Project and other fusion-related development projects. The FENDL activity [8-10] is supported by several IAEA Coordinated Research Programmes. Within the scope of the FENDL project [8-10], the International Atomic Energy Agency is committed to a program of nuclear data processing activities in order to create a modern and internationally available Fusion Evaluated Nuclear Data Library(FENDL). Several materials from ENDF/B-VI, JENDL-3.1 and BROND basic files have been processed using the 32 bit IBM-3091 mainframe computer available at the IAEA. The nuclear data processing code system NJOY developed at Los Alamos National laboratory, USA [2-7] with all modifications and improvements as available in the NJOY version 89.80+ is employed in this study. A coupled neutron-gamma library for use in transport codes and a point library for use in Monte-Carlo code, in particular the MCNP code, will be produced and made freely available internationally to users as results of this program of nuclear data processing activity. The Nuclear Data Section has the goal of producing FENDL/M-1, a multigroup library in MATXS format, with a tentative target completion date of July 1992.

2.1 Source of basic data for FENDL:

The coupled neutron-gamma data files for elements and isotopes of FENDL will be derived from ENDF/B-VI, JENDL-3.1 and BROND for the following materials following the recommendation of the FENDL meetings [8-10]:

ENDF/B-VI: ^{1}H, ^{3}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, C, ^{16}O, ^{19}F, P, S, Cl, K, ^{55}V, $^{50,52-54}Cr$, ^{55}Mn, $^{54,56-58}Fe$, ^{59}Co, $^{58,60-62,64}Ni$, $^{63,65}Cu$, $^{134-138}Ba$, $^{182-184,186}W$, $^{206-208}Pb$.

JENDL 3.1: ^{23}Na, Mg, ^{27}Al, Ca, Ti, ^{55}Mn, Mo, ^{181}Ta, ^{209}Bi.

BROND: ^{2}H, ^{14}N, ^{15}N, Si, $^{90-92,94,96}Zr$, ^{93}Nb, Sn.

2.2.Specifications for multigroup processing:

The specifications of multigroup processing as used in the NJOY runs for the FENDL project to produce a coupled neutron-gamma library is given below:

Neutron Groups: 175 (Vitamin-J structure)

Gamma groups: 42 (Vitamin-J structure)

Neutron weight function:

Thermal + 1/E +Fission + Fusion (IWT=6 in NJOY)

Gamma weight function:

1/E with rolloffs (IWT=3 in NJOY)

Legendre order for neutrons :P_6 for transport correction to P_5

Legendre order for gammas :P_8 for transport correction to P_7

Temperatures: 300, 900 and 1500 Kelvin

Dilution factors: 10^0, 10^1, 10^2, 10^3, 10^4, and 10^{10} barns

Reconstruction, linearization and thinning tolerances: 0.1 %

Thermal Scattering law included for Be in Be metal, C in graphite and H in water.

In spite of the limited manpower available for processing activities at the IAEA, evaluated files for most of the materials of FENDL have been successfully processed, and including up to the generation of Group ENDF or "GENDF" files. A coupled neutron-gamma library in MATXSR format for use in transport codes and a point library for use in Monte-Carlo code, in particular the MCNP code, will be produced and made freely available internationally to users as results of this program of nuclear data processing activity. However, the progress towards this goal is hampered at the time of writing this report by compatibility problems between the GROUPR and MATXSR modules of NJOY and between MATXSR and TRAMIX (TRANSX) post-processing programs. The NDS will be obtaining consulting assistance from the NJOY and TRANSX author R.E. MacFarlane on these problems so that the above stated target completion date still appears realistic.

3. IAEA CODE VERIFICATION PROJECT

The section briefly reviews the present status of the activities of the IAEA nuclear data processing code verification project [11-13]. We present some typical samples of our comparisons of line shapes produced for FENDL materials by both NJOY 89.31 and RECENT to see if both these codes produce essentially identical results.

The main conclusions are that, with an IBM mainframe, one needs to employ double precision in NJOY for the energy variable, and that there are other ambiguities, in addition, in the ENDF/B basic file and in the processing of unresolved resonance region etc. Thus there are

are many data processing issues and related physics still to be addressed. In spite of all this, we feel that this project is making considerable progress toward its main goal, namely, to make the nuclear data processing codes much more reliable. The IAEA code verification project [11-13] is a continuing activity at the Agency and the verification exercise will extend to other modules of processing. Any one interested to participate in the processing code verification project should please contact the first author of this report. Note that the IAEA code verification project [11-13] is being carried out primarily through correspondence and at no cost to the Agency.

3.1 Accuracy of reconstruction of line shapes

In the comparisons presented here, a reconstruction tolerance of 0.1% was employed as input in each of the processing modules RECONR and BROADR of the NJOY code system and similarly in the case of D.E. Cullen's codes LINEAR/RECENT/FIXUP/SIGMA1 [14-17].

3.2 Materials for which line shapes were compared

The following materials of ENDF/B-VI are covered:

^{1}H, ^{2}H, ^{3}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, C, ^{14}N, ^{15}N, ^{16}O, ^{19F}, ^{27}Al, Si, Ti, ^{55}V, $^{50,52-54}$Cr, ^{55}Mn, $^{54,56-58}$Fe, ^{59}Co, $^{58,60-62,64}$Ni, ^{63,65}Cu, $^{90-92,94,96}$Zr, ^{93}Nb, Mo, Sn, $^{134-138}$Ba, $^{182-184,186}$W, $^{206-208}$Pb, ^{209}Bi, ^{241}Pu, ^{232}Th and ^{238}U

The IAEA pre-processing codes LINEAR/RECENT/FIXUP/SIGMA1 and NJOY code system should, in principle, produce identical results (i.e. cross section line shapes), as both these processing code systems start from the same basic data file ENDF/B-VI and employ similar resonance reconstruction strategies.

3.3. Main results of intercomparison

All line shapes were intercompared using the COMPLOT program [17] in considerable detail using, in many cases, the "zooming" option. The results are presented in Figs. 1-163 of the unpublished report [13] and are not reproduced to save space. We have communicated the main discrepancies to R.E. MacFarlane at Los Alamos, D.E. Cullen at Lawrence Livermore Laboratory, and C. L. Dunford at Brookhaven National Laboratory, USA. We would like to acknowledge with thanks D. E. Cullen and R.E. MacFarlane for their important contributions to and active collaboration in this code verification project and for other useful feedback. Some of the interesting observations are as follows:

The cross section line shapes produced by NJOY89.31 and Red Cullen's codes LINEAR/RECENT/FIXUP/SIGMA1 showed, in general, in most of the energy regions, for most of the reactions in the case of most of the isotopes, excellent or perfect agreement. For

example, we see, for instance, in Fig. 1 and Fig. 2 that the results for ^{241}Pu are in good agreement, except at the boundaries of resolved and unresolved resonance region. It should be borne in mind that both NJOY [2-7] and the IAEA codes [14-17] were developed over a period of 10-15 years and it is extremely satisfying that, for the newly released ENDF/B-VI file, these code systems produce essentially identical results for most of the nuclear reaction cross sections. Selected results of comparisons are presented where, in some of these graphs, there are differences that cannot be ignored. We stress that since these comparisons were made, NJOY89.31 has been updated by R.E. MacFarlane and presently NJOY91.13 is available for distribution by Radiation Shielding and Information Center, Oak Ridge National laboratory, U.S.A. With this version of NJOY most of the differences have been eliminated. However, if the reader is using an older version of NJOY, he/she may still encounter these problems.

a. Resolved resonance region; potential scattering cross section

One of the most interesting discrepancies occurred in the case of ^{207}Pb as shown in Fig. 3. The potential cross section calculated by NJOY and RECENT differed substantially from each other. Cullen pointed to the fact that the large differences in the elastic cross section is due to different treatments of the j-multiplicity for both L=1 and L=2, which is adequately treated by RECENT. A memorandum clarifying the related issues is available from the authors [18].

b. Doppler broadening effects

The Doppler broadened line shapes at 300 Kelvin fail to achieve perfect agreement in many energy regions for many isotopes[13] but to save space we describe below only one interesting experience. More comparisons will be performed in the near future and results reported. The reason that the Doppler broadening aspects cannot be adequately presented here is that such discussions would be a premature mixture of the effects of differences in 300 Kelvin line shapes due to differences is zero Kelvin line shapes themselves plus differences if any due to the Doppler broadening modules themselves. In some cases the zero Kelvin cross sections agreed but not the higher temperature line shapes. Only one such sample is discussed below as a typical example: The 300 Kelvin (n,gamma) cross section data of ^{28}Si (Fig. 4) showed up some new structures for some of the narrow peaks in the higher energy (MeV) region at 300 K as compared to zero K line shapes. This non-physical Doppler broadening effect was successfully traced to a bug in BROADR module of NJOY by R.E. Macfarlane. The bug has been corrected by R.E.MacFarlane already, and we confirmed that it does not occur with our NJOY 89.80+ version.

c. Effects due to precision of IBM

1) NJOY was designed to operate on long word-length computers such as CDC and Cray. 2) RECENT was designed to operate on either long word length computers using single precision arithmetic or on short word length computers. (e.g., IBM) using double precision arithmetic.

For ^{60}Ni the NJOY results using double precision arithmetic on an IBM-3081 agree with the NJOY-Cray and RECENT results, bringing us to a clear conclusion that the user of NJOY should not use NJOY in single precision on IBM mainframe computers but go always to use double precision. The IBM-3081 employs 32-bit arithmetic, and as a result, in the reconstruction of sharp resonances in the resolved resonance region, NJOY is limited on this machine to a maximum of 6 digits in the single precision representation of the energy variable, whereas RECENT uses up to 9 digits of accuracy. We investigated this further in collaboration with Riyanto Raharjo of Indonesia as follows. Using an automatic compiler option available in IBM compiler, we created a double precision version of NJOY driver module and of RECONR, and tested it for ^{60}Ni data of ENDF/B-VI. The differences seen in Figs. 5-7 between NJOY(RECONR) and RECENT for ^{60}Ni essentially disappear when 7 digits are employed in the double precision version of NJOY. The results for even-even actinides such as ^{232}Th and ^{238}U distinctly showed the effect of using 9 digits in RECENT as compared to 6 digits in RECONR in many sharp resonances. The implications of 6 digits on Doppler changes can be significant as found earlier [12]. Figure 8 compares the results of a Cray run with 7 digits accuracy with RECENT for a p-wave resonance in ^{232}Th. The discrepancy (Fig. 9) almost disappears with the use of 7 digits. In summarizing this section, we state that, in many cases of isotopes, for zero Kelvin line shapes, NJOY(IBM-3081) differs significantly from RECENT unless double precision is used. On the other hand, there are cases such as ^{241}Pu where the resonances are not so sharp as to demand more than 6 digits of accuracy. In such cases the NJOY(IBM) and RECENT agree. See Fig. 1 and Fig. 2.

d. Unresolved resonance region

There were differences in the average 'point' cross sections calculated by the two processing modules RECONR and RECENT at zero K in the unresolved resonance region (URR) for some isotopes, namely, ^{238}U, Mo, W, and ^{184}W [Figs. 10-13]. In the case of Mo, as shown in Fig. 11, differences of -5.71% to +3.2% is seen for (n,gamma) cross sections in URR. For W, a clear discrepancy is seen (Fig. 12) in the unresolved resonance region. When the cross sections calculated by NJOY and RECENT agree in the URR (as in case of last three isotopes mentioned above) at only specific nodes, it can be deduced that the reason for the differences in the URR is due to different procedures or logic followed by NJOY and RECENT. Figure 10 gives the comparison for the ^{238}U (n,gamma) cross section at zero degree Kelvin. The 7% difference in the unresolved resonance region for capture was due to a bug in NJOY 89.31 and has been removed already by R.E. MacFarlane in NJOY 89.62 version.

e. Interpolation law for total cross section

For some isotopes (see Fig. 14 for ^{14}N and Fig. 15 for Si), the line shapes calculated by RECENT and RECONR did not agree for the total cross section in the lower energy region. The reason is that RECENT reconstructs the total cross section respecting the interpolation law specified for the total in the basic file, while the RECONR module of NJOY defines the total to be the exact sum of the reconstructed partials. The conclusion is that the interpolation law for total cross section in ENDF/B-VI is inadequate for such cases. More examples and discussions on this point are found elsewhere [13].

f. The 'artifacts' in comparison plots

There are 'artificial' discrepancies due to a convention of RECENT using repeated energy points and NJOY not using this convention at the boundary of resonance region. RECENT interprets the data on the two sides of the boundary as two completely different types of data which need not be continuous at the boundary. It seems unlikely that these differences could significantly affect calculations of integrals in the two systems.

g. Concluding remarks on the IAEA code verification project

The potential users of ENDF/B processing codes should be aware of possible errors that can arise in their processing of ENDF/B library.

NJOY is designed for long word-length computers and as such the readers should be aware of the approximations involved in using NJOY on short word-length machines.

Reactor physics teams working on different reactor concepts around the world using NJOY or RECENT (either recent or earlier version) will be interested to see the comparison plots obtained for many materials in this intercomparison study, apart from alerting the user that the accuracy of data processing cannot be taken for granted for all isotopes, in all energy regions, and for all reactions.

This section also distinguishes between differences due to the codes themselves and differences due to inconsistencies in the basic ENDF/B-VI evaluations- for example, as was pointed out in the text of this report, the differences in the unresolved region and in the definition of the total cross section are due to inconsistencies in the basic evaluations which have allowed NJOY and RECENT to each interpret the data in a non-unique way leading to different results- the method to eliminate these differences should not focus only on having NJOY and RECENT do exactly the same thing (which authors of NJOY and RECENT can agree to do) but focus on clarifying and documenting the ENDF/B conventions and procedures so that any other code will also calculate the same results.

4. WIMS LIBRARY UPDATE PROJECT

The International Atomic Energy Agency has initiated a project to update the multigroup nuclear data input library of the WIMS reactor physics code (in short: WIMS Library Update Project). The WIMS code is one of the most widely used thermal reactor physics codes and is of interest especially to reactor physics groups in developing countries. The WIMS Library Update project is principally conceived to proceed through a series of thermal reactor benchmark calculations using the evaluated nuclear data libraries, nuclear data processing codes and the WIMS code, with a gradual replacement of old by new nuclear data, and, including at each step, a checking of the reliability of the calculational results. Deviations between calculated and experimental benchmark data will be used to remedy inaccuracies in the calculations and/or nuclear data input and will also be fed back to the originators of the codes and/or evaluated nuclear data for review and improvement. The final outcome of this project will thus be a reliable up-to-date nuclear data base for the WIMS code in its present 69 energy groups format for all materials based on the newly released basic evaluated data files. Project participants in particular those from the developing countries will acquire a detailed knowledge of nuclear data relevant to thermal reactor physics as well as a capability for reliable use of an important reactor physics computer code and associated nuclear data processing codes. M. Ravnik and A. Trkov from the Josef Stefan Institute in Ljubljana, Slovenia are responsible for the technical co-ordination of this project. The status reports for the first two stages have been written [19,20]. One of the authors (S. Ganesan) is in charge of this project at the Agency. The project is being carried out primarily through correspondence and at no cost to the Agency.

The processing part of WLU project involves the use of available processing codes including NJOY and several related and interesting code developments. For instance, the non-availability of a WIMSR module prior to NJOY 91.0 has led some teams to develop their own post-processors (e.g., WIMSLIC developed in Korea [21]) to post-process the output of POWR module of NJOY. Care should be taken to obtain consistency between the options used in NJOY and the post-processor to the definitions of group constants as needed by the WIMS code. The details of this project and the current status are outlined by M. Ravnik and A. Trkov at this meeting in their presentation.

5. TRAINING ACTIVITIES ON NJOY

An in-house group fellowship training on nuclear data processing and reactor applications was organized at the IAEA Nuclear Data Section by the Agency during the period March - June 1991 in which six IAEA fellows successfully participated: The training program, which was conducted by D.W Muir and S. Ganesan and the staff of Nuclear Data Section, involved the following IAEA Fellows:

1. Fortunato AGUILAR HERNANDEZ (Mexico)
2. Vesselin LALOV (Bulgaria)
3. Abderrahmane MALKI (Algeria)
4. Muhammad ARSHAD (Pakistan)
5. Shafiqul Islam BHUIYAN (Bangladesh)
6. Riyanto RAHARJO (Indonesia)

The training program consisted of several informal lectures on ENDF/B formats and procedures, physical meaning of the input options used in NJOY for the generation of PENDF and GENDF files and practical computer exercises using the NJOY system. The version NJOY 89.31 was extensively used during that period by the Fellows to obtain experience in the use of NJOY to generate PENDF and GENDF files from ENDF/B-VI and JENDL-3 files for a few selected isotopes. A preliminary generation of 69 group constants in WIMS format was also attempted with some success for some light isotopes. It is planned to continue this training activity on NJOY in the future, depending on the level of interest from the developing countries and the availability of funds. One of the future activities of the Agency in the area of nuclear data processing will be to provide selected PENDF and GENDF files produced as a result of these training activities for free distribution to those who are interested to post-process such files to suit their specific application requirements. Such in-house fellowship training on NJOY is recognized as very useful to scientists even if they are interested to undertake only post-processing in their countries, where the resources are limited in terms of computer resources and manpower to undertake a complete NJOY computation starting from the basic evaluated data file.

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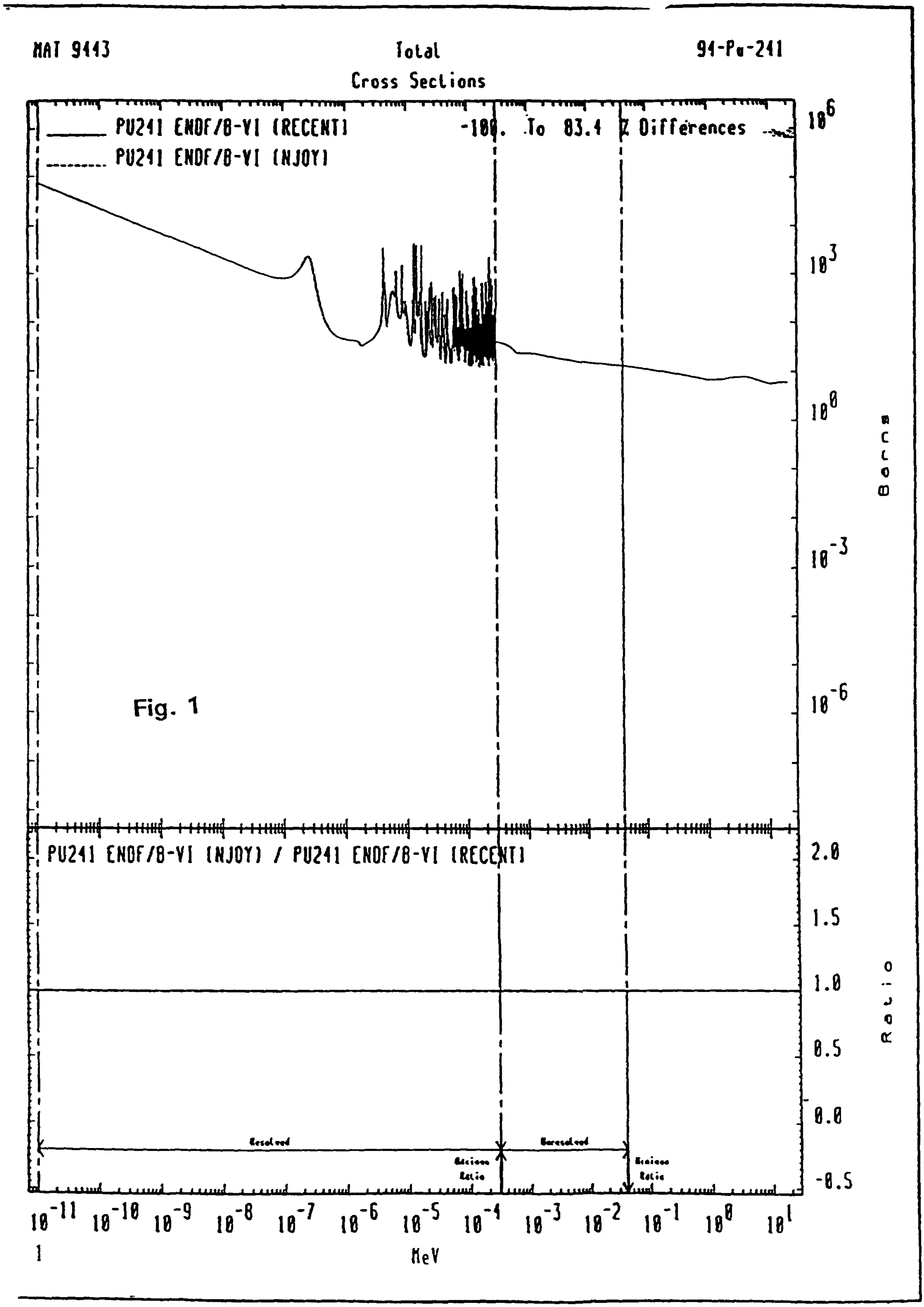
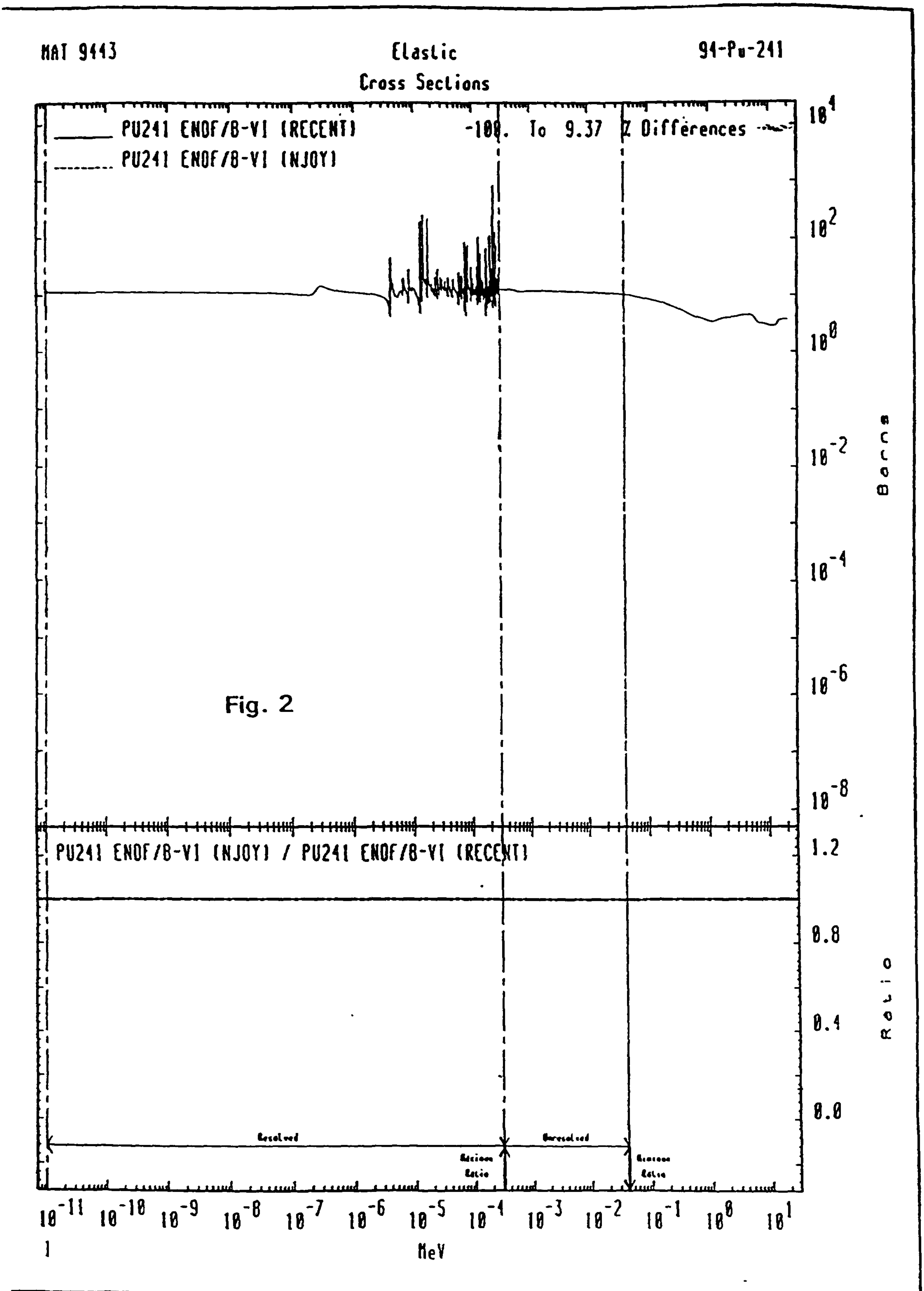

MAT 9443
Total
Cross Sections
94-Pu-241
PU241 ENDF/B-VI (RECENT)
PU241 ENDF/B-VI (NJOY)
-100. To 83.4 % Differences
10^6
10^3
10^0
10^-3
10^-6
Barns
PU241 ENDF/B-VI (NJOY) / PU241 ENDF/B-VI (RECENT)
2.0
1.5
1.0
0.5
0.0
-0.5
Ratio
10^-11 10^-10 10^-9 10^-8 10^-7 10^-6 10^-5 10^-4 10^-3 10^-2 10^-1 10^0 10^1
1
MeV

Fig. 1



MAT 9443
Elastic
Cross Sections
94-Pu-241
PU241 ENDF/B-VI (RECENT)
PU241 ENDF/B-VI (NJOY)
-100. To 9.37 % Differences
PU241 ENDF/B-VI (NJOY) / PU241 ENDF/B-VI (RECENT)
Resolved
Unresolved
Barns
Ratio
MeV

Fig. 2

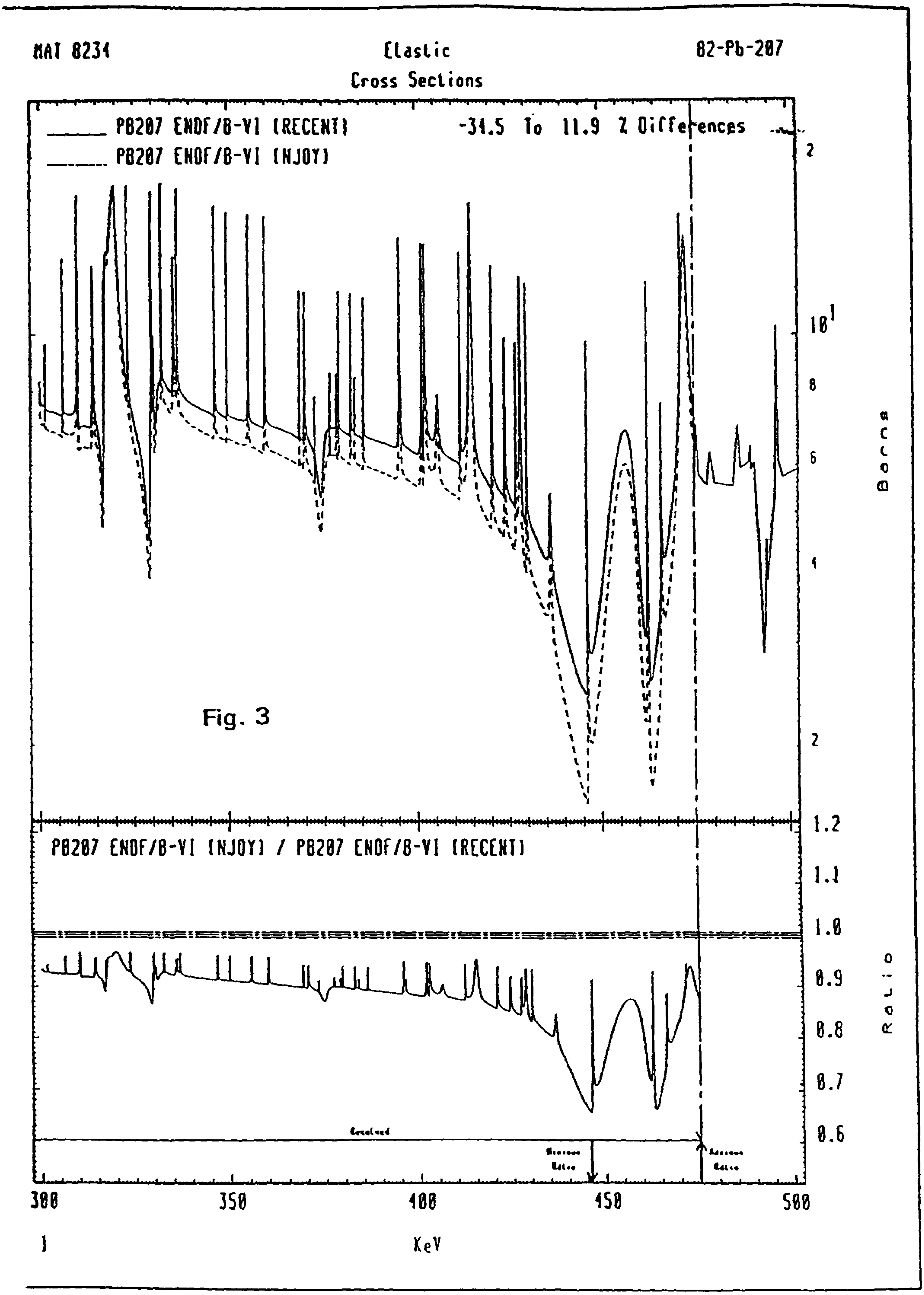

MAT 8234
Elastic
Cross Sections
82-Pb-207
PB207 ENDF/B-VI (RECENT)
PB207 ENDF/B-VI (NJOY)
-34.5 To 11.9 % Differences
PB207 ENDF/B-VI (NJOY) / PB207 ENDF/B-VI (RECENT)
Barns
Ratio
2
10^1
8
6
4
2
1.2
1.1
1.0
0.9
0.8
0.7
0.6
300
350
400
450
500
1
KeV

Fig. 3

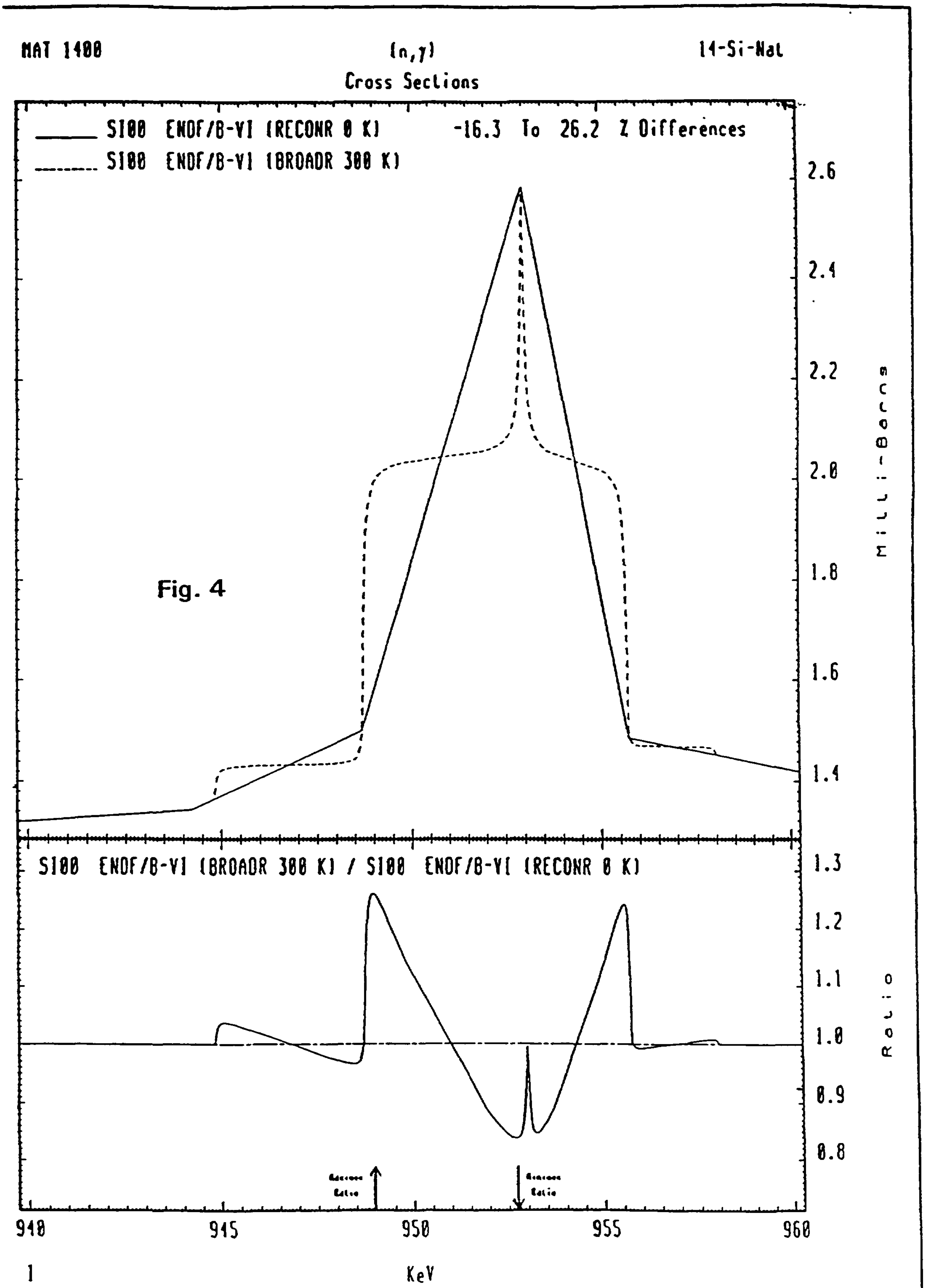

MAT 1400
(n,γ)
14-Si-Nat
Cross Sections
S100 ENDF/B-VI (RECONR 0 K)
-16.3 To 26.2 % Differences
S100 ENDF/B-VI (BROADR 300 K)
2.6
2.4
2.2
2.0
1.8
1.6
1.4
Milli-Barns
S100 ENDF/B-VI (BROADR 300 K) / S100 ENDF/B-VI (RECONR 0 K)
1.3
1.2
1.1
1.0
0.9
0.8
Ratio
940
945
950
955
960
1
KeV

Fig. 4

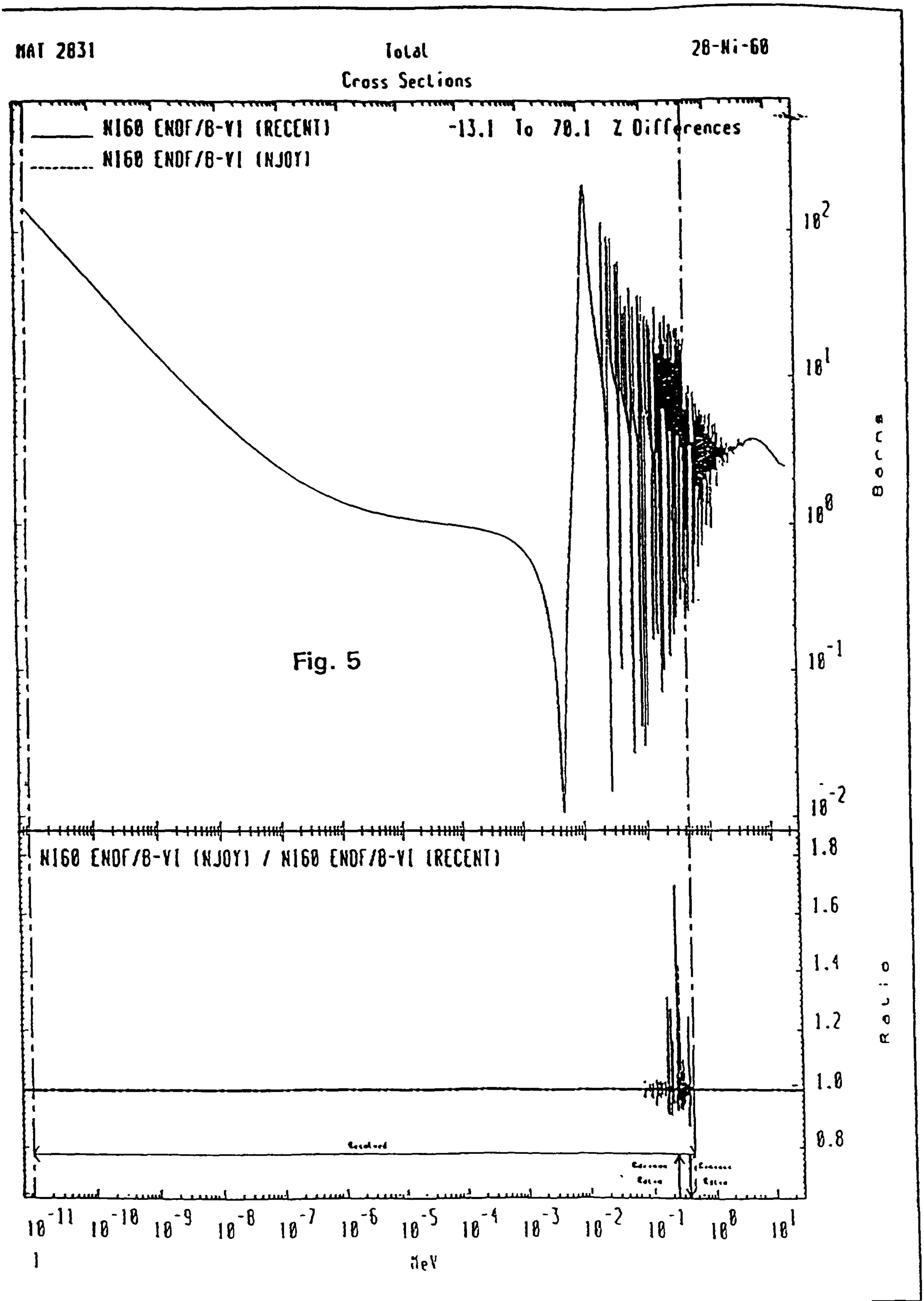

MAT 2831
Total
Cross Sections
28-Ni-60
NI60 ENDF/B-VI (RECENT)
NI60 ENDF/B-VI (NJOY)
-13.1 To 70.1 % Differences
Barns
NI60 ENDF/B-VI (NJOY) / NI60 ENDF/B-VI (RECENT)
Ratio
MeV

Fig. 5

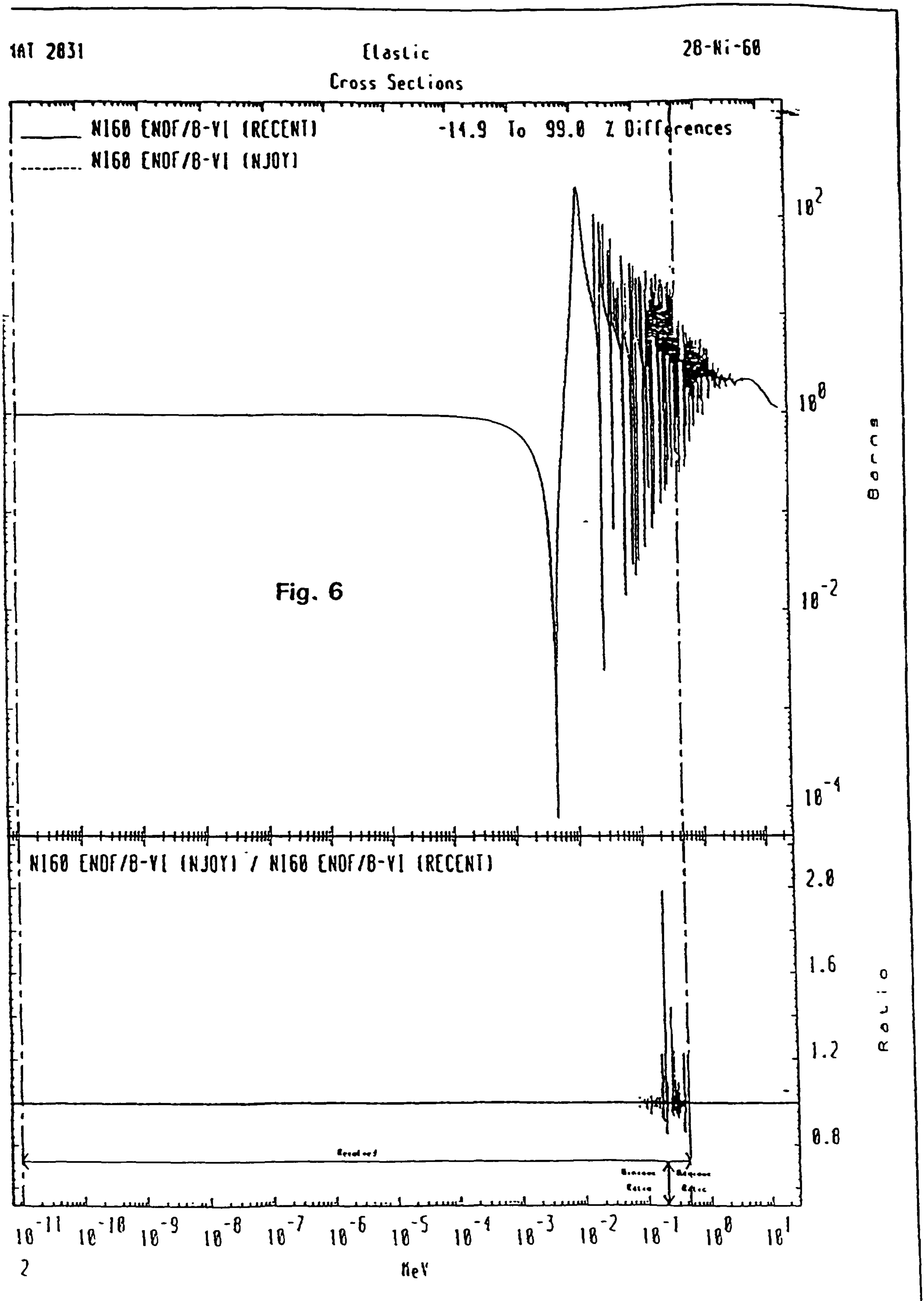

MAT 2831
Elastic
Cross Sections
28-Ni-60
NI60 ENDF/B-VI (RECENT)
NI60 ENDF/B-VI (NJOY)
-14.9 To 99.0 % Differences
10^{2}
10^{0}
10^{-2}
10^{-4}
Barns
NI60 ENDF/B-VI (NJOY) / NI60 ENDF/B-VI (RECENT)
2.0
1.6
1.2
0.8
Ratio
10^{-11} 10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1}
2
MeV

Fig. 6

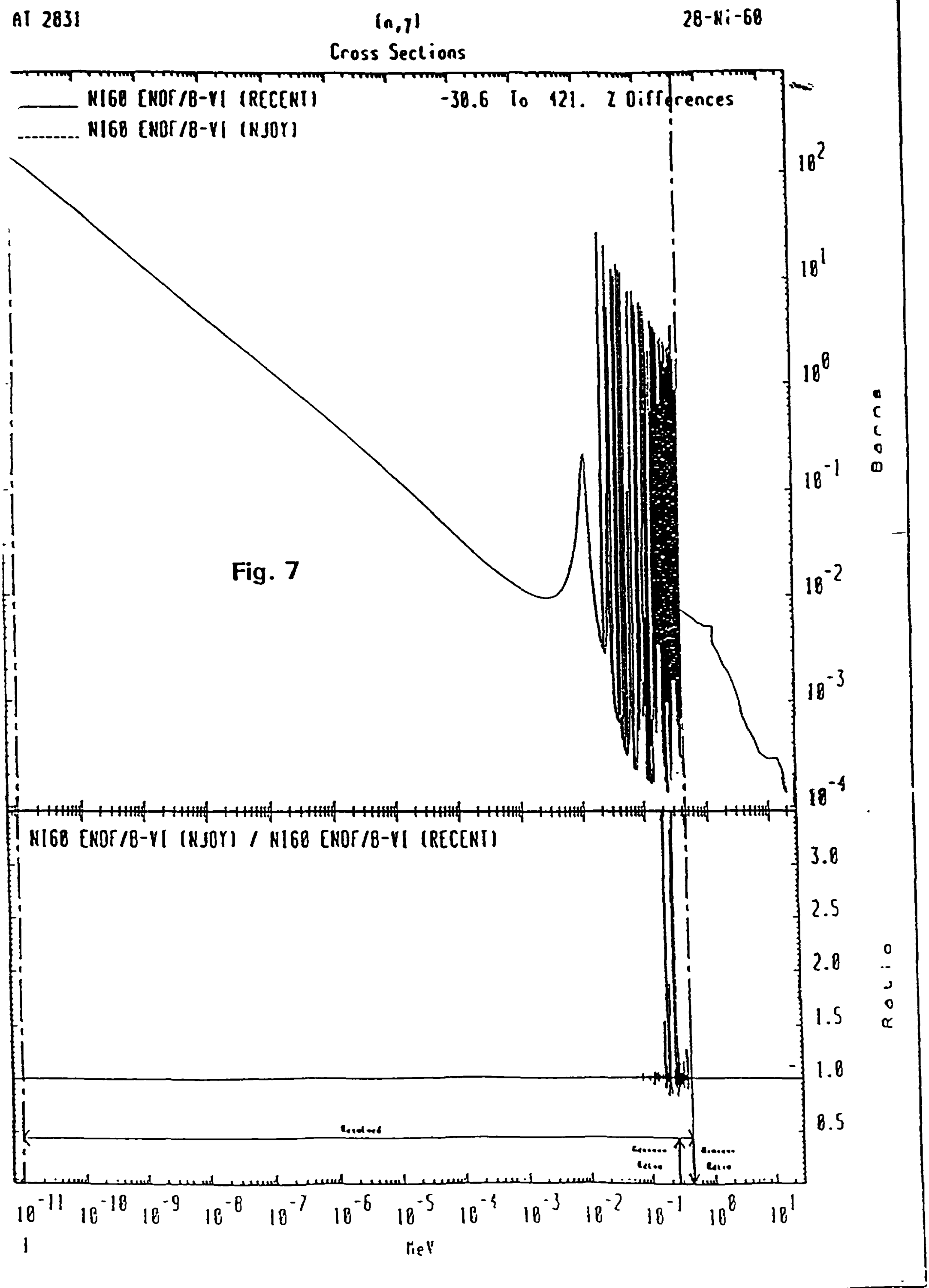
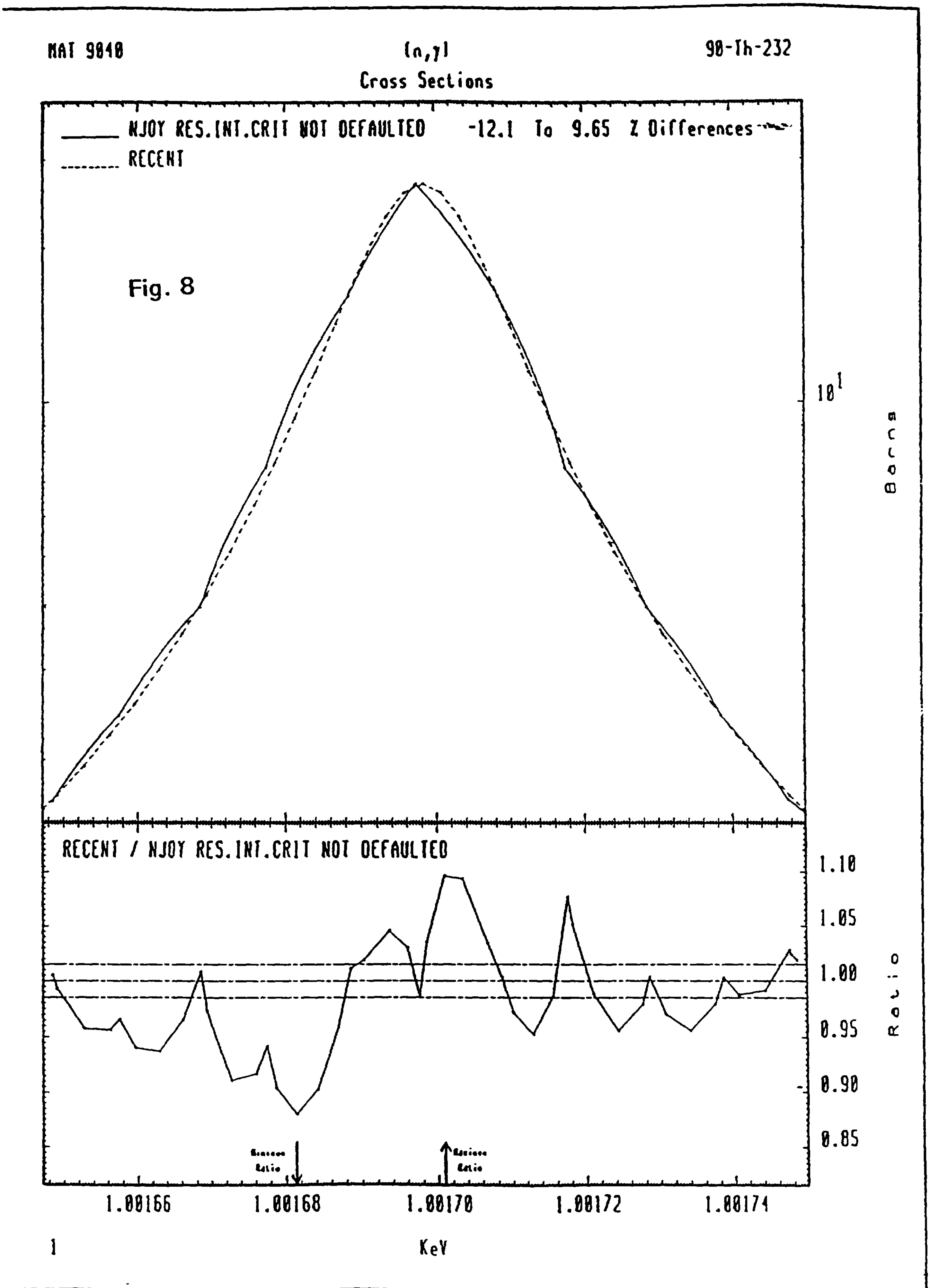

AT 2831
(n,γ)
Cross Sections
28-Ni-60
NI60 ENDF/B-VI (RECENT)
NI60 ENDF/B-VI (NJOY)
-30.6 To 421. % Differences
Barns
NI60 ENDF/B-VI (NJOY) / NI60 ENDF/B-VI (RECENT)
Ratio
Resolved
MeV

Fig. 7


MAT 9040
(n,γ)
90-Th-232
Cross Sections
NJOY RES.INT.CRIT NOT DEFAULTED -12.1 To 9.65 % Differences
RECENT
Fig. 8
10¹
Barns
RECENT / NJOY RES.INT.CRIT NOT DEFAULTED
1.10
1.05
1.00
0.95
0.90
0.85
Ratio
1.00166
1.00168
1.00170
1.00172
1.00174
1
KeV

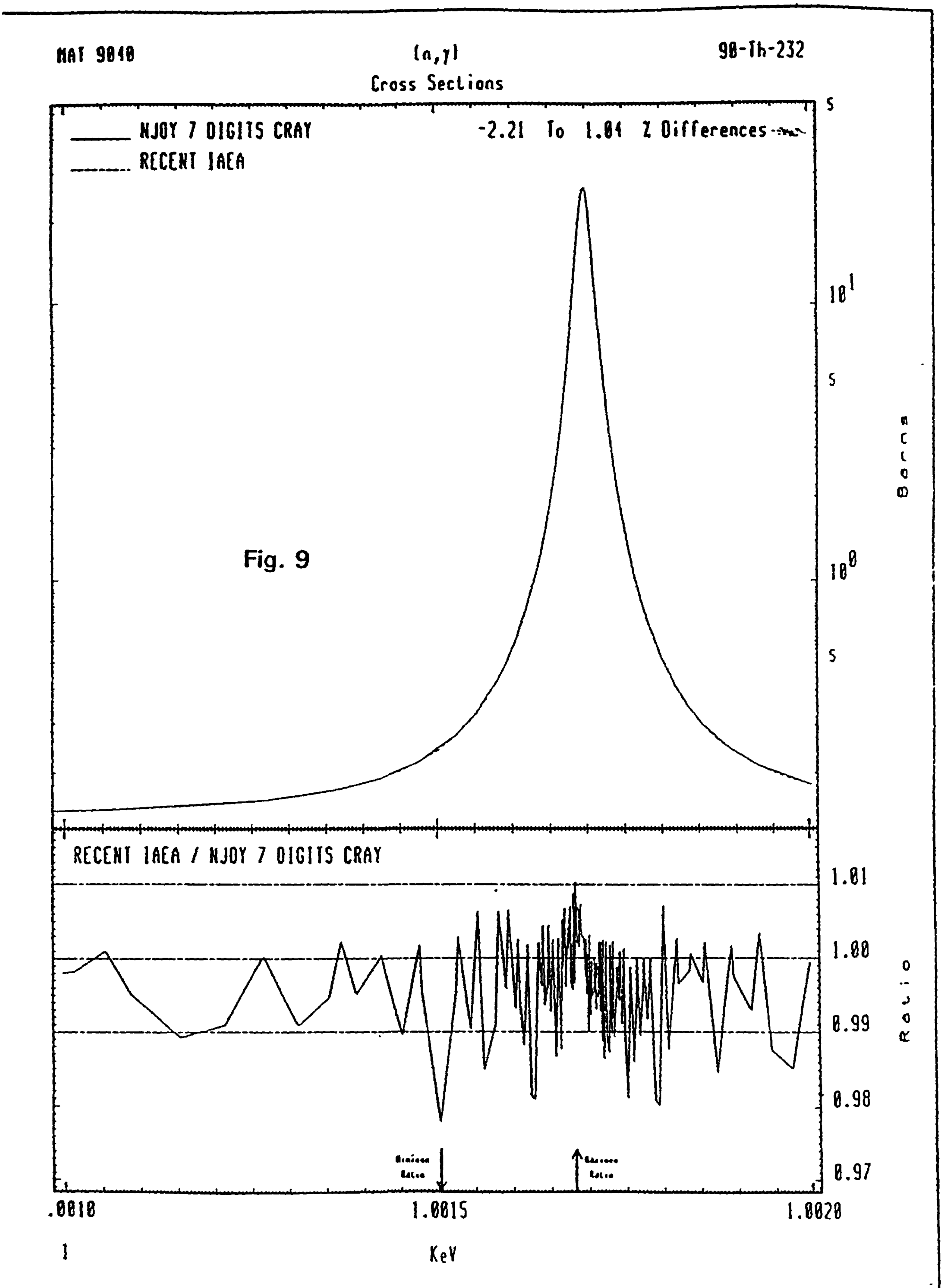

MAT 9040
(n,γ)
90-Th-232
Cross Sections
NJOY 7 DIGITS CRAY
RECENT IAEA
-2.21 To 1.04 % Differences
10^1
5
10^0
5
Barns
RECENT IAEA / NJOY 7 DIGITS CRAY
1.01
1.00
0.99
0.98
0.97
Ratio
.0010
1.0015
1.0020
1
KeV

Fig. 9

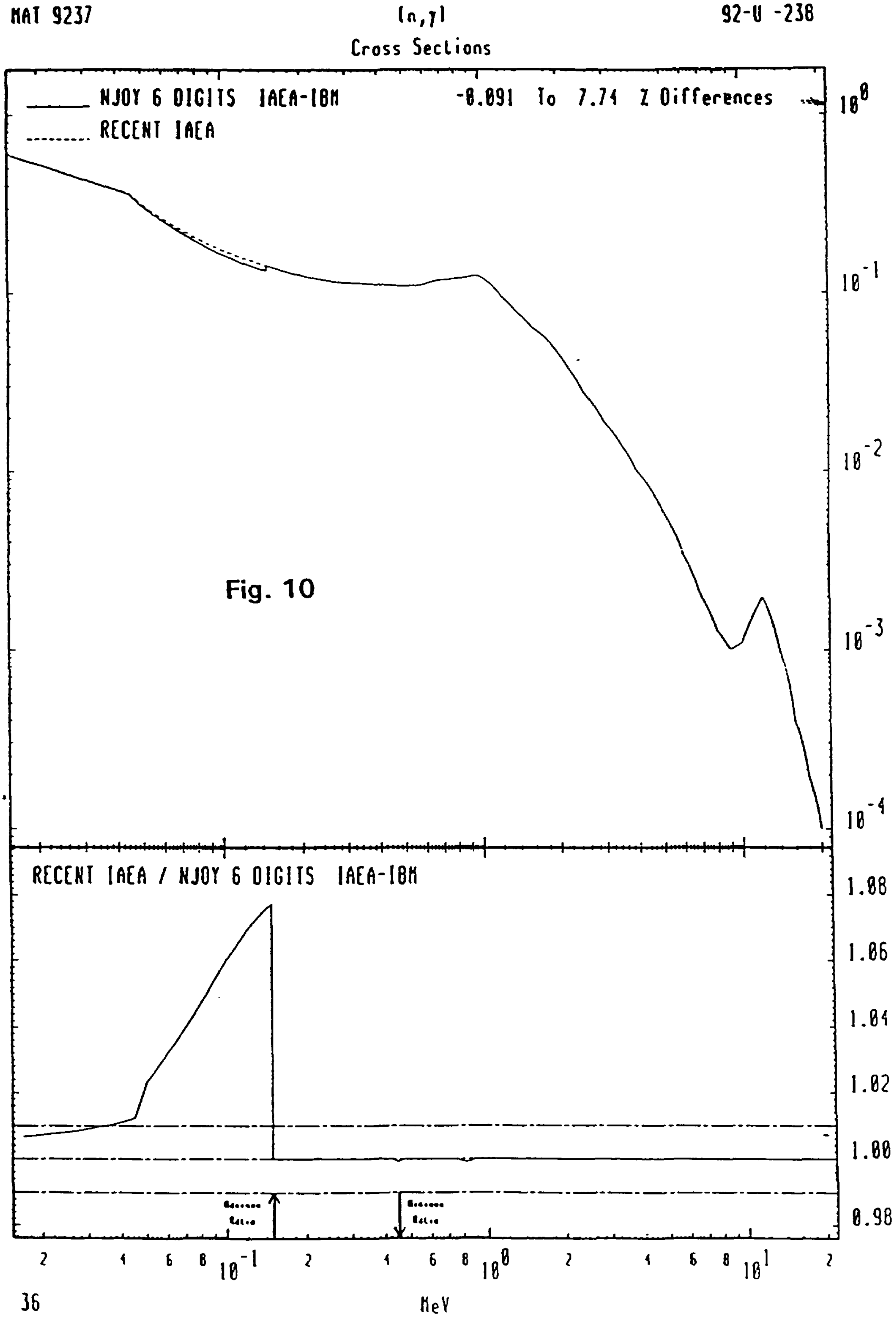

MAT 9237
(n,γ)
92-U -238
Cross Sections
NJOY 6 DIGITS IAEA-10M
RECENT IAEA
-0.091 To 7.74 % Differences
10^0
10^-1
10^-2
10^-3
10^-4
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-10M
1.08
1.06
1.04
1.02
1.00
0.98
Ratio
2 4 6 8 10^-1 2 4 6 8 10^0 2 4 6 8 10^1 2
MeV

Fig. 10

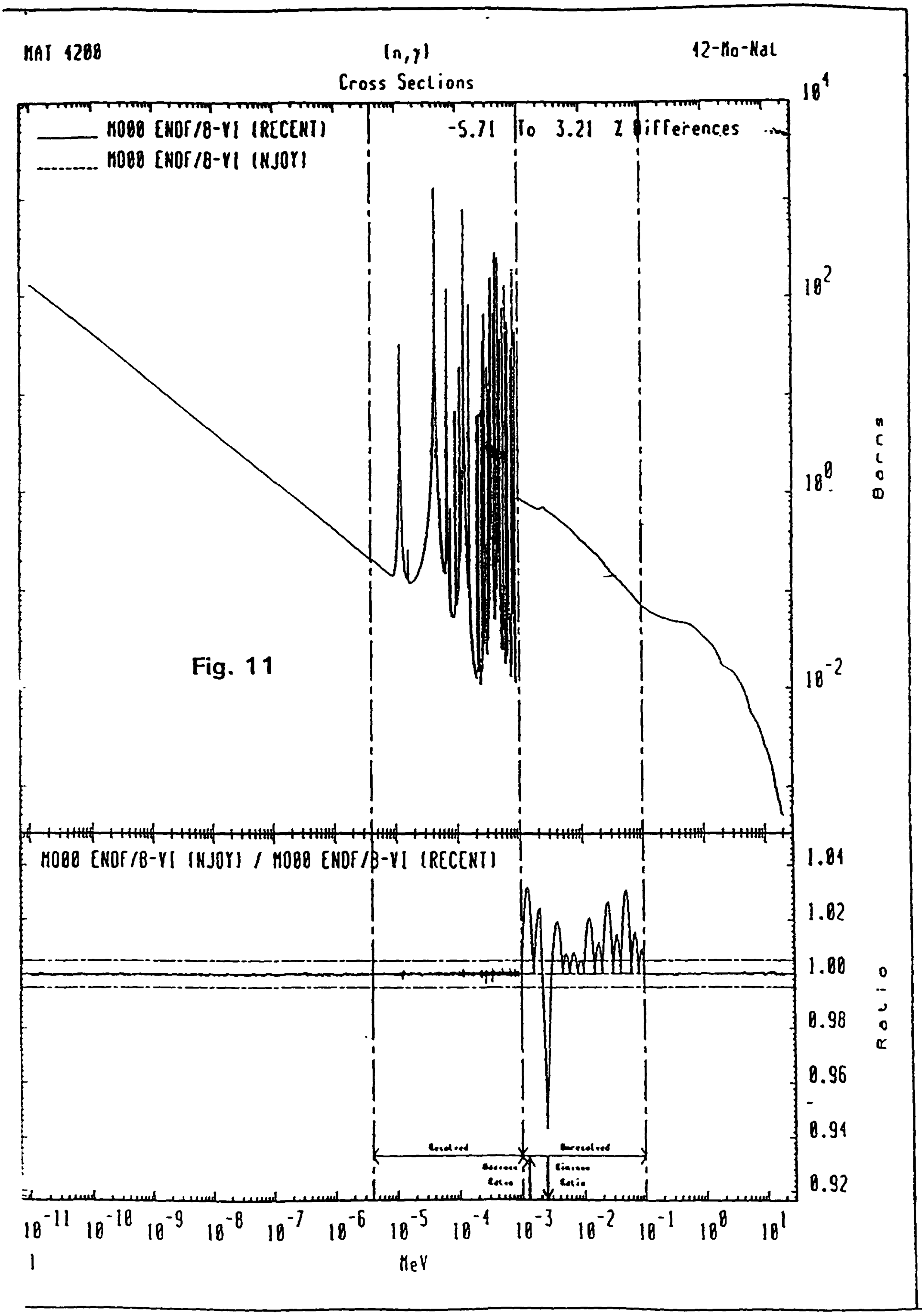

MAT 4200
(n,γ)
42-Mo-Nat
Cross Sections
M000 ENDF/B-VI (RECENT)
M000 ENDF/B-VI (NJOY)
-5.71 To 3.21 % Differences
Barns
M000 ENDF/B-VI (NJOY) / M000 ENDF/B-VI (RECENT)
Ratio
Resolved
Unresolved
MeV

Fig. 11

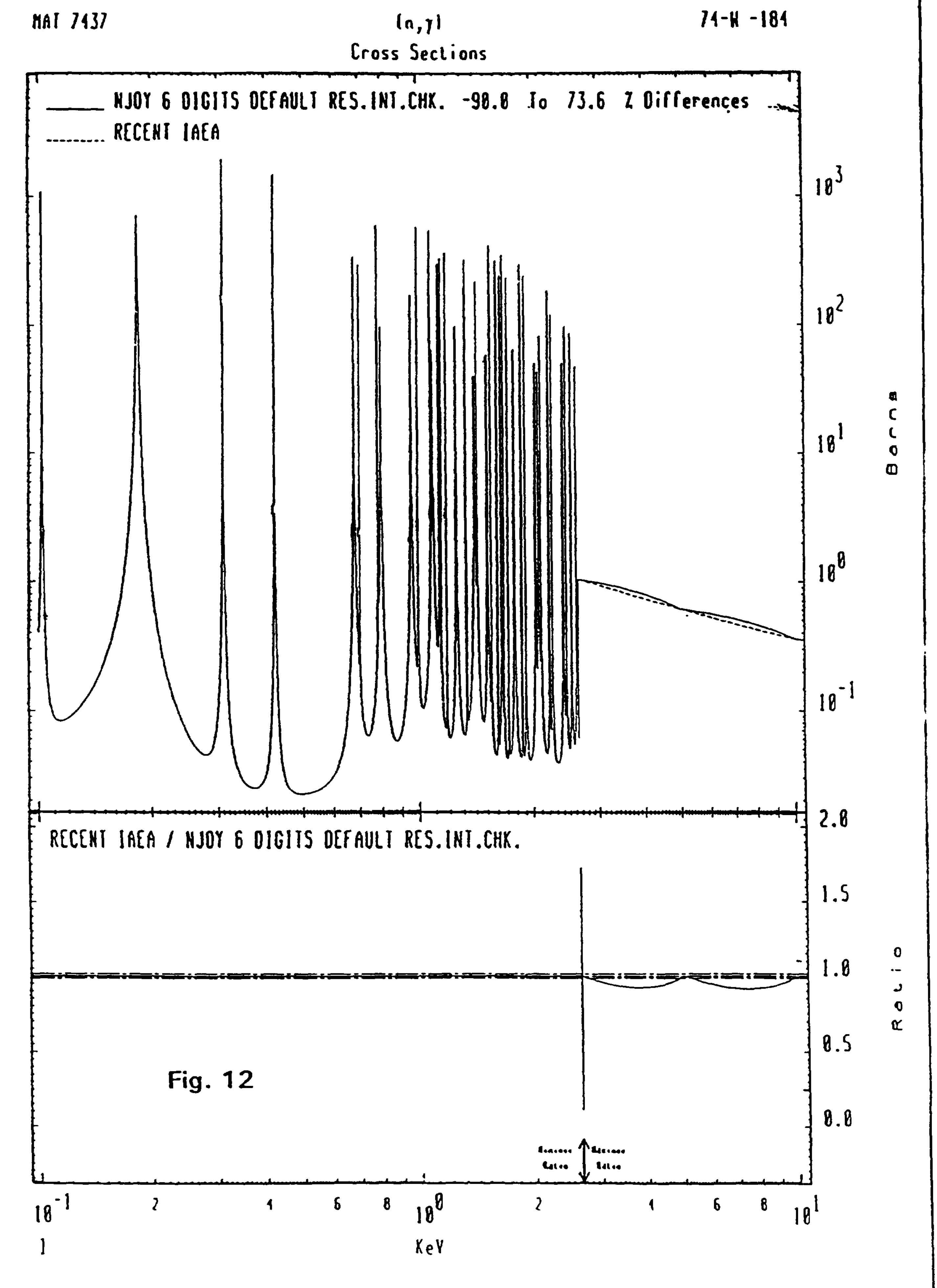

MAT 7437
(n,γ)
74-W -184
Cross Sections
NJOY 6 DIGITS DEFAULT RES.INT.CHK. -98.8 To 73.6 % Differences
RECENT IAEA
Barns
RECENT IAEA / NJOY 6 DIGITS DEFAULT RES.INT.CHK.
2.0
1.5
1.0
0.5
0.0
Ratio
KeV

Fig. 12

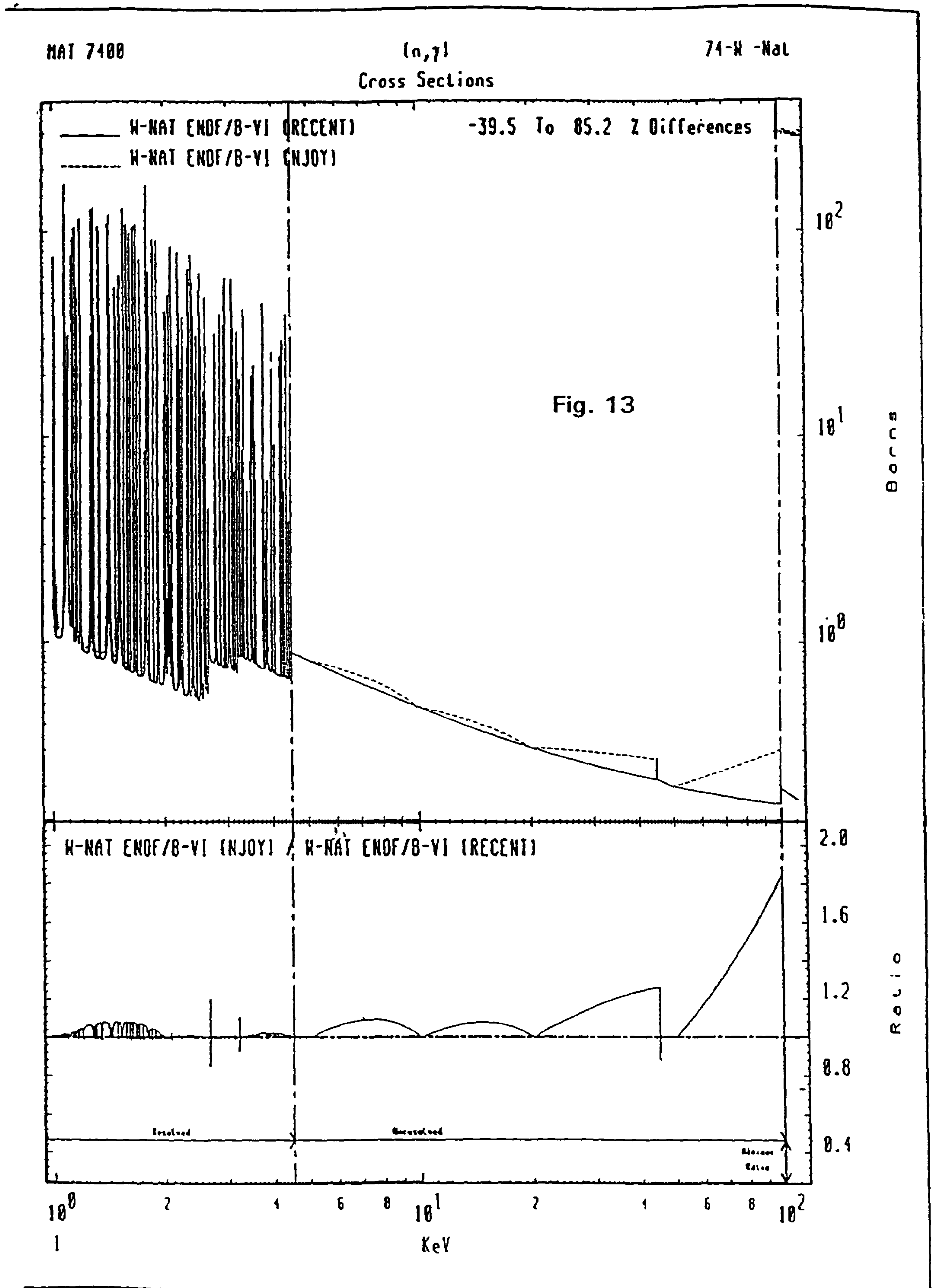

MAT 7400
(n,γ)
74-W -Nat
Cross Sections
W-NAT ENDF/B-VI (RECENT)
W-NAT ENDF/B-VI (NJOY)
-39.5 To 85.2 % Differences
W-NAT ENDF/B-VI (NJOY) / W-NAT ENDF/B-VI (RECENT)
10^2
10^1
10^0
Barns
2.0
1.6
1.2
0.8
0.4
Ratio
10^0
2
4
6
8
10^1
2
4
6
8
10^2
1
KeV

Fig. 13

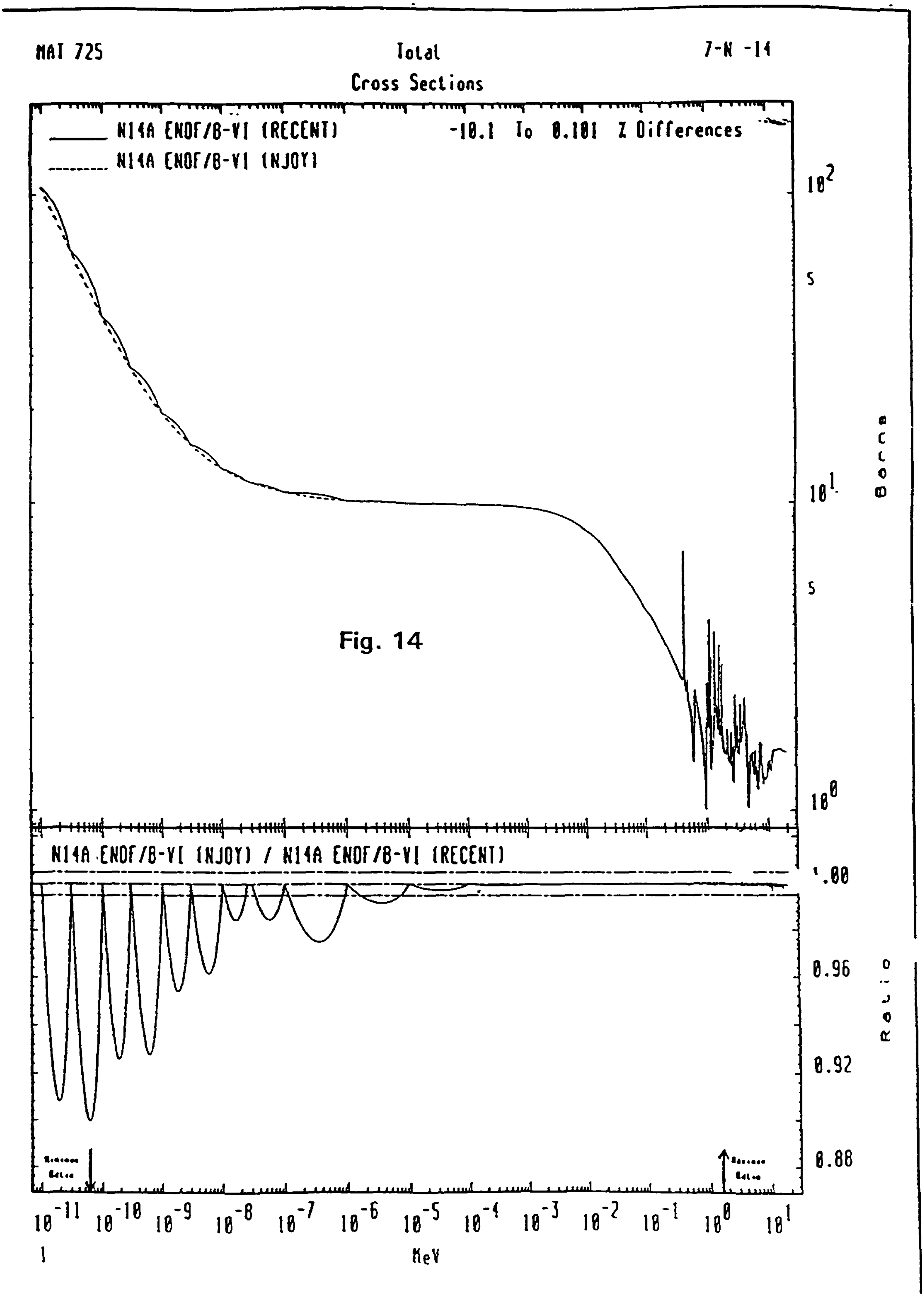
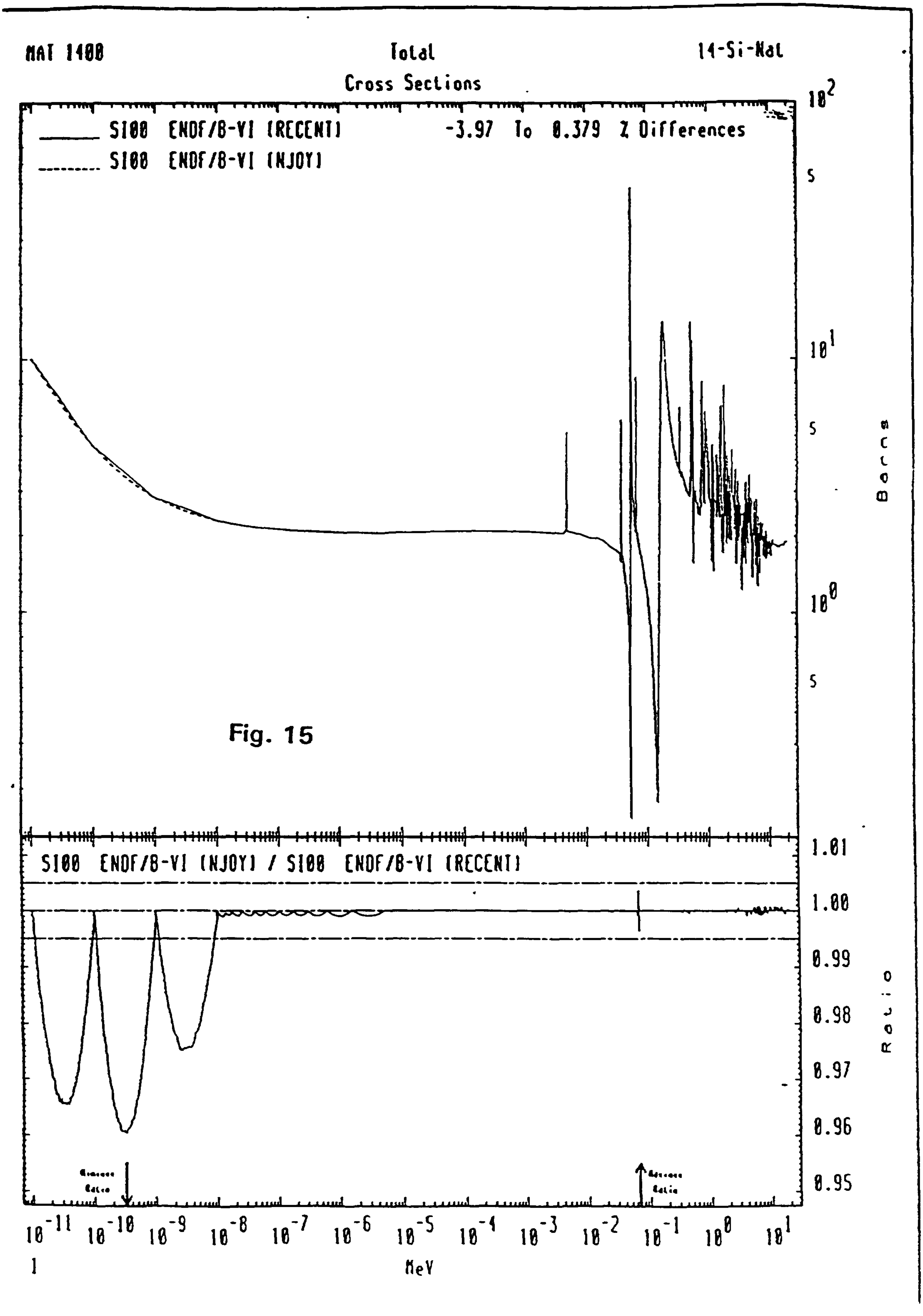

MAT 725
Total
Cross Sections
7-N -14
N14A ENDF/B-VI (RECENT)
N14A ENDF/B-VI (NJOY)
-10.1 To 0.101 % Differences
N14A ENDF/B-VI (NJOY) / N14A ENDF/B-VI (RECENT)
Barns
Ratio
MeV

Fig. 14



MAT 1400
Total
Cross Sections
14-Si-Nat
S100 ENDF/B-VI (RECENT)
-3.97 To 0.379 % Differences
S100 ENDF/B-VI (NJOY)
S100 ENDF/B-VI (NJOY) / S100 ENDF/B-VI (RECENT)
Barns
Ratio
MeV

Fig. 15

International Workshop on Nuclear Data for Fusion Reactor Technology

Del Mar, California, U.S.A
3-6 May 1993

Current Status of Production of Coupled Neutron-photon Multigroup Cross Section Libraries of FENDL for Use in Fusion Neutronics Calculations

by

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E-Mail (Earn-Bitnet): RNQ@IAEA1

Abstract: Selected neutron reaction nuclear data libraries and photon-atomic interaction cross section libraries for elements of interest to the IAEA's program on Fusion Evaluated Nuclear Data Library (FENDL) have been processed into GENDF and further into MATXS format using the NJOY system on the VAX4000 computer of the IAEA. The FENDL multigroup library may be post-processed using TRANSX to produce cross section tables compatible with many discrete-ordinates (S_N) and diffusion codes for neutron, photon or coupled transport for fusion neutronics calculations. The paper briefly describes the data processing actvities within the scope of the FENDL project of the Agency, lists the multigroup data libraries generated thus far at the Agency, and, presents an account of current and planned future data testing activities. All the multigroup data generated thus far at the Agency in the form of GENDF and MATXS files are available cost-free upon request from the IAEA Nuclear Data Section.

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1. INTRODUCTION AND BACKGROUND

The IAEA Nuclear Data Section, in co-operation with several national nuclear data centers and research groups, is creating an internationally available Fusion Evaluated Nuclear Data Library (FENDL), which will serve as a comprehensive source of processed and tested nuclear data tailored to the requirements of the Engineering and Development Activities (EDA) of the International Thermonuclear Experimental Reactor (ITER) Project and other fusion-related development projects (see for example refs.1-10) .

The FENDL activity [11-16] is supported by several IAEA Coordinated Research Programs. A series of international meetings in 1986, 1987, 1989, 1990, 1991 and 1992 and projected to continue with about the same frequency in the next few years, has been organized by the International Atomic Energy Agency with the goal of assembling, processing and testing a comprehensive, fusion-relevant Fusion Evaluated Nuclear Data Library with unrestricted international distribution. The fusion data experts at these meetings have addressed in detail, a. the nuclear data requirements and status of available nuclear data for integral calculations for blanket, shielding, and activation problems in fusion reactors; b. status of differential data, theory and possibilities to meet data needs; c. the creation of International fusion nuclear data file, and, d. IAEA sponsored international comparison of benchmark measurements and calculations in the subject of fusion neutronics.

FENDL library is composed of the several sublibraries describing the transport of both the plasma-source neutrons and secondary gamma rays through fusion reactor components, as well as the resulting radiation effects, such as nuclear heating, tritium breeding, activation and material damage. Also included are cross sections for fusion and other important charged-particle nuclear reactions of the plasma constituents, as well as data for fusion-relevant neutron dosimetry. The sublibraries of FENDL are:

1. Coupled 175-group neutron - 42-group gamma cross section sets (VITAMIN-J structure) processed with the NJOY system for neutron and gamma-ray transport calculations for 65 elements and isotopes of primary interest.

2. The most important neutron activation cross sections for the estimation of radiation hazards.

3. Charged particle nuclear reaction cross sections of the D-T plasma constituents p, d, T, ^{3}He and ^{4}He.

4. Fusion relevant neutron dosimetry cross sections.

This paper deals mainly with the tasks related to the production and testing of item 1 mentioned above. Within the scope of the FENDL project, the International Atomic Energy Agency is committed to a program of nuclear data processing activities in order to create a modern and internationally available Fusion Evaluated Nuclear Data Library(FENDL). The nuclear data processing code system NJOY developed at Los Alamos National Laboratory, USA [17] with all modifications and improvements as available is employed in this study. Selected neutron interaction libraries and photon-atomic interaction cross section libraries for elements of interest to the IAEA's program on FENDL retrieved from basic evaluated data files ENDF/B-VI, JENDL-3.1 and BROND-2, have been processed into "MATXS" format using the NJOY system on the VAX4000 computer of the IAEA. The paper briefly describes the data processing actvities within the scope of the FENDL project of the Agency, lists the multigroup data libraries generated thus far at the Agency, and, presents an account of current and planned future data testing activities.

2. SOURCE OF BASIC DATA FOR FENDL AND CURRENT STATUS OF PROGRESS IN PROCESSING

With the welcomed release [18] of ENDF/B-VI, JENDL-3.1, BROND-2, CENDL-2 and JEF-2, the FENDL project has turned from its earlier emphasis on the review and selection of candidate neutron-interaction evaluations to (a) processing the basic evaluated data files into MATXS format and integral testing of multigroup cross sections for neutrons and gamma-ray transport and (b) assembling, processing and testing of large special-application files to supplement the available files especially in the field of activation and decay data. Another paper [10] presented at this workshop deals with the status of data in the evaluated files for the most important neutron reactions in fusion materials.

The Consultants Meeting [20] organized by the IAEA and held in Vienna during 25-28 June 1990 on "First Results of FENDL-1 Testing and Start of FENDL-2" performed a critical review of FENDL-1 general purpose evaluations identified at previous meetings and summarized its recommendations for the selected candidate evaluations for various FENDL materials. The status of the evaluations already identified for FENDL-1 was reviewed, with particular attention directed at the completeness of the files. In particular, the data files for each material was checked for the presence of gamma-ray production data (cross sections and spectra), correlated energy-angle emission data (MF=6), specification of energy spectra for secondary charged particles, presence of complete covariance data, and consistency of the cross section data with evaluations chosen for the FENDL-1 activation and dosimetry files.

Additionally, comments were solocited and assembled regarding any known or suspected problems in the files. The complete reults of this recommendation is reproduced in Table 1 of Appendix I. The meeting also took into account the recommendation made at the ITER Specialists' Meeting on Shielding calculations held at Garching, 12-14 February 1990, that eight additional materials (Na, Mg, P, S, Cl, K, Ca and Ta) be added to the FENDL-1 library. The Consultants Meeting identified evaluations to satisfy this recommendation as presented in Table 2 of Appendix I together with comments similar to Table 1. Following these expert recommendations, the coupled neutron-gamma data files for elements and isotopes of FENDL are to be derived from ENDF/B-VI, JENDL-3.1 and BROND-2 for the following materials:

NEUTRON INTERACTION AND PHOTON PRODUCTION CROSS SECTIONS:

ENDF/B-VI: ^{1}H, ^{3}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, C, ^{14}N, ^{16}O, ^{19}F, P, S, Cl,

K, ^{55}V, $^{50,52\text{-}54}Cr$, ^{55}Mn, $^{54,56\text{-}58}Fe$, ^{59}Co, $^{58,60\text{-}62,64}Ni$,

$^{63,65}Cu$, $^{134\text{-}138}Ba$, $^{182\text{-}184,186}W$, $^{206\text{-}208}Pb$.

JENDL 3.1: ^{23}Na, Mg, ^{27}Al, Ca, Ti, ^{55}Mn, Mo, ^{181}Ta, ^{209}Bi.

BROND-2: ^{2}H, ^{14}N, ^{15}N, Si, $^{90\text{-}92,94,96}Zr$, ^{93}Nb, Sn.

PHOTON-ATOMIC INTERACTION CROSS SECTIONS

ENDF/B-VI: H, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zr, Nb, Mo, Sn, Ba, Ta, W, Pb, Bi.

The basic evaluated data ENDF/B-VI, JENDL-3.1 and BROND-2 are drawn from the basic libraries available from the NDS [18]. Photon-atomic interaction cross sections of ENDF/B-VI [19] was selected for ALL of the materials in the neutron interaction data.

2.1 On the use of the NJOY code system in the FENDL project

The NJOY system [17] has been under continuous development at the Los Alamos National Laboratory since 1974. During the last 16 years it has gone through a number of revisions, in response to the development of new ENDF formats, in order to add new processing capabilities, in response to changing computer systems and in order to fix errors. It should be noted that the NJOY code system is, by necessity, complex and large with over 65000 lines of Fortran instructions. NJOY has been widely used around the world in many leading laboratories and has served successfully as a general-purpose link between ENDF-formatted evaluated nuclear data files and important applications such as shield design, thermal-reactor core design, fusion-reactor blanket design, radiotherapy facility design and many others. A retrieval search, performed by the author, of bibliography from International Nuclear Information System showed that over 150 papers/reports dealing with applications using NJOY have been published and made available as entries in INIS at the time of writing this paper. The part of the FENDL project which is directed towards creating a coupled neutron gamma multigroup libarary enjoys therfore the major advantage of employing the widely used NJOY code system which has been checked in a variety of applications.

2.2 Verification of the accuracy of calculated line shapes at zero Kelvin.

The IAEA Nuclear Data Section is commited to the creation and distribution of FENDL multigroup library in the best possible form that can be described as one with the best quality keeping the errors in processing of the basic evaluated data to the minimum. A comparative study has been made between the zero kelvin cross section line shapes generated by the IAEA preprocessing codes [21] and the latest version of NJOY (i.e NJOY91.38) obtained from the Radiation Shielding and Information Center (RSIC), USA, for several materials from ENDF/B-VI. This intercomparison study is briefly described in Appendix II. Significant differences were found in the elastic cross sections calculated for the isotopes of Cr, Ni etc. The discrepancies were brought to the attention of the author of NJOY in mid 1992. The Nuclear Data Section of the agency has, in the mean time, used LINEAR / RECENT / FIXUP (LRF) benchmark Codes to obtain the zero kelvin line shapes as described in Appendix II. These pre-processed files were then processed by the complete NJOY system. At the time of writing this report, as described in Appendix II, both the RECONR module of NJOY and RECENT have now been independently updated and the results intercompared to assure that they are now both properly processing the ENDF/B-VI data for all the FENDL materials [23,24].

2.3 Current status of production of GENDF and MATXS files

The specifications of multigroup processing and the card image of the actual input deck used in the NJOY runs are presented in Appendix III. At the time of writing this report, production of all the 'point' ENDF i.e. files in 'PENDF' format, all the 'group' ENDF i.e. files in 'GENDF' format and in 'MATXS' format for all above mentioned nuclides except ^{19}F from ENDF/B-VI, and, ^{2}H ^{14}N, ^{93}Nb and Sn from BROND-2 have been generated. Note that the coupled library i.e. the 'MATXS' files (P-5 neutron interaction, photon production and photon interactions) derived from the neutron interaction cross section files of ENDF/B-VI, JENDL-3.1 and BROND-2 uses ENDF/B-VI for photon interaction data.

The following five different multigroup files are available for each isotope:

GENDF Formatted files:

1. GENDF files for neutron interaction cross sections and photon production cross section data (output of GROUPR module).

2. GENDF files for photon interaction cross section data (output of GAMINR module).

'MATXS' formatted files:

The above mentioned GENDF files have been post-processed into 'MATXS' format. Generated and made available are the following three types of multigroup data files in MATXSR format.

3. Photon interaction cross section data, P-8 Legendre order, 42 energy groups in

VITAMIN-J group structure derived from ENDF/B-VI for all the FENDL elements mentioned in the text.

4. Neutron interaction cross section data and photon production cross section data, P-5 Legendre order, 175 energy groups in VITAMIN-J group structure derived from ENDF/B-VI, JENDL-3.1 or BROND-2.

5. A coupled neutron-gamma, 175 neutron -42 photon groups, P-5 Legendre order, for neutron interaction cross section data derived from ENDF/B-VI, JENDL-3.1 or BROND-2, and, photon production cross section data and photon interaction cross section data derived from ENDF/B-VI.

The details of sizes of these files are given in Appendix IV. The code TRANSX 2.0 (ref. 22), for instance, serves to interface MATXS cross section libraries to nuclear transport codes such as ANISN. TRANSX reads nuclear data from a library in MATXS format and produces transport tables compatible with many discrete-ordinates (S_N) and diffusion codes. The FENDL multigroup library may be post-processed using TRANSX to produce tables for neutron, photon or coupled transport for specific application calculations.

Presently MATXSR module of NJOY does not permit the use of different Legendre orders for neutrons and photons. Users interested to maintain a higher Legendre order for photon interactions in their neutronic calculations may have to perform a photon source term calculations using P-5 'MATXS' files for neutron interactions and photon production and follow it up with a P-8 calculation for photon transport subsequently.

Currently, efforts towards production of a point library for use in Monte-Carlo code, in particular the MCNP code, have not yet been made due to limitation of resources, and due to the fact that both the ACER module of NJOY which formats the point data for MCNP and the MCNP code themselves are under continuous development.

3. FUTURE TASKS AND ADDITIONS TO PROCESSING TASKS IN THE FENDL PROJECT :

As pointed out earlier, the FENDL multigroup library should be post-processed by codes such as TRANSX to generate problem-dependent multigroup cross section tables for specific mixtures for input to neutronic codes such as ANISN, DOT 3.5 etc. While it is considered that the task of generation of multigroup library is completed to a considerable extent, it can be certified that the FENDL multigroup library is usable in fusion neutronics, including applications to practical design calculations such as in ITER only after successful analysis of several fusion related experimental and calculational benchmarks. In order to accelerate the process of integral testing of FENDL multigroup library, the multigroup library for a few selected high priority isotopes have been sent to a few interested colleagues. The feedback and contributions of members of several laboratories (**H.MAEKAWA** and **J. PULPAN**, FNS, JAERI, **J.E. WHITE**, ORNL, USA, **U. FISCHER**, KFK, Germany, **G. C. PANINI**, ENEA, Italy, **S. PELLONI**, Switzerland, and many others) who have started to check the FENDL multigroup library for consistency and its usability in fusion neutronic calculations will be very useful in thios regard. The photon production cross sections may be a problem in the GENDF and MATXS files for some of the isotopes as per the preliminary observation by J.E. White and J. Pulpan. The task of generation of multigroup library has been automated on the VAX4000 system at the Agency so that the repeat runs of NJOY can be done if necessary for any specific isotope in a very user-friendly manner. Future updates to the GENDF and MATXS files, if any, will be announced depending on the need to update FENDL multigroup library, based on feedback from the users of FENDL. Suggestions are most welcome. The task of generation of multigroup library can be said to have been completed only after the users certify that the FENDL multigroup library is usable in fusion neutronics calculations. This stage is expected to be reached in the near future.

During the IAEA Advisory Group Meeting [13] on "FENDL-2 and associated benchmark calculations," held in Vienna during 18-22 November 1991, the discussions which were held with the representatives of CENDL, JENDL, EFF, BROND and ENDF/B showed that, for several materials, new evaluations will become available for consideration for the next version of FENDL, i.e. FENDL/E-2. These materials are presented in Table 1 of Appendix V, along with the sources of new evaluations. For these additional evaluations, the generation of multigroup library using NJOY is planned to be carried out at the Agency in the near future. In addition to this list, W. Daenner and Y. Gohar provided a list of prioritized user needs for information identified as deficient in FENDL/E-1. This list is presented in Table 2 of Appendix V.

4. BENCHMARK EXPERIMENTS AND DATA TESTING OF FENDL

Much work is being reported [see, for example, refs. 25-49] on a large number of experimental and calculational benchmarks to validate the predictional capability of fusion neutronics methods and nuclear data. The IAEA Advisory Group Meeting (AGM) on "Nuclear Data for Neutron Multiplication in Fusion-Reactor First-Wall and Blanket Materials" held at Chengdu, China, 19-21 November 1990 endorsed the specifications of multigroup processing including the provision of self-shielding factors in the library. The working group [31] discussed the data processing issues and endorsed that the FENDL multigroup library be distributed in BCD (card-image) form as single-isotope (or material) NJOY group output (GENDF) and NJOY continuous-energy output (ACER). It will be left to the user to perform calculations to assemble working libraries in smaller number of energy groups if needed on their local computers. Presently, as results of this processing activity, both GENDF and the MATXS libraries have been generated and the FENDL multigroup library is thus available in GENDF as well as in MATXS format.

The fusion experts of the IAEA AGM held at Chengdu [31] have recommended the following. The IAEA should organize a data testing activity within the FENDL programme. The data testing activity should include the compilation and publication of complete specifications of fusion-relevant benchmark experiments. These specifications should include a complete description of the experiment, the measured results and the measurement uncertainties. In addition, it has been recommended that such a benchmark specification include a simple-geometry approximation to the actual, usually 3-dimensional, geometry of the experiment, together with the measured results "corrected" to equivalent values expected for direct measurements on the simple-geometry model. The specifications of Pb, Be and Fe experimental benchmarks submitted to the Agency by H. Maekawa on a diskette are available for distribution from the IAEA Nuclear Data Section upon request. The fusion experts of the IAEA AGM held at Chengdu [31] have recommended that the analysis of the documented benchmarks be organized as a sub-group of the FENDL activity.

ACKNOWLEDGEMENT

A large number of people have participated and/or are continuing to participate in this huge task of generation of multigroup library. **The following list is by no means complete.** In particular, the author of this documentation wishes to express his sincere thanks to **D.W. MUIR**, (Los Alamos National Laboratory, USA) for his excellent guidance and active participation in this task until he left the Nuclear Data Section of the Agency in May 1992. The valuable guidance and consultancy services from the author of NJOY, **R.E. MaCFARLANE**, (Los Alamos National Laboratory, USA) when problems developed during processing of the files at various stages are gratefully acknowledged with thanks.

Many persons have participated in the verification of the accuracy of processing of basic evaluated data files which greatly helped to assure quality control in the generation of zero Kelvin line shapes and the Doppler broadened cross section line shapes. In particular, the author of this documentation would like to thank **Red CULLEN** (Lawrence Livermore National Laboratory), USA, for his valuable contributions and guidance.

Many verification calculations for zero Kelvin line shapes and Doppler broadened line shapes were made on the IBM mainframe initially for the modules RECONR and BROADR of NJOY by the IAEA Fellows (March-June 1991) **Fortunato AGUILAR HERNANDEZ, Vesselin LALOV, Abderrahmane MALKI, Muhammad ARSHAD, Shafiqul Islam BHUIYAN and Riyanto RAHARJO**. In 1992-1993, **Tahar ZIDI**, IAEA Fellow, significantly contributed to the verification of the accuracy of data processing for some modules of the NJOY code system on the VAX4000 computer system at the Agency. The interactions with those using NJOY for their non-fusion applications were also very useful. Special mention should be made of the interactions with **Caroline RAEPSAT** (France), and **Andrej TRKOV** (Slovenia), in this respect. The feedback from many of the users of NJOY was generally very useful to get confidence in the results of generated multigroup constants and their usability. **Jaroslav PULPAN** contributed significantly to the preliminary checking of the consistency of the FENDL library by trying to analyze a lead benchmark.

The feedback and contributions of members of several laboratories (**H.MAEKAWA**, FNS, JAERI, **J.E. WHITE**, ORNL, USA, **U. FISCHER**, KFK, Germany, **G.C. PANINI**, ENEA, Italy, **S. PELLONI**, Switzerland, and many others) who have started to check the FENDL multigroup library for consistency and its usability in fusion neutronic calculations are expected to be very valuable. The task of generation of multigroup library can be said to have been completed only after the users certify that the library is usable. This stage is expected to be reached in the near future.

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A P P E N D I X I

TABLE I: Results of Review of FENDL-1 General Purpose Evaluations Identified at Previous Meetings +

Element	Library	γ-Ray Data	MF6 Data	Chg.Part. Spectra	Covariance Data	Act./Dos. Consistency	Comments
H	V6	Y	NA	Y	Y	–	Correct AWR for nuclear rather than atomic mass. Consider use of MF=30 for covariances.
D	BROND	Y	Y	Y	N	–	Several improvements have been made to the file since last meeting.
T	V6	Y	N	N	N	–	
Li-6	V6	Y	N*	NC	NC	–	
Li-7	V6	Y	N*	NC	Y	–	EFF-2/V6.1 will be considered for FENDL-2 after testing.
Be-9	V6	Y	Y	Y	N	–	Neutron emission spectra appear to be underestimated at back angles.
B-10	V6	Y	N*	NC	NC	–	
B-11	V6	Y	Y	Y	N	–	
C	V6	Y	N*	NC	Y	–	
N-14	BROND	Y	Y	Y	N	–	
N-15	BROND	Y	Y	Y	N	–	
O-16	V6	Y	N*	NC	N	–	
F-19	V6	Y	Y	Y	Y	N?	New BROND analysis using Pade approximates should be compared. (n,2n) cross sections might not be consistent with activation file.

Table I is continued on following page.

+ For explanations see end of Table I.

TABLE I (Contd.): Results of Review of FENDL-1 General Purpose Evaluations Identified at Previous Meetings +

Element	Library	γ-Ray Data	MF6 Data	Chg.Part. Spectra	Covariance Data	Act./Dos. Consistency	Comments
Al-27	JENDL-3	Y	N	N	N	N	
Si	BROND	Y	NC	Y	N	-	Use EFF-2 if completed in time. V6 isotopic evaluations will be available for consideration for FENDL-2.
Ti	JENDL-3	Y	N	NC	N	N	Ti-47 (n,p) not consistent with activation file.
V-51	V6	Y	N	N	Y	Y	
Cr-50, 52-54	V6	Y	Y	Y	Y	Y	Questions raised regarding resonance region for even Cr isotopes that should be checked.
Mn-55	V6/ JENDL-3	Y	Y	Y	Y	Y	Collaborative evaluation but only V6 contains MF=6 data.
Fe-54, 56-58	V6	Y	Y	Y	Y	Y	14 MeV neutron emission spectrum at 30° higher than Takahashi data in pre-equilibrium region. Should be checked.
Co-59	V6	Y	N	N	Y	Y	
Ni-58, 60-62,64	V6	Y	Y	Y	Y	Y	Check first few resonances in Ni isotopes for completeness.
Cu-63,65	V6	Y	Y	Y	Y	Y	
Zr-90-92, 94,96	BROND	Y	Y	Y	N	N	Cheng recommended that isotopic evaluations be used. Zr-90(n,2n) not consistent with activation file.

Table I is continued on following page.
+ For explanations see end of Table I.

TABLE I (Contd.): Results of Review of FENDL-1 General Purpose Evaluations Identified at Previous Meetings +

Element	Library	γ-Ray Data	MF6 Data	Chg.Part. Spectra	Covariance Data	Act./Dos. Consistency	Comments
Nb-93	BROND	Y	Y	N	N	NC	Nb-93(n,n')Nb-93m and (n,2n)Nb-92m should be added from activation/dosimetry files.
Mo	JENDL-3	Y	N	N	N	N	Isotopic evaluations do not include γ-ray data. Recommend addition of γ-ray data before FENDL-2.
Sn	BROND	Y	N	Y	N	N	MF=3 is combination of full evaluation of major isotopes. MF=4,5 based on calculations for two isotopes.
Ba-134- -138	V6	N	N	N	N	-	Fission product evaluations of limited scope.
W-182-184, 186	V6	Y	N	N	N	N	Some improvement in 14-MeV-neutron emission spectra possibly needed. Use of isotopic evaluations recommended by Cheng.
Pb-206- -208	V6	Y	Y	N	Y	N	Pb-206(n,alpha) not consistent with activation file. Pb-204 evaluation is encouraged.
Bi-209	JENDL-3	Y	N	N	N	N	Bi-209(n,2n) and (n,γ) not consistent with activation file.

+ Table Explanation

Y = Yes, data present
N = No, data not present
* = Indicates excitation energy bins (pseudo levels used in lieu of MF=6)
NC = not complete but some data present
NA = not applicable

TABLE II: Additional Evaluations Recommended for FENDL-I+

Element	Library	γ-Ray Data	MF6 Data	Chg.Part. Spectra	Covariance Data	Act./Dos. Consistency	Comments
Na-23	JENDL-3	Y	N	N	N	N	
Mg	JENDL-3	Y	N	N	N	N	
P-31	V6	Y	N	N	N	Y	JENDL-3 only includes files thru MF=5 - no γ-ray data.
S	V6	Y	N	N	N	N	JENDL-3 has no γ-ray data.
Cl	V6	Y	N	N	N	-	JENDL-3 has no γ-ray data.
K	V6	Y	N	N	N	-	JENDL-3 has no γ-ray data.
Ca	JENDL-3	Y	N	N	N	-	
Ta-181	JENDL-3	Y	N	N	N	N	Should be compared with BROND update.

+ Same symbols used as in Table I.

APPENDIX II

Intercomparison between NJOY 91.38+ And the IAEA pre-processing codes for some isotopes at zero kelvin line shapes of ENDF/B-VI.

The focus of this paper is not on the comparisons of RECONR module of NJOY with that of RECENT. The interested reader should contact the author [17,23] of the code system of NJOY and the author [21,24] of the IAEA preprocessing codes for additional details.

The IAEA Nuclear Data Section is commited to the creation and distribution of FENDL multigroup library in the best possible form that can be described as one with the best quality keeping the errors in processing of the basic evaluated data to the minimum.

A comparative study has been made between the zero kelvin cross section line shapes generated by the IAEA preprocessing codes and the latest version of NJOY (NJOY 91.38) obtained from the Radiation Shielding and Information Center (RSIC), USA, for several materials from ENDF/B-VI which are listed below:

^{1}H, ^{3}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, C, ^{16}O, ^{19}F, P, S, Cl, K, ^{55}V, $^{50,52-54}Cr$, ^{55}Mn, $^{54,56-58}Fe$, ^{59}Co, $^{58,60-62,64}Ni$,

In our processing of neutron interaction cross sections, the output of RECONR of NJOY has been compared with the output of RECENT. The reconstruction tolerance employed for both the RECONR module and the RECENT code is 0.1%. In principle, both the RECONR module of NJOY and RECENT must give identical results since they start from the same basic data file and employ similar resonance reconstruction strategies. A large number of plots was obtained using COMPLOT [21] comparing the two line shapes. This exercise indicated that the zero kelvin line shapes for potential scattering cross sections involved in the libraries were calculated incorrectly for several isotopes due to a bug in the updates to the RECONR module of NJOY. These discrepancies were communicated to the author of the NJOY code system and to the author of the IAEA pre-processing codes. At the time of writing this paper, the author of the NJOY code system, R.E. MacFarlane, confirmed that NJOY was giving incorrect answers for the elastic scattering cross section due to an error in coding that tried to determine the multiplicity for a particular IJ state. The materials that were affected are: $^{50,52-54}Cr$, ^{55}Mn, $^{54,56-58}Fe$, $^{58,60-62,64}Ni$, $^{63,65}Cu$, $^{206-208}Pb$. It was also discovered that RECENT was giving incorrect results for $^{54,56}Fe$ and ^{58}Ni as, for these nuclei, the l-dependency of the scattering radii was not considered.

In the mean time the Nuclear Data Section of the Agency has used LINEAR / RECENT / FIXUP (LRF) pre-processing Codes to obtain the zero kelvin line shapes. These "PENDF data" are then post-processed by the complete NJOY (version 91.38) system. In order to insure that using LRF data as input to NJOY is better than using RECONR directly, comparisons of LRF data with LRF-RECONR were made and satisfactory results were obtained.

Presently, R.E. MacFarlane, after a process of detailed verifications and interactions among J.E. White, D.E. Cullen, N.M. Larson, C.L. Dunford and R.E. MacFarlane, communicated [23, 24] that both the RECONR module of NJOY and RECENT have now been independently updated and the results intercompared to assure that they are now both properly processing the ENDF/B-VI data for all the FENDL materials. It should be stressed that the LRF route to generate zero kelvin cross section file was only a temporary approach as both RECONR. and LRF in the updated form give essentially the same results. It should be remembered for the sake of completeness that a comparison between the line shapes obtained by running LINEAR-RECENT-FIXUP and the output of the line shapes obtained by running the RECONR on the output of FIXUP, demonstrate that only the following differences persist between the line shapes of LINEAR-RECENT-FIXUP and that of LINEAR-RECENT-FIXUP-RECONR:

1. Differences due to the RECONR module recognizing only 7 digits of the output of FIXUP.

2. Differences at the boundary of the resolved/unresolved energy region due to the convention of NJOY not using repeated energy points and RECENT/FIXUP permitting a physical discontinuity.

The differences in the line shapes due to these two effects are found to be attenuated in the group cross sections. Therefore, such discrepancies may not significantly influence the integral results in many application calculations except being critical in certain specific studies where the cross section at a given energy play a sensitive role. One must always carefully investigate the limitations of any code system being used with regard to the specific application under consideration.

APPENDIX III

Specifications for multigroup processing

The specifications of multigroup processing as used in the NJOY runs for the FENDL project to produce a coupled neutron-gamma library is given below:

Neutron Groups: 175 (Vitamin-J structure)

Gamma groups: 42 (Vitamin-J structure)

Neutron weight function: Thermal + 1/E +Fission + Fusion (IWT=6 in NJOY)

Gamma weight function: 1/E with rolloffs (IWT=3 in NJOY)

Legendre order for neutrons: P_6 for transport correction to P_5

Legendre order for gammas: P_8 for transport correction to P_7

Temperatures: 300, 900 and 1500 Kelvin

Dilution factors: 10^0, 10^1, 10^2, 10^3, 10^4, and 10^{10} barns

Reconstruction, linearization and thinning tolerances used in LINEAR/RECENT/FIXUP: 0.2 %
No of digits for resonance reconstruction: up to 9 digits of accuracy. The NJOY system reads up to 7 digits, the maximum possible on the VAX system with NJOY at present).

Thermal Scattering law included for Be in Be metal, C in graphite and H in water.

INPUT DECK TO GENERATE GENDF LIBRARY FOR NEUTRON INTERACTION AND PHOTON PRODUCTION CROSS SECTIONS

```
 0
 6
*MODER*
20 -21
*RECONR*
-21 -22
*PENDF TAPE FOR FE56  FROM ENDF/B-VI */
 2631 3/
.001 0 7 .001 1.0E-15/
* FE56  FROM ENDF/B-VI */
*PROCESSED BY NJOY91.38 SYSTEM GANESAN IAEA NDS */
*RUN TO 7 DIGITS VAX FOR FENDL LIBRARY IAEA/NDS  15-JAN-1993 */
0/
*BROADR*
-22 -23
 2631 3 0 1 0 /
```

```
 .001 1.E6 /
 300. 900. 1500.
 0/
*UNRESR*
-21 -23 -24
 2631  3 6 1/
 300. 900. 1500./
 1.0E10  1.E4 1000. 100. 10. 1/
0/
 *HEATR*
 -21 -24 -26
  2631 2 0 0 0 0 /
 443 444/
 *GROUPR*
  -21 -26 0 -27
  2631 17 10 6 6 3 6 0
 *FE56  GROUPR N,NG DATA FOR FENDL*/
 300. 900. 1500.
 1.E10 1.E4 1000. 100. 10. 1
 3/
 3 251/
 3 252/
 3 253/
 3 259/
 3 301/
 3 443/
 3 444/
 6/
 16/
 0/
 3 1/
 3 2/
 3 102/
 3 301/
 3 443/
 3 444/
 6 2/
 0/
 3 1/
 3 2/
 3 102/
 3 301/
 3 443/
 3 444/
 6 2/
 0/
 0/
 *MODER*
 -27  40
```

```
*STOP*
```

INPUT DECK TO GENERATE MATXS LIBRARY FOR NEUTRON INTERACTION AND PHOTON PRODUCTION CROSS SECTIONS

```
0
6
 *MATXSR*
 32 0 42/
 1 *MATXSR FE56*/
 2 2 1 1/
 *MATXSR FE56 , NEUTRONS X'S, GAMMA PRODUCTION  15-JAN-1993 */
 *N* *G*/
 175 42/
 *NSCAT* *NG* /
 1 1 /
 1 2 /
 *FE56*   2631/
*STOP*
```

INPUT DECK TO GENERATE GENDF LIBRARY FOR PHOTON INTERACTION CROSS SECTIONS

```
 0
 6
 *RECONR*
 30 31
 *PENDF TAPE FOR FE  FROM ENDF/B-VI GAMMA-INT*/
 2600 3/
 .001 0/
 *FE  FROM ENDF/B-VI TAPE*/
 *PROCESSED NJOY91.++PROCESSING SYSTEM GANESAN 31-MAR-1993 VAX IAEA
NDS*/
 *SEE ORIGINAL ENDF/B-VI TAPE FOR DETAILS*/
 0/
  *GAMINR*
 30 31 0 32
 2600 10 3 8 1/
 * 42 GROUP FE  PHOTON INTERACTION GAMINR DATA ENDF6*/
  -1/
 0/
*STOP*
```

INPUT DECK TO GENERATE MATXS LIBRARY FOR PHOTON INTERACTION CROSS SECTIONS

```
0
6
 *MATXSR*
 0 32  42/
 1 *MATXSR FE*/
 1 1 1 1/
 *MATXSR FE ,PHOTON ATOMIC INT. CROSS SECTIONS. 31-MAR-1993 */
  *G*/
  42/
  *GSCAT*/
 1/
 1/
 *FE*   2600/
*STOP*
```

INPUT DECK TO GENERATE MATXS LIBRARY FOR NEUTRON INTERACTION, PHOTON PRODUCTION CROSS SECTIONS AND PHOTON INTERACTION CROSS SECTIONS

```
0
6
 *MATXSR*
  31 32  42/
 1 *MATXSR FE56*/
 2 3 1 1/
 *MATXSR FE56 , NEUTRONS X'S, GAMMA PRODUCTION  15-JAN-1993 */
 *N* *G*/
 175 42/
 *NSCAT* *NG* *GSCAT*/
 1 1 2/
 1 2 2/
 *FE56*   2631 2600/
*STOP*
```

APPENDIX IV

MATXSR formatted files:

DATA SET: UD4:[FENDL.MATXSR]xxx.MATXSR
('xxx' is the NDS internal name for the isotope)

Photon interaction cross section data, P-8 Legendre order, 42 energy groups in VITAMIN-J group structure derived from ENDF/B-VI for all the 34 FENDL elements mentioned in the text.

Number of 80 column records: 1006 each.

Element	NDS internal name
H	HG
Li	LIG
BE	BEG
B	BG
C	CG
N	NG
O	OG
F	FG
Na	NAG
Mg	MGG
Al	ALG
Si	SIG
P	PG
S	SG
Cl	CLG
K	KG
Ca	CAG
Ti	TIG
V	VG
Cr	CRG
Mn	MNG
Fe	FEG
Co	COG
Ni	NIG
Cu	CUG
Zr	ZRG
Nb	NBG
Mo	MOG
Sn	SNG
Ba	BAG
Ta	TAG
W	WG
Pb	PBG
Bi	BIG

MATXSR formatted files:

DATA SET: UD4:[FENDL.MATXSR]xxx.MATXSR_lib
('xxx' is the NDS internal name for the isotope and 'lib' is the library identifier)

lib = E6 for the ENDF/B-VI files
J3 for the JENDL-3.1 files
Br for the BROND-2 files

Neutron interaction cross section data and photon production cross section data, P-5 Legendre order, 175 energy groups in VITAMIN-J group structure derived from ENDF/B-VI, JENDL-3.1 or BROND-2.

Element	NDS internal name	Number of 80 column records	Basic File used
^{1}H	H1N	302827	ENDF/B-VI
^{2}H	H2N		BROND-2
^{2}H	H2N	117210	ENDF/B-VI
^{3}H	H3N	78699	ENDF/B-VI
^{6}Li	LI6N	73450	ENDF/B-VI
^{7}Li	LI7N	66606	ENDF/B-VI
^{9}Be	BE9N	38222	ENDF/B-VI
^{10}B	B10N	49742	ENDF/B-VI
^{11}B	B11N	44122	ENDF/B-VI
C	CN	32977	ENDF/B-VI
^{14}N	N14N	44749	ENDF/B-VI
^{15}N	N15N	33060	BROND-2
O	O16N	37944	ENDF/B-VI
^{23}Na	NA23N	37778	JENDL-3.1
Mg	MGN	40939	JENDL-3.1
^{27}Al	AL27N	31382	JENDL-3.1
Si	SiN	30730	BROND-2
^{31}P	P31N	20131	ENDF/B-VI
S	S00N	34903	ENDF/B-VI
Cl	CLN	22631	ENDF/B-VI
K	KN	22887	ENDF/B-VI
Ca	CAJ3N	38921	JENDL-3.1
Ti	TIJ3N	37828	JENDL-3.1
V	VN	26475	ENDF/B-VI

Element	NDS internal name	Number of 80 column records	Basic File used
^{60}Cr	CR50N	36495	ENDF/B-VI
^{62}Cr	CR52N	36505	ENDF/B-VI
^{63}Cr	CR53N	40926	ENDF/B-VI
^{64}Cr	CR54N	29422	ENDF/B-VI
^{66}Mn	MN55N	29718	JENDL-3.1
^{65}Mn	MN55N	47815	ENDF/B-VI
^{64}Fe	FE54N	36316	ENDF/B-VI
^{66}Fe	FE56N	43416	ENDF/B-VI
^{67}Fe	FE57N	41779	ENDF/B-VI
^{68}Fe	FE58N	34963	ENDF/B-VI
^{69}Co	CO59N	25314	ENDF/B-VI
^{68}Ni	NI58N	38714	ENDF/B-VI
^{60}Ni	NI60N	39247	ENDF/B-VI
^{61}Ni	NI61N	40859	ENDF/B-VI
^{62}Ni	NI62N	34723	ENDF/B-VI
^{64}Ni	NI64N	31994	ENDF/B-VI
^{63}Cu	CU63N	48810	ENDF/B-VI
^{65}Cu	CU65N	41415	ENDF/B-VI
^{90}Zr	ZR90N	17559	BROND-2
^{90}Zr	ZR91N	16993	BROND-2
^{92}Zr	ZR92N	18262	BROND-2
^{94}Zr	ZR94N	16566	BROND-2
^{96}Zr	ZR96N	14393	BROND-2
Mo	MoN	29736	JENDL-3.1
^{134}Ba	BA134N	13539	ENDF/B-VI
^{136}Ba	BA135N	14647	ENDF/B-VI
^{136}Ba	BA136N	14138	ENDF/B-VI
^{136}Ba	BA137N	13929	ENDF/B-VI
^{136}Ba	BA138N	14427	ENDF/B-VI
^{181}Ta	TA181N	30462	JENDL-3.1
^{182}W	W182N	34642	ENDF/B-VI

Element	NDS internal name	Number of 80 column records	Basic File used
^{183}W	W183N	34371	ENDF/B-VI
^{184}W	W184N	34737	ENDF/B-VI
^{186}W	W186N	35386	ENDF/B-VI
^{206}Pb	PB206N	37301	ENDF/B-VI
^{207}Pb	PB207N	37772	ENDF/B-VI
^{208}Pb	PB208N	27477	ENDF/B-VI
^{209}Bi	BI209N	23202	JENDL-3.1

MATXSR formatted files:

DATA SET: UD4:[FENDL.MATXSR]xxx.MATXSR_lib
('xxx' is the NDS internal name for the isotope and lib is the library identifier)

lib = E6 for the ENDF/B-VI files
J3 for the JENDL-3.1 files
Br for the BROND-2 files

A coupled neutron-gamma, 175 neutron - 42 photon groups, P-5 Legendre order, for neutron interaction cross section data derived from ENDF/B-VI, JENDL-3.1 or BROND-2, and, photon production cross section data and photon interaction cross section data derived from ENDF/B-VI.

Element	NDS internal name	Number of 80 column records	Basic File used
^{1}H	H1NG	303818	ENDF/B-VI
^{2}H	H2NG		BROND-2
^{2}H	H2NG	118201	ENDF/B-VI
^{3}H	H3NG	79690	ENDF/B-VI
^{6}Li	LI6NG	74441	ENDF/B-VI
^{7}Li	LI7NG	67597	ENDF/B-VI
^{9}Be	BE9NG	39213	ENDF/B-VI
^{10}B	B10NG	50733	ENDF/B-VI
^{11}B	B11NG	45113	ENDF/B-VI
C	CNG	33968	ENDF/B-VI
^{14}N	N14NG	45740	ENDF/B-VI
^{16}N	N15NG	34051	BROND-2
O	O16NG	38935	ENDF/B-VI
^{23}Na	NA23NG	38769	JENDL-3.1
Mg	MGNG	41930	JENDL-3.1
^{27}Al	AL27NG	32373	JENDL-3.1
Si	SiNG	31721	BROND-2
^{31}P	P31NG	21122	ENDF/B-VI
S	SOONG	35894	ENDF/B-VI
Cl	CLNG	23622	ENDF/B-VI
K	KNG	23878	ENDF/B-VI
Ca	CANG	39912	JENDL-3.1
Ti	TING	38819	JENDL-3.1

Element	NDS internal name	Number of 80 column records	Basic File used
V	VNG	27466	ENDF/B-VI
^{60}Cr	CR50NG	37487	ENDF/B-VI
^{62}Cr	CR52NG	37496	ENDF/B-VI
^{63}Cr	CR53NG	41917	ENDF/B-VI
^{64}Cr	CR54NG	30413	ENDF/B-VI
^{66}Mn	MN55NG	48806	ENDF/B-VI
^{66}Mn	MN55NG	30709	JENDL-3.1
^{64}Fe	FE54NG	37307	ENDF/B-VI
^{66}Fe	FE56NG	44407	ENDF/B-VI
^{67}Fe	FE57NG	42770	ENDF/B-VI
^{68}Fe	FE58NG	35954	ENDF/B-VI
^{69}Co	CO59NG	26305	ENDF/B-VI
^{68}Ni	NI58NG	39705	ENDF/B-VI
^{60}Ni	NI60NG	40238	ENDF/B-VI
^{61}Ni	NI61NG	41850	ENDF/B-VI
^{62}Ni	NI62NG	35714	ENDF/B-VI
^{64}Ni	NI64NG	32985	ENDF/B-VI
^{63}Cu	CU63NG	49801	ENDF/B-VI
^{66}Cu	CU65NG	42406	ENDF/B-VI
^{90}Zr	ZR90NG	18550	BROND-2
^{90}Zr	ZR91NG	17984	BROND-2
^{92}Zr	ZR92NG	19253	BROND-2
^{94}Zr	ZR94NG	17557	BROND-2
^{96}Zr	ZR96NG	15384	BROND-2
Mo	MoNG	30727	JENDL-3.1
^{134}Ba	BA134NG	14530	ENDF/B-VI
^{136}Ba	BA135NG	15638	ENDF/B-VI
^{136}Ba	BA136NG	15129	ENDF/B-VI
^{136}Ba	BA137NG	14920	ENDF/B-VI
^{138}Ba	BA138NG	15418	ENDF/B-VI
^{181}Ta	TA181NG	31453	JENDL-3.1

Element	NDS internal name	Number of 80 column records	Basic File used
^{182}W	W182NG	35633	ENDF/B-VI
^{183}W	W183NG	35362	ENDF/B-VI
^{184}W	W184NG	35728	ENDF/B-VI
^{186}W	W186NG	36377	ENDF/B-VI
^{206}Pb	PB206NG	38292	ENDF/B-VI
^{207}Pb	PB207NG	38763	ENDF/B-VI
^{208}Pb	PB208NG	28468	ENDF/B-VI
^{209}Bi	BI209NG	24193	JENDL-3.1

GENDF FILES: NEUTRON INTERACTION AND PHOTON PRODUCTION DATA

DATA SET: UD4:[FENDL.MATXSR]xxx.GROUPR_lib
('xxx' is the NDS internal name for the isotope and lib is the library identifier)

lib = E6 for the ENDF/B-VI files
J3 for the JENDL-3.1 files
Br for the BROND-2 files

Element	NDS internal name	Number of 80 column records	Basic File used
^{1}H	H1	317943	ENDF/B-VI
^{2}H	H2		BROND-2
^{2}H	H2	132103	ENDF/B-VI
^{3}H	H3	90689	ENDF/B-VI
^{6}Li	LI6	91031	ENDF/B-VI
^{7}Li	LI7	82980	ENDF/B-VI
^{9}Be	BE9	53232	ENDF/B-VI
^{10}B	B10	69055	ENDF/B-VI
^{11}B	B11	59243	ENDF/B-VI
C	C	47514	ENDF/B-VI
^{14}N	N14	45740	ENDF/B-VI
^{15}N	N15	34051	BROND-2
O	O	53037	ENDF/B-VI
^{23}Na	NA23	55196	JENDL-3.1
Mg	MG	60247	JENDL-3.1
^{27}Al	AL27	48110	JENDL-3.1
Si	Si	49885	BROND-2
^{31}P	P31	34559	ENDF/B-VI
S	S00	54736	ENDF/B-VI
Cl	CL	38486	ENDF/B-VI
K	K	38830	ENDF/B-VI
Ca	Ca	58575	JENDL-3.1
Ti	TI	58331	JENDL-3.1
V	V	44685	ENDF/B-VI
^{60}Cr	CR50	52330	ENDF/B-VI
^{62}Cr	CR52	52890	ENDF/B-VI

Element	NDS internal name	Number of 80 column records	Basic File used
^{63}Cr	CR53	58695	ENDF/B-VI
^{64}Cr	CR54	44662	ENDF/B-VI
^{66}Mn	MN55	69597	ENDF/B-VI
^{66}Mn	MN55	49540	JENDL-3.1
^{64}Fe	FE54	52092	ENDF/B-VI
^{66}Fe	FE56	62276	ENDF/B-VI
^{67}Fe	FE57	59087	ENDF/B-VI
^{68}Fe	FE58	49783	ENDF/B-VI
^{69}Co	CO59	43027	ENDF/B-VI
^{68}Ni	NI58	55258	ENDF/B-VI
^{60}Ni	NI60	56221	ENDF/B-VI
^{61}Ni	NI61	58485	ENDF/B-VI
^{62}Ni	NI62	50068	ENDF/B-VI
^{64}Ni	NI64	46714	ENDF/B-VI
^{63}Cu	CU63	69006	ENDF/B-VI
^{65}Cu	CU65	59930	ENDF/B-VI
^{90}Zr	ZR90	33879	BROND-2
^{90}Zr	ZR91	33864	BROND-2
^{92}Zr	ZR92	35319	BROND-2
^{94}Zr	ZR94	32974	BROND-2
^{96}Zr	ZR96	29524	BROND-2
Mo	Mo	52807	JENDL-3.1
^{134}Ba	BA134	29706	ENDF/B-VI
^{135}Ba	BA135	31748	ENDF/B-VI
^{136}Ba	BA136	30451	ENDF/B-VI
^{137}Ba	BA137	30437	ENDF/B-VI
^{138}Ba	BA138	29105	ENDF/B-VI
^{181}Ta	TA181	52001	JENDL-3.1
^{182}W	W182	52453	ENDF/B-VI
^{183}W	W183	53165	ENDF/B-VI
^{184}W	W184	52585	ENDF/B-VI

Element File	NDS internal name	Number of 80 column records	Basic used
^{186}W	W186	53707	ENDF/B-VI
^{206}Pb	PB206	60486	ENDF/B-VI
^{207}Pb	PB207	59855	ENDF/B-VI
^{208}Pb	PB208	43942	ENDF/B-VI
^{209}Bi	BI209	40316	JENDL-3.1

GENDF FILES: PHOTON INTERACTION DATA

DATA SET: UD4:[FENDL.GAMINR]Elxxx.GAMINR
('xxx' is the NDS internal name for the isotpe from the list below.)
Number of 80 coulumn records: 1673 for each.
All the GENDF files have been derived from ENDF/B-VI

Element	NDS internal name
H	H
Li	LI
Be	BE
B	B
C	C
N	N
O	O
F	F
Na	NA
Mg	MG
Al	AL
Si	SI
P	P
S	S
Cl	CL
K	K
Ca	CA
Ti	TI
V	V
Cr	CR
Mn	MN
Fe	FE
Co	CO
Ni	NI
Cu	CU
Zr	ZR
Nb	NB
Mo	MO
Sn	SN
Ba	BA
Ta	TA
W	W
Pb	PB
Bi	BI

A P P E N D I X V

TABLE I: Additional files proposed to be considered for inclusion in FENDL/E-2

Nuclide or Element	Library	γ-ray Data	File-6 Data	Chg.Part. Spectra	Covariance Data	Comments
^{1}H	CENDL-2	?	Y	Y	N	
^{2}H	CENDL-2	N	N	N	N	
^{3}He	CENDL-2	N	Y	N	Y	New eval. added for FENDL/E-2.
^{4}He	ENDF/B-VI	?	?	?	?	New eval. added for FENDL/E-2.
^{6}Li	JENDL-3 R2	Y	N	Y	N	
^{7}Li	JENDL-3 R1	Y	N*	Y	N	
^{7}Li	EFF-2	Y	Y	Y	N	
^{9}Be	EFF-2	Y	Y	Y	N	
^{9}Be	JENDL-3 R2	Y	N*	Y	N	Possibly completed.
^{14}N	ENDF/B-VI	Y	Y	Y	Y	
^{14}N	JENDL-3 R2	Y	N*	Y	N	
^{15}N	ENDF/B-VI	Y	Y	Y	Y	
^{27}Al	EFF-2	Y	Y	Y	N	
^{27}Al	JENDL-3 R2	Y	Y	Y	N	
^{28}Si	EFF-2	Y	Y	Y	N	
^{28}Si	ENDF/B-VI	Y	Y	Y	Y	

Table I is continued on following page.
+ For explanations see end of Table I.

TABLE I (Contd.): Additional files proposed to be considered for inclusion in FENDL/E-2

Nuclide or Element	Library	γ-ray Data	File-6 Data	Chg.Part. Spectra	Covariance Data	Comments
^{29}Si	ENDF/B-VI	Y	Y	Y	Y	
^{30}Si	ENDF/B-VI	Y	Y	Y	Y	
^{nat}Ca	JENDL-3 R2	Y	Y	Y	N	
^{isotopes}Ti	JENDL-3 R2	Y	Y	Y	N	
^{nat}Ti	JENDL-3 R2	Y	Y	Y	N	
^{52}Cr	EFF-2	Y	Y	Y	Y	
^{nat}Cr	JENDL-3 R2	Y	Y	Y	N	
^{56}Fe	EFF-2	Y	Y	Y	Y	
^{56}Fe	CENDL-2	Y	Y	Y	Y	
^{56}Fe	JENDL-3 R2	Y	Y	Y	N	
^{59}Co	JENDL-3 R2	Y	Y	Y	N	
^{58}Ni	EFF-2	Y	Y	Y	Y	
^{58}Ni	JENDL-3 R2	Y	Y	Y	N	
^{60}Ni	EFF-2	Y	Y	Y	Y	
^{nat}Cu	JENDL-3 R2	Y	Y	Y	N	
^{93}Nb	JENDL-3 R2	Y	Y	Y	N	
^{nat}Mo	JENDL-3 R2	Y	Y	Y	N	

Table I is continued on following page.
+ For explanations see end of Table I.

TABLE I (Contd.): Additional files proposed to be considered for inclusion in FENDL/E-2

Nuclide or Element	Library	γ-ray Data	File-6 Data	Chg.Part. Spectra	Covariance Data	Comments
^{nat}Pb	JENDL-3 R2	Y	Y	Y	N	
^{209}Bi	JENDL-3 R2	Y	Y	Y	N	

+ Table Explanation:

Y = Yes, data present
N = No, data not present
* = Indicates excitation energy bins (pseudo levels used en lieu of File-6)

APPENDIX V

TABLE II:

PRIORITIZED USER NEEDS FOR INFORMATION IDENTIFIED AS DEFICIENT IN FENDL/E-1

Data Types

	A	B	B	C
Priority	γ-ray Data	File-6 Data	Charged Particle Data	Covariance Data
I		Mo, W	C, ^{16}O, Mo, W, Pb	^{16}O, Mo, W
I	Re	Re	Re	Re
II		Al, Sn(?)	^{6}Li, ^{7}Li ^{10}B, Al	^{9}Be, ^{6}Li ^{27}Al, Si, Zr, Sn
III	Ba			

Priorities:

I Basic materials for ITER, completion desirable

I' Depends on choice of ITER divertor concept

II Needed in ITER only if driver blanket remains option

III Necessary only if Ba is used in biological shield

The different data types listed above are ranked in priority as follows: Priority (A) > Priority (B) > Priority (C).

International Workshop on Nuclear Data for Fusion Reactor Technology

Del Mar, California, U.S.A.

3-6 May 1993

Status of FENDL activation file and plans for future development

by

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Introduction

A series of international meetings, having taken place in 1986, 1987, 1989, 1990, 1991 and 1992 and projected to continue with about the same frequency in the next few years, has been organized by the International Atomic Energy Agency (IAEA), with goal of assembling, processing and testing a comprehensive, fusion-relevant Fusion Evaluated Nuclear Data Library (FENDL) with unrestricted international distribution [1-4].

FENDL is composed of "sublibraries" containing different data types, describing the transport of both the plasma-source neutrons and secondary gamma rays through reactor components, as well as the resulting radiation effects, such as nuclear heating, tritium breeding, activation and material damage. Also included are cross sections for fusion and other important charged-particle nuclear reactions of the plasma constituents, as well as data for fusion-relevant neutron dosimetry.

With the welcomed international release of ENDF/B-VI, JENDL-3 and BROND in early 1990, the FENDL project has turned from its earlier emphasis on the review and selection of candidate neutron-interaction evaluations to (a) processing and testing of cross sections for neutron and gamma-ray transport and (b) assembling, processing and testing of large special-application files needed to supplement the available files, especially in the field of activation and decay data.

1. FENDL activation sublibrary

1.1 FENDL/PA-1

The FENDL activation programme was started since May 1989 at the FENDL meeting [1], when the Working Group on Neutron Activation Data initiated an intercomparison of activation cross sections important for fusion reactor technology. It was agreed that national nuclear data centers and research laboratories will send to the NDS their contributions, according to a list of reactions selected on the basis of inventory calculations.

A list of 256 important reactions that are significant in producing activation both at short and long cooling times has been compiled by R. Forrest at Harwell Laboratory, UKAEA. The list was distributed to all interested parties and in response to this many activation data files have been received at the NDS from institutes participating in this exercise. Very detailed graphical intercomparisons have been prepared at the NDS, plotting, for each reaction, overlays of the various submitted evaluated data sets and experimental data from EXFOR.

Groups that were participating in the intercomparison are listed below, along with their libraries:

REAC-2 [5] (F.M. Mann, Hanford Engineering Development Laboratory)

REAC-ECN-5 [6] (J. Kopecky and H. Gruppelaar, Netherlands Energy Research Foundation)

ENDF/B-VI

All extracted individual reaction cross sections of the ENDF/B-6 general purpose files that are contained in the list of 256 high-priority reactions.

BOSPOR-86 [7,8]

BOSPOR, which means "library of evaluated threshold activation reaction cross sections", was organized in 1980 in the Obninsk Nuclear Data Centre. In 1986 the BOSPOR-80 library was revised and its new, extended version BOSPOR-86 was created in ENDF/B-5 File-3 format. Energy range is from threshold to 20 MeV.

SINCROSACT [9] (N. Yamamuro, Data Engineering, Inc.)

These activation data are almost all the cross-sections in ENDF-5 File-10 format for ^{59}Co, $^{64,66-68,70}Zn$, $^{58,60-62,64}Ni$, ^{63}Cu, $^{90-92,94,96}Zr$, ^{93}Nb, $^{92,94-98,100}Mo$, $^{107,109}Ag$, $^{121,123}Sb$, $^{185-187}Re$, ^{197}Au and $^{196,198-200,204}Hg$. Ground state production and isomeric state production cross-sections are given separately. The energy region covered is from threshold to 20 MeV.

ADL-90 [10]

The Activation Data Library (ADL-90), for calculation of activation and transmutation in materials used in fusion reactor technology, was created in Obninsk to contribute to the development of FENDL activation sublibrary. This version of library now contains cross sections for about 5000 (n,p), (n,α), (n,γ), (n,2n) and (n,3n) reaction, for all stable targets.

In addition data for a few reactions were taken from JENDL-3 [11] and BROND [12] libraries.

All data contributed by the participants were kept unchanged, except that the data format was in all cases changed to ENDF-6 [13] at the NDS. This review and intercomparison activity has the practical goal of creating an activation data sublibrary of FENDL. Selection of the 256 specific evaluations was made at the June 1990 FENDL meeting [2] after detailed discussions with the following fusion nuclear activation data and neutronics specialists:

E.T. Cheng, TSI Research, Inc., U.S.A.
R.A. Forrest, Harwell Laboratory, U.K.
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This selection was considerably aided by the availability of the large number of overlay plots mentioned above. This selected evaluations, with a few subsequent modifications, formed the basis of the first version of the FENDL pointwise activation sublibrary (FENDL/PA-1) which was issued in fall of 1991 [14].

The FENDL/PA-1 file contains cross-section data for 372 neutron induced activation reactions of 150 isotopes for incident neutron energies up to 20 MeV. When it was necessary, the initial data were processed to pointwise evaluated data which includes linearization, reconstruction of resonance data from resonance parameters and summation with the background cross-sections. This processing was done using the preprocessing codes LINEAR and RECENT by D.E. Cullen [15]. The pointwise cross-section data of this library are in ENDF-6 format, MF = 3. But the users of the file should pay attention to the fact that new MT numbers were introduced for the representation of the isomer production data [13] and should check whether their inventory codes handle them.

The list of reactions included in the FENDL/PA-1 activation file as well as sources of evaluations, MAT numbers and brief description of methods, used for data evaluations are given in [14].

The FENDL/PA-1 library contains 254233 records or 20 Mb of memory.

1.2 FENDL/PA-1 (Revised)

Version 1 of the FENDL pointwise activation sublibrary (FENDL/PA-1), consisting of "256 reactions" most important for activation, was reviewed in detail at the next FENDL meeting held in Vienna from 18-22 November 1991 [3]. The review and selection process has been renewed, using, as an additional source of data, the results of the IAEA Co-ordinated Research Programme on Activation Cross Sections for the Generation of Long-lived Radionuclides [16] and some new evaluations [17, 18]. The sources of data were agreed and this lead to the creation of a second version of activation sublibrary, FENDL/PA-1 (Revised), early in 1992. The following revisions of activation cross section data have been agreed and incorporated:

(1) New Data Sources Replacing Current Data in FENDL/PA-1 have been identified;

(2) evaluated (n,γ) data from REAC-ECN-5 which are the results of renormalization at 14.5 MeV to branching ratio BR = $\sigma^m/(\sigma^m+\sigma^g)$ = 0.5 have been replaced by EAF-2 [17];

(3) all BOSPOR-86 data have been replaced by ADL-91 data [18];

(4) all ADL-90 data have been replaced by ADL-91 data (except for Zr-93(n,α)).

1.3 FENDL/PA-1.1 and FENDL/GA-1.1 sublibraries

To enable realistic activation calculations to be performed by users the FENDL activation library should be as complete as possible (i.e., containing at least all targets with $T_{½}$ > 10 days and all reactions energetically possible for E_n < 20 MeV). In order to achieve this in reasonable time, all reactions data from the European Activation File version 2 (EAF-2) in pointwise form were made available by J. Kopecky at the IAEA/NDS in the middle of 1992. After analysis and minor corrections these EAF-2 data were converted to ENDF-6 format and combined with the above FENDL/PA-1 (Revised) sublibrary. Resulting from this the revised and extended FENDL/PA-1.1 pointwise activation library has been released early this year [19]. The FENDL/PA-1.1 file contains all stable and unstable targets with half-lifes longer than ½ day. If a reaction produces isomers the cross-sections for the ground- and isomeric-state are given separately. The FENDL/PA-1.1 includes 636 target nuclides with about 11,000 reactions with non-zero cross-sections below 20 MeV.

All materials that are represented in the FENDL/PA-1.1 library have been processed at the NDS into 175 Vitamin-J multigroup form [20] using the GROUPIE pre-processing code [15] on the IBM-3081 mainframe computer at the IAEA. This has lead to a drastic reduction of the size of the library and so-called FENDL/GA-1.1 groupwise activation file contains 289426 records or 23 Mb of memory. In order to accelerate the process of integral testing of FENDL activation library, FENDL/PA-1.1 and FENDL/GA-1.1 files have been, and, are being distributed to interested colleagues for the purpose of preliminary checks and integral testing. All the data generated are available cost-free upon request from the IAEA Nuclear Data Section.

1.4 FENDL/D-1.1

In order to use activation cross section data in inventory codes it is necessary to have a source of decay data. It was agreed at the FENDL meeting [3] that the decay data sublibrary (FENDL/D-1.1) should be based on the data library used by the REAC code and data system. Following this recommendation F. Mann has supplied to NDS by March 1992 his data library (which is, in turn, based on ENDF/B-VI and ENSDF) in ENDF/B-VI format for distribution by NDS to interested parties. Approximately 2900 nuclides are included.

2. Conclusion and Future Plans

The most important conclusion from the preceding sections is that at present as a result of international cooperation a first international full activation data file has been created. The first version FENDL/PA-1.1 already means a large improvement compared to the presently available activation cross section files. Advantages and shortcomings of FENDL activation library fully depends on the quality of contributed data files. The FENDL/PA-1.1 file is rather complete, but this file is still primarily recommended for fusion reactor activation calculations with a hard neutron spectrum. A major activity should now be devoted to improve its quality and to extend its range of application, in particular with respect to the low-energy cross-sections. The intercomparison analysis done at NDS [21] demonstrated that two major shortcomings characterize the present status of the contributed files illustrating the need for much further experimental and theoretical research:

- In view of large gaps in experimental data and the large number of reactions required, most cross sections were so far calculated with rather crude nuclear models and codes (e.g. with the THRESH code [22, 23] in order to satisfy short-term needs for feasibility studies.

- The intercomparison of data files show numerous large discrepancies in data for all reaction types, particularly for photon-production data and (n,α) cross sections. Illustrations of such discrepancies [21, 24] are given in figures 1 for ^{64}Zn(n,γ)^{65}Zn, 2 for ^{63}Cu(n,p)^{63}Ni, 3 for ^{62}Ni(n,α)^{59}Fe and 4 for ^{66}Zn(n,2n)^{65}Zn.

The existing FENDL activation programme may be further extended to form the basis for the production of FENDL/PA-2. There are teams of evaluators, experimentalists and users working on the project to create a second version of the file. This work concerning primarily the (n,gamma) and (n,n gamma) data is underway at Petten. Additional support could come from KFK and Obninsk, by adding charged-particle induced activation data and isomer production cross sections, respectively. It would be valuable to test the inventory codes and activation data libraries against recently performed experimental data. The TSI Research (E. Cheng) could coordinate the data testing activities involving both 14-MeV-neutron generating accelerators and high-flux-thermal and fast reactors. Arguments and proposals concerning a programme for activation code studies came from R. Forrest from AEA Harwell. In many discussions and mail contacts we have identified several areas in which a larger coordinated action may substantially improve and speed up future versions of activation files [25, 26, 27]:

- Investigation of methods for the fast and reliable prediction of neutron reaction cross sections that can be used with confidence when no experimental measurements exist. The methods should require minimum input so that use on a 'mass production' basis is feasible.

- To start the validation of data libraries (both cross section and decay data) against experimental irradiations of realistic materials in high neutron fluxes. Only by extending benchmarking of codes and data in this way can we have real confidence in their ability to predict activation on large scale fusion devices.

- To investigate the detail required for uncertainty data in the cross section libraries. It will be impossible at this stage to include uncertainty data in activation files in the same detail as in the general purpose files, but how much is required for activation, and for the unmeasured reactions how can we estimate it?

- Extension of the cross section libraries to higher energies to cover accelerator based applications, e.g. transmutation. The extension of the existing libraries above 20 MeV will require a large effort, and then these would also require comparison and validation.

- Investigation of the importance of other reactions apart from those directly induced by neutrons. The effects of sequential charged particle reactions are already recognised in certain materials, but no comprehensive library yet exists. Also photon induced reactions may in special cases be of importance [4].

The future work in the area of nuclear data for activation is of vital importance to:

- designers of fusion devices who require activation data for choice of existing materials;

- planners who must consider the management of waste (including decommisioning) arising from the operation of fusion reactors;

- the fusion community who have to convince funding bodies and the public that fusion power is (or can be) an environmentally benign and safe technology.

It must be stressed that data libraries and inventory codes require more than just "polishing up". Construction of quality assured libraries with suitable documentation is a major task and requires continued funding. The inadequacy of many existing codes and libraries to reproduce the benchmarks and experiments that have recently been studied [28, 29] is a concrete example of how difficult it is to accurately calculate activation and should be used to convince funding agencies that this area requires continued effort and support.

Since the available man power in laboratories active in this field is rather limited, a collaboration in an international frame would be very beneficial and probably also the fastest to obtain results. For this reasons the Nuclear Data Section initiated the Co-ordinated Research Programme (CRP) of the IAEA to support FENDL activation project and to form in the future the basis for production of improved versions of activation files.

3. The IAEA Co-ordinated Research Programme (CRP) on "Establishment of an International Reference Data Library of Nuclear Activation Cross Sections"

3.1 General information on the CRP

Where it is deemed desirable that several institutes co-operate in furthering research in a given field, Co-ordinated Research Programme (CRPs) represent an effective means to bring together researchers to collaborate in a well defined research topic. The role of the International Atomic Energy Agency (IAEA) is to define, co-ordinate and support the programme.

The duration of a CRP is generally 3 years, but an extension is possible, if recommended and approved by the IAEA. Research Co-ordination Meetings (RCMs) are generally convened at the beginning, in the middle and at the end of a CRP, with the purpose to define details of the programme, review the progress and formulate a final report.

In accordance with the proposal from the IAEA Nuclear Data Section [30] to support FENDL project and with endorsement by the International Nuclear Data Committee (INDC), an advisory body for the nuclear data programme of the IAEA, the proposed CRP on Establishment of an International Reference Data Library of Nuclear Activation Cross Sections was recommended to start in 1993.

3.2 Scientific Scope and Proposed Programme Goals

Following discussions at the 19th INDC Meeting in March 1993, the data base should satisfy the following requirements:

(a) it should include activation cross-sections, decay half-lives, branching ratios and energy spectra of emitted radiation;

(b) the data base should contain uncertainty estimates;

(c) it should be extensively tested against integral activation measurements;

(d) it should allow reliable estimation and prediction of radiation doses and health hazards from artificial radiation sources (radioactive waste, radioisotope applications, reactor decommissioning, fall-out of nuclear accidents, natural sources);

(e) it should cover initially incident particle energies up to 20 MeV with gradual extension (1995) to the intermediate energies.

The total size of the library is expected to comprize more than ten thousand activation reactions and associated nuclear decay data for more than thousand radioactive species.

4. Summary

The revised and extended FENDL/PA-1.1 (pointwise) and FENDL/GA-1.1 (groupwise) activation data libraries are described. The present FENDL activation library is rather complete but these files are still primarily recommended for fusion reactor activation calculations with a hard neutron spectrum. The existing FENDL activation programme to form the basis for the production of FENDL/PA-2 are briefly discussed. Several areas of coordinated actions to improve and speed up future versions of activation files are identified. This way FENDL/PA-2 will become a general activation file applicable for both fission and fusion reactor technology. Since the available man power in laboratories active in this field is rather limited, a collaboration in frame of the new IAEA Co-ordinated Research Programme (CRP), initiated in 1993 to support the FENDL project, would be very beneficial and probably the fastest to obtain results.

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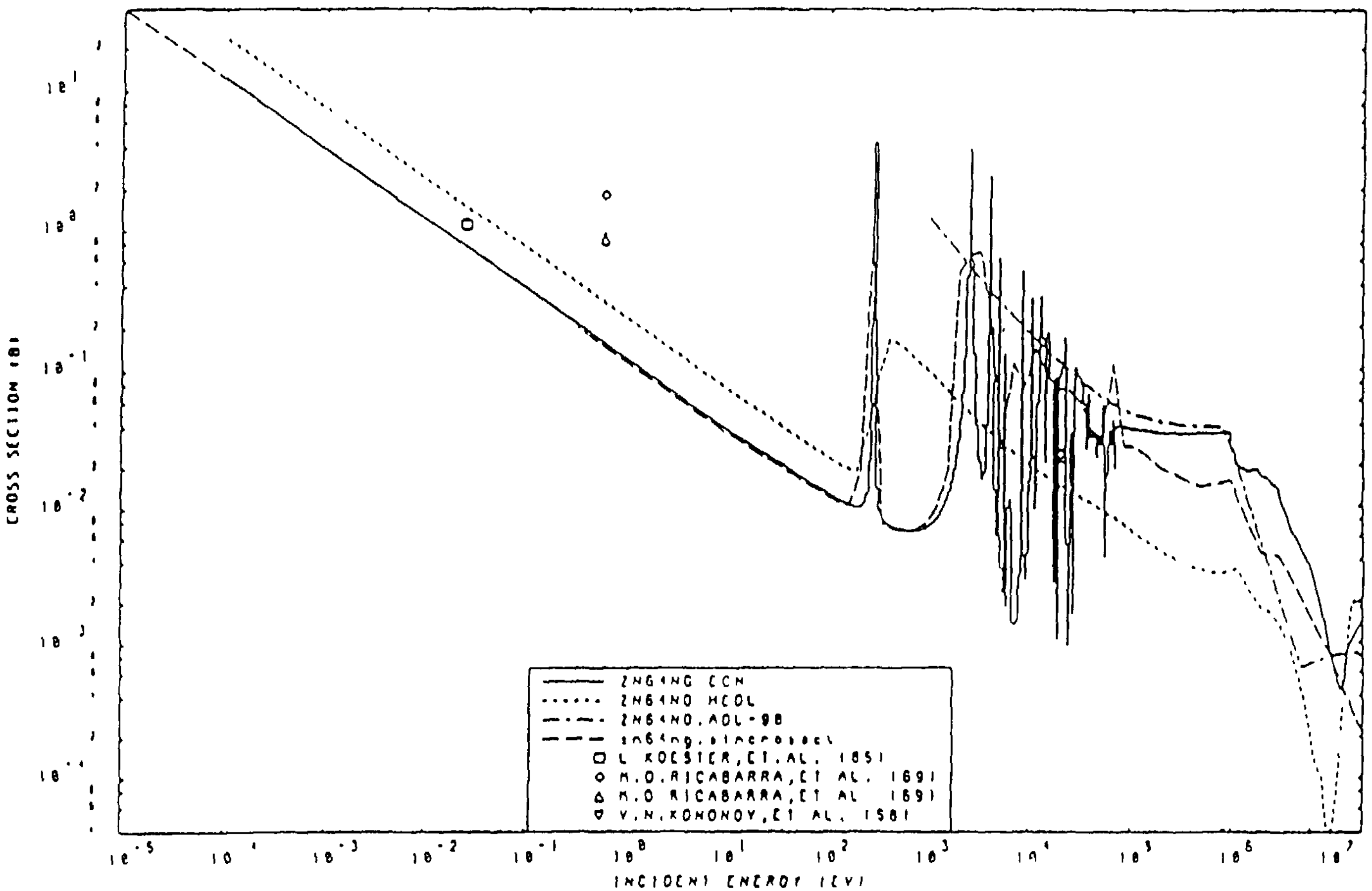

Fig. 1 Comparison of $^{64}Zn(n,gamma)^{65}Zn$ cross sections from various activation data files [21]

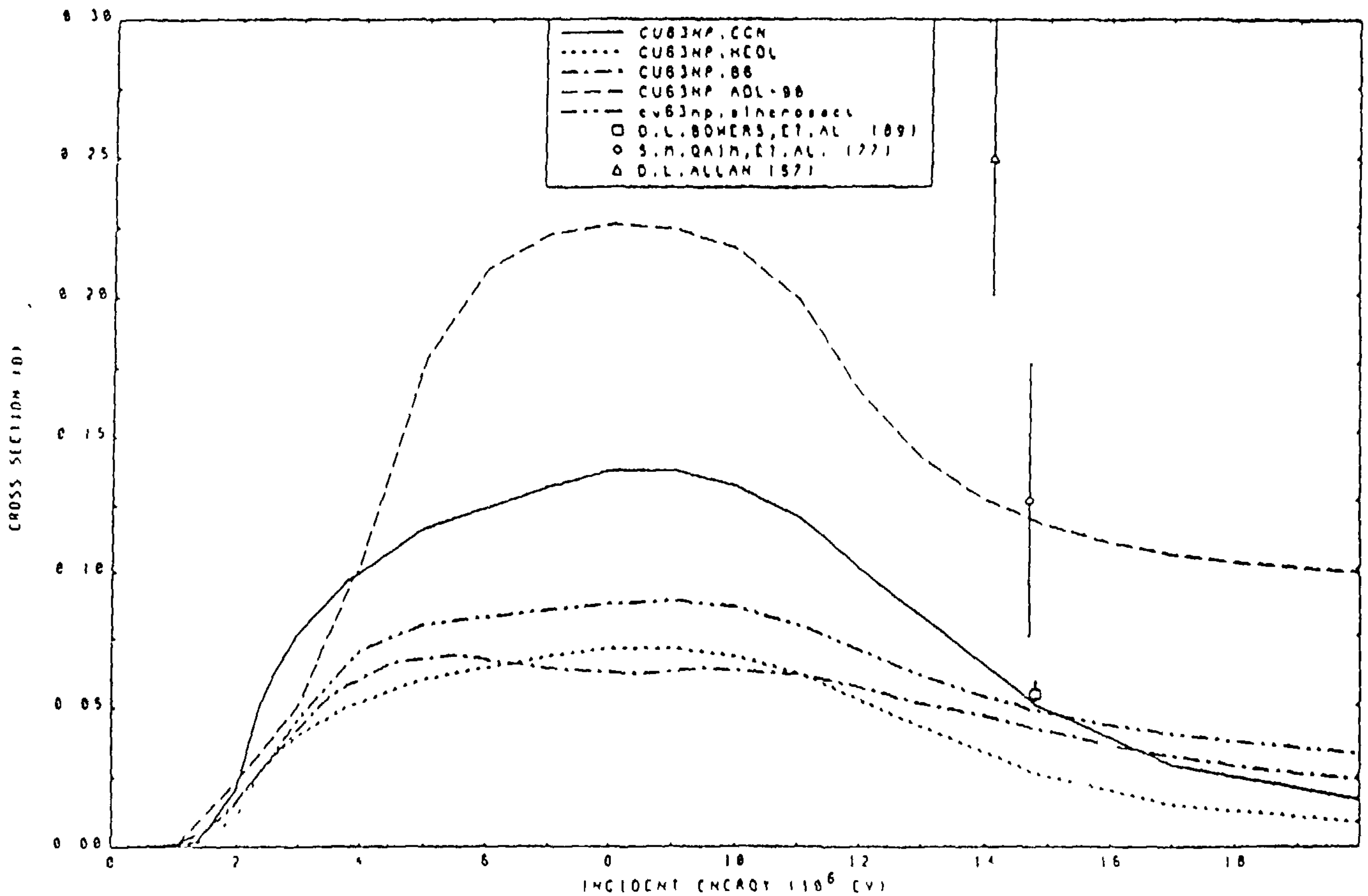

Fig. 2 Comparison of $^{63}Cu(n,p)^{63}Ni$ cross sections from various activation data files [21]

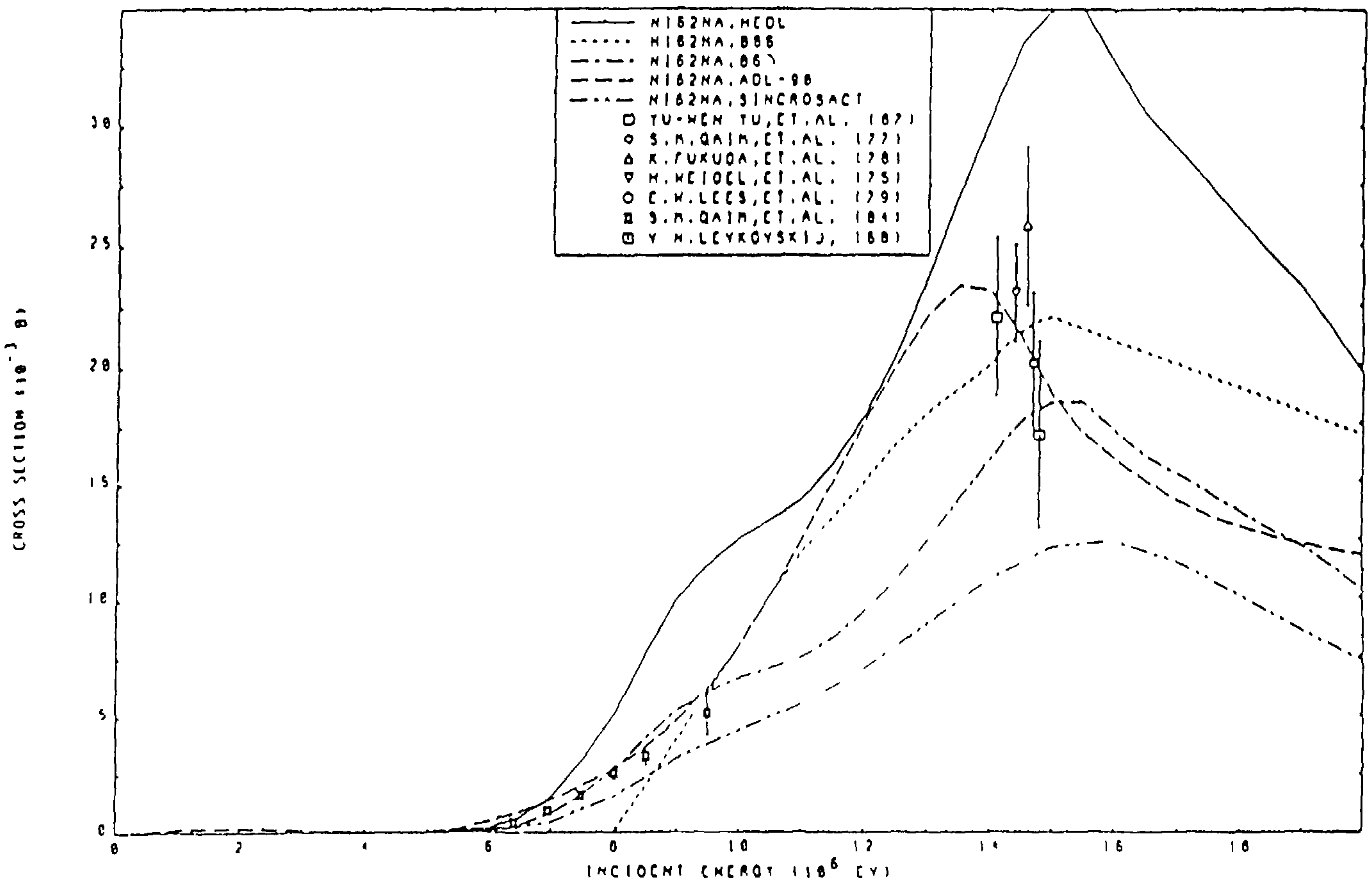

Fig. 3 Comparison of $^{62}Ni(n,alpha)^{59}Fe$ cross sections from various activation data files [21]

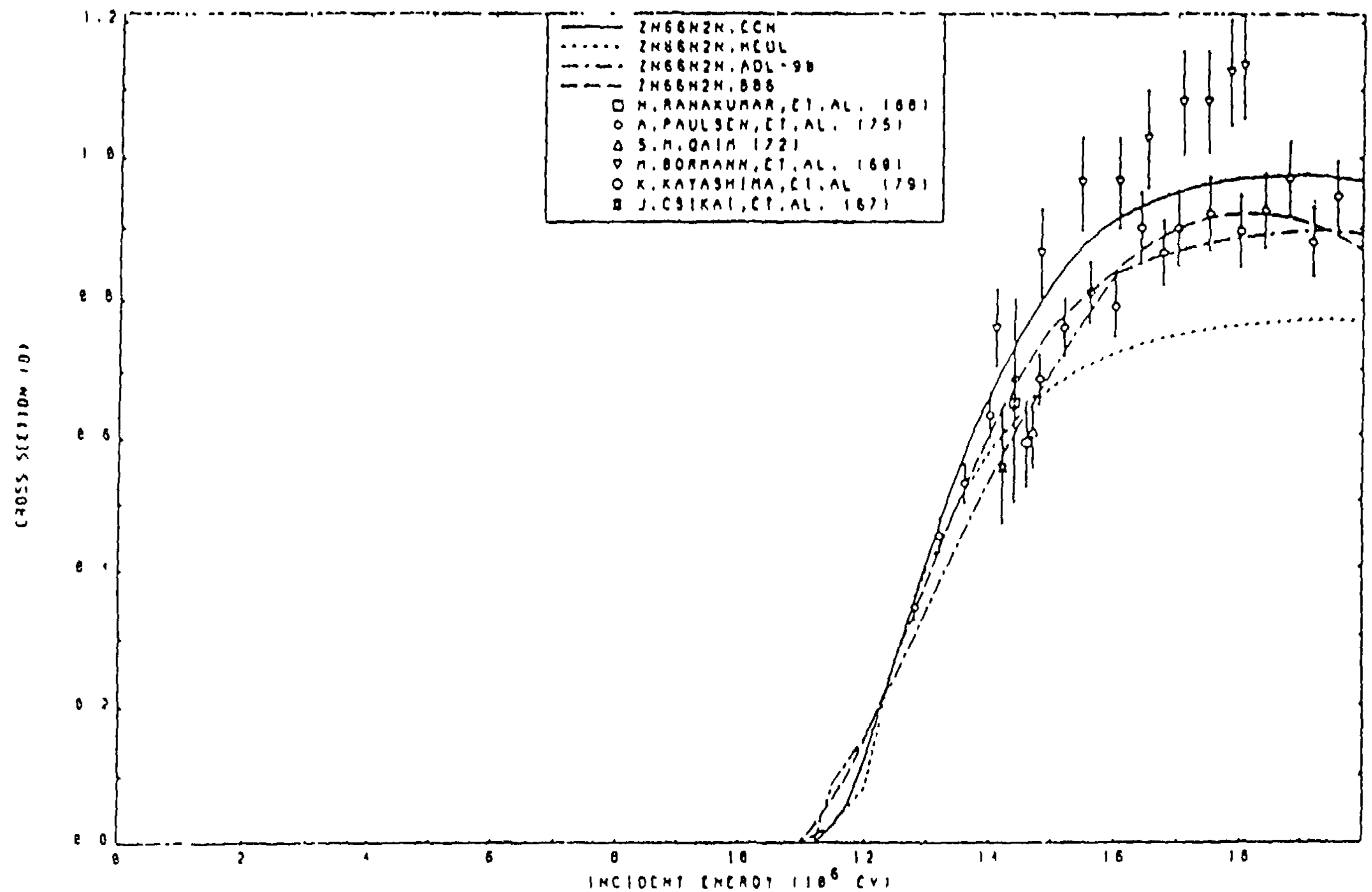

Fig. 4 Comparison of $^{66}Zn(n,2n)^{65}Zn$ cross sections from various activation data files [21]