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INTERNATIONAL ATOMIC ENERGY AGENCY

NUCLEAR DATA SERVICES

DOCUMENTATION SERIES OF THE IAEA NUCLEAR DATA SECTION

PEND-B6

Point cross-section data files derived from ENDF/B-6 basic data files

S. Ganesan, D.W. Muir and P.K. McLaughlin

Abstract

This document summarizes PEND-B6, a collection of resonance reconstructed (point) data files derived from ENDF/B-6 basic data files. The files are available free of charge from the IAEA Nuclear Data Section upon request.

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IAEA NUCLEAR DATA SECTION, P.O. BOX 100, A-1400 VIENNA

PEND-B6

Point cross-section data files derived from ENDF/B-6 basic data files

S. Ganesan, D.W. Muir and P.K. McLaughlin

At the present, the following two files for U-238 are considered in this document.

File	MAT nuclide	original library	code used	accuracy temperature	resulting file size	for details see page
1	9237 92-U-238	ENDF/B-6	LINEAR + RECENT	0.1 % 0 Kelvin	937 252 records 73 Mbytes	3
2	9237 92-U-238	ENDF/B-6	RECONR module of NJOY89.31	0.5 % 0 Kelvin	148 353 records 12 Mbytes	3

U-238 Point data files from ENDF/B-6

Introduction

The neutron-interaction cross section data of U-238 from ENDF/B-6 have been processed using IBM-3081 mainframe computer at the IAEA Nuclear Data Section (NDS). The file is available free of charge from the NDS on magnetic tape. The point data file at zero Kelvin was generated using both the NJOY 89.31 (Ref. 1) and LINEAR/RECENT (Ref. 2) code systems. Some differences were noted in the results of the two code systems.

Computer time:

The processing of ENDF/B-6 data for U-238 for the generation of PENDF file using NJOY 89.31 and the point file using LINEAR/RECENT code system turned out to be a very costly, requiring up to 20 hours of CPU time on the relatively fast IBM-3081 mainframe (14 MIPs).

The reason for the large running time is the presence of a large number of resonances in the resolved-resonance region, which extends upto 16.4 keV. The Reich-Moore formalism is employed in ENDF/B-6 for representing resonances in U-238.

The number of resonances are as follows:

Neutron angular momentum (ℓ)	No. of resonances
0 (s-wave)	801
1 (p-wave)	1 112

The last resolved s-wave resonance is at 16.393 keV and the last p-wave resonance (ℓ = 1) is at 14.1076 keV. Unresolved-resonance parameters are provided from 10 keV to 149.029 keV.

While LINEAR was run with 0.1 % accuracy followed by RECENT with 0.1 % accuracy, the code NJOY 89.31 was run with 0.5 % accuracy (by setting the input parameter ERR=0.005).

The CPU times used are as follows:

RECENT	1 172 minutes
RECONR	156 minutes.

In the case of RECONR, the module of NJOY that reconstructs resonance cross sections, default values were taken for both the resonance-integral check tolerance (ERRINT) and the maximum resonance-integral error (ERRMAX). The two results should, in principle, agree within the reconstruction tolerances specified. It was seen however that significant differences existed between these output files.

The sizes of the files obtained using RECONR of NJOY and RECENT are given below.

NJOY : Number of resonance points: 87 620

RECENT: total : 557 871 points
elastic: 557 949 points
capture: 557 883 points

Size of the PENDF file from RECONR: 148 353 cards

Size of the RECENT output file : 937 252 cards.

The size of data for individual reactions are enclosed.

The large number of energy points generated by RECENT is due to the combination of two effects. First a tighter error tolerance was employed (0.1 % vs. 0.5 %). Secondly unlike RECENT, RECONR treats the energy variable in single precision. This, in turn, requires that on our 32-bit computer, no more than 6 digits can be used by RECONR to represent any energy point. It is interesting to note that the ratio of running times of the two processing codes very nearly equal the ratio of the number of energy points generated.

Enclosed are the outputs of MERGER code giving details of reactions and number of records for the point data files.

Using COMPLOT program (Ref. 2) comparisons were made between RECENT output and RECONR output. The comparison graphs obtained using COMPLOT program are self-explanatory and are appended to this note.

Presently the authors of these two code systems have been informed about the differences in results. Until the reasons for the differences are fully understood, it is important to treat the following remarks as preliminary introductory in nature.

(1) The sharp resonances at high energies do not get represented completely adequately in the single precision NJOY calculation. It is well known that this difference between NJOY and RECENT does not significantly affect the group cross sections but may lead to different temperature dependence of self shielded cross sections (see for example ref. 3).

(2) There are a few-percent differences in the capture cross sections in the unresolved-resonance region. These differences which are exhibited also at the 640 group level are yet to be clearly understood.

References

(1) R.E. MacFarlane, D.W. Muir and R.M. Boicourt
The NJOY Nuclear Data Processing System, Volume II: The NJOY, RECONR, BROADR, HEATR, and THERMR Modules, LA-9303-M, Vol. II (ENDF-324), Los Alamos National Laboratory, May 1982

(2) D. E. Cullen, P. K. McLaughlin, S. Ganesan
The 1989 ENDF Pre-processing codes, IAEA-NDS-39 Rev. 6, IAEA Nuclear Data Section, Vienna, Austria

(3) S. Ganesan, V. Gopalakrishnan, M.M. Ramanadhan and D.E. Cullen
Verification of the Accuracy of Doppler Broadened, Self-Shielded Multigroup Cross Sections for Fast Power Reactor Applications, Ann. Nucl. Energy, Vol. 15, No. 3, pp. 113-140, 1988

Appendices

```
MERGE ENDF/B DATA INTO MAT/MF/MT ORDER (MERGER 89-1)
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INTERPRETATION OF INPUT PARAMETERS
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MERGED TAPE UNIT NUMBER------          20
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RETRIEVAL REPORT UNIT NUMBER-           0 (REPORT WILL NOT BE WRITTEN)
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E6 U238 RECENT OUTPUT                                                  2000
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---------------------------------------------------------------------------
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TAPE CARDS 937252

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MERGED SECTIONS---- 115
MERGED CARDS------- 937252

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NOTE..THE CARD COUNT OF RETRIEVED DATA FOR EACH REQUEST DOES NOT INCLUDE FEND, MEND AND TEND CARDS. THEREFORE THE TOTAL NUMBER OF CARDS ACTUALLY RETRIEVED AND WRITTEN ON THE MERGED TAPE WILL BE MORE THAN THE SUM OF THE NUMBER OF CARDS FOR ALL REQUESTS.

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MERGE ENDF/B DATA INTO MAT/MF/MT ORDER (MERGER 89-1)
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MAT CARDS 148351

TAPE CARDS 148353

RETRIEVAL STATISTICS

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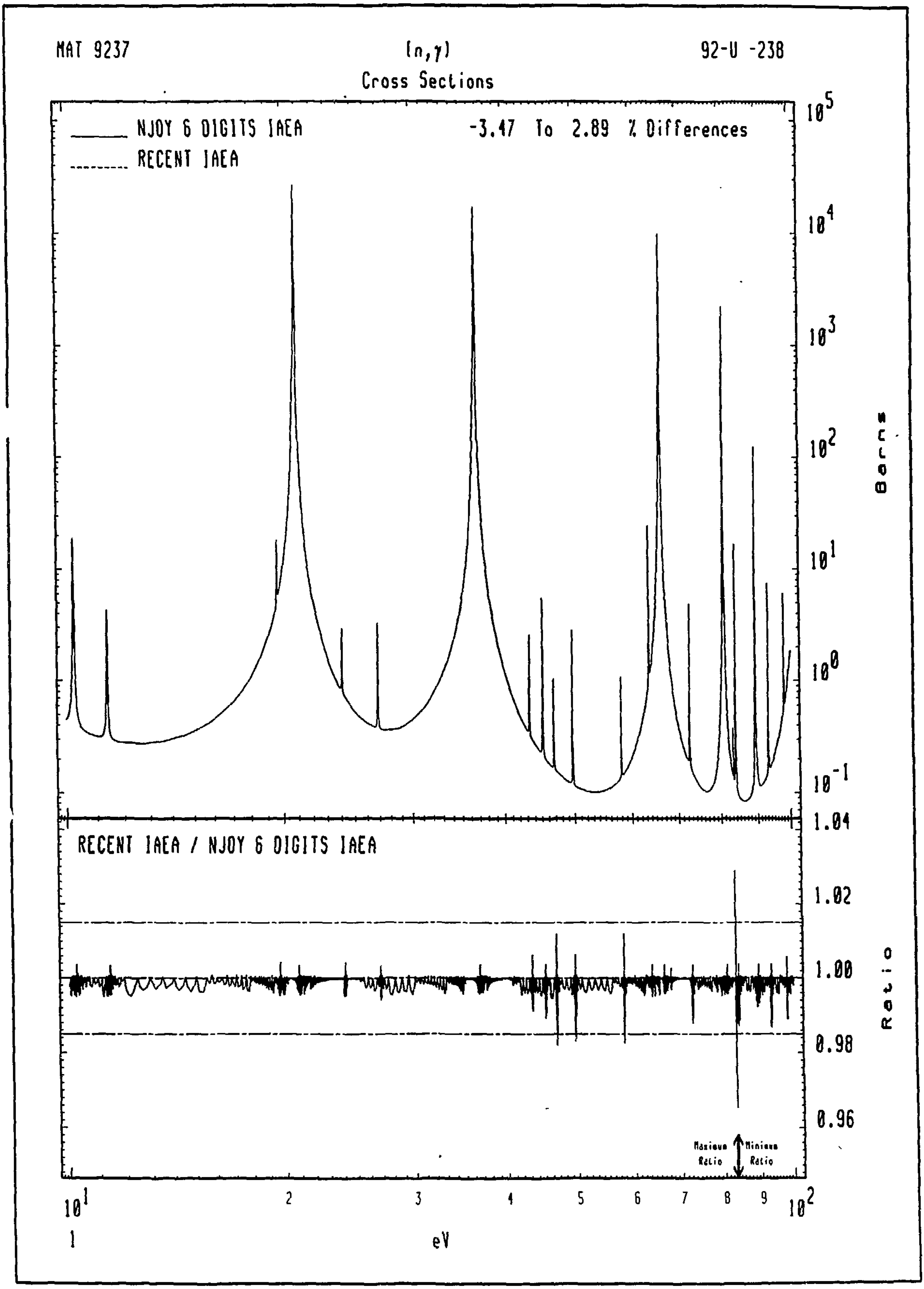
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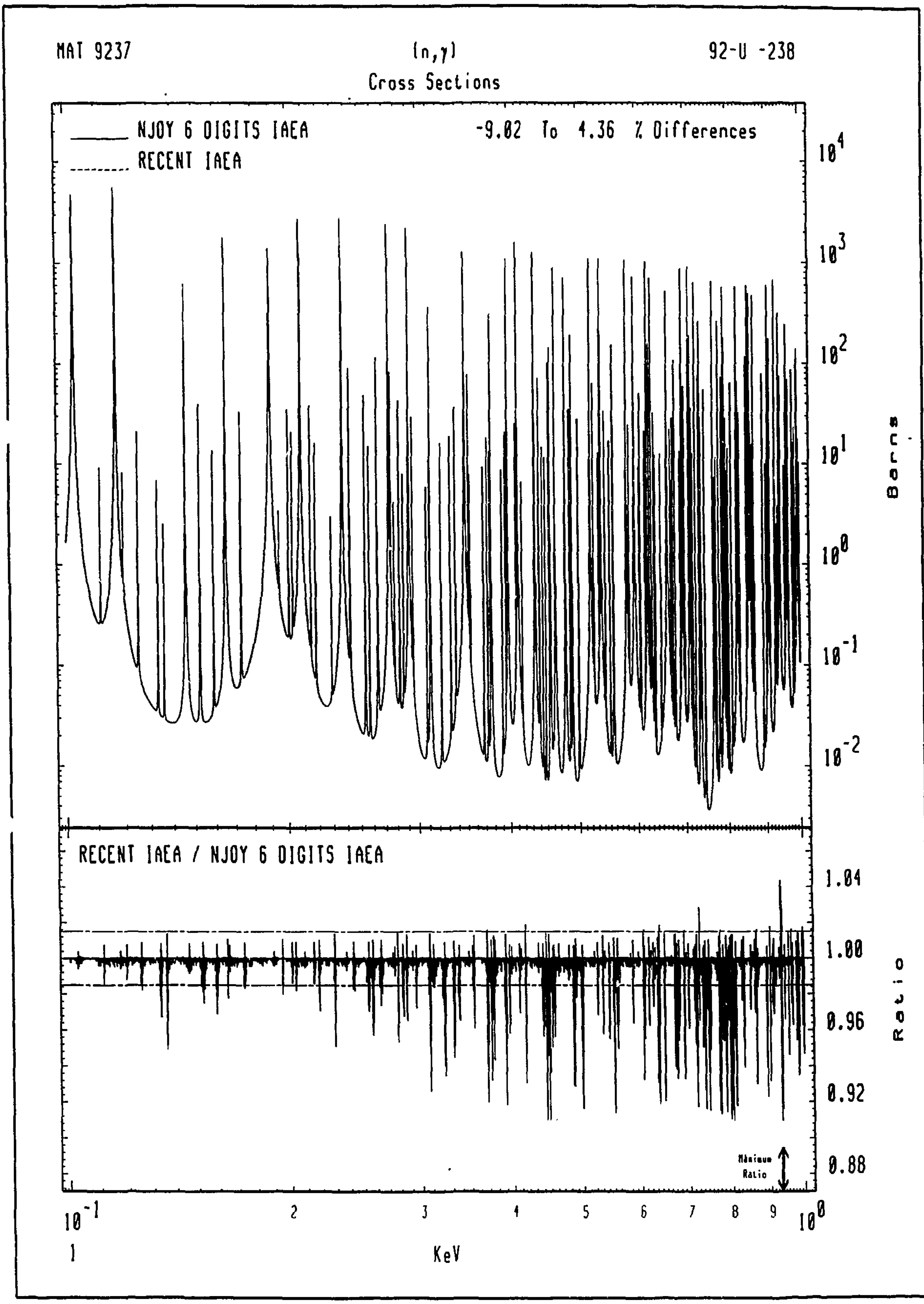
92-U -238
Cross Sections
NJOY 6 DIGITS IAEA
RECENT IAEA
-3.47 To 2.89 % Differences
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA
Ratio
Maximum Ratio
Minimum Ratio
eV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(n,γ)
92-U -238
Cross Sections
NJOY 6 DIGITS IAEA
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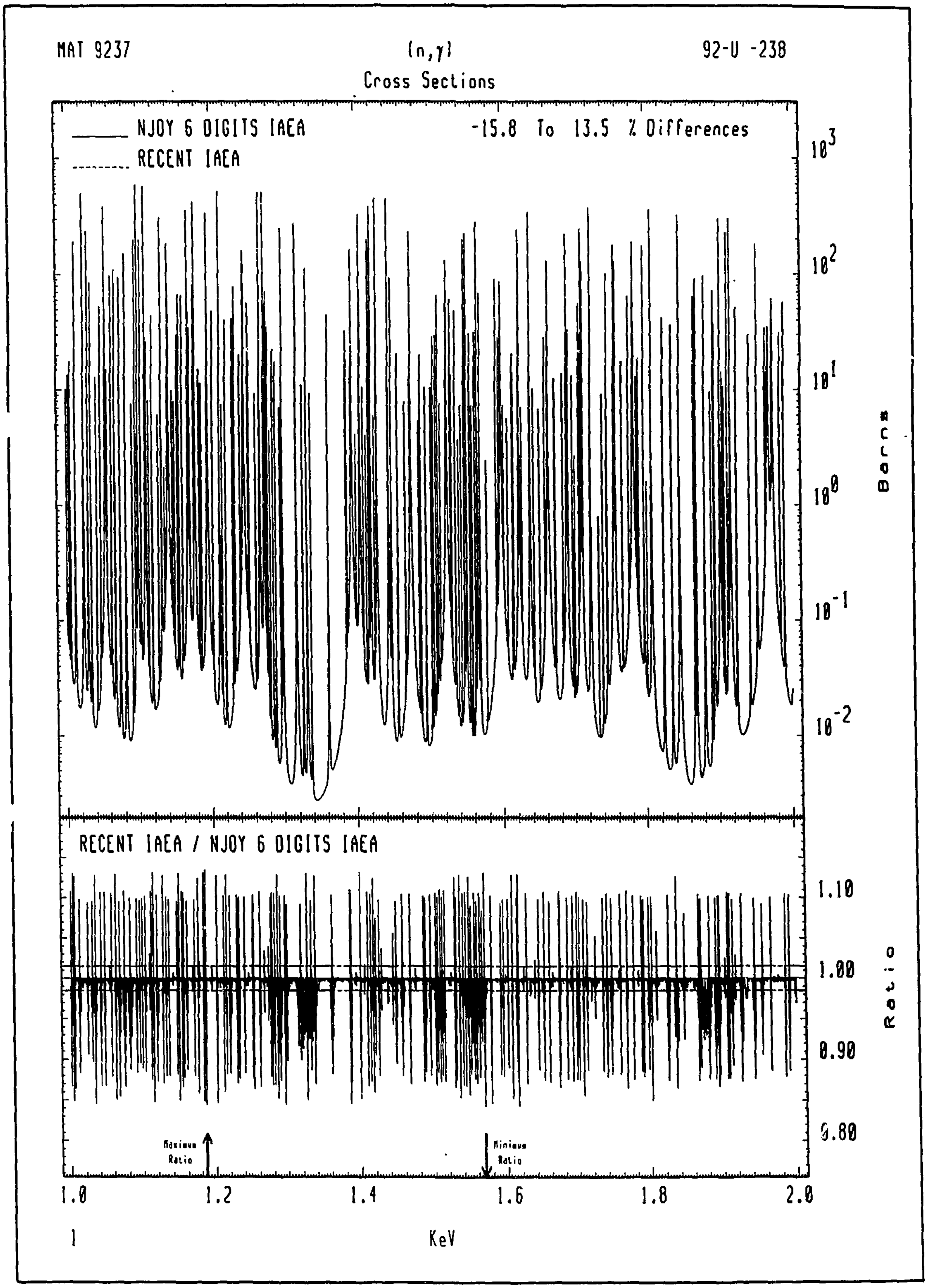
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA
Ratio
Maximum Ratio
KeV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(n,γ)
92-U -238
Cross Sections
NJOY 6 DIGITS IAEA
RECENT IAEA
-15.8 To 13.5 % Differences
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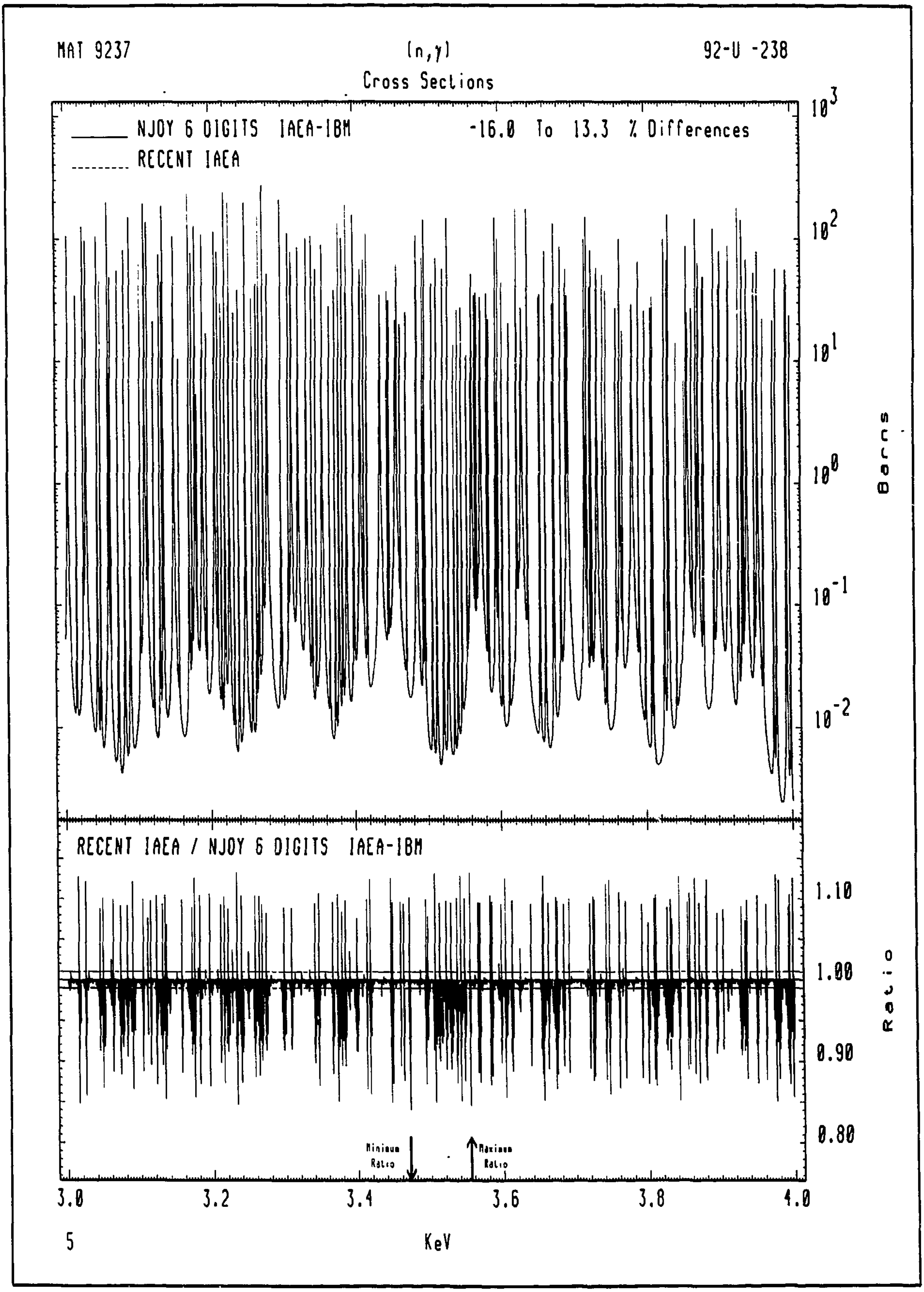
10^2
10^1
10^0
10^-1
10^-2
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA
1.10
1.00
0.90
0.80
Ratio
Maximum Ratio
Minimum Ratio
1.0
1.2
1.4
1.6
1.8
2.0
1
KeV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(n,γ)
92-U -238
Cross Sections
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RECENT IAEA
-16.0 To 13.3 % Differences
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10^2
10^1
10^0
10^-1
10^-2
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.10
1.00
0.90
0.80
Ratio
Minimum Ratio
Maximum Ratio
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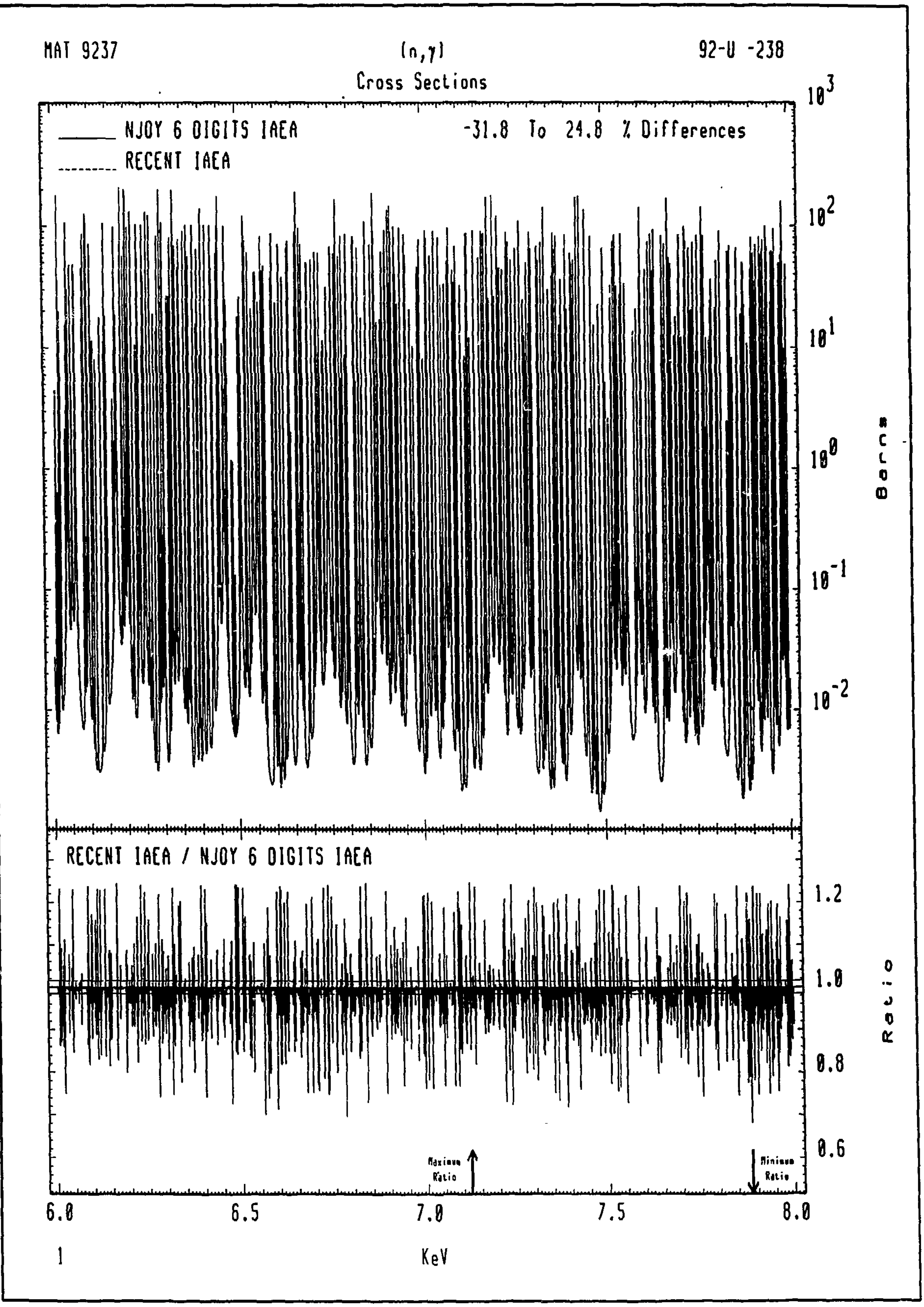
3.2
3.4
3.6
3.8
4.0
5
KeV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(n,γ)
92-U -238
Cross Sections
NJOY 6 DIGITS IAEA
RECENT IAEA
-31.8 To 24.8 % Differences
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10^2
10^1
10^0
10^-1
10^-2
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA
1.2
1.0
0.8
0.6
Ratio
Maximum Ratio
Minimum Ratio
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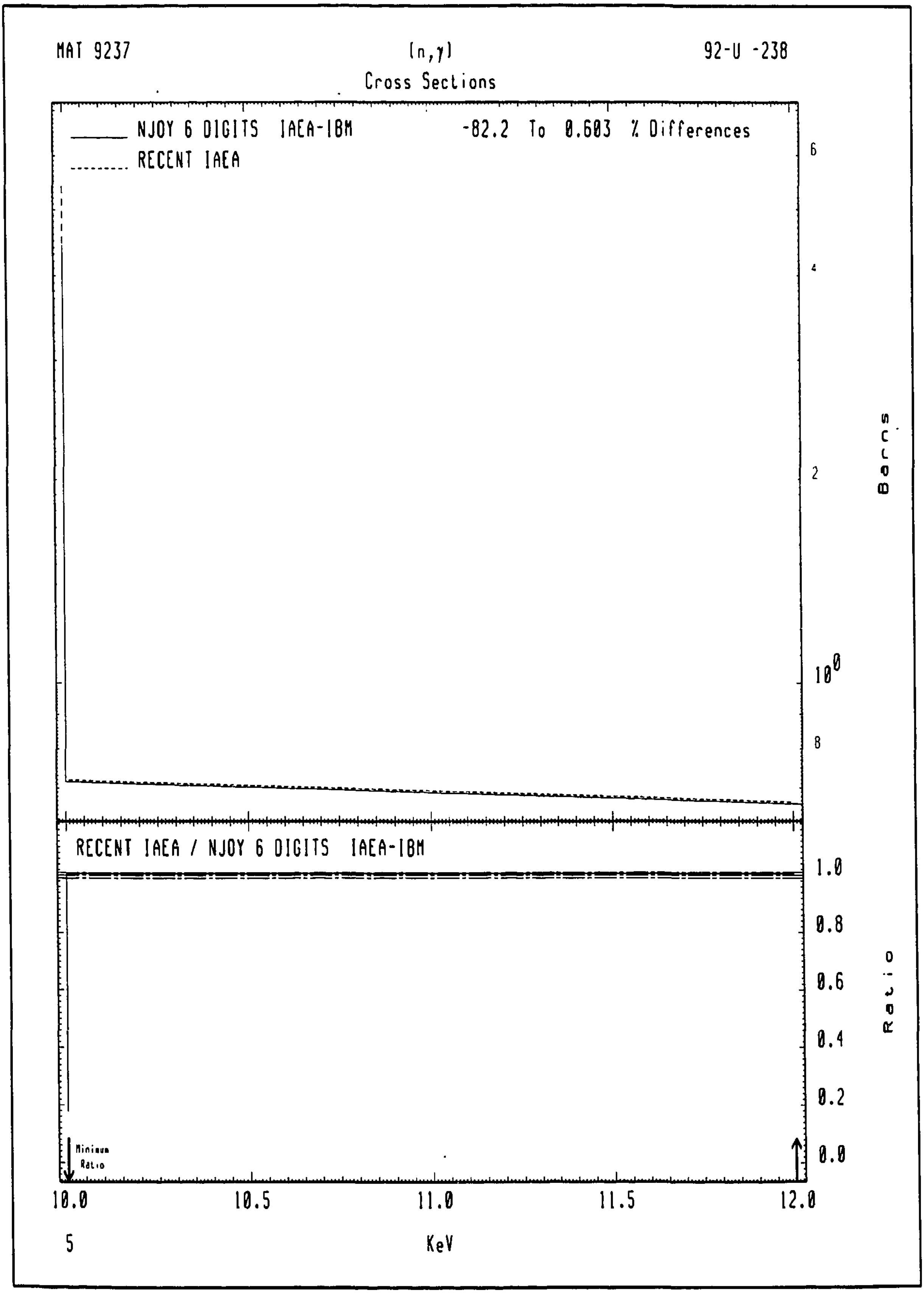
6.5
7.0
7.5
8.0
1
KeV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(n,γ)
92-U -238
Cross Sections
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-82.2 To 0.603 % Differences
6
4
2
10^0
8
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.0
0.8
0.6
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0.2
0.0
Ratio
Minimum Ratio
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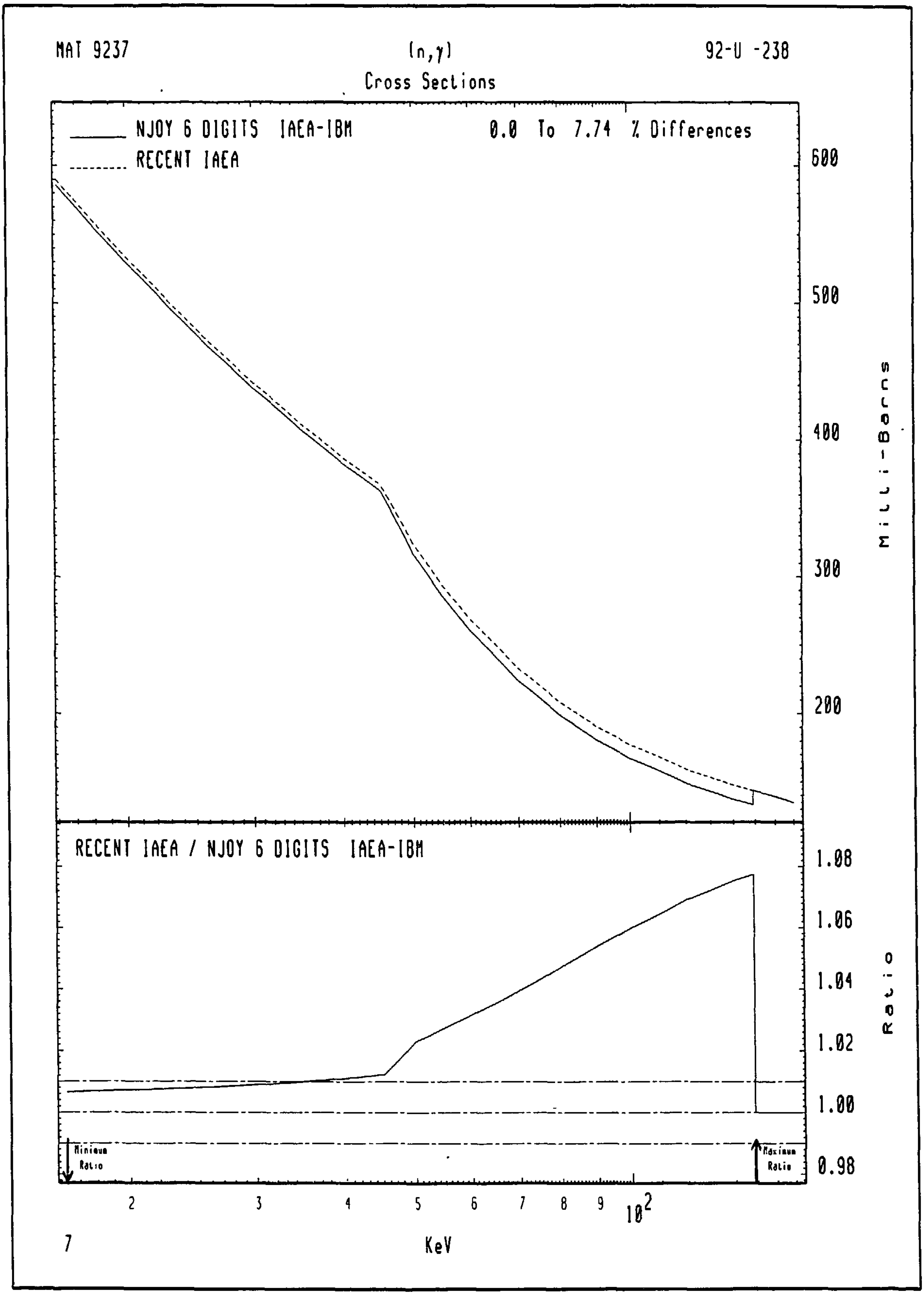
10.5
11.0
11.5
12.0
5
KeV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(n,γ)
92-U -238
Cross Sections
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
0.0 To 7.74 % Differences
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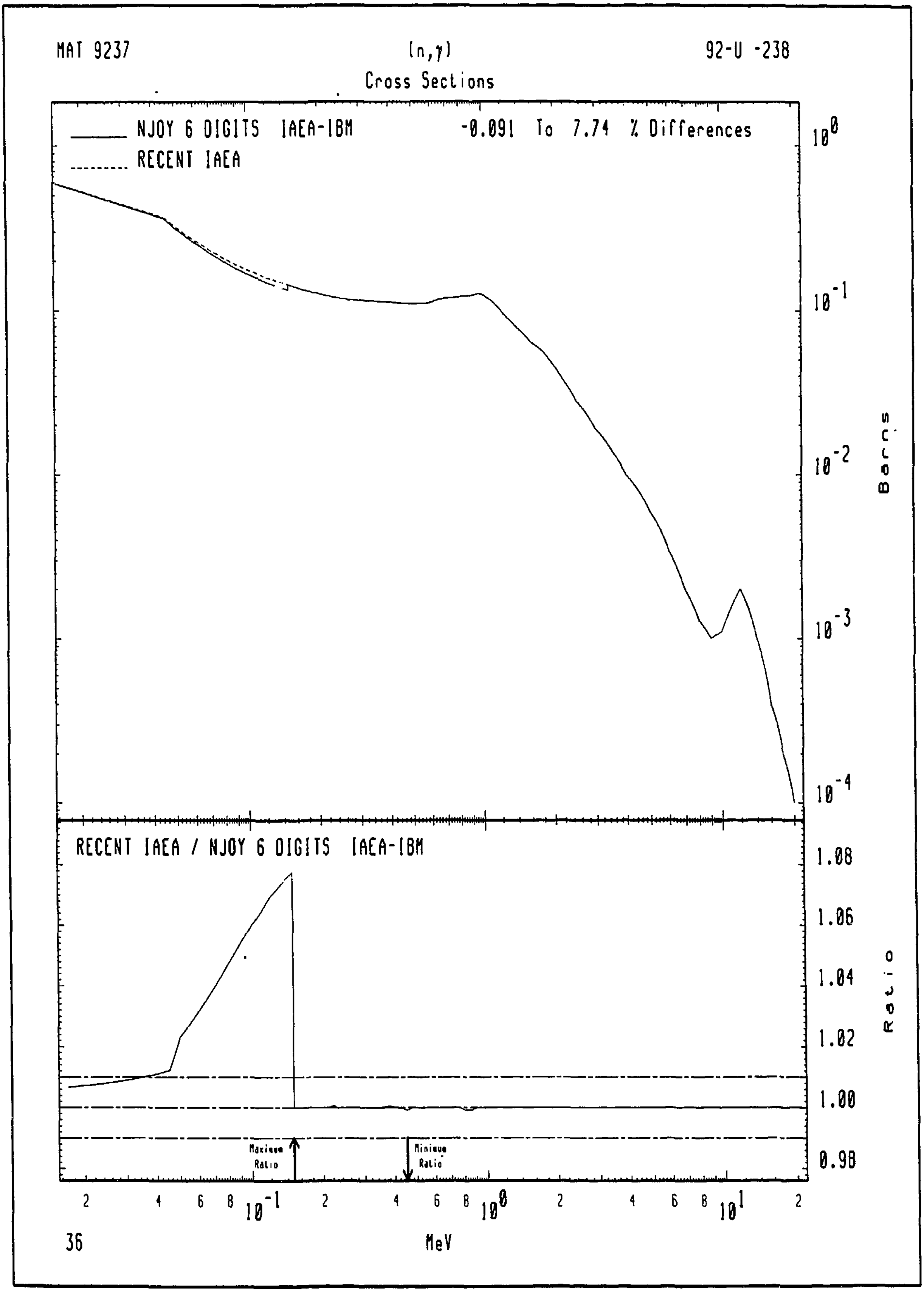
500
400
300
200
Milli-Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.08
1.06
1.04
1.02
1.00
0.98
Ratio
Minimum Ratio
Maximum Ratio
2
3
4
5
6
7
8
9
10^2
7
KeV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(n,γ)
92-U -238
Cross Sections
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RECENT IAEA
-0.091 To 7.74 % Differences
10^0
10^-1
10^-2
10^-3
10^-4
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.08
1.06
1.04
1.02
1.00
0.98
Ratio
Maximum Ratio
Minimum Ratio
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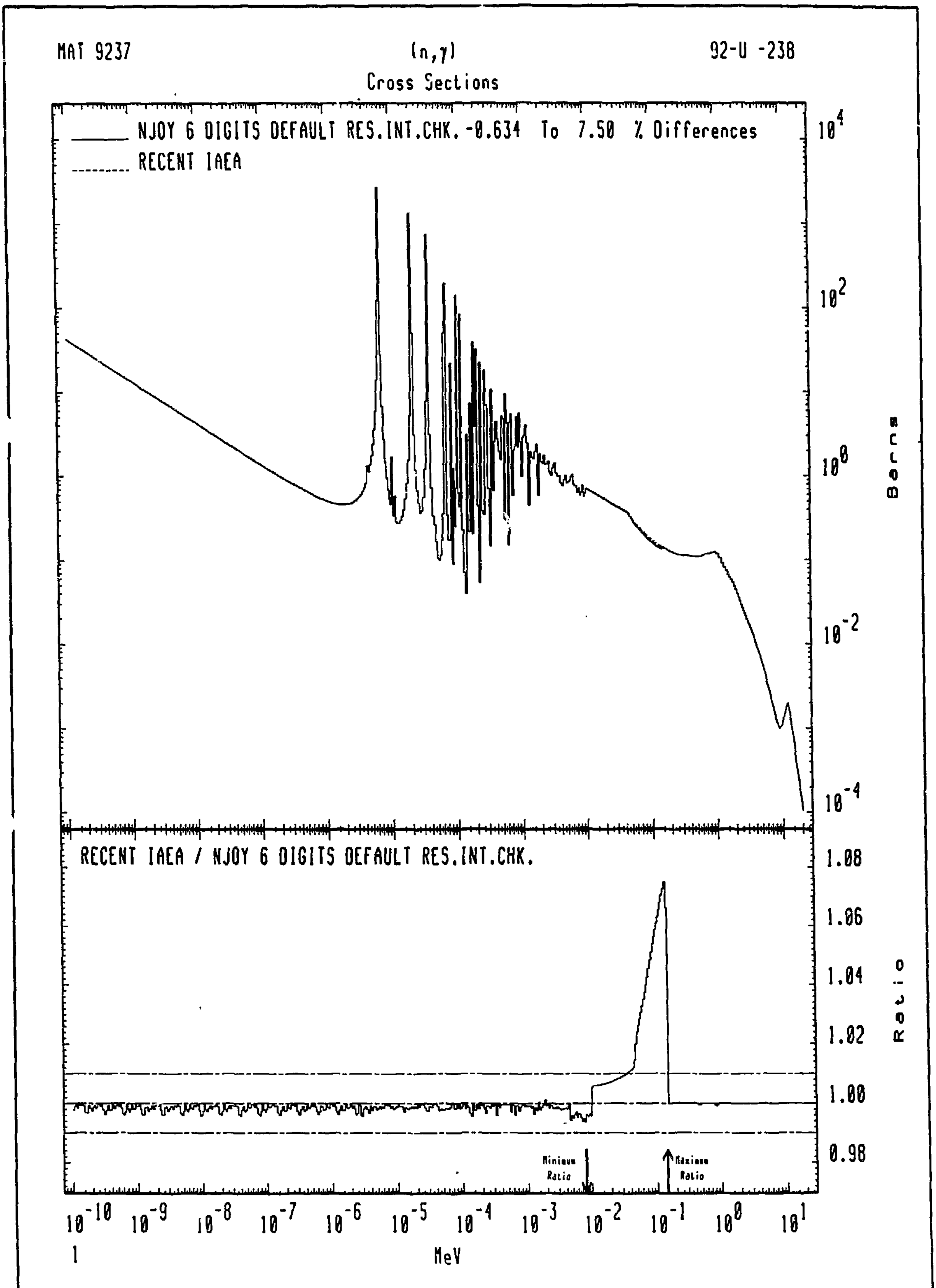
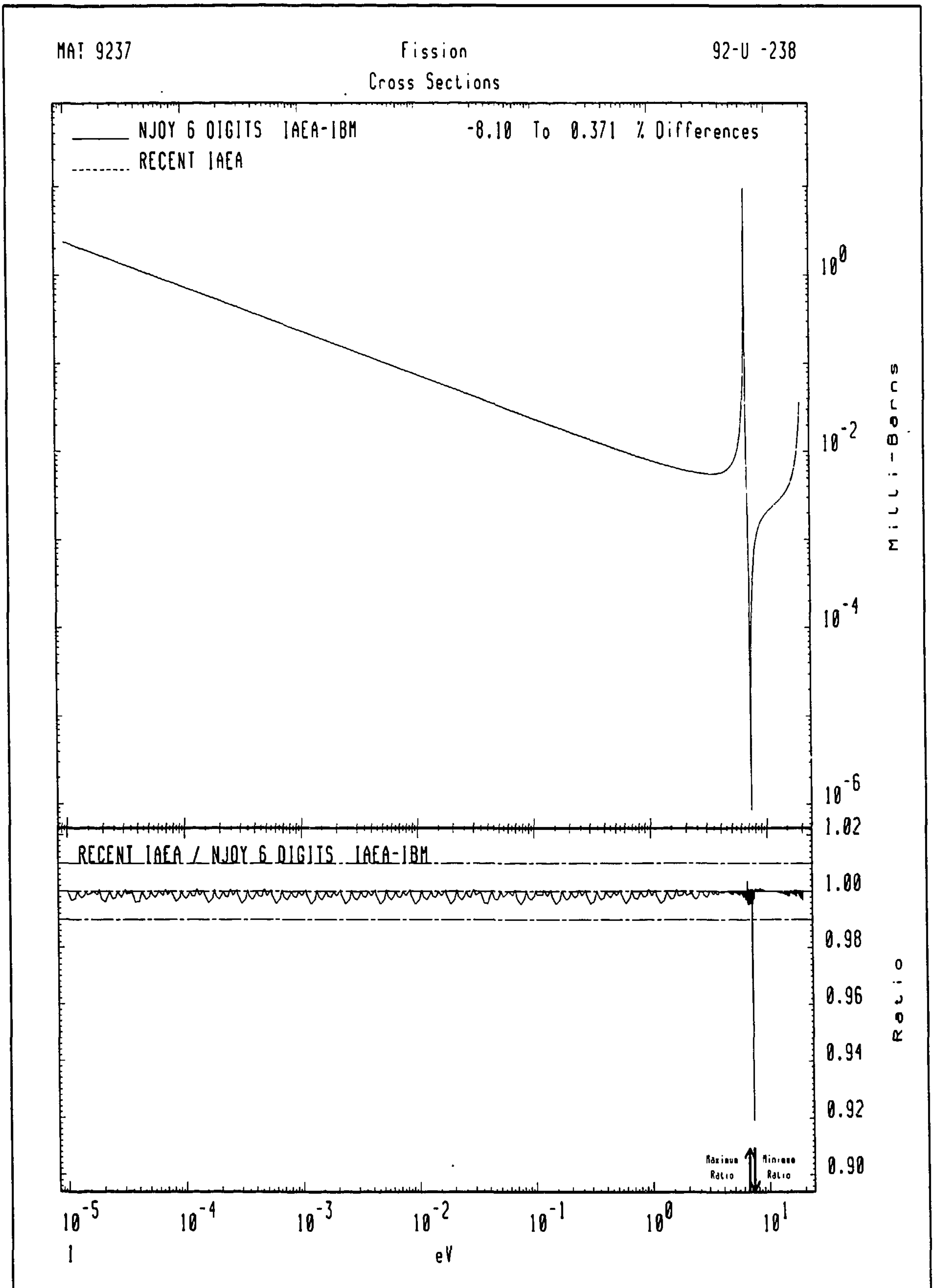
36
MeV



MAT 9237
(n,γ)
92-U -238
Cross Sections
NJOY 6 DIGITS DEFAULT RES.INT.CHK. -0.634 To 7.50 % Differences
RECENT IAEA
RECENT IAEA / NJOY 6 DIGITS DEFAULT RES.INT.CHK.
10^4
10^2
10^0
10^-2
10^-4
Barns
1.08
1.06
1.04
1.02
1.00
0.98
Ratio
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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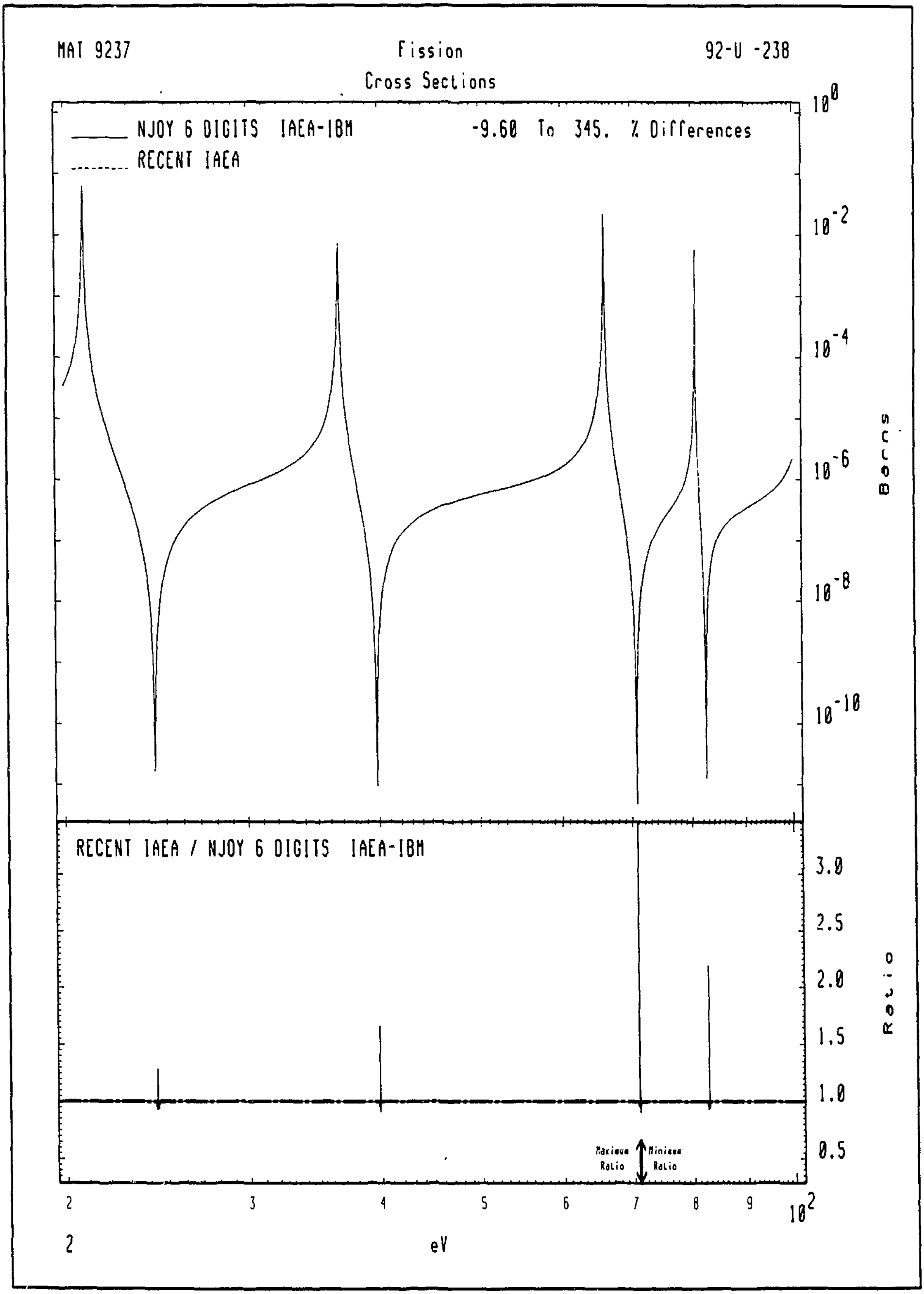
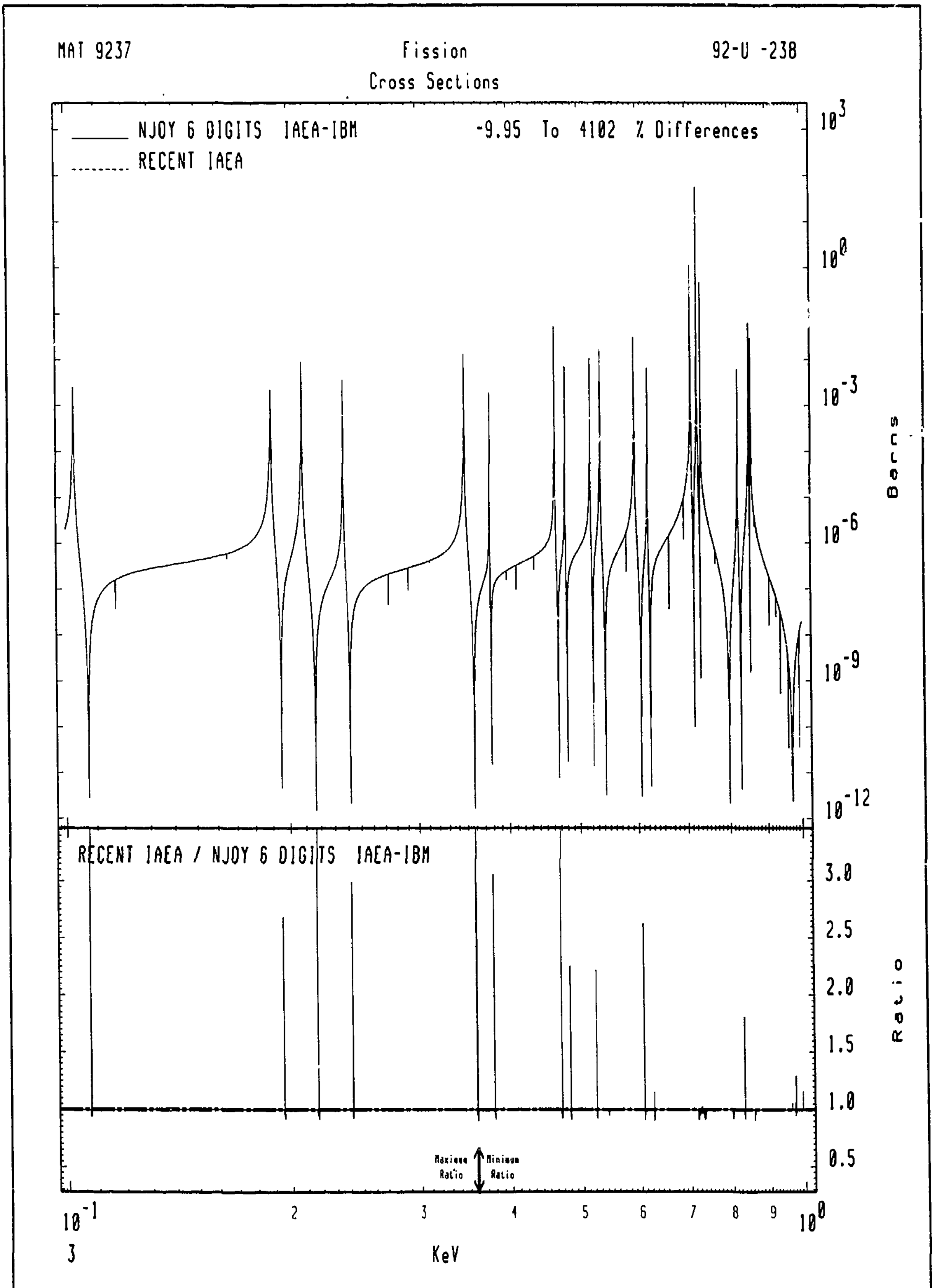
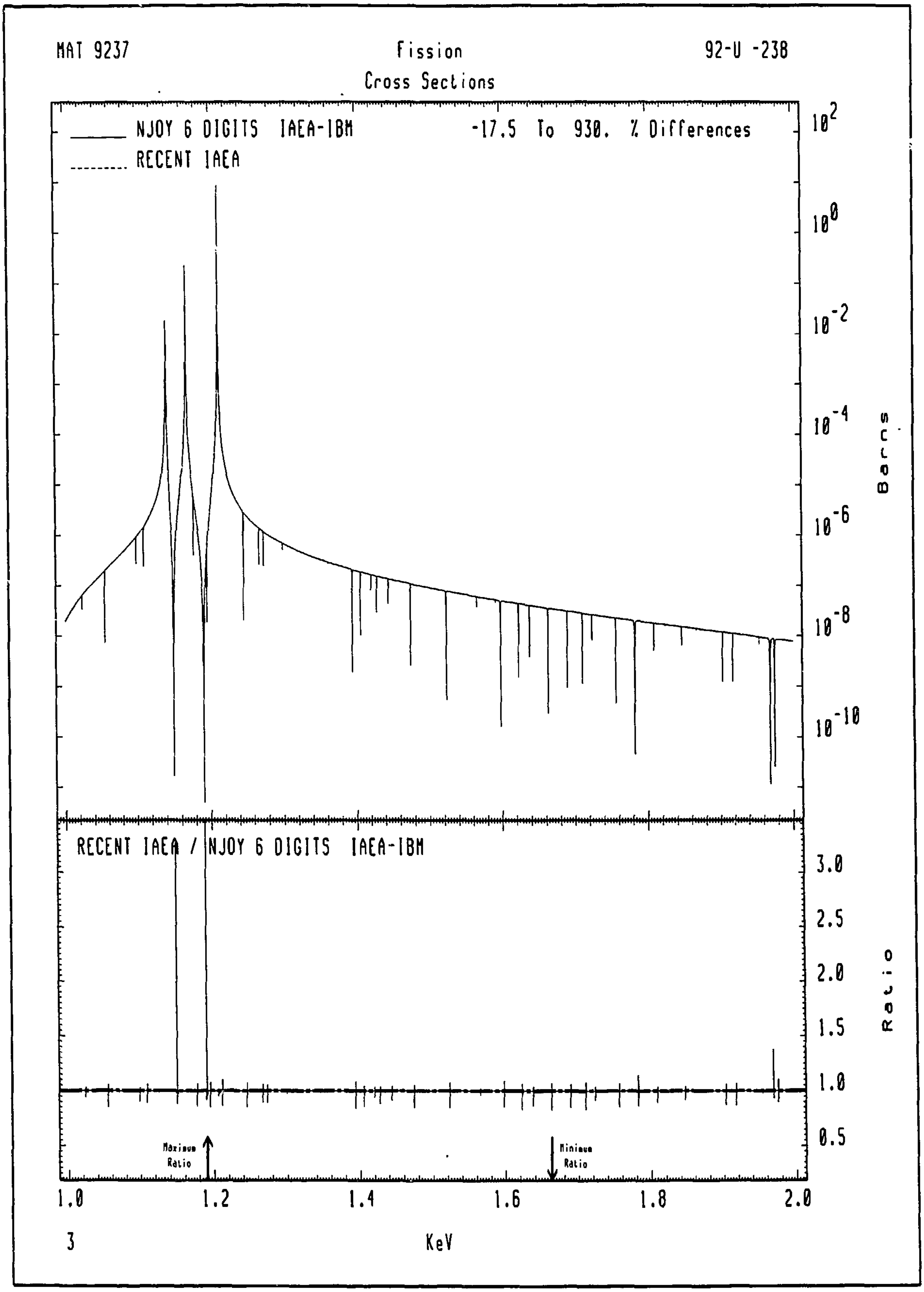
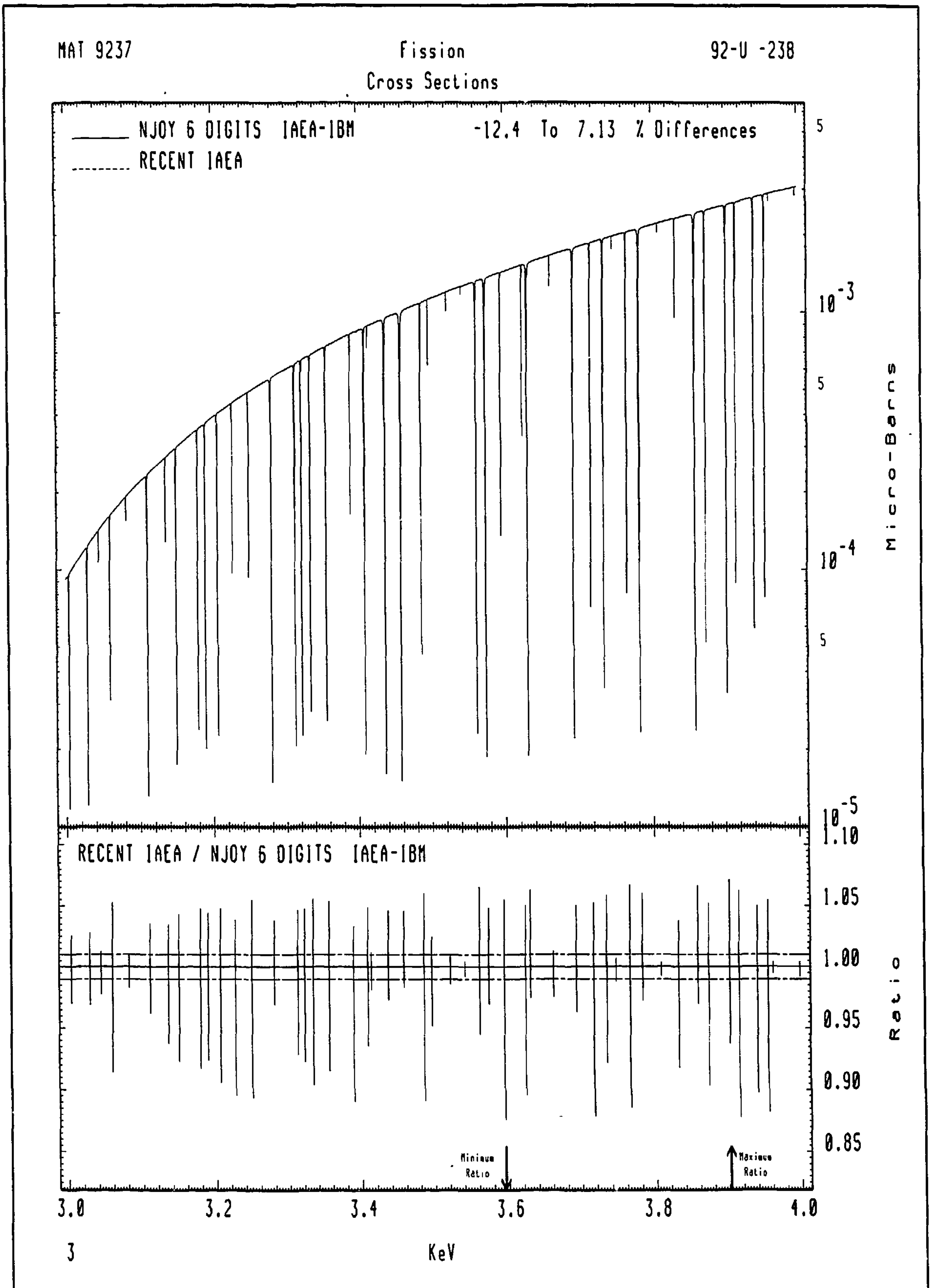
Fission
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-8.10 To 0.371 % Differences
Milli-Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
Ratio
1.02
1.00
0.98
0.96
0.94
0.92
0.90
Maximum Ratio
Minimum Ratio
eV

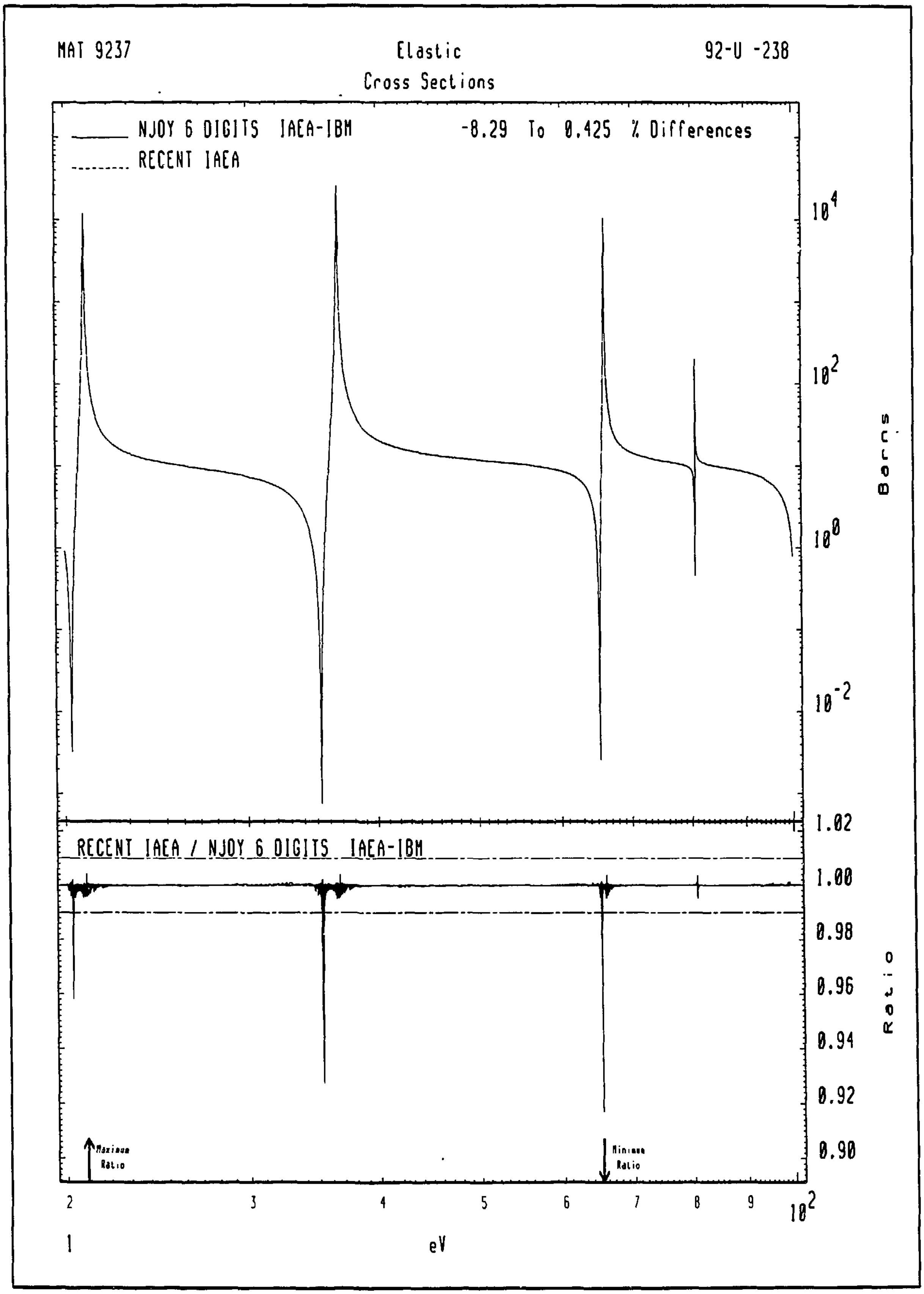

MAT 9237
Fission
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-9.60 To 345. % Differences
10^0
10^-2
10^-4
10^-6
10^-8
10^-10
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
3.0
2.5
2.0
1.5
1.0
0.5
Ratio
Maximum Ratio
Minimum Ratio
2
3
4
5
6
7
8
9
10^2
2
eV

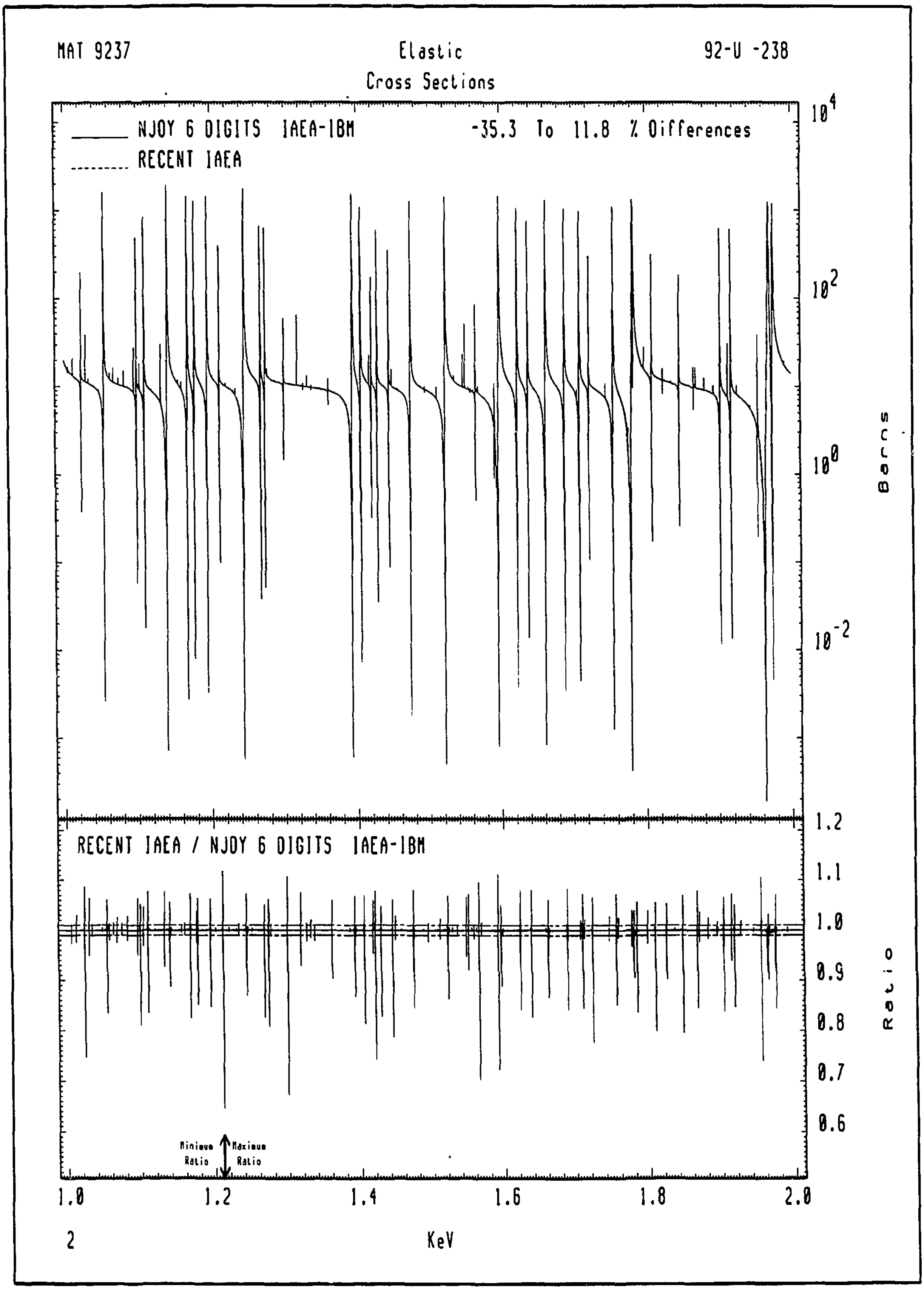

MAT 9237
Fission
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-9.95 To 4102 % Differences
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
Maximum Ratio
Minimum Ratio
Barns
Ratio
KeV
10^{3}
10^{0}
10^{-3}
10^{-6}
10^{-9}
10^{-12}
3.0
2.5
2.0
1.5
1.0
0.5
10^{-1}
2
3
4
5
6
7
8
9
10^{0}
3

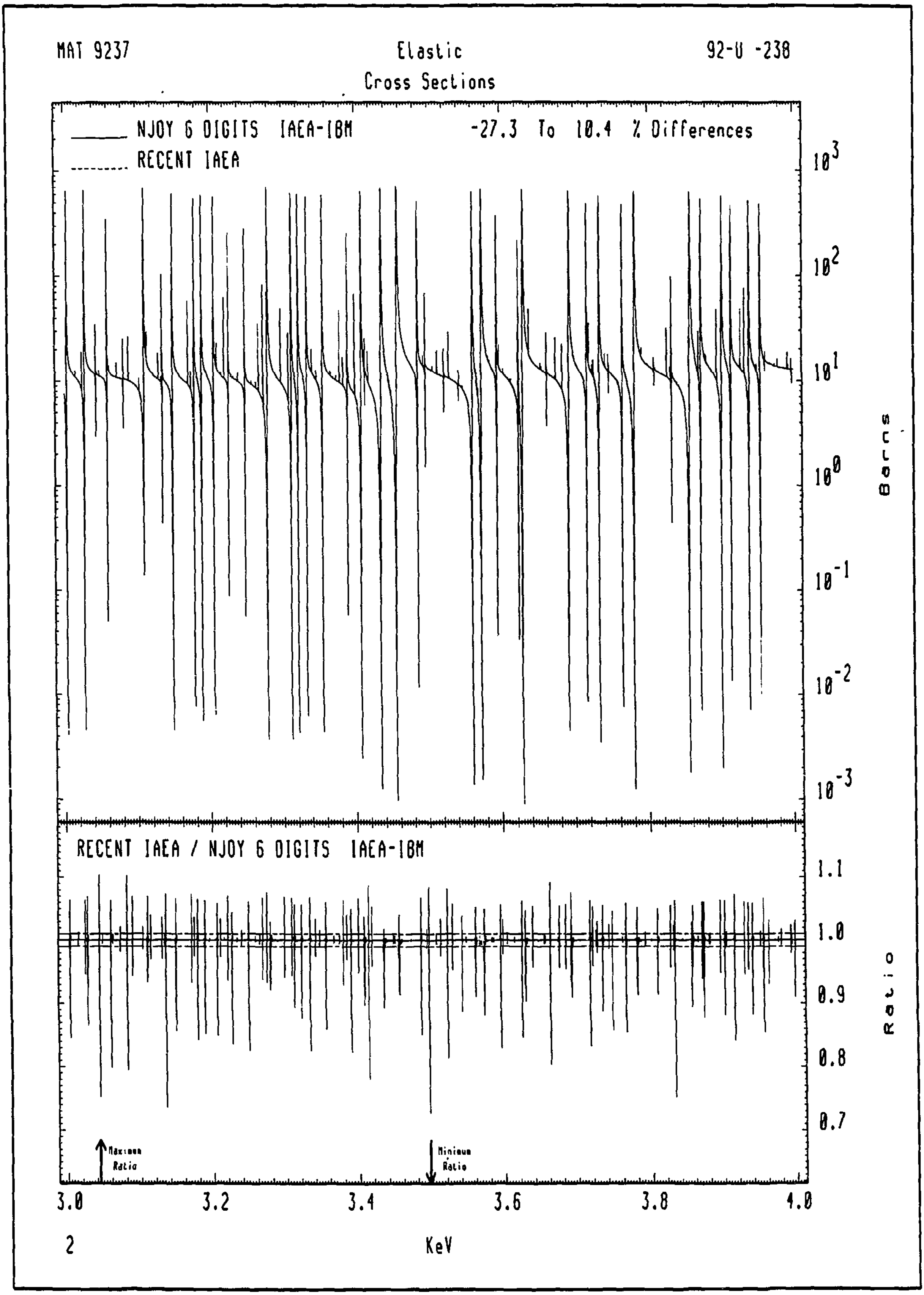

MAT 9237
Fission
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-17.5 To 930. % Differences
10^2
10^0
10^-2
10^-4
10^-6
10^-8
10^-10
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
3.0
2.5
2.0
1.5
1.0
0.5
Ratio
Maximum Ratio
Minimum Ratio
1.0
1.2
1.4
1.6
1.8
2.0
3
KeV

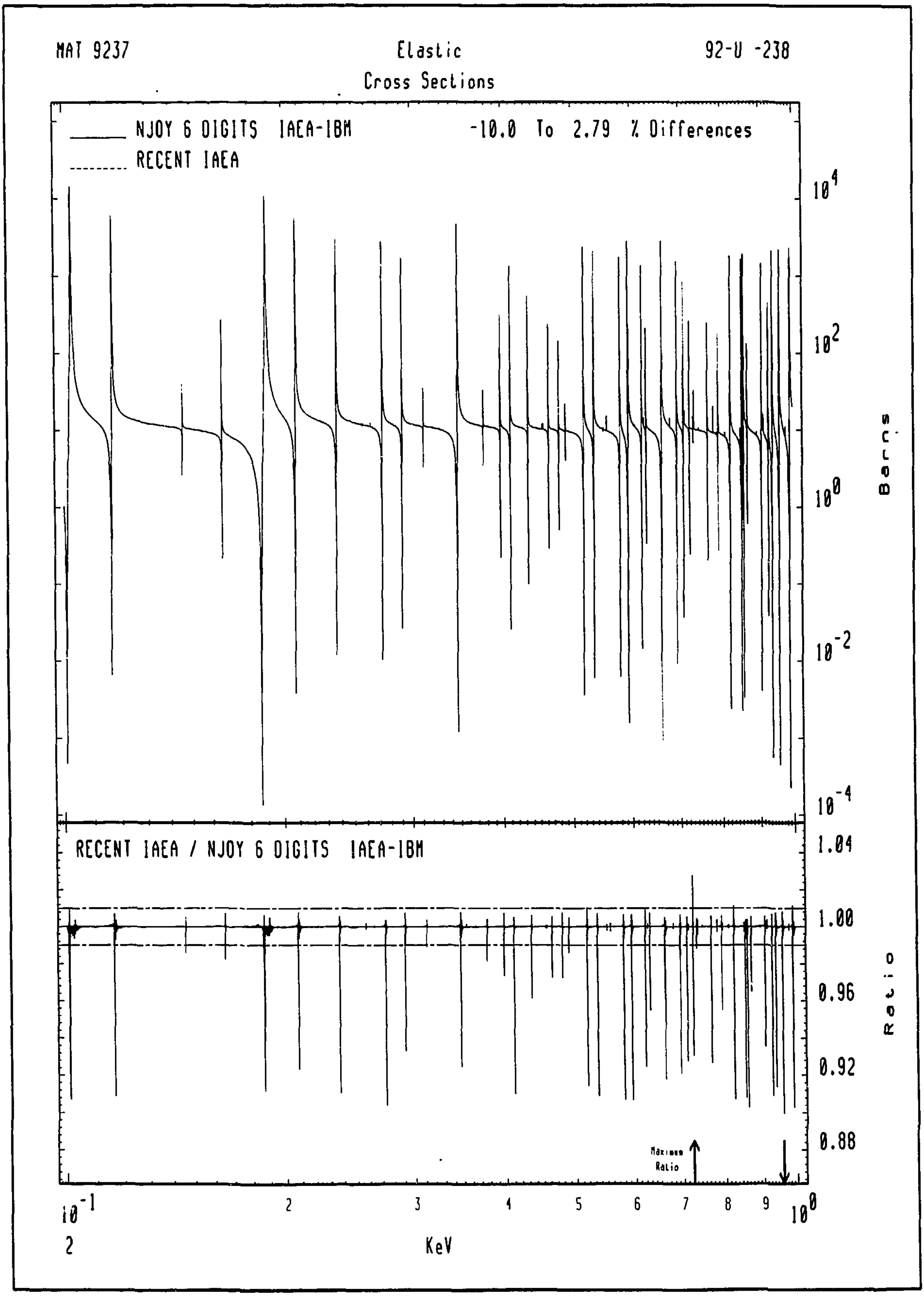
H T 728

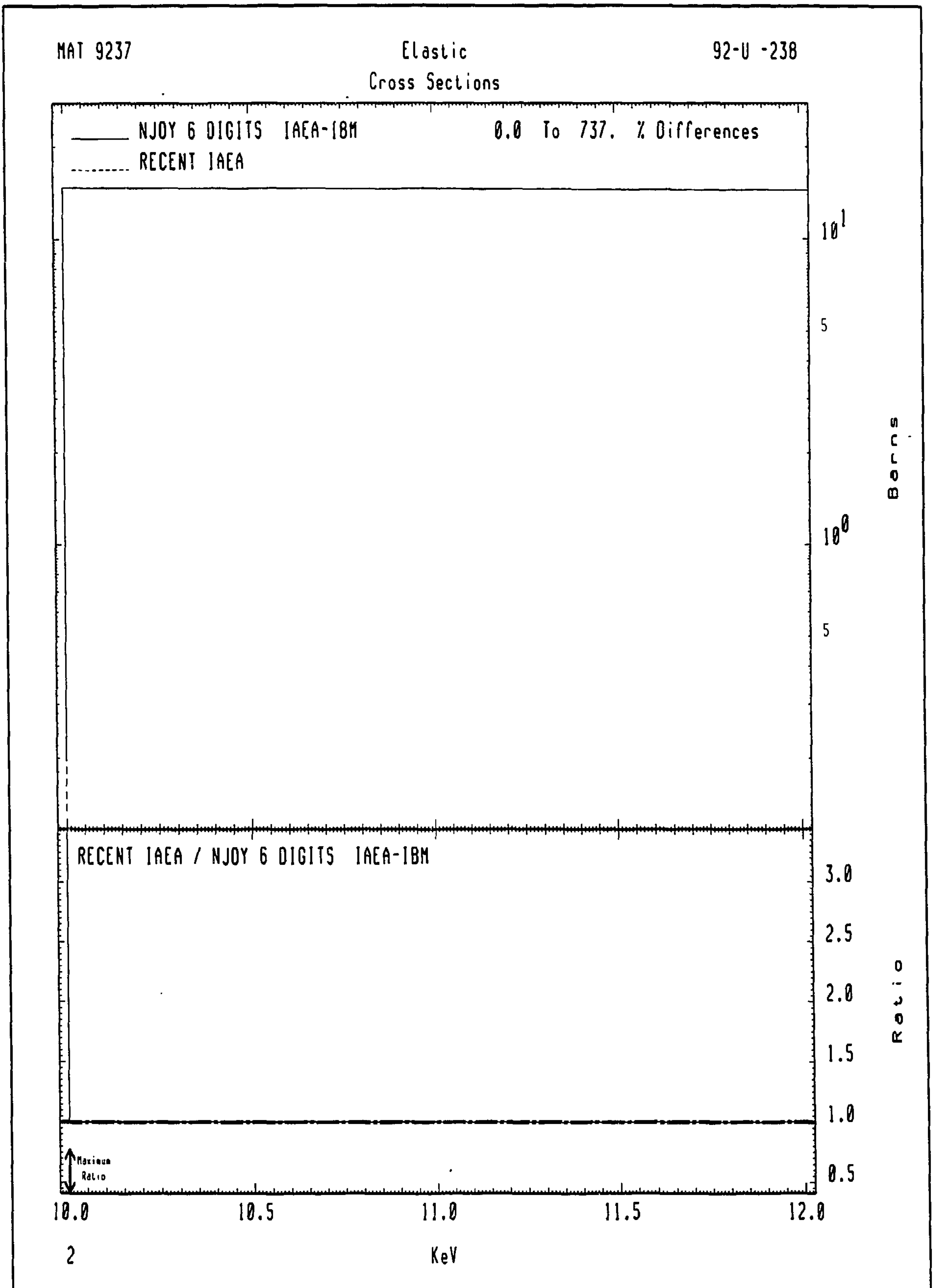

MAT 9237
Fission
92-U -238
Cross Sections
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-12.4 To 7.13 % Differences
5
10^-3
5
10^-4
5
10^-5
Micro-Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.10
1.05
1.00
0.95
0.90
0.85
Ratio
Minimum Ratio
Maximum Ratio
3.0
3.2
3.4
3.6
3.8
4.0
3
KeV

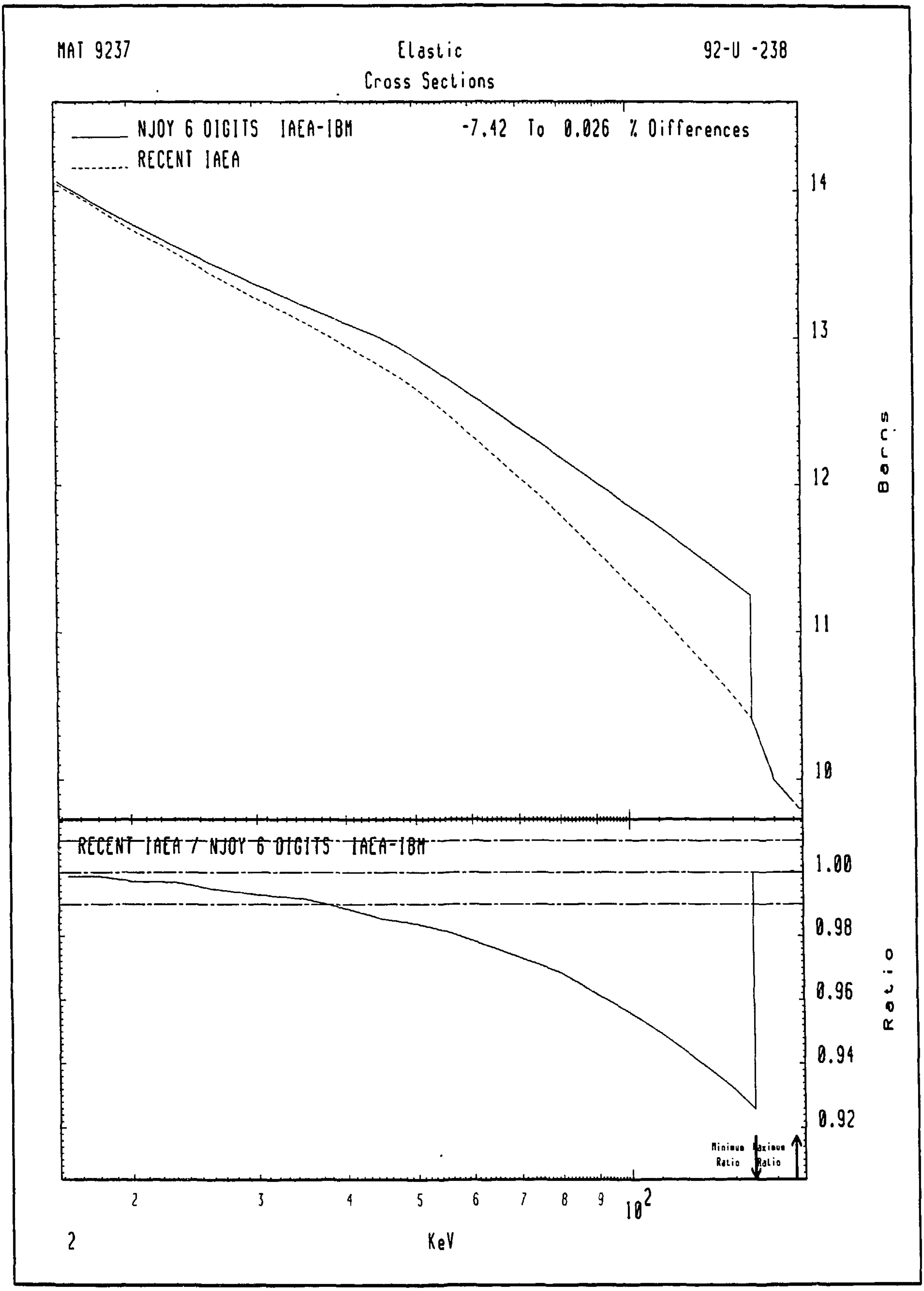

MAT 9237
Elastic
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-8.29 To 0.425 % Differences
10^4
10^2
10^0
10^-2
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.02
1.00
0.98
0.96
0.94
0.92
0.90
Ratio
Maximum Ratio
Minimum Ratio
2
3
4
5
6
7
8
9
10^2
1
eV

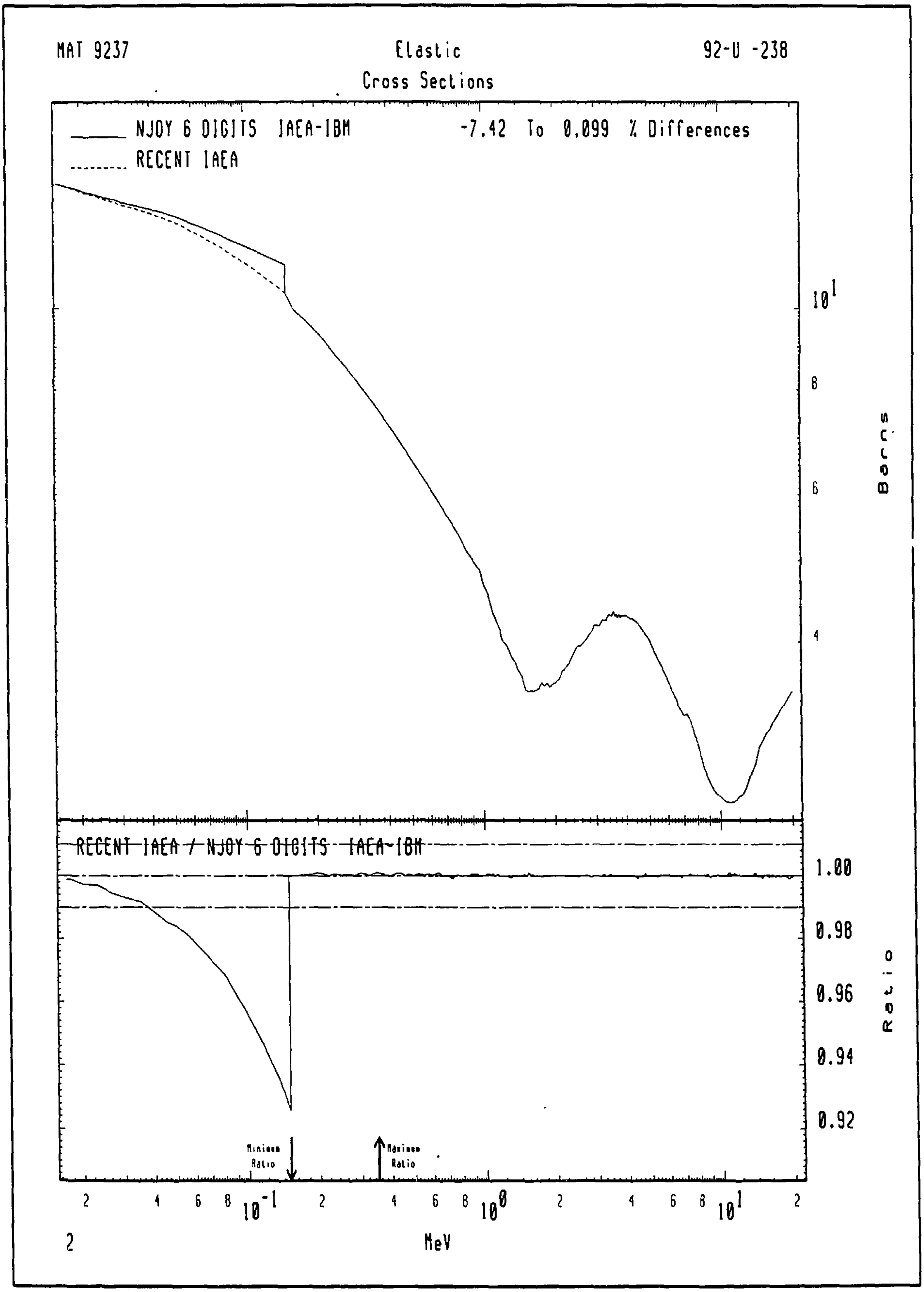

MAT 9237
Elastic
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-35.3 To 11.8 % Differences
10^4
10^2
10^0
10^-2
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.2
1.1
1.0
0.9
0.8
0.7
0.6
Ratio
Minimum Ratio
Maximum Ratio
1.0
1.2
1.4
1.6
1.8
2.0
2
KeV

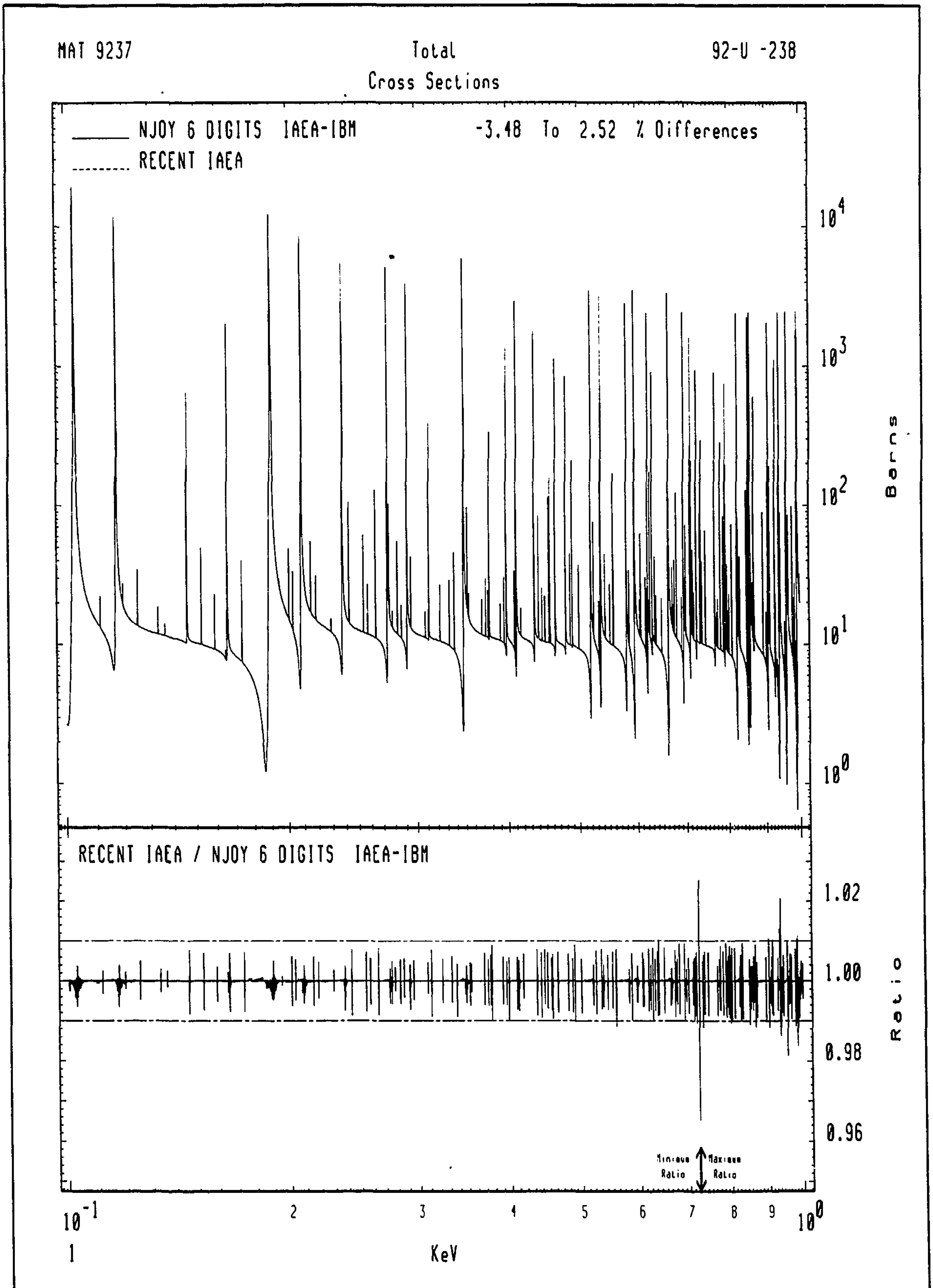

MAT 9237
Elastic
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-27.3 To 10.4 % Differences
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.1
1.0
0.9
0.8
0.7
Ratio
Maximum Ratio
Minimum Ratio
3.0
3.2
3.4
3.6
3.8
4.0
2
KeV

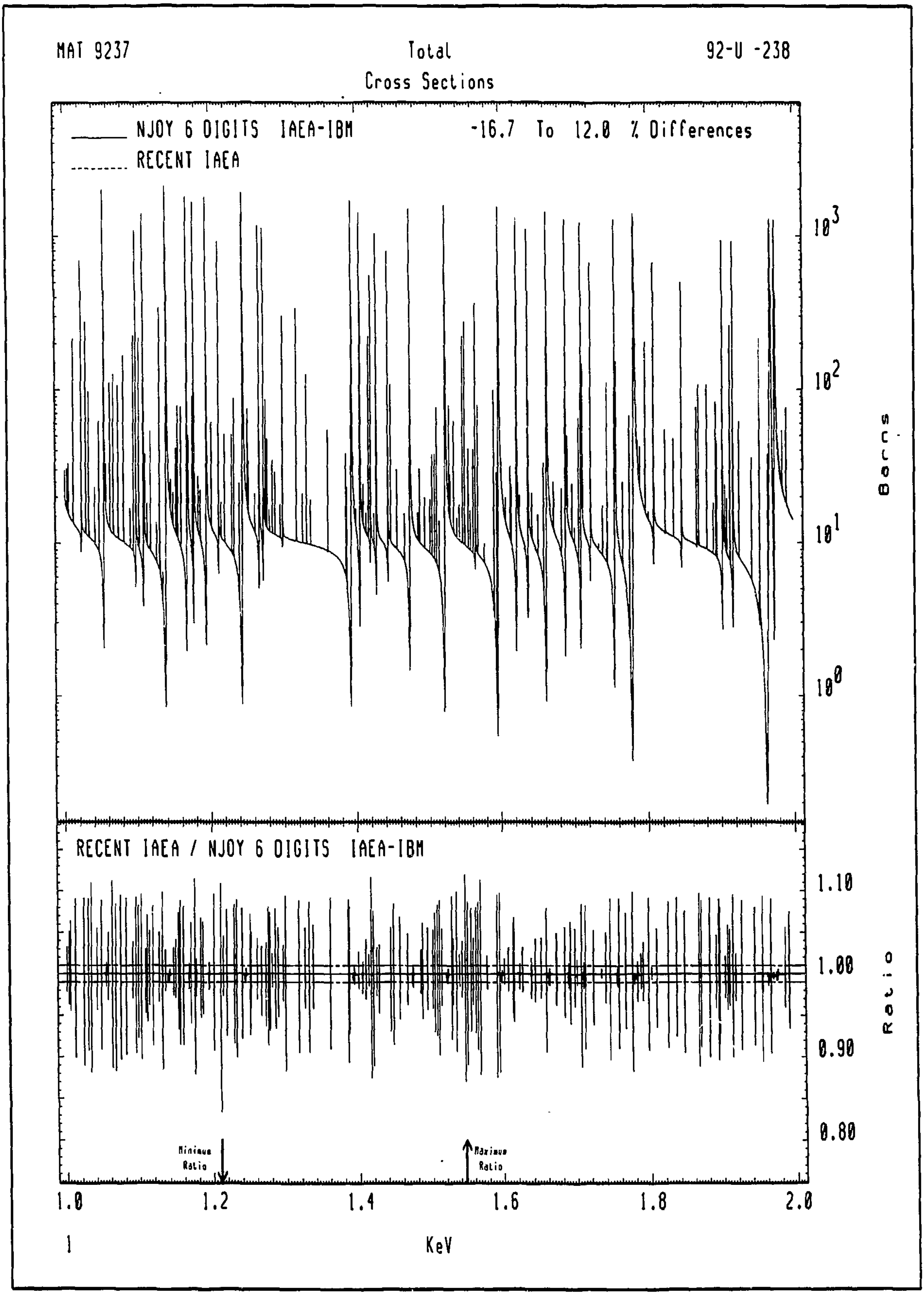

MAT 9237
Elastic
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-10.0 To 2.79 % Differences
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
Ratio
Maximum
Ratio
KeV

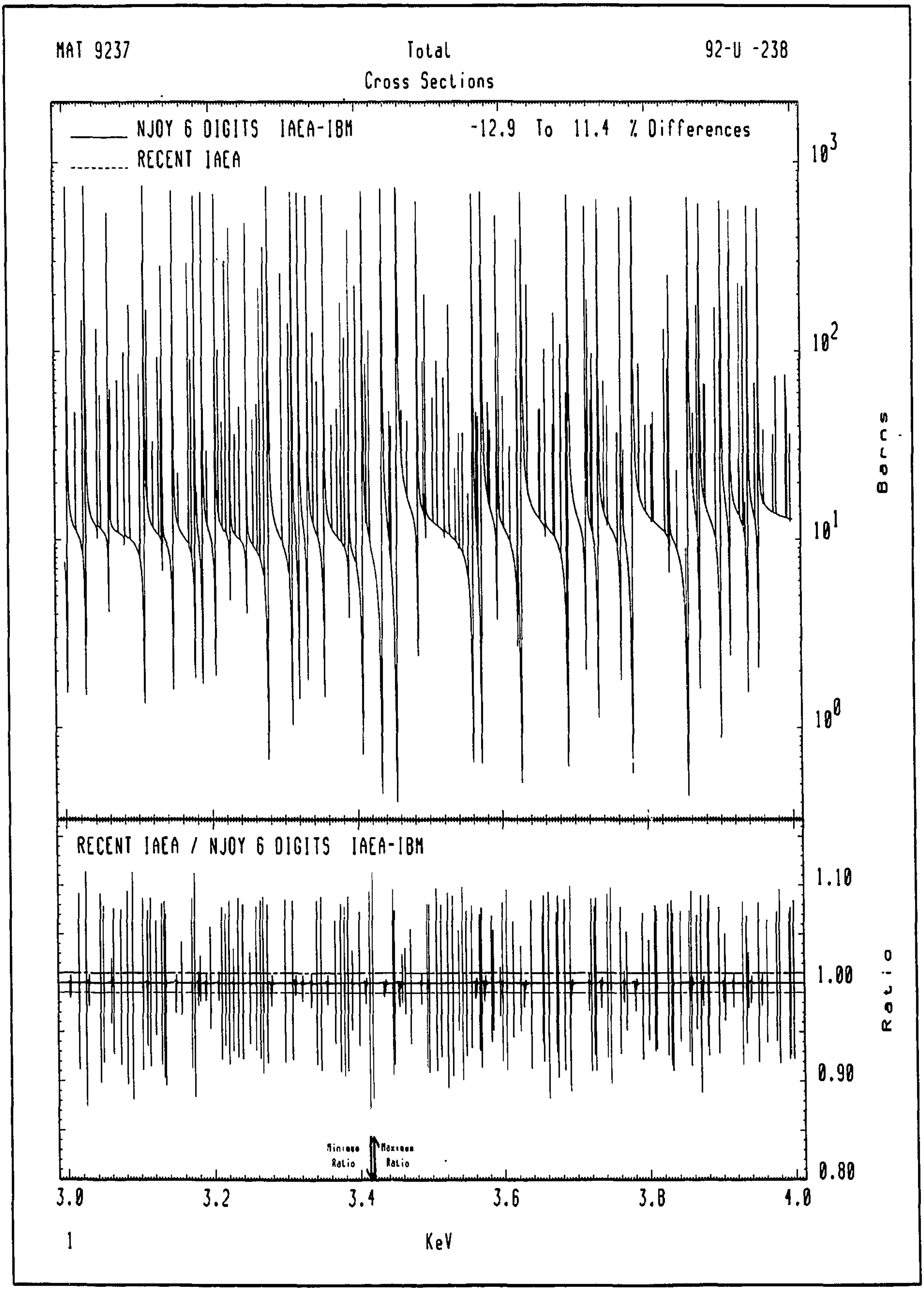

MAT 9237
Elastic
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
0.0 To 737. % Differences
10^1
5
10^0
5
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
3.0
2.5
2.0
1.5
1.0
0.5
Ratio
Maximum Ratio
10.0
10.5
11.0
11.5
12.0
2
KeV

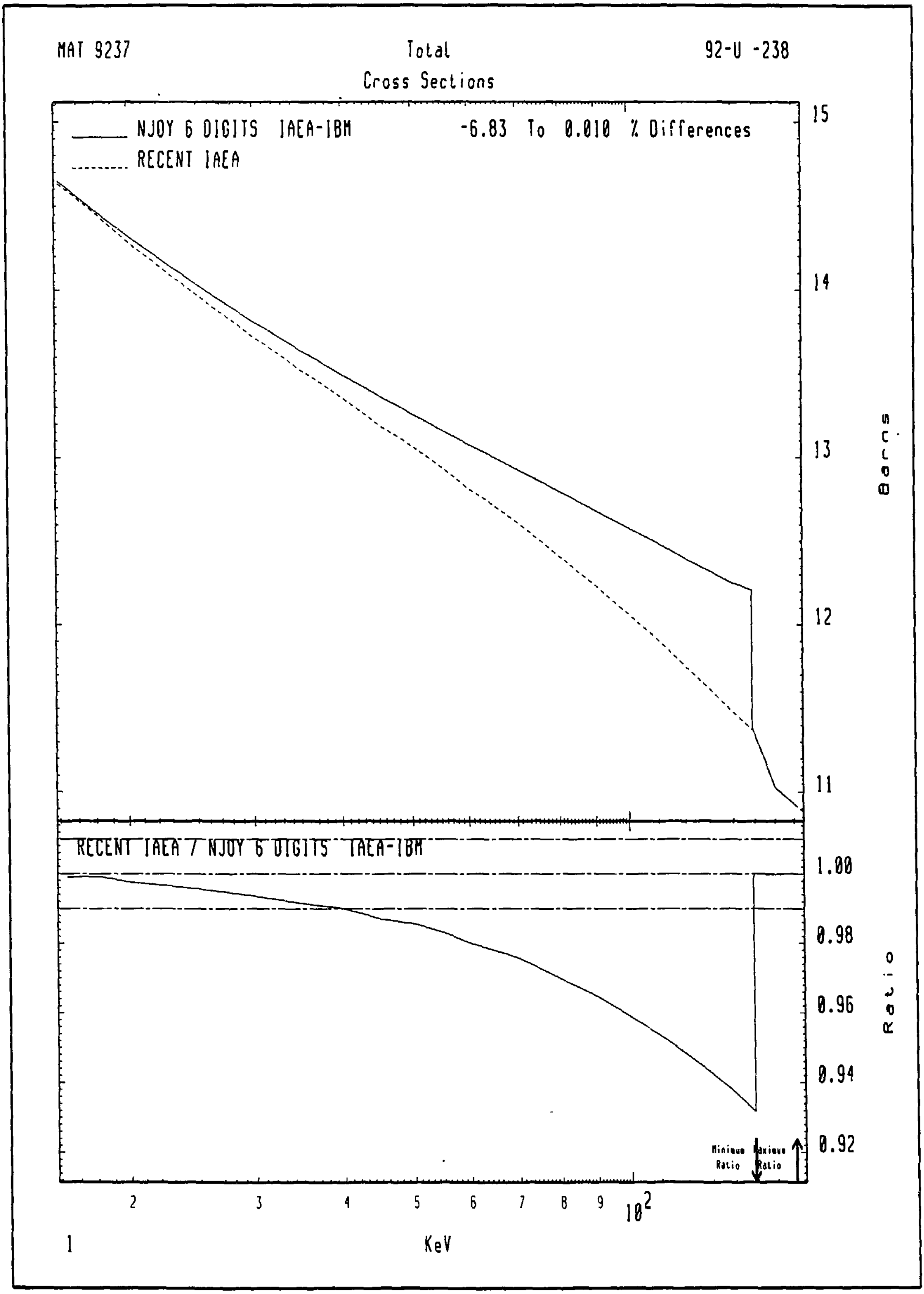

MAT 9237
Elastic
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-7.42 To 0.026 % Differences
14
13
12
11
10
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.00
0.98
0.96
0.94
0.92
Ratio
Minimum Ratio
Maximum Ratio
2
3
4
5
6
7
8
9
10^2
2
KeV

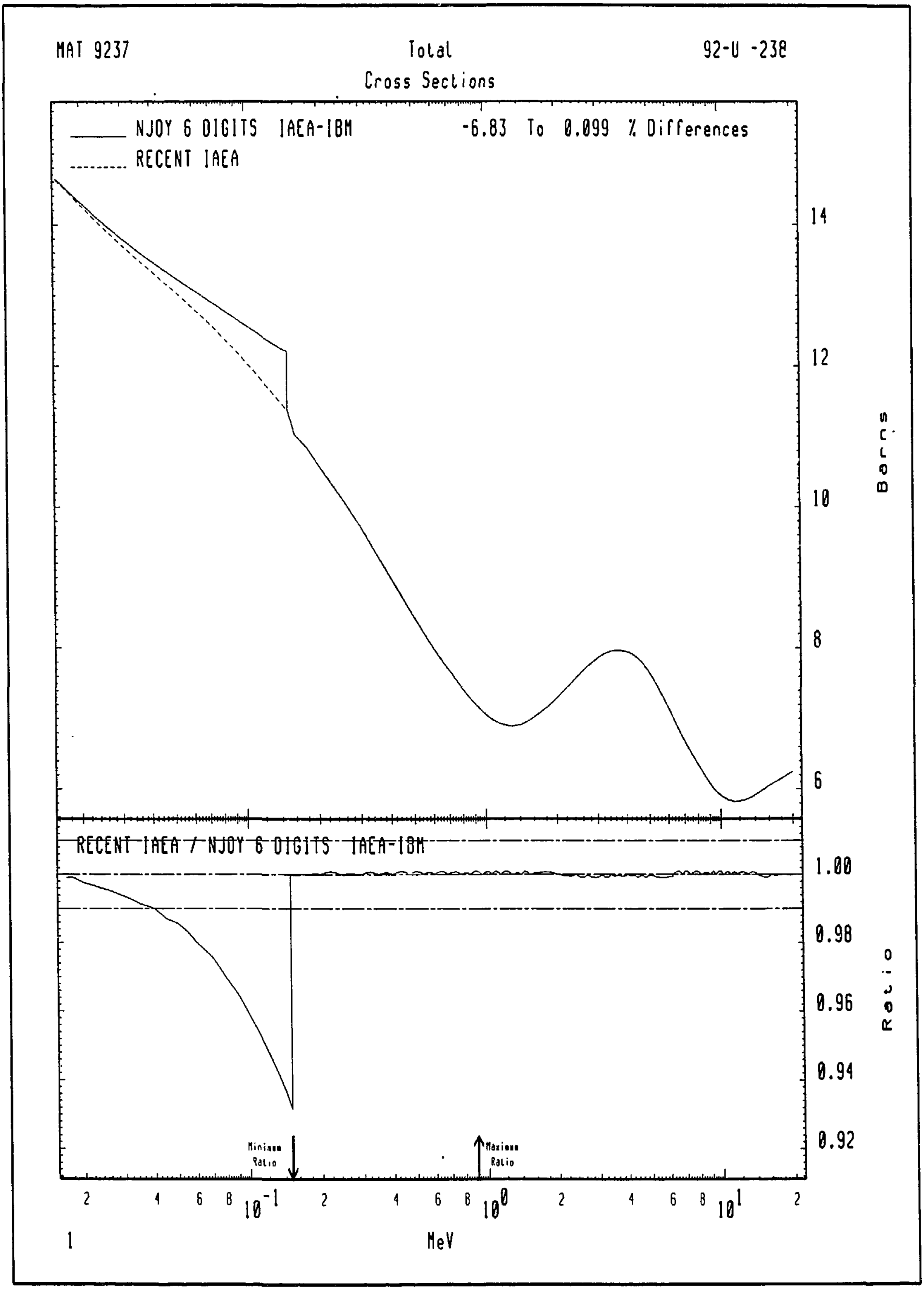

MAT 9237
Elastic
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-7.42 To 0.099 % Differences
10^1
8
6
4
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.00
0.98
0.96
0.94
0.92
Ratio
Minimum Ratio
Maximum Ratio
2 4 6 8 10^-1 2 4 6 8 10^0 2 4 6 8 10^1 2
2
MeV


MAT 9237
Total
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-3.48 To 2.52 % Differences
10^4
10^3
10^2
10^1
10^0
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.02
1.00
0.98
0.96
Ratio
Minimum Ratio
Maximum Ratio
10^{-1}
2
3
4
5
6
7
8
9
10^0
1
KeV


MAT 9237
Total
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-16.7 To 12.0 % Differences
10^3
10^2
10^1
10^0
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.10
1.00
0.90
0.80
Ratio
Minimum Ratio
Maximum Ratio
1.0
1.2
1.4
1.6
1.8
2.0
1
KeV


MAT 9237
Total
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-12.9 To 11.4 % Differences
10^3
10^2
10^1
10^0
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.10
1.00
0.90
0.80
Ratio
Minimum Ratio
Maximum Ratio
3.0
3.2
3.4
3.6
3.8
4.0
1
KeV


MAT 9237
Total
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-6.83 To 0.010 % Differences
15
14
13
12
11
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.00
0.98
0.96
0.94
0.92
Ratio
Minimum Ratio
Maximum Ratio
2
3
4
5
6
7
8
9
10^2
1
KeV


MAT 9237
Total
Cross Sections
92-U -238
NJOY 6 DIGITS IAEA-IBM
RECENT IAEA
-6.83 To 0.099 % Differences
14
12
10
8
6
Barns
RECENT IAEA / NJOY 6 DIGITS IAEA-IBM
1.00
0.98
0.96
0.94
0.92
Ratio
Minimum Ratio
Maximum Ratio
2 4 6 8 10^{-1} 2 4 6 8 10^{0} 2 4 6 8 10^{1} 2
1
MeV