June 24, 1996

Verification of Evaluated Nuclear Data File for Vanadium

A.Trkov, G.Reffo

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1 General

To summarize the analysis of the contents of evaluated nuclear data files, the layout of the report has been adopted, which includes the requirements for the Review Kit for the FENDL-2 candidate evaluations, as defined at the meeting in Del Mar [1].

Detailed comparison of the cross section data for Vanadium from ENDF/B-VI and JENDL-3 evaluated nuclear data files has been presented in reports [2, 3]. These documents served to select the starter file for a new Vanadium evaluation which was performed at ENEA Bologna to remove some of the shortcommings, particularly to add the double differential cross sections and the total gamma ray emission spectra. In this report the current status of the EFF-3 file for Vanadium is described and some additional comments are made for the convenience of the reviewer.
According to the document [1] the review kit should contain:

1. General description, outlining the improvements with respect to FENDL-1.
2. Comparison plots with FENDL-1 and other candidate evaluations.
3. Comparison with experimental data.
4. Legendre coefficients of the angular distributions (MF 4) data.
5. Energy/angle correlated distributions (MF 6) data, giving energy distributions of neutrons, charged particles and recoils at 8, 11 and 14.1 MeV. Particularly:
   a. Neutron spectra are to be compared to the data of Vonach, Takahashi and others, where possible.
   b. Charged particle data are to be compared with the Grimes and Haight data at 14.1 MeV where possible.
   c. The integrated gamma ray production cross section at incident neutron energies of 8, 11 and 14.1 MeV.
   d. Capture gamma ray spectra at least at thermal neutron energy is to be presented.
   e. If uncertainty files are present, compare the variance as a function of neutron energy for MF 33.

The results of the analysis of the EFF-3 Vanadium evaluation are given in the following sections.

2 Format and Data Consistency

Testing procedures, which are usually applied at ENEA for Quality Assurance purposes, have revealed some minor problems with data consistency. This information is not explicitly requested for the FENDL-2 review kit, but it is presented for completeness.

The Nuclear Data File locally named: "`/data/189/work/V_51/V_51.eff3`" is Revision 3 of an Evaluated Nuclear Data File for (supposedly) Vanadium-51, MAT=2351. It was assembled at ECN, Petten (Holland) by Dr. Gruppelaar et.al., based on the work by M. Herman, F. Fabbri and G. Reffo at ENEA-Bologna in February 1995. The file was retreived from ECN-Petten by FTP on February 15, 1996.

The comments related to warnings and error messages obtained in the ENEA evaluated data file verification procedure are as follows:

- Considering that the evaluation is declared to correspond to the isotope ^{51}V, there should be resonance parameters in file MF=2 for a single isotope (`NIS=1` and `ABN=1.0`). From the comment section in the file (MF=1, MT=451) it can be seen that the starter file was the ENDF/B-VI evaluation, which is given for the natuaral vanadium. The file description is therefore inconsistent with the data.

- In the covariance data (MF=33) there are subsections with `LB=8` missing for the total, (n,2n), (n,α) and (n,p) reactions (MT=1, 16, 103 and 107, respectively).

- A possible inconsistency of the Q value for the radiative capture reaction (MT=102) is reported.

- There are some energy balance problems in the ($n, n\alpha$) reaction (MT=22) amounting to 6.5% (see also the last paragraph in Section 3. Energy balance is conserved for all other reactions to better than 2% except near thresholds.

- The sum of the partial resonance widths differs from the total. The difference arises only due to the numerical roundoff errors in the data representation and can be ignored.

- In some cases the reactions start below the threshold energy. In all such cases the difference from the threshold energy is negligible.

3 Review kit information

3.1 Cross sections comparison with FENDL-1

The data adopted for EFF-3 use ENDF/B-VI as the starter file without modifications. The cross sections sets are therefore identical.

3.2 Cross section comparison with experimental data

The plots comparing the data retrieved from the EXFOR data base with the data from the EFF-3 Vanadium evaluated nuclear file are given in the Appendix A.2 on page 7. For further details consult documents [2, 3].

3.3 Energy/Angle distributions

Comparison of the energy/angle correlated distributions is fairly difficult to manage due to various possibilities of data representation and the need to sum the contributions from different reactions for comparison with the measured values. In order to bring the evaluated nuclear data from different sources to the same basis, they were processed with `NJOY94.35` [4] to generate particle production matrices in the Vitamin-J 175-group structure for neutrons and 94-groups for photons. The following observations are made:

- The neutron emission spectra from incident neutrons at about 14 MeV (group energy interval $13.840 - 14.191$ MeV) are compared to the data measured by Takahashi et.al. [5]. The differences between the EFF-3 and ENDF/B-VI are rather small and it would be difficult to choose between the two. At lower energies no experimental data were found.

- In the ENDF/B-VI file the photon emission spectra are given entirely in the non-elastic cross section data set. The data for the (n, γ) reaction are given separately, but it is not clear if they need to be added to the non-elastic contribution, since in principle tha later is redundant and should include the contribution from the (n, γ) reaction.

- The photon emission spectrum due to incident neutrons at about 14 MeV from EFF-3 has a pronounced structure and agrees in many details with the measurements of Newman & Morgan [6] (taken from the incident neutron energy bin from $14 - 17$ MeV), particularly the strongly pronounced peaks below 2 MeV. The photon spectrum shape is slightly too low for intermediate photon energies and too high for high photon energies compared to the measurements and even to ENDF/B-VI. On the other hand, at lower incident neutron energies the ENDF/B-VI spectra decrease rapidly above a certain photon cutoff energy, while the agreement between the EFF-3 data and the measurements improves. The diagrams of the photon emission spectra are shown in Appendix A.3 on page 22.

- In the EFF-3 file the data for the photon spectra from the inelastic scattering into discrete levels are not included. Their contribution is therefore missing in the diagrams in Appendix A.3.

- No proton and alpha spectra are given in the ENDF/B-VI file.

During the analysis it was also observed that the $(n, n\alpha)$ reaction in the EFF-2 file has no photon data. Furthermore, the non-elastic data are redundant and inconsistent with the outgoing particle distributions calculated by summing the partial contributions.

4 Conclusion

The EFF-3 evaluated nuclear data file for Vanadium requires some improvements.

- It is recommended to declare the evaluation to correspond to the natural Vanadium rather than the ^{51}V isotope, since the presence of 0.25 % of the isotope ^{50}V in the natural element is not expected to affect the angular distributions, but it can affect significantly the cross sections in the resonance region. The MAT number and the corresponding ZA designation shold be changed. Alternatively, the resonance data should be reviewed, removing the contribution form the ^{50}V isotope.

- The addition of the photon production data to the $(n, n\alpha)$ energy/angle distribution data (MF6) could remove the energy balance problems.

- The photon production matrices from the inelastic scattering into discrete levels can not be generated because file-12 and 14 (MF12, MF14) data are not included. They should be added.

- The energy and angle distributions of the outgoing particles are given in the redundant non-elastic reaction (MT3), inherited from ENDF/B-VI. They are inconsistent with the distributions obtained by summing the contributions from the individual reactions. It is suggested that the MT3 energy and angle distribution data for the outgoing particles (MF13, 14, 15) should be removed from the file.

Apart from the deficiencies mentioned above, the improvements to the starter file are substantial and significantly improve the quality of the data contained in the evaluated nuclear data file.

References

[1] A.B.Pashchenko (Compiled by:) *Summary Report on the Completion of FENDL-1 and Start of FENDL-2*, Advisory Group Meeting, 5-9 Dec.1995, Del Mar, California, INDC(NDS)-352 (Draft).

[2] G.Reffo, M.Herman, F.Fabbri: *A Study for Possible Adjustment to the Vanadium File*, European Fusion File Meeting, paris, 8-9 Dec.1994.

[3] G.Reffo, M.Herman, F.Fabbri: *Review of Existing Evaluations for V, Zr, Nb, Ta*, EFF-DOC-78, (1991).

[4] R.E.MacFarlane, D.W.Muir: `The NJOY Nuclear Data Processing System`, Los Alamos National Laboratory, New Mexico, LA-12740-M, Oct.1994).

[5] A.Takahashi, E.Ichimura,Y.Sasaki, H.Sugimoto: *Double and Single Differential Neutron Emission Cross Sections at 14.1 MeV*, (R,OKTAV-A-87-03,8711), (S,INDC(YUG)-010/G,8605), (S,INDC(JAP)-106/L,86), EXFOR data retrieval.

[6] E.Newman, G.L.Morgan: *The V (n,x gamma) Reaction Cross Section for Incident Neutron Energies Between 0.2 and 20.0 MeV*, (R,ORNL-TM-5299,7604), (J,NSE,62,515,7703), EXFOR data retrieval.

APPENDIX

A.1 General information section of the EFF-3 Vanadium data file

```
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 EFF-DOC              DIST-OCT91 REV2-OCT91                      2351 1451    6
-----EFF-2            MATERIAL 2351        REVISION 2            2351 1451    7
-----INCIDENT NEUTRON DATA                                      2351 1451    8
------ENDF-6 FORMAT                                            2351 1451    9
**********************************************************************2351 1451   10
*                                                                    *2351 1451   11
*    EEEEEEEE    FFFFFFFF    FFFFFFFF    3333333        000        *2351 1451   12
*    E           F           F                 3      0   0        *2351 1451   13
*    E           F           F                 3     0     0       *2351 1451   14
*    EEEEEE      FFFFFF      FFFFFF      3333333   *  0     0       *2351 1451   15
*    E           F           F                 3     0     0       *2351 1451   16
*    E           F           F                 3      0   0        *2351 1451   17
*    EEEEEEEE    F           F           3333333        000        *2351 1451   18
*                                                                    *2351 1451   19
**********************************************************************2351 1451   20
                                                                     2351 1451   21
              EUROPEAN FUSION FILE VERSION 3.0                       2351 1451   22
              --------------------------------                       2351 1451   23
                                                                     2351 1451   24
The European Fusion File is a project of various European            2351 1451   25
laboratories and is sponsored by the European Fusion Programme of    2351 1451   26
the European Union.                                                  2351 1451   27
The data file EFF-3.0 is maintained at ECN-Petten. Contact:          2351 1451   28
                                                                     2351 1451   29
Dr. H. Gruppelaar                                                    2351 1451   30
ECN Nuclear Energy                                                   2351 1451   31
Netherlands Energy Research Foundation ECN                           2351 1451   32
P.O. Box 1                                                           2351 1451   33
1755 ZG Petten                                                       2351 1451   34
The Netherlands                                                      2351 1451   35
                                                                     2351 1451   36
**********************************************************************2351 1451   37
**    This evaluation has been selected from ENDF/B-6 library        2351 1451   38
**    by ENEA-BOLOGNA                                                2351 1451   39
                                                                     2351 1451   40
 Revision 3 by M.Herman, F.Fabbri and G.Reffo at ENEA-Bologna        2351 1451   41
                                                    feb. 1995        2351 1451   42
                                                                     2351 1451   43
 Double differential cross sections for MT=16,22,28,91,103,107       2351 1451   44
 (including recoil nuclei and gamma emission) added based on the     2351 1451   45
 compound nucleus and preequilibrium calculations performed with     2351 1451   46
 the ida code system.                                                2351 1451   47
                                                                     2351 1451   48
 Angular distributions (MF4) for discrete levels MT=51-63 taken      2351 1451   49
 from JENDL-3                                                        2351 1451   50
                                 1        451        108            12351 1451   51
                                 2        151        126            12351 1451   52
                                 3          1       2060            12351 1451   53
                                 3          2       2053            12351 1451   54
                                 3          4         31            12351 1451   55
                                 3         16         10            12351 1451   56
                                 3         22          8            12351 1451   57
                                 3         28          9            12351 1451   58
                                 3         32          5            12351 1451   59
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                                 3         53         13            12351 1451   62
                                 3         54         12            12351 1451   63
                                 3         55         10            12351 1451   64
                                 3         56         10            12351 1451   65
                                 3         57          9            12351 1451   66
                                 3         58          9            12351 1451   67
```

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4	51	113	12351 1451	95
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5	32	7	12351 1451	119
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6	22	154	12351 1451	121
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6	91	860	12351 1451	123
6	103	880	12351 1451	124
6	107	464	12351 1451	125
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14	102	1	12351 1451	129
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33	1	26	12351 1451	132
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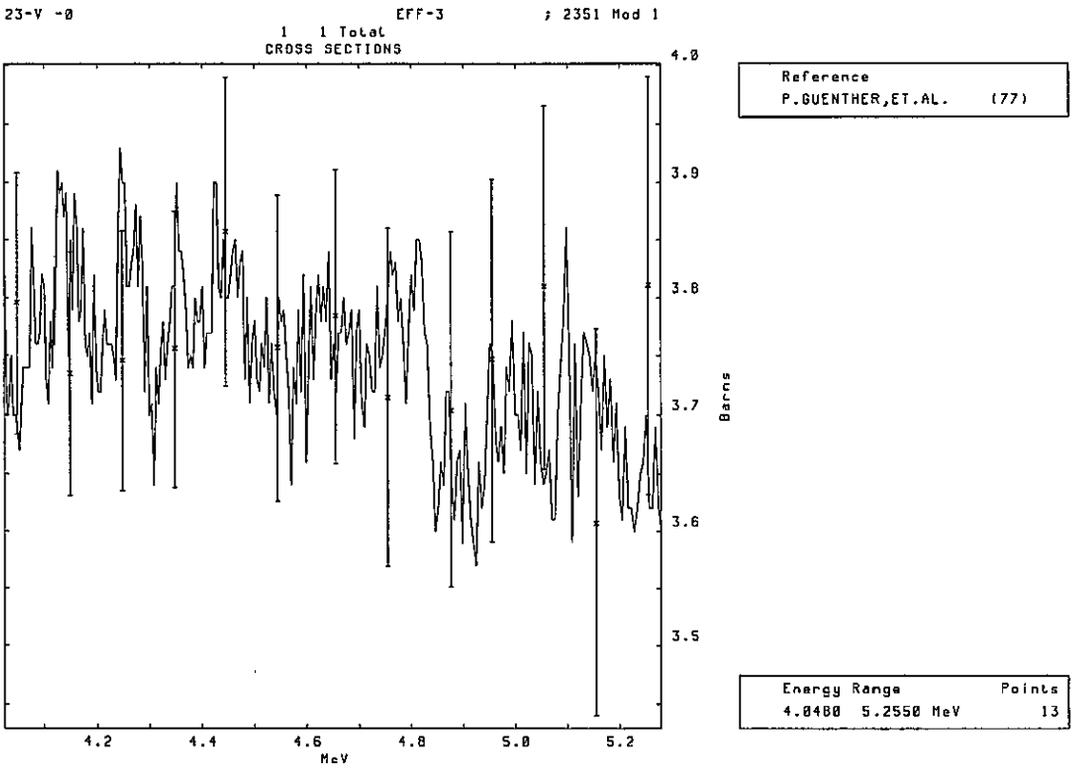
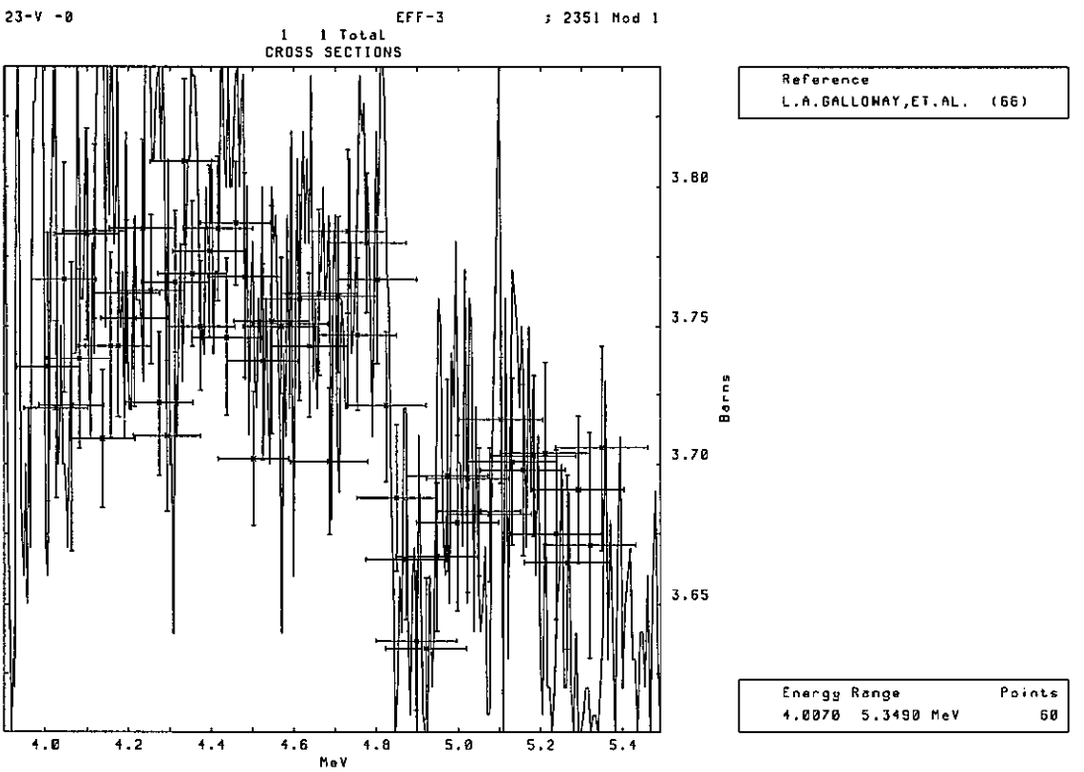
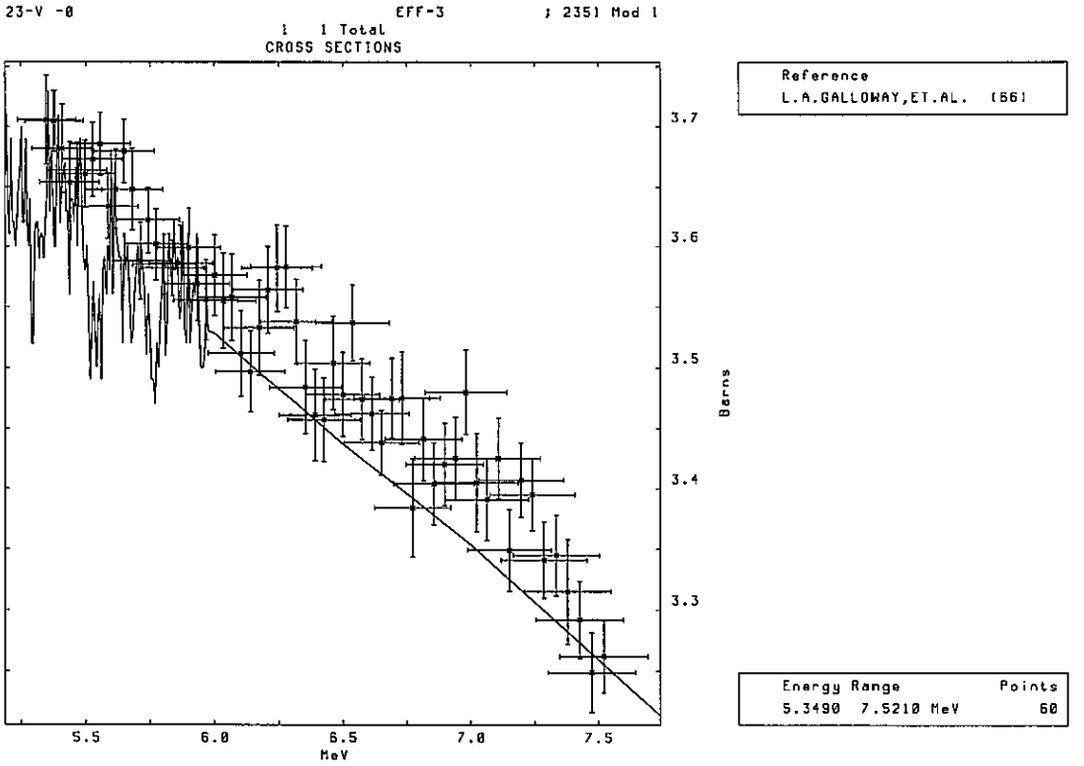
A.2 Cross sections comparison with measured data



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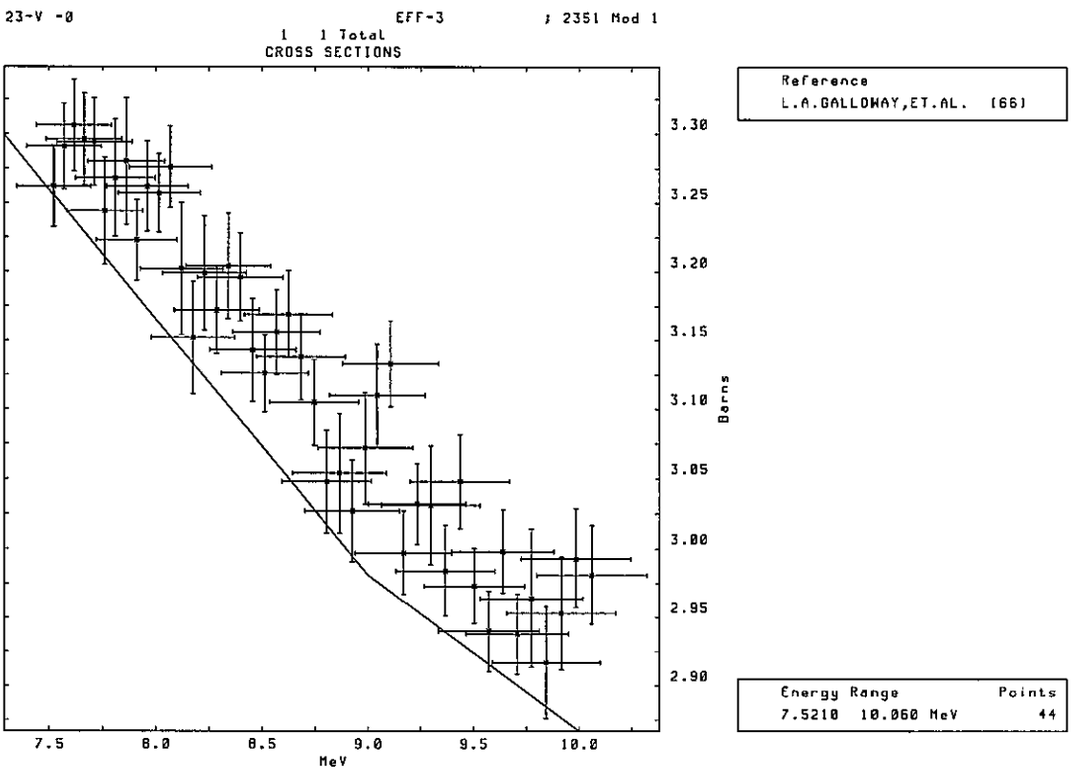
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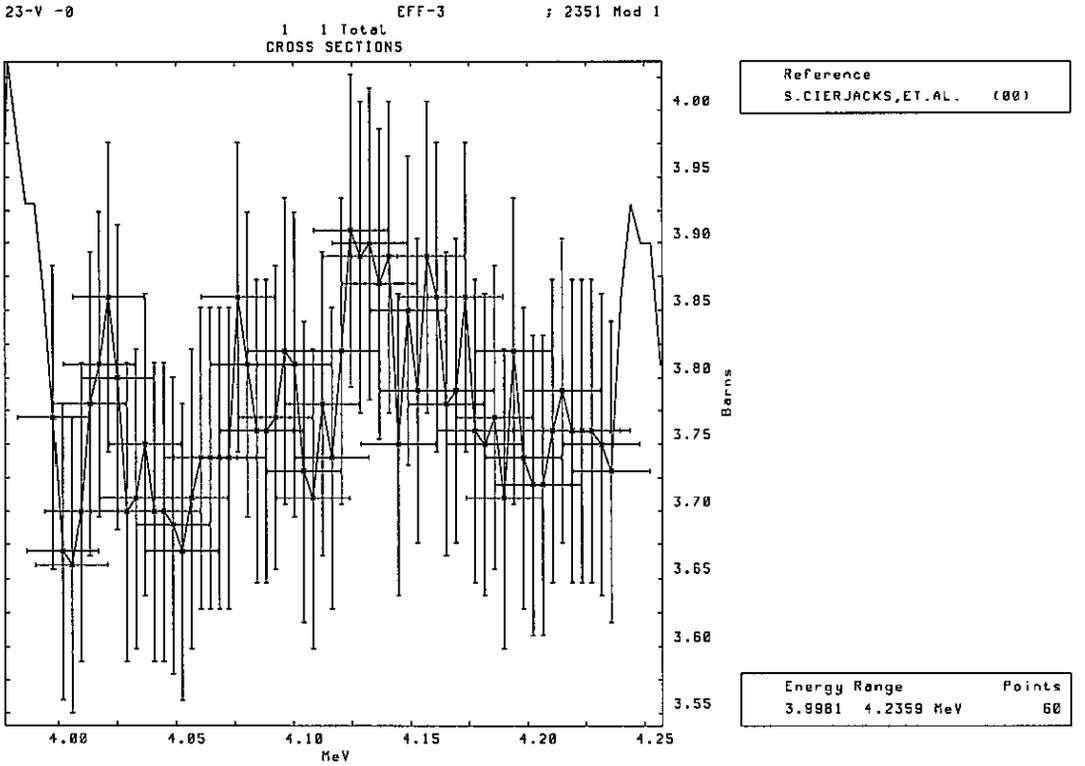
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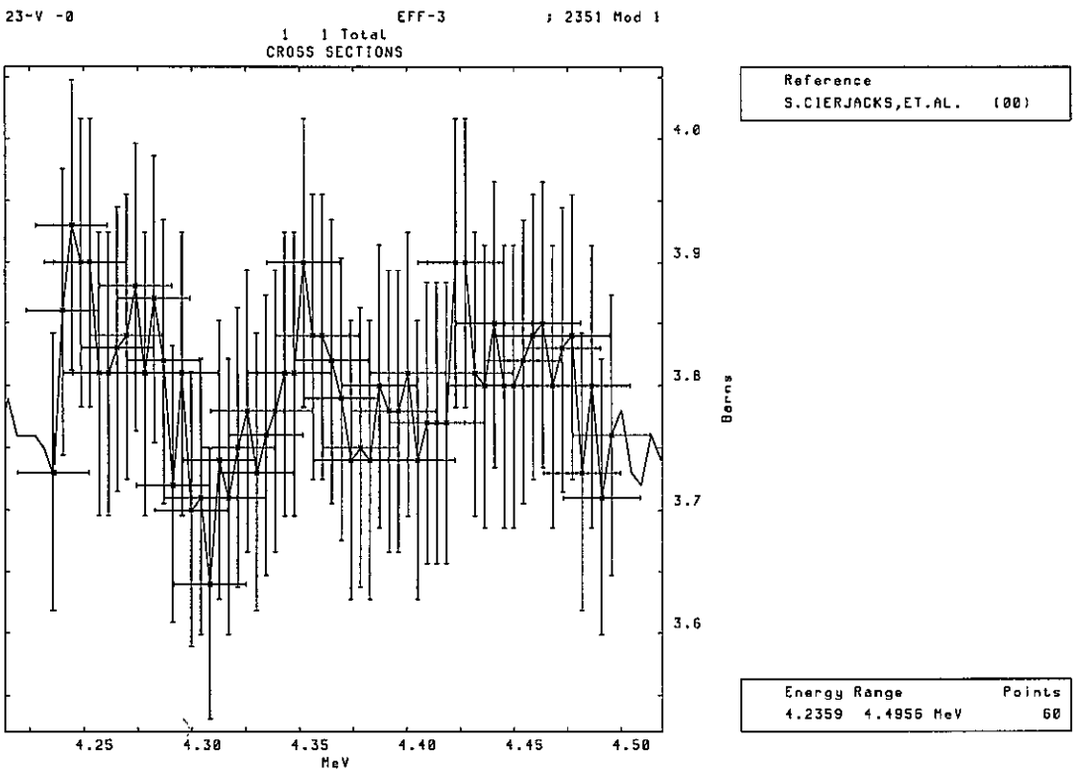
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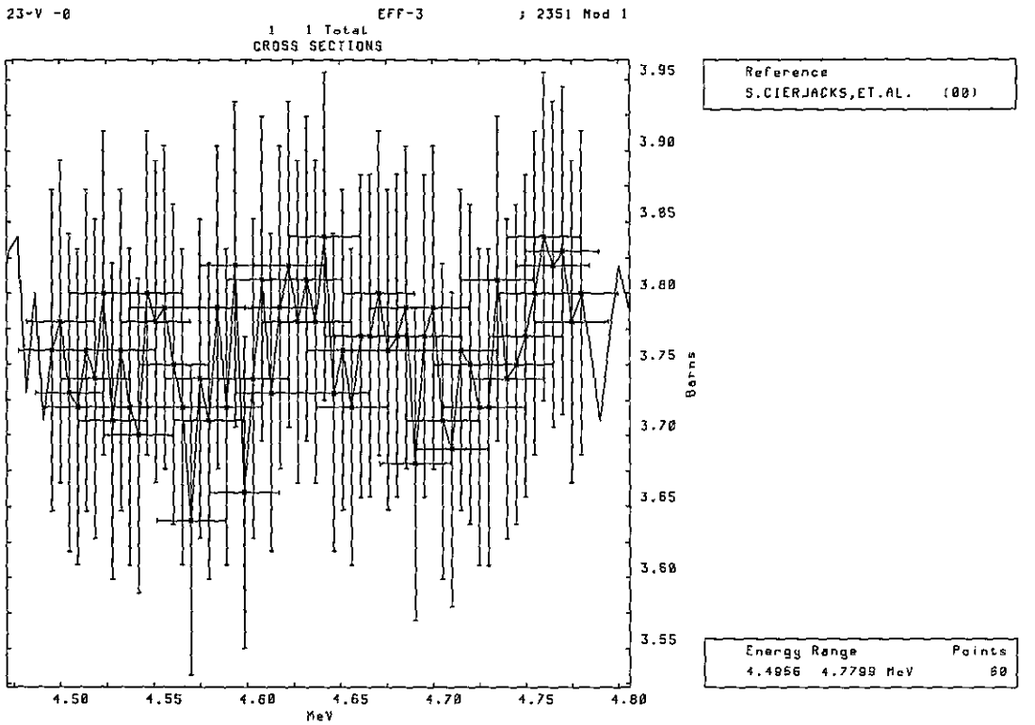
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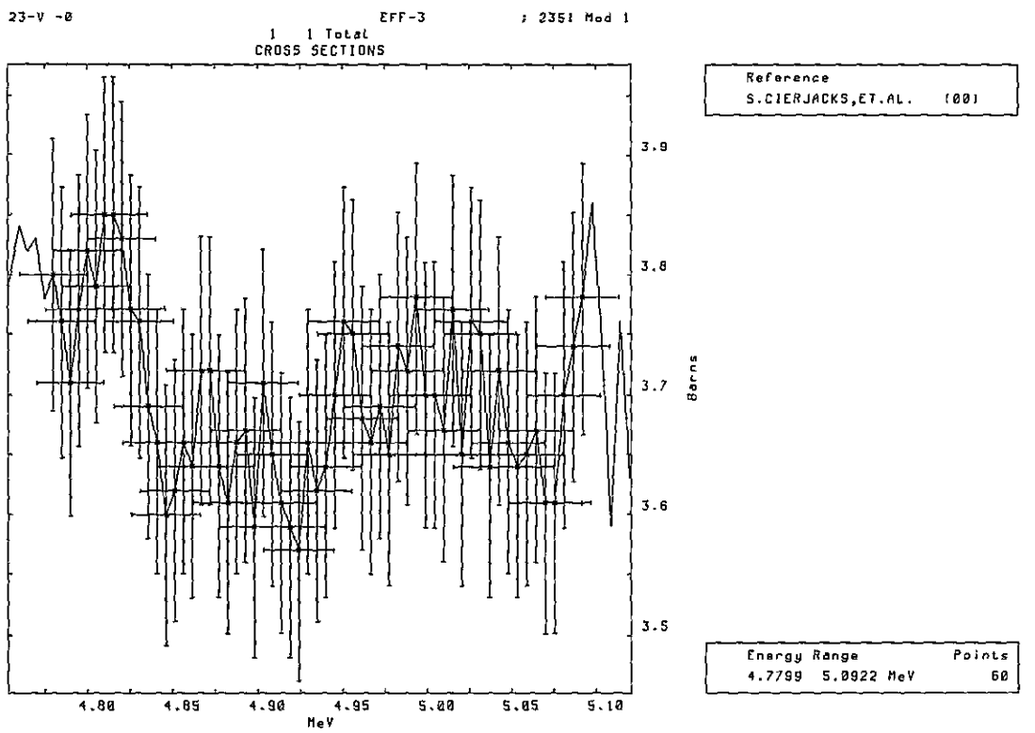
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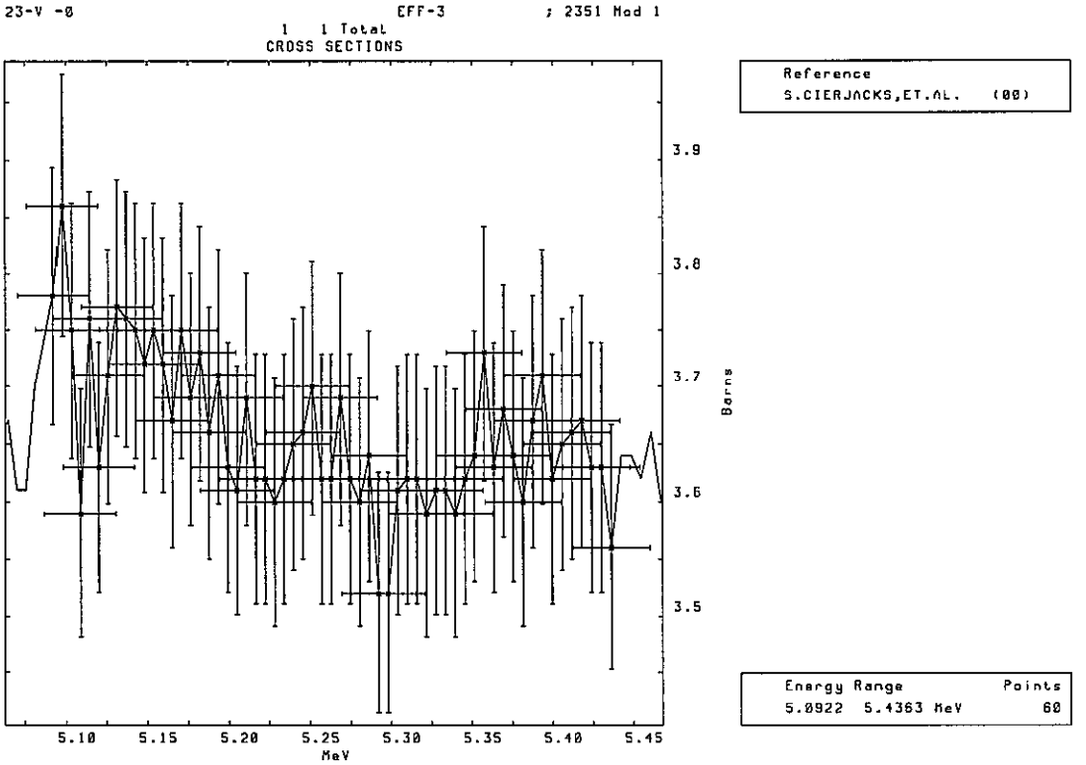
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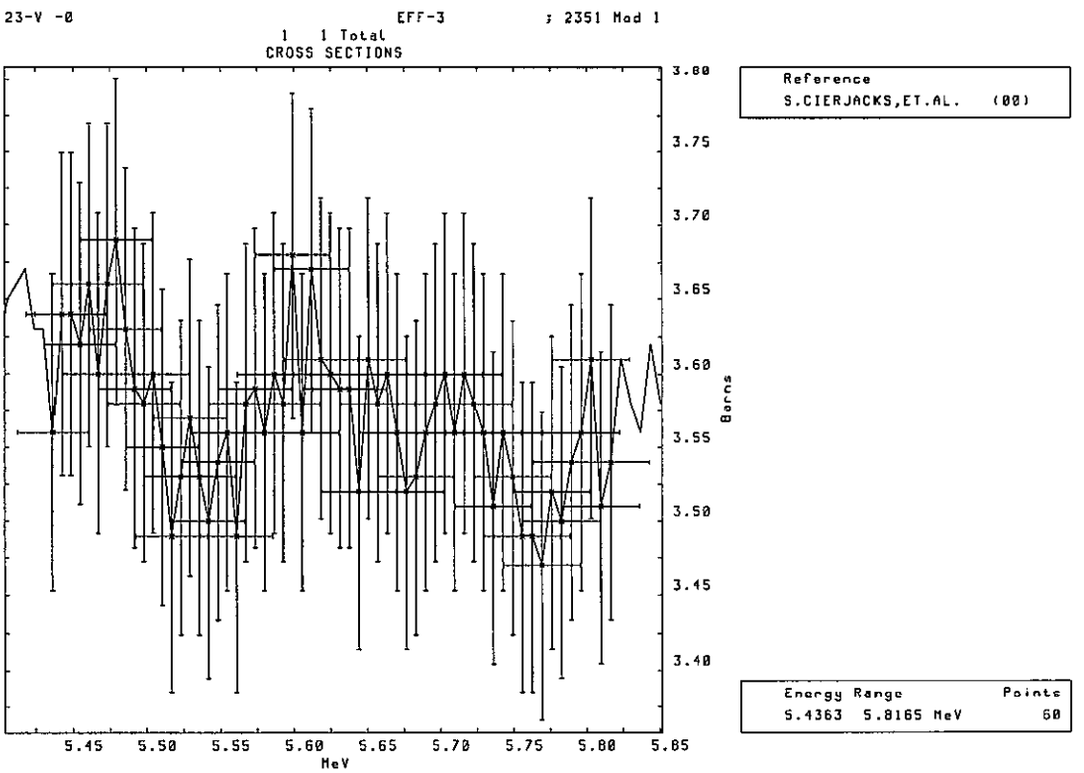
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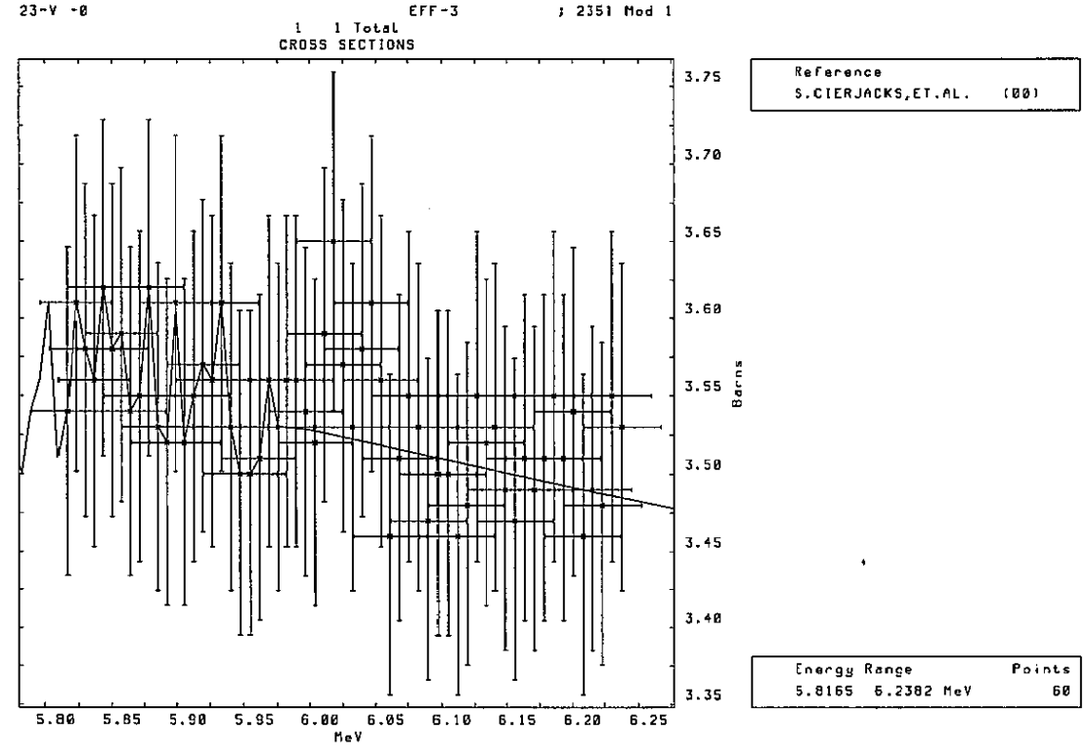
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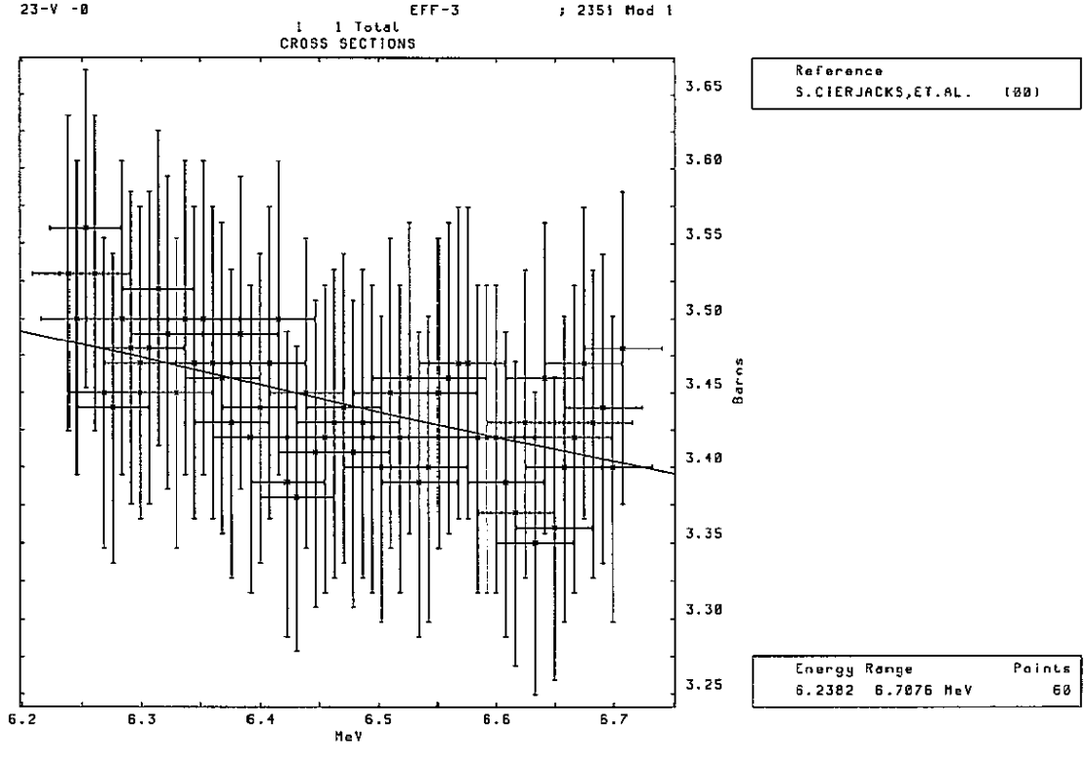
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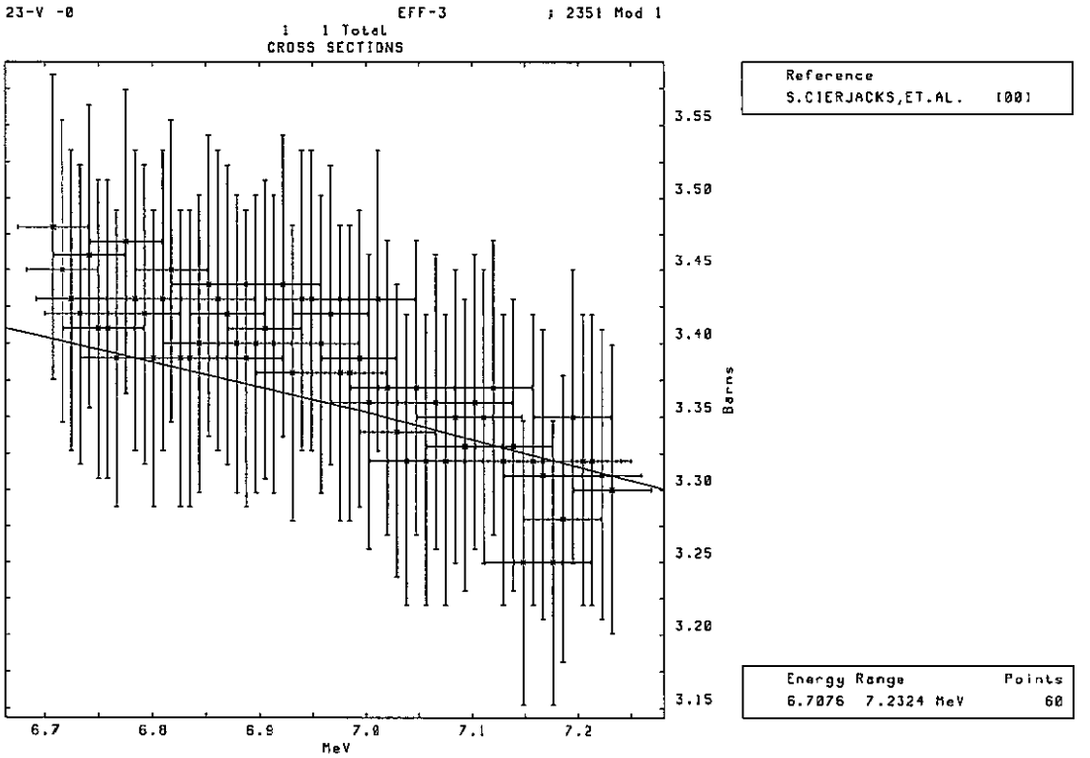
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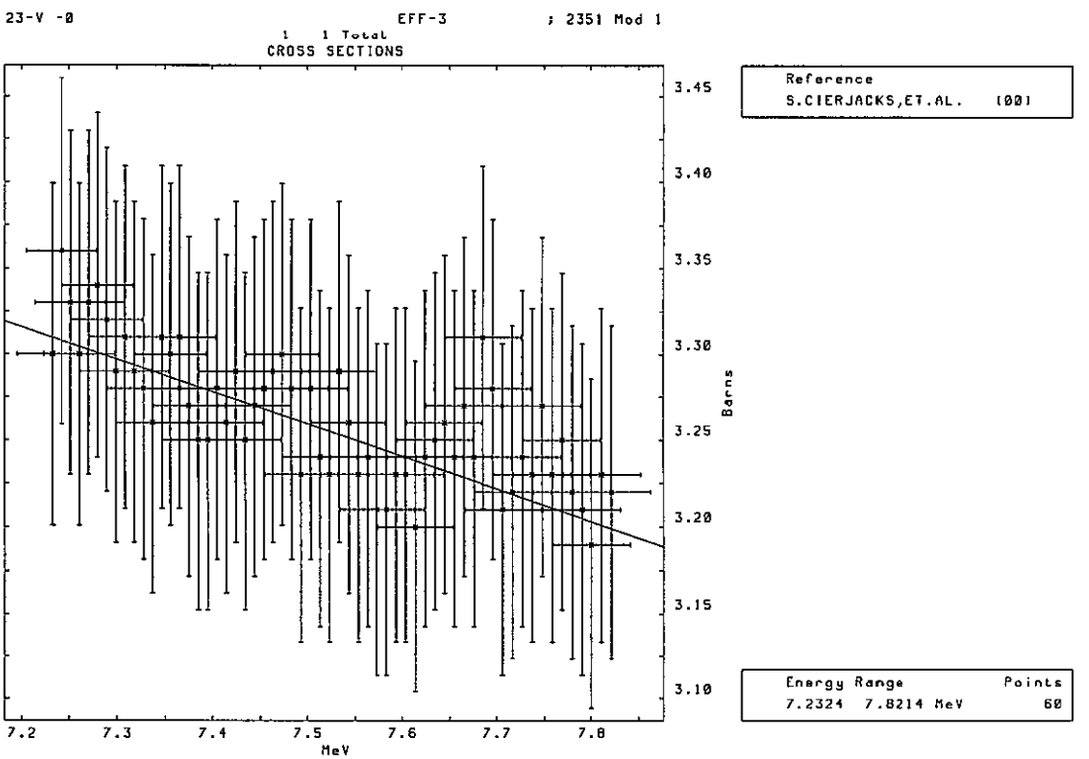
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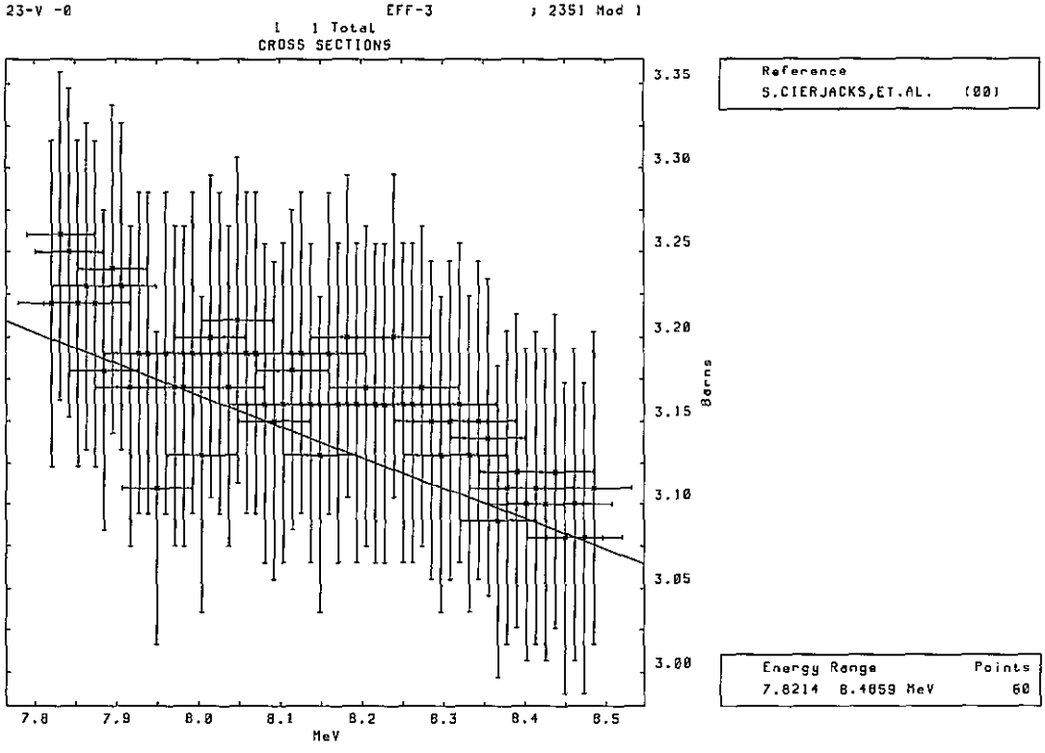
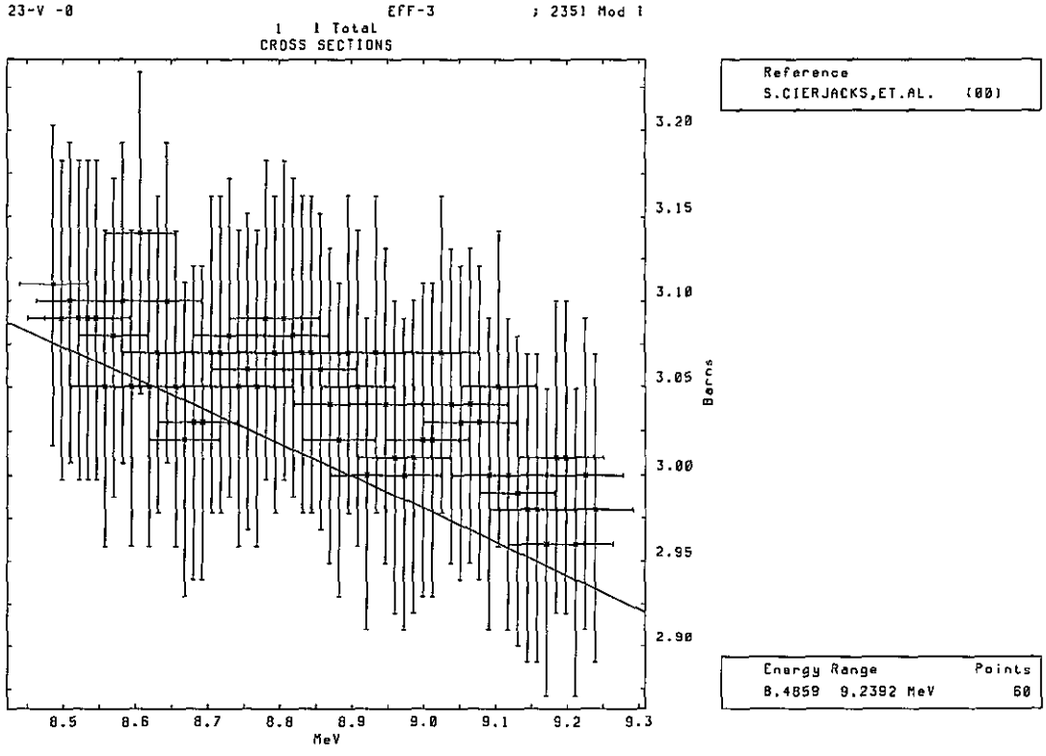
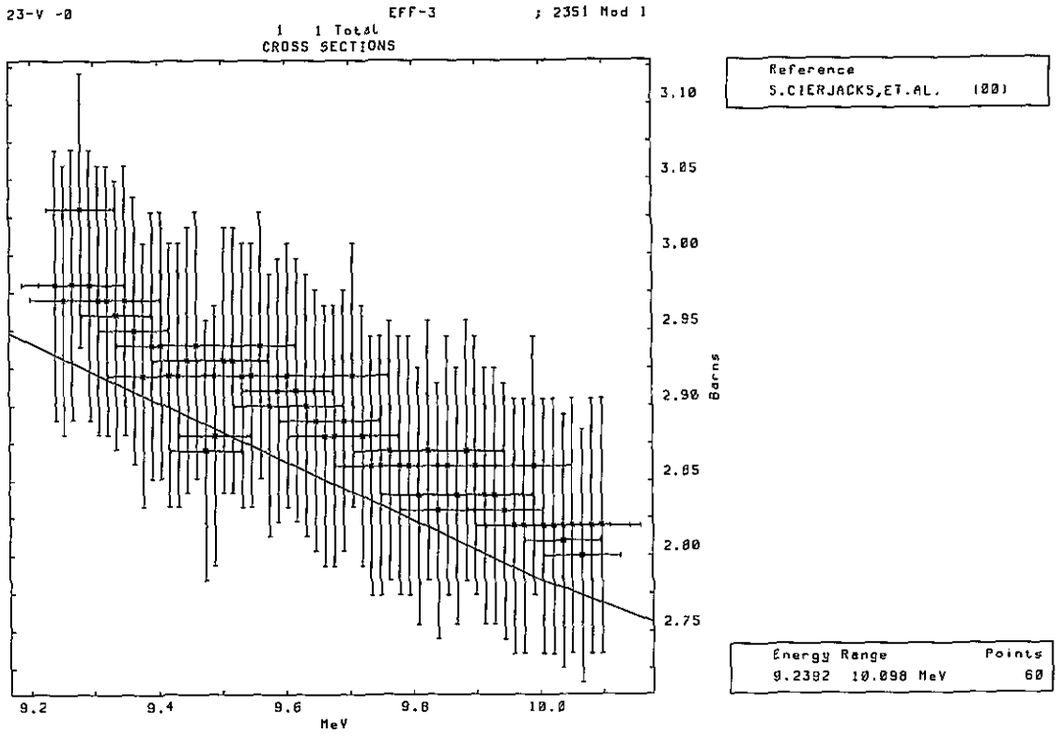
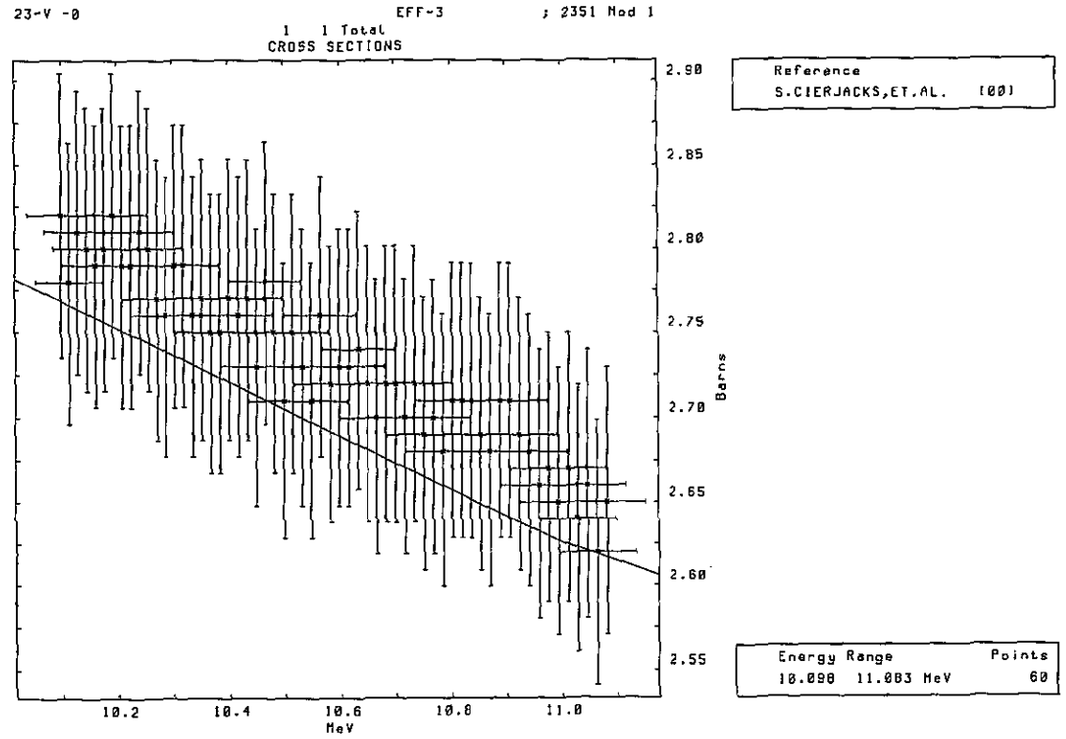
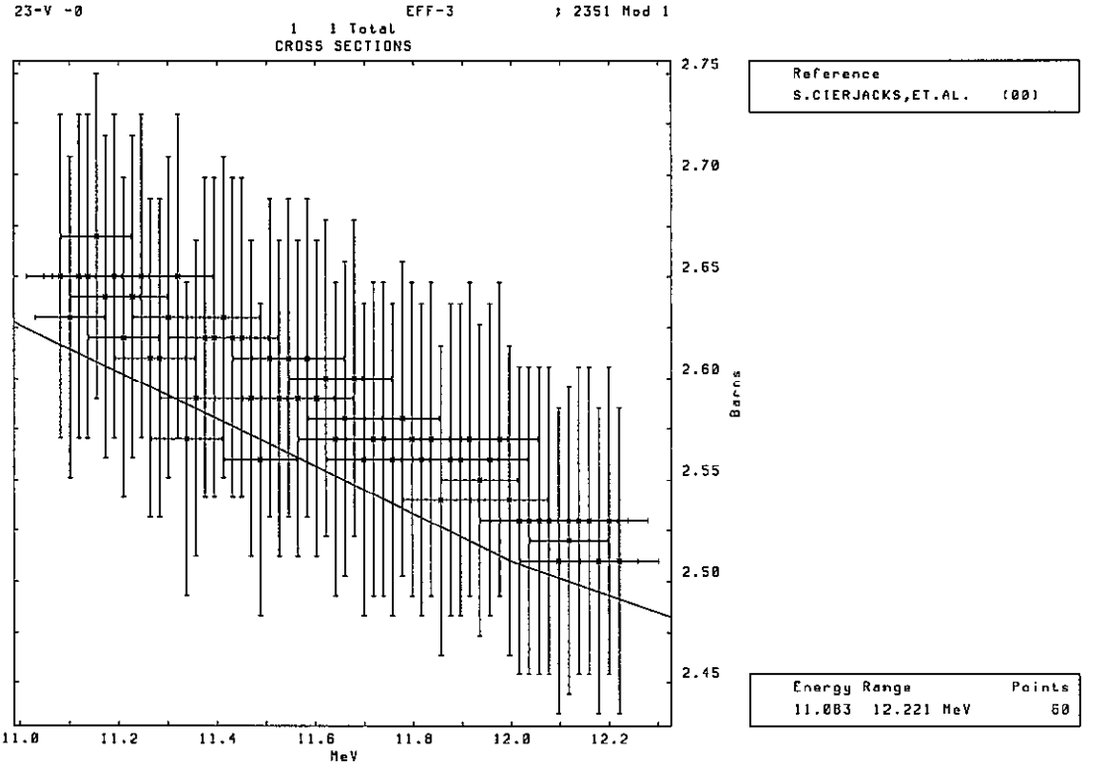
Barns
7.2
7.3
7.4
7.5
7.6
7.7
7.8
MeV
Energy Range Points
7.2324 7.8214 MeV 60

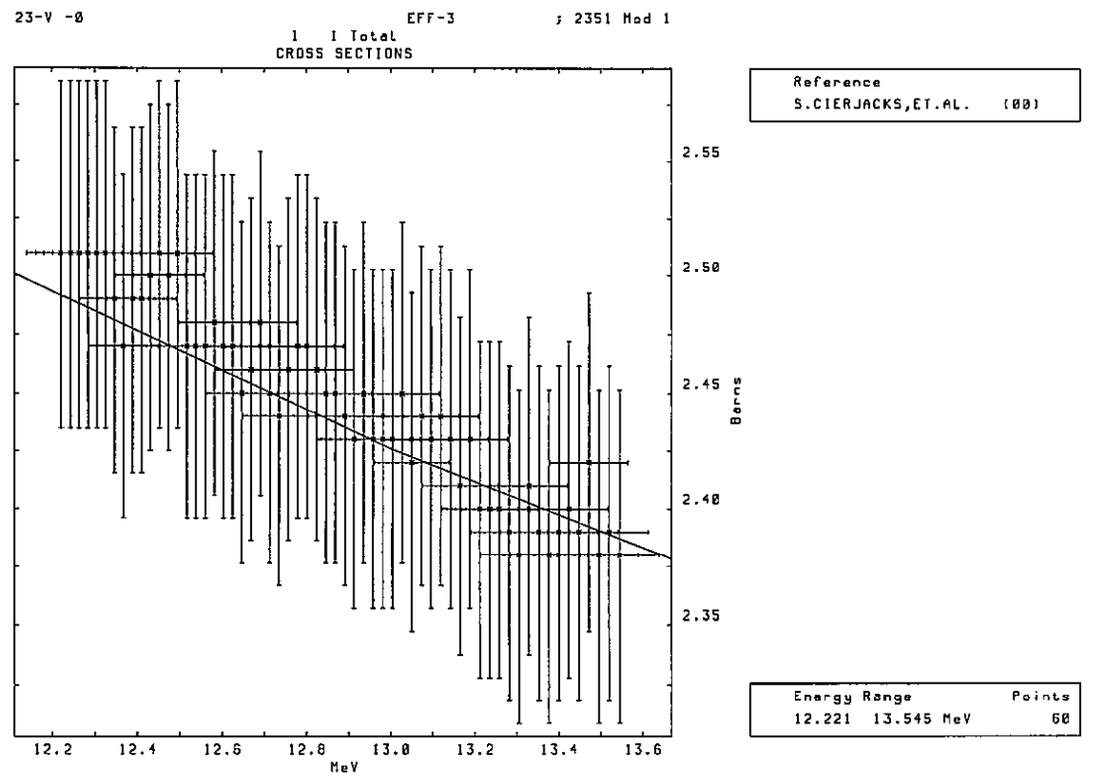

23-V -0 EFF-3 ; 2351 Mod 1
1 1 Total
CROSS SECTIONS
Reference
S.CIERJACKS,ET.AL. (00)
3.35
3.30
3.25
3.20
3.15
3.10
3.05
3.00
Barns
7.8
7.9
8.0
8.1
8.2
8.3
8.4
8.5
MeV
Energy Range Points
7.8214 8.4859 MeV 60

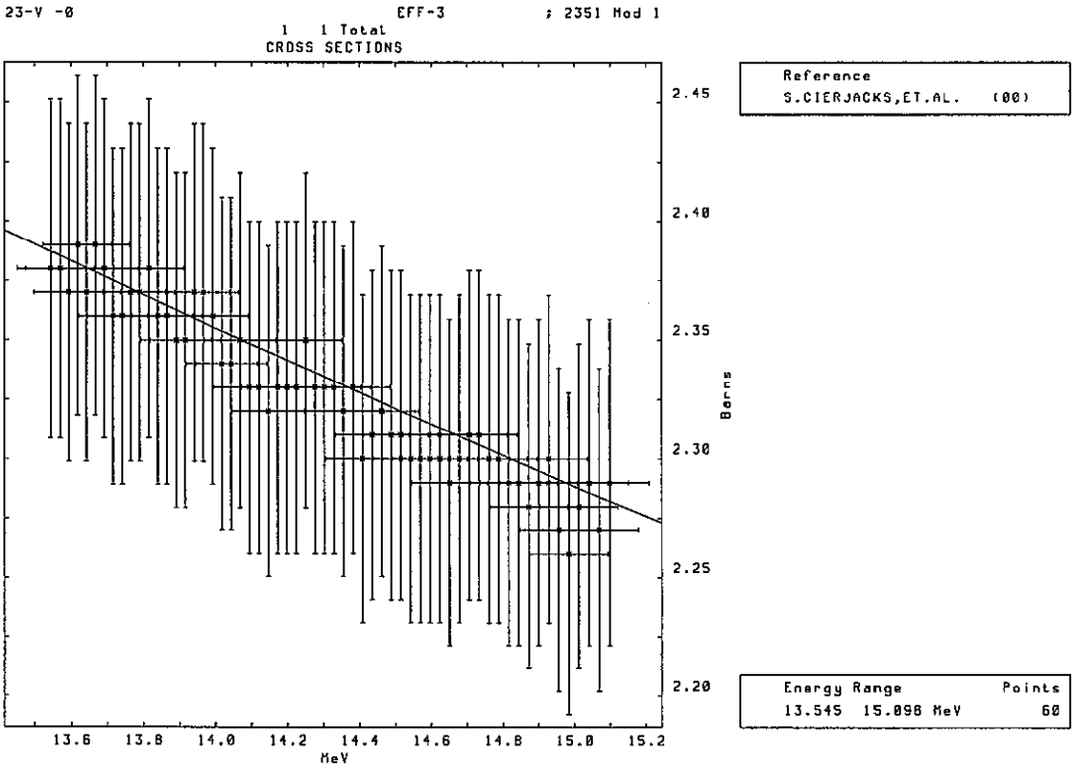

23-V -0 EFF-3 ; 2351 Mod 1
1 1 Total
CROSS SECTIONS
Reference
S.CIERJACKS,ET.AL. (00)
3.20
3.15
3.10
3.05
3.00
2.95
2.90
Barns
8.5
8.6
8.7
8.8
8.9
9.0
9.1
9.2
9.3
MeV
Energy Range Points
8.4859 9.2392 MeV 60

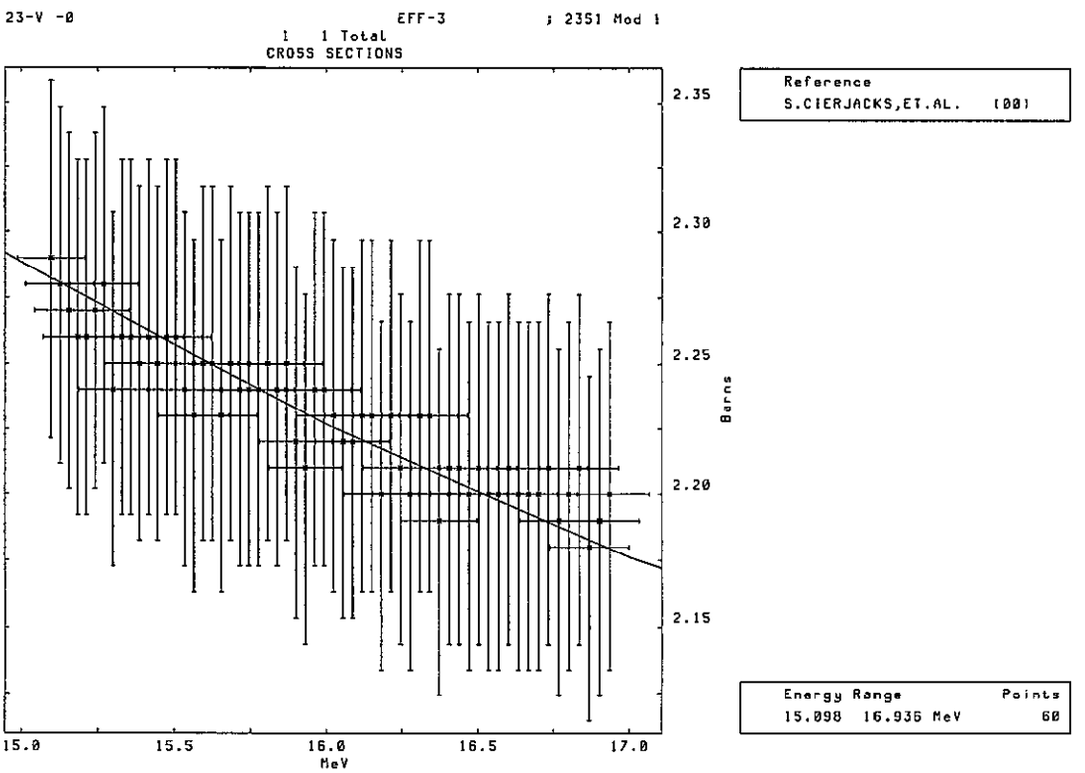

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
Reference
S.CIERJACKS,ET.AL. (00)
3.10
3.05
3.00
2.95
2.90
2.85
2.80
2.75
Barns
Energy Range
Points
9.2392 10.098 MeV
60
9.2
9.4
9.6
9.8
10.0
MeV

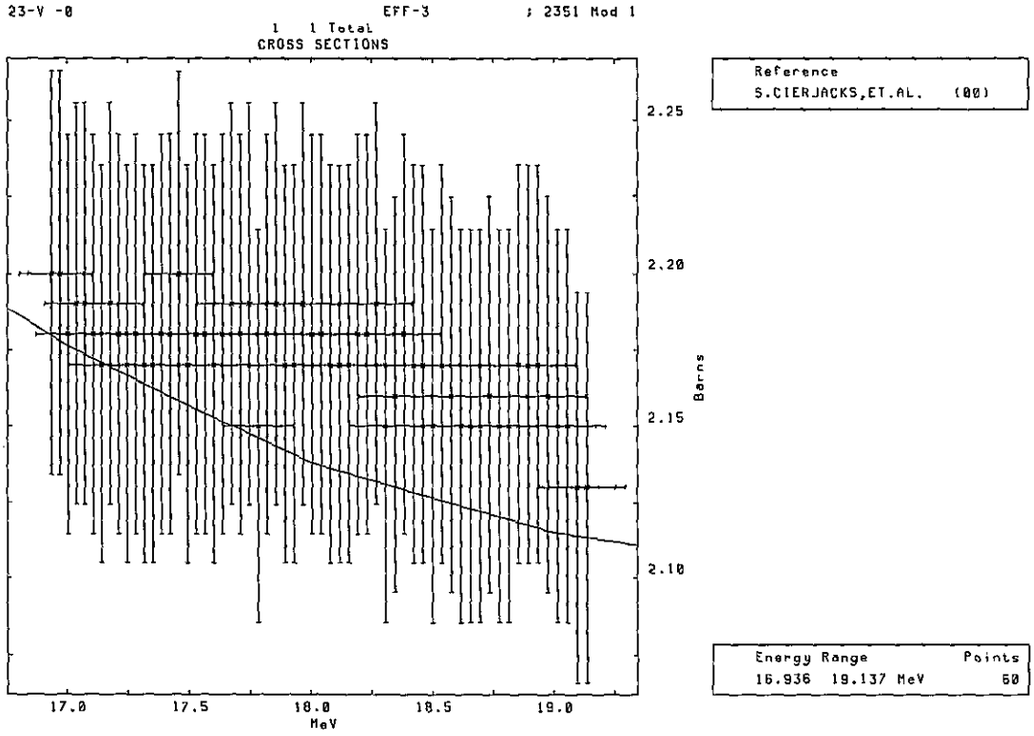

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
Reference
S.CIERJACKS,ET.AL. (00)
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
Barns
Energy Range
Points
10.098 11.083 MeV
60
10.2
10.4
10.6
10.8
11.0
MeV

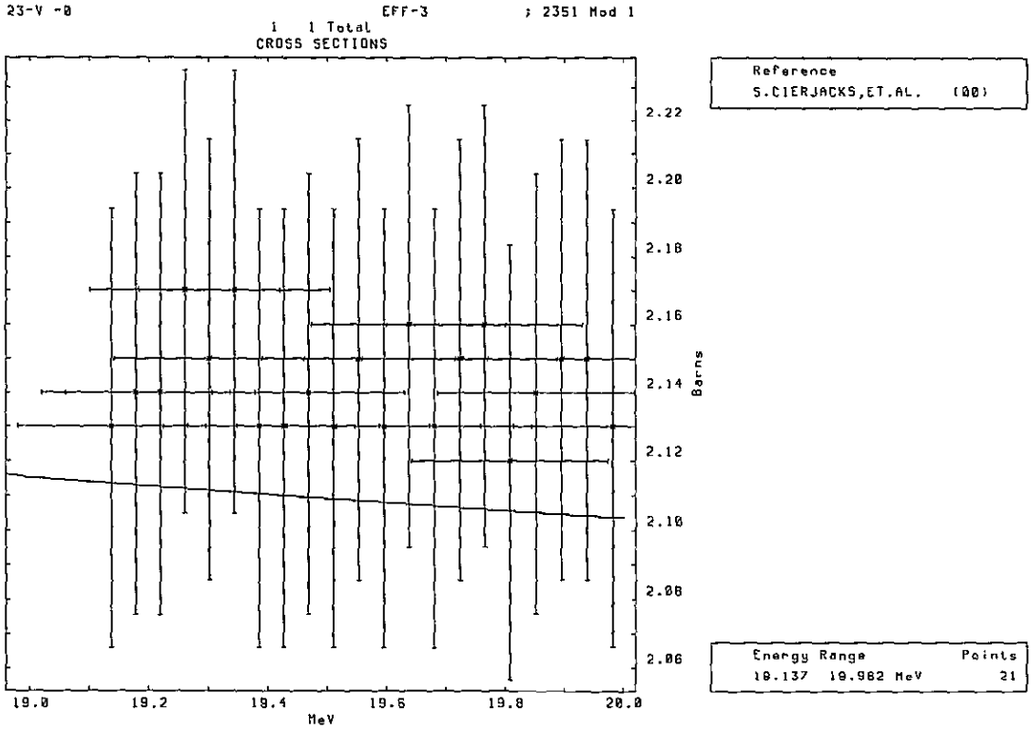

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
2.75
2.70
2.65
2.60
2.55
2.50
2.45
Barns
11.0
11.2
11.4
11.6
11.8
12.0
12.2
MeV
Reference
S.CIERJACKS,ET.AL. (00)
Energy Range
Points
11.083 12.221 MeV
60

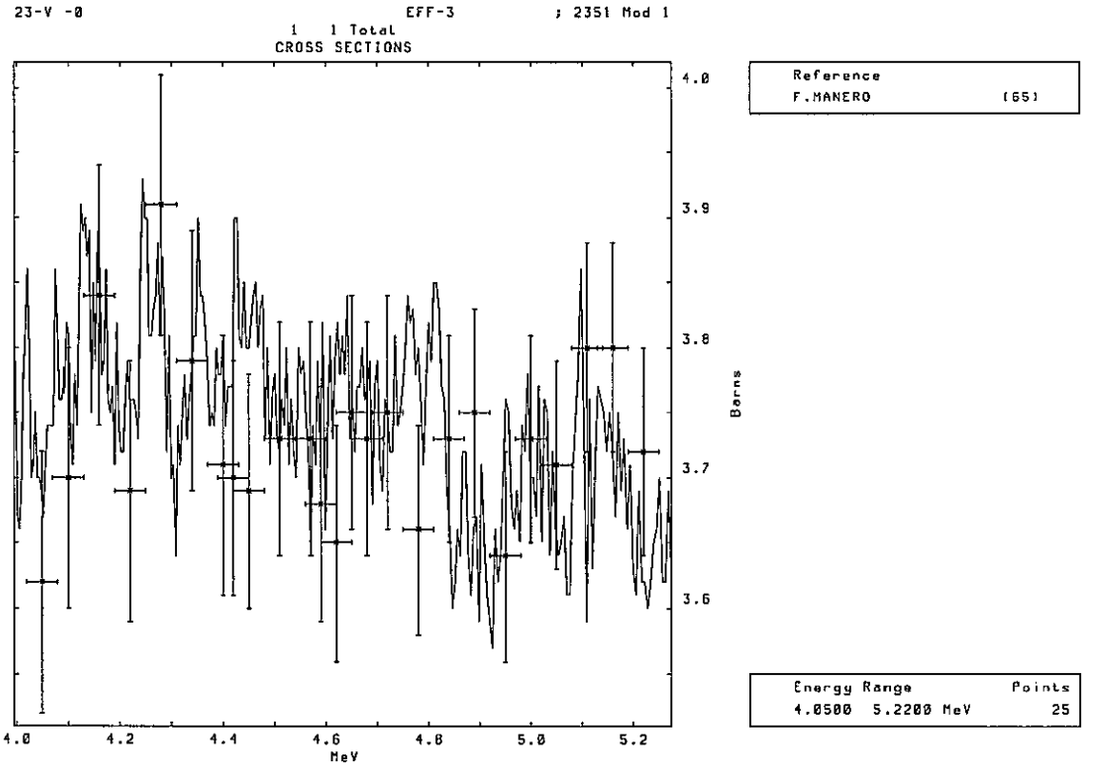

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
2.55
2.50
2.45
2.40
2.35
Barns
12.2
12.4
12.6
12.8
13.0
13.2
13.4
13.6
MeV
Reference
S.CIERJACKS,ET.AL. (00)
Energy Range
Points
12.221 13.545 MeV
60

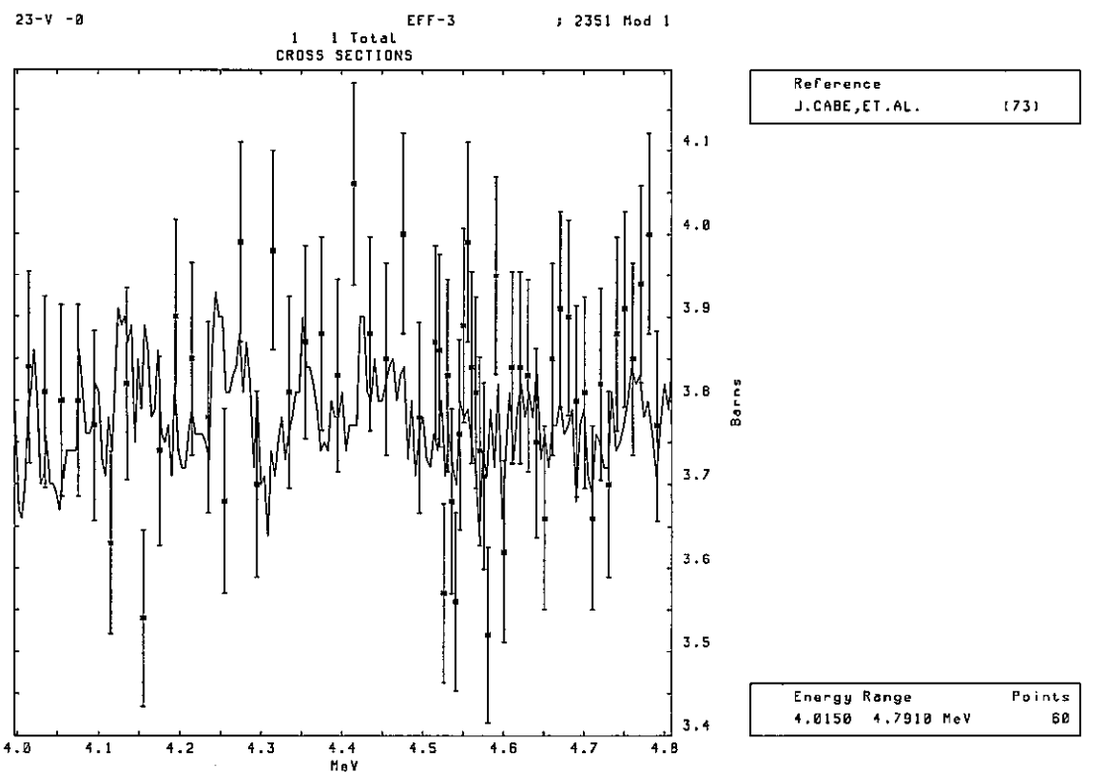

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
Reference
S.CIERJACKS,ET.AL. (00)
2.45
2.40
2.35
2.30
2.25
2.20
Barns
13.6
13.8
14.0
14.2
14.4
14.6
14.8
15.0
15.2
MeV
Energy Range Points
13.545 15.098 MeV 60

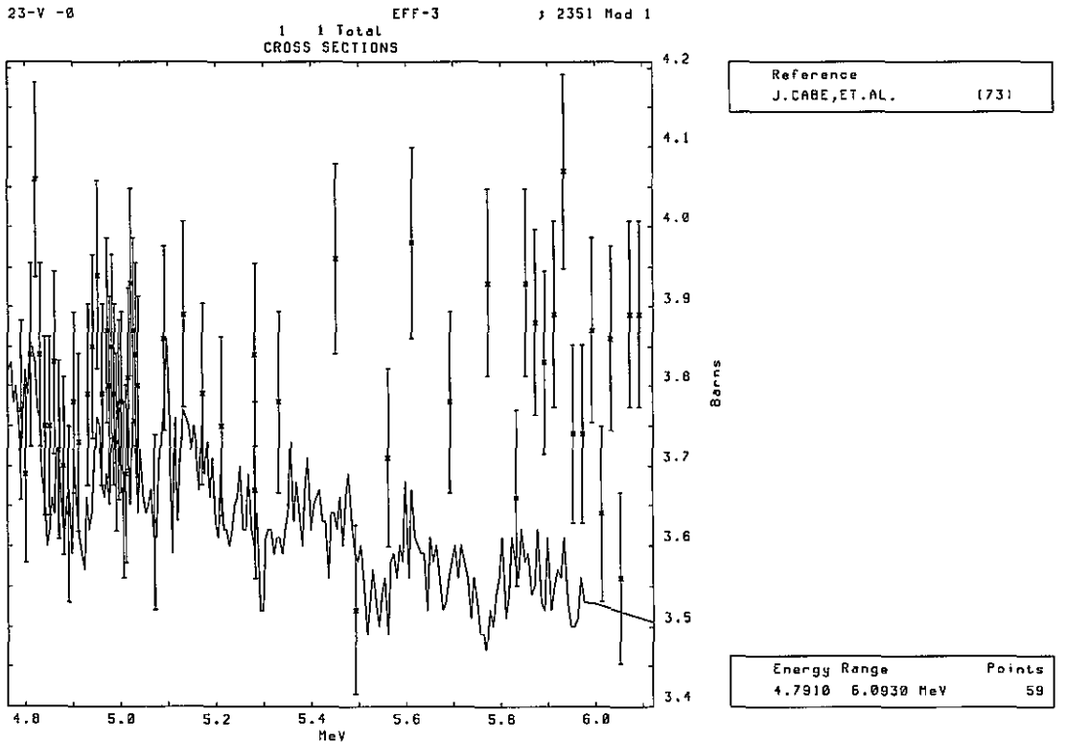

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
Reference
S.CIERJACKS,ET.AL. (00)
2.35
2.30
2.25
2.20
2.15
Barns
15.0
15.5
16.0
16.5
17.0
MeV
Energy Range Points
15.098 16.936 MeV 60

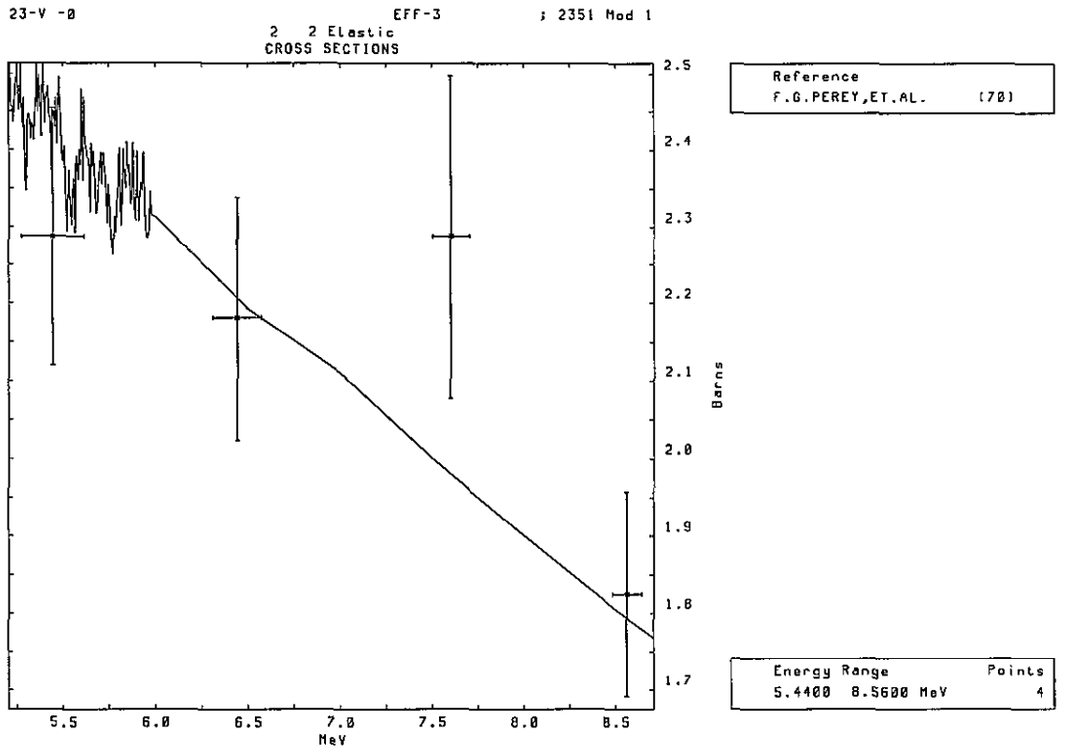

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
Reference
S.CIERJACKS,ET.AL. (00)
2.25
2.20
2.15
2.10
Barns
17.0
17.5
18.0
18.5
19.0
MeV
Energy Range
Points
16.936 19.137 MeV
60

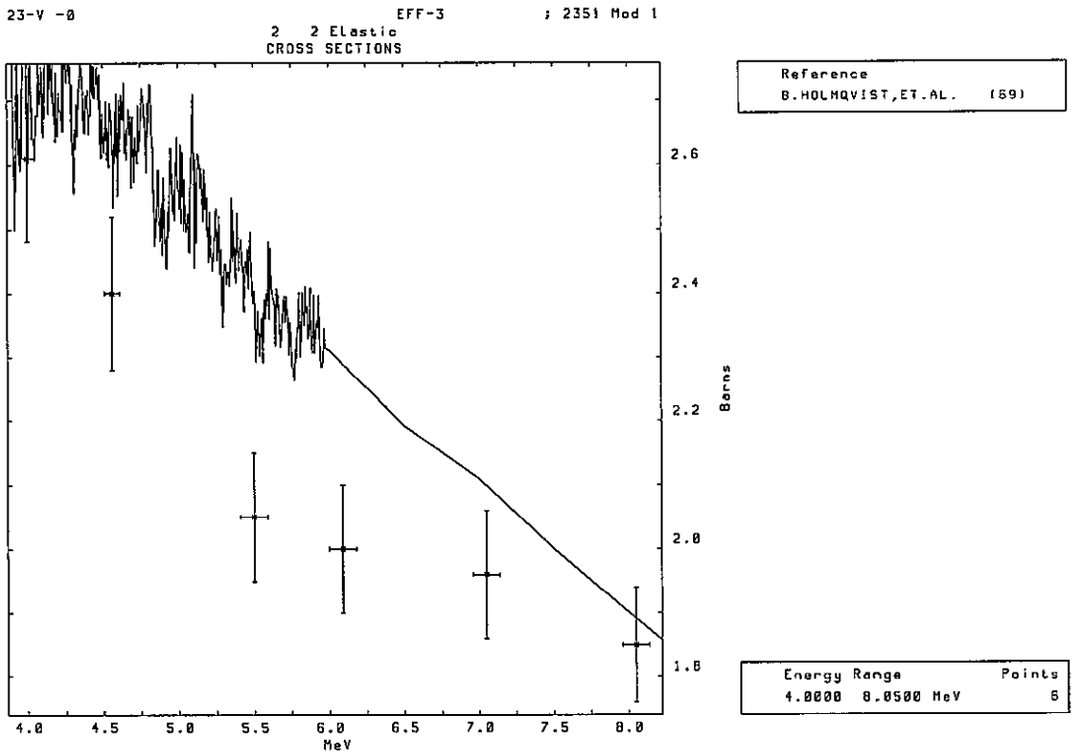

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
Reference
S.CIERJACKS,ET.AL. (00)
2.22
2.20
2.18
2.16
2.14
2.12
2.10
2.08
2.06
Barns
19.0
19.2
19.4
19.6
19.8
20.0
MeV
Energy Range
Points
19.137 19.982 MeV
21

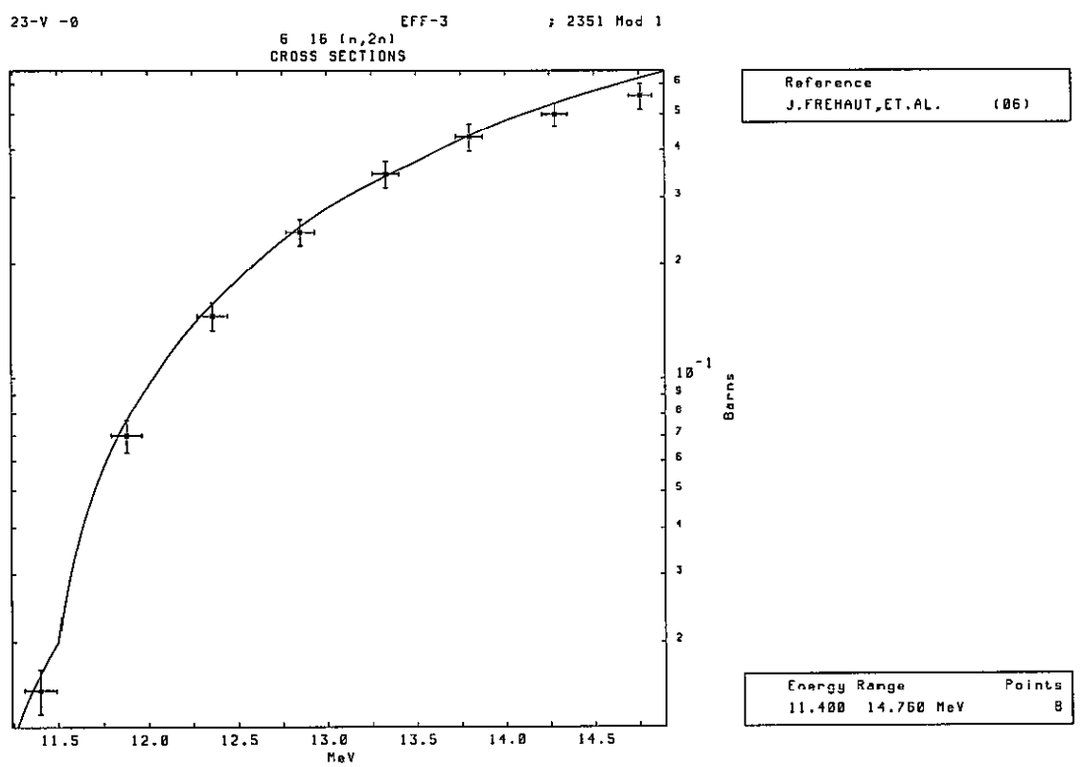

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
4.0
3.9
3.8
3.7
3.6
Barns
4.0
4.2
4.4
4.6
4.8
5.0
5.2
MeV
Reference
F.MANERO (65)
Energy Range Points
4.0500 5.2200 MeV 25


23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
Barns
4.0
4.1
4.2
4.3
4.4
4.5
4.6
4.7
4.8
MeV
Reference
J.CABE,ET.AL. (73)
Energy Range Points
4.0150 4.7910 MeV 60

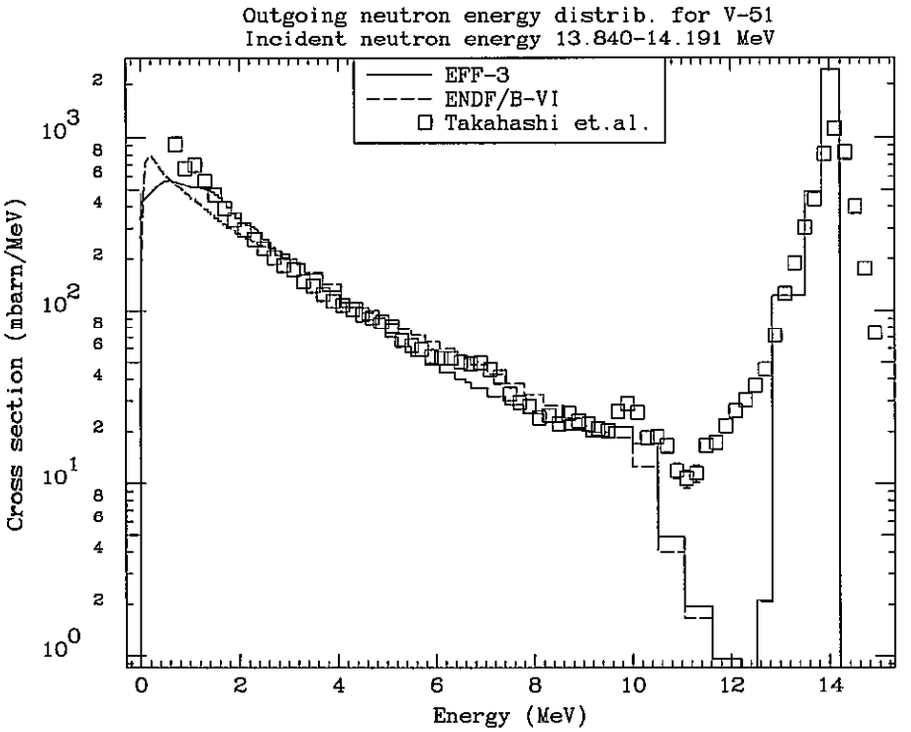

23-V -0
EFF-3
; 2351 Mod 1
1 1 Total
CROSS SECTIONS
Reference
J.CABE,ET.AL. (73)
Barns
MeV
Energy Range
4.7910 6.0930 MeV
Points
59

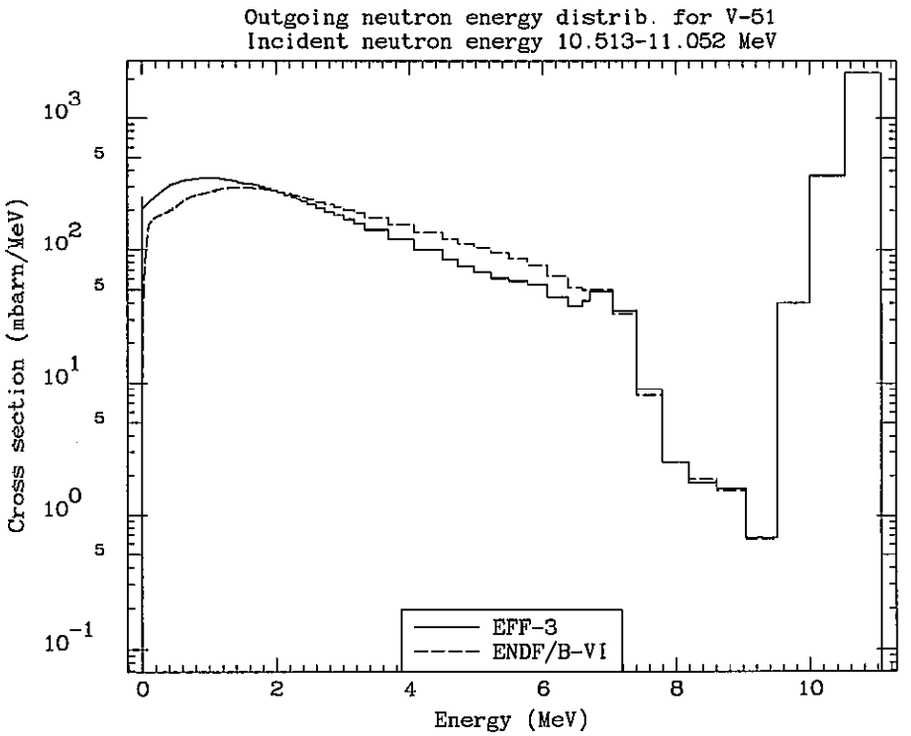

23-V -0
EFF-3
; 2351 Mod 1
2 2 Elastic
CROSS SECTIONS
Reference
F.G.PEREY,ET.AL. (70)
Barns
MeV
Energy Range
5.4400 8.5600 MeV
Points
4

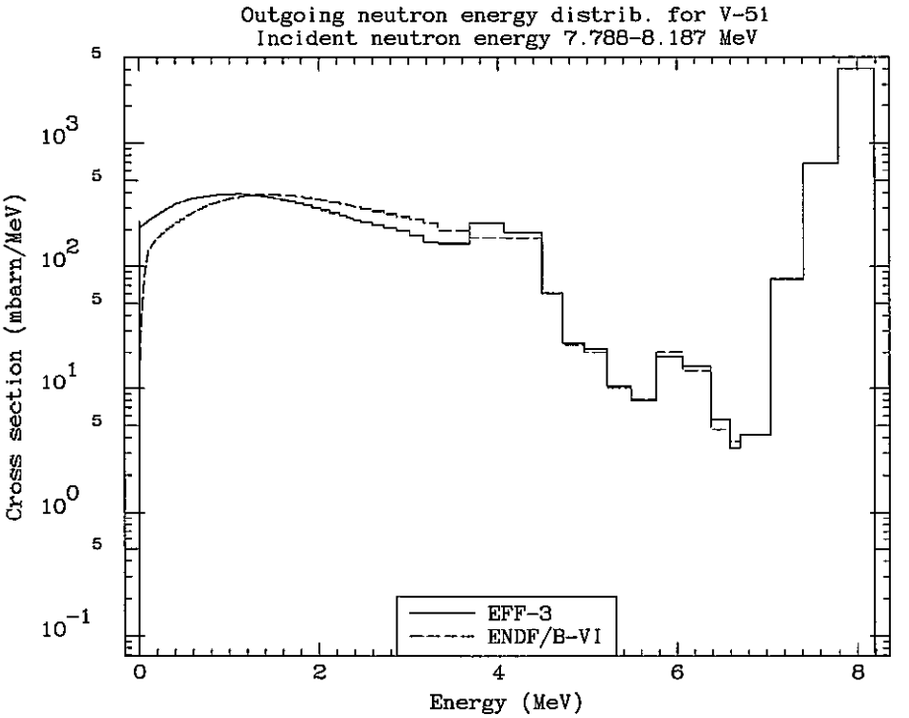

23-V -0
EFF-3
; 2351 Mod 1
2 2 Elastic
CROSS SECTIONS
Reference
B.HOLMQVIST,ET.AL. (69)
2.6
2.4
2.2
2.0
1.8
Barns
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
MeV
Energy Range
Points
4.0000 8.0500 MeV
6

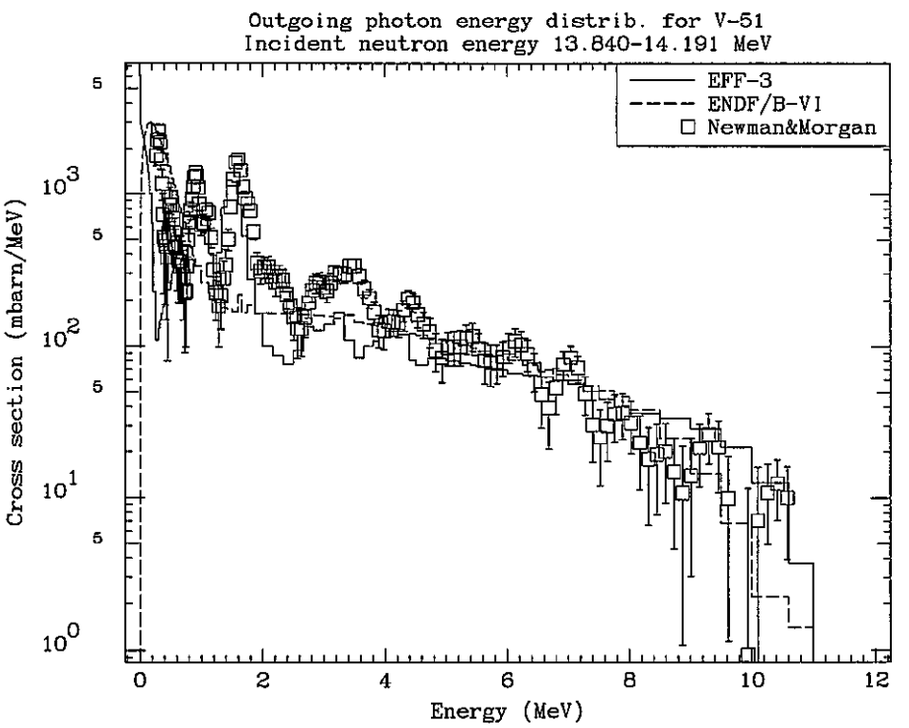

23-V -0
EFF-3
; 2351 Mod 1
6 16 (n,2n)
CROSS SECTIONS
Reference
J.FREHAUT,ET.AL. (86)
10^-1
Barns
11.5
12.0
12.5
13.0
13.5
14.0
14.5
MeV
Energy Range
Points
11.400 14.760 MeV
8

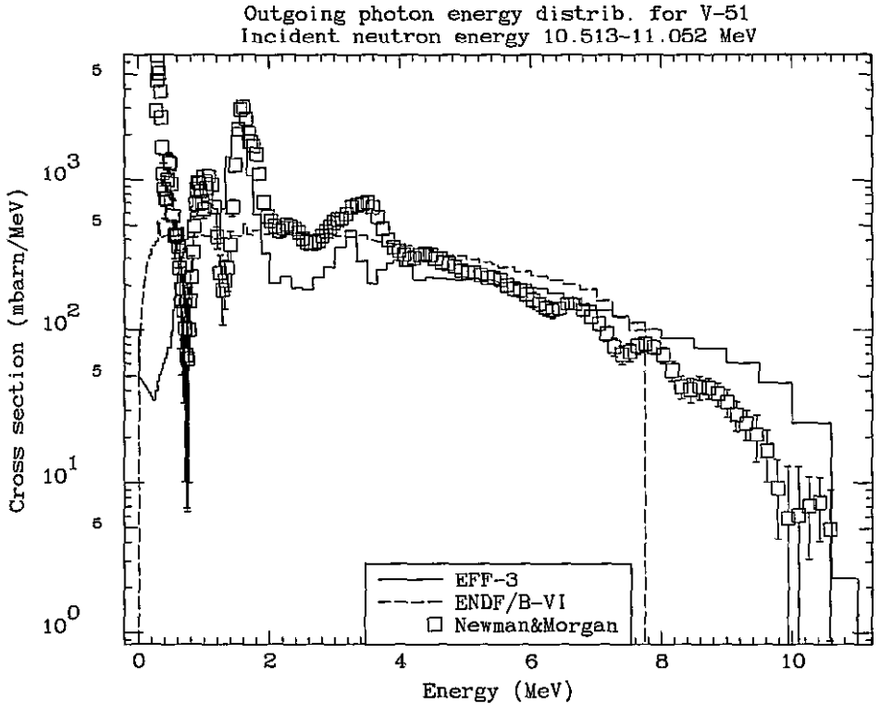
A.3 Outgoing particle spectra comparison

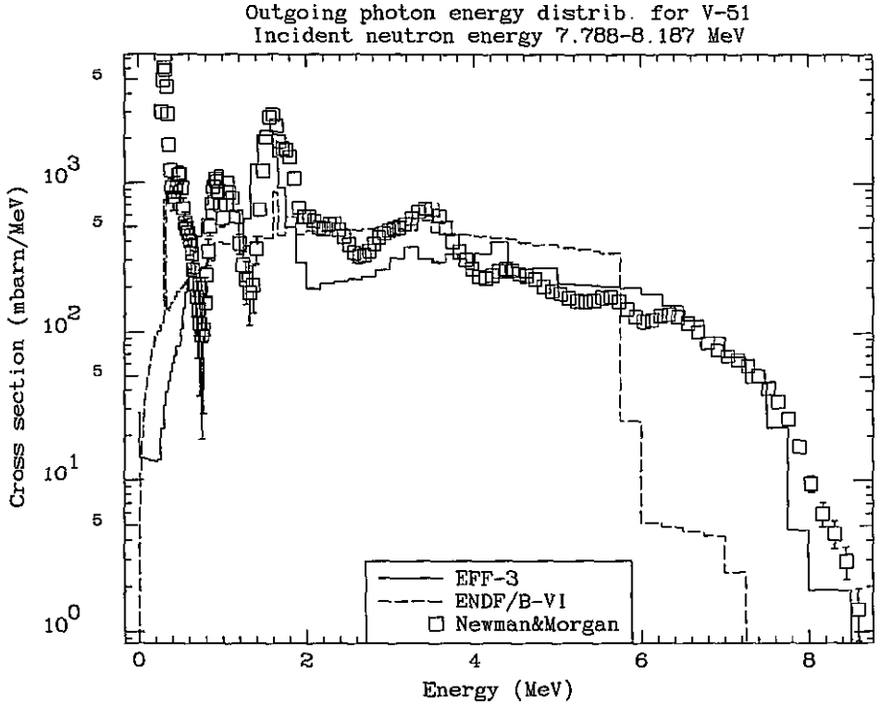


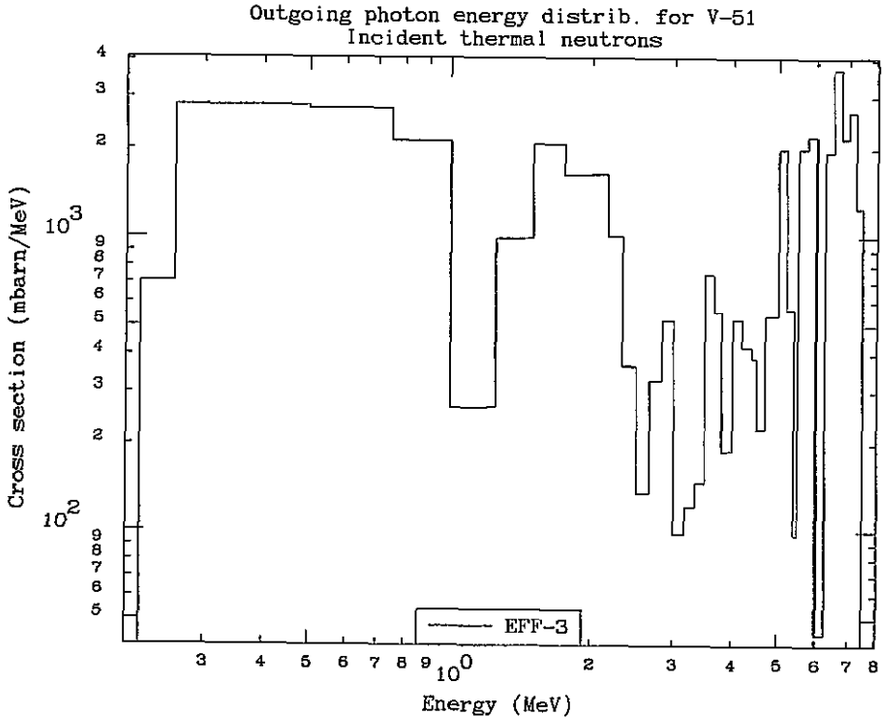


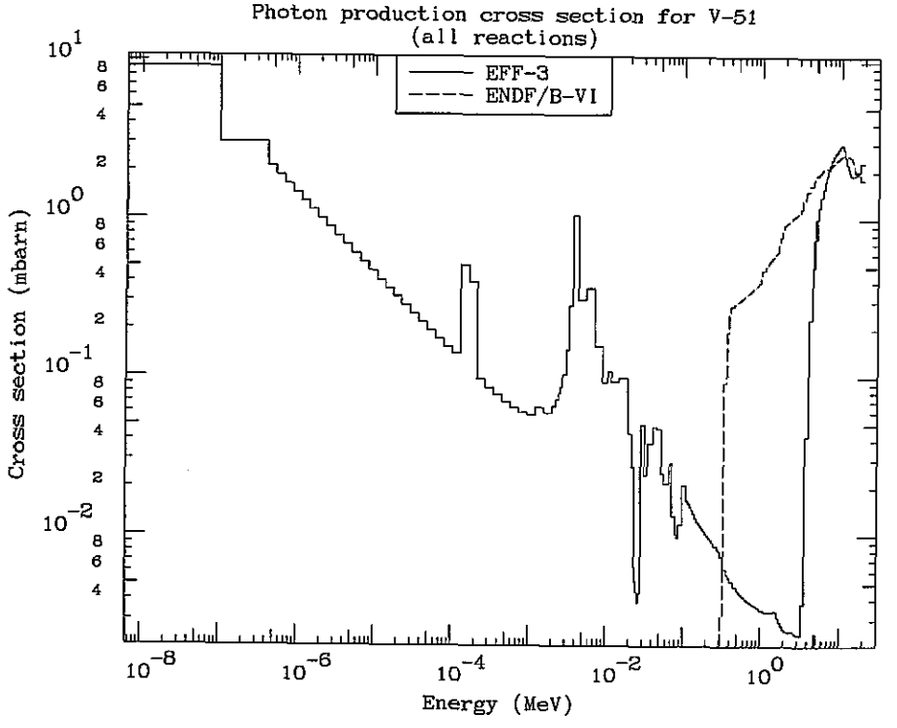

Outgoing neutron energy distrib. for V-51
Incident neutron energy 7.788-8.187 MeV
Cross section (mbarn/MeV)
Energy (MeV)
EFF-3
ENDF/B-VI

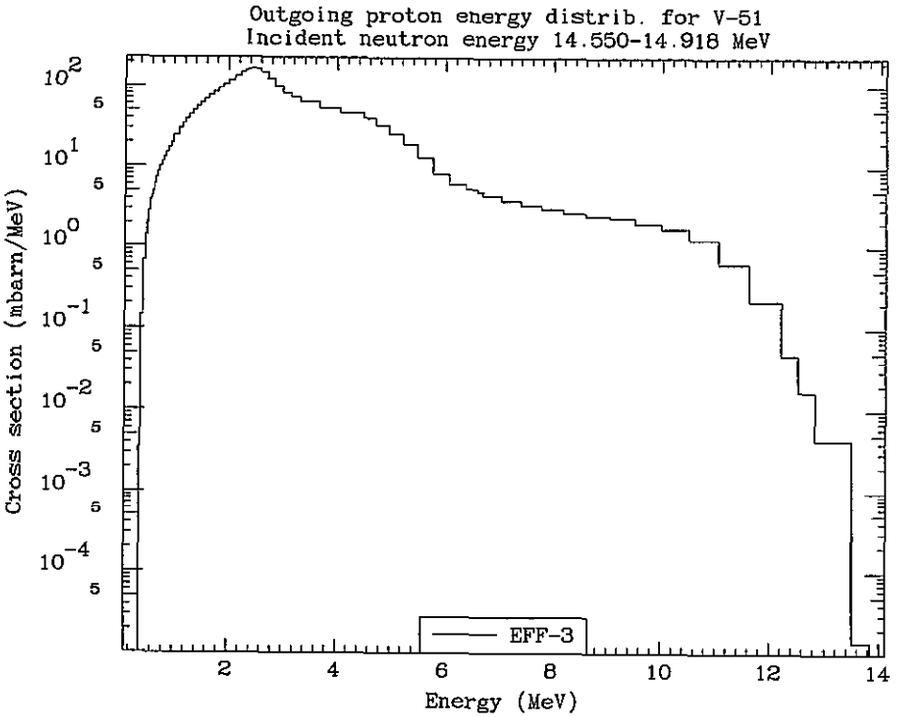

Outgoing photon energy distrib. for V-51
Incident neutron energy 13.840-14.191 MeV
Cross section (mbarn/MeV)
Energy (MeV)
EFF-3
ENDF/B-VI
Newman&Morgan

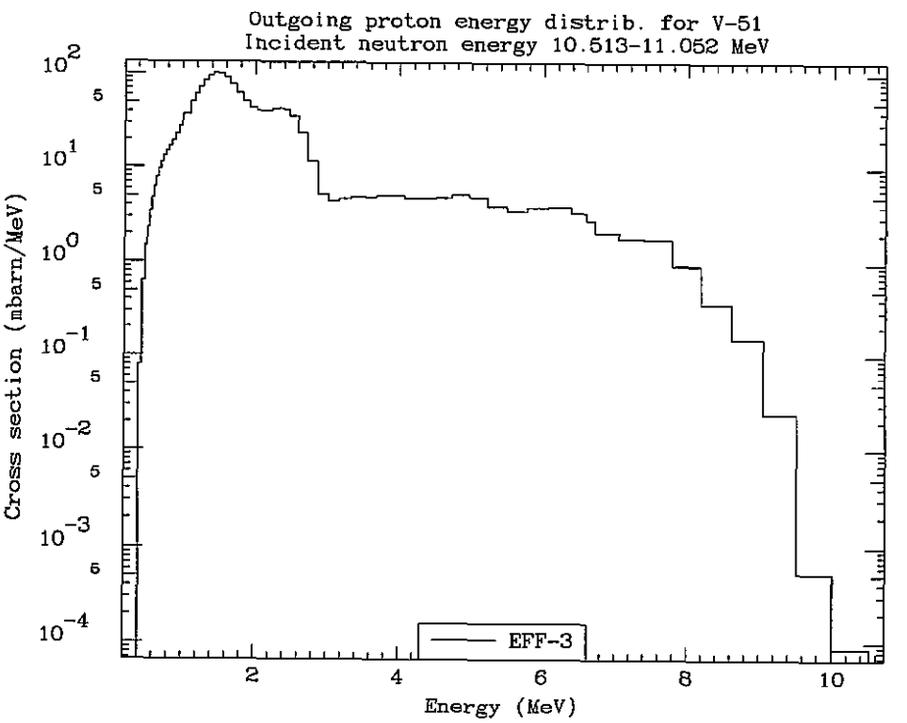

Outgoing photon energy distrib. for V-51
Incident neutron energy 10.513-11.052 MeV
Cross section (mbarn/MeV)
Energy (MeV)
EFF-3
ENDF/B-VI
Newman&Morgan

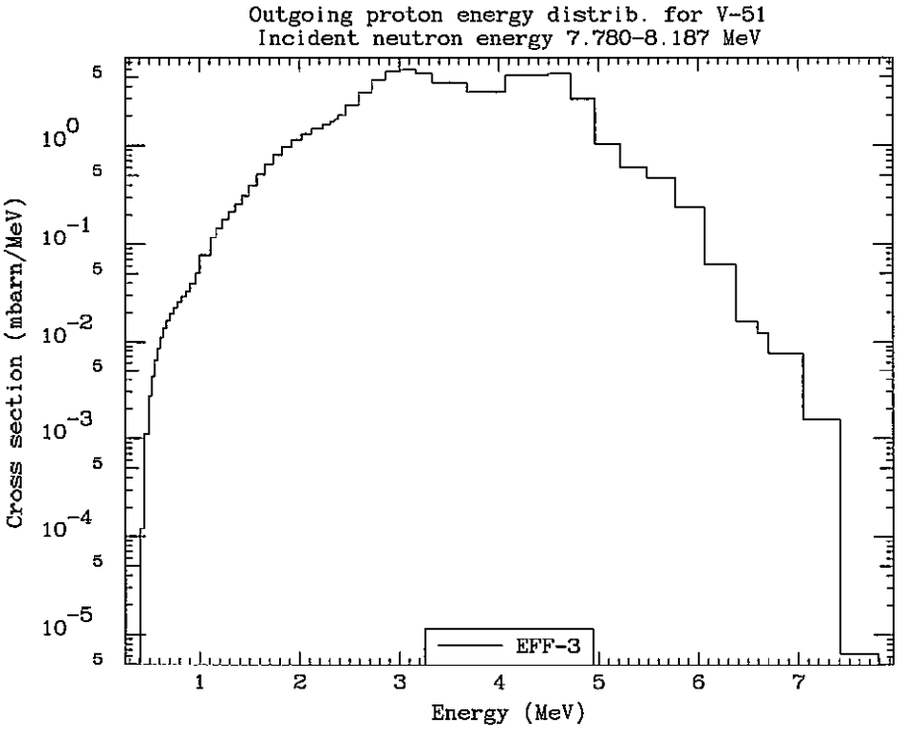

Outgoing photon energy distrib. for V-51
Incident neutron energy 7.788-8.187 MeV
Cross section (mbarn/MeV)
Energy (MeV)
EFF-3
ENDF/B-VI
Newman&Morgan


Outgoing photon energy distrib. for V-51
Incident thermal neutrons
Cross section (mbarn/MeV)
Energy (MeV)
EFF-3


Photon production cross section for V-51
(all reactions)
EFF-3
ENDF/B-VI
Cross section (mbarn)
Energy (MeV)


Outgoing proton energy distrib. for V-51
Incident neutron energy 14.550-14.918 MeV
Cross section (mbarn/MeV)
Energy (MeV)
EFF-3


Outgoing proton energy distrib. for V-51
Incident neutron energy 10.513-11.052 MeV
Cross section (mbarn/MeV)
Energy (MeV)
EFF-3


Outgoing proton energy distrib. for V-51
Incident neutron energy 7.780-8.187 MeV
Cross section (mbarn/MeV)
Energy (MeV)
EFF-3