



**Validation Study of UNIVAC-1110 Version of the  
CTR-PMCS-Nuclear Data Library & Codes  
Package**

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***FUSION TECHNOLOGY INSTITUTE  
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Validation Study of the UNIVAC 1110 Version of  
The CTR-PMCS - Nuclear Data  
Library and Codes Package

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## ABSTRACT

A validation effort for the AMPC interface version of the CTR-PMCSL library and codes adaptation for the UNIVAC-1110 computer is reported. In addition, results from two different blankets are presented. The first is the standard blanket<sup>(1)</sup> (Bench Mark Problem) and the second is the UWMAK-III blanket. Integral and differential quantities are compared with the results from using different libraries (DLC-37B and DLC-20). The comparison shows good agreement between the CTR-PMCSL and DLC-37B libraries.

## INTRODUCTION

A validation effort for the AMPX interface version of the CTR-PMCSL<sup>(1)</sup> (Processed Multigroup Cross Section Library) and codes adaptation for the UNIVAC-1110 computer is reported. Two problems are investigated using different libraries based on ENDF/B-III and IV.

The first problem is a standard blanket which was considered as a benchmark problem by Steiner<sup>(2)</sup>. Tritium production from  ${}^6\text{Li} (n,\alpha)\text{t}$  and  ${}^7\text{Li}(n,n'\alpha)\text{t}$  reactions and neutron multiplication from the  $(n,2n)$  reaction have been compared on total and per zone bases. Neutron spectra from the different libraries have been considered to detect changes in the data sets.

The second problem employs the UWMAK-III design which includes the use of the ISSEC concept<sup>(3)</sup> (internal spectral shifter and energy converter) and it has the characteristic of a shielding problem. The tritium and helium production, and neutron multiplication have been investigated. Group cross section plots for the materials under consideration are shown to explain the differences in the results from the different libraries.

### Multigroup Cross Section Data Sets

Three different multigroup data sets have been used. The first data set, DLC-2D is based on the ENDF/B-III library as processed by the SUPERTOG<sup>(4)</sup> code. The second data set DLC-37B is based on ENDF/B-IV and generated by the AMPX<sup>(5)</sup> system at 800°K except for Nb. The Nb cross sections were generated from ENDF/B-III. The third data set, CTR-PMCSL is based on ENDF/B-IV but is generated by the MINX<sup>(6)</sup> neutron processor coupled with the AMPX system.

DLC-2D and DLC-37B libraries were obtained from RSIC in a form which required only a minor effort to generate group independent cross sections for neutron and gamma transport calculations. On the other hand, the CTR-PMCSL library required a significant amount of work to produce a working version of the library. The conversion to the working library requires the use of several computer codes<sup>(1)</sup> (AIM,CHOX, MALOCS, DIAL, RADE, NITWAL, and GIP). These codes have been modified to operate on the UNIVAC system (since they were originally written for the IBM system). This new version of the codes is available from RSIC. As a result, the user has more options to generate suitable libraries for different purposes.

### The Bench Mark Problem

The geometry, the materials, and the parameters used in this calculation are given in Table 1 and Figure 1. This information was taken from reference 1. The angular quadrature sets used in the  $S_n$  calculation are given in table 2. The weighted model has been employed to correct for negative fluxes during the calculations. The ANISN<sup>(7)</sup> program was used to perform the calculations.

### Results of the Bench Mark Calculations

The  $S_4$ - $P_3$  results using different data sets are given in Tables 3 to 7 and Figures 2 to 5. Table 3 presents the tritium breeding ratio from the blanket by zone. Tables 4 and 5 give the  ${}^6\text{Li} (n,\alpha)t$  and  ${}^7\text{Li} (n,n'\alpha)t$  reactions per zone per fusion neutron. Tables 6 and 7 give the  $(n,2n)$  reaction per zone per fusion neutron from Nb and all other materials. Figures 2 to 5 show  $\text{Li} (n,t)$ ,  ${}^6\text{Li} (n,\alpha)t$ ,  ${}^7\text{Li} (n,n'\alpha)t$  and the  $(n,2n)$  reactions as a function of radius per fusion neutron. Table 8 lists the tritium production results from different calculations<sup>(8,9)</sup>. The LLL results for the standard blanket using the monte carlo code TART with different data sets are listed. These data sets were generated by the CLYDE system with both the ENDF/B-III and ENDF/B-IV libraries. Table 9 shows the relative percent difference between the different results using the CTR-PMCSL results as the reference case. The neutron spectra at different positions through the blanket are given in Figures 6 to 13. Figures 14 to 21 give the absorption and the total cross section for  ${}^6\text{Li}$ ,  ${}^7\text{Li}$ , Nb and C used in the calculations from ENDF/B-III and ENDF/B-IV.

### Discussion of the Standard Blanket Results

The first look at the CTR-PMCSL results indicate that the breeding ratio is about 3.6 to 7.5% higher than the values predicted by libraries based on ENDF/B-III. The breeding in  ${}^7\text{Li}$  is  $\sim 8$  to 10% greater than the value based on the ENDF/III library. This increase in the  ${}^7\text{Li}$  breeding indicates that the  ${}^7\text{Li}(n,n'\alpha)t$  may have been changed, particularly if figure 4 is taken into consideration. Figure 4 shows the  ${}^7\text{Li} (n,n'\alpha)t$  reaction rate as a function of distance through the blanket. Figures 16 and 17 show the absorption and the total cross sections for  ${}^7\text{Li}$ . Although Figures 16 and 17 show no change in these cross sections, the reaction rate shows changes. A close look at the neutron spectra shows the same difference, particularly in the energy range



of interest from the spectrum (greater than 0.55 Mev). This change in the spectrum is related to the change in the Nb cross section, particularly the elastic scattering cross section. Figure 19 shows clearly that for neutron energies greater than 0.55 Mev, the current total cross section for Nb is less than the one based on ENDF/B-III.

The breeding based on the CTR-PMCSL library is  $\sim 3.2$  to  $6.4\%$  higher than the value predicted by the calculations which were based on ENDF/B-III. A close look shows the  ${}^6\text{Li}$  cross section is unchanged. On the other hand, the Nb cross section changes, particularly the elastic and the absorption cross section influence this reaction rate. The change in the Nb absorption cross section is not in one direction, increasing or decreasing over the neutron energy range of interest. In fact, the Nb absorption cross section decreases in the energy range 0.5 to 3.0 Mev and increases in the energy range 0.2 to 0.5 Mev. The elastic scattering cross section is changed by a factor of five in the energy range 0.1 to 0.5 Mev and the ratio of the scattering to the absorption in this particular range of energy is  $\sim 100$ . This results in an increase in the neutron spectrum over the energy range from 0.01 to 0.001 Mev. Figures 6 to 13 show a decrease in the neutron spectrum for neutron energies less than 0.001 Mev. The net effect is a slight increase in the  ${}^6\text{Li}$  breeding, since the increase in the higher energy range dominates the effect at the lower energy. In addition, the increase in the (n,2n) reaction rates has a positive effect on the  ${}^6\text{Li}$  breeding.

#### UWMAK-III Blanket

The UWMAK-III blanket and shield has been described in detail elsewhere (10,11). The reactor geometry, materials and the calculational procedure in considering the different aspects of UWMAK-III are given in the references (10,12), particularly with regard to the asymmetry in the poloidal direction and the source distribution. Figure 22 shows schematically the reactor geometry

and the materials used in the calculations. Two sets of calculations have been carried out based on the DLC-37B and the CTR-PMCSL data sets. The ANISN code has been used to perform the calculations in the  $S_6$ - $P_3$  approximation. The number densities of the materials used are listed in Table 10.

#### Results of the UWMAK-III Neutronic Calculation

Tables 11 to 13 give the breeding ratio, and the  ${}^6\text{Li}(n,\alpha)t$  and  ${}^7\text{Li}(n,n'\alpha)t$  reaction rates per fusion neutron. Neutron multiplication through  $(n,2n)$  reactions per fusion neutron are given in Table 14. Table 15 presents the percentage difference in the calculated parameters relative to the CTR-PMCSL results. Figures 23 and 24 show the absorption and the total cross sections for Molybdenum used in the calculations. Figures 25 to 33 show the neutron spectra at selected positions in the blanket. These positions are given in Table 17.

#### Discussion of the UWMAK-III Results

The tritium breeding ratio based on CTR-PMCSL is  $\sim 5\%$  less than the value based on the DLC-37B library. The relative difference in the  ${}^7\text{Li}$  breeding is  $\sim 1.5\%$  (0.0080 reactions/fusion neutron), and 8.6% (0.0643 reactions/fusion neutron) in the  ${}^6\text{Li}$  breeding. The  $(n,2n)$  reactions show a 2.1% relative increase which seems to contradict the decrease in the  ${}^6\text{Li}$  breeding. A close look at the Mo cross sections shows an increase in the absorption and total cross sections in the energy range from 0.001 to 0.1 Mev as shown in Figures 23 and 24. These changes in the Mo cross sections explain the changes in neutron spectra shown in Figures 25 to 33 between the calculations based on CTR-PMCSL and DLC-37B. The neutron spectra based on the CTR-PMCSL library is less in the energy range  $< 0.1$  Mev, particularly in the zones with a high percentage of Mo. These changes in the Mo cross sections are related to the neutron processing code MINX<sup>(1)</sup>. A comparison between the absorption and total cross sections from MINX and the corresponding cross sections from DLC-37B shows

the cross sections from the MINX processor are higher, and this in turn explains the difference in the breeding ratio. Table 16 shows Helium production rates from  $^6\text{Li}$ ,  $^7\text{Li}$  and C. The Helium production from the carbon ISSEC shows good agreement between CTR-PMCSL and DLC-37.

### Computer Codes

A UNIVAC version of the computer code package with the CTR-PMCSL library has been developed. This version of the package was generated from the IBM version. Two types of modification were carried out. The first modification is related to the difference between the IBM and UNIVAC systems. As an example of this type, the IBM system stores four characters per word while UNIVAC stores six characters per word. This difference in the manner of storage requires the changing of all alphanumeric data statements and the sub-routine calls with strings of characters and the input, output format for the alphanumeric data. The second type of modification is related to the efficiency of the programs (memory size, input, output and speed). An example of this type is the dynamic allocation of the required memory using a fortran sub-routine in a standard way which is independent of the system to save on the memory required. The input data for these codes are unchanged, which eliminates the need for new user manuals.

The only exception is the NITWAL program where some assembly routines were written to take of direct access input output. The details of this particular case is given in the code itself, since it is necessary only for code operation.

### Conclusions

Analysis of the calculations identified some real changes in the processed data and the effects on the neutronic performance of fusion reactors. Some problems are also indicated which require more precise processing of the data. Thus further attention should be given to validation efforts covering different materials existing in the library.

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Table 1. Nuclide Number Densities for the Materials of the Standard Blanket

Material	Constituent	Number Density/CC $\times 10^{-24}$
A	Isotropic source of neutrons in vacuum	0.0
B	Vacuum	0.0
C	Niobium	0.05556
D	Niobium	0.003334
	Lithium-6	0.003234
	Lithium-7	0.04038
E	Carbon	0.0804

Table 2.  $S_4$  and  $S_6$  Angular Quadrature Set

$S_4$		$S_6$	
Cosine	Weight	Cosine	Weight
-0.508374	0.0	-0.963797	0.0
-0.359475	0.173927	-0.926181	0.0880632
0.359475	0.173927	-0.681508	0.0786035
-0.940432	0.0	-0.266635	0.0880632
-0.868845	0.163036	0.266635	0.0880632
-0.359887	0.163036	0.681508	0.0786035
0.359887	0.163036	0.926181	0.0880632
0.868845	0.163036	-0.731811	0.0
		-0.681508	0.0786035
		-0.266635	0.0786035
		0.266635	0.0786035
		0.681508	0.0786035
		-0.377079	0.0
		-0.266635	0.0880631
		0.266635	0.0880631

Table 3. Comparison of Total Tritium Breeding by Zone

Zone	ORNL-III <sup>(1)</sup>	UW-III <sup>(2)</sup>	UW-IV-1 <sup>(3)</sup>	UW-IV-2 <sup>(4)</sup>
3				
4	0.1286	0.1280	0.1276	0.1346
5				
6	0.5724	0.5818	0.5795	0.6143
7	0.3462	0.3476	0.3460	0.3704
8	0.3402	0.3211	0.3522	0.3574
9				
10	0.0643	0.0497	0.0831	0.0675
Total	1.4517	1.4282	1.4884	1.5442

1) Results from Reference 1.

2) Results using DLC-2 Library.

3) Results using DLC-37 Library.

4) Results using CTR-PMCSL Library.

Table 4. Comparison of  ${}^6\text{Li}$  (n, $\alpha$ )t Reaction Rate  
by Zone

Zone	ORNL-III	UW-III	UW-IV-1	UW-IV-2
3				
4	0.0480	0.0483	0.0480	0.0500
5				
6	0.2912	0.2945	0.2921	0.3020
7	0.2364	0.2375	0.2351	0.2455
8	0.2944	0.2777	0.3079	0.3053
9				
10	0.0634	0.0490	0.0823	0.0664
Total	0.9334	0.9070	0.9654	0.9692



Table 5. Comparison of  ${}^7\text{Li}$  ( $n, n'\alpha$ ) $\gamma$  Reaction Rate  
by Zone

Zone	ORNL-III	UW-III	UW-IV-1	UW-IV-2
3				
4	0.0806	0.0797	0.0796	0.0846
5				
6	0.2812	0.2873	0.2874	0.3123
7	0.1098	0.1101	0.1109	0.1249
8	0.0458	0.0434	0.0443	0.0521
9				
10	0.0009	0.0007	0.0008	0.0011
Total	0.5183	0.5213	0.5230	0.5750

Table 6. Comparison of Nb(n,2n) Reactions  
by Zone

Region	ORNL-III	UW-III	UW-IV-1	UW-IV-2
3	0.0575	0.0556	0.0557	0.0635
4		0.0168	0.0169	0.0196
5	0.0394	0.0392	0.0396	0.0467
6		0.0485	0.0495	0.0617
7		0.0143	0.0151	0.0208
8		0.0048	0.0052	0.0078
9				
10		0.0001	0.0001	0.0001
Total		0.0193	0.1821	0.2202

Table 7. Comparison of (n,2n) Reaction by Zone  
From all the Materials

Zone	ORNL-III	UW-III	UW-IV-1	UW-IV-2
3	0.0582	0.0556	0.0557	0.0635
4	0.0289	0.0221	0.0222	0.0251
5	0.0395	0.0392	0.0396	0.0467
6	0.0793	0.0644	0.0657	0.0790
7	0.0240	0.0192	0.0203	0.0267
8	0.0086	0.0066	0.0070	0.0100
9				
10	0.0001	0.0001	0.0001	0.0001
Total	0.2386	0.2072	0.2106	0.2511

Table 8. Comparison of  ${}^6\text{Li}$  ( $n,\alpha$ ) $t$ ,  ${}^7\text{Li}$  ( $n,n'\alpha$ ) $t$ , and Total Breeding Ratio From Different References for the Standard Blanket

Method	Reference	Data Set Origin	${}^6\text{Li}$ ( $n,\alpha t$ )	${}^7\text{Li}$ ( $n,n'\alpha t$ )	B.R.
Monte Carlo	LLL ( )	ENDF/B-III	$0.938 \pm 0.013$	$0.528 \pm 0.006$	$1.466 \pm 0.013$
$S_4$ -P <sub>3</sub>	ORNL (1)	ENDF/B-III	0.933	0.518	1.452
$S_4$ -P <sub>3</sub>	UW	ENDF/B-III	0.907	0.521	1.428
Monte Carlo	LLL ( )	ENDF/B-IV	$0.956 \pm 0.013$	$0.579 \pm 0.006$	$1.535 \pm 0.013$
$S_4$ -P <sub>3</sub>	ORNL ( )	ENDF/B-IV	0.969	0.575	1.544
$S_4$ -P <sub>3</sub>	UW	ENDF/B-IV	0.969	0.575	1.544

Table 9. The Relative Change in the Different  
Parameters in % Relative to the CTR-PMCSL Library Results

Parameter	ORNL-III	UW-III	LLL-III	UW-IV-1	LLL-IV
Breeding Ratio	-6.0	-7.5	-5.0	-3.6	-0.6
$^6\text{Li}$ (n, $\alpha$ t)	-3.7	-6.4	-3.2	-0.4	-1.4
$^7\text{Li}$ (n,n' $\alpha$ t)	-9.9	-9.4	-8.2	-9.0	+0.7
Nb (n,2n)	-	-18.6	-21.4	-17.3	-5.5
Total (n,2n)	-4.9	-17.5	-	-16.1	-

Table 10. Nuclide Number Densities for the  
Material of UWMAK-III

Material	Constituent	Number Density X $10^{-24}$
A	Carbon	0.08023
B	Molybdenum	0.06403
C	Molybdenum	0.00192
	Lithium - 6	0.00331
	Lithium - 7	0.04131
D	Carbon	0.07943
	Molybdenum	0.00064
E	Molybdenum	0.0525
	Aluminum	0.0043
	Silicon	0.0043
	Oxygen	0.0109

Table 11. Comparison of the Total Tritium  
Breeding by Zone

Zone	UW-IV-1	UW-IV-2
8	1.3052	1.2395
10	0.0590	0.0584
Totals	1.3642	1.2979

Table 12. Comparison of  ${}^6\text{Li}$  (n, $\alpha$ )t reaction  
per Zone

Zone	UW-IV-1	UW-IV-2
8	0.7568	0.6934
10	0.0572	0.0563
Totals	0.8140	0.7497



Table 13. Comparison of  $^7\text{Li}$  (n,n' $\alpha$ )t Reaction  
per Zone

Zone	UW-IV-1	UW-IV-2
8	0.5484	0.5461
10	0.0018	0.0021
Totals	0.5402	0.5482

Table 14. Comparison of (n,2n) and Absorption  
Reactions per Zone

Zone	UW-IV-1		UW-IV-2	
	n,2n	Absorption	n,2n	Absorption
1	0.0133	0.1261	0.0165	0.1281
2	0.0013	0.0214	0.0016	0.0205
3		0.0408		0.0421
7	0.0223	0.0117	0.0256	0.0169
8	0.0920	0.0995	0.1058	0.1491
9	0.0005	0.0385	0.0007	0.0442
10	0.0002	0.0048	0.0003	0.0052
11		0.0030		0.0035
Totals	0.1296	0.3458	0.1505	0.4096

Table 15. Relative Changes in Reaction Rates  
Relative to CTR-PMCSC Library Results

Parameter	UW-IV-1
Total Breeding Ratio	5.1
${}^6\text{Li} (n,\alpha)t$	8.6
${}^7\text{Li} (n,n'\alpha)t$	-1.5
$(n,2n)$	13.8
Absorption	15.6

Table 16. Comparison of Helium Production by Zone

Zone	$^6\text{Li}$		$^7\text{Li}$		$^{12}\text{C}$		TOTAL	
	UW-IV-1	UW-IV-2	UW-IV-1	UW-IV-2	UW-IV-1	UW-IV-2	UW-ID-1	UW-ID-2
3	--	--	--	--	0.2688	0.2560	0.2688	0.2560
8	0.7626	0.6993	0.5766	0.5759	--	--	1.3392	1.2752
9	--	--	--	--	0.0331	0.0377	0.0331	0.0377
10	0.0572	0.0563	0.0019	0.0022	--	--	0.0591	0.0585
11	--	--	--	--	0.0018	0.0024	0.0018	0.0024
Total	0.8198	0.7556	0.5785	0.5781	0.3037	0.2961	1.7020	1.6298

Table 17: The Positions of the Neutron Spectra  
Given in Figures 25 to 33.

Position	Interval
1	71
2	76
3	86
4	96
5	136
6	52
7	44
8	36
9	27

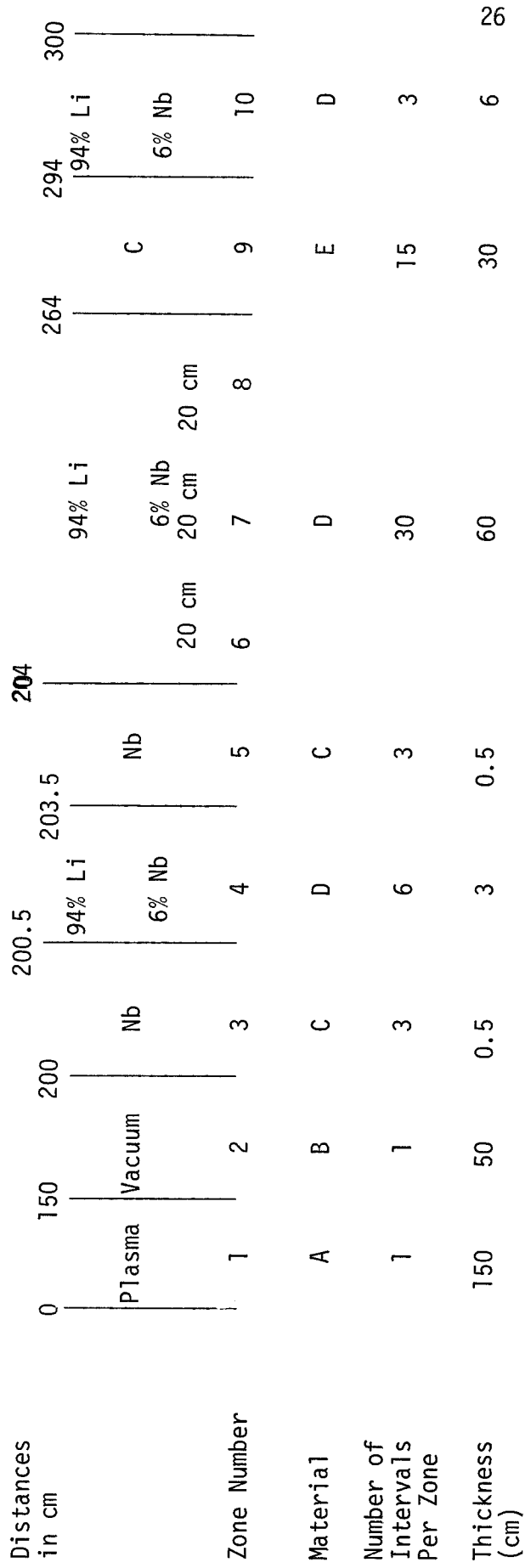
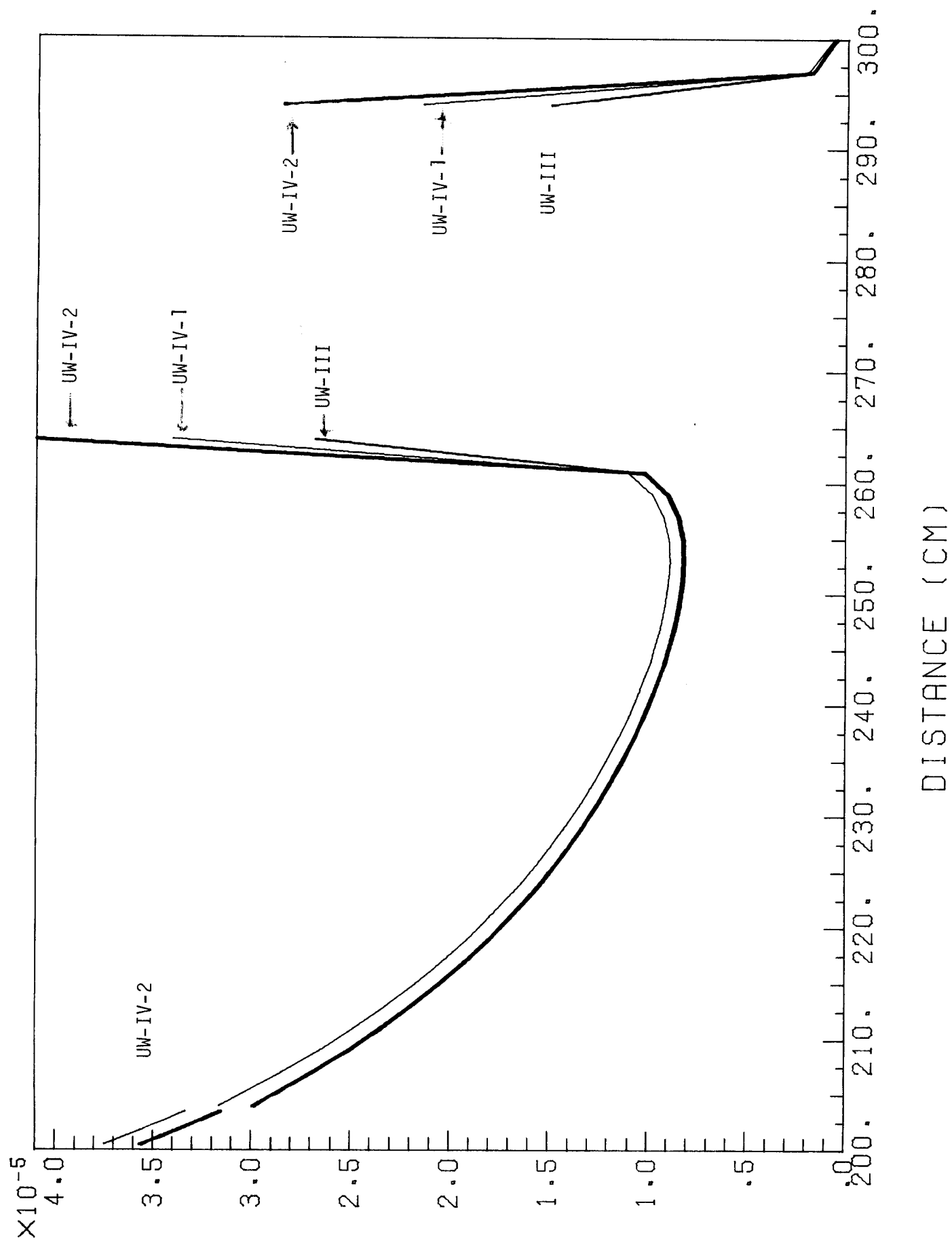


Fig. 1. A Schematic of the Standard Blanket

Figure 2. Tritium Production Rate



LI(N,AT) PLUS LI(N,N'AT) REACTION/CM<sup>3</sup>. FUSION NEUTRON

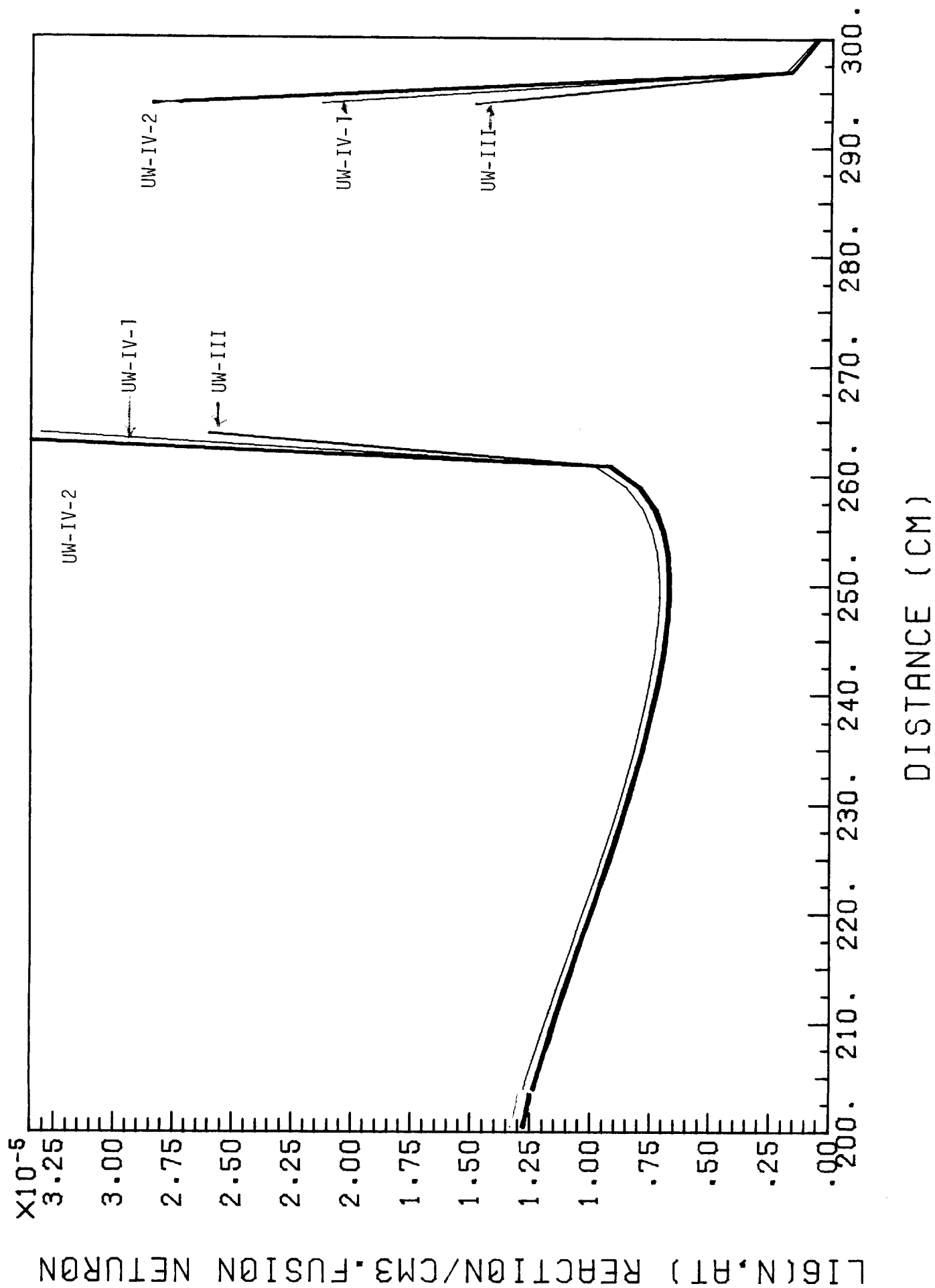
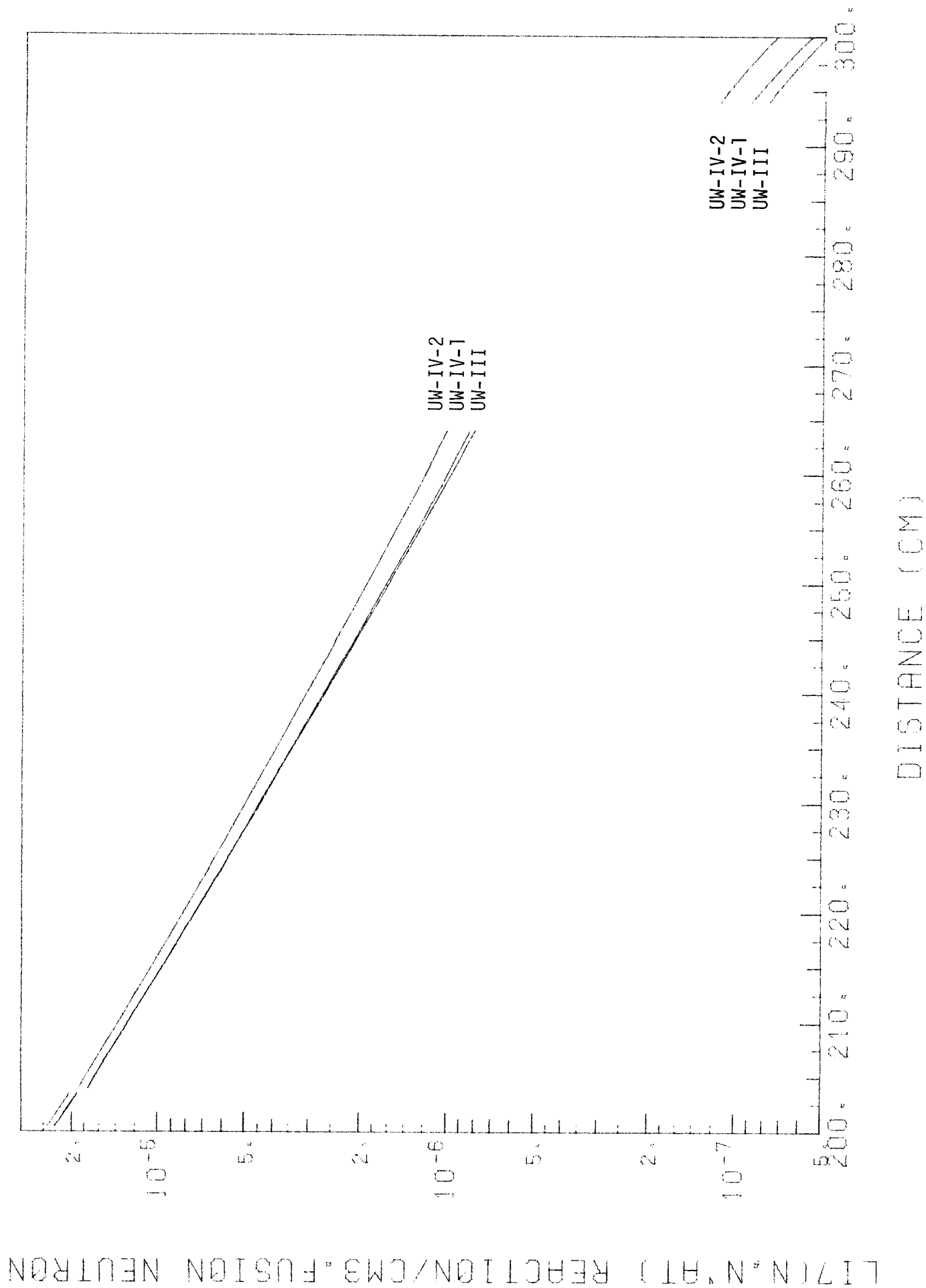
Figure 3. Tritium Production Rate From  ${}^6\text{Li}$ .



Figure 4. Tritium Production Rate from  $^7\text{Li}$ .

L17(N, N'AT) REACTION/CM3 \* FUSION NEUTRON

Figure 5. Neutron Multiplication Rate From (N,2N) Reaction

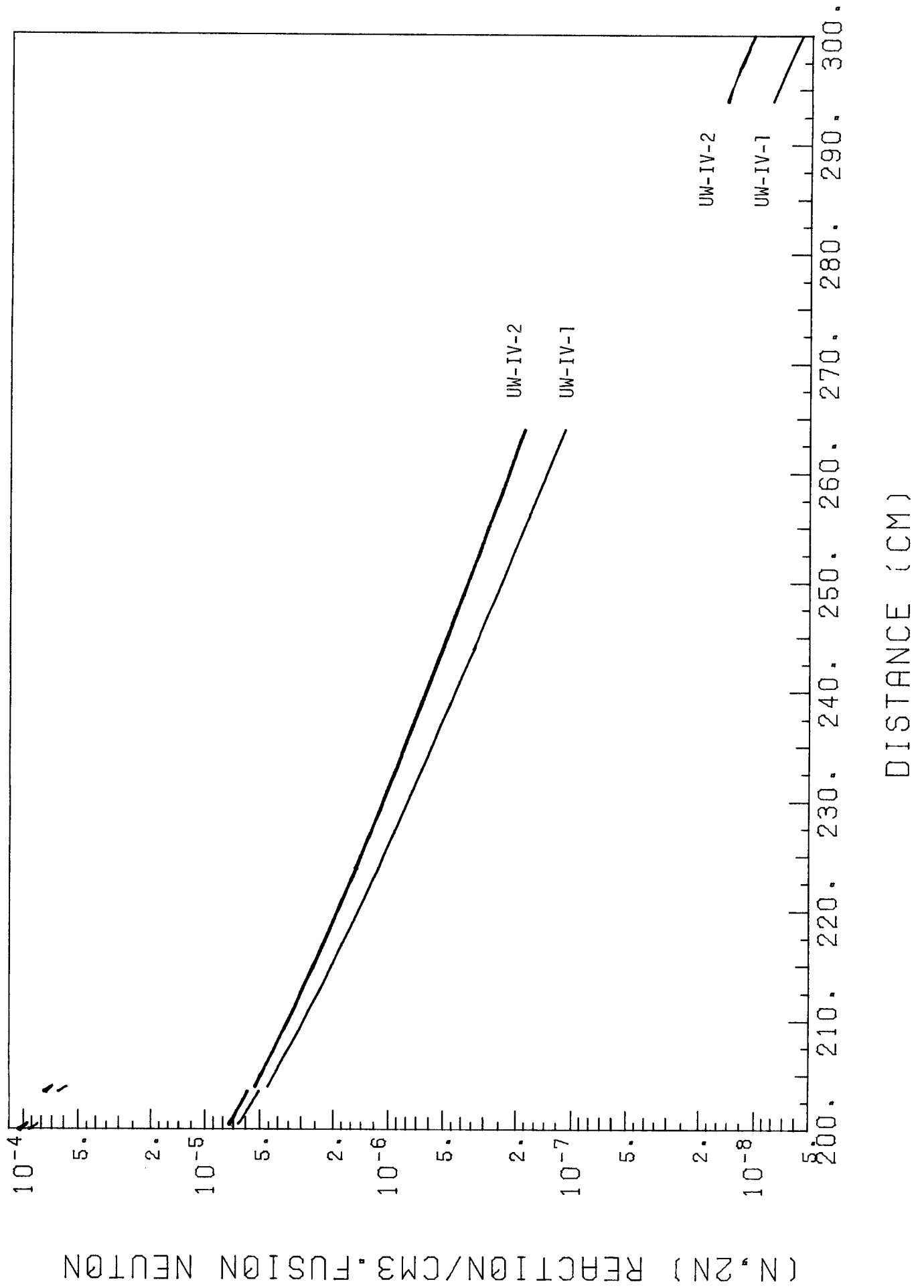


Figure 6. Neutron Spectrum at Interval 4.

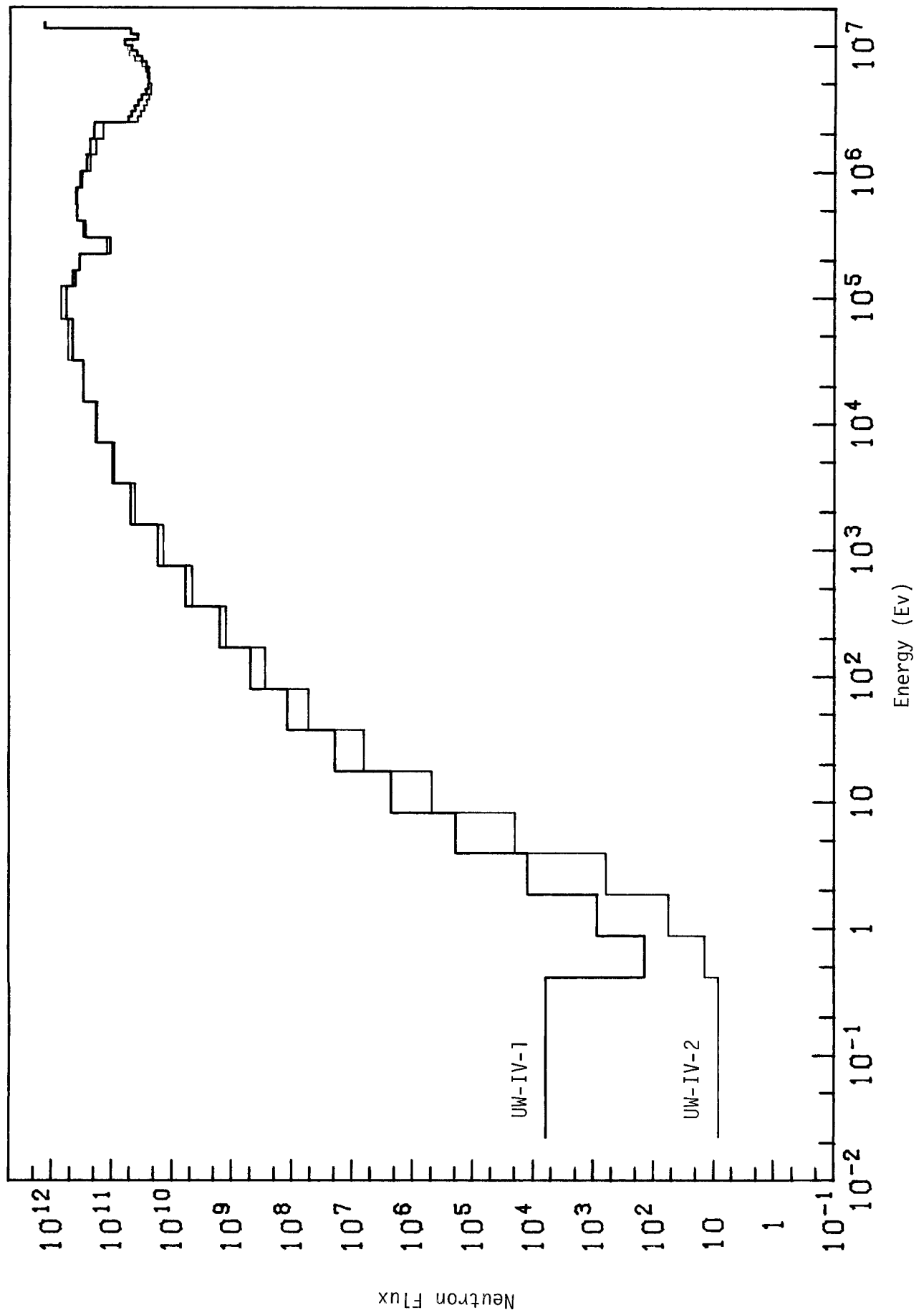


Figure 7. Neutron Spectrum at Interval 8.

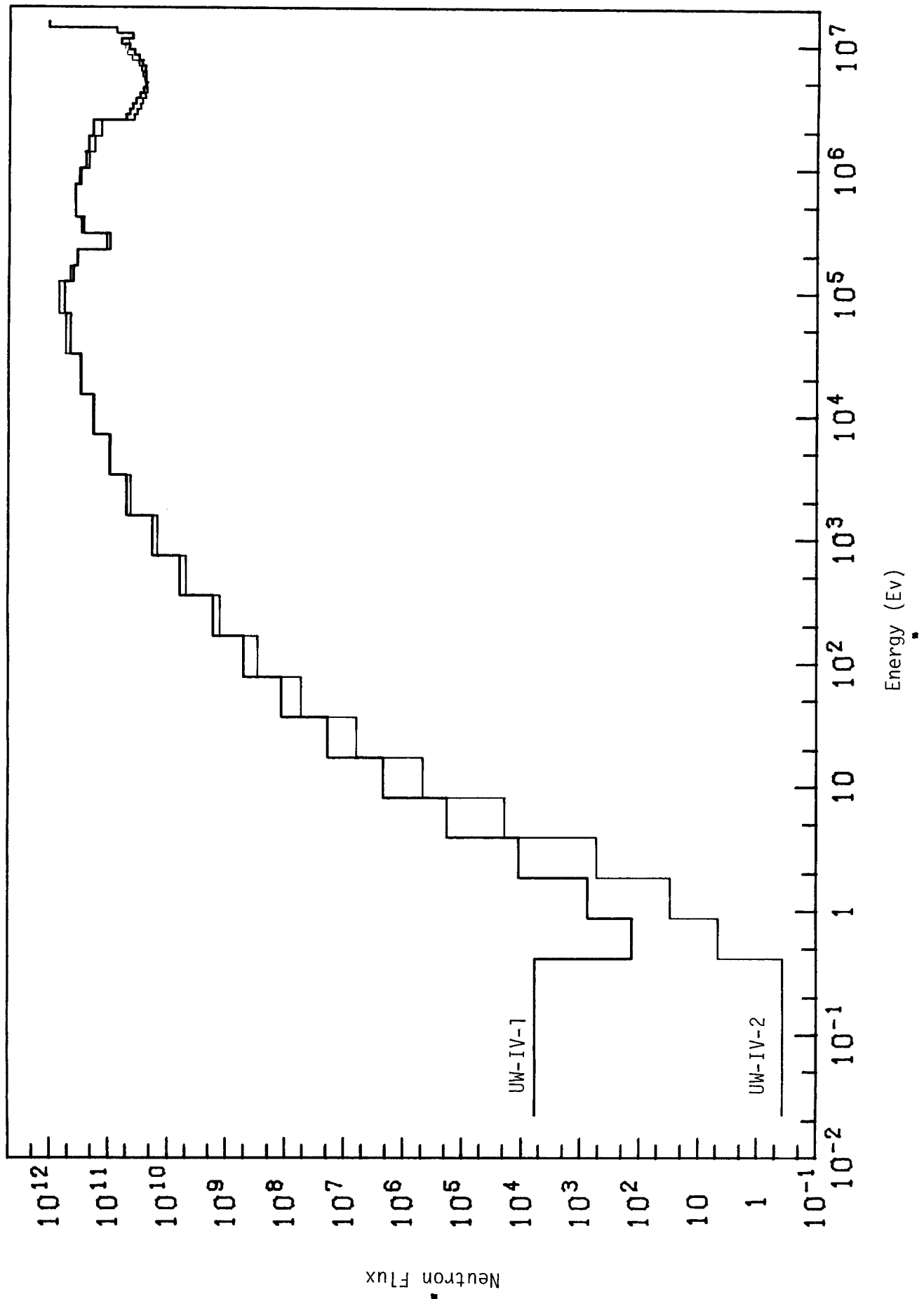


Figure 8. Neutron Spectrum at Interval 13.

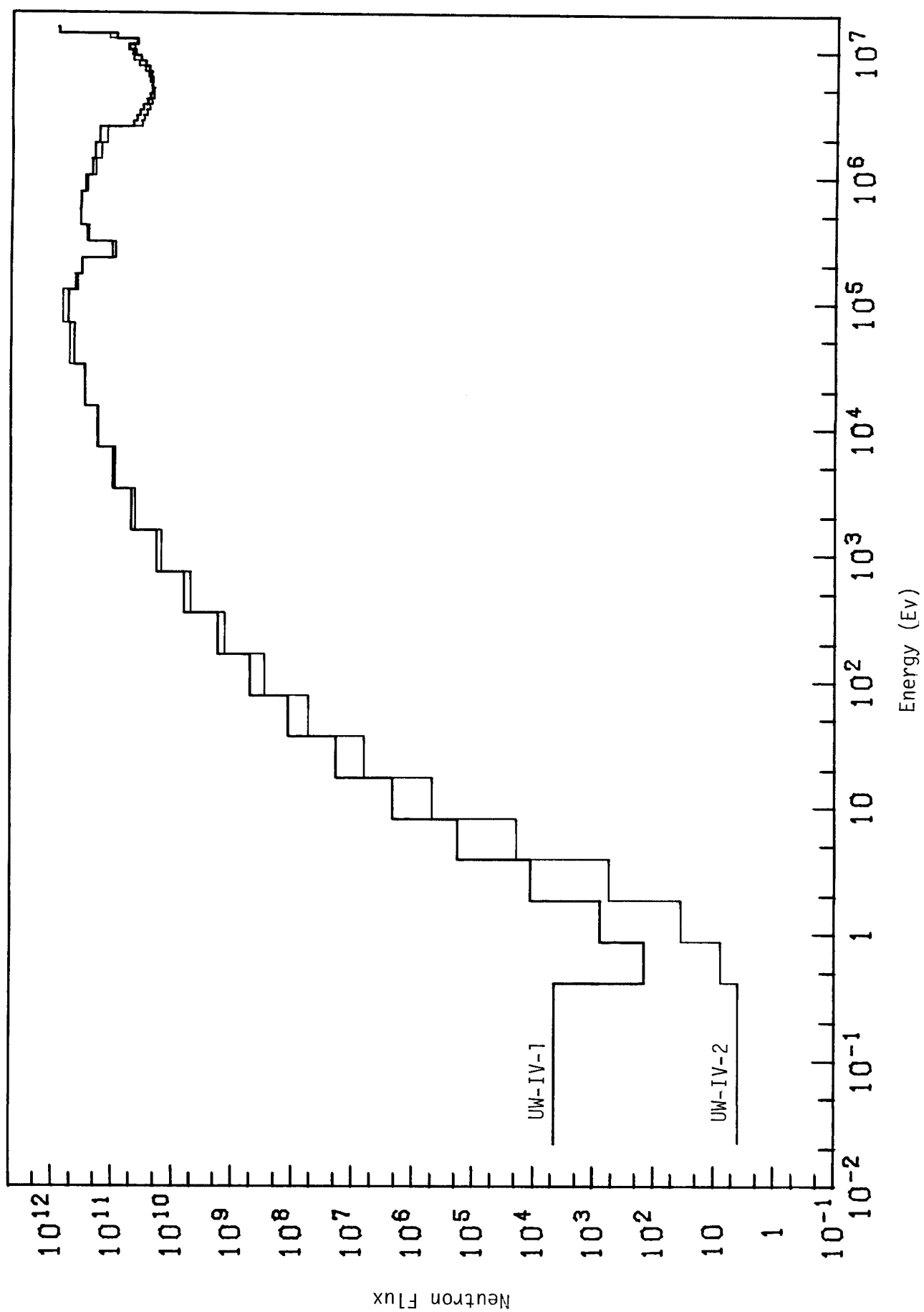


Figure 9. Neutron Spectrum at Interval 19.

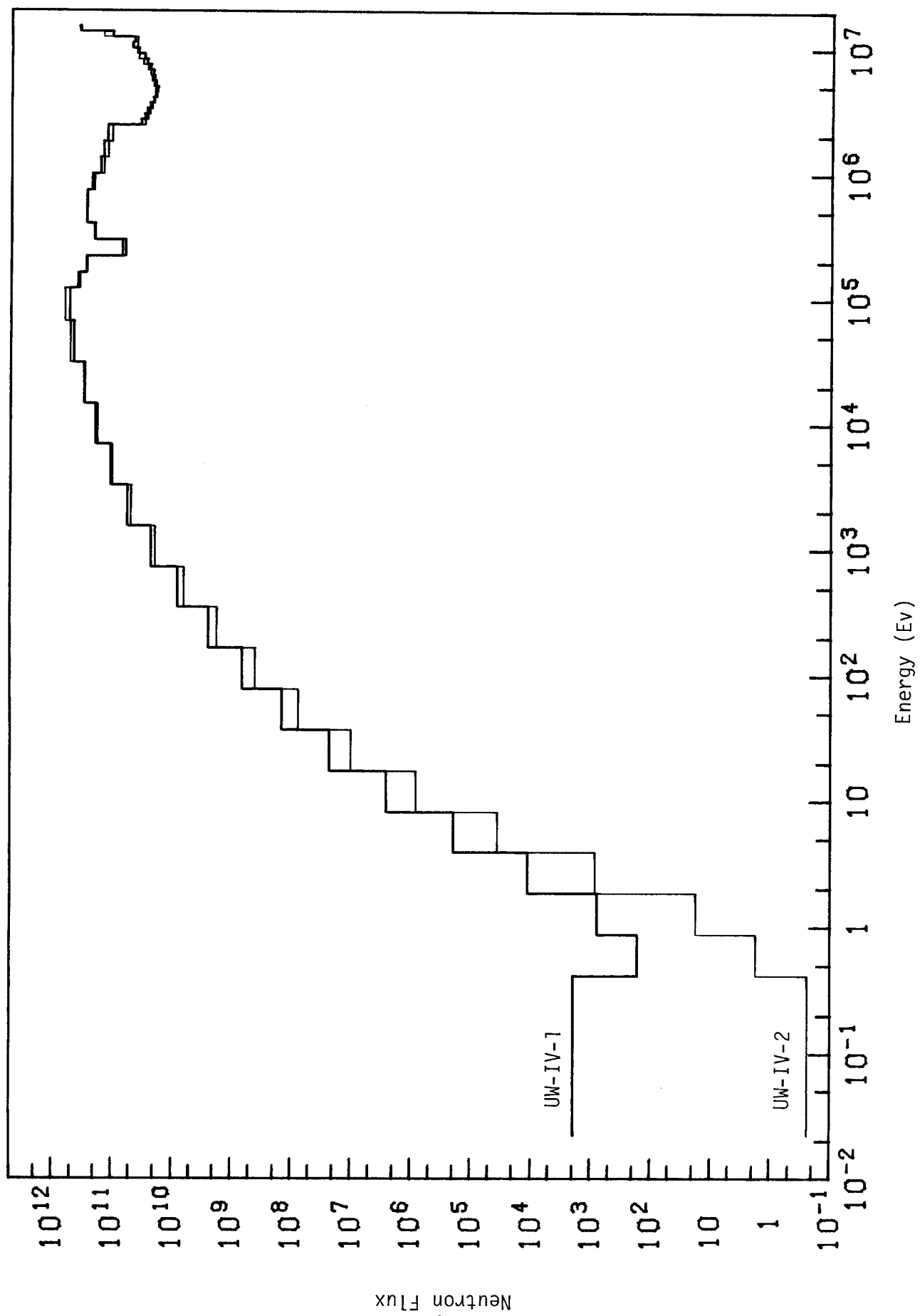


Figure 10. Neutron Spectrum at Interval 29.

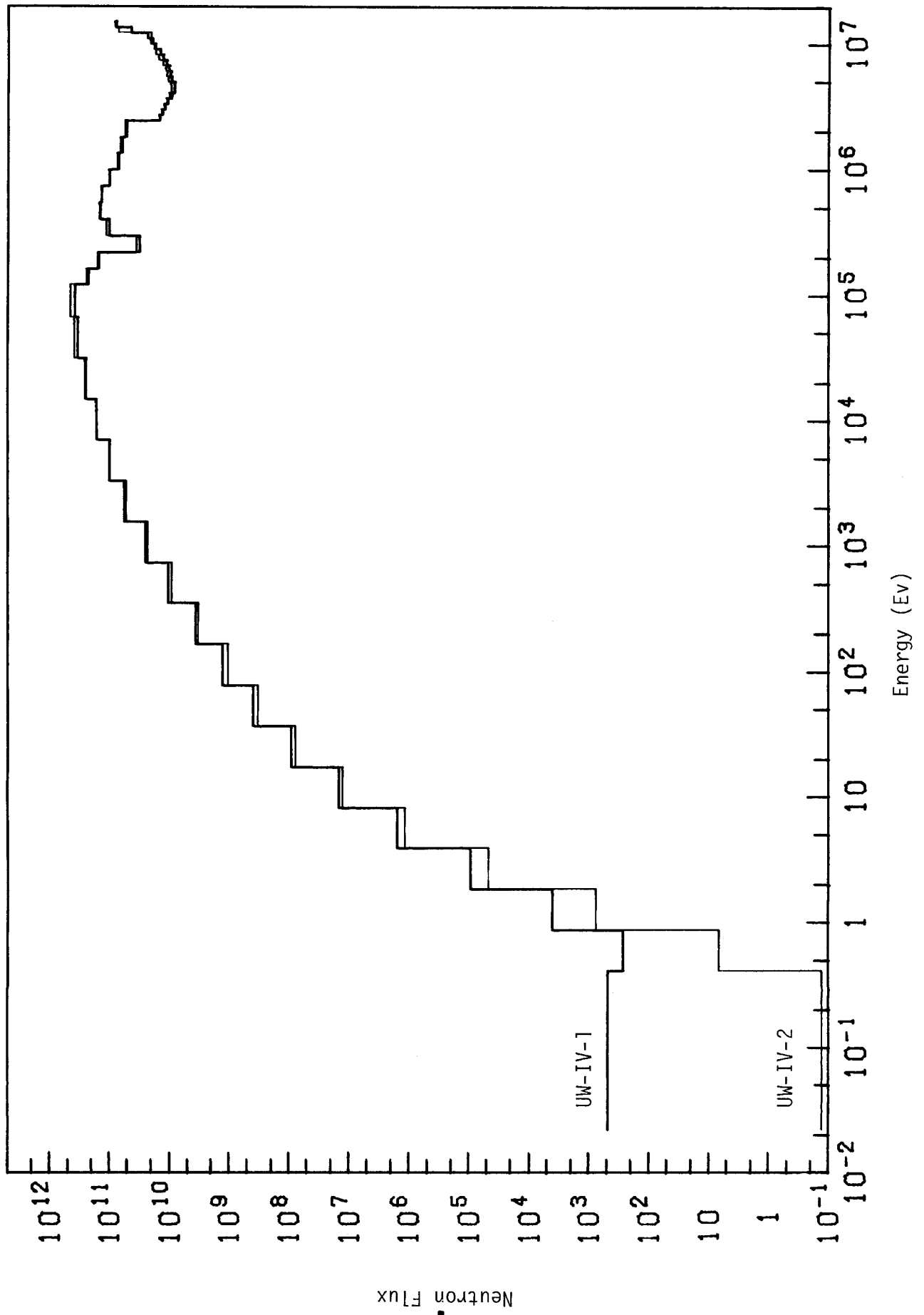


Figure 11. Neutron Spectrum at Interval 39.

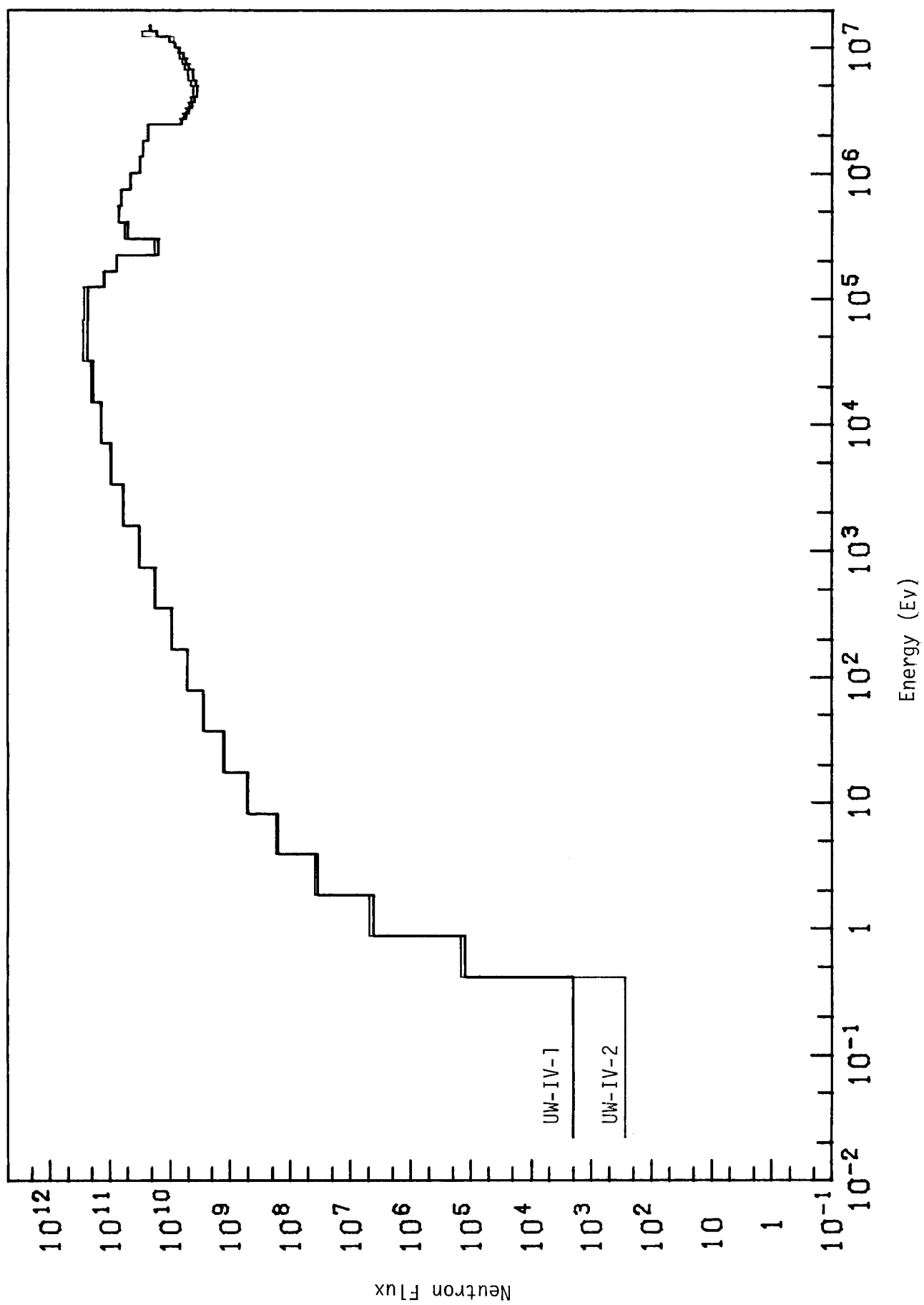




Figure 12. Neutron Spectrum at Interval 52.

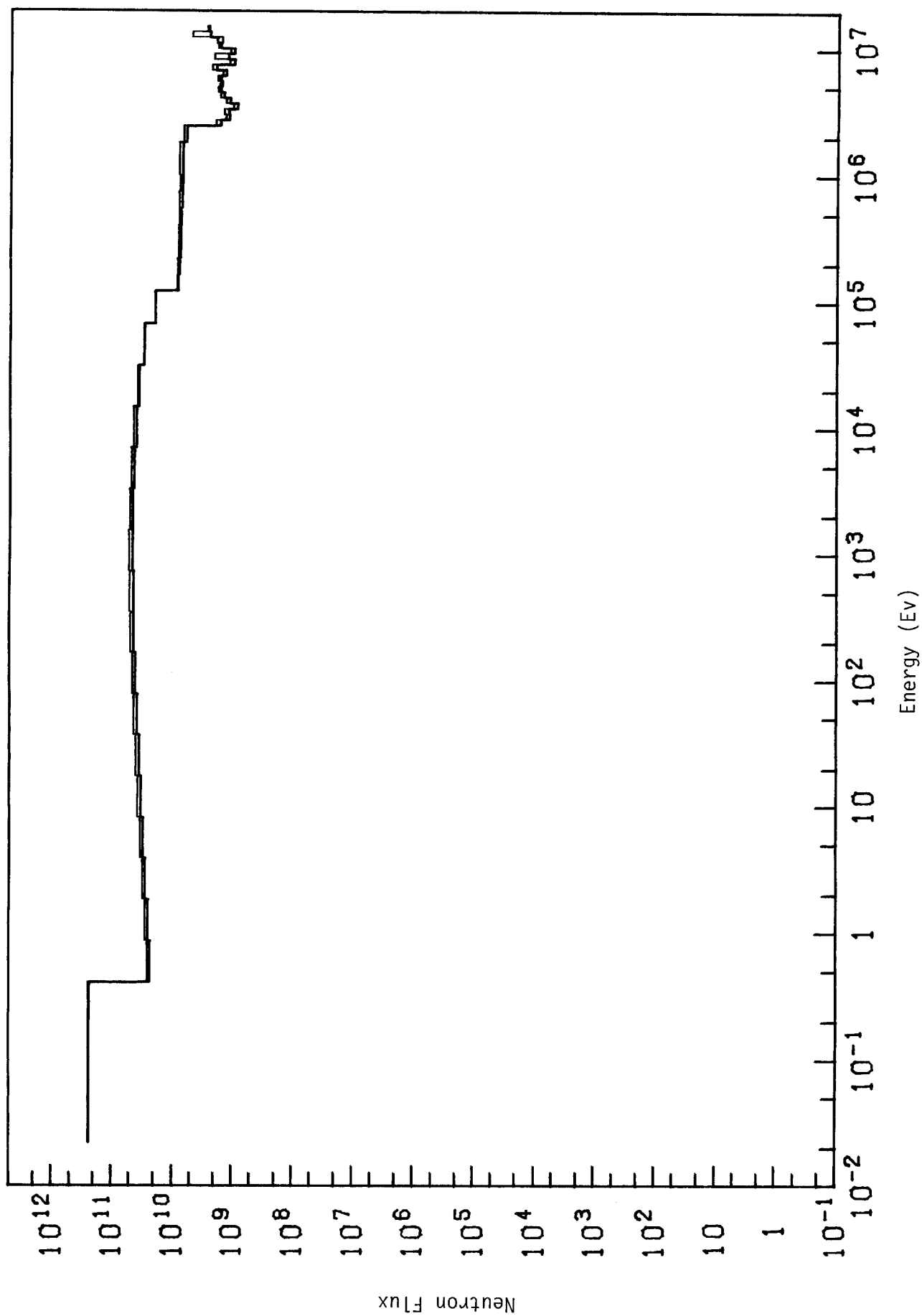


Figure 13. Neutron Spectrum at Interval 61.

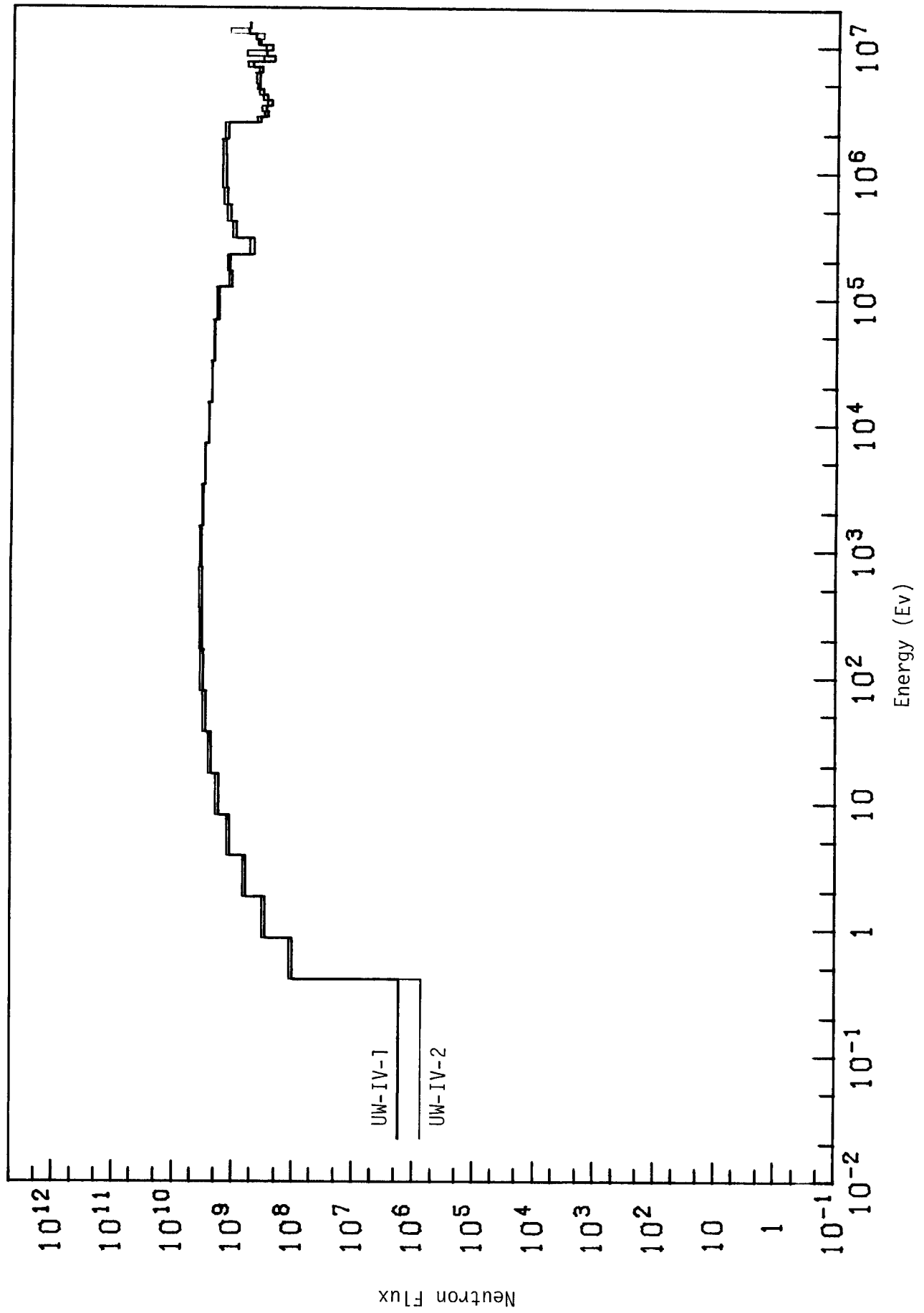
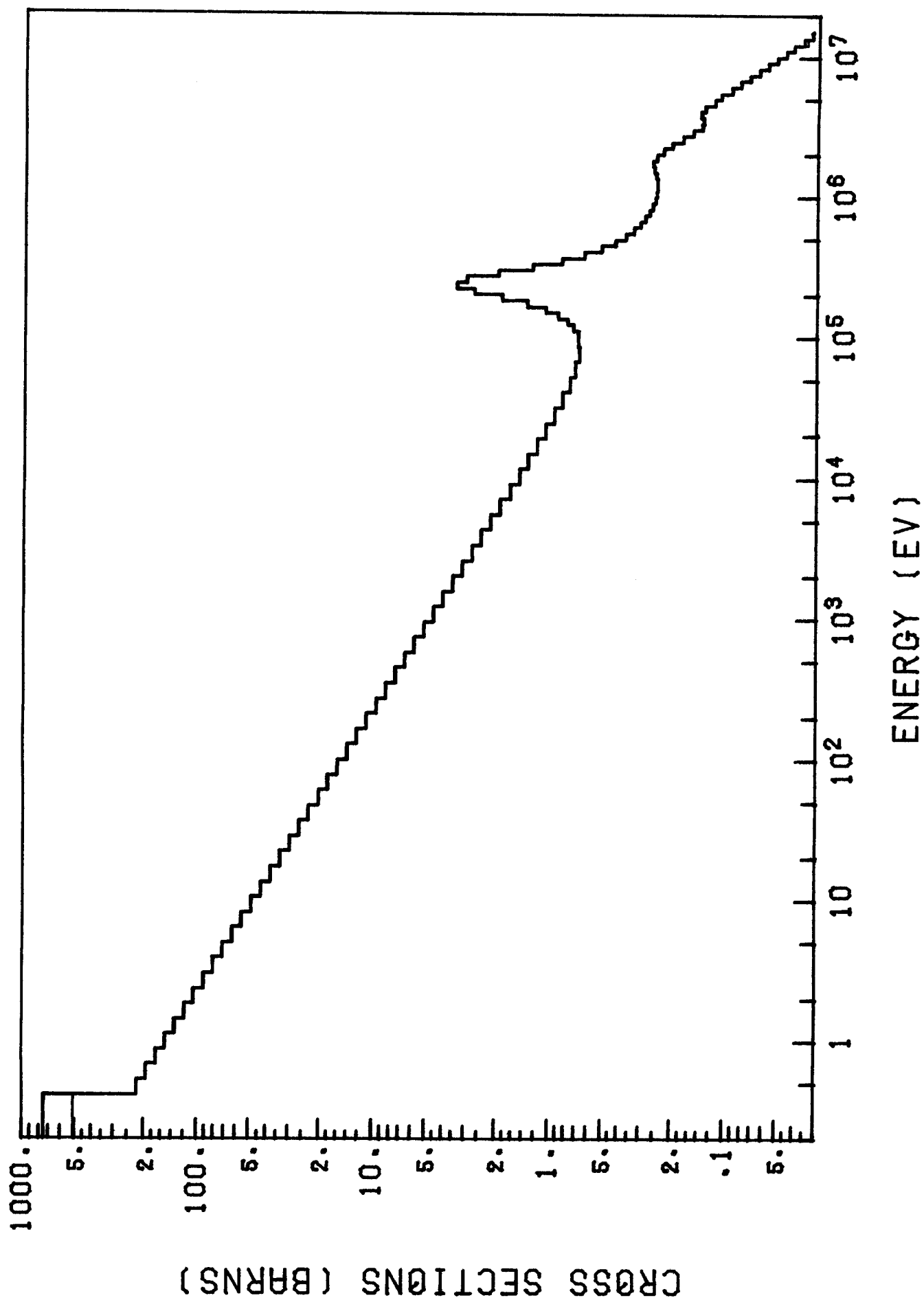


Figure 14. LI - 6 ABSORPTION CROSS SECTIONS



## LI - 6 TOTAL CROSS SECTIONS

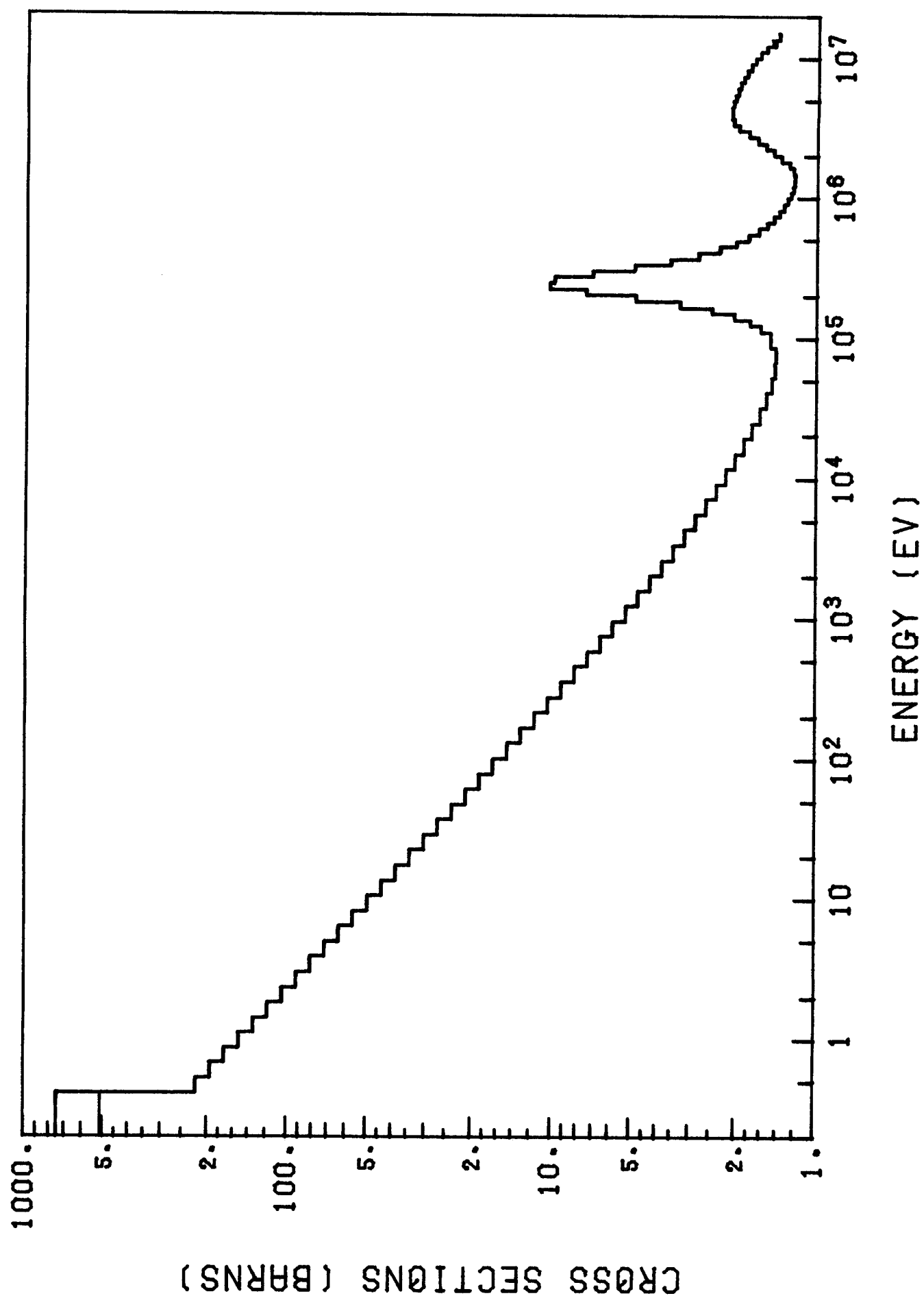
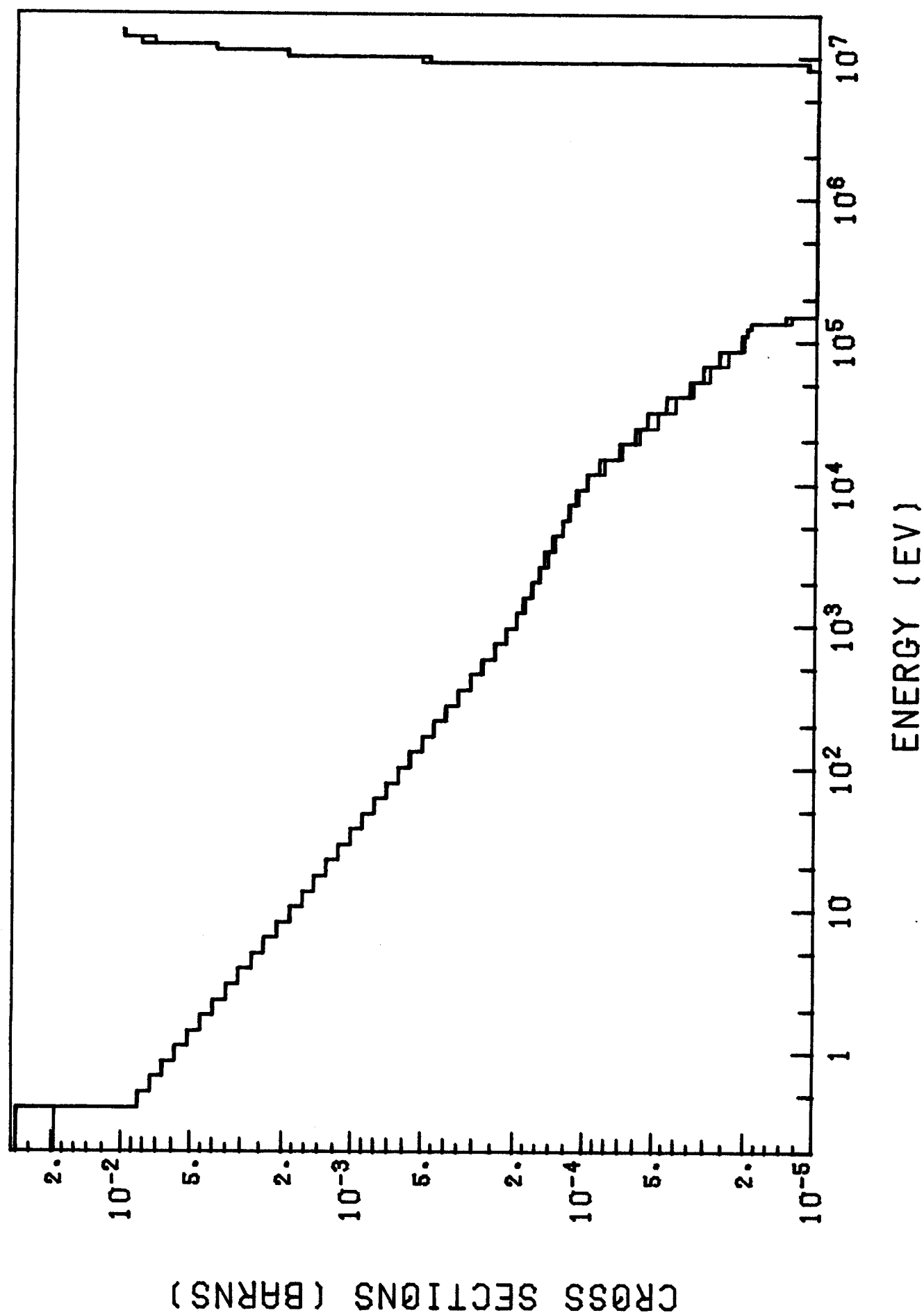


Figure 16. LI - 7 ABSORPTION CROSS SECTIONS



## LI - 7 TOTAL CROSS SECTIONS

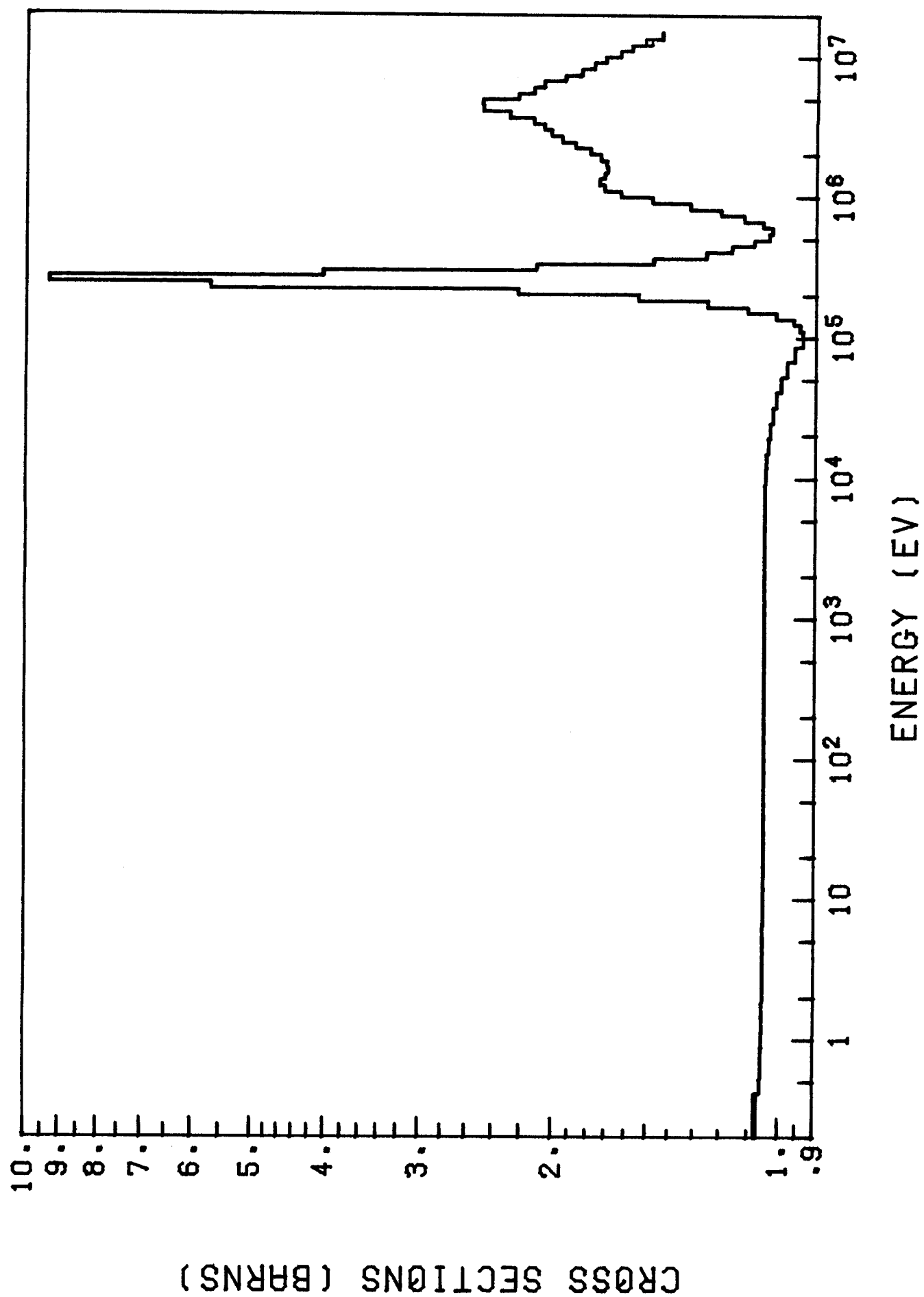
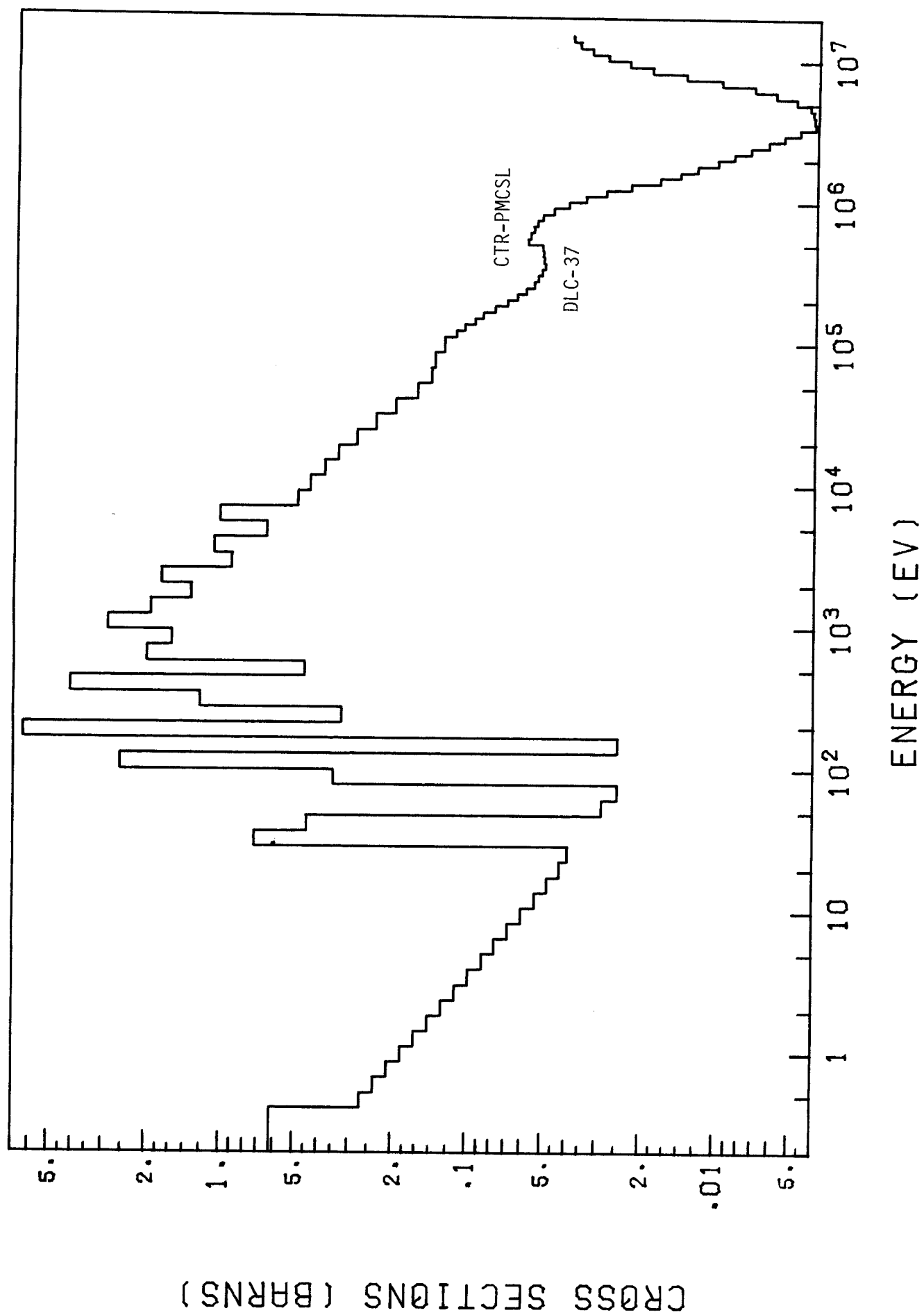
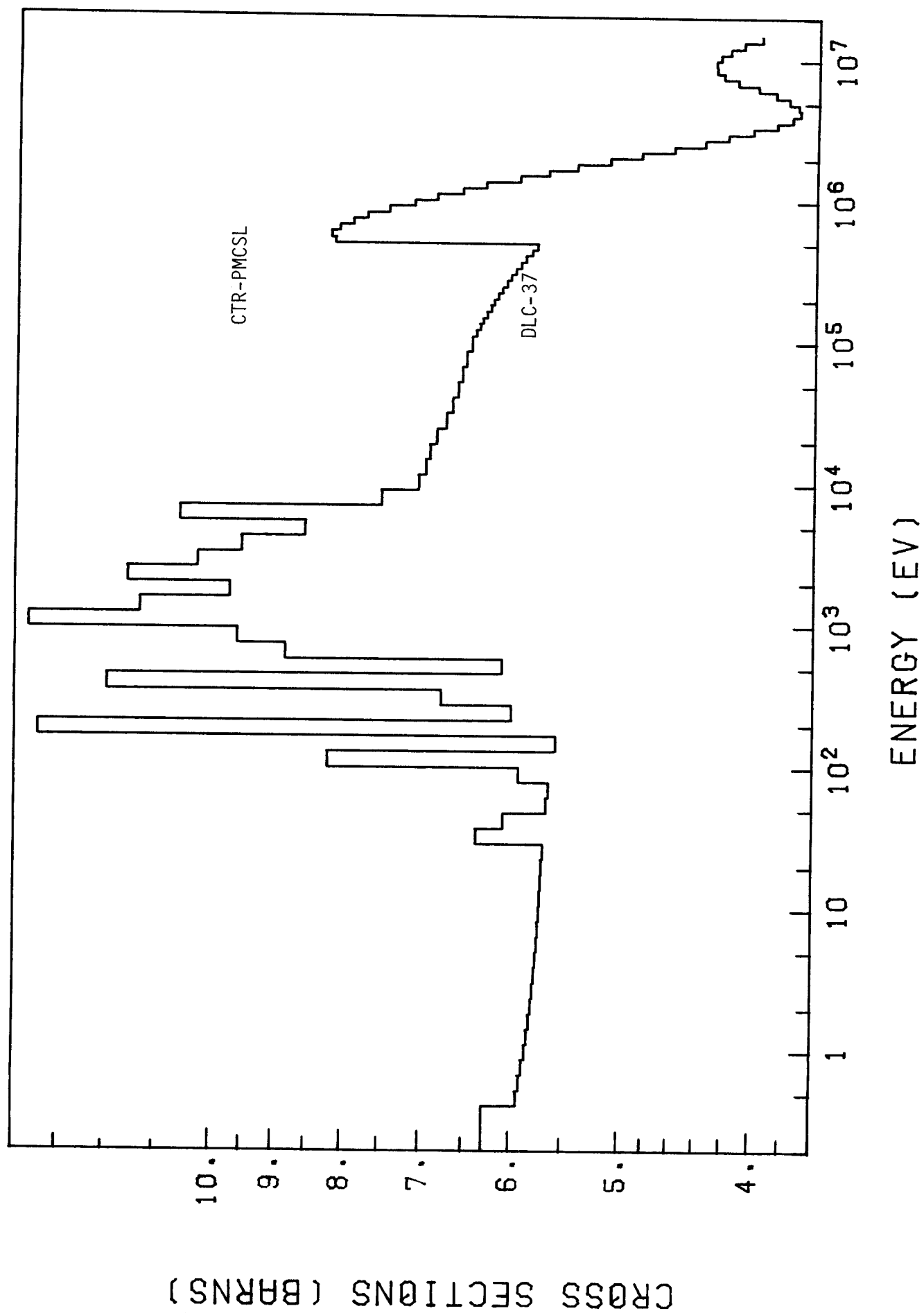


Figure 18. NB ABSORPTION CROSS SECTIONS



## NB TOTAL CROSS SECTIONS

Figure 19.





## C ABSORPTION CROSS SECTIONS

Figure 20.

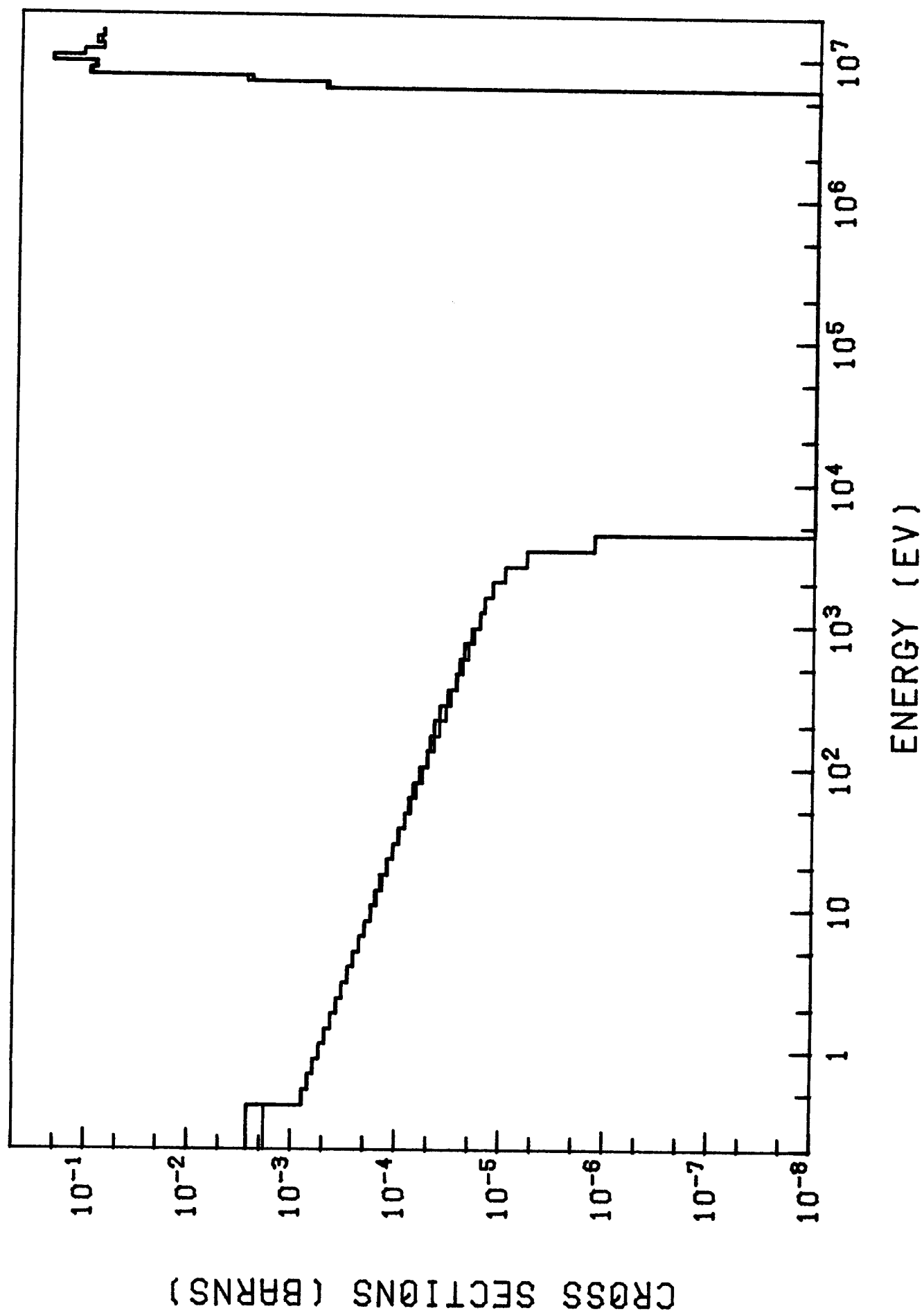


Figure 21.

C TOTAL CROSS SECTIONS

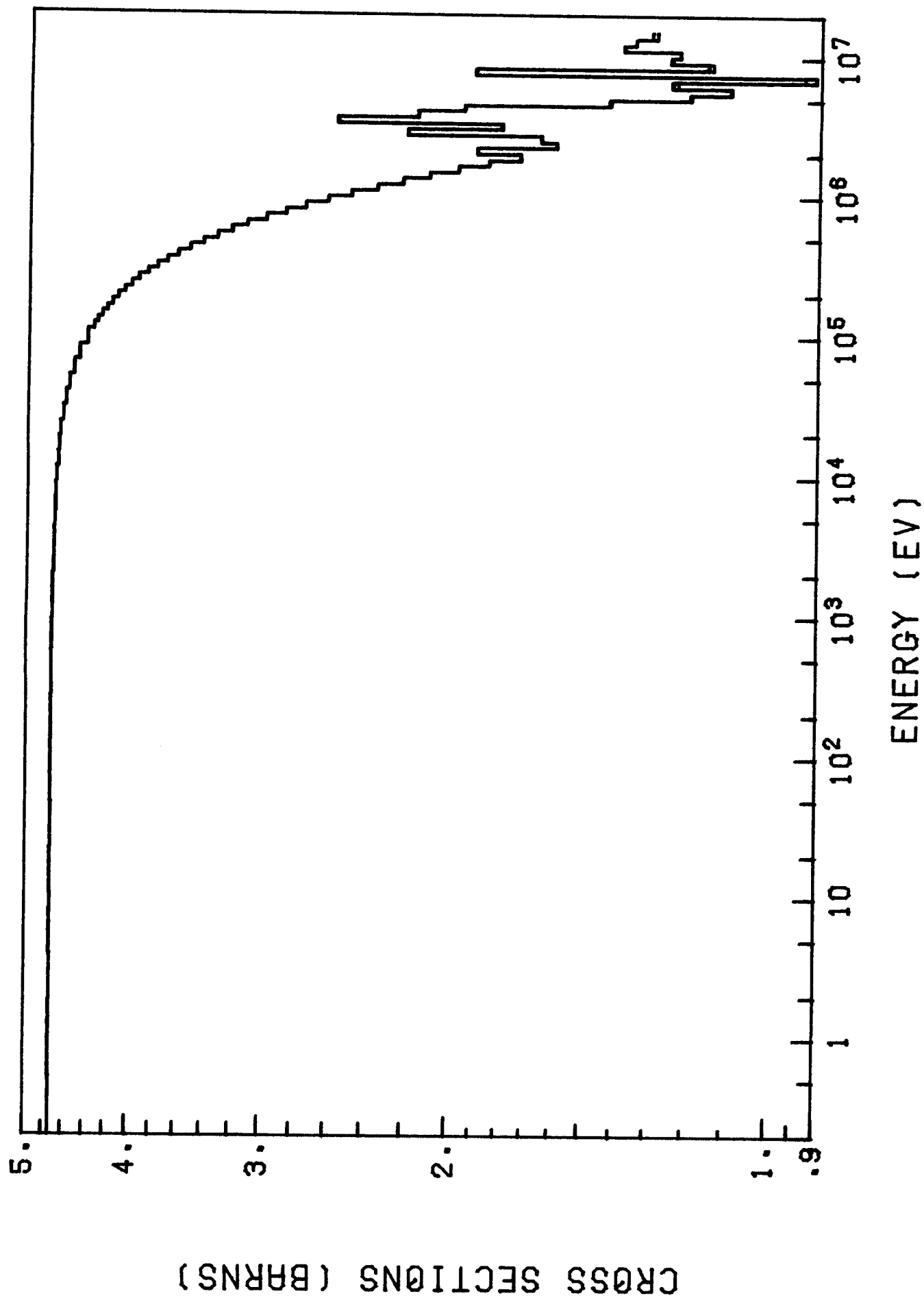
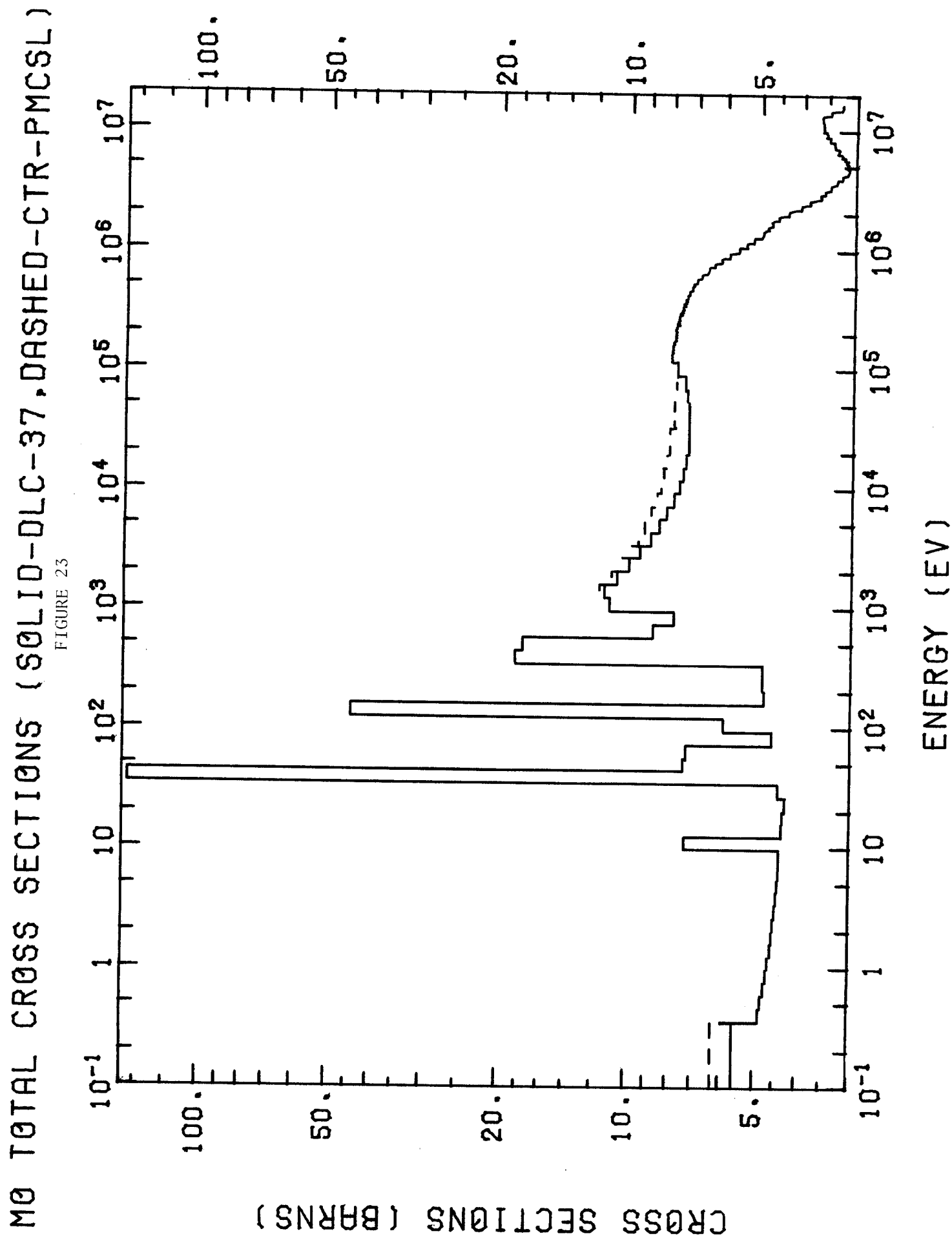


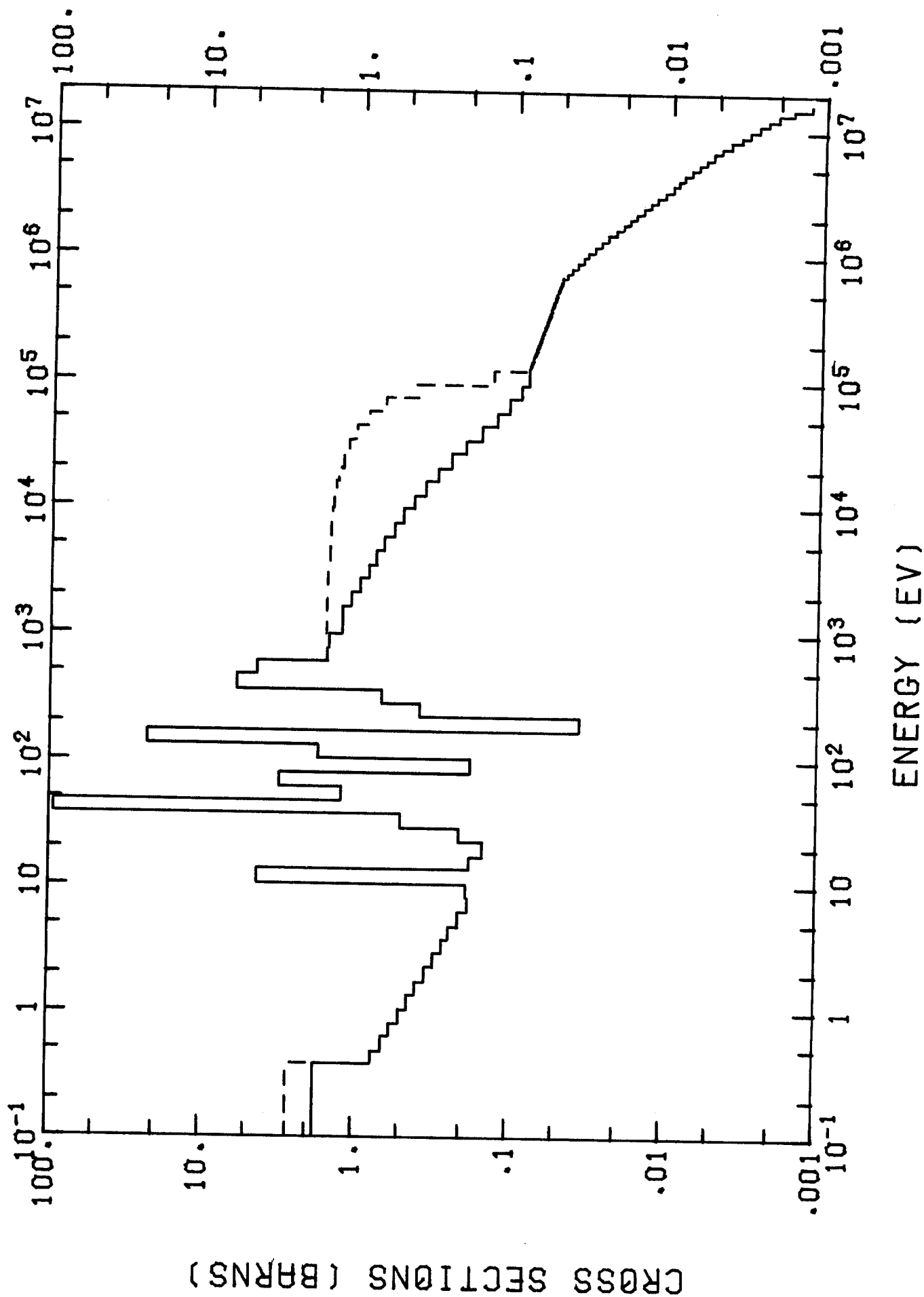
Figure 22. A Schematic of the UWMAK-III Blanket

Distance in cm	444.5	494.5	495.0	520.0	540.0	1079.85	1129.85	1130	1190	1220	1230	1250
	82% Mo. + 18% Al <sub>2</sub> O <sub>3</sub> 2 SiO <sub>2</sub>	100% Mo	100% C	Vacuum	Plasma	Vacuum	Mo	97% Li + 3% Mo	99% C + 1% Mo	97% Li + 3% Mo	99% C + 1% Mo	
Zone Number	1	2	3	4	5	6	7	8	9	10	11	
Material	V	II	I				II	III	IV	III	IV	
Number of Intervals per Zone	25	2	25	1	26	1		30	30	10	20	
Density Factor	0.86	1	1				1	1	0.9	1.0	0.9	
Thickness (cm)	50	0.5	25	20	529.85	50	0.15	60	30	10	20	



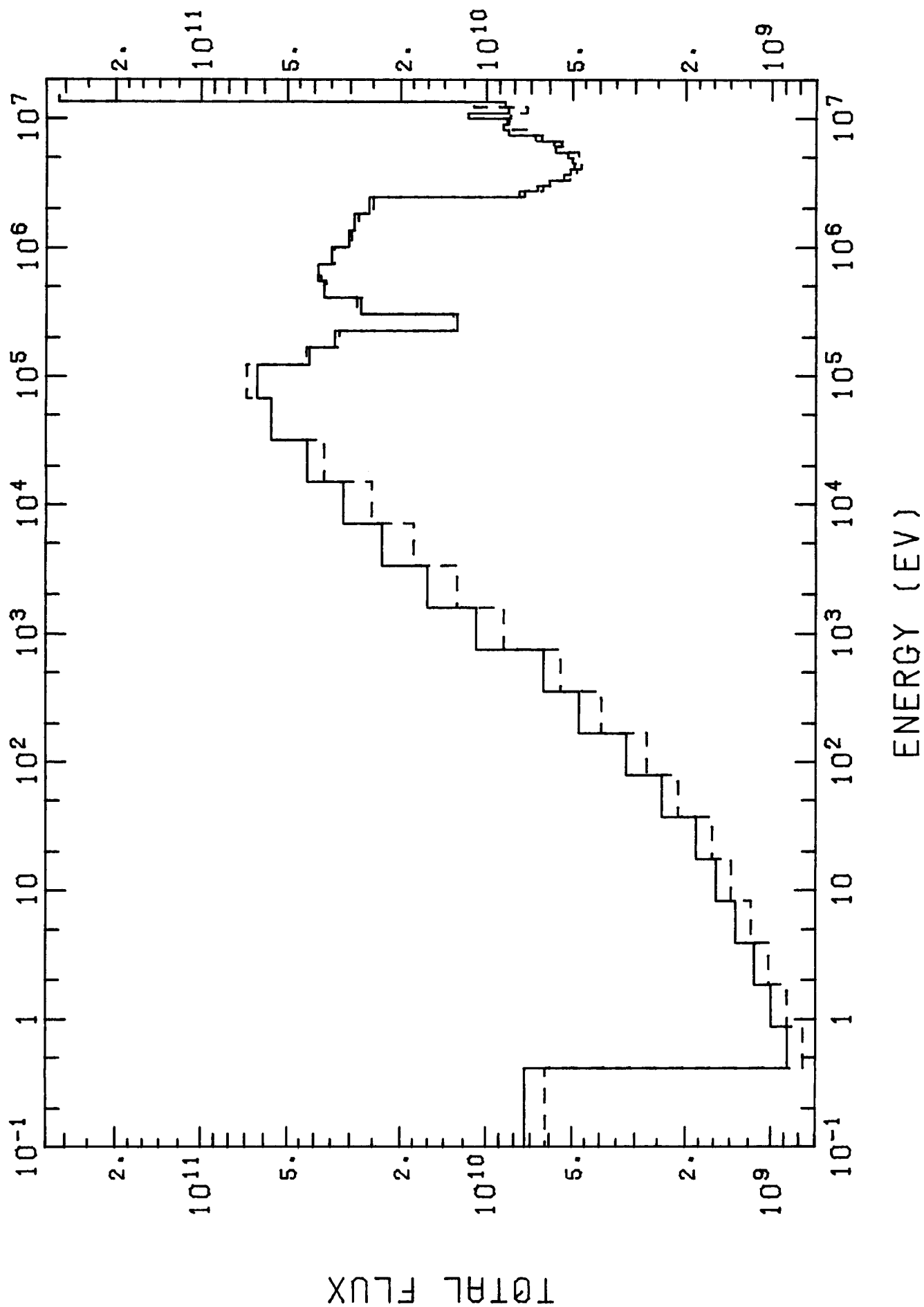
MO ABSORPTION CROSS SECTIONS (SOLID-DLC-37, DASHED-CTR-PMCSL)

FIGURE 24

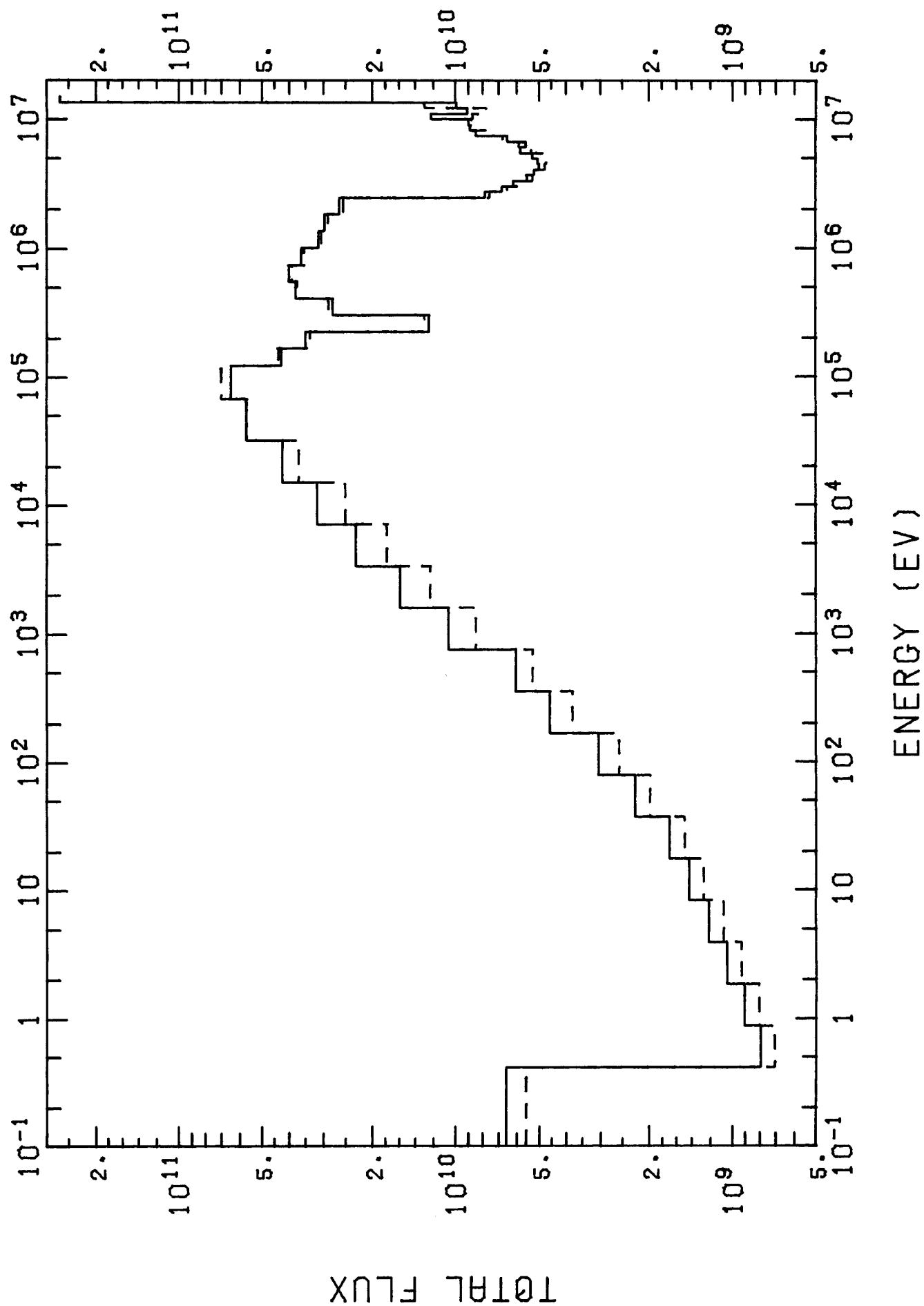


# UWMAK-3 NEUTRON FLUX, POSITION 1

Figure 25.

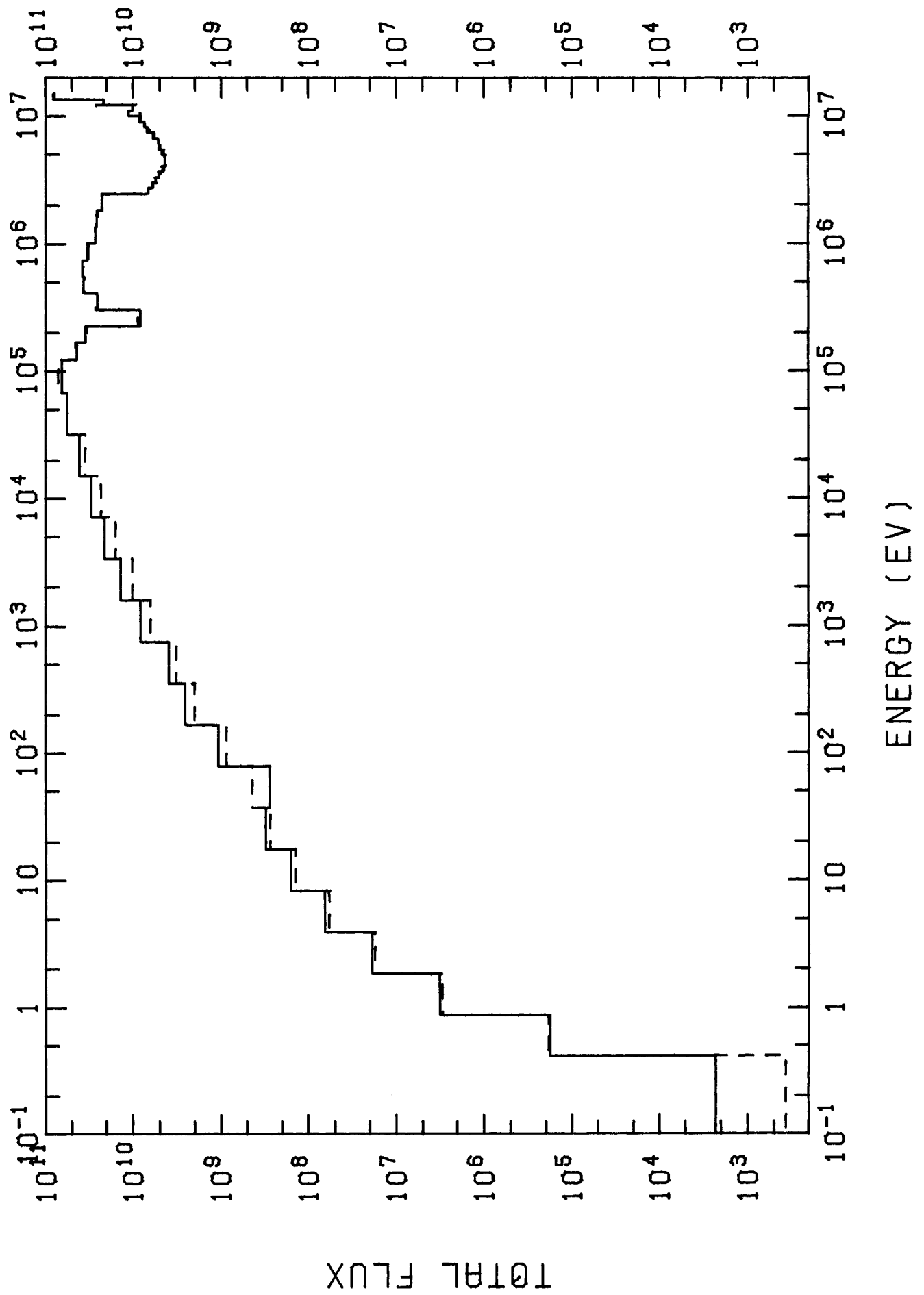


## UWMAK-3 NEUTRON FLUX, POSITION 2



## UWMAK-3 NEUTRON FLUX, POSITION 3

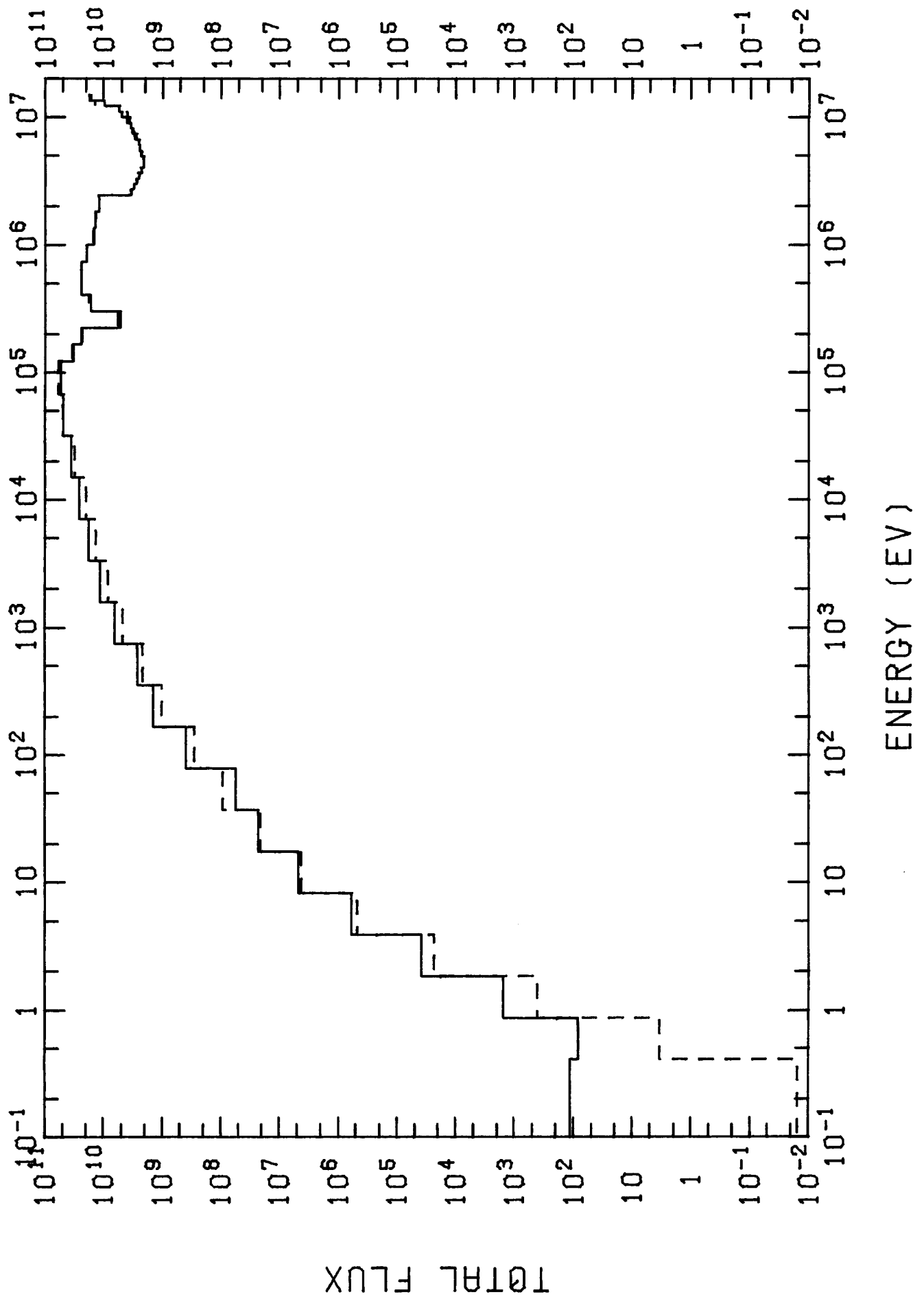
Figure 27.





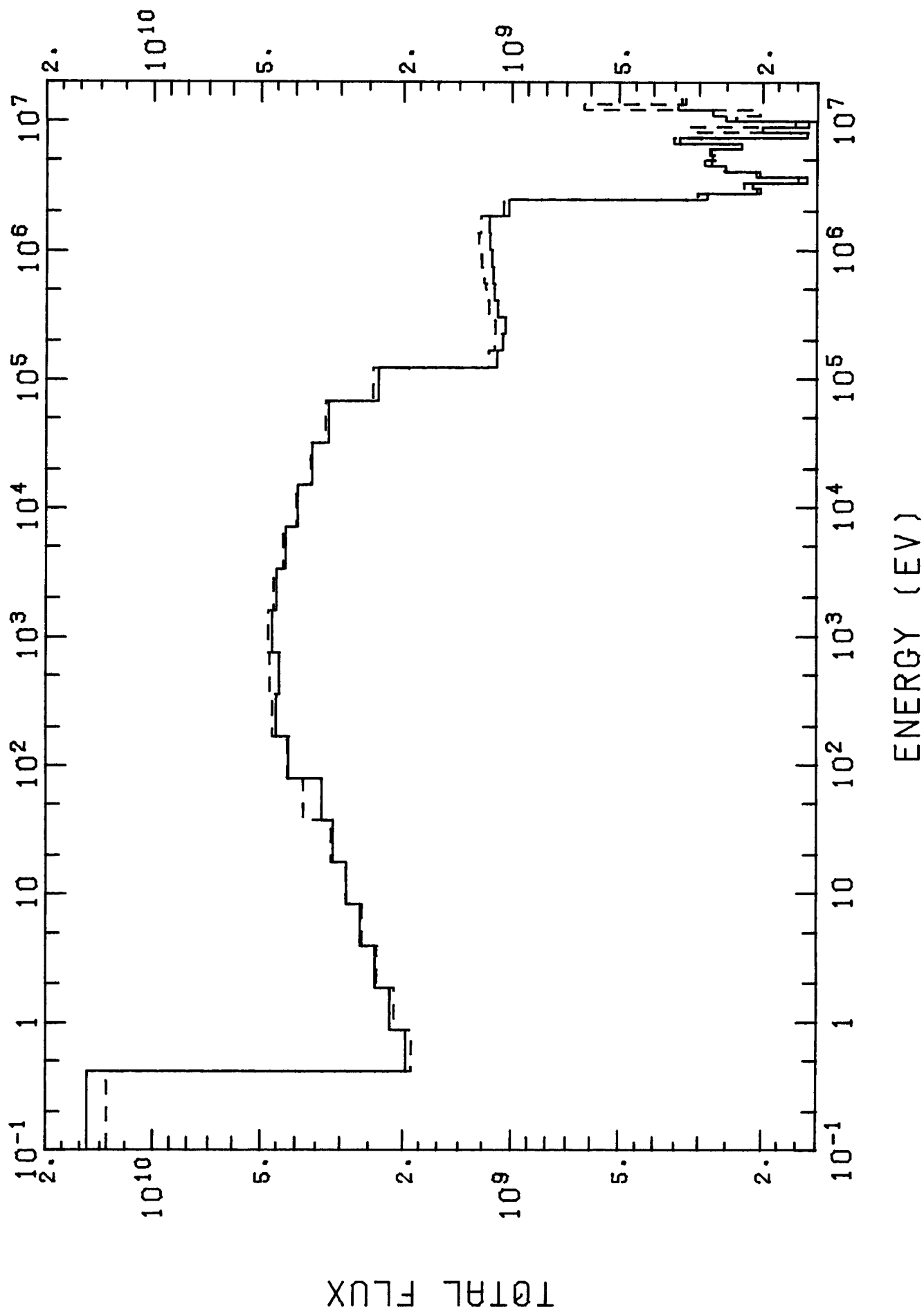
## UWMAK-3 NEUTRON FLUX, POSITION 4

Figure 28.



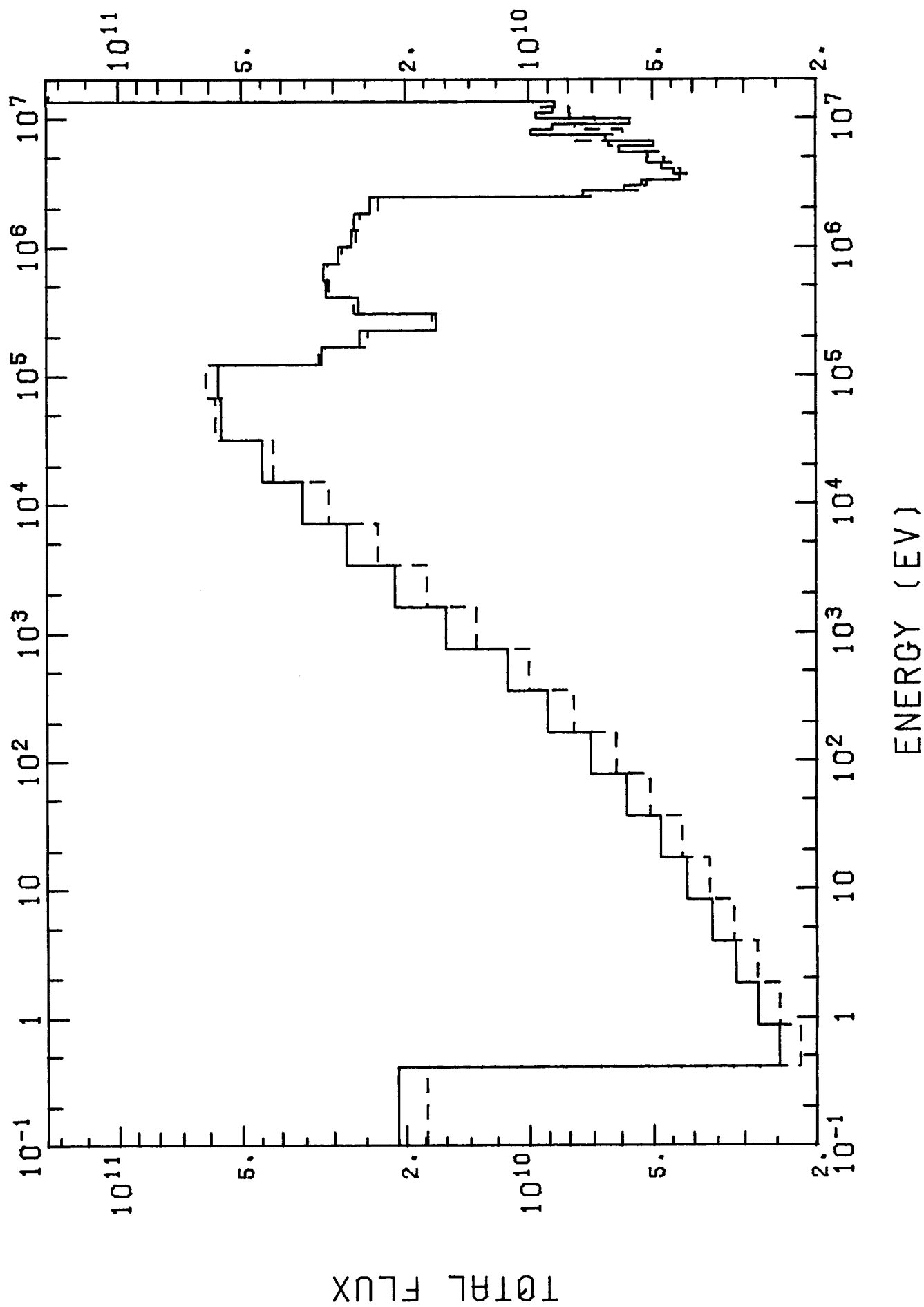
# UWMAK-3 NEUTRON FLUX, POSITION 5

Figure 29.

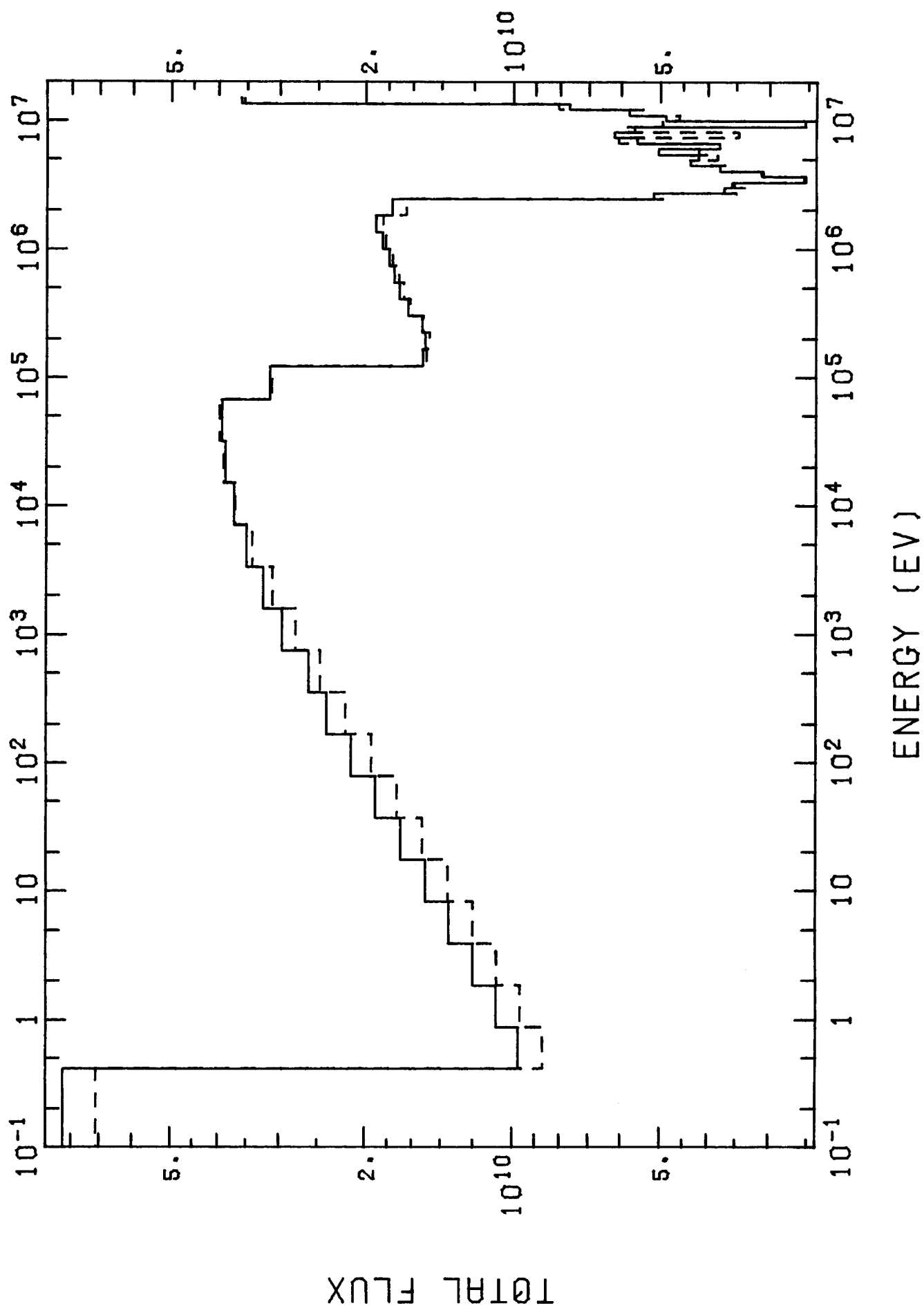


## UWMAK-3 NEUTRON FLUX, POSITION 6

Figure 30.

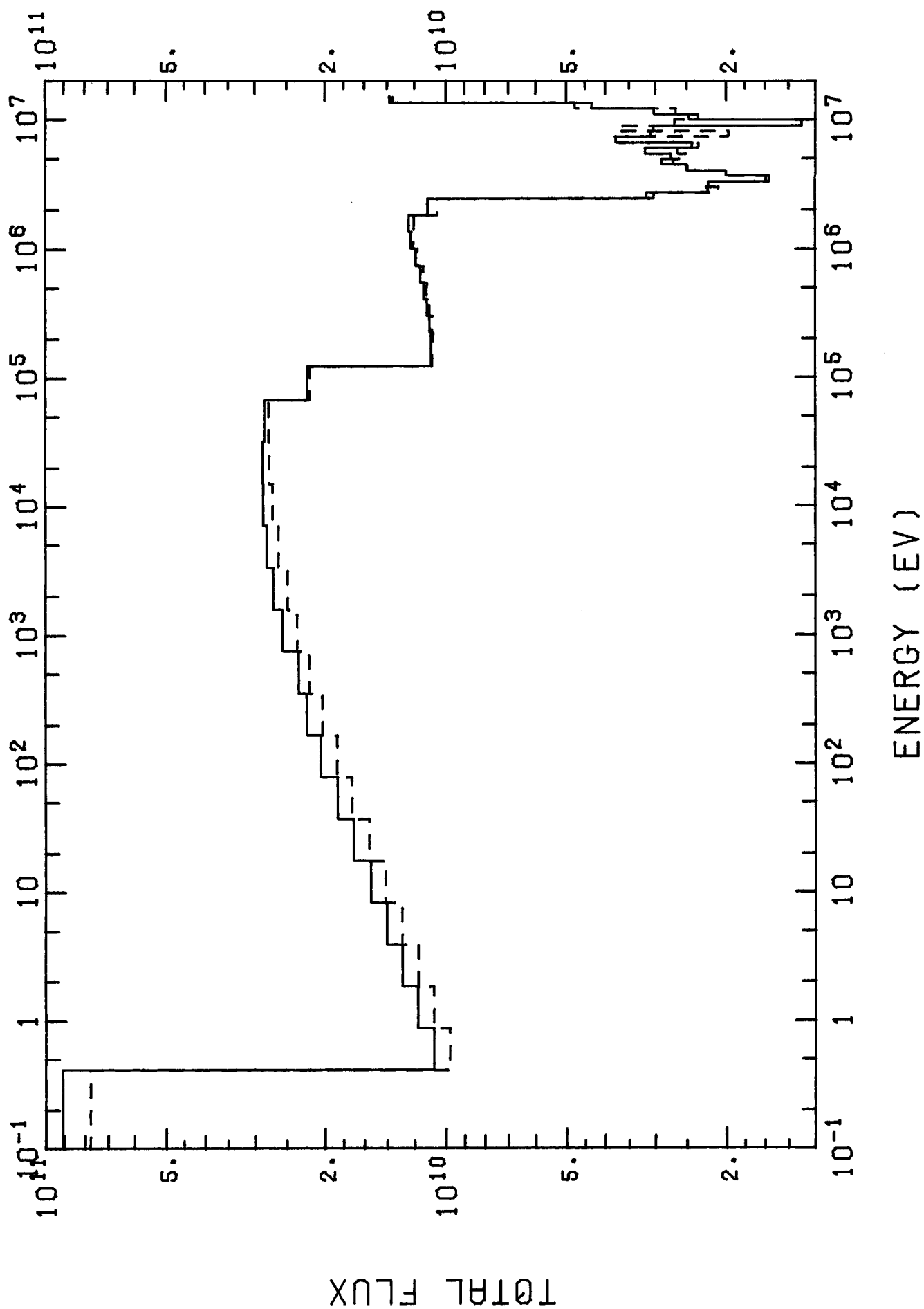


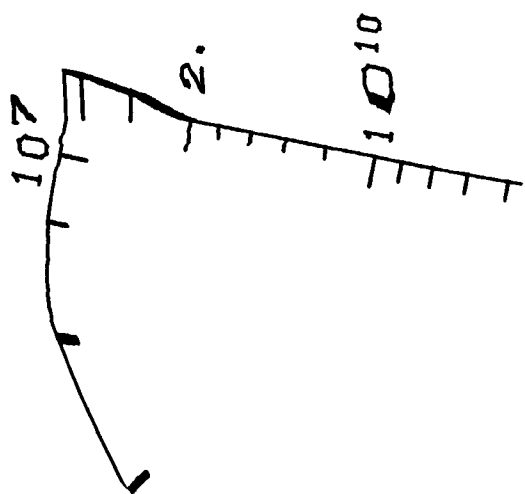
## UWMAK-3 NEUTRON FLUX, POSITION 7



## UWMAK-3 NEUTRON FLUX, POSITION 8

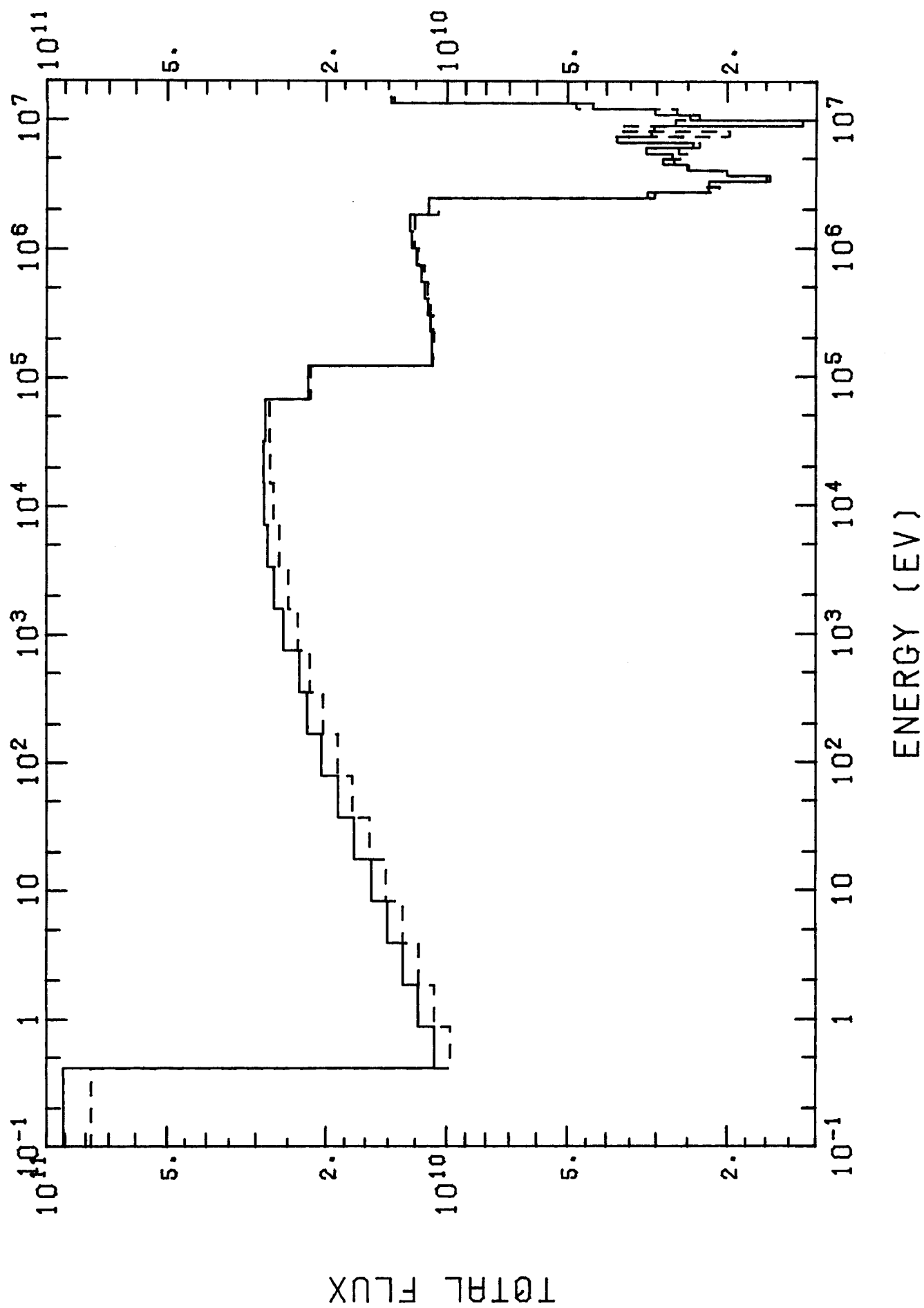
Figure 32.





## UWMAK-3 NEUTRON FLUX, POSITION 8

Figure 32.



## UWMAK-3 NEUTRON FLUX, POSITION 9

Figure 33.

