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## The LAW Library—A Multigroup Cross-Section Library for Use in Radioactive Waste Analysis Calculations

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Computing Applications Division

**THE LAW LIBRARY — A MULTIGROUP CROSS-SECTION LIBRARY  
FOR USE IN RADIOACTIVE WASTE ANALYSIS CALCULATIONS**

N. M. Greene, J. W. Arwood, R. Q. Wright, C. V. Parks

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## ABSTRACT

The 238-group LAW Library is a new multigroup neutron cross-section library based on ENDF/B-V data, with five sets of data taken from ENDF/B-VI ( $^{14}\text{N}_7$ ,  $^{15}\text{N}_7$ ,  $^{16}\text{O}_8$ ,  $^{154}\text{Eu}_{63}$ , and  $^{155}\text{Eu}_{63}$ ). These five nuclides are included because the new evaluations are thought to be superior to those in Version V. The LAW Library contains data for over 300 materials and will be distributed by the Radiation Shielding Information Center, located at Oak Ridge National Laboratory. It was generated for use in neutronics calculations required in radioactive waste analyses, although it has equal utility in any study requiring multigroup neutron cross sections.



## 1. INTRODUCTION

In the latter part of 1988, an effort was initiated to produce a multigroup neutron cross-section library to be used in calculations associated with radioactive waste analyses. The impetus was twofold:

1. A new version of the AMPX<sup>1</sup> system had been implemented on the IBM and CRAY computers at Oak Ridge. The new library would, therefore, be able to take advantage of extensions and improvements provided in this system.
2. The analysis of radioactive waste requires cross sections for a very large number of isotopes. The new library was to contain data for as many nuclides as could be found in the ENDF/B-V<sup>2</sup> data collections. It also contains data for <sup>14</sup>N<sub>7</sub>, <sup>15</sup>N<sub>7</sub>, <sup>16</sup>O<sub>8</sub>, <sup>154</sup>Eu<sub>63</sub>, and <sup>155</sup>Eu<sub>63</sub>, taken from ENDF/B-VI.<sup>3</sup>

A natural course of action would have been to start with the 227-group library<sup>4</sup> that was produced several years earlier because it was based on ENDF/B-V data and already contained data for 130 materials. However, it was recognized that several improvements had been made to the processing codes, especially in the processing of resonance data. These improvements, combined with a desire to produce a library with all the traceability required by present quality assurance procedures, led to a decision to produce new values for all materials included in the library. The new library has been named the LAW Library, or Library to Analyze Radioactive Waste. Alternatively, the LAW Library is referred to as the SCALE-238 Library because of its group structure and use of SCALE nuclide identifiers.

### 1.1 THE SCALE SYSTEM

The SCALE<sup>5</sup> modular code system was developed with support from the U.S. Nuclear Regulatory Commission (NRC) for use in the evaluation and study of the nuclear aspects of fuel cycle facilities and transportation packages. The system is ideal for criticality, shielding, and source term (radiation, decay heat, isotopic concentrations) analyses related to radioactive waste and spent fuel. The modules of the system can be used individually or the user can access one of the standard analysis sequences that can help facilitate the analysis.

Even though the new cross sections will be used in SCALE, they can also be output in a variety of alternative formats that are used by several major independent programs, such as DOT,<sup>6</sup> ANISN,<sup>7</sup> VENTURE,<sup>8</sup> MORSE,<sup>9</sup> etc.

### 1.2 THE AMPX SYSTEM

The LAW Library was produced by the AMPX-77 system.<sup>1</sup> The library will be distributed in the AMPX master library format. AMPX-77 is a version of AMPX which uses FORTRAN-77 and contains the latest versions of the ever-evolving codes in the systems.

AMPX was developed for the Defense Nuclear Agency to provide an integrated capability to produce multigroup cross sections for use in various shielding and radiation effects studies. It is a modular system and, in addition to the codes that produce multigroup data, includes several routines for manipulating and further processing multigroup data, including

codes to convert cross sections from its master library format to the formats used in the codes described in refs. 6-9.

AMPX was developed in the early 1970s on IBM computers. Subsequently, partial implementations of the system have been made on other computing systems, such as CDC, Prime, and UNIVAC, though never in anything approaching a full implementation.

An effort was completed in October 1988 to convert the existing AMPX modules from the IBM FORTRAN-H dialect to the newer FORTRAN-77. This new version of the system was fully implemented on both IBM and CRAY systems. The bulk of the LAW Library was produced on the CRAY version of the system, although several nuclides (as described below) have been reprocessed using higher accuracy data and procedures on the IBM-3090 at Oak Ridge National Laboratory (ORNL). The CRAY version was not used because these new data were produced after retirement of the CRAY in September 1992.

The new version of AMPX has been made available to the Radiation Shielding Information Center (RSIC) located at ORNL, along with an updated User's Guide.

### 1.3 EXISTING MULTIGROUP CROSS-SECTION LIBRARIES FOR THE SCALE SYSTEM

The SCALE system provides several multigroup cross-section libraries in the AMPX master library format for its neutronics calculations:

1. a 16-group library based primarily on Hansen-Roach<sup>10</sup> data, augmented by sets produced from various versions of ENDF/B data;
2. a 123-group library formed from 99-group GAM-II<sup>11</sup> cross sections coupled to 30-group THERMOS<sup>12</sup> libraries produced at ORNL;
3. a 218-group library<sup>13</sup> produced by AMPX from Version IV ENDF/B data;
4. a 27-group library produced by collapsing the 218-group library; and
5. an alternative version of the 27-group library supplemented with fission-product data.

The 16- and 123-group libraries have been used extensively and produce good results for many applications, probably because they have been adjusted to fit a variety of experiments.

The 218-group library is based on ENDF/B evaluations. One of the major tenets of ENDF is to reject adjustments that make evaluations produce "correct" results. This approach is taken to ensure that evaluations improve because of advances in the evaluation art and not because of some fortuitous (and often misunderstood) change in an associated calculational procedure. In this spirit, our ENDF/B-derived libraries are never adjusted.

The 218-group and its 27-group derivative have been benchmarked against some 400 or 500 critical experiments, including both uranium- and plutonium-fueled assemblies. Comparisons of calculations<sup>13</sup> with both multigroup and point Monte Carlo calculations verified the processing of the library and established calculational biases that were due to inadequacies in the Version IV ENDF/B evaluations.

A 227-group ENDF/B-V library and a 27-group derivative were produced and had some benchmarking performed, although not nearly as much as the 218-group data. These libraries were produced during a period of austere support and, because of limited benchmarking, were never released to the public.

Taking into account the differences between Versions IV and V of ENDF/B, the 227- and 218-group libraries have been shown to produce results that compare favorably with other published results for the same criticals. However, note that the 27-group library, derived from the 218-group library, produces more consistent results than does the 27-group library derived from the 227-group library.

An examination of the procedures used to collapse the two libraries reveals the reason the older 27-group library gives better results.

Many of the important nuclides in the 218-group library were collapsed using a spectrum consisting of a Maxwellian spectrum below 0.12 eV, coupled to a  $1/(E\sigma_f)$  spectrum extending to 67 keV, and coupled to a fission spectrum above that. The 227-group library used a similar scheme, except that the region between 0.12 eV and 67 keV used a  $1/E$  spectrum. Either of these weighting schemes is generally adequate for the fine-group libraries. As noted below, the  $1/E$  spectrum was applied in this energy range for generating the LAW Library. Certainly for nuclides with strong resonances, all of these libraries will have additional weighting with a resonance self-shielding calculation. For the 27-group libraries, broad-group collapsing used the fine-group weighting spectra. However, since the weighting spectrum of the 218-group library contained a  $1/(E\sigma_f)$  part, and since this is closer to a "real" flux (especially when the nuclide is important) than the  $1/E$  variation in the 227-group library spectrum, the older 27-group library based on ENDF/B-IV produced better results.

It was probably a mistake to make it so easy (in the AMPX MALOCS module) to collapse a fine-group library using the spectrum that produced the fine-group library. The option was programmed primarily for testing collapsing procedures and not as a recommended way to make broad-group libraries. In any event, any future broad-group libraries derived from the new 238-group LAW Library will be collapsed over "real" spectra, produced from transport calculations for representative systems. (See Sect. 2.4 for a description of a set of characteristic weighting spectra derived from realistic cases.)

## 2. CHARACTERISTICS OF THE LAW LIBRARY

The LAW Library uses the 238-group energy structure shown in Table 1. The structure contains all the boundaries of the 227-group structure.<sup>4</sup> The extra group boundaries are all in the thermal range and were included for two principal reasons:

1. A boundary was added at 0.625 eV to hit the cadmium-cutoff, thereby making it more convenient to calculate resonance integrals.
2. Several very low energy boundaries were added so that the group structure would adequately support calculations needing detailed structures at low energies, such as the Advanced Neutron Source Reactor.<sup>14</sup>

Table 1. Group structure for the 238-group LAW Library

Group	Upper energy boundary						
1	2.0000E+07	41	2.7000E+05	81	1.8600E+02	121	2.0000E+01
2	1.7333E+07	42	2.0000E+05	82	1.2200E+02	122	1.9000E+01
3	1.5683E+07	43	1.5000E+05	83	1.1900E+02	123	1.8500E+01
4	1.4550E+07	44	1.2830E+05	84	1.1500E+02	124	1.7000E+01
5	1.3840E+07	45	1.0000E+05	85	1.0800E+02	125	1.6000E+01
6	1.2840E+07	46	8.5000E+04	86	1.0000E+02	126	1.5100E+01
7	1.0000E+07	47	8.2000E+04	87	9.0000E+01	127	1.4400E+01
8	8.1873E+06	48	7.5000E+04	88	8.2000E+01	128	1.3750E+01
9	6.4340E+06	49	7.3000E+04	89	8.0000E+01	129	1.2900E+01
10	4.8000E+06	50	6.0000E+04	90	7.6000E+01	130	1.1900E+01
11	4.3040E+06	51	5.2000E+04	91	7.2000E+01	131	1.1500E+01
12	3.0000E+06	52	5.0000E+04	92	6.7500E+01	132	1.0000E+01
13	2.4790E+06	53	4.5000E+04	93	6.5000E+01	133	9.1000E+00
14	2.3540E+06	54	3.0000E+04	94	6.1000E+01	134	8.1000E+00
15	1.8500E+06	55	2.5000E+04	95	5.9000E+01	135	7.1500E+00
16	1.5000E+06	56	1.7000E+04	96	5.3400E+01	136	7.0000E+00
17	1.4000E+06	57	1.3000E+04	97	5.2000E+01	137	6.7500E+00
18	1.3560E+06	58	9.5000E+03	98	5.0600E+01	138	6.5000E+00
19	1.3170E+06	59	8.0300E+03	99	4.9200E+01	139	6.2500E+00
20	1.2500E+06	60	6.0000E+03	100	4.8300E+01	140	6.0000E+00
21	1.2000E+06	61	3.9000E+03	101	4.7000E+01	141	5.4000E+00
22	1.1000E+06	62	3.7400E+03	102	4.5200E+01	142	5.0000E+00
23	1.0100E+06	63	3.0000E+03	103	4.4000E+01	143	4.7500E+00
24	9.2000E+05	64	2.5800E+03	104	4.2400E+01	144	4.0000E+00
25	9.0000E+05	65	2.2900E+03	105	4.1000E+01	145	3.7300E+00
26	8.7500E+05	66	2.2000E+03	106	3.9600E+01	146	3.5000E+00
27	8.6110E+05	67	1.8000E+03	107	3.9100E+01	147	3.1500E+00
28	8.2000E+05	68	1.5500E+03	108	3.8000E+01	148	3.0500E+00
29	7.5000E+05	69	1.5000E+03	109	3.7000E+01	149	3.0000E+00
30	6.7900E+05	70	1.1500E+03	110	3.5500E+01	150	2.9700E+00
31	6.7000E+05	71	9.5000E+02	111	3.4600E+01	151	2.8700E+00
32	6.0000E+05	72	6.8300E+02	112	3.3750E+01	152	2.7700E+00
33	5.7300E+05	73	6.7000E+02	113	3.3250E+01	153	2.6700E+00
34	5.5000E+05	74	5.5000E+02	114	3.1750E+01	154	2.5700E+00
35	4.9952E+05	75	3.0500E+02	115	3.1250E+01	155	2.4700E+00
36	4.7000E+05	76	2.8500E+02	116	3.0000E+01	156	2.3800E+00
37	4.4000E+05	77	2.4000E+02	117	2.7500E+01	157	2.3000E+00
38	4.2000E+05	78	2.1000E+02	118	2.5000E+01	158	2.2100E+00
39	4.0000E+05	79	2.0750E+02	119	2.2500E+01	159	2.1200E+00
40	3.3000E+05	80	1.9250E+02	120	2.1000E+01	160	2.0000E+00

Table 1 (continued)

Group	Upper energy boundary						
161	1.9400E+00	181	1.0900E+00	201	6.0000E-01	221	6.0000E-02
162	1.8600E+00	182	1.0800E+00	202	5.5000E-01	222	5.0000E-02
163	1.7700E+00	183	1.0700E+00	203	5.0000E-01	223	4.0000E-02
164	1.6800E+00	184	1.0600E+00	204	4.5000E-01	224	3.0000E-02
165	1.5900E+00	185	1.0500E+00	205	4.0000E-01	225	2.5300E-02
166	1.5000E+00	186	1.0400E+00	206	3.7500E-01	226	1.0000E-02
167	1.4500E+00	187	1.0300E+00	207	3.5000E-01	227	7.5000E-03
168	1.4000E+00	188	1.0200E+00	208	3.2500E-01	228	5.0000E-03
169	1.3500E+00	189	1.0100E+00	209	3.0000E-01	229	4.0000E-03
170	1.3000E+00	190	1.0000E+00	210	2.7500E-01	230	3.0000E-03
171	1.2500E+00	191	9.7500E-01	211	2.5000E-01	231	2.5000E-03
172	1.2250E+00	192	9.5000E-01	212	2.2500E-01	232	2.0000E-03
173	1.2000E+00	193	9.2500E-01	213	2.0000E-01	233	1.5000E-03
174	1.1750E+00	194	9.0000E-01	214	1.7500E-01	234	1.2000E-03
175	1.1500E+00	195	8.5000E-01	215	1.5000E-01	235	1.0000E-03
176	1.1400E+00	196	8.0000E-01	216	1.2500E-01	236	7.5000E-04
177	1.1300E+00	197	7.5000E-01	217	1.0000E-01	237	5.0000E-04
178	1.1200E+00	198	7.0000E-01	218	9.0000E-02	238	1.0000E-04
179	1.1100E+00	199	6.5000E-01	219	8.0000E-02		1.0000E-05
180	1.1000E+00	200	6.2500E-01	220	7.0000E-02		

The selection criteria for the 227-group structure (and its predecessor 218-group structure) are documented in ref. 4.

All nuclides in the 238-group LAW Library use the same weighting spectrum, consisting of

1. Maxwellian spectrum (peak at 300 K) from  $10^{-5}$  to 0.125 eV,
2. a  $1/E$  spectrum from 0.125 eV to 67.4 keV,
3. a fission spectrum (effective temperature at 1.273 MeV) from 67.4 keV to 10 MeV, and
4. a  $1/E$  spectrum from 10 MeV to 20 MeV.

A plot of this spectrum is shown in Fig. 1.

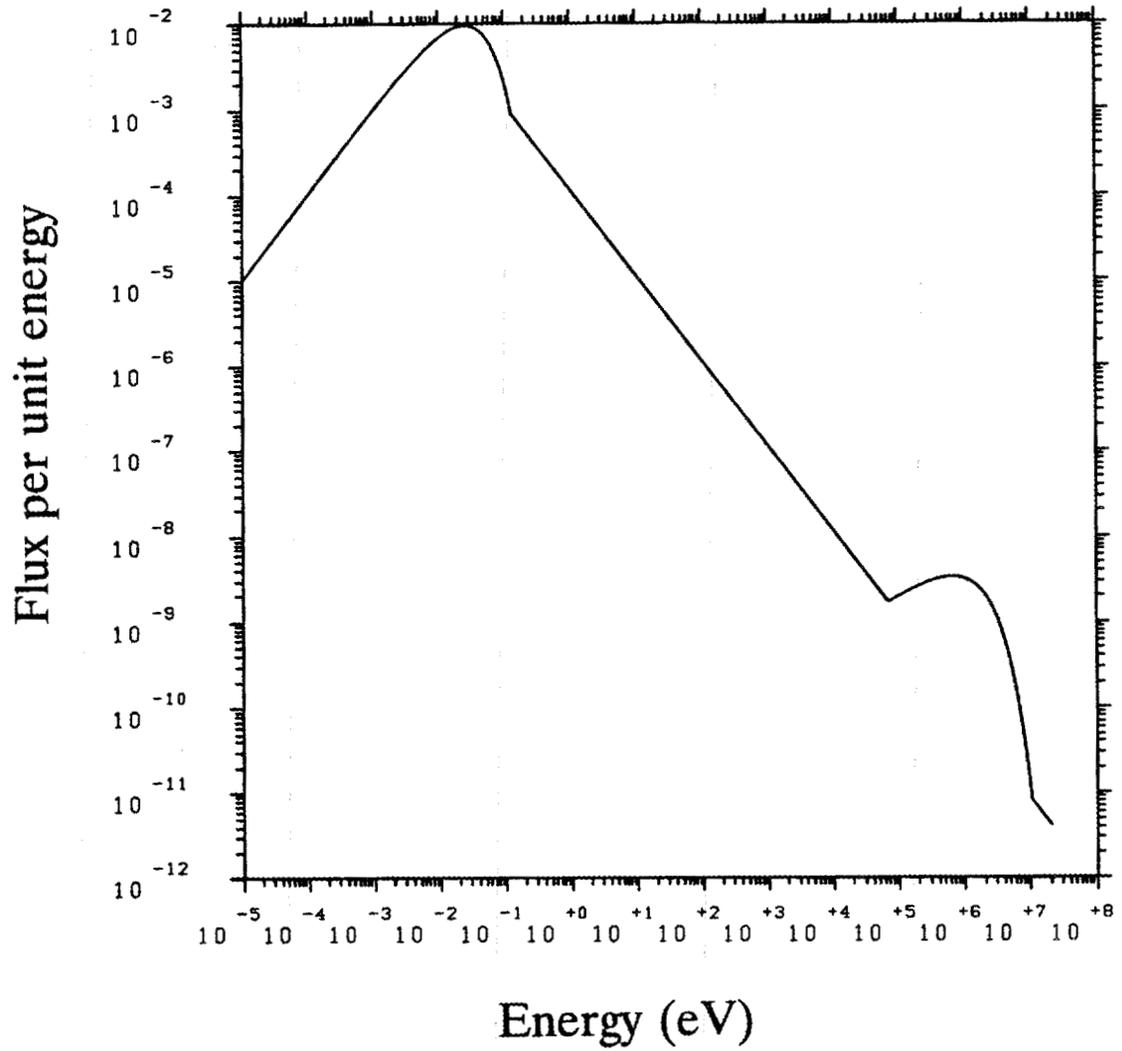


Fig. 1. Weighting function for 238-group LAW Library.

Even though the choice of the parameters that define this weighting spectra is somewhat arbitrary, the 238-group mesh is fine enough to help ensure that the library it produces is suitable for the class of problems it is intended to solve.

All nuclides use a  $P_5$  Legendre expansion to fit the elastic and discrete level inelastic scattering processes, thereby making the library suitable for both reactor and shielding applications. A  $P_3$  fit was used for thermal-scattering matrices. All other scattering processes use  $P_0$  fits.

## 2.1 NUCLIDES IN THE LAW LIBRARY

Prior to initiating the production of the LAW Library, a task was completed to combine all complete ENDF/B evaluations from the ENDF/B-V General-Purpose, Fission Product, and Actinide files. The combined file contained about 300 sets of data. It also contains sets of data from the ENDF/B-VI file for  $^{14}\text{N}_7$ ,  $^{15}\text{N}_7$ ,  $^{16}\text{O}_8$ ,  $^{154}\text{Eu}_{63}$ , and  $^{155}\text{Eu}_{63}$ .

The contents of the LAW Library are shown in Table 2. Note that the common ZA (atomic number Z, atomic mass A) notation is used to identify cross-section sets, whenever possible. Nuclides with MAT-numbers (the ENDF/B nuclide identifier) in the 1000 range were taken from the General-Purpose file, while those from the Actinide file are in the 8000 range, and those from the Fission Product File are in the 9000 range. The "MOD" is the revision number for the set of data; the "DATE" is the evaluation date. The cryptic notation under "RESONANCE DATA" tells what kind of resonance data, if any, are contained in the ENDF file. For example, SL17 indicates the evaluation contains 17 single-level Breit-Wigner resonances, ML17 would indicate 17 multilevel Breit-Wigner resonances, and UN indicates the evaluation has unresolved resonance data. In the case of  $^{233}\text{U}$  and  $^{241}\text{Pu}$ , the AA indicates the evaluation uses the Adler-Adler formalism. A notation of BF implies this nuclide has Bondarenko factors for all energy groups.

In addition to the data on the combined ENDF file, a small number of materials require thermal-scattering law data that exist on a separate ENDF/B file. Separate sets of hydrogen were made for consideration of hydrogen bound in a water molecule, hydrogen bound in a polyethylene molecule, hydrogen bound in benzene, and hydrogen as a free gas. Deuterium sets are available for deuterium bound in  $\text{D}_2\text{O}$  and for the free-gas case. A set of beryllium data considers the thermal effects existing in beryllium metal. Carbon cross sections are given in one set that has thermal data based on thermal graphite data and another based on the free-gas model. In the case of graphite, the set of cross sections uses a new graphite evaluation<sup>15</sup> performed by J.-P. Renier, who noted that the previous evaluation, based on calculations performed by the GASKET<sup>16</sup> code, although based on input data that are thought to be reasonable, were not converged to a reasonable level.

A special set, identified by 900, contains dose factors based on the ANSI/ANS 6.1.1-1977 standard. Dose factors based on the more recent ANSI/ANS 6.1.1-1991 standard are also included and identified by 9031.

Table 2. Contents of 238-group LAW Library

Nuclide	LAW identifier	ENDF MAT	MOD	Eval. date	Resonance data	Thermal MAT
47-Ag-107	47107	1407	2	Jun 1983	ML74	
47-Ag-109	47109	1409	2	Jun 1983	ML83	
47-Ag-111	47111	9415	1	Dec 1979		
13-Al-27	13027	1313	1	Dec 1973	BF	
95-Am-241	95241	1361	2	Apr 1978	SL66,UN	
95-Am-242	95242	8542	1	Aug 1975	SL82,UN	
95-Am-242m	95601	1369	1	Apr 1978	SL6,UN	
95-Am-243	95243	1363	2	Apr 1978	SL220,UN	
33-As-75	33075	9071	1	Apr 1974	SL32	
79-Au-197	79197	1379	3	Feb 1977	ML263	
5-B-10	5010	1305	1	Dec 1976		
5-B-11	5011	1160	1	Sep 1971		
56-Ba-134	56134	9684	1	Apr 1974	SL8	
56-Ba-135	56135	9685	1	Apr 1974	SL13	
56-Ba-136	56136	9687	1	Apr 1974	SL3	
56-Ba-137	56137	9689	1	Apr 1974	SL8	
56-Ba-138	56138	1353	1	Aug 1978		
56-Ba-140	56140	9693	1	Dec 1979		
4-Be-9	4009	1304	2	Oct 1976		
Be-metal	4309	1304	2			1064
83-Bi-209	83209	1375	1	Apr 1980		
97-Bk-249	97249	8749	1	Jul 1976	SL91,UN	
35-Br-79	35079	9113	1	Apr 1974	SL13	
35-Br-81	35081	9117	1	Apr 1974	SL5	
6-C	6012	1306	2	Dec 1973		
Graphite	6000	1306	2			1065
20-Ca	20000	1320	3	Aug 1971		
48-Cd	48000	1281	1	May 1974		
48-Cd-106	48106	9440	2	Feb 1980		
48-Cd-108	48108	9442	1	Apr 1974		
48-Cd-110	48110	9444	1	Apr 1974	SL68	
48-Cd-111	48111	9445	1	Apr 1974	SL125	
48-Cd-112	48112	9447	1	Apr 1974	SL55	
48-Cd-113	48113	1318	1	Nov 1978	SL12,UN	
48-Cd-114	48114	9450	1	Apr 1974	SL33	
48-Cd-115	48601	9452	1	Dec 1979		
48-Cd-116	48116	9453	1	Apr 1974	SL12	
58-Ce-140	58140	9724	1	Apr 1974		
58-Ce-141	58141	9725	1	Dec 1979		
58-Ce-142	58142	9726	1	Apr 1974		
58-Ce-143	58143	9727	1	Dec 1979		
58-Ce-144	58144	9728	1	Dec 1979		

Table 2. (continued)

Nuclide	LAW identifier	ENDF MAT	MOD	Eval. date	Resonance data	Thermal MAT
98-Cf-249	98249	8849	1	Jul 1976	SL53,UN	
98-Cf-250	98250	8850	1	Jul 1976	SL20,UN	
98-Cf-251	98251	8851	1	Jul 1976	SL20,UN	
98-Cf-252	98252	8852	1	Jul 1976	SL21,UN	
98-Cf-253	98253	8853	1	Dec 1975	SL120,UN	
17-Cl	17000	1149	1	Feb 1967		
96-Cm-241	96241	8641	1	Apr 1978		
96-Cm-242	96242	8642	1	Apr 1978	SL21,UN	
96-Cm-243	96243	1343	1	Apr 1978	SL16,UN	
96-Cm-244	96244	1344	2	Apr 1978	SL38,UN	
96-Cm-245	96245	1345	2	Jan 1979	SL39,UN	
96-Cm-246	96246	1346	1	Jul 1976	SL10,UN	
96-Cm-247	96247	8647	1	Jul 1976	SL35,UN	
96-Cm-248	96248	8648	1	Apr 1978	SL46,UN	
27-Co-59	27059	1327	3	Jun 1977	ML180	
24-Cr	24000	1324	2	Dec 1977	SL183	
24-Cr(1/E* $\sigma_i$ )	24301	1324	2	Dec 1977	SL183	
24-Cr(1/E* $\sigma_i$ (SS304))	24304	1324	2	Dec 1977	SL183	
55-Cs-133	55133	1355	1	Nov 1978	SL123	
55-Cs-134	55134	9663	1	Dec 1979		
55-Cs-135	55135	9665	1	Dec 1979		
55-Cs-136	55136	9667	1	Dec 1979	SL7	
55-Cs-137	55137	9669	1	Dec 1979		
29-Cu	29000	1329	1	Dec 1973	ML48	
1-D-2	1802	1302	2	Nov 1967		
Deuterium	1002	1302	2			1004
66-Dy-160	66160	9864	1	Apr 1974	SL3	
66-Dy-161	66161	9865	1	Apr 1974	SL27	
66-Dy-162	66162	9866	1	Apr 1974	SL8	
66-Dy-163	66163	9867	1	Apr 1974	SL60	
66-Dy-164	66164	1031	1	Jun 1967	SL2,UN	
68-Er-166	68166	9875	1	Apr 1974	SL51	
68-Er-167	68167	9876	1	Apr 1974	SL32	
99-Es-253	99253	8953	1	Jul 1976	SL27,UN	
63-Eu	63000	1463	1	Aug 1981	ML164	
63-Eu-151	63151	1357	1	Dec 1977	SL92,UN	
63-Eu-152	63152	1292	2	Dec 1973	SL93,UN	
63-Eu-153	63153	1359	1	Feb 1978	ML72,UN	
63-Eu-154	63154	Version 6 of ENDF/B				
63-Eu-154	631541	1293	1	Dec 1973	SL72,UN	
63-Eu-155	63155	Version 6 of ENDF/B				
63-Eu-155	631551	9832	1	Dec 1979		

Table 2. (continued)

Nuclide	LAW identifier	ENDF MAT	MOD	Eval. date	Resonance data	Thermal MAT
63-Eu-156	63156	9833	1	Dec 1979		
63-Eu-157	63157	9834	1	Feb 1980		
9-F-19	9019	1309	3	Jul 1974	BF	
26-Fe	26000	1326	3	Oct 1977	ML314	
26-Fe(1/E* $\sigma_i$ )	26301	1326	3	Oct 1977	ML314	
26-Fe(1/E* $\sigma_i$ (SS304))	26301	1326	3	Oct 1977	ML314	
31-Ga-11	31000	1358	1	May 1980		
64-Gd-152	64152	1362	2	Jan 1977	ML18	
64-Gd-154	64154	1364	1	Jan 1977	ML49	
64-Gd-155	64155	1365	1	Jan 1977	ML92	
64-Gd-156	64156	1366	2	Jan 1977	ML30,UN	
64-Gd-157	64157	1367	1	Jan 1977	ML56	
64-Gd-158	64158	1368	1	Jan 1977	ML93,UN	
64-Gd-160	64160	1370	1	Jan 1977	ML44	
32-Ge-72	32072	9050	1	Apr 1974	SL8	
32-Ge-73	32073	9051	1	Apr 1974	SL10	
32-Ge-74	32074	9053	1	Apr 1974	SL3	
32-Ge-76	32076	9056	1	Apr 1974	SL4	
1-H-1	1801	1301	1	Aug 1970		
H in C6H6	1901	1301	1			1095
H in CH2	2801	1301	1			1114
H in H2O	1001	1301	1			1002
2-He-3	2003	1146	1	Jun 1968		
2-He-4	2004	1270	0	Oct 1973		
72-Hf	72000	1372	1	Apr 1976	SL236	
72-Hf-174	72174	1374	1	Apr 1976	SL10,UN	
72-Hf-176	72176	1376	1	Apr 1976	SL22,UN	
72-Hf-177	72177	1377	1	Apr 1976	SL99,UN	
72-Hf-178	72178	1378	1	Apr 1976	SL25,UN	
72-Hf-179	72179	1383	1	Apr 1976	SL49,UN	
72-Hf-180	72180	1384	1	Apr 1976	SL31,UN	
67-Ho-165	67165	9872	1	Apr 1974	SL29	
53-I-127	53127	9606	1	Feb 1980	SL79	
53-I-129	53129	9608	1	Feb 1980	SL5	
53-I-130	53130	9609	1	Dec 1979		
53-I-131	53131	9611	1	Dec 1979		
53-I-135	53135	9618	1	Dec 1979		
49-In-113	49113	9473	1	Apr 1974	SL9	
49-In-115	49115	9477	1	Dec 1979	SL91	
19-K	19000	1150	1	Feb 1967		
36-Kr-78	36078	1330	1	Apr 1978	SL4	
36-Kr-80	36080	1331	1	Apr 1978	SL5	
36-Kr-82	36082	1332	1	Apr 1978	SL2	
36-Kr-83	36083	1333	1	Apr 1978	SL3	

Table 2. (continued)

Nuclide	LAW identifier	ENDF MAT	MOD	Eval. date	Resonance data	Thermal MAT
36-Kr-84	36084	1334	1	Apr 1978	SL3	
36-Kr-85	36085	9145	1	Dec 1979		
36-Kr-86	36086	1336	1	Jul 1972	SL1	
57-La-139	57139	9707	1	Feb 1980	SL69	
57-La-140	57140	9708	1	Dec 1979		
3-Li-6	3006	1303	1	Sep 1977		
3-Li-7	3007	1397	1	Dec 1981	BF	
71-Lu-175	71175	1032	1	Jun 1967	SL17,UN	
71-Lu-176	71176	1033	1	Jun 1967	SL21,UN	
12-Mg	12000	1312	1	Feb 1978		
25-Mn-55	25055	1325	2	Mar 1977	ML141	
42-Mo	42000	1321	1	Feb 1979	SL46	
42-Mo-92	42092	9278	1	Feb 1980	SL28	
42-Mo-94	42094	9281	1	Feb 1980	SL10	
42-Mo-95	42095	9282	1	Feb 1980	SL55	
42-Mo-96	42096	9283	1	Feb 1980	SL15	
42-Mo-97	42097	9284	1	Feb 1980	SL64	
42-Mo-98	42098	9285	1	Feb 1980	SL22	
42-Mo-99	42099	9286	1	Dec 1979		
42-Mo-100	42100	9287	1	Feb 1980	SL17	
7-N-14	70141	1275	2	Jul 1973		
7-N-14	7014	Version 6 of ENDF/B				
7-N-15	70151	1307	1	Mar 1977		
7-N-15	7015	Version 6 of ENDF/B				
11-Na-23	11023	1311	3	Dec 1977	ML23	
41-Nb-93	41093	1189	1	May 1974	SL218,UN	
41-Nb-94	41094	9251	1	Dec 1979	SL2	
41-Nb-95	41095	9253	1	Dec 1979		
60-Nd-142	60142	9763	1	Apr 1974	SL17	
60-Nd-143	60143	9764	1	Feb 1980	SL18	
60-Nd-144	60144	9765	1	Feb 1980	SL19	
60-Nd-145	60145	9766	1	Feb 1980	SL79	
60-Nd-146	60146	9767	1	Feb 1980	SL18	
60-Nd-147	60147	9768	1	Dec 1979		
60-Nd-148	60148	9769	1	Feb 1980	SL12	
60-Nd-150	60150	9771	1	Feb 1980	SL15	
28-Ni	28000	1328	2	Mar 1977	SL294	
28-Ni(1/E* $\sigma_i$ )	28301	1328	2	Mar 1977	SL294	
28-Ni(1/E* $\sigma_i$ (SS304))	28304	1328	2	Mar 1977	SL294	
93-Np-237	93237	1337	2	Apr 1978	SL169,UN	
93-Np-238	93238	8338	1	Aug 1975	SL95,UN	
8-O-16	80161	1276	2	Aug 1973		
8-O-16	8016	Version 6 of ENDF/B				
8-O-17	8017	1317	1	Jan 1978		

Table 2. (continued)

Nuclide	LAW identifier	ENDF MAT	MOD	Eval. date	Resonance data	Thermal MAT
15-P-31	15031	1315	1	Oct 1977		
91-Pa-231	91231	8131	1	Nov 1977	SL31,UN	
91-Pa-233	91233	1391	2	May 1978	SL34,UN	
82-Pb	82000	1382	2	Jul 1971		
46-Pd-102	46102	9379	2	Feb 1980		
46-Pd-104	46104	9381	1	Feb 1980	SL1	
46-Pd-105	46105	9382	1	Feb 1980	SL9	
46-Pd-106	46106	9383	1	Feb 1980	SL1	
46-Pd-107	46107	9384	1	Feb 1980		
46-Pd-108	46108	9386	1	Feb 1980	SL3	
46-Pd-110	46110	9389	1	Feb 1980		
61-Pm-147	61147	9783	1	Feb 1980	SL14	
61-Pm-148	61148	9784	1	Dec 1979		
61-Pm-148m	61601	9785	1	Dec 1979	SL1	
61-Pm-149	61149	9786	1	Dec 1979		
61-Pm-151	61151	9788	1	Dec 1979		
59-Pr-141	59141	9742	1	Feb 1980	SL15	
59-Pr-142	59142	9743	1	Dec 1979		
59-Pr-143	59143	9745	1	Dec 1979		
94-Pu-236	94236	8436	1	Apr 1978	SL21,UN	
94-Pu-237	94237	8437	1	Apr 1978		
94-Pu-238	94238	1338	3	Apr 1978	SL16,UN	
94-Pu-239	94239	1399	2		SL128,UN	
94-Pu-240	94240	1380	3	Apr 1977	ML201,UN	
94-Pu-241	94241	1381	2	Oct 1977	AA83,UN	
94-Pu-242	94242	1342	2	Oct 1978	SL68,UN	
94-Pu-243	94243	8443	1	Jul 1976	SL41,UN	
94-Pu-244	94244	8444	1	Apr 1978	SL21,UN	
37-Rb-85	37085	1360	1	Oct 1979	ML88	
37-Rb-86	37086	9161	1	Dec 1979		
37-Rb-87	37087	1341	1	Oct 1979	ML15	
75-Re-185	75185	1083	1	Jan 1968	SL30,UN	
75-Re-187	75187	1084	1	Jan 1968	SL25,UN	
45-Rh-103	45103	1310	1	Nov 1978	SL119,UN	
45-Rh-105	45105	9355	2	Dec 1979		
44-Ru-96	44096	9325	2	Feb 1980		
44-Ru-98	44098	9327	2	Feb 1980		
44-Ru-99	44099	9328	1	Apr 1974	SL5	
44-Ru-100	44100	9329	1	Feb 1980	SL1	
44-Ru-101	44101	9330	1	Feb 1980	SL7	
44-Ru-102	44102	9331	1	Feb 1980	SL3	
44-Ru-103	44103	9332	1	Dec 1979		
44-Ru-104	44104	9333	1	Feb 1980	SL4	
44-Ru-105	44105	9334	1	Dec 1979		
44-Ru-106	44106	9335	1	Dec 1979		
16-S	16000	1347	1	Apr 1979	ML118	
16-S-32	16032	1316	1	Oct 1977		

Table 2. (continued)

Nuclide	LAW identifier	ENDF MAT	MOD	Eval. date	Resonance data	Thermal MAT
51-Sb-121	51121	9548	1	Feb 1980	SL82	
51-Sb-123	51123	9551	1	Feb 1980	SL63	
51-Sb-124	51124	9552	1	Dec 1979		
51-Sb-125	51125	9555	1	Dec 1979		
51-Sb-126	51126	9556	1	Dec 1979		
34-Se-74	34074	9089	2	Feb 1980	SL7	
34-Se-76	34076	9091	1	Apr 1974	SL17	
34-Se-77	34077	9092	1	Apr 1974	SL31	
34-Se-78	34078	9094	1	Apr 1974	SL12	
34-Se-80	34080	9097	1	Apr 1974	SL7	
34-Se-82	34082	9100	1	Apr 1974	SL4	
14-Si	14000	1314	3	Feb 1974	BF	
62-Sm-144	62144	9803	2	Feb 1980		
62-Sm-147	62147	9806	2	Feb 1980	SL59	
62-Sm-148	62148	9807	1	Feb 1980		
62-Sm-149	62149	1319	1	Nov 1978	ML30,UN	
62-Sm-150	62150	9809	1	Apr 1974	SL12	
62-Sm-151	62151	9810	1	Feb 1980	SL8	
62-Sm-152	62152	9811	1	Feb 1980	SL57	
62-Sm-153	62153	9812	1	Dec 1979		
62-Sm-154	62154	9813	1	Apr 1974	SL18	
50-Sn-112	50112	9513	2	Feb 1980	SL12	
50-Sn-114	50114	9516	2	Feb 1980	SL5	
50-Sn-115	50115	9517	1	Apr 1974	SL3	
50-Sn-116	50116	9518	1	Apr 1974	SL8	
50-Sn-117	50117	9519	1	Apr 1974	SL25	
50-Sn-118	50118	9521	1	Apr 1974	SL8	
50-Sn-119	50119	9522	1	Apr 1974	SL10	
50-Sn-120	50120	9524	1	Apr 1974	SL48	
50-Sn-122	50122	9527	1	Apr 1974	SL6	
50-Sn-123	50123	9528	1	Dec 1979		
50-Sn-124	50124	9530	1	Apr 1974	SL5	
50-Sn-125	50125	9531	1	Dec 1979		
50-Sn-126	50126	9533	1	Dec 1979		
38-Sr-84	38084	9179	2	Feb 1980	SL10	
38-Sr-86	38086	9182	1	Apr 1974	SL24	
38-Sr-87	38087	9183	1	Apr 1974	SL22	
38-Sr-88	38088	9185	1	Apr 1974	SL16	
38-Sr-89	38089	9186	1	Dec 1979		
38-Sr-90	38090	9187	1	Dec 1979		
1-T-3	1003	1169	2	Feb 1965		
73-Ta-181	73181	1285	2	Jan 1972	ML76,UN	
73-Ta-182	73182	1127	1	Apr 1971	ML10,UN	
65-Tb-159	65159	9857	1	Feb 1980	SL23	
65-Tb-160	65160	9858	1	Dec 1979		

Table 2. (continued)

Nuclide	LAW identifier	ENDF MAT	MOD	Eval. date	Resonance data	Thermal MAT
43-Tc-99	43099	1308	2	Nov 1978	SL68,UN	
52-Te-120	52120	9576	2	Feb 1980		
52-Te-122	52122	9579	1	Apr 1974	SL22	
52-Te-123	52123	9580	1	Apr 1974	SL26	
52-Te-124	52124	9582	1	Apr 1974	SL36	
52-Te-125	52125	9583	1	Apr 1974	SL33	
52-Te-126	52126	9585	1	Apr 1974	SL21	
52-Te-127	52601	9587	1	Dec 1979		
52-Te-128	52128	9588	1	Apr 1974	SL9	
52-Te-129	52611	9590	1	Dec 1979		
52-Te-130	52130	9591	1	Apr 1974	SL22	
52-Te-132	52132	9594	1	Dec 1979		
90-Th-230	90230	8030	1	Nov 1977	SL22	
90-Th-232	90232	1390	2	Dec 1977	ML435,UN	
22-Ti	22000	1322	1	Aug 1977		
92-U-232	92232	8232	1	Nov 1977	SL13,UN	
92-U-233	92233	1393	2	Dec 1978	AA83,UN	
92-U-234	92234	1394	3	Jul 1978	ML119,UN	
92-U-235	92235	1395	3	Apr 1977	SL130,UN	
92-U-236	92236	1396	3	Jul 1978	ML191,UN	
92-U-237	92237	8237	1	Jul 1976	SL27,UN	
92-U-238	92238	1398	3	Jun 1977	ML444,UN	
23-V	23000	1323	1	Jan 1977		
74-W	74000	1474	1	Mar 1982	ML197	
74-W-182	74182	1475	2	Dec 1980	ML69,UN	
74-W-183	74183	1476	2	Dec 1980	ML50,UN	
74-W-184	74184	1477	2	Dec 1980	ML38,UN	
74-W-186	74186	1478	2	Dec 1980	ML40,UN	
54-Xe-124	54124	1335	1	Mar 1978	ML4	
54-Xe-126	54126	1339	1	Mar 1978	ML4	
54-Xe-128	54128	1348	1	Mar 1978	ML10	
54-Xe-129	54129	1349	1	Mar 1978	ML70	
54-Xe-130	54130	1350	1	Mar 1978	ML12	
54-Xe-131	54131	1351	1	Mar 1978	ML40	
54-Xe-132	54132	1352	2	Mar 1978	ML4	
54-Xe-133	54133	9643	1	Dec 1979		
54-Xe-134	54134	1354	1	Mar 1978	ML3	
54-Xe-135	54135	1294	1	Jun 1967		
54-Xe-136	54136	1356	1	Mar 1978		
39-Y-89	39089	9202	1	Apr 1974	SL16	
39-Y-90	39090	9204	1	Dec 1979		
39-Y-91	39091	9206	1	Dec 1979		

Table 2. (continued)

Nuclide	LAW identifier	ENDF MAT	MOD	Eval. date	Resonance data	Thermal MAT
40-Zr	40000	1340	2	Apr 1976	ML397	
40-Zr-90	40090	1385	2	Apr 1976	ML123	
40-Zr-91	40091	1386	2	Apr 1976	ML94	
40-Zr-92	40092	1387	2	Apr 1976	ML79	
40-Zr-93	40093	9232	1	Dec 1979		
40-Zr-94	40094	1388	2	Apr 1976	ML71	
40-Zr-95	40095	9234	1	Dec 1979		
40-Zr-96	40096	1389	2	Apr 1976	ML30	
1/v set	999					
Dose factors	900					
Weighting spectra*	99					

\*See Sect. 2.4.

## 2.2 RESONANCE SELF-SHIELDING THE LAW LIBRARY

A Nordheim Integral Treatment<sup>17</sup> calculation is typically used for self-shielding resolved resonances with the LAW Library; the Bondarenko treatment<sup>18</sup> is typically employed for unresolved resonance self-shielding. In the AMPX system, the ROLAIDS module provides a multizone, one-dimensional integral transport calculation for resolved resonance self-shielding. This module can be used with the LAW Library if the situation is such that the much simpler Nordheim Treatment is inadequate.

Nuclides that use single or multilevel Breit-Wigner data will have the information necessary for a Nordheim calculation placed on the AMPX master library. Those nuclides with unresolved data will also contain Bondarenko factor data.

The two nuclides, <sup>233</sup>U and <sup>241</sup>Pu, that used Adler-Adler data were processed as "infinite dilution" by AMPX to produce sets that require a ROLAIDS calculation to be made, if used in a situation that requires them to be resonance self-shielded. They were also processed using the NJOY<sup>19</sup> system to produce sets that contain Bondarenko data for all energy groups and can therefore be self-shielded in both the resolved and unresolved region using the Bondarenko method.

Four nonresonance nuclides were specially processed to take into account possible self-shielding effects arising from resonance structure in the point data. These were <sup>7</sup>Li, <sup>19</sup>F, <sup>27</sup>Al, and <sup>14</sup>Si. These nuclides contain Bondarenko data for all energy groups.

Nuclides with unresolved data contain Bondarenko factors for self-shielding in this energy range, with a few exceptions. The nuclides W, Eu, Hf, and Mo all contain unresolved data. However, they are multi-isotope evaluations and do not have Bondarenko data on the master library because the unresolved resonance region varies from isotope to isotope. Our present Bondarenko treatment program (BONAMI) allows the factors to be given for an arbitrary energy range, but only one range can be specified in a cross-section set. The same is not true for the

resolved range where the Nordheim calculation, as implemented in NITAWL, can treat variable ranges. The data for these sets in the LAW Library are, therefore, infinite dilution in the unresolved range with full self-shielding capabilities in the resolved range. Generally, this situation will not create a problem because sets of data are also provided for most isotopes that are part of the natural elemental form of these nuclides.

In the original version of the LAW-238 library, only *s*-wave resonance data were included in the resonance parameters that were passed to the Nordheim treatment in NITAWL. Subsequently, applications have been encountered, notably involving transport through iron and zirconium, whereby experimentally adding *d*-wave resonance data changed results by several percent. As a result, a special program was written to scan the ENDF/B-V library to locate all nuclides with *d*-wave and *p*-wave resonances, and to extract these data in a format which would allow them to be included in the 238-group library. A total of 21 nuclides was involved, as listed in Table 3. (Note that the self-shielding of these higher-order parameters is not automatic in NITAWL; the IQM parameter in the 1\$ array is used to request their usage.)

### 2.3 THERMAL-SCATTERING PROCESSING

As mentioned earlier, several of the sets of data required the use of the ENDF/B scattering law data files. For all other nuclides,  $P_3$ -scattering matrices were generated based on free-gas scattering. For all nuclides except those noted below, thermal-scattering matrices were generated at 300, 500, and 900 K.

For water-bound hydrogen (ID = 1001) and D<sub>2</sub>O-bound deuterium (ID = 1002), thermal matrices are given at 296, 350, 400, 450, 500, 600, 800, and 1000 K.

For polyethylene-bound hydrogen (ID = 1901), thermal matrices are given at 296 and 350 K.

For beryllium in metallic form (ID = 4309), thermal matrices are given at 296, 400, 500, 600, 700, 800, 1000, and 1200 K.

For carbon in graphite (ID = 6000), thermal matrices are given at 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, and 2000 K.

### 2.4 SPECIAL WEIGHTING FUNCTIONS PROVIDED TO COLLAPSE 238-GROUP LIBRARY

A special material is included in the LAW Library with an identifier of 99, which contains 238-group weighting spectra for a variety of situations one might find of interest.

As mentioned in Sect. 1.3, it is easy to tell the AMPX MALOCS module to collapse the cross-section sets in a library over the spectrum that was used to obtain the 238-group library. An option is also provided, wherein one can select a function from any set of data on the library and use this spectrum to collapse all nuclides on the library. This latter option is useful for producing an "application-specific" collapsed library.

Table 3. ENDF/B-V nuclides with p- and d-wave resonance parameters

Nuclide	Identifier	MAT	Isotope	Abundance	s-wave	p-wave	d-wave	Energy range
Co-59	27059	1327	59	1.0	72	107		$1 \times 10^{-5}$ - $8.5 \times 10^4$
Cr	24000	1324	50	0.043	38	20		$1 \times 10^{-5}$ - $6.93 \times 10^5$
			52	0.838	14	59		
			53	0.095	15	10		
			54	0.024	10	14		
Fe	26000	1326	54	0.058	16	58	56	$155-4 \times 10^5$
			56	0.917	15	69	43	
			57	0.022	21	29		
			58	0.003	5			
Mn-55	25055	1325	55	1.0	43	96		$1.0 \times 10^{-5}$ - $1.3 \times 10^5$
Mo	42000	1321	92	0.158	1			4-1000
			94	0.090	1			
			95	0.157	7	11		
			96	0.165	1	1		
			97	0.095	10	7		
			98	0.238	4	1		
Na-23	11023	1311	23	1.0	4	12	7	$600-5 \times 10^5$
			100	0.096	1	1		
Nb-93	41093	1189	93	1.0	95	123		$1 \times 10^{-5}$ -7500
Ni	28000	1328	58	0.681	30	36		$1 \times 10^{-5}$ - $6.9 \times 10^5$
			60	0.265	40	49		
			62	0.040	35	35		
			64	0.015	24	44		
Rb-85	37085	1360	85	1.0	75	12		$1 \times 10^{-5}$ - $2 \times 10^4$
Rb-87	37087	1341	87	1.0	14	1		$1 \times 10^{-5}$ - $3 \times 10^4$
Rh-103	45103	1310	103	1.0	59	60		$1 \times 10^{-5}$ -1500
S	32000	1347	32	0.950	5	92	16	$1 \times 10^{-5}$ - $1.1 \times 10^6$
			33	0.008	6	33		
			34	0.042	4	9		
			99	1.0	42	25		
Tc-99	43099	1308	99	1.0	42	25		$1 \times 10^{-5}$ -800
Th-232	90232	1390	232	1.0	241	192		5-4000
U-238	92238	1398	238	1.0	116	280		1-4000
Zr	40000	1340	90	0.515	34	84	5	$1 \times 10^{-5}$ - $9 \times 10^4$
			91	0.112	35	58		$1 \times 10^{-5}$ - $2.45 \times 10^4$
			92	0.171	15	63		$1 \times 10^{-5}$ - $9 \times 10^4$
			94	0.174	22	48		$1 \times 10^{-5}$ - $9 \times 10^4$
			96	0.028	8	21		$1 \times 10^{-5}$ - $9 \times 10^4$
Zr-90	40090	1385	90	1.0	34	84	5	$1 \times 10^{-5}$ - $9 \times 10^4$
Zr-91	40091	1386	91	1.0	35	58		$1 \times 10^{-5}$ - $2.45 \times 10^4$
Zr-92	40092	1387	92	1.0	15	63		$1 \times 10^{-5}$ - $9 \times 10^4$
Zr-94	40094	1388	94	1.0	22	48		$1 \times 10^{-5}$ - $9 \times 10^4$
Zr-96	40096	1389	96	1.0	8	21		$1 \times 10^{-5}$ - $9 \times 10^4$

Several spectra are included, as listed below:

1. spectrum based on a fuel cell from a  $17 \times 17$  Westinghouse light-water-reactor (LWR) assembly and identified by 9001,
2. spectrum designed for use with the Molten Salt Reactor Experiment (MSRE) fuel storage tanks at ORNL and identified by 9002,
3. average spectrum in a 27-cm carbon steel for use in cask shielding studies and identified by 9003,
- 4,5. average spectra in an 18.6-cm lead/13-cm resin shield for use in shielding cask studies (the flux in the lead region is identified by 9004 and that in the resin region by 9005), and
6. average spectrum in a 50-cm concrete shield for cask shielding studies and identified by 9006.

In the latter four cases, the spent fuel source is a Westinghouse  $15 \times 15$  assembly with initial enrichment of 3.0 wt % and burned to 30 gigawatt days per metric ton of uranium (30 GWd/MTU) and cooled for 5 years.

### 3. LIBRARY PRODUCTION PROCEDURES

A sequence of three programs was run for each set of data on the LAW Library. The XLACS program reads ENDF/B data and produces a set of multigroup cross sections in AMPX library format. The RADE program was used to perform quality and consistency checks on the multigroup data. The VASELINE program was used to make plots of the multigroup and point data, as a further aid to testing.

In the case of nuclides with unresolved resonance data, this sequence of three programs was augmented by three more programs. PRUDE processes unresolved data into a point format, TABU processes these point data into Bondarenko factors, and, finally, the UNITAB program couples the Bondarenko factors with the master library produced by XLACS.

Figure 2 is a flow chart of the above procedure.

As mentioned earlier,  $^{233}\text{U}$  and  $^{241}\text{Pu}$  were processed by NJOY. In these cases, the sequence of NJOY modules—RECONR, BROADR, UNRESR, THERMR, GROUPT, and AMPXR—was run. RECONR is used to produce a "point" ENDF file with data at 0 K from the basic ENDF file. BROADR takes this file and Doppler-broadens the data to 300, 500, 900 and 2100 K. UNRESR processes the unresolved ENDF parameters and produces self-shielded point files at the temperatures mentioned above and for background cross-section values of 1, 10, 100, 1000,  $10^4$ ,  $10^5$ , and  $10^{10}$  barns. THERMR produced thermal-scattering matrices based on the free-gas model at 300, 500, 900, and 2100 K. GROUPT reduces the point data to group-averaged form, and, finally, AMPXR converts from the GENDF format written by GROUPT to the AMPX master format. This procedure is shown schematically in Fig. 3.

After all nuclides were produced, the AJAX program was used to collect all sets of data into a single AMPX master library. This library was subsequently run through the COMET program that forces consistency between group-averaged scattering cross sections and scattering transfer arrays. Subsequently, it writes a new master library.

The final operation for the library is one required for the thermal-scattering matrices. The familiar free-gas treatment assumes a constant value of the free-atom cross section at energies well above thermal. The equations that arise combine this constant cross section with free-gas-scattering kinematics and Doppler broadening. Unfortunately, many nuclides have resonances that are located in or near the thermal region. Even nuclides that have flat scattering cross sections have their cross-section values affected by resonances away from the thermal range.

Since thermal scattering is not that important for most heavier nuclides (which are the nuclides with low-energy resonances), the following simple scheme was selected. The thermal-scattering matrices are generated by using a free-atom cross section derived from using the scattering radius given as part of the resonance data on an ENDF/B evaluation. These matrices are then normalized to the group-averaged values determined by Doppler broadening and weighting point ENDF/B data. This method is a crude way of producing matrices. However, it includes the effects of thermal resonance structure, Doppler broadening, and thermal-scattering kinematics. This last normalization is performed by the FRESH program. The library it produces is the 238-group LAW Library.

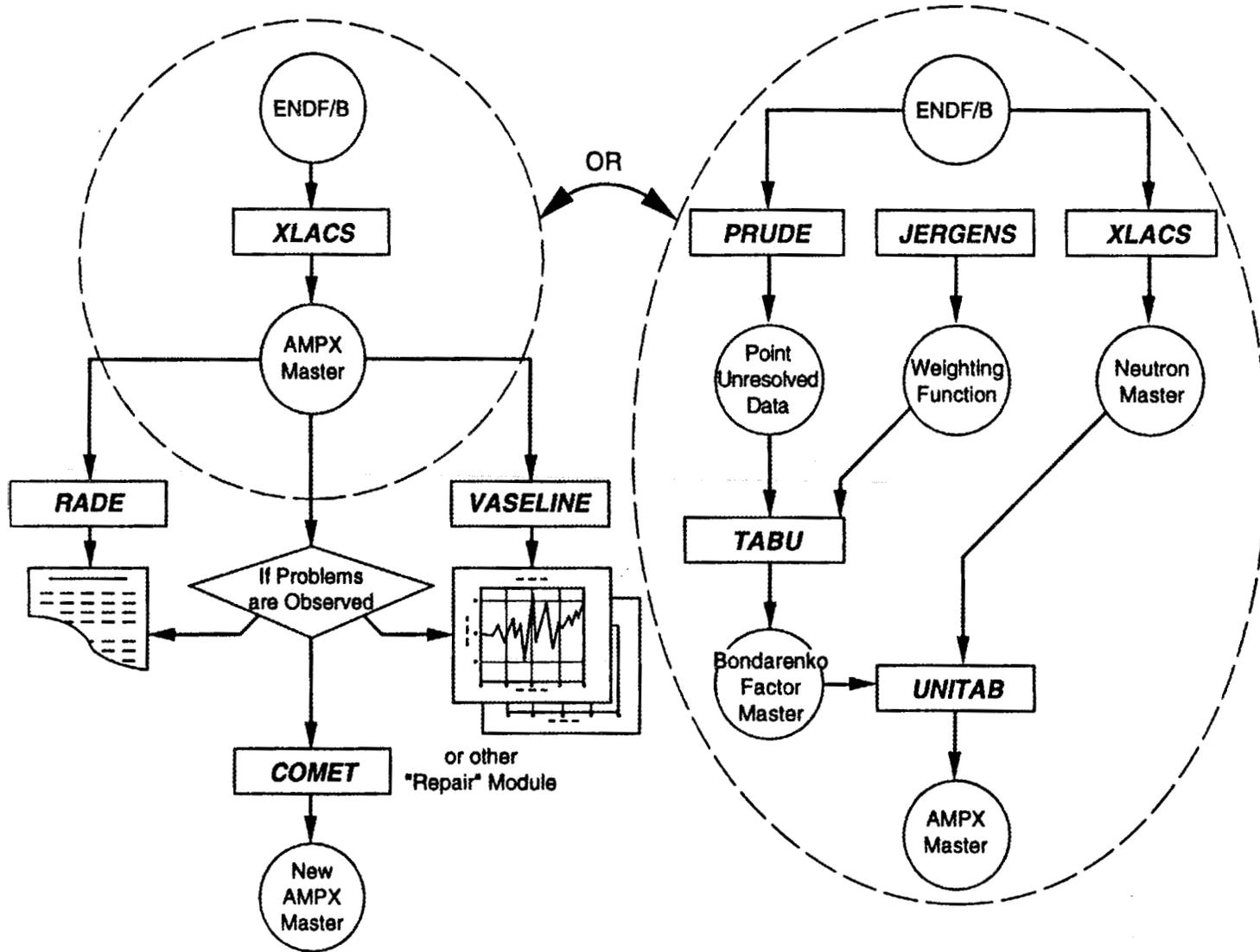


Fig. 2. Neutron production path for most nuclides in the 238-group library.

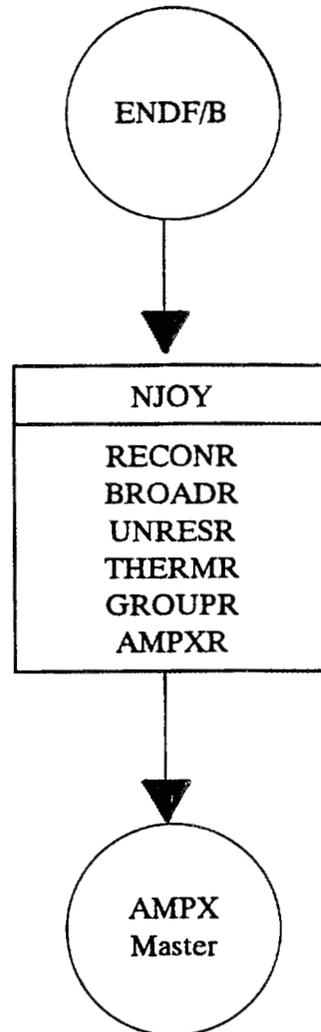


Fig. 3. Processing procedure for  $^{233}\text{U}_{92}$  and  $^{241}\text{Pu}_{94}$ .

## 4. LIBRARY TESTING AND CONCLUSIONS

### 4.1 HISTORY OF ENDF/B-V DATA TESTING

The ENDF/B-V Cross-Section Library<sup>2</sup> was released in 1980, and the ENDF/B-V Benchmark Data Testing Report<sup>20</sup> was published in August 1982. The <sup>239</sup>Pu evaluation was revised in June 1983 (ENDF/B-V Revision 2). Additional ENDF/B-V data testing was done to assess the impact of the revised <sup>239</sup>Pu evaluation.

### 4.2 DATA TESTING OF THE LAW-238 LIBRARY

The objective of the present data testing effort is to verify the new cross-section processing procedures used in generating the LAW-238 multigroup cross sections. The LAW-238 testing to date includes calculations for 7 Pu-fueled, 1 <sup>233</sup>U-fueled, and 25 <sup>235</sup>U-fueled benchmarks. There are 15 fast and 18 thermal benchmarks. Of these 33 benchmarks, 28 can be considered to be CSEWG benchmarks. We were able to demonstrate that, for most benchmarks, the calculations using the LAW-238 cross-section library give results that are very close to those obtained with other ENDF/B-V-based libraries. The results discussed in Sects. 4.3–4.4 were performed after initial preparation of the LAW library. Oxygen data from ENDF/B-V were used in this initial testing except as noted in Sect. 4.4.7. The analyses were repeated after selected resonance nuclides were modified to add p-wave and d-wave resonance data and selected nonresonance nuclides were modified to include shielding factors for high-energy resonance-like structure. No significant changes in the results or the observations noted below were seen in the final analyses. Results from the final test analyses are shown in Appendix A and compared to the initial test results discussed below.

### 4.3 FAST-REACTOR BENCHMARKS

Specifications for the CSEWG fast reactor benchmarks are given in ref. 21 and will not be given in this document. Calculations have been done for ten of the CSEWG fast benchmarks. The values of  $k_{\text{eff}}$  using the LAW-238 Library are shown in Table 4 and are compared with calculated values using the 174-group VITAMIN-E Library<sup>22</sup> and with results from Bob MacFarlane<sup>23</sup> of Los Alamos National Laboratory. For eight of the ten benchmarks in Table 4, the calculated  $k_{\text{eff}}$  values are in good agreement with the other two ENDF/B-V calculations. The LAW-238 calculated value for the JEZEBEL benchmark is a little lower than the corresponding values from the other calculations. By calculating a sphere of pure <sup>239</sup>Pu with a radius of 4.967 cm and <sup>239</sup>Pu density of 19.70 gm/cc, we were able to show that the JEZEBEL LAW-238/VITAMIN-E difference of 0.4% is due to differences in the <sup>239</sup>Pu cross sections in the two libraries since the numerical benchmark (pure <sup>239</sup>Pu) is also different by the same amount. The calculated  $k_{\text{eff}}$  for ZPR-6/6A using the LAW-238 Library is 0.31% higher than both the VITAMIN-E and LANL calculations.

Table 4. Fast-reactor benchmarks

Benchmark	VITAMIN-E 174-GROUP	LANL 80-GROUP	LAW-238
JEZEBEL <sup>a</sup>	0.9983	0.9961	0.9944
JEZEBEL-PU	1.0021	0.9999	0.9986
JEZEBEL-23 ( <sup>238</sup> U)	0.9935	0.9940	0.9959
GODIVA <sup>b</sup>	0.9966	0.9973	0.9963
FLATTOP-25	1.0047	1.0065	1.0046
BIG TEN <sup>c</sup>	1.0103	1.0121	1.0103
ZPR-3/11	1.0126		1.0119
ZPR-3/12	1.0047		1.0068
ZPR-6/6A	0.9921	0.9922	0.9952
ZPR-6/7	1.0037	0.9975	1.0022

<sup>a</sup>S<sub>16</sub> to S<sub>∞</sub> correction: -0.0021 was applied.

<sup>b</sup>S<sub>16</sub> to S<sub>∞</sub> correction: -0.0017 was applied.

<sup>c</sup>LANL calculations for BIG TEN used 175 groups.

#### 4.4 THERMAL REACTOR BENCHMARKS

Data testing of ENDF/B-V for thermal reactors is reported in ENDF-311.<sup>20</sup> In the present work, a subset of the cases considered in ref. 20 will be considered. The main emphasis will be for <sup>235</sup>U-fueled benchmarks, with only limited coverage of Pu-fueled assemblies.

##### 4.4.1 ORNL Spheres (uranyl nitrate in water)

Benchmark specifications for the ORNL spheres are available in ENDF-202.<sup>21</sup> A detailed analysis of these systems is given in ref. 24. This series of benchmarks consists of five unreflected spheres of <sup>235</sup>U (as uranyl nitrate) in water, three of them poisoned with boron. The <sup>235</sup>U enrichment is approximately 93%. Values of k<sub>eff</sub> calculated by XSDRNPM for S<sub>8</sub>, P<sub>3</sub> using the LAW-238 Library are given in Table 5. Calculations of the ORNL spheres were also done with the ANSL-V 39- and 99-group libraries<sup>25</sup> and for ORNL-1, -2, and -10 by Bob MacFarlane<sup>26</sup> using 187 groups. The other results are compared with the LAW-238 values in Table 5. We note

Table 5. ORNL spheres (uranyl nitrate in water)

BENCHMARK	ANSL-V 39-GROUP	ANSL-V 99-GROUP	LANL 187-GROUP	LAW-238
ORNL-1	1.0025	1.0012	1.0008	1.0007
ORNL-2	1.0023		1.0005	1.0005
ORNL-3	0.9993			0.9975
ORNL-4	1.0007			0.9989
ORNL-10	1.0012	1.0002	0.9980	0.9993

a trend for the calculated  $k_{\text{eff}}$  of a given benchmark to decrease by about 0.2% as the number of groups is increased (from 39 to 187 or 238). Also, the LANL-187 and LAW-238 values are in excellent agreement for ORNL-1 and ORNL-2. For some reason, the agreement for ORNL-10 is not quite as good.

#### 4.4.2 Uranium Lattice Benchmark Testing

Benchmark specifications for TRX-1 and TRX-2 and the BAPL-1, -2, and -3 lattices are given in ENDF-202.<sup>21</sup> The benchmarks are H<sub>2</sub>O-moderated lattices of slightly enriched (1.3 wt %) uranium rods in a triangular pattern. The TRX rods are uranium metal, and the BAPL rods are uranium oxide. The clad is aluminum for all of these lattices. The lattices directly test the <sup>235</sup>U fission-resonance integral and thermal-fission cross section. They also test <sup>238</sup>U shielded resonance capture and the thermal-capture cross section. They are sensitive to the <sup>238</sup>U fast-fission cross section, <sup>238</sup>U inelastic scattering, and the <sup>235</sup>U fission spectrum. The scattering and thermal absorption cross sections of H<sub>2</sub>O are also important. To account for leakage, an homogenized B-3 calculation with an input "height" corresponding to the total buckling of each lattice was done. For the BAPL lattices, a two-region correction was added to the calculated  $k_{\text{eff}}$  values. For TRX-1 and TRX-2, the two-region corrections are small and were assumed to be zero.

Values of  $k_{\text{eff}}$  calculated by XSDRNPM using the ANSL-V (99-group) and the LAW-238 libraries are given in Table 6. Calculations of TRX-1 and BAPL-1 were also done with the "NMG" 99-group library (same specifications as for LAW-238 but in the ANSL-V 99-group structure). The LAW-238 and ANSL-V results agree to within 0.15% for all five lattices shown in Table 6. We note that for TRX-1, the LAW-238 and "NMG-99" values are exactly the same while for BAPL-1 the NMG-99  $k_{\text{eff}}$  is higher by +0.0018. Thus we appear to have a group structure effect for BAPL-1 but not for TRX-1. The TRX and BAPL lattices were calculated by Don Craig<sup>27</sup> in 1982 and are documented in AECL-7690. Craig's results are also included in Table 6. Craig's calculations were made using the integral transport code RAHAB<sup>28</sup> with the

Table 6. Uranium-H<sub>2</sub>O-moderated lattices

Benchmark	ANSL-V			
	99-GROUP	NMG-99	CRAIG <sup>a</sup>	LAW-238
TRX-1	0.9901	0.9915	0.9951	0.9920
TRX-2	0.9970		0.9971	0.9962
BAPL-1	0.9986	0.9999	1.0011	0.9986
BAPL-2	1.0001		1.0015	1.0002
BAPL-3	1.0024		1.0022	1.0024

<sup>a</sup>Data taken from ref. 9.

resonance reaction rates being obtained from the OZMA<sup>29</sup> program for the most important nuclides (i.e., <sup>235</sup>U and <sup>238</sup>U for these lattices). OZMA solves the neutron transport equation for a unit cell; the discrete-ordinates option was used in Craig's work. OZMA is similar to ROLAIDS in that <sup>235</sup>U/<sup>238</sup>U resonance overlap effects are accounted for. In this respect, the OZMA calculation is more accurate than NITAWL, which only treats one resonance nuclide at a time. Eighty-nine energy groups were used for RAHAB, with 42 groups in the thermal range below 4 eV; neutron upscattering was included up to 4 eV. These choices appear to be entirely adequate for these calculations. Craig's calculated  $k_{\text{eff}}$  for TRX-1 is 0.31% higher than the LAW-238 value, and his BAPL-1 calculated value is 0.25% higher. The other lattices agree to within 0.13% or better. The LAW-238 values for the BAPL lattices have a significant trend with H<sub>2</sub>O/fuel ratio, while Craig's results show a much smaller variation.

A trend for the U-metal lattices to be about 0.3% lower than the uranium-oxide lattices is also observed in Table 6. The combined methods and differential data estimated uncertainty for the TRX-2 lattice was 0.5% in ref. 20. The impact of uncertainties in <sup>238</sup>U resonance parameters (i.e., the <sup>238</sup>U shielded capture) on the performance parameters of the TRX-1 and BAPL-1 lattices was investigated in a 1983 paper.<sup>30</sup> The <sup>238</sup>U resonance parameter sensitivities for the TRX-1 and BAPL-1 lattices were found to be almost identical. Thus, the TRX-1/BAPL-1  $\Delta k$  of about 0.3% cannot be eliminated by changing the <sup>238</sup>U resonance parameters, and some other explanation must be sought. We should consider the possibility that the resonance shielding method used in NITAWL may be contributing to the bias between the TRX and BAPL lattices.

#### 4.4.3 Uranyl Fluoride (UO<sub>2</sub>F<sub>2</sub>)/H<sub>2</sub>O Moderator

The L-series, Table 7, meet the requirements for benchmarks and are recognized as good candidates for data testing by the Thermal Reactor Data Testing and Applications Subcommittee of CSEWG. The L-series benchmarks are documented in EPRI NP-5058.<sup>31</sup> The LAW-238 calculated  $k_{\text{eff}}$  values in Table 7 are in good agreement with the LANL 187-group values.<sup>26</sup> The calculated leakage for these benchmarks<sup>31</sup> varies from 0.1742 for L-9 to 0.4687 for L-7. The calculations with the LAW-238 cross sections show a trend with leakage. This trend was not seen in the calculations by Schmidt and Rose (see Table 2-2 of ref. 31) using the SAM-CE Monte Carlo program, but has been seen by other data testers (e.g., the LANL-187 values in Table 8). A plot of the LAW-238 calculated  $k_{\text{eff}}$  vs leakage is given in Fig. 4. The slope of the line in Fig. 4 is 0.0115, which shows the trend of  $k_{\text{eff}}$  to increase with leakage. This is excellent agreement with the LANL-187 results (compare the calculated  $k_{\text{eff}}$  values for the L-9 and L-7 cases) which show a slope of 0.0157. The trend with leakage is also seen by other CSEWG data testers and is generally accepted by the Thermal Reactor Data Testing and Applications Subcommittee. The impact of the ENDF/B-VI <sup>16</sup>O evaluation will be to lower the calculated  $k_{\text{eff}}$  values of the L-series benchmarks and also to lower the slope of the line in Fig. 4. The L-series benchmark calculations were repeated using the ENDF/B-VI oxygen cross sections and are discussed in Sect. 4.4.7.

Table 7. Uranyl fluoride (UO<sub>2</sub>F<sub>2</sub>)/H<sub>2</sub>O moderator

Benchmark	LANL-187	LAW-238
L-7	1.0099	1.0081
L-8	1.0090	1.0088
L-9	1.0053	1.0052
L-10		1.0090
L-11		1.0036

Table 8. Homogeneous Pu-H<sub>2</sub>O assemblies

Benchmark	LANL <sup>a</sup>	LAW-238
PNL-3	1.0003 ± 0.0023	0.9982
PNL-6B	1.0118 ± 0.0024	1.0102
PNL-11	1.0098 ± 0.0022	1.0023 ± 0.0034

<sup>a</sup>Data taken from ref. 23.

# L-Series Benchmarks

## $k_{\text{eff}}$ vs Leakage

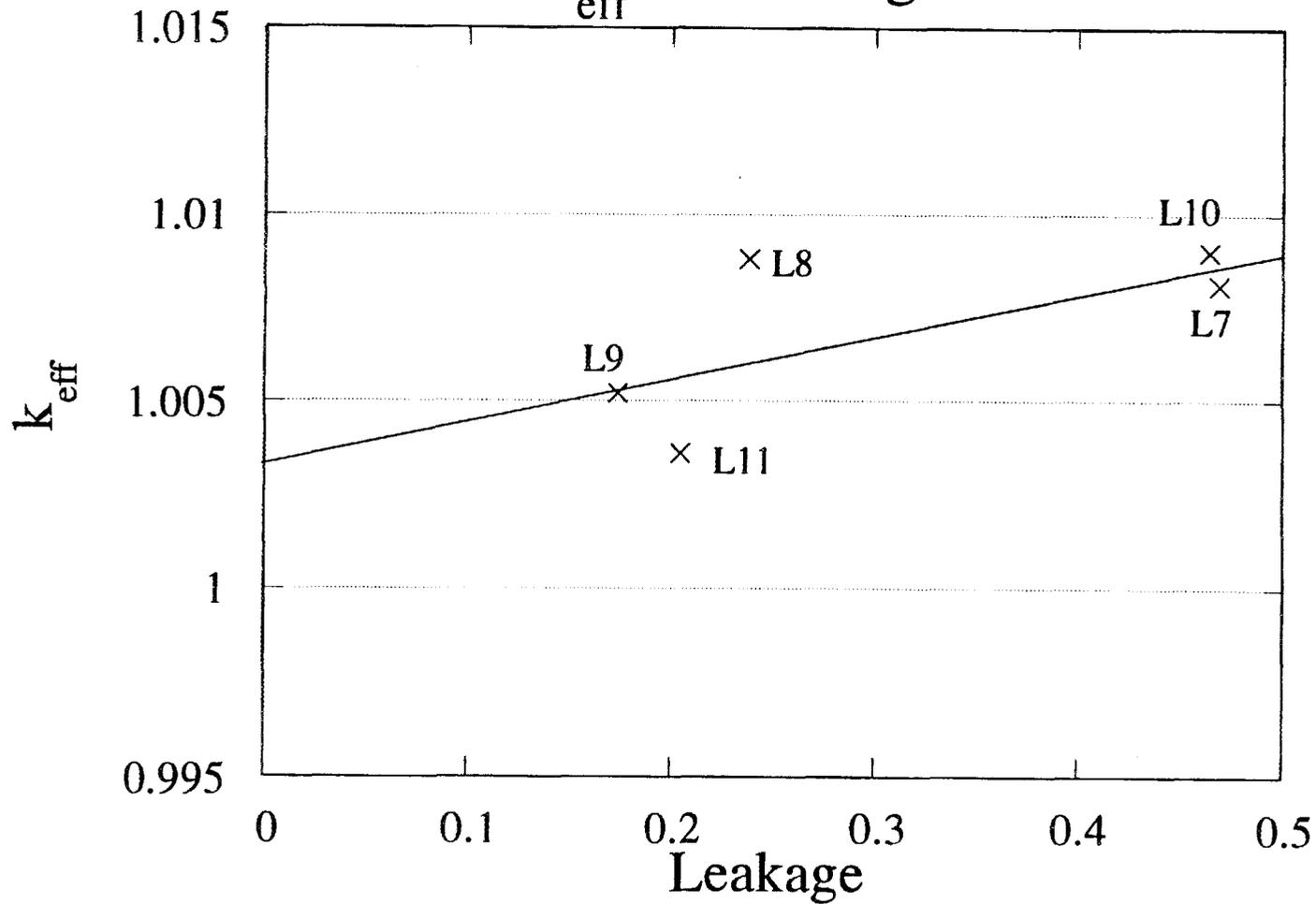


Fig. 4. Calculated  $k_{\text{eff}}$  vs leakage.

#### 4.4.4 Homogeneous Pu-H<sub>2</sub>O Assemblies

As noted previously, the main emphasis in this work is for <sup>235</sup>U benchmarks with only limited coverage of Pu-fueled assemblies. Three homogeneous Pu-H<sub>2</sub>O assemblies have been calculated using the LAW-238 Library. KENO V.a was used for the PNL-11 calculation. The calculated  $k_{\text{eff}}$  values are compared in Table 8 with values from LANL (see ref. 20). When the Monte Carlo uncertainties are taken into account, the level of agreement between the LAW-238 and LANL values is fairly good. Based on the limited amount of testing done thus far, results obtained for these homogeneous Pu-H<sub>2</sub>O assemblies are in good agreement with those obtained by other ENDF/B-V data testers.

#### 4.4.5 Other Fast Benchmarks

Five additional uranium benchmarks have also been analyzed. Even though they are not CSEWG benchmarks, they are of interest for ENDF/B-V data testing. The H2OX-1 benchmark was analyzed by Slater.<sup>25</sup> Systems similar to H2OX-1 are of considerable interest to the criticality safety community (e.g., accident analysis of the ANS reactor). The two uranium hydride cases, UH3-UR and UH3-NI, differ significantly from the fast benchmarks considered in Table 4. The HISS(HUG) and HISS(HPG) benchmarks are sensitive to <sup>235</sup>U fission and <sup>239</sup>Pu fission in the resolved resonance range and as such are unique in this respect and thus represent a valuable addition to the benchmarks considered.

Calculated  $k_{\text{eff}}$  values for these five additional benchmarks are given in Table 9. The H2OX-1 benchmark is a light-water-reflected U-metal sphere;<sup>25,32</sup> the calculated value of  $k_{\text{eff}}$  from ref. 25 is given in Table 9. We note that the ANSL-V 39-group calculated  $k_{\text{eff}}$ , 1.0029, is slightly better (i.e., closer to 1) than the LAW-238 value. The impact of the ENDF/B-VI oxygen cross sections will be to lower the H2OX-1 calculated  $k_{\text{eff}}$  values slightly (see Appendix A).

Table 9. Other fast benchmarks

	VITAMIN-E 174 GRP	ANSL-V 39 GRP	LAW-238
H2OX-1		1.0029	1.0047
UH3-UR	1.0065		1.0098
UH3-NI	1.0137		1.0245
HISS(HUG)	1.0258		1.0241
HISS(HPG)	0.9949		1.0005

The UH3-UR and UH3-NI benchmarks are enriched-uranium-hydride critical assemblies with natural uranium and nickel reflectors, respectively. These critical experiments were done on the Topsy machine.<sup>33</sup> In the initial calculation of the UH3-NI benchmark we determined that the Ni cross sections were being treated as infinitely dilute. After investigation we found that CSASN had identified Ni as a nonresonance material. We also found that both Ni and Cr were treated as nonresonance materials in some of the fast benchmarks in Table 4. Some other materials were also incorrectly flagged as nonresonance materials. CSASN was revised to correctly set the resonance flags for a number of materials, and the ZPR-3/11, ZPR-3/12, ZPR-6/6A, and ZPR-6/7 cases were reexecuted. Results given in Table 4 are from the corrected cases. The UH3-NI case has been executed using ID 28301, which is weighted using  $1/(E\sigma_T)$  weighting. This adjusted value will be closer to the correct weighting for Ni in the resonance range. However, in the fission spectrum range the weighting should be more like a fission spectrum divided by  $\sigma_T$ . The value of  $k_{\text{eff}}$  given in Table 9 for the UH3-NI benchmark was obtained using ID 28301 [i.e., for  $1/(E\sigma_T)$  weighting]. The calculated  $k_{\text{eff}}$  for the UH3-NI benchmark using VITAMIN-E is 1.0137, which gives a  $\Delta k$  of 0.0109 compared with the LAW-238 value. Another result of interest for the UH3-NI benchmark is that the leakage fraction using VITAMIN-E cross sections is 33.18%, compared with only 30.02% leakage with the LAW-238 Library. The VITAMIN-E/LAW-238  $\Delta k$  can be explained primarily as a leakage effect that is due to "group structure" differences. This is illustrated in Figs. 5 and 6, which show the Ni total cross sections from the LAW-238 and VITAMIN-E libraries, respectively.

The HISS benchmarks are documented in ref. 34. HISS(HUG) has homogeneous uranium-graphite fuel; the HISS(HPG) benchmark has homogeneous plutonium-graphite fuel. The HISS cases are modeled as an infinite homogeneous medium. In other words, the calculation is  $k_{\infty}$  rather than  $k_{\text{eff}}$ . The HISS cases have also been executed using VITAMIN-E cross sections. We note that the HISS(HUG) benchmark calculated  $k_{\infty}$  is about 1.0250 with both LAW-238 and VITAMIN-E cross sections, which can be compared with the "experimental" value of  $1.0000 \pm 0.0040$ .<sup>34</sup> The HISS(HPG)-calculated  $k_{\infty}$  using the LAW-238 cross sections is 1.0005; the corresponding VITAMIN-E value is 0.9949. The  $\Delta k$  for LAW-238 vs VITAMIN-E is thus 0.0056, which is a rather large difference for an infinite medium calculation. Additional study to understand this difference is suggested since the HISS(HUG) calculated  $k_{\infty}$  values are in excellent agreement.

#### 4.4.6 Fission Rate Plots

A valuable aid to the understanding and analysis of the fast- and thermal-reactor benchmarks considered in this study is to obtain a plot of the fission rate in the fuel zone. Actually, we have plotted fissions/unit lethargy. This method has an advantage of removing the group width ( $\Delta U$ ) so that each group is on the same basis. The fission rate/unit lethargy plots give an indication of which energy range is important for a given benchmark, but, of course, slowing down is almost always an important consideration so that, for example, scattering in water could be important at higher energies where fissions/unit lethargy may be small. Plots for six fast and three thermal benchmarks are shown in Figs. 7 through 18. For the L11 critical solution benchmark, only 2.1% of the fissions are above 0.625 eV. For the L7 benchmark, the

# SCALE-238 Ni Total Cross-Section (UH3UR Benchmark)

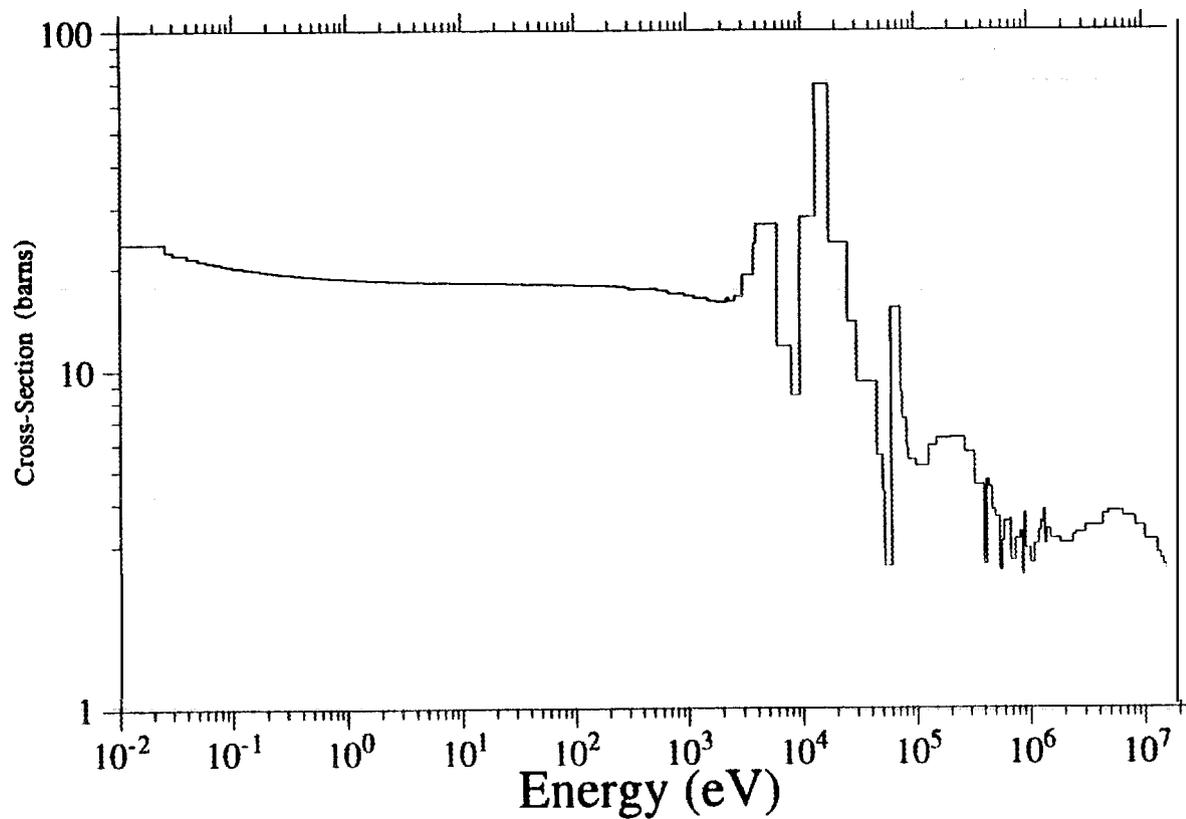


Fig. 5. UH3-NI/SCALE-238 Ni total cross section

# VITAMIN-E Ni Total Cross-Section (UH3UR Benchmark)

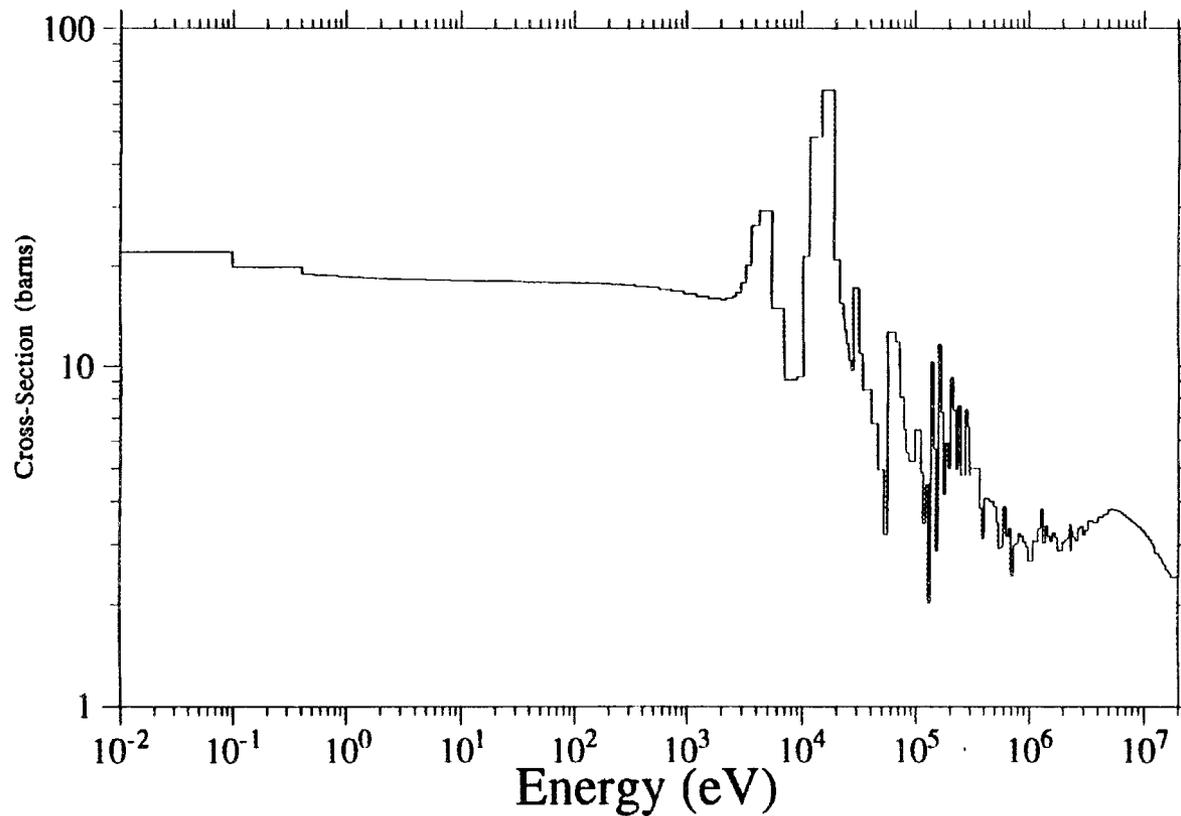


Fig. 6. UH3-NI/VITAMIN-E Ni total cross section

# L11CSB BENCHMARK

SCALE-238 Library

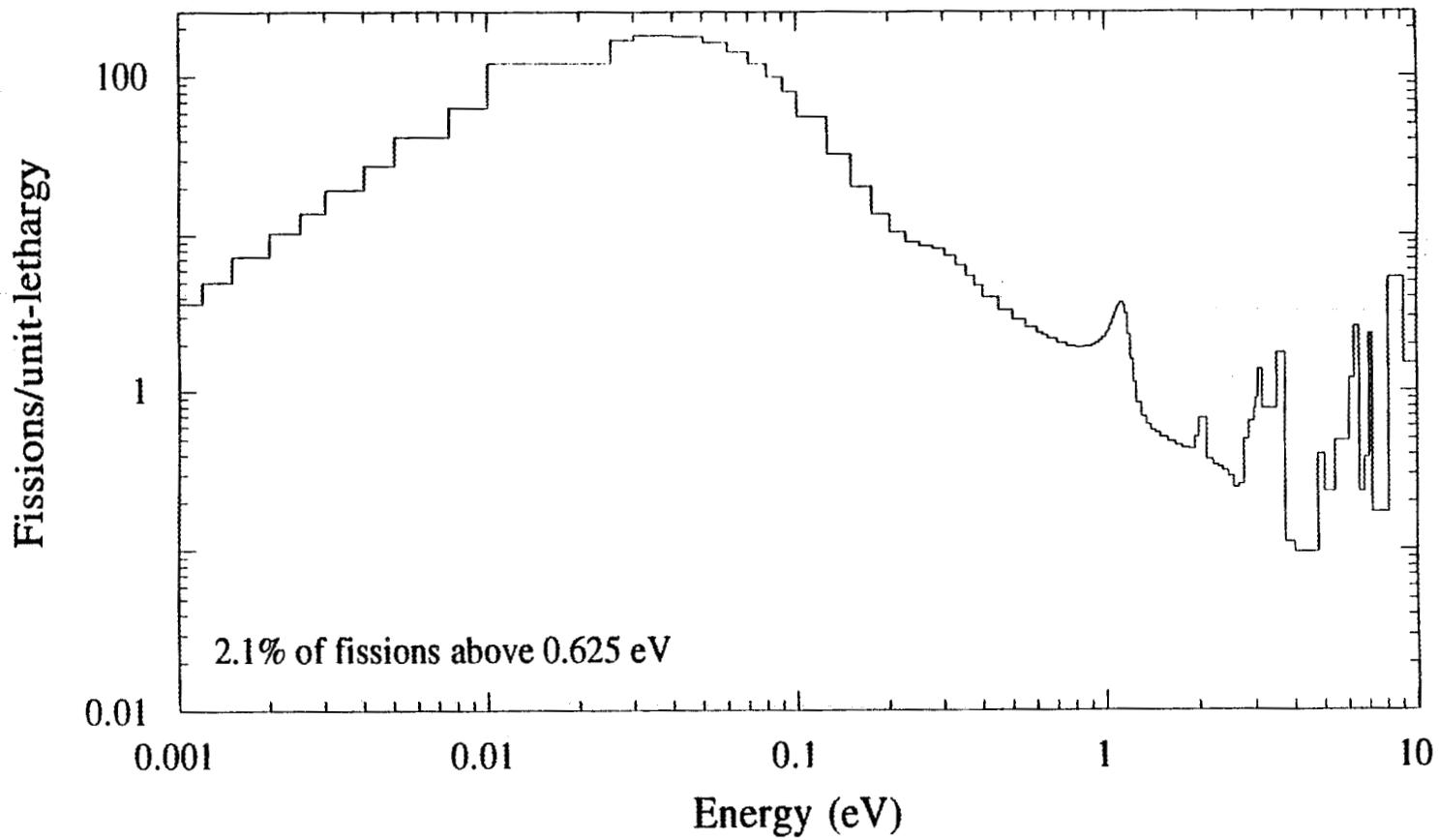


Fig. 7. L11CSB fission rate for 0.001 to 10 eV.

# L7CSB BENCHMARK

## SCALE-238 Library

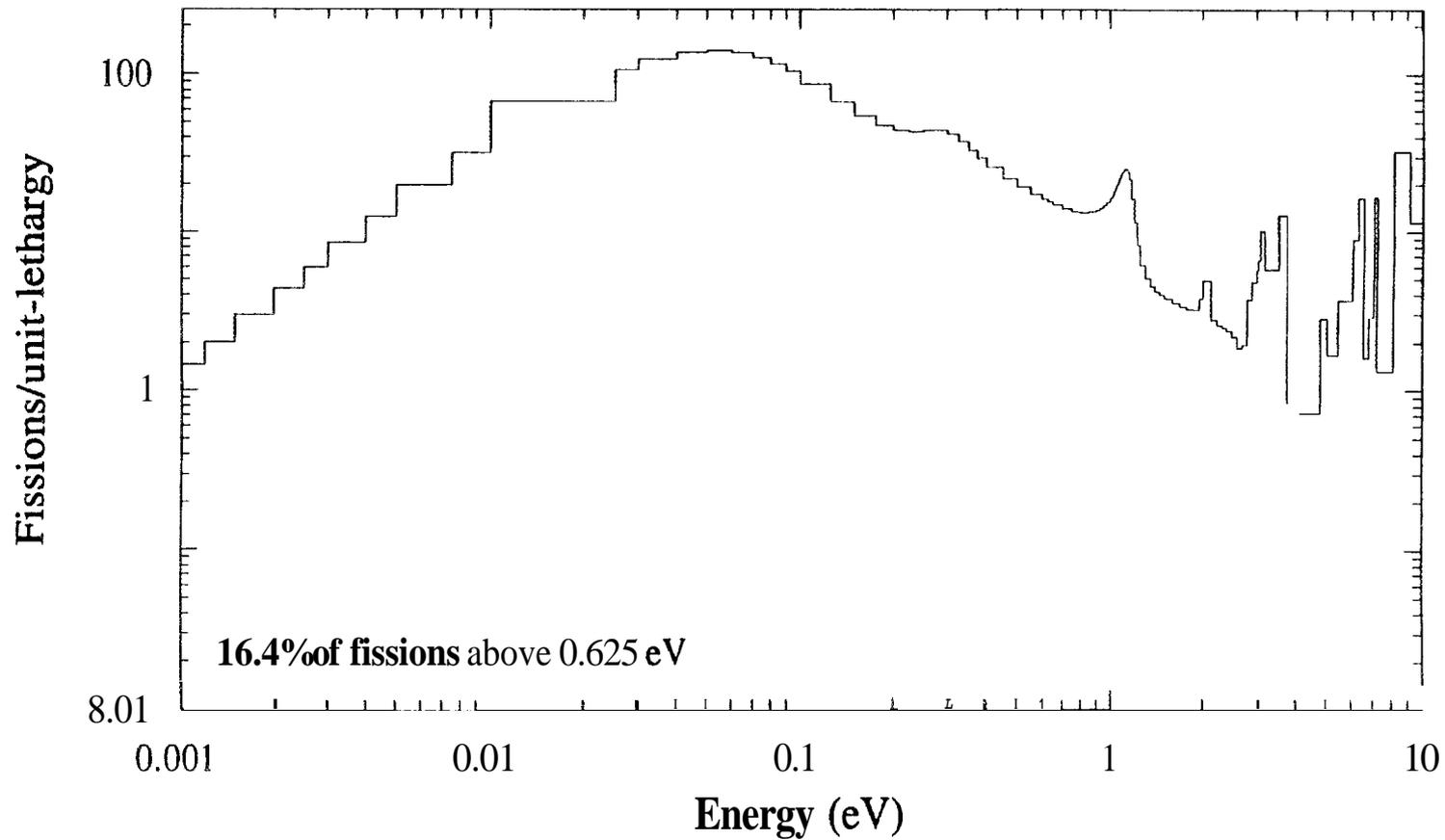


Fig. 8. L7CSB fission rate for 0.001 to 10 eV.

# HI240R BENCHMARK

## SCALE-238 Library

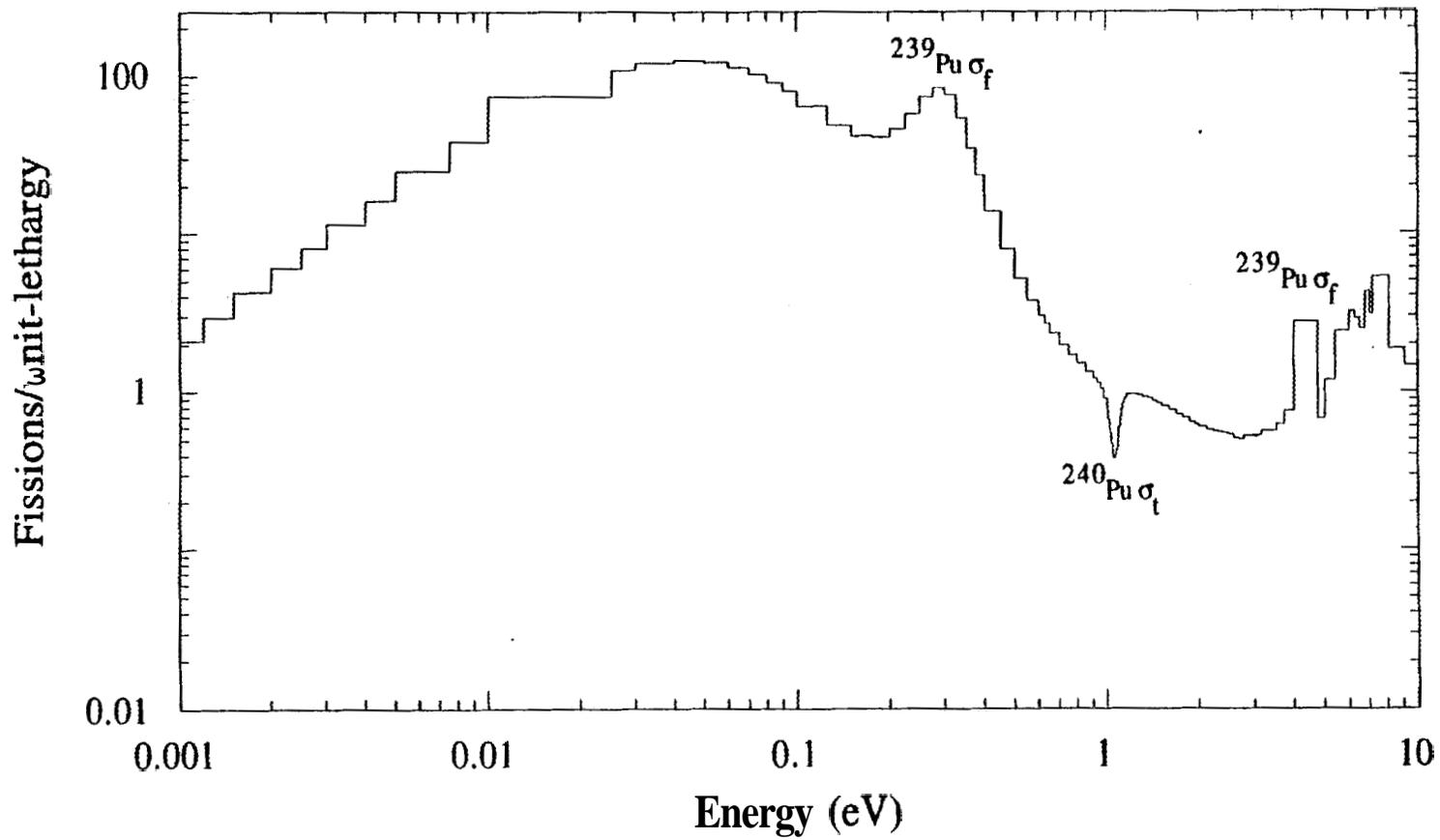


Fig. 9. HI240R fission rate for 0.001 to 10 eV.

# H2OX1 BENCHMARK

## SCALE-238 Library

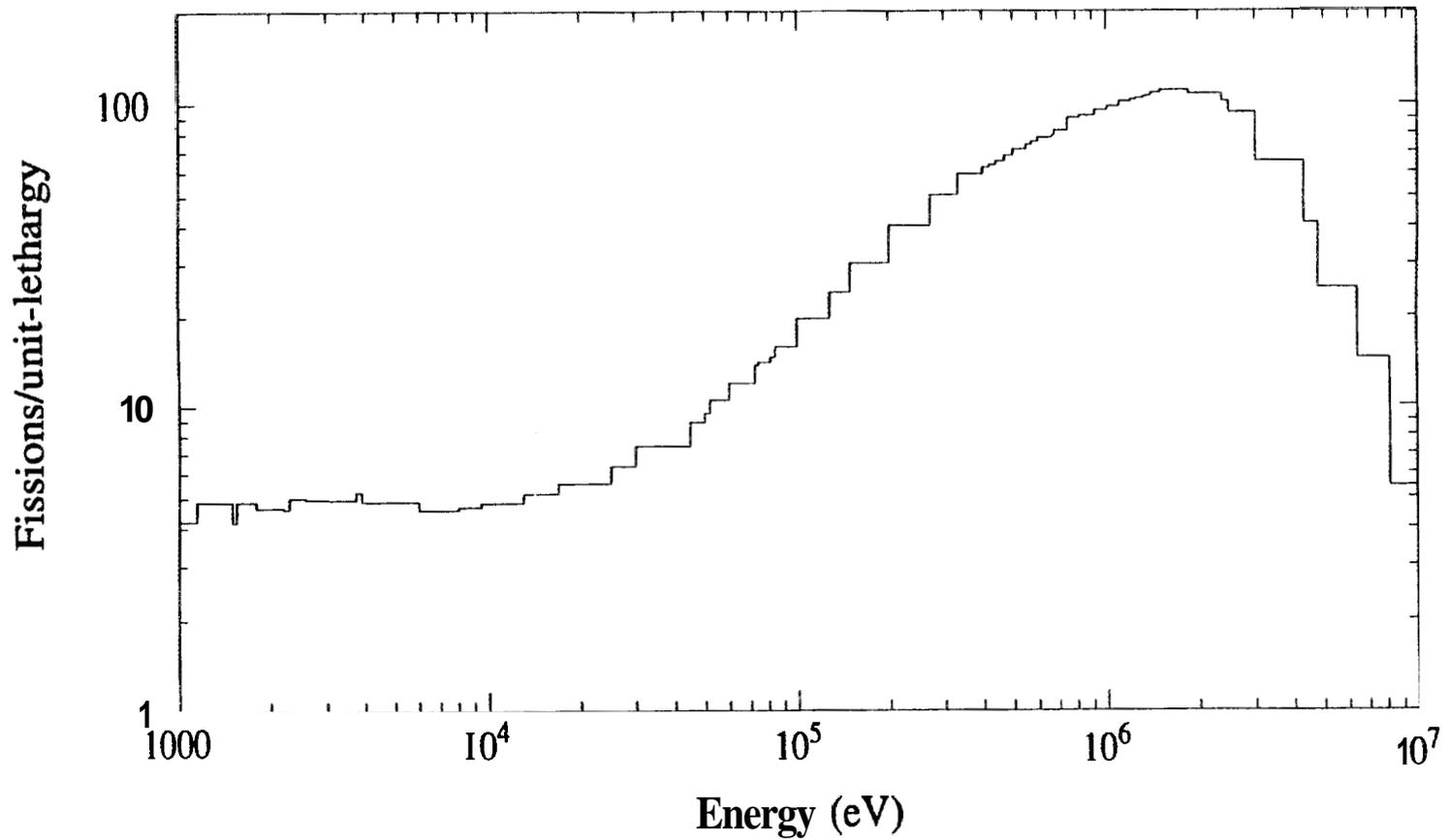


Fig. 10. H2OX1 fission rate for 0.001 to 10 MeV.

# H2OX1 BENCHMARK

SCALE-238 Library

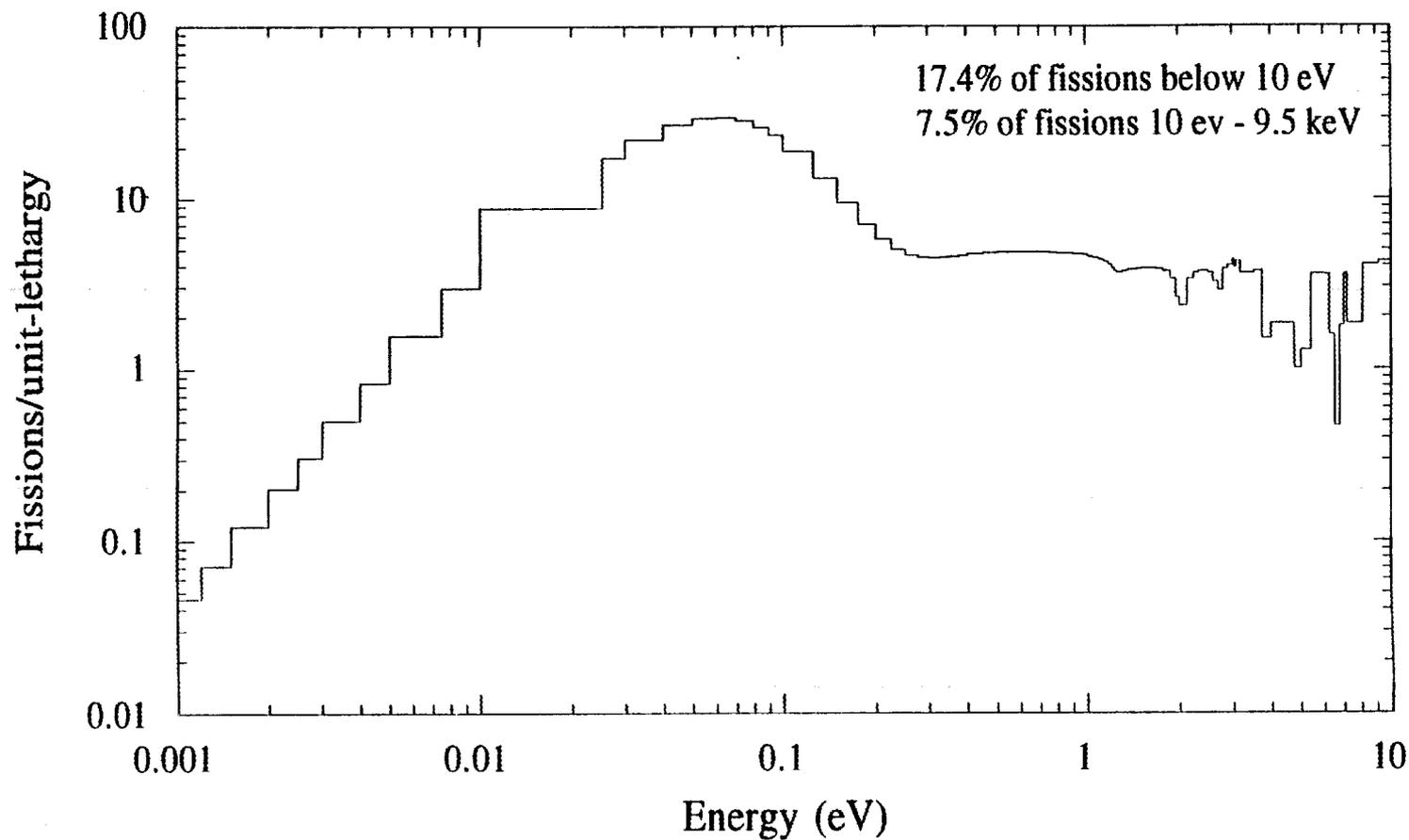


Fig. 11. H2OX1 fission rate for 0.001 to 10 eV.

# UH3NI BENCHMARK

## SCALE-238 Library

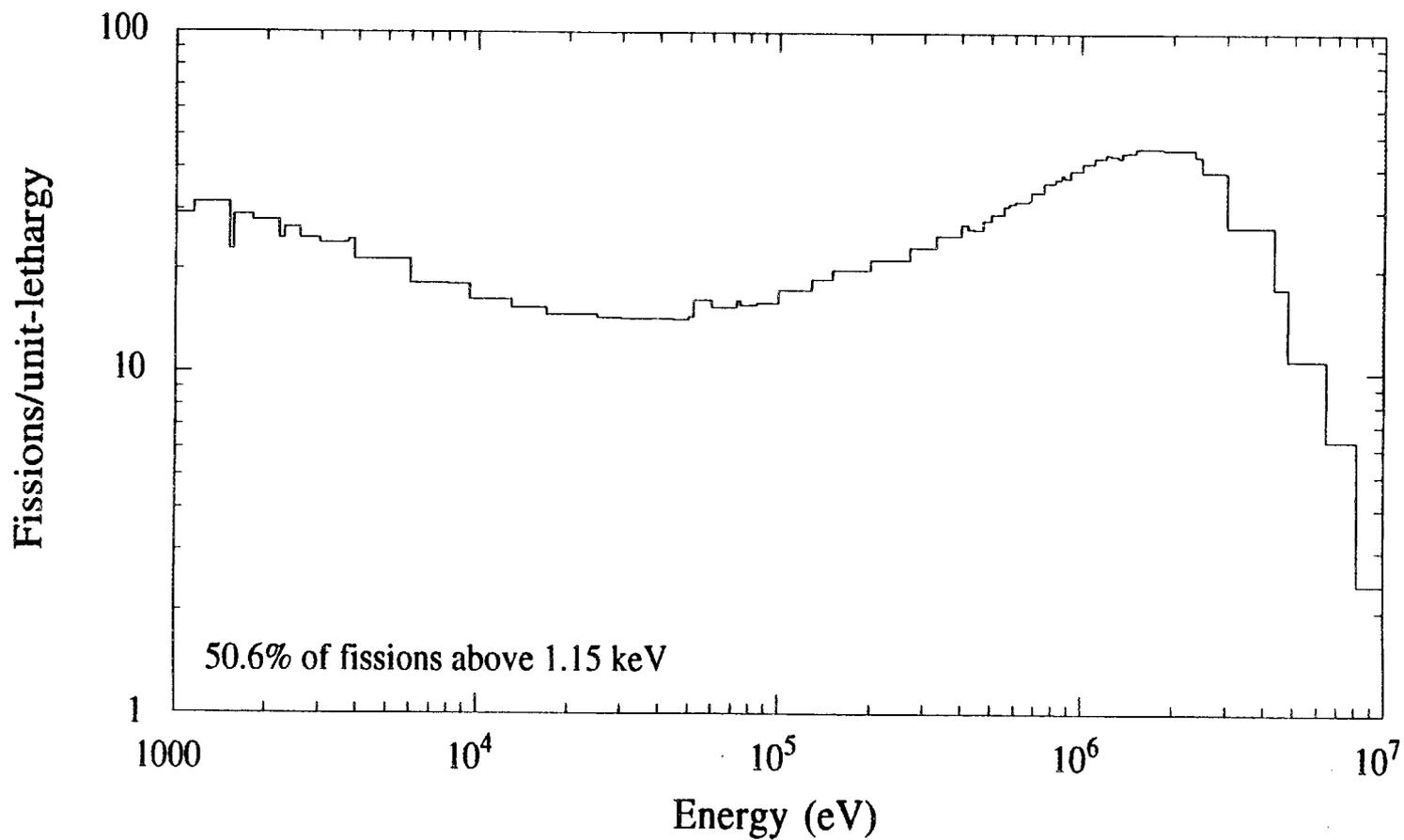


Fig. 12. UH3NI fission rate for 0.001 to 10 MeV.

# UH3NI BENCHMARK

## SCALE-238 Library

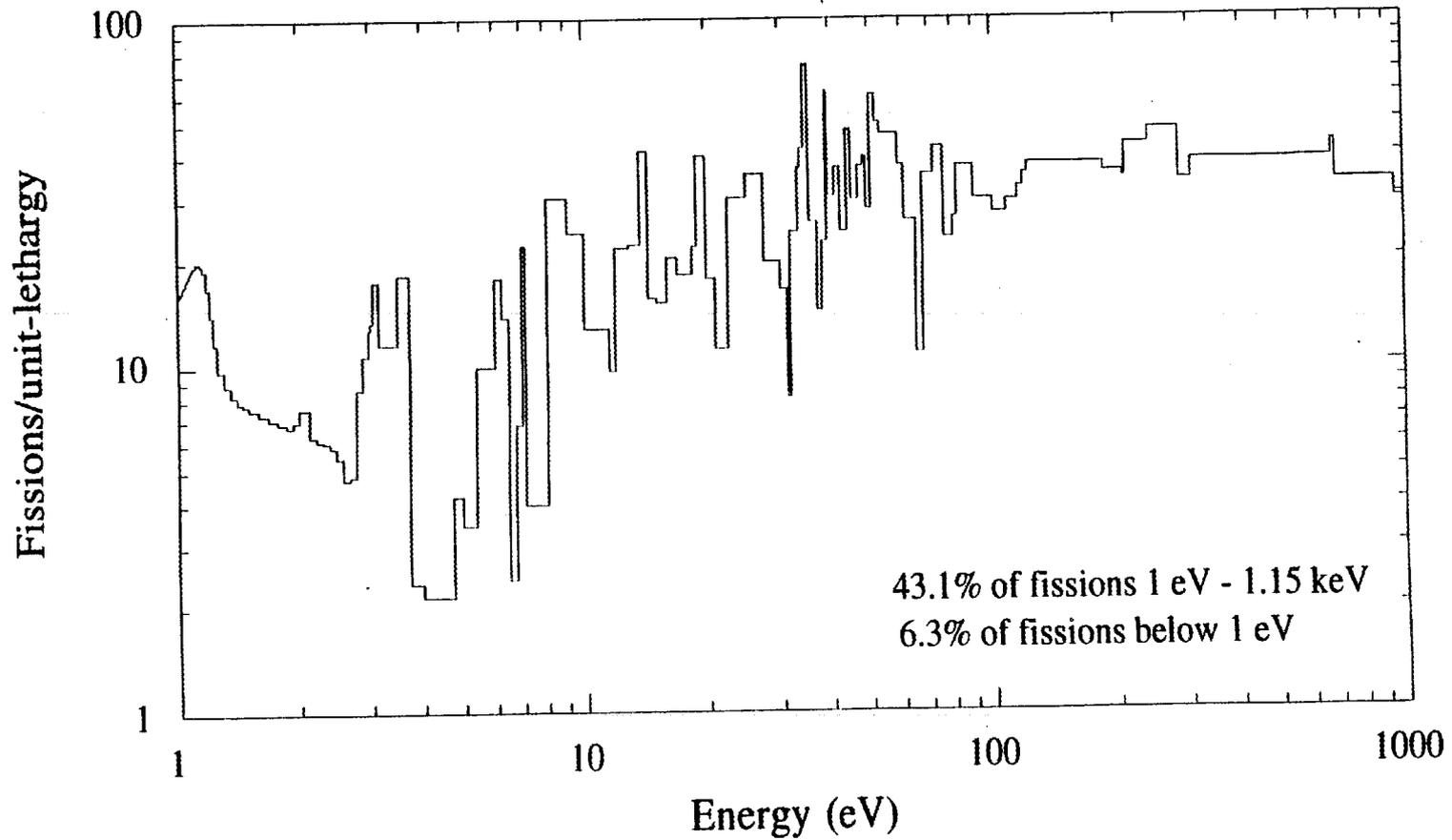


Fig. 13. UH3NI fission rate for 1 to 1000 eV.

# HISS (HUG) BENCHMARK

## SCALE-238 Library

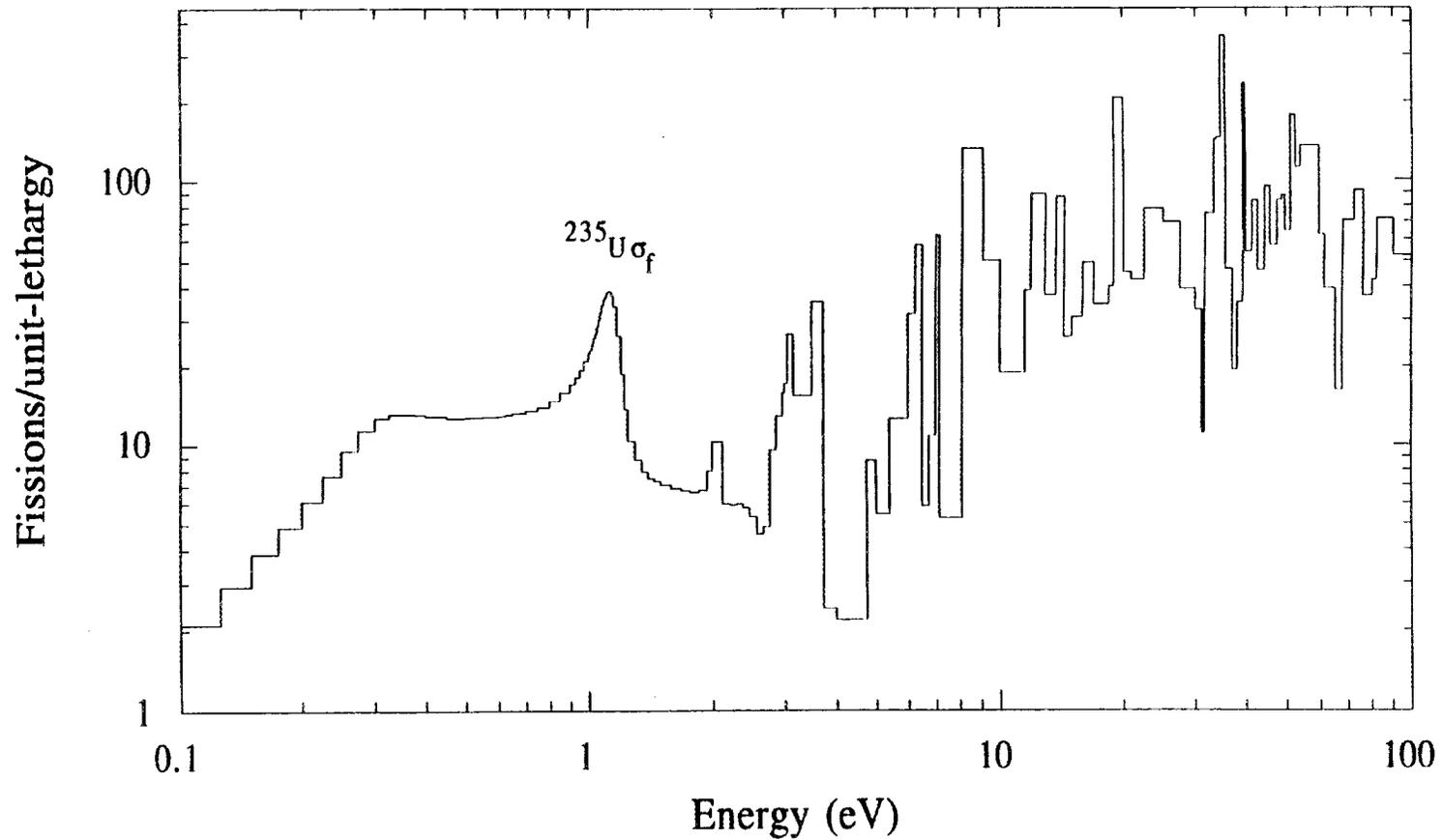


Fig. 14. HISS(HUG) fission rate for 0.1 to 100 eV.

# HISS (HUG) BENCHMARK

## SCALE-238 Library

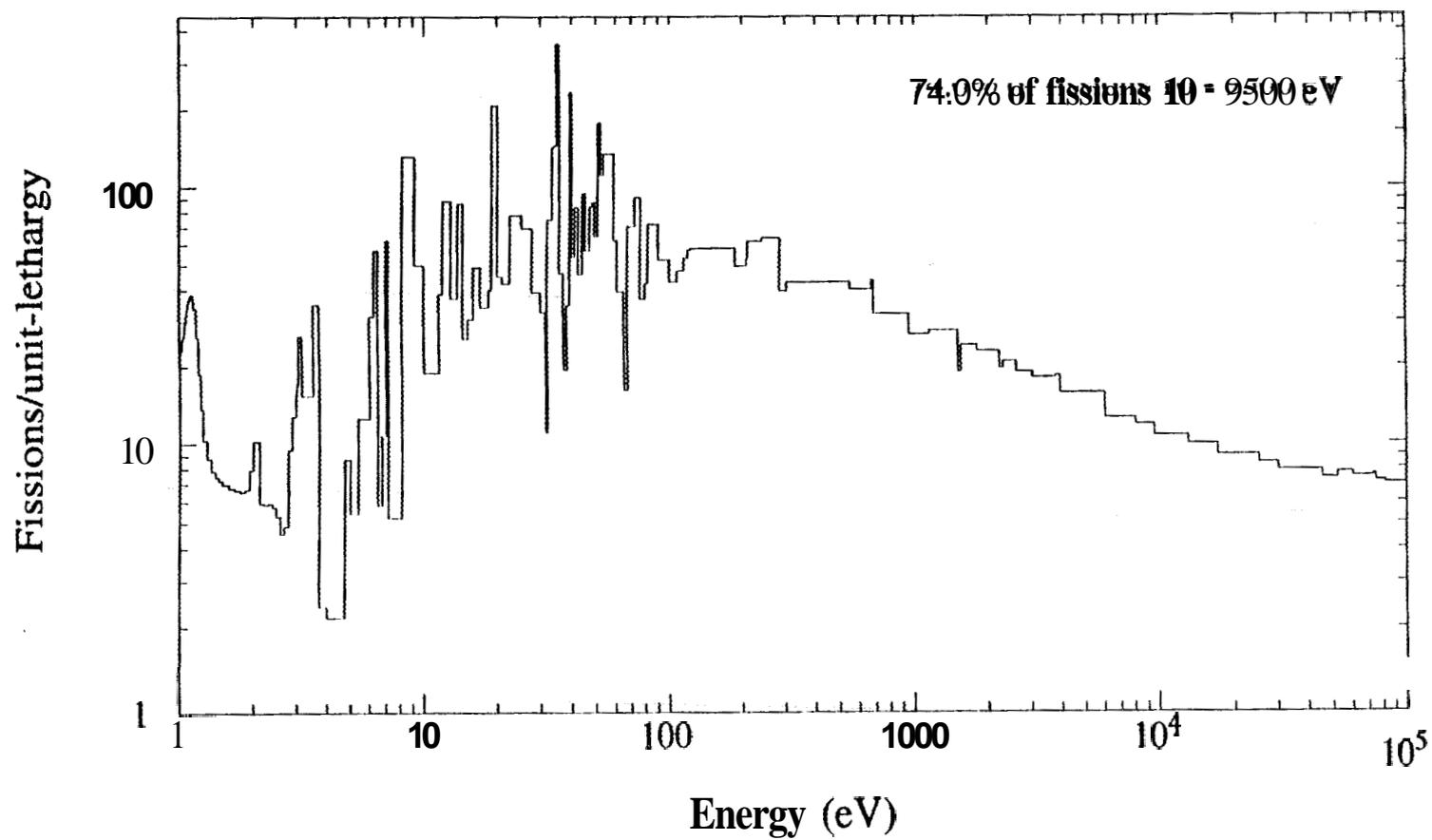


Fig. 15. HISS(HUG) fission rate for 1 to 100,000 eV.

# HISS (HPG) BENCHMARK

## SCALE-238 Library

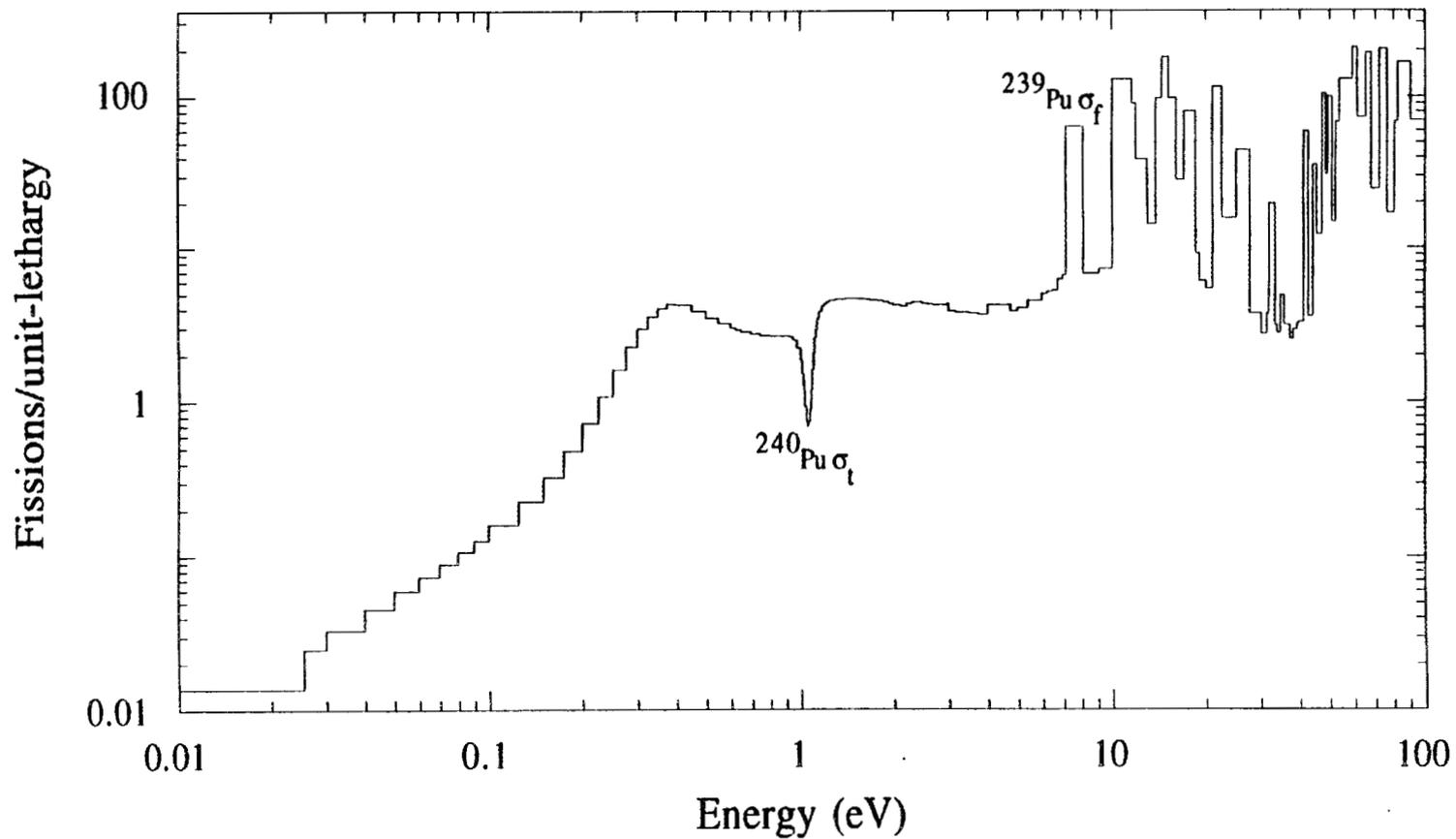


Fig. 16. HISS(HPG) fission rate for 0.1 to 100 eV.

# ZPR-3/12 BENCHMARK

SCALE-238 Library

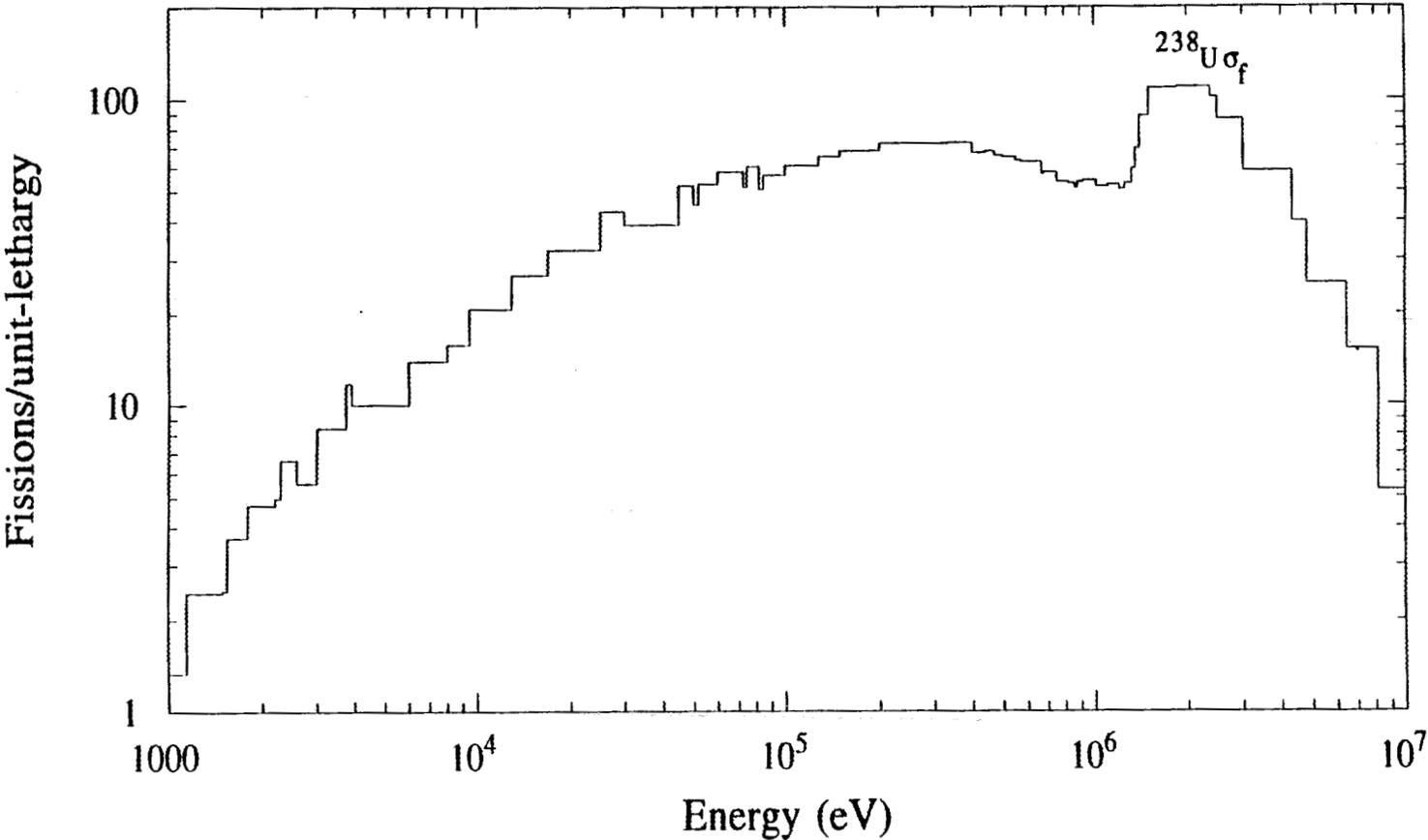


Fig. 17. ZPR-3/12 fission rate for 0.001 to 10 MeV.

# ZPR-6/6A BENCHMARK

SCALE-238 Library

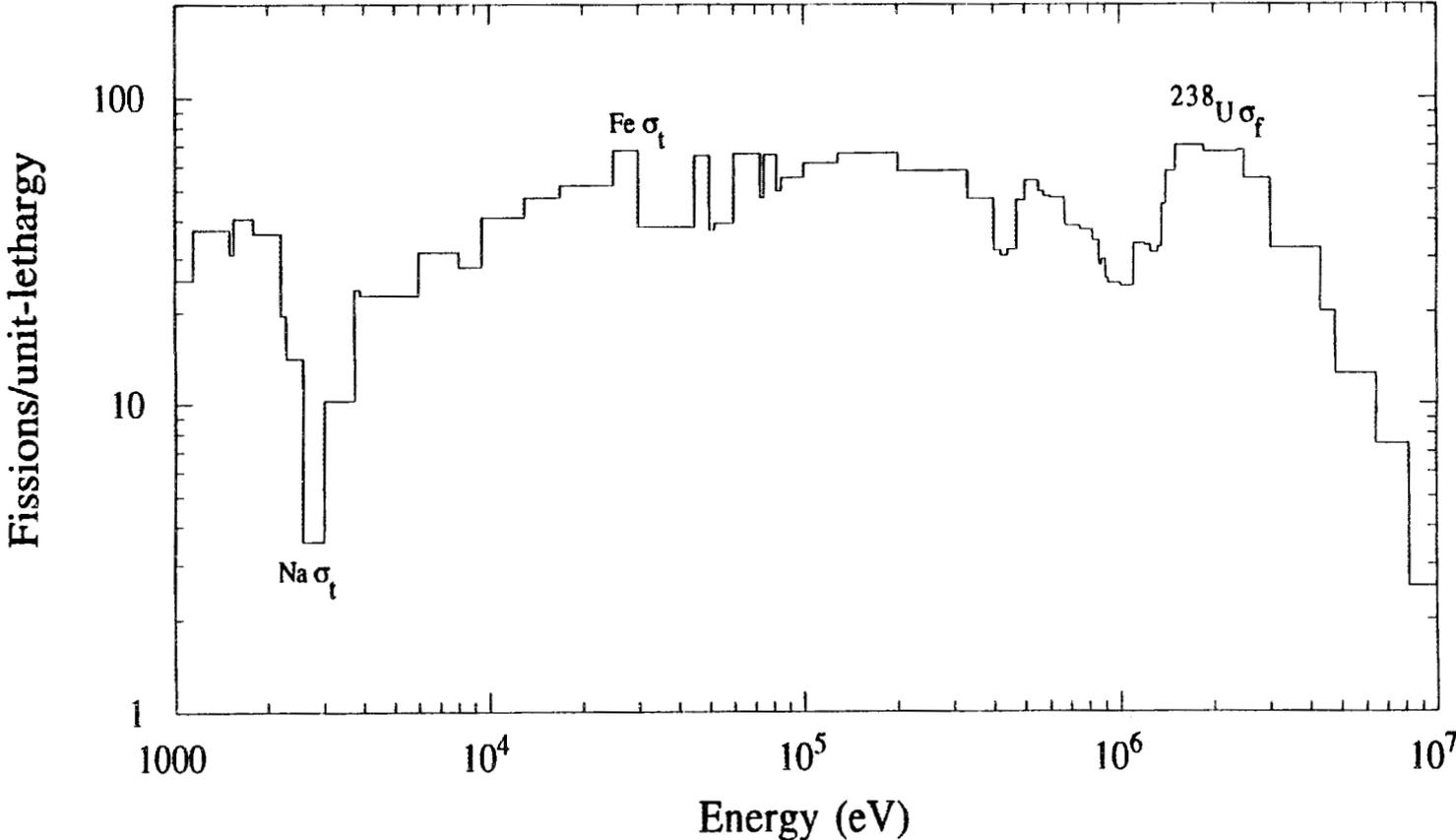


Fig. 18. ZPR-6/6A fission rate for 0.001 to 10 MeV.

benchmark similar to PNL-11 which requires a KENO V.a model. The HI240R benchmark is based on the XSDRNPM spherical approximation to the KENO V.a model. Three interesting features are apparent in the HI240R fission rate plot:  $^{239}\text{Pu}$  fission resonance at 0.3 eV;  $^{240}\text{Pu}$  resonance at 1.057 eV; and the  $^{239}\text{Pu}$  fission resonance at 7.82 eV.

The H2OX1 benchmark is 94% enriched U-metal with  $\text{H}_2\text{O}$  reflector. We find that 75.1% of the fissions are above 9.5 keV, and 24.9% are below. The UH3NI benchmark has uranium hydride fuel with a Ni reflector. We find that 50.6% of the fissions are above 1.15 keV, but 43.1% of the fissions are in the energy range 1 eV to 1.15 keV. Thus, the  $^{235}\text{U}$  fission cross section is relatively important in this energy range (i.e., the  $^{235}\text{U}$  resolved and unresolved resonance range). For the HISS (HUG) benchmark (homogeneous uranium graphite with a large amount of boron), the fissions/unit lethargy peak in the energy range 30 to 300 eV; 74% of the fissions are in the range 10 to 9500 eV. Fissions/unit lethargy fall off below 1 eV because of the high boron content. For the HISS (HPG) benchmark (i.e., homogeneous plutonium graphite with boron), fissions/unit lethargy peak in the energy range 10 to 100 eV. ZPR-3/12 is a 4:1 uranium:graphite system, the blanket consists primarily of depleted uranium. The ZPR-6/6A benchmark is a uranium-oxide-fueled fast critical assembly. The reflector is 33.81 cm of depleted uranium. The ZPR-6/6A fuel is enriched uranium with a  $^{238}\text{U}$  to  $^{235}\text{U}$  ratio of about 5:1. The fuel also contains Na, O, and Fe, with small amounts of Ni, Cr, and Mn. A number of features are evident in the fission rate plot (e.g., the sodium resonance at 2.85 keV, the iron window at 24 keV, and the peak in the fission rate at 2 MeV which is due to  $^{238}\text{U}$  fission).

#### 4.4.7. Calculations with ENDF/B-VI Oxygen

Calculations for ten of the thermal benchmarks using the LAW-238 Library with ENDF/B-VI cross sections for  $^{16}\text{O}$  were also done as part of this study. The results are compared with the previous ENDF/B-V calculated values in Table 10. The results using the ENDF/B-VI oxygen are from 0.13 to 0.45% lower relative to the corresponding ENDF/B-V values. A plot of  $k_{\text{eff}}$  vs leakage for the L-series benchmarks is shown in Fig. 19; the corresponding ENDF/B-V results are shown in Fig. 4. On the basis of results shown in Fig. 19, the trend for  $k_{\text{eff}}$  to increase with leakage is almost eliminated using the ENDF/B-VI oxygen. We note that in Table 10,  $k_{\text{eff}}$  for L-9 is 0.45% higher than for ORNL-1. The reason for this bias is not understood. In any case, it does not seem correct to include the ORNL spheres with the L-series cases in order to show a trend with leakage since each set, by itself, shows almost no trend with leakage. Also, on the basis of the results from this study, the use of ENDF/B-VI cross sections for  $^{16}\text{O}$  in the LAW-238 Library is highly recommended.

#### 4.4.8. Conclusions

A number of conclusions have been reached concerning the results using the LAW-238 Library in this study. These conclusions are summarized in Table 11. The most important of these is for the UH3-NI benchmark. The LAW-238 group structure is not adequate for the NI reflector of the UH3-NI benchmark. Note the JEZEBEL benchmark (see Table 4); also ZPR-6/6A (Table 4) capture, to agree with the HISS(HUG) experimental value of  $^{235}\text{U}$  alpha

Table 10. Thermal benchmarks with ENDF/B-VI  $^{16}\text{O}$ 

Benchmark	All ENDF/B-V	ENDF/B-VI $^{16}\text{O}$	% Diff.
L-7	1.0081	1.0036	-0.45
L-8	1.0088	1.0065	-0.23
L-9	1.0052	1.0032	-0.20
L-10	1.0090	1.0046	-0.44
L-11	1.0036	1.0013	-0.23
ORNL-1	1.0007	0.9987	-0.20
ORNL-10	0.9993	0.9980	-0.13
TRX-1	0.9920	0.9907	-0.13
PNL-3	0.9982	0.9951	-0.31
PNL-6B	1.0102	1.0057	-0.45

# L-Series Benchmarks

## $k_{eff}$ vs. Leakage

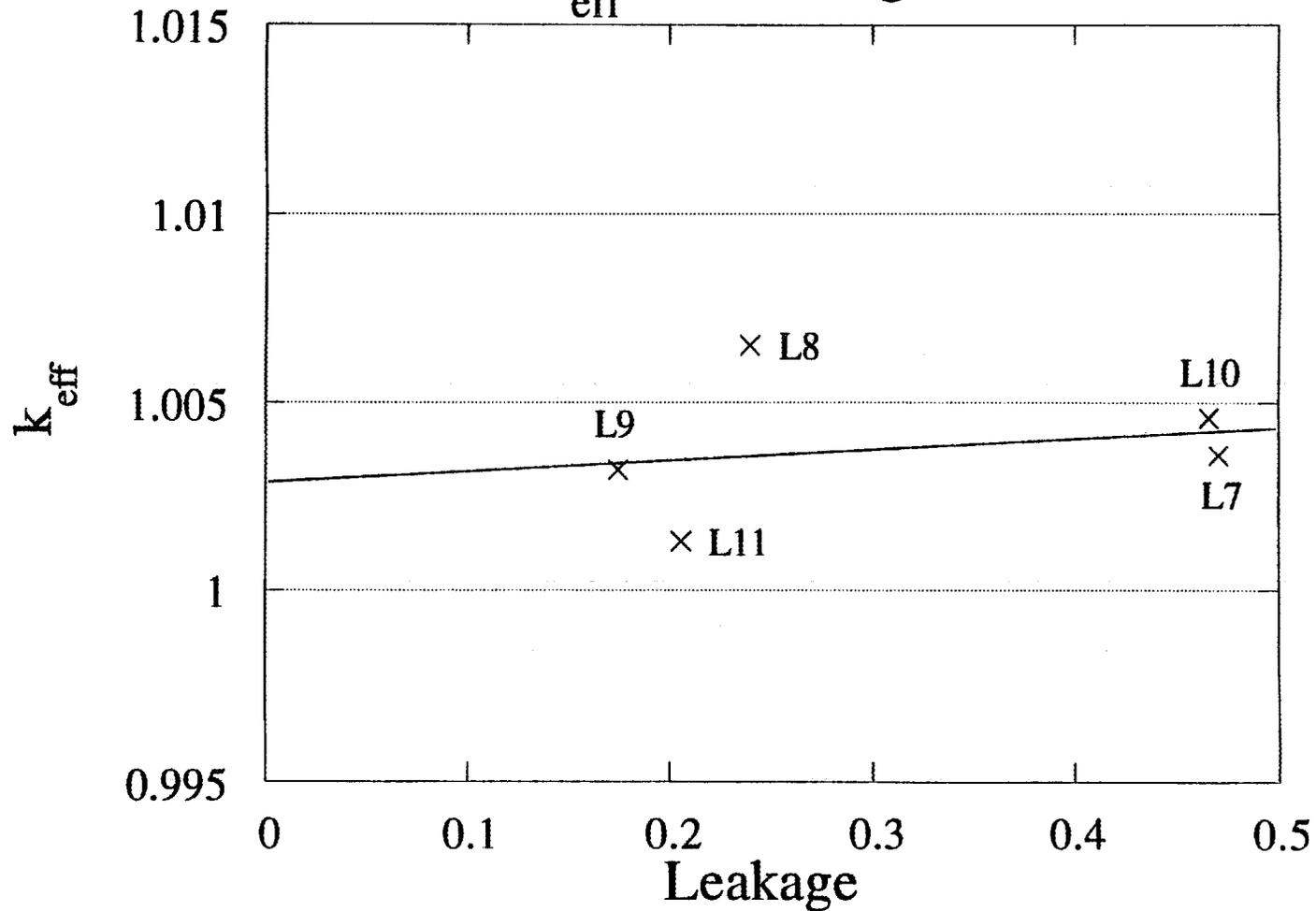


Fig. 19.  $k_{eff}$  vs leakage with ENDF/B-VI  $^{16}\text{O}$ .

Table 11. Benchmarks for which further study is recommended

Benchmark	Comment
JEZEBEL	LAW-238 value low relative to other ENDF/B-V calculations
ZPR-6/6A	LAW-238 value is slightly high relative to other calculations
TRX-1	LAW-238 $k_{\text{eff}}$ is 0.80% low relative to the experimental value. See discussion in the section on uranium lattice benchmark testing for details
UH3-NI	LAW-238 group structure is not adequate for the NI reflector. Also calculate benchmark with ENDF/B-VI cross sections
HISS(HUG)	ENDF/B-V $^{235}\text{U}$ fission cross section should be lower? ENDF/B-VI not as good
HISS(HPG)	LAW-238 value is 0.0056 higher than VITAMIN-E

(capture/fission ratio), would significantly improve the agreement between the HISS(HUG) calculated and experimental parameters.

Data testing has been done for 33 benchmarks, including 28 CSEWG benchmarks. Results obtained for these benchmarks are very close to those obtained by other data testers using different ENDF/B-V-based cross-section libraries. There is considerable improvement in the trend of  $k_{\text{eff}}$  vs leakage obtained with the use of the ENDF/B-VI oxygen evaluation. The use of the ENDF/B-VI cross sections for  $^{16}\text{O}$  in the LAW-238 Library is highly recommended. The LAW-238 Library appears to be acceptable for general use in criticality and reactor physics applications. The library has had minimal testing for shielding applications and should be evaluated by the user for applicability.

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## APPENDIX A

### NEW RESONANCE DATA

ENDF/B-V cross-section evaluations include resolved resonance parameters for higher-order resonances than have historically been included in AMPX and SCALE cross-section libraries. Although Level 0 (s-wave) resonances have always been available for resolved-resonance isotopes, the later ENDF releases have included Level 1 (p-wave), and in some cases Level 2 (d-wave), resonance parameters for a limited number of isotopes. The SCALE LAW-238 cross-section library contains higher-order resonance data not available in earlier SCALE cross-section libraries. The isotopes and the corresponding resonance levels available in the LAW-238 library are given in Table 3 of the text. However, for versions of SCALE prior to and including Version 4.2, the analysis sequences were designed to retrieve only Level 0 data during NITAWL resonance processing. Hence, these versions of SCALE are unable to access the higher-order resonances.

Results presented in this report are based on calculations performed with SCALE 4.2 and therefore include only s-wave ( $L=0$ ) resonances. However, each of these cases has been recomputed using a modified version of SCALE 4.2 in which the analysis sequence modules have been updated to allow Level-1 and -2 data processing for isotopes for which these data are available. (These modifications will be included in future releases of SCALE, along with enhancements to NITAWL to enable more efficient processing of the higher-order resonances.) Table A.1 compares  $k_{\text{eff}}$  values computed using Level-0 data only, as reported in the body of this report, relative to results based on Level-0, -1, and -2 resonance data. These results indicate that use of the higher-order resonance data results in an average decrease in the value of  $k_{\text{eff}}$  by approximately 0.2%. However, the higher-order resonances can have a much larger effect on the  $k_{\text{eff}}$  value for intermediate energy systems where these nuclides are significant contributors. Inclusion of the higher-order resonances can affect a dry iron/<sup>235</sup>U mixture by several percent.

Table A.1. Comparisons of results using L=0 and L=0, 1, and 2 resonance data

Case designation	$k_{\text{eff}}$ (L=0 only)	$k_{\text{eff}}$ (L=0, 1, and 2 data)	% change
JEZEBEL	0.9944	0.9965	0.21
JEZEBEL-PU	0.9986	0.9983	-0.03
JEZEBEL-23	0.9959	0.9939	-0.20
GODIVA	0.9963	0.9980	0.17
FLATTOP-25	1.0046	1.0046	0.00
BIG TEN	1.0103	1.0103	0.00
ZPR-3/11	1.0119	1.0119	0.00
ZPR-3/12	1.0068	1.0071	0.03
ZPR-6/6A	0.9952	0.9981	0.29
ZPR-6/7	1.0022	0.9967	-0.55
ORNL-1	1.0007	0.9987	-0.20
ORNL-2	1.0005	0.9985	-0.20
ORNL-3	0.9975	0.9955	-0.20
ORNL-4	0.9989	0.9969	-0.20
ORNL-10	0.9993	0.9980	-0.13
TRX-1	0.9920	0.9908	-0.12
TRX-2	0.9962	0.9946	-0.16
BAPL-1	0.9986	0.9921	-0.65
BAPL-2	1.0002	0.9938	-0.64
BAPL-3	1.0024	0.9963	-0.61
L-7	1.0081	1.0031	-0.50
L-8	1.0088	1.0064	-0.24
L-9	1.0052	1.0032	-0.20
L-10	1.0090	1.0042	-0.48
L-11	1.0036	1.0012	-0.24
PNL-3	0.9982	0.9951	-0.31
PNL-6B	1.0101	1.0057	-0.44
PNL-11	1.0023 ± 0.0034	1.0000 ± 0.0034	-0.23
H2OX-1	1.0047	1.0006	-0.41
UH3-UR	1.0098	1.0112	0.14
UH3-NI	1.0245	1.0223	-0.21
HISS(HUG)	1.0241	1.0241	0.00
HISS(HPG)	1.0005	1.0005	0.00
<b>Average</b>	<b>1.0034</b>	<b>1.0015</b>	<b>-0.19</b>
<b>Maximum</b>	<b>1.0245</b>	<b>1.0241</b>	
<b>Minimum</b>	<b>0.9920</b>	<b>0.9908</b>	

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96. J. R. Thornton, Duke Engineering & Services, Inc., 2300 S. Tryon St., P.O. Box 1004, Charlotte, NC 28201-1004
97. H. Toffer, Westinghouse Hanford Company, P.O. Box 1970, HO-38, Richland, WA 99352
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