

10/9/92 JPSQ  
12

ornl

ORNL/TM-12230

OAK RIDGE  
NATIONAL  
LABORATORY

MARTIN MARIETTA

Specifications for the Development  
of BUGLE-93: An ENDF/B-VI  
Multigroup Cross Section Library  
for LWR Shielding and Pressure  
Vessel Dosimetry

J. E. White  
R. Q. Wright  
R. W. Roussin  
D. T. Ingersoll

MANAGED BY  
MARTIN MARIETTA ENERGY SYSTEMS, INC.  
FOR THE UNITED STATES  
DEPARTMENT OF ENERGY

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from the Office of Scientific and Technical Information, P.O. Box 62, Oak Ridge, TN 37831; prices available from (615) 576-8401, FTS 626-8401.

Available to the public from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161.

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ORNL/TM--12230

DE93 004028

**Engineering Physics and Mathematics Division**

**SPECIFICATIONS FOR THE DEVELOPMENT OF  
BUGLE-93: AN ENDF/B-VI MULTIGROUP CROSS SECTION  
LIBRARY FOR LWR SHIELDING AND PRESSURE VESSEL  
DOSIMETRY**

**J. E. White  
R. Q. Wright  
R. W. Roussin  
D. T. Ingersoll**

**NOTICE** This document contains information of a preliminary nature.  
It is subject to revision or correction and therefore does not represent a  
final report.

**Date Published: November 1992**

**Prepared for the  
U.S. Nuclear Regulatory Commission  
Washington, DC 20555  
under Interagency Agreement DOE 41 80 41 5B 1**

**NRC FIN B0415**

**Prepared by the  
OAK RIDGE NATIONAL LABORATORY  
Oak Ridge, Tennessee 37831  
managed by  
MARTIN MARIETTA ENERGY SYSTEMS, INC.  
for the  
U.S. DEPARTMENT OF ENERGY  
under contract DE-AC05-84OR21400**

**MASTER**

**DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED**

## Contents

<b>ABSTRACT</b> . . . . .	1
<b>INTRODUCTION</b> . . . . .	1
<b>FINE-GROUP SPECIFICATIONS</b> . . . . .	2
A. Name . . . . .	2
B. Materials, Temperatures and Background Cross Sections . . . . .	2
C. Energy Group Structure . . . . .	9
D. Weighting Function . . . . .	14
E. Legendre Order of Scattering . . . . .	14
F. Convergence Parameters . . . . .	14
G. Processing Codes . . . . .	15
<b>BROAD-GROUP SPECIFICATIONS</b> . . . . .	17
A. Name . . . . .	17
B. Materials and Energy Group Structure . . . . .	17
C. Weighting Spectra . . . . .	19
D. Output Format . . . . .	21
E. Response Functions and Source Spectra . . . . .	21
<b>DATA TESTING PROGRAM</b> . . . . .	22
A. Processing Methods . . . . .	22
B. Thermal and Fast Reactor Data Testing Benchmarks . . . . .	23
C. Shielding Benchmarks . . . . .	24
<b>ACKNOWLEDGEMENTS</b> . . . . .	26
<b>REFERENCES</b> . . . . .	27

## ABSTRACT

Specifications have been developed for a new multigroup cross section library based on ENDF/B-VI data for light water reactor shielding and reactor pressure vessel dosimetry applications. The resulting broad-group library and an intermediate fine-group library are defined by the specifications provided in this report. Processing ENDF/B-VI into multigroup format for use in radiation transport codes will provide radiation shielding analysts with the most currently available nuclear data. It is expected that the general nature of the specifications will be useful in other applications such as reactor physics.

## INTRODUCTION

Ten years ago the ANS 6.1 Working Group issued a standard describing the methodology for producing multigroup cross sections for nuclear power plant shielding analyses. This standard, ANSI/ANS 6.1.2, explicitly describes the fine-group VITAMIN-C cross-section library and the derived broad-group BUGLE-80 library as satisfying the preferred processing methodology. These libraries, derived from version 4 of the Evaluated Nuclear Data File (ENDF/B-IV), are now in need of updating with more modern and accurate nuclear data.

The United States Cross-Section Evaluation Working Group (CSEWG) has released a new Evaluated Nuclear Data Library (ENDF/B-VI) that contains significant improvements, particularly for structural materials (Cr, Fe, Mn, Ni) and better representations of collision processes for all materials. Processing ENDF/B-VI into multigroup format for use in radiation transport codes will provide analysts with the most currently available nuclear data and should help to reduce design biases and uncertainties.

Previous multigroup cross section development efforts<sup>1-7</sup> have demonstrated that the generation of fine-group, pseudo problem-independent data using the VITAMIN concept is a very effective approach for a wide variety of applications (e.g. fusion reactor neutronics, LMFBR core physics analysis, radiation effects of nuclear weapons, and light water reactor shielding and dosimetry). The approach used is to generate a multigroup library with a large number of energy groups over a range of temperatures and resonance self-shielding conditions. The resulting library is called a "pseudo problem-independent," fine-group, cross-section library because it has been prepared with enough detail in energy, temperatures, and resonance self-shielding so as to be applicable to a wide range of specific problems. The specific problems can be solved with a "problem-dependent" library derived from the fine-group library by applying temperature and resonance self-shielding information and collapsing to a smaller number of groups. The result is called a broad-group problem-dependent library (e.g., BUGLE).

Past VITAMIN libraries were created using a combination of AMPX<sup>8</sup> and MINX<sup>9</sup> for reference nuclear data based on ENDF/B-IV and later ENDF/B-V. Format changes in ENDF-6, which allow improved representations of nuclear data, require corresponding changes to the processing codes. For this project, advances in cross section processing methods have led to the selection of NJOY<sup>10-15</sup> as the ENDF/B-VI processing code for neutron interaction, gamma-ray production, and gamma-ray interaction data in ENDF-6 format.<sup>16</sup>

The calculational approach for developing this new ENDF/B-VI library will be consistent with the ANS 6.1.2 standard and is based on the successful development and application of the VITAMIN-C and VITAMIN-E pseudo problem-independent, fine-group cross-section libraries. The primary cross-section processing will be performed by the modular NJOY91 system with RECONR, BROADR, THERMR, UNRESR, GROUPR, and GAMINR playing major roles. Selected modules from the AMPX77 system<sup>17</sup> will be used to perform the manipulations necessary to make problem-dependent working libraries that can be used in shielding applications using ANISN, DORT, TORT, MORSE, and other multigroup radiation transport codes. The SMILER<sup>18</sup> module in the AMPX77 system will be used to translate the intermediate NJOY91 file named GENDF into the AMPX master library format.

## FINE-GROUP SPECIFICATIONS

### A. Name.

The fine-group pseudo problem-independent library in AMPX master library format will be called VITAMIN-B6.

### B. Materials, Temperatures and Background Cross Sections.

The initial set of materials to be processed for VITAMIN-B6 are listed in Table 1, which also indicates the ENDF/B-VI MAT numbers for each particular isotope or element, and the ENDF/B-VI tape number. When significant changes to an evaluation are available, the latest version will be used for this project. The BUGLE-80 nuclides,<sup>19</sup> identified by 'X' in Table 1, will be the minimum set of nuclides in the new broad-group library and will be processed with the highest priority. The other nuclides in Table 1 will be processed as time and resources allow. Materials in the BUGLE-80 library that are not available in ENDF/B-VI will be carried over to make the final broad-group library complete. Since many other data sets are available in ENDF/B-VI, this list will be expanded as required by data testing activities or by programmatic objectives.

Table 1. ENDF/B-VI materials expected to be processed for the fine-group library.

Z	Material	MAT	ENDF tape	BUGLE-80 materials
1	H-1 ( $H_2O$ )	125/1	120/118	X
	H-1 ( $CH_2$ )	125/37	120/118	
	H-2 ( $D_2O$ )	128/11	116/118 <sup>a</sup>	
	H-3	131	101	X
2	He-3	225	120	
	He-4	228	101	X
3	Li-6	325	120	X
	Li-7	328	100	X
4	Be-9	425	100	X
	Be-9 (Thermal)	425/26	100/118	
5	B-10	525	120	X
	B-11	528	100	X

Table 1. (contd.)

Z	Material	MAT	ENDF tape	BUGLE-80 materials
6	C	600	120	X
	C (Graphite)	600/31	120/118 <sup>a</sup>	
7	N-14	725	116	X
	N-15	728	116	
8	O-16	825	116	X
	O-17	828	101	
9	F-19	925	115	X
11	Na-23	1125	120	X
12	Mg	1200	101	X
13	Al-27	1325	101	X
14	Si	1314	116	X
15	P-31	1525	101	X
16	S	1600	101	X
	S-32	1625	101	
17	Cl	1700	101	
19	K	1900	101	X
20	Ca	2000	101	X
22	Ti	2200	102	X
23	V	2300	103	X
24	Cr-50	2425	122	X
	Cr-52	2431	122	X
	Cr-53	2434	122	X
	Cr-54	2437	122	X
25	Mn-55	2525	114	X
26	Fe-54	2625	123	X
	Fe-56	2631	123	X
	Fe-57	2634	123	X
	Fe-58	2637	123	X
27	Co-59	2725	103	X
28	Ni-58	2825	124	X
	Ni-60	2831	124	X
	Ni-61	2834	124	X
	Ni-62	2837	124	X
	Ni-64	2843	124	X
29	Cu-63	2925	114	X
	Cu-65	2931	114	X
31	Ga	3100	102	
39	Y-89	3925	103	
40	Zr	4000	120	X
41	Nb-93	4125	120	X
42	Mo	4200	104	X

Table 1. (contd.)

Z	Material	MAT	ENDF tape	BUGLE-80 materials
47	Ag-107	4725	104	X
	Ag-109	4731	104	X
48	Cd	4800	104	X
49	In	4900	116	
63	Eu-151	6325	103	X
	Eu-152	6328	103	X
	Eu-153	6331	103	X
	Eu-154	6334	103	X
	Eu-155	6337	120	
	Hf	7200	106	
72	Hf-174	7225	106	
	Hf-176	7231	106	
	Hf-177	7234	106	
	Hf-178	7237	106	
	Hf-179	7240	106	
	Hf-180	7243	120	
	Ta-181	7328	106	X
73	Ta-182	7331	106	
74	W	7400	120	
	W-182	7431	107	X
	W-183	7434	107	X
	W-184	7437	107	X
	W-186	7443	107	X
	Re-185	7525	115	
75	Re-187	7531	115	
	Au-197	7925	120	
82	Pb-206	8231	115	X
	Pb-207	8234	120	X
	Pb-208	8237	115	X
	Bi-209	8325	108	
90	Th-230	9034	110	
	Th-232	9040	109	X
91	Pa-231	9131	109	
	Pa-233	9137	110	
92	U-232	9219	109	
	U-233	9222	109	X
	U-234	9225	109	X
	U-235	9228	121	X
	U-236	9231	108	X
	U-237	9234	109	
	U-238	9237	121	X

Table 1. (contd.)

Z	Material	MAT	ENDF tape	BUGLE-80 materials
93	Np-237	9346	121	
	Np-238	9349	109	
	Np-239	9352	108	
94	Pu-236	9428	110	
	Pu-237	9431	110	
	Pu-238	9434	109	X
	Pu-239	9437	117	X
	Pu-240	9440	121	X
	Pu-241	9443	121	X
	Pu-242	9446	109	X
	Pu-243	9449	110	
	Pu-244	9452	110	
95	Am-241	9543	108	X
	Am-242	9546	121	
	Am-242m	9547	121	
96	Am-243	9549	108	
	Cm-241	9628	110	
	Cm-242	9631	109	
	Cm-243	9634	110	
	Cm-244	9637	110	
	Cm-245	9640	109	
	Cm-246	9643	110	
	Cm-247	9646	110	
	Cm-248	9649	110	

\*It is anticipated that improved thermal scattering law data from ORNL will be used.

All materials will be processed at temperatures of 300, 600, 1000, and 2100 K. The range of background cross sections is summarized in Table 2. Based on previous experience, we have found that about 6 to 8 values of  $\sigma_0$  are adequate for any given material. Generally, multigroup libraries include the following values: 1, 10, 100,  $1.0e+3$ ,  $1.0e+4$ , and  $1.0e+10$ . These values are probably adequate for most materials. Some multigroup libraries do not include Bondarenko factors for the light materials (e.g., Z less than 12), because infinitely dilute cross sections are generally adequate for these materials. For VITAMIN-B6, we will use infinitely dilute cross sections for Z less than 7 with the exception of  $^{11}B$ . For most of the remaining materials we will use 7 values of  $\sigma_0$ . These include the 6 values listed above as well as  $1.0e+5$ . The reason for including  $1.0e+5$  is to improve slightly the accuracy of the cross section interpolation in the range  $1.0e+4$  to  $1.0e+10$ . For a few materials, values are included for  $\sigma_0 = 30$  and/or 300. Again the rationale is to improve slightly the accuracy of the cross section interpolation in the range 1 to 100 and/or 100 to 1000 for these materials. These values are based on experience obtained in the utilization of VITAMIN-E, which uses the Bondarenko (f-factor) method for handling resonance self-shielding and temperature effects. The thermal

scattering law data for graphite, polyethylene, beryllium metal, heavy water, and water will be processed at all temperatures available on the ENDF tape.

Table 2. Background cross section values at which Bondarenko factors are tabulated in the VITAMIN-B6 fine group library.

Material	Background cross sections (barns)											Temp*	Legendre order
	10+10 <sup>a</sup>	10+6	10+5	10+4	1000	300	100	50	10	1			
H-1	X										4	7	
H-2	X										4	7	
H-3	X										4	7	
He-3	X										4	7	
He-4	X										4	7	
Li-6	X										4	7	
Li-7	X										4	7	
Be-9	X										4	7	
B-10	X										4	7	
B-11	X			X		X		X	X		4	7	
C	X										4	7	
N-14	X				X		X		X	X	4	7	
N-15	X				X		X		X	X	4	7	
O-16	X				X		X		X	X	4	7	
O-17	X				X		X		X	X	4	7	
F-19	X				X		X		X	X	4	7	
Na-23	X				X	X	X	X	X	X	4	7	
Mg	X		X	X	X		X		X	X	4	7	
Al-27	X		X	X	X		X	X	X	X	4	7	
Si	X		X	X	X		X		X	X	4	7	
P-31	X		X	X	X		X		X	X	4	7	
S	X		X	X	X		X		X	X	4	7	
S-32	X		X	X	X		X		X	X	4	7	
Cl	X		X	X	X		X		X	X	4	7	
K	X		X	X	X		X		X	X	4	7	
Ca	X		X	X	X		X		X	X	4	7	
Ti	X		X	X	X		X		X	X	4	7	
V	X		X	X	X		X		X	X	4	7	
Cr-50	X		X	X	X		X		X	X	4	7	
Cr-52	X		X	X	X		X		X	X	4	7	

Table 2. (contd.)

Material	Background cross sections (barns)											
	10+10 <sup>a</sup>	10+6	10+5	10+4	1000	300	100	50	10	1	Temps <sup>b</sup>	Legendre order
Cr-53	X		X	X	X		X		X	X	4	7
Cr-54	X		X	X	X		X		X	X	4	7
Mn-55	X		X	X	X		X		X	X	4	7
Fe-54	X		X	X	X		X		X	X	4	7
Fe-56	X		X	X	X		X	X	X	X	4	7
Fe-57	X		X	X	X		X		X	X	4	7
Fe-58	X		X	X	X		X		X	X	4	7
Co-59	X		X	X	X		X		X	X	4	7
Ni-58	X		X	X	X		X	X	X	X	4	7
Ni-60	X		X	X	X		X	X	X	X	4	7
Ni-61	X		X	X	X		X		X	X	4	7
Ni-62	X		X	X	X		X		X	X	4	7
Ni-64	X		X	X	X		X		X	X	4	7
Cu-63	X		X	X	X		X		X	X	4	7
Cu-65	X		X	X	X		X		X	X	4	7
Ga	X		X	X	X		X		X	X	4	7
Y-89	X		X	X	X		X		X	X	4	7
Zr	X		X	X	X		X		X	X	4	7
Nb-93	X		X	X	X		X		X	X	4	7
Mo	X		X	X	X		X				4	7
Ag-107	X		X	X	X		X		X	X	4	7
Ag-109	X		X	X	X		X		X	X	4	7
Cd	X		X	X	X		X		X	X	4	7
In	X		X	X	X		X		X	X	4	7
Eu-151	X		X	X	X		X	X			4	7
Eu-152	X	X	X	X	X		X				4	7
Eu-153	X		X	X	X		X	X			4	7
Eu-154	X	X	X	X	X		X				4	7
Eu-155	X	X	X	X	X		X				4	7
Hf	X		X	X	X		X		X	X	4	7
Hf-174	X		X	X	X		X		X	X	4	7
Hf-176	X		X	X	X		X		X	X	4	7
Hf-177	X		X	X	X		X	X			4	7

Table 2. (contd.)

Material	Background cross sections (barns)												Legendre order
	$10+10^*$	$10+6$	$10+5$	$10+4$	1000	300	100	50	10	1	Temp <sup>b</sup>		
Hf-178	X		X	X	X		X		X	X	4		7
Hf-179	X		X	X	X		X	X			4		7
Hf-180	X		X	X	X		X		X	X	4		7
Ta-181	X		X	X	X		X	X			4		7
Ta-182	X		X	X	X		X	X			4		7
W	X		X	X	X		X		X	X	4		7
W-182	X		X	X	X		X		X	X	4		7
W-183	X		X	X	X		X	X			4		7
W-184	X		X	X	X		X		X	X	4		7
W-186	X		X	X	X		X		X	X	4		7
Re-185	X	X	X	X	X		X				4		7
Re-187	X	X	X	X	X		X				4		7
Au-197	X		X	X	X		X		X	X	4		7
Pb-206	X		X	X	X		X		X	X	4		7
Pb-207	X		X	X	X		X		X	X	4		7
Pb-208	X		X	X	X		X		X	X	4		7
Bi-209	X		X	X	X		X		X	X	4		7
Th-230	X	X	X	X	X		X				4		7
Th-232	X			X	X	X	X	X	X	X	4		7
Pa-231	X		X	X	X		X	X			4		7
Pa-233	X		X	X	X		X	X			4		7
U-232	X		X	X	X		X		X	X	4		7
U-233	X		X	X	X		X	X			4		7
U-234	X		X	X	X		X		X	X	4		7
U-235	X	X	X	X	X		X	X			4		7
U-236	X		X	X	X		X		X	X	4		7
U-237	X		X	X	X		X	X			4		7
U-238	X			X	X	X	X	X	X	X	4		7
Np-237	X		X	X	X		X		X	X	4		7
Np-238	X		X	X	X		X	X			4		7
Np-239	X		X	X	X		X	X			4		7
Pu-236	X		X	X	X		X		X	X	4		7
Pu-237	X		X	X	X		X	X			4		7

Table 2. (contd.)

Material	Background cross sections (barns)											
	$10+10^a$	$10+6$	$10+5$	$10+4$	1000	300	100	50	10	1	Temps <sup>b</sup>	Legendre order
Pu-238	X		X	X	X		X		X	X	4	7
Pu-239	X		X	X	X		X	X			4	7
Pu-240	X		X	X	X		X		X	X	4	7
Pu-241	X		X	X	X		X	X			4	7
Pu-242	X		X	X	X		X		X	X	4	7
Pu-243	X		X	X	X		X	X			4	7
Pu-244	X		X	X	X		X		X	X	4	7
Am-241	X		X	X	X		X	X			4	7
Am-242	X		X	X	X		X	X			4	7
Am-242m	X		X	X	X		X	X			4	7
Am-243	X		X	X	X		X	X			4	7
Cm-241	X		X	X	X		X	X			4	7
Cm-242	X		X	X	X		X		X	X	4	7
Cm-243	X		X	X	X		X	X			4	7
Cm-244	X		X	X	X		X		X	X	4	7
Cm-245	X		X	X	X		X	X			4	7
Cm-246	X		X	X	X		X		X	X	4	7
Cm-247	X		X	X	X		X	X			4	7
Cm-248	X		X	X	X		X		X	X	4	7

<sup>a</sup>Read as  $i \times 10^{10}$ , etc.<sup>b</sup>4 temperatures implies Bondarenko factors at 300, 600, 1000, and 2100 K.

### C. Energy Group Structure.

Feedback from users of previous VITAMIN libraries, which were developed for "fast" neutron applications, indicated that advantages could be gained by refining the neutron group structure in the thermal energy range. With regard to thermal data, experience with a 27n/18g broad-group library from the SCALE system has been very favorable for many years. This cross-section library is based on ENDF/B-IV (1974) data and was developed primarily for criticality safety and shielding analyses for out-of-core applications. The group structure for this library is especially fine in the thermal range, but lacks adequate resolution in the high energy range ( $E > 0.1$  MeV). The VITAMIN-B6 neutron energy group structure is a compromise and improvement over the 174n (group structure used for VITAMIN-E) and the 27n group structures. The 36 groups in the VITAMIN-B6 thermal energy range are shown in Table 3, which also labels corresponding boundaries from the VITAMIN-E and 27-group libraries. The earlier VITAMIN libraries concentrated on detailed resolution in the keV and MeV energy range. The boundaries for VITAMIN-C and VITAMIN-E were selected to resolve

resonance minima that are important for shielding calculations overlaid upon the 100 group equal lethargy structure used for many applications in reactor physics. These complementary characteristics suggested that we combine the features of the VITAMIN and 27 group neutron energy grid to maximize our options for creating the best problem-independent energy grid for a variety of reactor designs including graphite moderated systems. In this manner, problem-dependent libraries can be derived without having to repeat the multigroup averaging for a different group structure.

Table 3. VITAMIN-B6 thermal energy range.

Group	Energy (eV)	$\Delta u^a$	Group	Energy (eV)	$\Delta u^a$
164	5.0435*	0.25	182	0.36680	0.121
165	3.9279*	0.25	183	0.3250#	0.167
166	3.0590*	0.250	184	0.2750	0.201
167	2.3824*	0.250	185	0.2250#	0.210
168	1.8554*	0.250	186	0.1840	0.204
169	1.4450*	0.106	187	0.1500	0.182
170	1.3000#	0.144	188	0.1250	0.223
171	1.1253*	0.041	189	0.1000*#	0.357
172	1.0800	0.038	190	0.0700	0.366
173	1.0400	0.039	191	0.0500#	0.223
174	1.0000#	0.132	192	0.0400	0.288
175	0.87643*	0.091	193	0.0300#	0.357
176	0.8000#	0.159	194	0.0210	0.370
177	0.68256*	0.088	195	0.0145	0.372
178	0.62506	0.162	196	0.0100#	0.693
179	0.53158*	0.061	197	0.0050	0.916
180	0.5000	0.188	198	0.0020	1.386
181	0.41399*	0.121	199	0.0005	3.912
					0.00001*#

<sup>a</sup> $\Delta u$  is the group lethargy width.

\*VITAMIN-E boundary.

#27-group SCALE boundary.

The VITAMIN-B6 full neutron energy group structure is given in Table 4. The 199 group boundaries are based on the 175 groups in VITAMIN-J (a European library based on the VITAMIN-C and VITAMIN-E structures) and the 27 groups used in the SCALE shielding library, with deference given to the VITAMIN-J boundaries at higher energies when the energy values are slightly different. The thermal energy range will have 5.043 eV as the uppermost boundary.

The photon energy group structure is given in Table 5. It is based on a combination of the 42 gamma-ray groups in VITAMIN-J and the 18 groups in the SCALE shielding library. The top energy group extends to 30 MeV, which allows proper representation of high energy gamma rays

Table 4. Neutron group energy boundaries for VITAMIN-B6.

Fine group	Upper energy (eV)	Upper lethargy	Fine group	Upper energy (eV)	Upper lethargy
1	1.9640E+07	-6.7498E-01	42	2.5924E+06	1.3500E+00
2	1.7332E+07	-5.4997E-01	43	2.4660E+06	1.4000E+00
3	1.6905E+07	-5.2502E-01	44	2.3852E+06	1.4333E+00
4	1.6487E+07	-4.9999E-01	45	2.3653E+06	1.4417E+00
5	1.5683E+07	-4.4999E-01	46	2.3457E+06	1.4500E+00
6	1.4918E+07	-3.9998E-01	47	2.3069E+06	1.4667E+00
7	1.4550E+07	-3.7501E-01	48	2.2313E+06	1.5000E+00
8	1.4191E+07	-3.5002E-01	49	2.1225E+06	1.5500E+00
9	1.3840E+07	-3.2498E-01	50	2.0190E+06	1.6000E+00
10	1.3499E+07	-3.0003E-01	51	1.9205E+06	1.6500E+00
11	1.2840E+07	-2.4998E-01	52	1.8268E+06	1.7000E+00
12	1.2523E+07	-2.2498E-01	53	1.7377E+06	1.7500E+00
13	1.2214E+07	-2.0000E-01	54	1.6530E+06	1.8000E+00
14	1.1618E+07	-1.4997E-01	55	1.5724E+06	1.8500E+00
15	1.1052E+07	-1.0003E-01	56	1.4957E+06	1.9000E+00
16	1.0513E+07	-5.0028E-02	57	1.4227E+06	1.9500E+00
17	1.0000E+07	0.0000E+00	58	1.3534E+06	2.0000E+00
18	9.5123E+06	4.9999E-02	59	1.2874E+06	2.0500E+00
19	9.0484E+06	9.9997E-02	60	1.2246E+06	2.1000E+00
20	8.6071E+06	1.5000E-01	61	1.1648E+06	2.1500E+00
21	8.1873E+06	2.0000E-01	62	1.1080E+06	2.2000E+00
22	7.7880E+06	2.5000E-01	63	1.0026E+06	2.3000E+00
23	7.4082E+06	3.0000E-01	64	9.6164E+05	2.3417E+00
24	7.0469E+06	3.5000E-01	65	9.0718E+05	2.4000E+00
25	6.7032E+06	4.0000E-01	66	8.6294E+05	2.4500E+00
26	6.5924E+06	4.1667E-01	67	8.2085E+05	2.5000E+00
27	6.3763E+06	4.5000E-01	68	7.8082E+05	2.5500E+00
28	6.0653E+06	5.0000E-01	69	7.4274E+05	2.6000E+00
29	5.7695E+06	5.5000E-01	70	7.0651E+05	2.6500E+00
30	5.4881E+06	6.0000E-01	71	6.7206E+05	2.7000E+00
31	5.2205E+06	6.4999E-01	72	6.3928E+05	2.7500E+00
32	4.9659E+06	6.9999E-01	73	6.0810E+05	2.8000E+00
33	4.7237E+06	7.4999E-01	74	5.7844E+05	2.8500E+00
34	4.4933E+06	8.0000E-01	75	5.5023E+05	2.9000E+00
35	4.0657E+06	9.0000E-01	76	5.2340E+05	2.9500E+00
36	3.6788E+06	1.0000E+00	77	4.9787E+05	3.0000E+00
37	3.3287E+06	1.1000E+00	78	4.5049E+05	3.1000E+00
38	3.1664E+06	1.1500E+00	79	4.0762E+05	3.2000E+00
39	3.0119E+06	1.2000E+00	80	3.8774E+05	3.2500E+00
40	2.8651E+06	1.2500E+00	81	3.6883E+05	3.3000E+00
41	2.7253E+06	1.3000E+00	82	3.3373E+05	3.4000E+00

Table 4. (contd.)

Fine group	Upper energy (eV)	Upper lethargy	Fine group	Upper energy (eV)	Upper lethargy
83	3.0197E+05	3.5000E+00	126	1.5034E+04	6.5000E+00
84	2.9849E+05	3.5116E+00	127	1.1709E+04	6.7500E+00
85	2.9721E+05	3.5159E+00	128	1.0595E+04	6.8500E+00
86	2.9452E+05	3.5250E+00	129	9.1188E+03	7.0000E+00
87	2.8725E+05	3.5500E+00	130	7.1017E+03	7.2500E+00
88	2.7324E+05	3.6000E+00	131	5.5308E+03	7.5000E+00
89	2.4724E+05	3.7000E+00	132	4.3074E+03	7.7500E+00
90	2.3518E+05	3.7500E+00	133	3.7074E+03	7.9000E+00
91	2.2371E+05	3.8000E+00	134	3.3546E+03	8.0000E+00
92	2.1280E+05	3.8500E+00	135	3.0354E+03	8.1000E+00
93	2.0242E+05	3.9000E+00	136	2.7465E+03	8.2000E+00
94	1.9255E+05	3.9500E+00	137	2.6126E+03	8.2500E+00
95	1.8316E+05	4.0000E+00	138	2.4852E+03	8.3000E+00
96	1.7422E+05	4.0500E+00	139	2.2487E+03	8.4000E+00
97	1.6573E+05	4.1000E+00	140	2.0347E+03	8.5000E+00
98	1.5764E+05	4.1500E+00	141	1.5846E+03	8.7500E+00
99	1.4996E+05	4.2000E+00	142	1.2341E+03	9.0000E+00
100	1.4264E+05	4.2500E+00	143	9.6112E+02	9.2500E+00
101	1.3569E+05	4.3000E+00	144	7.4852E+02	9.5000E+00
102	1.2907E+05	4.3500E+00	145	5.8295E+02	9.7500E+00
103	1.2277E+05	4.4000E+00	146	4.5400E+02	1.0000E+01
104	1.1679E+05	4.4500E+00	147	3.5357E+02	1.0250E+01
105	1.1109E+05	4.5000E+00	148	2.7536E+02	1.0500E+01
106	9.8037E+04	4.6250E+00	149	2.1445E+02	1.0750E+01
107	8.6517E+04	4.7500E+00	150	1.6702E+02	1.1000E+01
108	8.2503E+04	4.7975E+00	151	1.3007E+02	1.1250E+01
109	7.9499E+04	4.8346E+00	152	1.0130E+02	1.1500E+01
110	7.1998E+04	4.9337E+00	153	7.8893E+01	1.1750E+01
111	6.7379E+04	5.0000E+00	154	6.1442E+01	1.2000E+01
112	5.6562E+04	5.1750E+00	155	4.7851E+01	1.2250E+01
113	5.2475E+04	5.2500E+00	156	3.7266E+01	1.2500E+01
114	4.6309E+04	5.3750E+00	157	2.9023E+01	1.2750E+01
115	4.0868E+04	5.5000E+00	158	2.2603E+01	1.3000E+01
116	3.4307E+04	5.6750E+00	159	1.7604E+01	1.3250E+01
117	3.1828E+04	5.7500E+00	160	1.3710E+01	1.3500E+01
118	2.8501E+04	5.8604E+00	161	1.0677E+01	1.3750E+01
119	2.7000E+04	5.9145E+00	162	8.3153E+00	1.4000E+01
120	2.6058E+04	5.9500E+00	163	6.4760E+00	1.4250E+01
121	2.4788E+04	6.0000E+00	164	5.0435E+00	1.4500E+01
122	2.4176E+04	6.0250E+00	165	3.9279E+00	1.4750E+01
123	2.3579E+04	6.0500E+00	166	3.0590E+00	1.5000E+01
124	2.1875E+04	6.1250E+00	167	2.3824E+00	1.5250E+01
125	1.9305E+04	6.2500E+00	168	1.8554E+00	1.5500E+01

Table 4. (contd.)

Fine group	Upper energy (eV)	Upper lethargy	Fine group	Upper energy (eV)	Upper lethargy
169	1.4450E+00	1.5750E+01	185	2.2500E-01	1.7610E+01
170	1.3000E+00	1.5856E+01	186	1.8400E-01	1.7811E+01
171	1.1253E+00	1.6000E+01	187	1.5000E-01	1.8015E+01
172	1.0800E+00	1.6041E+01	188	1.2500E-01	1.8198E+01
173	1.0400E+00	1.6079E+01	189	1.0000E-01	1.8421E+01
174	1.0000E+00	1.6118E+01	190	7.0000E-02	1.8777E+01
175	8.7643E-01	1.6250E+01	191	5.0000E-02	1.9114E+01
176	8.0000E-01	1.6341E+01	192	4.0000E-02	1.9337E+01
177	6.8256E-01	1.6500E+01	193	3.0000E-02	1.9625E+01
178	6.2506E-01	1.6588E+01	194	2.1000E-02	1.9981E+01
179	5.3158E-01	1.6500E+01	195	1.4500E-02	2.0352E+01
180	5.0000E-01	1.6811E+01	196	1.0000E-02	2.0723E+01
181	4.1399E-01	1.7000E+01	197	5.0000E-03	2.1416E+01
182	3.6680E-01	1.7121E+01	198	2.0000E-03	2.2333E+01
183	3.2500E-01	1.7242E+01	199	5.0000E-04	2.3719E+01
184	2.7500E-01	1.7409E+01		1.0000E-05	2.7631E+01

Table 5. Photon group energy boundaries for VITAMIN-B6.

Fine group	Upper energy (eV)	Fine group	Upper energy (eV)	Fine group	Upper energy (eV)
1	3.0000E+07	15	3.5000E+06	29	4.5000E+05
2	2.0000E+07	16	3.0000E+06	30	4.0000E+05
3	1.4000E+07	17	2.5000E+06	31	3.0000E+05
4	1.2000E+07	18	2.0000E+06	32	2.0000E+05
5	1.0000E+07	19	1.6600E+06	33	1.5000E+05
6	8.0000E+06	20	1.5000E+06	34	1.0000E+05
7	7.5000E+06	21	1.3400E+06	35	7.5000E+04
8	7.0000E+06	22	1.3300E+06	36	7.0000E+04
9	6.5000E+06	23	1.0000E+06	37	6.0000E+04
10	6.0000E+06	24	8.0000E+05	38	4.5000E+04
11	5.5000E+06	25	7.0000E+05	39	4.0000E+04
12	5.0000E+06	26	6.0000E+05	40	3.0000E+04
13	4.5000E+06	27	5.1200E+05	41	2.0000E+04
14	4.0000E+06	28	5.1000E+05	42	1.0000E+04 1.0000E+03

from neutron capture at high energies. Although the cross-section for capture at neutron energies between 20 and 30 MeV is small, such a reaction in some materials could produce gamma rays with energies between 20 and 30 MeV (VITAMIN-E gamma-ray groups only went up to 20 MeV).

#### D. Weighting Function.

The neutron weighting function is of the form typically chosen for fission reactor shielding problems. The breakpoint energies for the 3-region spectrum are similar to those used in VITAMIN-C. The breakpoint energy between the Maxwellian and 1/E shapes is 0.125 eV. The fission temperature has been adjusted to better reflect the neutron spectrum in a thermal reactor ( $\theta = 1.273$  MeV versus  $\theta = 1.41$  MeV for VITAMIN-E). The use of a large number of energy groups should make the exact functional form and energy break points less important compared to generating a broad-group library directly from ENDF/B data.

	<u>Functional form</u>	<u>Energy limits</u>	<u>Group No. (see Table 4)</u>
1)	Maxwellian Thermal Spectrum $W_1(E) = C_1 E e^{-E/\theta}$	$10^5$ eV to 0.125 eV	188-199
2)	"1/E" slowing-Down Spectrum $W_2(E) = C_2/E$	0.125 eV to 820.8 keV	67-187
3)	Fission Spectrum ( $\theta = 1.273$ MeV) $W_3(E) = C_3 E^{1/2} e^{-E/\theta}$	820.8 keV to 20 MeV	1-66

The photon weighting spectrum will be 1/E plus rolloffs (IWT=3 in the NJOY module GAMINR).

#### E. Legendre Order of Scattering.

The order of scattering used for both neutrons and photons will be  $P_7$ . Most calculations are likely to be done with  $P_3$  scattering, but for some problems, e.g., when single scatter events dominate, higher order may be required.

#### F. Convergence Parameters.

The fractional error tolerances, which are input parameters to NJOY, have been chosen based on our experiences with the VITAMIN libraries and the experiences of NJOY users. As a result, the resolved resonance reconstruction tolerance of 0.2% will be used for all nuclides. The tolerances for linearization 0.2%, thinning 0.2%, and integration 0.1% will be the same as was used for VITAMIN-E. In summary:

Reconstruction	0.2%
Linearization	0.2%
Thinning	0.2%
Integration	0.1%

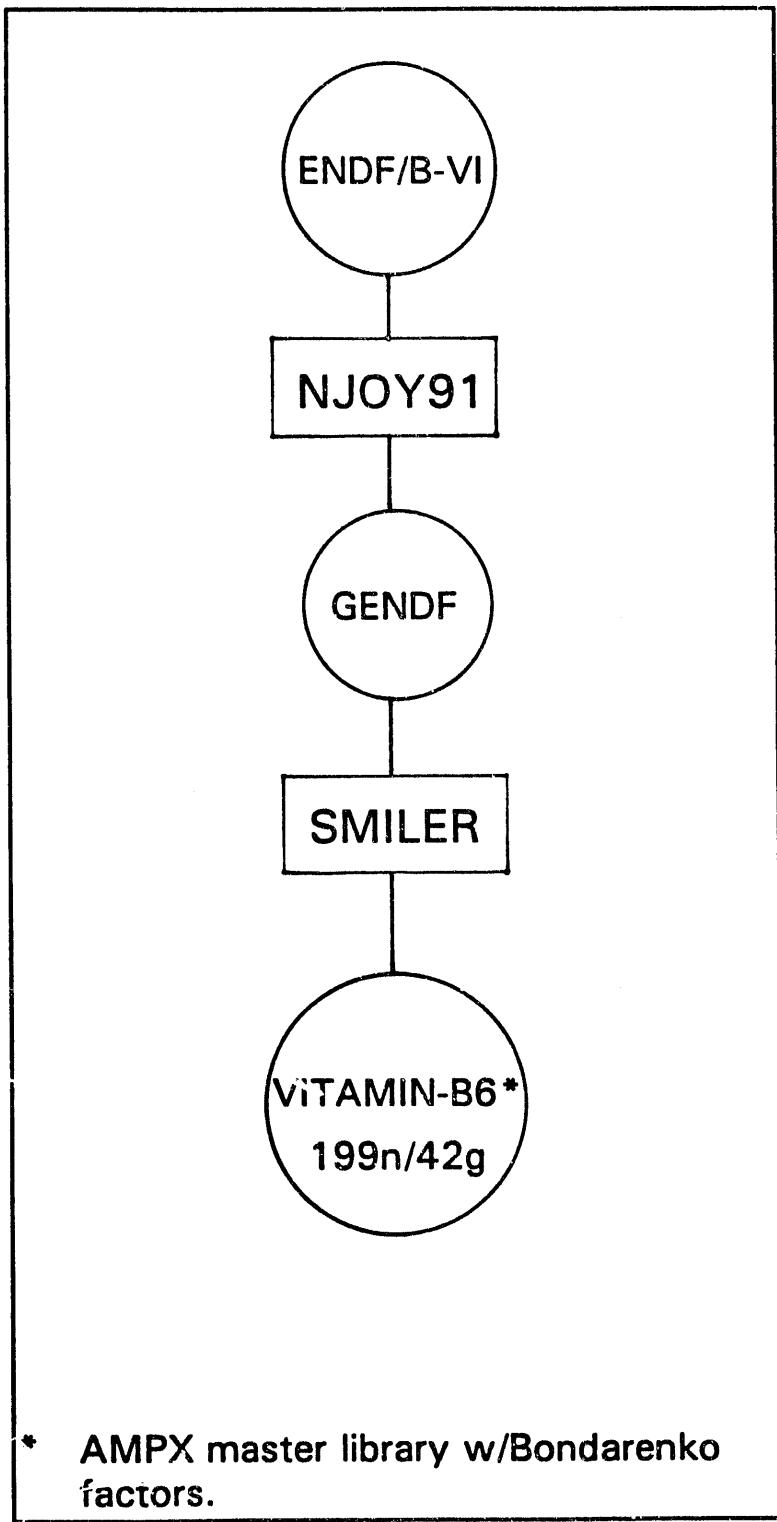
## G. Processing Codes

The NJOY91 processing system will be used to produce the point data and to produce multi-group averaged data in GENDF format. The SMILER code will then be used to translate the multigroup data into AMPX master library format. The AMPX77 system will form the basis of the post-processing codes that will self-shield, temperature-correct, and collapse the fine-group library into broad-group working library forms.

A schematic diagram illustrating the link between the NJOY91 and AMPX77 code systems is provided in Fig. 1. MODER, RECONR, BROADR, UNRESR, HEATR, THERMR, GROUPR, and GAMINR are modules in the NJOY nuclear data processing system that will play the dominant role in the fine-group averaging task. These modules are described in Table 6.

Table 6. Modules from the NJOY91 nuclear cross section processing system.

NJOY Module	Function
MODER	Convert between ENDF/B standard coded mode and the NJOY blocked binary mode.
RECONR	Reconstruct pointwise cross sections from ENDF/B resonance parameters and interpolation schemes.
BROADR	Doppler broaden and thin pointwise cross sections.
UNRESR	Compute effective pointwise self-shielded cross sections in the unresolved energy range.
HEATR	Generates pointwise heat production cross sections (KERMA factors) and radiation-damage-production cross sections.
THERMR	Generate neutron scattering cross sections and point-to-point scattering kernels in the thermal range for free or bound atoms.
GROUPR	Generate self-shielded multigroup cross sections and group-to-group scattering and photon production matrices.
GAMINR	Compute multigroup photon interaction cross sections, scattering matrices, and heat production.



**Figure 1.** Calculational flow used to produce self-shielded multigroup cross sections from ENDF/B-VI data.

A large number of supporting roles will be played by various modules of the AMPX77 system. The names and a brief description of the AMPX77 modules are given in Table 7. A key module for interpolating thermal scattering matrices with upscattering, called WORKER, is a new member of the AMPX77 system.

Table 7. Post-processing codes from AMPX77.

AMPX77 Module	Function
AIM	BCD-to-binary (or vice-versa) conversion.
AJAX	Merging and deleting operations.
UNITAB	Combining neutron and gamma-ray files.
MALOCS	Energy group collapsing.
BONAMI-S	Perform interpolation on Bondarenko factors to self-shield reaction cross sections.
RADE	Perform tests on multigroup libraries.
ALPO	Produce ANISN library from AMPX working library format.
ALE	Display information contained on either an AMPX master or working library.
WORKER	Prepare working libraries for use in transport calculations. Interpolate thermal scattering matrices; particularly nuclides with upscattering.
XSDRNP	Performs a one-dimensional discrete-ordinates or diffusion theory calculation using cross sections on an AMPX working library. Also, performs spacial cross-section weighting.
SMILER	Translate GENDF files produced by NJOY into AMPX master interface format.

## BROAD-GROUP SPECIFICATIONS

### A. Name

The problem-dependent broad-group cross sections derived from VITAMIN-B6 will be designated as BUGLE-93 and will consist of 47 neutron and 20 gamma-ray groups.

### B. Materials and Energy Group Structure

BUGLE-93 will contain all nuclides available in the fine-group (VITAMIN-B6) library. Both neutron and gamma-ray group structures will be consistent with the previously developed BUGLE-80 library. The relationship between BUGLE-93 and VITAMIN-B6 is provided in Table 8 which also illustrates the 47 neutron structure. The corresponding 20 gamma-ray group structure is given in Table 9.

Table 8. Neutron group energy boundaries for BUGLE-93.

Broad group	Upper energy (eV)	Upper lethargy	VITAMIN-B6 groups
1	1.7332E+07	-5.4997E-01	2-7
2	1.4191E+07	-3.5002E-01	8-12
3	1.2214E+07	-2.0000E-01	13-16
4	1.0000E+07	0.0000E+00	17-19
5	8.6071E+06	1.5000E-01	20-22
6	7.4082E+06	3.0000E-01	23-27
7	6.0653E+06	5.0000E-01	28-31
8	4.9659E+06	6.9999E-01	32-35
9	3.6788E+06	1.0000E+00	36-38
10	3.0119E+06	1.2000E+00	39-40
11	2.7253E+06	1.3000E+00	41-42
12	2.4660E+06	1.4000E+00	43-44
13	2.3653E+06	1.4417E+00	45
14	2.3457E+06	1.4500E+00	46-47
15	2.2313E+06	1.5000E+00	48-50
16	1.9205E+06	1.6500E+00	51-53
17	1.6530E+06	1.8000E+00	54-57
18	1.3534E+06	2.0000E+00	58-62
19	1.0026E+06	2.3000E+00	63-66
20	8.2085E+05	2.5000E+00	67-68
21	7.4274E+05	2.6000E+00	69-72
22	6.0810E+05	2.8000E+00	73-76
23	4.9787E+05	3.0000E+00	77-80
24	3.6883E+05	3.3000E+00	81-84
25	2.9721E+05	3.5159E+00	85-94
26	1.8316E+05	4.0000E+00	95-104
27	1.1109E+05	4.5000E+00	105-110
28	6.7379E+04	5.0000E+00	111-114
29	4.0868E+04	5.5000E+00	115-116
30	3.1828E+04	5.7500E+00	117-119
31	2.6058E+04	5.9500E+00	120-121
32	2.4176E+04	6.0250E+00	122-123
33	2.1875E+04	6.1250E+00	124-125
34	1.5034E+04	6.5000E+00	126-129
35	7.1017E+03	7.2500E+00	130-133
36	3.3546E+03	8.0000E+00	134-140
37	1.5846E+03	8.7500E+00	141-145
38	4.5400E+02	1.0000E+01	146-148
39	2.1445E+02	1.0750E+01	149-151
40	1.0130E+02	1.1500E+01	152-155
41	3.7266E+01	1.2500E+01	156-160
42	1.0677E+01	1.3750E+01	161-163
43	5.0435E+00	1.4500E+01	164-167

Table 8. (contd.)

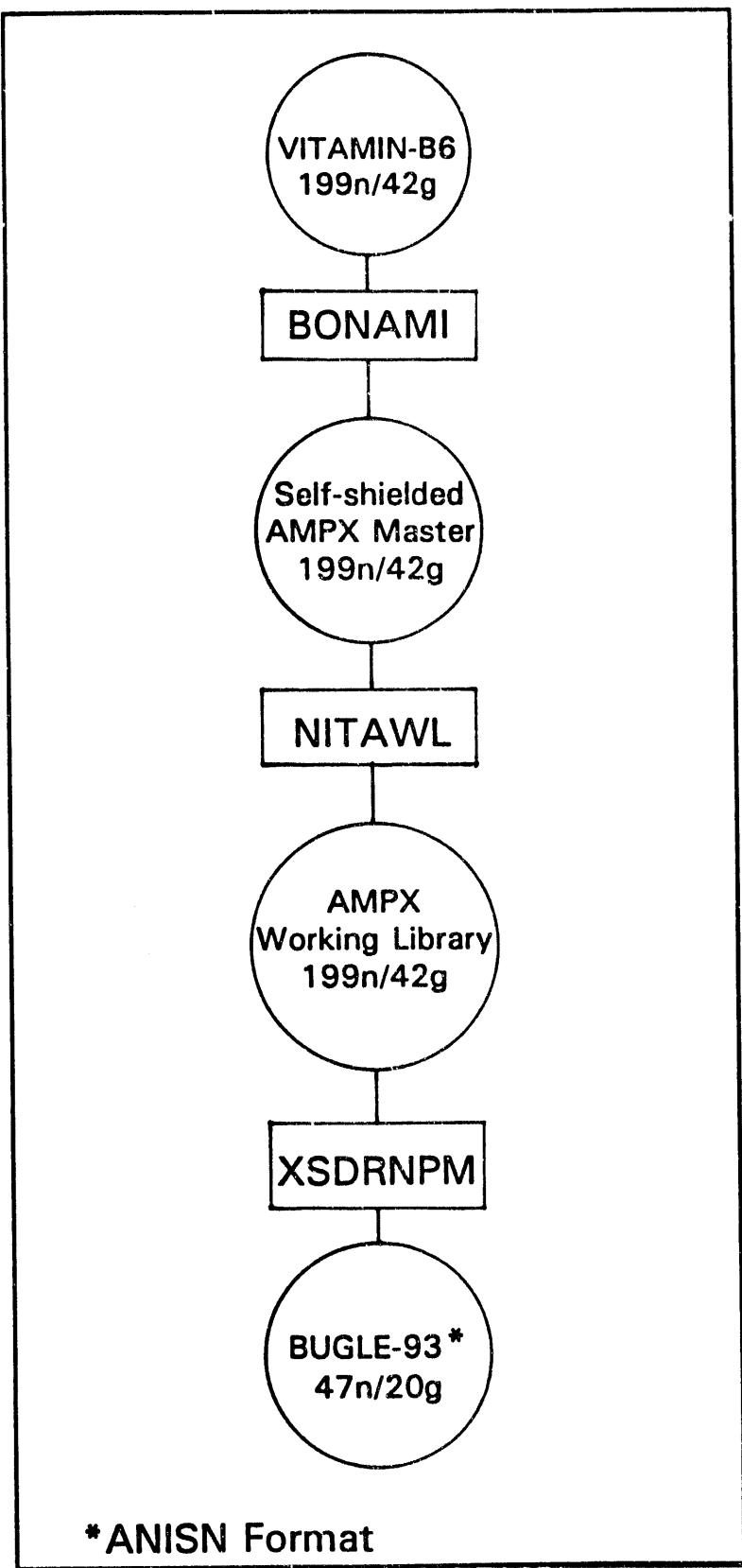
Broad group	Upper energy (eV)	Upper lethargy	VITAMIN-B6 groups
44	1.8554E+00	1.5500E+01	168-174
45	8.7643E-01	1.6250E+01	175-180
46	4.1399E-01	1.7000E+01	181-188
47	1.0000E-01	1.8421E+01	189-199
	1.0000E-05	2.7631E+01	

Table 9. Photon group energy boundaries for BUGLE-93

Broad group	Upper energy (eV)	VITAMIN-B6 groups	Broad group	Upper energy (eV)	VITAMIN-B6 groups
1	1.4000E+07	3-4	11	1.0000E+06	23
2	1.0000E+07	5	12	8.0000E+05	24
3	8.0000E+06	6-7	13	7.0000E+05	25
4	7.0000E+06	8-9	14	6.0000E+05	26-29
5	6.0000E+06	10-11	15	4.0000E+05	30-31
6	5.0000E+06	12-13	16	2.0000E+05	32-33
7	4.0000E+06	14-15	17	1.0000E+05	34-36
8	3.0000E+06	16-17	18	6.0000E+04	37-39
9	2.0000E+06	18-19	19	3.0000E+04	40
10	1.5000E+06	20-22	20	2.0000E+04	41
				1.0000E+04	

### C. Weighting Spectra

BUGLE-93 will be produced by collapsing the fine-group (VITAMIN-B6) library with the same methodology and reactor models used for both BUGLE-80 and SAILOR.<sup>20</sup> Five separate sets of broad-group cross sections will be generated. All nuclides in VITAMIN-B6 will be collapsed to (47n/20g) using a weighting spectrum based on the flux in the concrete shield of a PWR model. Also, selected materials will be resonance self-shielded, corrected for temperature effects, and collapsed for BWR fuel cell, PWR fuel cell, steel-water mixture, and PWR pressure vessel. The computational procedure, which was developed for the SAILOR library, is given in Fig. 2. A series of one-dimensional calculations with XSDRNPM using VITAMIN-B6 will be performed to obtain the flux spectrum for the appropriate group collapsing.



**Figure 2.** Generic scheme used to produce broad-group cross-sections for BUGLE-93 from VITAMIN-B6.

## D. Output Format.

The resulting broad-group library will be made available in ANISN format.

## E. Response Functions and Source Spectra

The following response functions and source spectra will be included with BUGLE-93 and also with VITAMIN-B6:

1. Total kerma factors for neutrons and photons calculated with the HEATR module of NJOY.
2. Dosimetry reaction cross sections based on ENDF/B-VI evaluations. At a minimum, the 45 neutron responses in the SAILOR library, which are listed in Table 10, will be made available.
3. Tissue dose response functions based on ANSI/ANS 6.1.1-1991, the latest Standard recommended by ANSI-6.1.
4. Group form of the VITAMIN-B6 weighting function.
5. VITAMIN-B6 neutron and photon group boundaries, midpoint energy values, energy intervals, lethargy intervals, etc.
6. Sources (group integrals) for the various benchmarks that will be used to test VITAMIN-B6.

Table 10. Neutron response functions

1	Group maximum energy (MeV)	24	Ni-58 (n,2n)
2	Fission spectrum	25	Ni-60 (n,p)
3	Li-6 (n,alpha)	26	Cu-63 (n,alpha)
4	B-10 (n,alpha)	27	Cu-65 (n,2n)
5	Th-232 (n,fission)	28	In-115 (n,n')
6	U-235 (n,fission)	29	I-127 (n,2n)
7	U-238 (n,fission)	30	Sc-45 (n,g)
8	Np-237 (n,fission)	31	Na-24 (n,g)
9	Pu-239 (n,fission)	32	Fe-58 (n,g)
10	Al-27 (n,p)	33	Co-59 (n,g)
11	Al-27 (n,alpha)	34	Cu-63 (n,g)
12	S-32 (n,p)	35	In-115 (n,g)
13	Ti-46 (n,p)	36	Au-197 (n,g)
14	Ti-47 (n,p)	37	Th-232 (n,g)
15	Ti-47 (n,n'p)	38	U-238 (n,g)
16	Ti-48 (n,p)	39	Square root (E)
17	Ti-48 (n,n'p)	40	Constant
18	Mn-55 (n,2n)	41	U-234 (n,fission)
19	Fe-54 (n,p)	42	U-236 (n,fission)
20	Fe-56 (n,p)	43	Pu-240 (n,fission)
21	Co-59 (n,2n)	44	Pu-241 (n,fission)
22	Co-59 (n,alpha)	45	Pu-242 (n,fission)
23	Ni-58 (n,p)		

## DATA TESTING PROGRAM

Because of the complexity of processing evaluated nuclear data into the multigroup formats used by the applications codes, it is important that the cross-section libraries be tested in their final format using accepted integral benchmarks. The amount of effort, however, can be extensive due to the vast number of nuclear interactions which comprise the cross sections and due to the broad range of shielding applications. The integral testing effort is then forced to be a compromise between thoroughness and affordability.

The integral testing serves not only to identify data processing mistakes, but also helps to assess the potential impact of the new cross sections for specific applications.

### A. Processing Methods

The data testing activities for this cross-section development task will begin after the initial creation of a preliminary fine-group shielding library consisting of a limited set of materials. This data testing will include the use of several diagnostic modules in the AMPX77 system. An example of cross-section checks performed by one of these modules, RADE, is provided in Table 11. In addition, plotting either pointwise or multigroup data and comparing with ENDF/B-V results for key reactions will be performed where necessary.

Some comparisons of the new BUGLE-93 and the previous BUGLE-80 broad-group libraries will be made by checking calculated group fluxes in several one-dimensional transport problems. Any significant differences not consistent with changes in the basic ENDF data will be investigated and reconciled before BUGLE-93 is finalized.

The calculation of criticality benchmarks<sup>21</sup> will help to establish the reliability of the resulting fine-group cross-section library and the cross section processing methods. The testing will include the calculation of CSEWG fast and thermal critical experiments where we have significant nuclear data performance experience. Successful results will assure that systems for self-shielding and coupling the neutron, gamma-ray production, and photon interaction cross-section interfaces have been implemented correctly.

After the initial testing is performed as part of the fine-group production task, the preliminary library will be released to shielding analysts for further testing and benchmark verification. Close cooperation and coordination with the shielding analysts will be maintained so that pertinent changes/additions to the specifications can be incorporated into the final version of VITAMIN-B6 library.

Table 11. Cross section checks<sup>a</sup> performed by RADE on  
AMPX master interface files.

---

1.  $\sigma_i = \sigma_a + \sigma_s$ .
2.  $\sigma_{in} = \sum \sigma_{in}^{\text{partial}}$ .
3.  $\sigma_a = \sigma_c + \sigma_f$ .
4.  $\sigma_c = \sigma_{n\gamma} + \sigma_{na} + \sigma_{np} + \sigma_{nd} + \dots$ .
5.  $\sigma_{el}^s = \sum_{g'} \sigma_{el,g}(g \rightarrow g')$  (also made on all processes with a scattering matrix).
6.  $\sigma_o(g \rightarrow g') > 0$ .
7.  $\sigma_i, \sigma_a, \sigma_f, \sigma_{na}, \sigma_{np}, \dots > 0$ .
- 8.<sup>b</sup>  $-1 \leq \left\{ \bar{\mu}(g \rightarrow g') = \frac{\sigma_l(g \rightarrow g')}{(2l+1)\sigma_o(g \rightarrow g')} \right\} \leq 1$ , for all odd  $l$ .

---

<sup>a</sup>Deviations between the right- and left-hand sides of the above relationships are printed if greater than a user supplied tolerance.

<sup>b</sup>For even  $l$ , the left-hand side of this inequality is given by the table:

$l$	$\bar{\mu}(g \rightarrow g')$
2	-0.5
4	-0.433
6	-0.419
8	-0.414

## B. Thermal and Fast Reactor Data Testing Benchmarks

The following benchmarks will be analyzed.

### 1. Thermal Reactor Benchmarks:

ORNL-1, -2, -3, -4, and -10: unreflected spheres of U-235 (as uranyl nitrate) in H<sub>2</sub>O. These benchmarks are useful for testing H<sub>2</sub>O fast scattering data, U-235 absorption, and neutron capture in hydrogen.

TRX-1 and TRX-2: H<sub>2</sub>O moderated uranium lattices. These lattices directly test U-235 resonance fission integral and thermal fission cross section. Also, U-238 shielded resonance capture and thermal neutron capture will be tested. These benchmarks are sensitive to U-235 fission spectrum and U-238 fast fission and inelastic scattering cross section.

BAPL-1, -2, and -3: H<sub>2</sub>O moderated uranium oxide critical lattices in a triangular pattern.

PNL-3: unreflected plutonium sphere.

PNL-6, and -11: homogeneous aqueous plutonium nitrate spheres and cylinders. These benchmarks are useful for testing  $H_2O$  scattering data, cross sections for resonance and thermal fission of Pu-239 and the Pu-239 fission spectrum.

ORNL-7, -8, 9, -10, -11: reflected and unreflected spheres of U-235 (as uranyl fluoride) in  $H_2O$ .

## 2. Fast Benchmarks:

JEZEBEL: a bare sphere of plutonium metal.

JEZEBEL-PU: a bare sphere of plutonium metal containing 20.1% Pu-240.

JEZEBEL-23: a bare sphere of U (98.13 at % U-233) metal.

GODIVA: a bare sphere of enriched uranium metal.

FLATTOP-25: a reflected sphere of enriched uranium metal.

BIG TEN: a reflected cylinder of uranium containing 10% U-235.

ZPR-3/11: fertile to fission uranium metal ratio of 7:1 with U-238 reflector.

ZPR-3/12: U-fueled assembly with uranium-graphite ratio of 4:1, U-238 blanket.

ZPR-6/6A: a uranium oxide fueled fast critical assembly.

ZPR-6/7: a large (3100 liter) plutonium oxide fueled fast critical assembly.

## 3. Other Benchmarks:

The following non-CSEWG benchmarks may be useful for ENDF/B-VI data testing. ENDF/B-V results are available for these benchmarks.

H2OX-1, UH3-UR, UH3-NI, HISS(HUG), HISS(HPG).

## C. Shielding Benchmarks

Several integral benchmarks have been identified as useful for testing the VITAMIN-B6 and BUGLE-93 cross-section libraries to be generated under this project. While some benchmarks are sensitive to specific nuclear data, others are more directed toward LWR shielding and pressure vessel dosimetry applications. The benchmarks are divided into three categories. The first two categories represent organizations which have sponsored and/or approved benchmark activities for the purpose of testing nuclear data and numerical methods. The third category represents additional benchmarks which have been generally accepted and are expected to be helpful in assessing the quality and adequacy of the new cross-section libraries.

**1. Cross Section Evaluation Working Group (CSEWG):**

**SDT1-5: "Broomstick" Experiments for Iron, Oxygen, Nitrogen, Sodium, and Stainless Steel.**

**SDT11: ORNL Benchmark for Iron and Stainless Steel.**

**SB2: Secondary Gamma-Ray Production for Thermal Neutron Spectrum.**

**SB3: Secondary Gamma-Ray Production for Fast Neutron Spectrum.**

**SB5: ORNL 14-MeV Stainless Steel/Borated Polyethylene Slab Experiment.**

**SB6: ORNL 14-MeV Iron Duct Experiment.**

**2. These benchmarks are now under the auspices of the Nuclear Energy Agency Nuclear Science Committee (NEANSC). They were formerly known as NEACRP benchmarks:**

**Winfirth Iron Benchmark Experiment.**

**Winfirth Water Benchmark Experiment.**

**PWR Shielding Benchmark (Computational).**

**LMFBR Shielding Benchmark (Computational).**

**3. Other Relevant Benchmarks:**

**University of Illinois Iron Sphere Benchmarks (14-MeV and Cf-252).**

**PCA-PV "Blind Test" Benchmark.**

**Winfirth NESDIP2 and NESDIP3 Radial Shield and Cavity Experiments.**

**LWR Shielding Benchmark (Computational).**

**CTR Standard Blanket Benchmark (Computational).**

## ACKNOWLEDGEMENTS

These specifications were developed from previous cross section processing experience performed at Oak Ridge National Laboratory. The authors are indebted to earlier contributors for many of the technical details included in this report. For the current work, we wish to acknowledge our indebtedness to Professor Mark Williams of Louisiana State University, R. E. MacFarlane of Los Alamos National Laboratory, and N. M. Greene of Oak Ridge National Laboratory for many valuable discussions and useful feedback on the initial draft report.

## REFERENCES

1. R. W. Roussin, et al, "Experience in Developing and Using the VITAMIN-C 171-Neutron, 36-Gamma-Ray Group Cross-Section Library," p. 107 in *A Review of Multigroup Nuclear Cross-Section Processing, Proceedings. of a Seminar-Workshop*, Oak Ridge National Laboratory report ORNL/RSIC-41 (October 1978).
2. C. R. Weisbin, R. W. Roussin, J. E. White, and R. Q. Wright, *Specification for Pseudo-Composition-Independent Fine-Group and Composition Dependent Fine- and Broad-Group LMFBR Neutron-Gamma Libraries at ORNL*, ORNL/TM-5142(ENDF-224) (December 1975).
3. R. W. Roussin, et al, *The CTR Processed Multigroup Cross-Section Library for Neutronics Studies*, ORNL/RSIC-37 (1978).
4. C. R. Weisbin, et al, "The Role of 'Standard' Fine-Group Cross-Section Libraries in Shielding Analysis," in *Proc. 5th ICNS*, Science Press, Princeton (1977).
5. *VITAMIN-C: 171 Neutron, 36 Gamma-Ray Group Cross-Sections in AMPX and CCCC Interface Formats for Fusion and LMFBR Neutronics*, RSIC Data Library Collection, DLC-41 (1978).
6. C. R. Weisbin, et al, *VITAMIN-E: An ENDF/B-V Multigroup Cross Section Library for LMFBR Core and Shield, LWR Shield, Dosimetry and Fusion Blanket Technology*, ORNL-5505(ENDF-274) (February 1979).
7. *VITAMIN-E: A Coupled 174-Neutron, 38-Gamma-Ray Multigroup Cross Section Library for Deriving Application-Dependent Working Libraries for Radiation Transport Calculations*, RSIC Data Library Collection, DLC-113 (1987).
8. N. M. Greene, et al, *AMPX: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B*, ORNL/TM-3706 (1976).
9. C. R. Weisbin, et al, *MINX, A Multigroup Interpretation of Nuclear Cross Section*, LA-6486-MS (1976).
10. R. E. MacFarlane, *Introducing NJOY 89*, LA-UR 89-2057 (June 1989).
11. R. E. MacFarlane and D. W. Muir, "NJOY 87.0," Los Alamos National Laboratory Memo T-2-L-10991 (June 1987).
12. R. E. MacFarlane, D. W. Muir, and R. M. Boicourt, *The NJOY Nuclear Data Processing System, Volume I: User's Manual*, LA-9303-M, Vol. I(ENDF-324) (May 1982).
13. R. E. MacFarlane, D. W. Muir, and R. M. Boicourt, *The NJOY Nuclear Data Processing System, Volume II: The NJOY, RECONR, BROADR, HEATR, and THERMR Modules*, LA-9303-M, Vol. II(ENDF-324) (May 1982).
14. R. E. MacFarlane and D. W. Muir, *The NJOY Nuclear Data Processing System, Volume III: The GROUPR, GAMINR, and MODER Modules*, LA-9303-M, Vol. III(ENDF-324) (October 1987).

15. R. E. MacFarlane and D. W. Muir, *The NJOY Nuclear Data Processing System, Volume IV: The ERROR and COVR Modules*, LA-9303-M, Vol. IV(ENDF-324) (December 1985).
16. P. F. Rose and C. L. Dunford, *Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6*, BNL-NCS-44945(ENDF 102) (July 1990).
17. Oak Ridge National Laboratory, *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-200, Revision 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (draft February 1990).
18. N. M. Greene, W. E. Ford, III, L. M. Petrie, and J. W. Arwood, *AMPX-77: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Cross-Section Libraries from ENDF/B-IV and/or ENDF/B-V*, ORNL/CSD/TM-283.
19. *BUGLE-80: Coupled 47 Neutron, 20 Gamma-Ray, P<sub>s</sub>, Cross-Section Library for LWR Shielding Calculations*, Radiation Shielding Information Center Data Library Collection, DLC-075 (1980).
20. *SAILOR: Coupled, Self-Shielded, 47-Neutron, 20-Gamma-Ray, P<sub>s</sub>, Cross Section Library for Light Water Reactors*, RSIC Data Library Collection DLC-076 (1985).
21. *ENDF-202, Cross-Section Evaluation Working Group Benchmark Specifications*, BNL-19302, Volume II, November 1974.

## INTERNAL DISTRIBUTION

1-2.	Central Research Library	22.	J. P. Renier
3.	Document Reference Section	23-27.	R. W. Roussin
4-5.	Laboratory Records Department	28.	R. T. Santoro
6.	Laboratory Records, ORNL—RC	29.	C. O. Slater
7.	ORNL Patent Section	30.	R. C. Ward
8.	B. R. Appleton	31.	R. M. Westfall
9.	B. L. Broadhead	32-36.	J. E. White
10.	J. A. Bucholz	37-41.	R. Q. Wright
11.	N. M. Greene	42.	R. W. Brockett (Consultant)
12-16.	D. T. Ingersoll	43.	J. J. Dorning (Consultant)
17.	F.B.K. Kam	44.	J. E. Leiss (Consultant)
18.	J. V. Pace	45.	N. Moray (Consultant)
19.	C. V. Parks	46.	M. F. Wheeler (Consultant)
20.	R. T. Primm	47.	EPMD Reports Office
21.	C. E. Pugh		

## EXTERNAL DISTRIBUTION

48. S. L. Anderson, Westinghouse Electric Corp., Radiation and Environmental Systems, Monroeville Nuclear Center MNC-436, P.O. Box 355, Pittsburgh, PA 15230.
49. John Carew, Brookhaven National Laboratory, Dept. of Nuclear Energy, Building 130, Upton, NY 11973.
50. L. R. Greenwood, Battelle Pacific Northwest Laboratory, MS. P7-22, P.O. Box 999, Richland, WA 99352.
51. Donald R. Harris, Dept. of Nuclear Engineering, Rensselaer Polytechnic Inst., Troy, NY 12181.
52. W. C. Hopkins, Bechtel Corp., 15740 Shady Grove Road, Gaithersburg, MD 20877-1454.
53. R. E. MacFarlane, Los Alamos National Laboratory, MS 243B, P.O. Box 1663, Los Alamos, NM 87545.
54. M. E. Mayfield, U. S. Nuclear Regulatory Commission, Washington, DC 20555.
55. E. D. McGarry, National Institute of Standards and Technology, Building 235, Room 2155, Gaithersburg, MD 20899.
56. Norm Snidow, Babcock & Wilcox co., P.O. Box 11165, Lynchburg, VA 24506-1165.
57. A. Taboada, U. S. Nuclear Regulatory Commission, Washington, DC 20555.
58. M. L. Williams, Louisiana State University, Nuclear Science Center, Baton Rouge, LA 70803.
59. DOE, Office of Advanced Reactor Programs, NE-45, Washington, D.C. 20585.
60. DOE, Assistant Manager for Energy Research and Development, Oak Ridge Operations Office, P.O. Box 2008, Oak Ridge, Tennessee 37831-6269.
- 61-70. DOE, Office of Scientific and Technical Information, P.O. Box 62, Oak Ridge, Tennessee 37831.

**DATE  
FILMED  
01/10/93**

