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VITAMIN-E: An ENDF/B-V Multigroup Cross-Section Library for LMFBR Core and Shield, LWR Shield, Dosimetry and Fusion Blanket Technology

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ABSTRACT

The Department of Energy (DOE) Office of Fusion Energy (OFE) and the Division of Reactor Research and Technology (DRRT) jointly sponsored the development of a coupled fine-group cross section library. This 171-neutron, 36-gamma-ray group library was based upon ENDF/B-IV and was intended to be applicable to fusion reactor neutronics and LMFBR core and shield analysis. Versions of the library are available from the Radiation Shielding Information Center (RSIC) at the Oak Ridge National Laboratory in both AMPX and CCCC formats. Computer codes for energy group collapsing, interpolation on Bondarenko factors for resonance self-shielding and temperature corrections, and various other useful data manipulations are also available.

The experience gained in the generation, validation and utilization of this library along with its broad range of applicability has led to the request for updating this data set using ENDF/B-V. Additional support in this regard has been provided by the Defense Nuclear Agency (DNA) and by the Electric Power Research Institute (EPRI) in support of weapons analyses and light water reactor shielding and dosimetry problems, respectively. The purpose of this report is to provide detailed specifications and rationale for the proposed ENDF/B-V update (designated VITAMIN-E) to the VITAMIN-C library.

I. Introduction

The Department of Energy (DOE) Office of Fusion Energy (OFE) and the Division of Reactor Research and Technology (DRRT) jointly sponsored the development of a coupled fine-group cross section library.[1,2,3,4] This 171-neutron, 36-gamma-ray group library was based upon ENDF/B-IV and was intended to be applicable to fusion reactor neutronics and LMFBR core and shield analysis. Versions of the library are available from the Radiation Shielding Information Center (RSIC) at the Oak Ridge National Laboratory in both AMPX (DLC-41/VITAMIN-C) and CCCC (DLC-53/VITAMIN-4C) formats. Computer codes for energy group collapsing, interpolation on Bondarenko factors for resonance self-shielding and temperature corrections, and various other useful data manipulations are also available via the PSR-63/AMPX-II and PSR-117/MARS packages.

The experience gained in the generation, validation, and utilization of this library along with its broad range of applicability has led to the request for updating this data set using ENDF/B-V. Additional support in this regard has been provided by the Defense Nuclear Agency (DNA) and by the Electric Power Research Institute (EPRI) in support of weapons analyses and light water reactor shielding and dosimetry problems, respectively. The purpose of this report is to provide detailed specifications and rationale for the proposed ENDF/B-V update (designated VITAMIN-E) to the VITAMIN-C library.

Later reports will outline specifications for the broad-group, application-dependent libraries which are to be derived from the fine-group master library discussed in this report. Some of the pertinent experience obtained in the development of VITAMIN-C is reviewed and some explanation for particular revisions or refinements to the library is provided in Section II. Section III contains the resulting specifications for the fine-group update based upon ENDF/B-V. Finally, a report on the proposed library testing program and anticipated near term applications is given in Section IV.

II. Rationale for Changes from the VITAMIN-C Specifications

A. Name. The development of a major library of this magnitude certainly warrants the consideration of a new name. The new library will be called VITAMIN-E, the E (the fifth letter of the alphabet) standing for ENDF/B Version V (the fifth version of ENDF/B).

B. Materials/Temperatures/Background Cross Sections. VITAMIN-C currently contains more than 66 materials which permits a broad spectrum of applications. ENDF/B Version V contains a significant expansion of this nuclear data base, particularly for the actinides (including the Th cycle materials). All materials in the General Purpose file will be processed for VITAMIN-E.[a] Regarding temperatures, the values of 0°, 300°, 900°, and 2100°K for the VITAMIN-C library were found to be quite satisfactory. There is a possibility that future Doppler calculations may require higher temperatures for certain selected materials, but this will be treated later on a case by case basis. A similar situation exists for the values of σ_0, the background cross section. Most users were satisfied with the values employed in VITAMIN-C. Hence, although the selection of σ_0's can clearly be improved with respect to particular applications, the generality of the library and earlier work (there will undoubtedly be many comparisons of Version IV and V cross sections) tend to lead us to draw upon our previous experience, supplementing additional σ_0 values where necessary. For example, we have added entries for ∞ dilution ($\sigma_0=10^7$; actually in this case an analytic form is used) and pure concentration ($\sigma_0=0$; actually approximated as $\sigma_0=10^{-6}$ to avoid problems taking logarithms).

C. Group Structure. For the intended range of application (LMFBR core physics and shielding, LWR shielding and dosimetry, fusion blanket technology), the 171/36 group structure has been favorably received. Only

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[a] Additional special purpose files (e.g. actinide, dosimetry, activation, etc.) will be processed at room temperature and infinite dilution. The ENDF/B-V fission product library has also been updated; accordingly, the ORYX library[5] will be updated with fine group fission product cross sections. The ORYX data can be collapsed to the group quantities required by ORIGEN[6] to obtain lumped fission products for fuel calculations.

minor adjustments to formally include energy boundaries of the DNA broad group library[7] and to extend the energy range to ∿ 20 MeV will be made. Synthesis with higher energy libraries (> 20 MeV), primarily for CTR applications, will be performed in a separate step as done previously. Finally, the group boundaries will include the break points used to describe the multi-region weighting function. The gamma-ray energy group structure has been extended to 20 MeV with a single minor change to one energy boundary (75 keV → 70 keV) for compatibility with the DNA γ-ray group structure.

D. Weighting Function. Several considerations enter into the selection of a smooth weighting function, W(E). Experience in Cooperative Processing Methods Testing has shown that the use of a more realistic smooth weighting function would help in assuring computation of proper group constants. In particular, below ∿ 25 keV the weighting function used previously was 1/E while we know that typical LMFBR spectra in this energy range are roughly constant and do not increase with decreasing energy. Similarly, the point at which the 1/E spectrum was joined to the fission spectrum was 821 keV in the VITAMIN-C library, while testing has shown that a higher value might be more reasonable. One must be quite careful with these types of arguments however, since for typical shielding situations the flux spectrum is often 1/E and sometimes even $1/E^n$, where $n > 1$. Also, it is perceived that the use of any particular reactor-dependent weighting function may detract from the generality of the resulting shielding factor library. Finally, built-in spectral corrections (e.g. elastic removal) are intended to account for some of these effects and the associated theories are currently based on a 1/E model.[8] It is also recognized that in special circumstances other sets of weighting functions may be required.

Thus, the weighting function specified in the next section obviously represents a set of compromises which hopefully can provide adequate accuracies over the range of intended applications. Basically, the energy at which the fission spectrum can be smoothly joined to the 1/E spectrum (i.e. where flux/lethargy is constant) is found to be equal to 3/2 of the fission spectrum temperature (taken here as $\theta \simeq 1.4$ MeV). *To provide consistency with the selected energy group boundaries, the (1/E)/fission spectrum cutpoint was raised to 2.1225 MeV, a boundary equal*

to 3/2 θ (θ = 1.415 MeV). Below this energy and above 0.414 eV, the W(E) spectrum is assumed to be 1/E with the knowledge that elastic removal corrections may be used to improve estimates of flux shapes. Shielding and thermal reactor problems also favor this shape. It should also be noted whereas the *Maxwellian temperature in the thermal group was fixed at 300°K for the VITAMIN-C library, it will be temperature dependent in the VITAMIN-E library.* For the 0° temperature, the smooth flux spectrum temperature is still set at 300°K. However, for the 300°, 900°, and 2100°K cases the spectrum temperature will be changed to the respective temperatures. The cutpoint for the Maxwillian and 1/E shapes is fixed at 0.414 eV independent of temperature (the original 5kT guideline was only nominal).

The weighting function for the γ-ray interaction cross sections is to be constant in energy.

E. Legendre Order of Scattering. The P_3 expansion of the group-to-group neutron transfer matrix was found to be quite acceptable for most applications. High energy transport in lighter materials (e.g. Na, Fe) is better represented by a P_5 expansion, although we do not have the quantified information at this time regarding the expected accuracy improvement for deep penetration problems. In the lack of further information, neutron cross sections for all materials will be processed with a P_3 expansion except for Na, Fe, H, Li, Si, N, and O which will be processed using a P_5 expansion. The γ-ray expansion will continue to be set at P_5.

F. Convergence Parameter Requirements. To improve accuracy we have reduced the tolerance on resonance reconstruction from 1% to 0.5% and that for linearization from 0.5% to 0.2%. The linearization tolerance was reduced below 0.5% without significant computational penalty. The cumulative uncertainty is a complex combination of all of these approximations; there is currently no methodology used to systematically combine these various sources of error.

G. Processing Codes. The following codes (or code systems) will be used to process the cross sections: Neutrons - MINX[9]
Gamma Rays - AMPX[10]
Covariance Files - PUFF[11]

The processing codes have been upgraded to handle Version V formats and tested as part of the CSEWG Data Testing Process. Multigroup neutron cross sections will be generated with MINX while the gamma-ray production and interaction cross sections will be generated with the LAPHNGAS and SMUG modules of the AMPX system. This system was chosen because of its successful performance in the generation of VITAMIN-C, the experience obtained by ORNL and General Electric as part of the preliminary ENDF/B-V Data Testing,[12] and the improvements to the modules as described below:

(1) Inclusion[13] of competitive widths, interference scattering, and resonance overlap in the unresolved energy region derived from modified versions of the MC^2-2 algorithm.[14] This was done for the total, elastic, fission, and capture cross sections.

(2) A current weighting of the total cross section including competitive widths, interference scattering, within sequence and sequence-sequence overlap corrections.[13]

(3) An auxiliary f-factor checking module[15] has been derived which provides best upper and lower bounds for the f-factors.

(4) Improvement of the numerical procedure employed in MINX to obtain the infinitely-dilute group averaged cross section in the unresolved energy region.

(5) Upgrade to handle Version V formats
   (a) Energy dependent Watt fission spectra are read. As in VITAMIN-C, *only the 1 MeV spectrum will be placed in the VITAMIN-E library* (MINX does not currently process fission matrices).
   (b) MOD number insert
   (c) Isotropic flag in file 4
   (d) Addition of competitive width processing.

(6) New and upgraded modules for Doppler broadening, linearization, and thinning which:
   (a) Thin the 0° data before broadening. This process saves enormous amounts of computing time.

(b) Guarantee of a sufficient number of points in the Doppler broadened tape such that linear interpolation is accurate to within a fixed input criteria.

(7) Added capability to process elastic removal f-factors.

(8) Improvements to Gamma Ray Production Processing.

(a) Experience with ENDF/B-IV gamma ray production processing led to linearization and normalization of the weight function to help improve the precision of the LAPHNGAS calculation.

(b) A coding change was made to the LAPHNGAS code to allow better precision when an input weighting spectrum is used (the case for VITAMIN-C). The change improves the integration scheme by incorporating the weighting function energy grid into the energy grid used by LAPHNGAS to calculate the group averaged multiplicities or gamma-ray production cross sections.

(c) A feature was also added to LAPHNGAS to allow calculation of multi-group multiplicities for materials without resonance parameters. This permits self shielding of gamma-ray production cross sections, e.g., from capture, using the Bondarenko scheme.

(9) A MINX change was made to permit the smooth energy weighting function to be temperature dependent in the thermal range.

(10) Work is currently underway to upgrade the PUFF processing code to handle ENDF/B-V covariance formats including energy dependent derived cross sections, correlations to standards, and uncertainties in resonance parameters. Infinitely dilute covariance matrices will also be processed in the fine-group structure for subsequent collapse.

H. Output Formats. Having the data available in CCCC and AMPX master formats, with auxiliary handling codes, was found to be quite acceptable. A new program has been written to provide a conversion capability between AMPX master format and a new format (MATXS) developed at Los Alamos Scientific Laboratory. For a first order check, plots of point versus multigroup data will be prepared. Finally, the covariance files will be output in COVERX format.[16]

I. Handling Codes for the Library. Two different sequences of handling codes for retrieving, manipulating, converting, editing, collapsing, self-shielding, etc., the libraries are available depending upon whether one needs to work in the CCCC or AMPX code systems. Codes for handling AMPX format are available in PSR-63/AMPX-II, and codes for handling CCCC format are available in PSR-117/MARS. Both computer code packages are available from RSIC. The various programs and functions are listed in Table VI of Section III of this report.

All the codes in MARS are operational on the IBM-360/91. The CCCC codes were written for the CDC-7600 and were converted for IBM-360/91 use at ORNL. Some AMPX modules useful for handling DLC-41 have been converted to CDC and UNIVAC machines by the user community and are available from RSIC in PSR-112/MAME.

III. Detailed Specifications for the ENDF/B-V Fine Group Library

A. Name. VITAMIN-E

B. Materials/Temperatures/Background Cross Sections. All materials on the General Purpose file will be processed at 0°, 300°, 900°, and 2100°K. The selection of σ_0's was modified from VITAMIN-C based upon experience[1,17] and extended to include values of $\sigma_0=0$ (actually $\sigma_0=10^{-6}$ is used to avoid problems using logarithms) and $\sigma_0=10^7$. Table I lists the materials which include all those in the General Purpose ENDF/B-V file. Table II lists the materials contained in the ENDF/B-V actinide file for which only partial evaluations (e.g. (n,γ) only) may be available. Final ENDF/B-V MAT numbers have not yet been assigned. *Special purpose files (e.g. actinides, dosimetry, etc.) will be processed at room temperature and infinite dilution.* Table III lists the background cross sections to be used in processing the General Purpose file materials.

Evaluations for the materials ^{99}Tc, ^{103}Rh, ^{107}Ag, ^{109}Ag, ^{113}Cd, ^{133}Cs, and ^{149}Sm have not been received at BNL as of this writing, but it is assumed that they are forthcoming. Additional materials not in this issue of ENDF/B include Ar, Ga, and Sn. These will be taken from the ENDL library.[19] All reactions will be processed including the covariance

files.

More than one hundred additional evaluations (with cross sections and decay data) are present on the ENDF/B-V fission product file. Several hundred more are provided with decay data only. The complete fission product file will form the basis for our update to ORYX-E.

Table I. VITAMIN-E Materials from the ENDF/B-V General Purpose File

Material	Material	Material	Material	Material
1. H-1	23. Cl	45. Zr-96	67. Gd-156	89. Au-197
2. H-2	24. K	46. Nb-93	68. Gd-157	90. Pb
3. H-3	25. Ca	47. Mo	69. Gd-158	91. Th-232
4. He-3	26. Ti	48. Cd	70. Gd-160	92. Pa-233
5. He-4	27. V	49. Xe-124	71. Dy-164	93. U-233
6. Li-6	28. Cr	50. Xe-126	72. Lu-175	94. U-234
7. Li-7	29. Mn-55	51. Xe-128	73. Lu-176	95. U-235
8. Be-9	30. Fe	52. Xe-129	74. Hf	96. U-236
9. B-10	31. Co-59	53. Xe-130	75. Hf-174	97. U-238
10. B-11	32. Ni	54. Xe-131	76. Hf-176	98. Np-237
11. C	33. Cu	55. Xe-132	77. Hf-177	99. Pu-238
12. N-14	34. Kr-78	56. Xe-134	78. Hf-178	100. Pu-239
13. N-15	35. Kr-80	57. Xe-135	79. Hf-179	101. Pu-240
14. O-16	36. Kr-82	58. Xe-136	80. Hf-180	102. Pu-241
15. O-17	37. Kr-83	59. Ba-138	81. Ta-181	103. Pu-242
16. F-19	38. Kr-84	60. Eu-151	82. Ta-182	104. Am-241
17. Na-23	39. Kr-86	61. Eu-152	83. W-182	105. Am-242
18. Mg	40. Zr	62. Eu-153	84. W-183	106. Am-243
19. Al	41. Zr-90	63. Eu-154	85. W-184	107. Cm-243
20. Si	42. Zr-91	64. Gd-152	86. W-186	108. Cm-244
21. P-31	43. Zr-92	65. Gd-154	87. Re-185	109. Cm-245
22. S-32	44. Zr-94	66. Gd-155	88. Re-187	110. Cm-246

Table II. VITAMIN-E Materials from the ENDF/B-V Actinide File

Material	Material	Material	Material
1. Tl-208	11. Pa-231	21. Pu-237	31. Cm-248
2. Pb-212	12. Pa-232	22. Pu-243	32. Cm-249
3. Bi-212	13. U-232	23. Pu-244	33. Bk-249
4. Po-216	14. U-237	24. Am-240	34. Bk-250
5. Rn-220	15. U-239	25. Am-242 m	35. Cf-249
6. Ra-224	16. Np-236	26. Am-244	36. Cf-250
7. Th-228	17. Np-236 m	27. Am-244 m	37. Cf-251
8. Th-230	18. Np-238	28. Cm-241	38. Cf-252
9. Th-231	19. Np-239	29. Cm-242	39. Cf-253
10. Th-233	20. Pu-236	30. Cm-247	40. Es-253

Table IIIa. Background Cross Sections (σ_0) to be Used In Processing the General Purpose File

Number	Material	10^7	10^5	10^4	10^3	10^2	10^1	10^0	10^{-1}	10^{-6}
1	H-1	X			X	X	X	X	X	X
2	H-2	X			X	X	X	X	X	X
3	H-3	X			X	X	X	X	X	X
4	He-3	X		X	X	X	X	X		X
5	He-4	X		X	X	X	X	X	X	X
6	Li-6	X			X	X	X	X	X	X
7	Li-7	X			X	X	X	X	X	X
8	Be-9	X			X	X	X	X	X	X
9	B-10	X			X	X	X	X		X
10	B-11	X	X	X	X	X	X	X		X
11	C	X			X	X	X	X	X	X
12	N-14	X			X	X	X	X	X	X
13	N-15	X		X	X	X	X	X		X
14	O-16	X			X	X	X	X	X	X
15	O-17	X		X	X	X	X	X		X
16	F-19	X		X	X	X	X	X	X	X
17	Na-23	X			X	X	X	X	X	X
18	Mg	X		X	X	X	X	X	X	X
19	Al	X		X	X	X	X	X		X
20	Si	X			X	X	X	X	X	X
21	P-31	X			X	X	X	X	X	X
22	S-32	X			X	X	X	X	X	X
23	Cl	X			X	X	X	X	X	X
24	K	X			X	X	X	X	X	X
25	Ca	X			X	X	X	X	X	X
26	Ti	X		X	X	X	X	X		X
27	V	X		X	X	X	X	X		X
28	Cr	X			X	X	X	X	X	X
29	Mn-55	X		X	X	X	X	X		X
30	Fe	X			X	X	X	X	X	X
31	Co-59	X			X	X	X	X	X	X
32	Ni	X			X	X	X	X	X	X
33	Cu	X			X	X	X	X	X	X
34	Kr-78	X			X	X	X	X	X	X
35	Kr-80	X			X	X	X	X	X	X
36	Kr-82	X			X	X	X	X	X	X
37	Kr-83	X			X	X	X	X	X	X
38	Kr-84	X			X	X	X	X	X	X
39	Kr-86	X			X	X	X	X	X	X
40	Zr	X			X	X	X	X	X	X
41	Zr-90	X			X	X	X	X	X	X
42	Zr-91	X			X	X	X	X	X	X
43	Zr-92	X			X	X	X	X	X	X
44	Zr-94	X			X	X	X	X	X	X
45	Zr-96	X			X	X	X	X	X	X

Table IIIa. (continued)

Number	Material	10^{7}	10^{5}	10^{4}	10^{3}	10^{2}	10^{1}	10^{0}	10^{-1}	10^{-6}
46	Nb-93	X		X	X	X	X	X		X
47	Mo	X		X	X	X	X	X		X
48	Cd	X			X	X	X	X	X	X
49	Xe-124	X			X	X	X	X	X	X
50	Xe-126	X			X	X	X	X	X	X
51	Xe-128	X			X	X	X	X	X	X
52	Xe-129	X			X	X	X	X	X	X
53	Xe-130	X			X	X	X	X	X	X
54	Xe-131	X			X	X	X	X	X	X
55	Xe-132	X			X	X	X	X	X	X
56	Xe-134	X			X	X	X	X	X	X
57	Xe-135	X		X	X	X	X	X		X
58	Xe-136	X		X	X	X	X	X		X
59	Ba-138	X			X	X	X	X	X	X
60	Eu-151	X		X	X	X	X	X		X
61	Eu-152	X		X	X	X	X	X		X
62	Eu-153	X		X	X	X	X	X		X
63	Eu-154	X		X	X	X	X	X		X
64	Gd-152	X		X	X	X	X	X		X
65	Gd-154	X		X	X	X	X	X		X
66	Gd-155	X		X	X	X	X	X		X
67	Gd-156	X		X	X	X	X	X		X
68	Gd-157	X		X	X	X	X	X		X
69	Gd-158	X		X	X	X	X	X		X
70	Gd-160	X		X	X	X	X	X		X
71	Dy-164	X		X	X	X	X	X		X
72	Lu-175	X		X	X	X	X	X		X
73	Lu-176	X		X	X	X	X	X		X
74	Hf	X		X	X	X	X	X		X
75	Hf-174	X		X	X	X	X	X		X
76	Hf-176	X		X	X	X	X	X		X
77	Hf-177	X		X	X	X	X	X		X
78	Hf-178	X		X	X	X	X	X		X
79	Hf-179	X		X	X	X	X	X		X
80	Hf-180	X		X	X	X	X	X		X
81	Ta-181	X			X	X	X	X	X	X
82	Ta-182	X			X	X	X	X	X	X
83	W-182	X		X	X	X	X	X		X
84	W-183	X		X	X	X	X	X		X
85	W-184	X		X	X	X	X	X		X
86	W-186	X		X	X	X	X	X		X
87	Re-185	X		X	X	X	X	X		X
88	Re-187	X		X	X	X	X	X		X
89	Au-197	X		X	X	X	X	X		X
90	Pb	X			X	X	X	X	X	X

Table IIIa. (continued)

Number	Material	10^7	10^5	10^4	10^3	10^2	10^1	10^0	10^{-1}	10^{-6}
91	Th-232	X		X	X	X	X	X	X	X
92	Pa-233	X		X	X	X	X	X		X
93	U-233	X		X	X	X	X	X	X	X
94	U-234	X		X	X	X	X	X		X
95	U-235	X		X	X	X	X	X	X	X
96	U-236	X		X	X	X	X	X		X
97	U-238	X		X	X	X	X	X	X	X
98	Np-237	X		X	X	X	X	X		X
99	Pu-238	X		X	X	X	X	X		X
100	Pu-239	X		X	X	X	X	X	X	X
101	Pu-240	X		X	X	X	X	X		X
102	Pu-241	X		X	X	X	X	X		X
103	Pu-242	X		X	X	X	X	X		X
104	Am-241	X		X	X	X	X	X		X
105	Am-242	X		X	X	X	X	X		X
106	Am-243	X		X	X	X	X	X		X
107	Cm-243	X		X	X	X	X	X		X
108	Cm-244	X		X	X	X	X	X		X
109	Cm-245	X		X	X	X	X	X		X
110	Cm-246	X		X	X	X	X	X		X

Table IIIb. Background Cross Sections (σ_0) to be Used In Processing. Materials Soon to be Added to ENDF/B-V or Taken from ENDL.

Additional Materials	10^7	10^5	10^4	10^3	10^2	10^1	10^0	10^{-1}	10^{-6}
Tc-99	X		X	X	X	X	X		X
Rh-103	X		X	X	X	X	X		X
Ag-107	X		X	X	X	X	X		X
Ag-109	X		X	X	X	X	X		X
Cd-113	X			X	X	X	X	X	X
Xe-127	X			X	X	X	X	X	X
Cs-133	X		X	X	X	X	X		X
Sm-149	X		X	X	X	X	X		X
Ar	X		X	X	X	X	X		X
Ga	X		X	X	X	X	X		X
Sn	X		X	X	X	X	X		X

C. Group Structure. The 174 neutron group structure is given in Table IV, the 37 gamma-ray group structure is given in Table V.

Table IV. Neutron Energy Group Structure for VITAMIN-E

	Upper Energy (eV)	Lethargy		Upper Energy (eV)	Lethargy
1	0.19640E+08	-0.67500E+00	46	0.23069E+07	0.14667E+01
2	0.17333E+08	-0.55000E+00	47	0.22313E+07	0.15000E+01
3	0.16905E+08	-0.52500E+00	48	0.21225E+07	0.15500E+01
4	0.16487E+08	-0.50000E+00	49	0.20190E+07	0.16000E+01
5	0.15683E+08	-0.45000E+00	50	0.19205E+07	0.16500E+01
6	0.14918E+08	-0.40000E+00	51	0.18268E+07	0.17000E+01
7	0.14550E+08	-0.37500E+00	52	0.17377E+07	0.17500E+01
8	0.14191E+08	-0.35000E+00	53	0.16530E+07	0.18000E+01
9	0.13840E+08	-0.32500E+00	54	0.15724E+07	0.18500E+01
10	0.13499E+08	-0.30000E+00	55	0.14957E+07	0.19000E+01
11	0.12523E+08	-0.22500E+00	56	0.14227E+07	0.19500E+01
12	0.12214E+08	-0.20000E+00	57	0.13534E+07	0.20000E+01
13	0.11618E+08	-0.15000E+00	58	0.12873E+07	0.20500E+01
14	0.11052E+08	-0.10000E+00	59	0.12246E+07	0.21000E+01
15	0.10513E+08	-0.50000E-01	60	0.11648E+07	0.21500E+01
16	0.10000E+08	0.	61	0.11080E+07	0.22000E+01
17	0.95123E+07	0.50000E-01	62	0.10026E+07	0.23000E+01
18	0.90484E+07	0.10000E+00	63	0.96164E+06	0.23417E+01
19	0.86071E+07	0.15000E+00	64	0.90718E+06	0.24000E+01
20	0.81873E+07	0.20000E+00	65	0.86294E+06	0.24500E+01
21	0.77880E+07	0.25000E+00	66	0.82085E+06	0.25000E+01
22	0.74082E+07	0.30000E+00	67	0.78082E+06	0.25500E+01
23	0.70469E+07	0.35000E+00	68	0.74274E+06	0.26000E+01
24	0.67032E+07	0.40000E+00	69	0.70651E+06	0.26500E+01
25	0.65924E+07	0.41667E+00	70	0.67206E+06	0.27000E+01
26	0.63763E+07	0.45000E+00	71	0.63928E+06	0.27500E+01
27	0.60653E+07	0.50000E+00	72	0.60810E+06	0.28000E+01
28	0.57695E+07	0.55000E+00	73	0.57844E+06	0.28500E+01
29	0.54881E+07	0.60000E+00	74	0.55023E+06	0.29000E+01
30	0.52205E+07	0.65000E+00	75	0.52340E+06	0.29500E+01
31	0.49659E+07	0.70000E+00	76	0.49787E+06	0.30000E+01
32	0.47237E+07	0.75000E+00	77	0.45049E+06	0.31000E+01
33	0.44933E+07	0.80000E+00	78	0.40762E+06	0.32000E+01
34	0.40657E+07	0.90000E+00	79	0.38774E+06	0.32500E+01
35	0.36788E+07	0.10000E+01	80	0.36883E+06	0.33000E+01
36	0.33287E+07	0.11000E+01	81	0.33373E+06	0.34000E+01
37	0.31664E+07	0.11500E+01	82	0.30197E+06	0.35000E+01
38	0.30119E+07	0.12000E+01	83	0.29850E+06	0.35116E+01
39	0.28650E+07	0.12500E+01	84	0.29720E+06	0.35159E+01
40	0.27253E+07	0.13000E+01	85	0.29452E+06	0.35250E+01
41	0.25924E+07	0.13500E+01	86	0.28725E+06	0.35500E+01
42	0.24660E+07	0.14000E+01	87	0.27324E+06	0.36000E+01
43	0.23852E+07	0.14333E+01	88	0.24724E+06	0.37000E+01
44	0.23653E+07	0.14417E+01	89	0.23518E+06	0.37500E+01
45	0.23457E+07	0.14500E+01	90	0.22371E+06	0.38000E+01
			91	0.21280E+06	0.38500E+01

Table IV. (continued)

	Upper Energy (eV)	Lethargy		Upper Energy (eV)	Lethargy
92	0.20242E+06	0.39000E+01	134	0.30354E+04	0.81000E+01
93	0.19255E+06	0.39500E+01	135	0.27465E+04	0.82000E+01
94	0.18316E+06	0.40000E+01	136	0.26126E+04	0.82500E+01
95	0.17422E+06	0.40500E+01	137	0.24852E+04	0.83000E+01
96	0.16573E+06	0.41000E+01	138	0.22487E+04	0.84000E+01
97	0.15764E+06	0.41500E+01	139	0.20347E+04	0.85000E+01
98	0.14996E+06	0.42000E+01	140	0.15846E+04	0.87500E+01
99	0.14264E+06	0.42500E+01	141	0.12341E+04	0.90000E+01
100	0.13569E+06	0.43000E+01	142	0.96112E+03	0.92500E+01
101	0.12907E+06	0.43500E+01	143	0.74852E+03	0.95000E+01
102	0.12277E+06	0.44000E+01	144	0.58295E+03	0.97500E+01
103	0.11679E+06	0.44500E+01	145	0.45400E+03	0.10000E+02
104	0.11109E+06	0.45000E+01	146	0.35358E+03	0.10250E+02
105	0.98037E+05	0.46250E+01	147	0.27536E+03	0.10500E+02
106	0.86517E+05	0.47500E+01	148	0.21445E+03	0.10750E+02
107	0.82500E+05	0.47975E+01	149	0.16702E+03	0.11000E+02
108	0.79500E+05	0.48346E+01	150	0.13007E+03	0.11250E+02
109	0.72000E+05	0.49337E+01	151	0.10130E+03	0.11500E+02
110	0.67379E+05	0.50000E+01	152	0.78893E+02	0.11750E+02
111	0.56562E+05	0.51750E+01	153	0.61442E+02	0.12000E+02
112	0.52475E+05	0.52500E+01	154	0.47851E+02	0.12250E+02
113	0.46309E+05	0.53750E+01	155	0.37267E+02	0.12500E+02
114	0.40868E+05	0.55000E+01	156	0.29023E+02	0.12750E+02
115	0.34307E+05	0.56750E+01	157	0.22603E+02	0.13000E+02
116	0.31828E+05	0.57500E+01	158	0.17603E+02	0.13250E+02
117	0.28500E+05	0.58604E+01	159	0.13710E+02	0.13500E+02
118	0.27000E+05	0.59145E+01	160	0.10677E+02	0.13750E+02
119	0.26058E+05	0.59500E+01	161	0.83153E+01	0.14000E+02
120	0.24788E+05	0.60000E+01	162	0.64760E+01	0.14250E+02
121	0.24176E+05	0.60250E+01	163	0.50435E+01	0.14500E+02
122	0.23579E+05	0.60500E+01	164	0.39279E+01	0.14750E+02
123	0.21875E+05	0.61250E+01	165	0.30590E+01	0.15000E+02
124	0.19305E+05	0.62500E+01	166	0.23824E+01	0.15250E+02
125	0.15034E+05	0.65000E+01	167	0.18554E+01	0.15500E+02
126	0.11709E+05	0.67500E+01	168	0.14450E+01	0.15750E+02
127	0.10595E+05	0.68500E+01	169	0.11254E+01	0.16000E+02
128	0.91188E+04	0.70000E+01	170	0.87642E+00	0.16250E+02
129	0.71017E+04	0.72500E+01	171	0.68256E+00	0.16500E+02
130	0.55308E+04	0.75000E+01	172	0.53156E+00	0.16750E+02
131	0.43074E+04	0.77500E+01	173	0.41399E+00	0.17000E+02
132	0.37074E+04	0.79000E+01	174	0.10000E+00	0.18421E+02
133	0.33546E+04	0.80000E+01		0.10000E-04	

Table V. Gamma Ray Energy Group Structure for VITAMIN-E

Group Number	Upper Energy (MeV)	Group Number	Upper Energy (MeV)
1	20.0	20	1.33
2	14.0	21	1.0
3	12.0	22	0.80
4	10.0	23	0.70
5	8.0	24	0.60
6	7.5	25	0.512
7	7.0	26	0.510
8	6.5	27	0.45
9	6.0	28	0.40
10	5.5	29	0.30
11	5.0	30	0.20
12	4.5	31	0.15
13	4.0	32	0.10
14	3.5	33	0.070
15	3.0	34	0.060
16	2.5	35	0.045
17	2.0	36	0.030
18	1.66	37	0.020
19	1.50		0.010

D. Weighting Function. The neutron and photon production weighting function is as follows:

	Functional Form	Energy Limits	Group No. (see Table IV)
1)	Maxwellian Thermal Spectrum $W_1(E) = C_1 E e^{-E/kT}$	10^{-5} eV to 0.414 eV	173-174
2)	"1/E" Slowing-Down Spectrum $W_2(E) = C_2/E$	0.414 eV to 2.12 MeV	48-172
3)	Fission Spectrum (Θ = 1.415 MeV) $W_3(E) = C_3 E^{1/2} e^{-E/\Theta}$	2.12 MeV to 10.0 MeV	16-47
4)	"1/E" Spectrum $W_4(E) = C_4/E$	10.0 MeV to 12.52 MeV	11-15
5)	Velocity Exponential Fusion Peak (E_p = 14.07 MeV) (kT = 0.025 MeV) $W_5(E) = C_5 \exp\left\{-\frac{5}{kT}(E^{1/2}-E_p^{1/2})^2\right\}$	12.52 MeV to 15.68 MeV	5-10
6)	"1/E" Spectrum $W_6(E) = C_6/E$	15.68 MeV to 19.64 MeV	1-4

The weighting function for the gamma-ray interaction cross sections is to be constant in energy.

E. Legendre Order of Scattering.

P_3: Neutrons (except for Na, Fe, H, Li, Si, N, and O which will be processed using P_5)

P_5: γ-rays

F. Convergence Parameters.

(1)	reconstruction	0.5%
(2)	linearization	0.2%
(3)	thinning	0.2%
(4)	integration	0.1%

G. Processing Codes.

Neutrons	- MINX
Gamma Rays	- AMPX (LAPHNGAS and SMUG modules)
Covariance Files	- PUFF

H. Output Formats. CCCC, AMPX master, and MATXS (also plots of point vs. multi-group data). The covariance files will be output in COVERX format. Special purpose files of elastic removal f-factors will also be provided.

I. Handling Codes for the Library. Handling programs for data in AMPX format are available as part of the PSR-63/AMPX-II package. For convenience, many of the AMPX modules have been selected from the PSR-63 package and placed in PSR-117/MARS along with handling programs for data in CCCC formats. The PSR-117/MARS package is thus designed to be used in conjunction with multigroup libraries in AMPX, CCCC, or a combination of the two formats.

Table VI contains a brief functional list of some of the programs included in PSR-117/MARS.

Table VI. Handling Codes from the MARS (PSR-117) Package of Software Support

AMPX Module	CCCC Computer Code	Function
AIM	BINX, LASIP-III	BCD-to-binary (or vice-versa) conversion.
AJAX	LINX, I2I, B2B	Merging and deleting operations.
CHOX		Combining neutron and gamma-ray files.
CHOXM		Combining self-shielding factors, neutron files, and gamma-ray files.
MALOCS	CINX	Energy group collapsing.
BONAMI	SPINX	Perform interpolation on Bondarenko factors.
NITAWL	I2D	Prepare working libraries for use in transport calculations.
RADE	---	Perform tests on multigroup libraries.

IV. Testing Program and Anticipated Schedule

The testing program will be intimately associated with feedback from sponsor application and participation in various cooperative national testing programs. Anticipated application includes continued analysis of the OFE integral experiments, analysis of LMFBR critical experiments and Large Plant Design Studies, analysis of experiments relevant to pressure vessel surveillance, and weapons related applications. Benchmark validation will include cooperative testing in the framework of the CSEWG Data Testing Subcommittee, the CEWG Processing Methods Testing Subcommittee, ANS-6.1.2 (LWR Shield Standard Cross Sections), and the OFE Validation Group.

Some of the more important materials for these applications will be processed with high priority as soon as they become available. Our

current estimate is that processed cross sections for some important materials will be available by approximately March 1979 but that the complete library will not be completed until early 1980. Extensions to the current effort will include the dosimetry, activation and gas production data, as they become available, kerma factors and response functions, and delayed data. Processing refinements and library improvements are thus expected to continue for at least 2-3 more years.

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REFERENCES

1. R. W. Roussin, C. R. Weisbin, J. E. White, R. Q. Wright, N. M. Greene, W. E. Ford, III, J. B. Wright, and B. R. Diggs, "Experience in Developing and Using the VITAMIN-C 171- Neutron, 36-Gamma-Ray Group Cross-Section Library," A Review of Multigroup Nuclear Cross-Section Processing, Proceedings of a Seminar-Workshop, ORNL/RSIC-41, page 107 (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, C. R. Weisbin, J. E. White, N. M. Greene, R. Q. Wright, and J. B. Wright, "The CTR Processed Multigroup Cross-Section Library for Neutronics Studies," ORNL/RSIC-37 (1978).

4. C. R. Weisbin, R. W. Roussin, E. M. Oblow, J. E. White, and R. Q. Wright, and D. E. Cullen, "The Role of "Standard" Fine-Group Cross-Section Libraries in Shielding Analysis," Proceedings of the Fifth International Conference on Reactor Shielding, Science Press, Princeton (1977).

5. "ORYX-E ORIGEN Yields and Cross Sections - Nuclear Transmutation and Decay Data from ENDF/B," DLC-38 RSIC Data Library Collection (Updated January 1976).

6. M. J. Bell, "ORIGEN - The ORNL Isotope Generation and Depletion Code," ORNL-4628, May 1973.

7. D. E. Bartine, J. R. Knight, J. V. Pace, III, and R. W. Roussin, "Production and Testing of the DNA Few-Group Coupled Neutron-Gamma Cross-Section Library," ORNL/TM-4840 (March 1977). Available from RSIC as DLC-31/(DPL-1/FEWG1).

8. C. L. Cowan, E. Kujawski, and R. Protsik, "Implementation of the Rapid Cross Section Adjustment Approach at General Electric," A Review of Multigroup Nuclear Cross-Section Processing, Proceedings of a Seminar-Workshop, ORNL/RSIC-41, page 97 (October 1978).

9. C. R. Weisbin, P. D. Soran, R. E. MacFarlane, D. R. Harris, R. J. LaBauve, J. S. Hendricks, J. E. White, and R. B. Kidman, "MINX, A Multigroup Interpretation of Nuclear Cross Sections," LA-6486-MS (1976).

10. N. M. Greene, J. L. Lucius, L. M. Petrie, W. E. Ford, III, J. E. White, and R. Q. Wright, "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B," ORNL/TM-3706 (1976).

11. C. R. Weisbin, E. M. Oblow, J. Ching, J. E. White, R. Q. Wright, and J. D. Drischler, "Cross Section and Method Uncertainties: The Application of Sensitivity Analysis to Study Their Relationship in Radiation Transport Benchmark Problems," ORNL/TM-4847 (ENDF-218), Oak Ridge National Laboratory (August 1975); see also, RSIC Code Collection PSR-93, Oak Ridge National Laboratory.

12. R. Q. Wright, J. E. White, D. G. Cacuci, and C. R. Weisbin, "ORNL Fast Reactor Data Testing Results Based on Pre-Preliminary ENDF/B-V Data," September 11, 1978, see "Report of the CSEWG Data Testing - Evaluator Meeting, September 11-13, 1978, Brookhaven National Laboratory, CSEWG Newsletter #57; see also E. Kujawski and S. L. Beamon, "Phase II Testing of Preliminary ENDF/B-V at GE-ARSK." Letter to the Cross Section Evaluation Working Group, (September 5, 1978).

13. D. G. Cacuci, "Cross Section Treatment in the Unresolved Energy Region at ORNL for ENDF/B-V Using MINX," September 7, 1978, Oak Ridge National Laboratory Internal Memorandum. See also J. Barhen and D. G. Cacuci, "Cross Section Processing for the Unresolved Energy Region," Oak Ridge National Laboratory Internal Memorandum, (December 4, 1978).

14. H. Henryson, II, B. J. Toppel, and C. G. Stenberg, "MC^2-2: A Code to Calculate Fast Neutron Spectra and Multigroup Nuclear Cross Section Processing," ANL-8144 (ENDF-239) (June 1976).

15. D. G. Cacuci and M. A. Bjerke, "Analytical Inequalities Satisfied by the Cross Section Self-Shielding Factors - Best Upper and Lower Bounds," A Review of Multigroup Nuclear Cross-Section Processing, Proceedings of a Seminar-Workshop, ORNL/RSIC-41, page 227 (October 1978).

16. J. D. Drischler and C. R. Weisbin, "Compilation of Multigroup Cross-Section Covariance Matrices for Several Important Reactor Materials," ORNL-5318 (ENDF-235) (October 1977).

17. R. B. Kidman and R. E. MacFarlane, "LIB-IV, A Library of Group Constants for Nuclear Reactor Calculations," LA-6260-MS (March 1976).

18. 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).

19. R. J. Howerton and M. H. MacGregor, "The LLL Evaluated Nuclear Data Library (ENDL): Descriptions of Individual Evaluations for Z=0-98," UCRL-50400 Volume 15 (May 1978).

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