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Specification of a Generally Useful Multigroup Structure for Neutron Transport

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Specification of a Generally Useful Multigroup Structure for Neutron Transport

by

C. R. Weisbin
R. J. LaBauve

LOS ALAMOS NATL. LAB. LIBS.
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This work supported by the US Atomic Energy Commission's Division of Reactor Development and Technology.

SPECIFICATION OF A GENERALLY USEFUL MULTIGROUP STRUCTURE FOR NEUTRON TRANSPORT

by

C. R. Weisbin and R. J. LaBauve

ABSTRACT

This report represents the work of a committee appointed and directed by the Codes and Formats Subcommittee of the Cross Section Evaluation Working Group and is parallel to that already completed for the thermal range. It is an attempt to suggest reasonable energy bounds, weighting function and output format for a "standardized" multigroup library in the fast energy range (>1 eV) to be prepared for general distribution. Although the emphasis is clearly directed toward the LMFBR program, the large number of groups (~250) has made it possible to include the majority of CTR, shielding, and weapons requirements with the notion that a problem dependent group structure can be obtained conveniently at run time by a simple collapsing procedure.

The new structure is compatible with past design experience and incorporates detailed representation for specific cross section features known to be important in a wide range of nuclear design applications.

I. INTRODUCTION

At the direction of the Codes and Formats Subcommittee of the Cross Section Evaluation Working Group (CSEWG), a committee has been formed to determine energy bounds, weighting function and output format for a generally applicable set of fine multigroup constants in the fast (and epithermal) energy range. The work of this committee is reported herein. Section II describes briefly the rationale behind the creation of such a problem independent file. Section III discusses the basis upon which rests the selection of particular energy cut-points and the total number of groups. Section IV describes the "sensitivity testing" phase in which group constants are computed in this multigroup structure and compared for several reasonable choices of within group weighting spectra. Section V describes the choice of fine group weighting and indicates a format useful for the description of the multigroup library.

II. THE *Raison d'Etre* FOR A GENERALLY APPLICABLE MULTIGROUP FILE

A. Economics

For routine design, parametric surveys, physics studies, etc., it is becoming increasingly expensive to reprocess multigroup constants from fundamental pointwise cross sections and resonance parameters in a group structure tailored for each specific problem of interest. Even when one restricts one's self to a "class" of problems (LMFBR, CTR, weapons output, etc.) one is immediately confronted with a group structure choice which depends upon source spectrum, detector response, composition changes, etc.

The reliance upon readily available, accurate, and appropriate fine multigroup sets, collapsed with a problem dependent flux spectrum is an effective means of carrying out design studies. The reduction of a fine group set to a broad group set is clearly a less time-consuming task when compared to reprocessing from fine-energy-detail data. Moreover, the need for multigroup code maintenance (as computing systems and ENDF/B formats change) and development at a large number of laboratories around the country would be lessened with the introduction and support of a "standardized" multigroup file. Finally, if a specific problem appears to require special treatment, one could always request that a special problem-dependent set be created. The existence of a basic multigroup data file does not, of course, require its sole usage.

B. Design Comparisons and Methods Testing

Specification of a fine multigroup data base would go a long way toward resolving discrepancies that may arise between design and methods calculations performed at different installations. For a given problem, broad group structure, and flux spectrum estimate, design differences associated with differing integration techniques, various transport approximations, different resonance and kinematic treatments would no longer mask differences in design performance.

C. Feedback from a Wide Variety of Users

The fast breeder reactor, thermal reactor, fusion reactor and nuclear weapon system communities have many common data areas of interest, although there may be different energy regions on which emphasis must be placed. In all cases, the methods and techniques involved are basically the same. Therefore, since the fine multigroup data base is going to be collapsed in application, a generally useful and still reasonably sized set can be formed containing the "union" of the objectives of the agencies involved. Fast reactor designers may choose to have the energy groups above 10 MeV collapsed into a single group. The weapons community may choose, for specific design problems, to collapse all energy groups below 1 keV. Clearly, with the premise that the data set will be collapsed for application, the needs of the various organizations are not mutually exclusive. Moreover, the wide diversity of interests involved will test the data over most of its energy range. It is precisely the common comparison of calculations against experiment and as-built product which is required to provide a useful data base for nuclear design. To illustrate this feedback, the addition of high energy groups for the benefit of the weapons designer is no great practical burden on the fast reactor designer and the addition of these groups encourage the weapons designer to feed his experience in the keV and low MeV range back to the fast reactor designer, for in this range their interest are similar.

III. GUIDING PRINCIPLES FOR THE SELECTION OF ENERGY BOUNDARIES

A. Begin with a Design Based Structure

Several multigroup libraries presently exist[1-5] and are in widespread use. A number of other multigroup libraries exist and are used locally.[6-7] Almost all are structured upon some basic increment in lethargy. Although this selection of cut-points may have little significance in the source region, the design experience obtained heretofore was judged to be indispensable. Therefore, the development of the generalized file proposed in this work began with consideration of the GAM-II structure.[2]

The base lethargy mesh above ~100 keV was reduced to .05 to include the GAM-I points not appearing in the GAM-II set. The finer mesh permits a better resonance scattering treatment for light and medium weight nuclei (A>50). Certain threshold and source phenomena are better treated by the finer mesh. Furthermore, such a scheme is an attempt to be consistent with measured energy resolution of ~5% as in the German 208 group set[8] and to produce ultimately a group set containing approximately 200 fine groups. Between ~1 and 100 keV, the GAM-II base lethargy step of .25 was narrowed to .125.

Physics considerations not appropriately accounted for in the GAM-II structure are included, where possible, by insertion of additional points. In order for MC^2-II[9] to be able to generate multigroup cross sections in the standard CSEWG structure, it was required to relocate all energy bounds such that they lie as integral multiples of the MC^2-II ultra fine group lethargy width (1/120). This has been done in all cases with the single exception of the MUFT[3] boundary at lethargy 16.588 rather than the MC^2-II point at 16.583. The 16.588 lethargy corresponds to .625 eV, an energy frequently used to join the fast and thermal cross section sets. With these additions the new file is *compatible* with past design experience; the file is collapsable to GAM-I, GAM-II, CSEWG Data Testing Structure, LASL 30 Group, MUFT, Shielding Subcommittee Structure, etc.*

B. Incorporation of Specific Cross Section Features

Due to the much wider energy range encountered and the diversity of problems addressed in the fast energy range, merely taking the union of all previous design meshes (as done for the Standard Thermal Structure) was not deemed to be adequate. Hence, letters and telephone solicitations were sent to a wide community of applications oriented evaluators, methods developers, and nuclear designers in an attempt to document past experience and recommendations regarding physical phenomena important in calculations in a wide range of nuclear design applications. Responses were such that particular attention has been paid to the cross section features and energy ranges described in Appendix A and Appendix B. Figures 1 and 2 illustrate the group divisions about the 24 keV iron minima and 2.85 keV sodium resonance as examples. No attempt was made to reflect the rapid cross section fluctuations in the resonance range for the heavy nuclides.

IV. SENSITIVITY TESTING

A. Flux Independence

The result of incorporating the suggestions made in Section III-B into the basic GAM-II structure yields a structure which must be tested to demonstrate its utility for a wide variety of problems. The fundamental considerations for "general" applicability is that the structure must be chosen so that *group constants are relatively insensitive to reasonable choices of the within-group weighting spectra*; that is, a spread of values is observed which does not exceed the recognized uncertainties in nuclear data. The sensitivity of measured parameters (reaction rate ratios, k_{eff}, etc.) to variations in the group constants with changes in flux weighting must be determined by a series of computer investigations for important problems. However, the magnitude of these variations is straightforward to calculate and can serve directly as a guide. This limited "testing" is presently underway. Stacey et al.[10] have already tried such a scheme and found certain group constants quite sensitive to changes in group structure. However, they were examining structures of .1 and .25 which are relatively coarse compared to the structure proposed herein. With our energy bounds, one anticipates changes of less than 1% in group constants for reasonable choices of the infinitely dilute weighting function. The variation in group constants for U^{235} (MAT 1157) total, fission, elastic scattering and capture to weighting spectra of 1/E, constant, and fission spectra have been investigated.[11]

B. Composition Factors

For the Bondarenko pseudo-composition independent cross section representation, the "standard" library can be tested directly in the sense that the energy dependence of the background total cross section/absorbed atom must be minimal. The probability of significant energy variation in the background total cross section across an energy group is generally assumed to be small. This is to be checked quantitatively for several assumed mixture concentrations.

V. FINE GROUP WEIGHTING AND OUTPUT FORMAT

A. Fine Group Weighting

For those libraries created in the Bondarenko format[12] (infinitely dilute cross sections and self shielding factors tabulated for various temperatures and background cross section) it is suggested that the smooth flux variation consist of a 1/E slowing down spectrum tied to a fission spectrum and joined (at energies $\geq$10 MeV) to a fusion spectrum.

The self shielding in this model is taken into account through division by the total cross section.

The motivation for the inclusion of a (D,T) source variation at high energies is simply that most applications where these energies are of interest involve a thermonuclear source. Many LMFBR reactor applications presently treat this energy region rather cavalierly; however, this energy region is crucial to CTR and weapon problems. Thus, the proposed weighting function is again motivated by the desire to make the resulting multigroup data set as generally useful as possible.

*The new structure is based upon .05 lethargy widths down to ~100 keV, .125 lethargy widths to ~1 keV and .25 lethargy units below.

B. Output Format

The output format proposed herein is the CCCC[13] format for ease in interfacing the data file directly into a larger code system and because this multigroup file is already formatted. Another feature of this format is the suppression of superfluous zeroes in transfer matrix arrays.

VI. CONCLUSION

The energy bounds for a generally applicable set of fine multigroup constants in the fast (and epithermal) energy range are given in Table I. These have been derived by consideration of past design experience and particular cross section features known to be important in neutron transport calculations. It is suggested that if the Bondarenko flux model is adopted, the smooth flux variation for within group weighting be a 1/E slowing down spectrum tied to a fission spectrum and joined (at energies $\geq$ 10 MeV) to a fusion spectrum. Self shielding in this case is taken into account through division by the total cross section. Another alternative would be to calculate, in detail, the flux thought to be appropriate for a large class of problems. It is recommended that the standardized multigroup file be output in the CCCC format.

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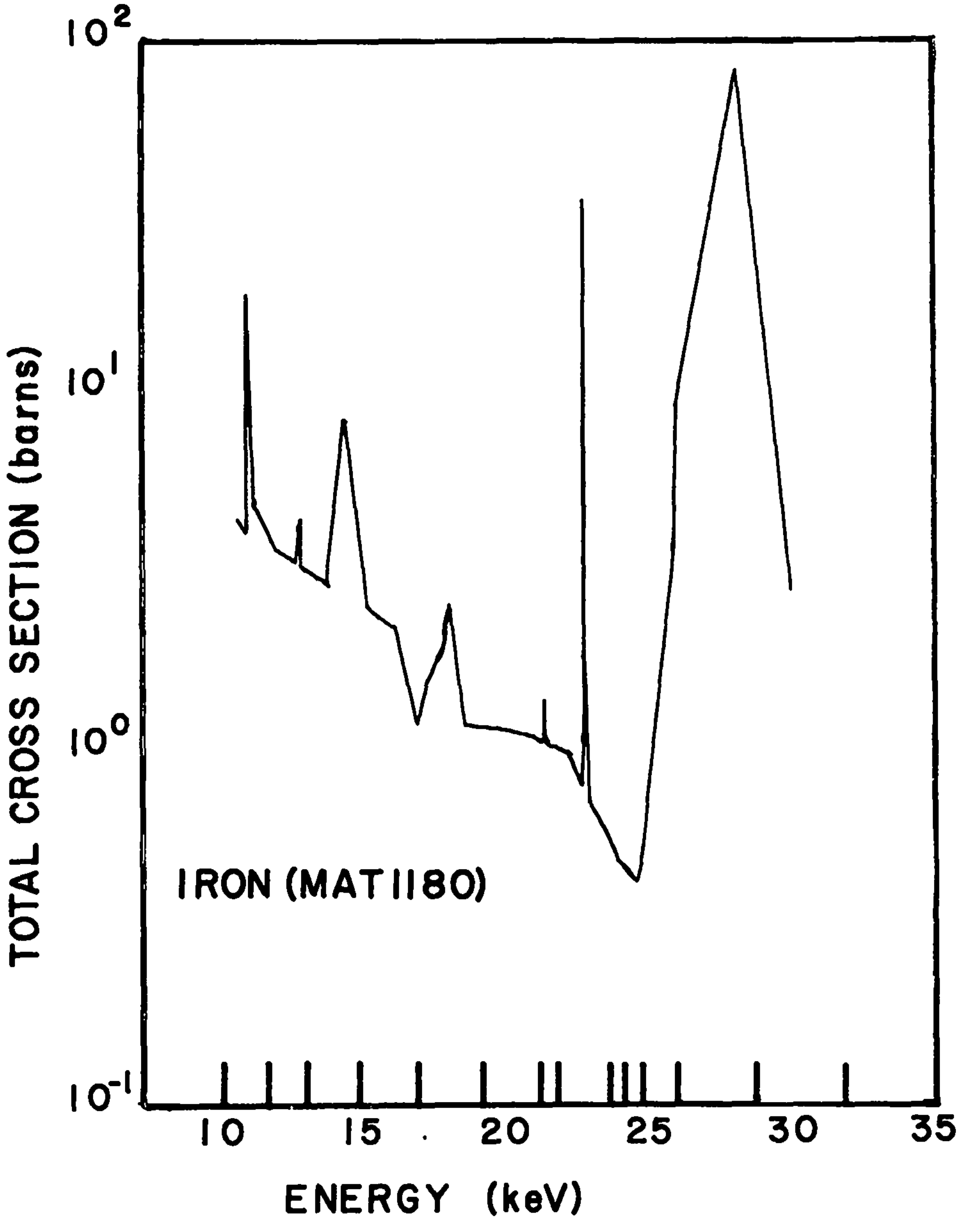

Fig. 1. Proposed CSEWG Standard Structure in the Vicinity of 24 keV Iron Minima (Group Boundaries Indicated by Tick Marks on Abscissa).

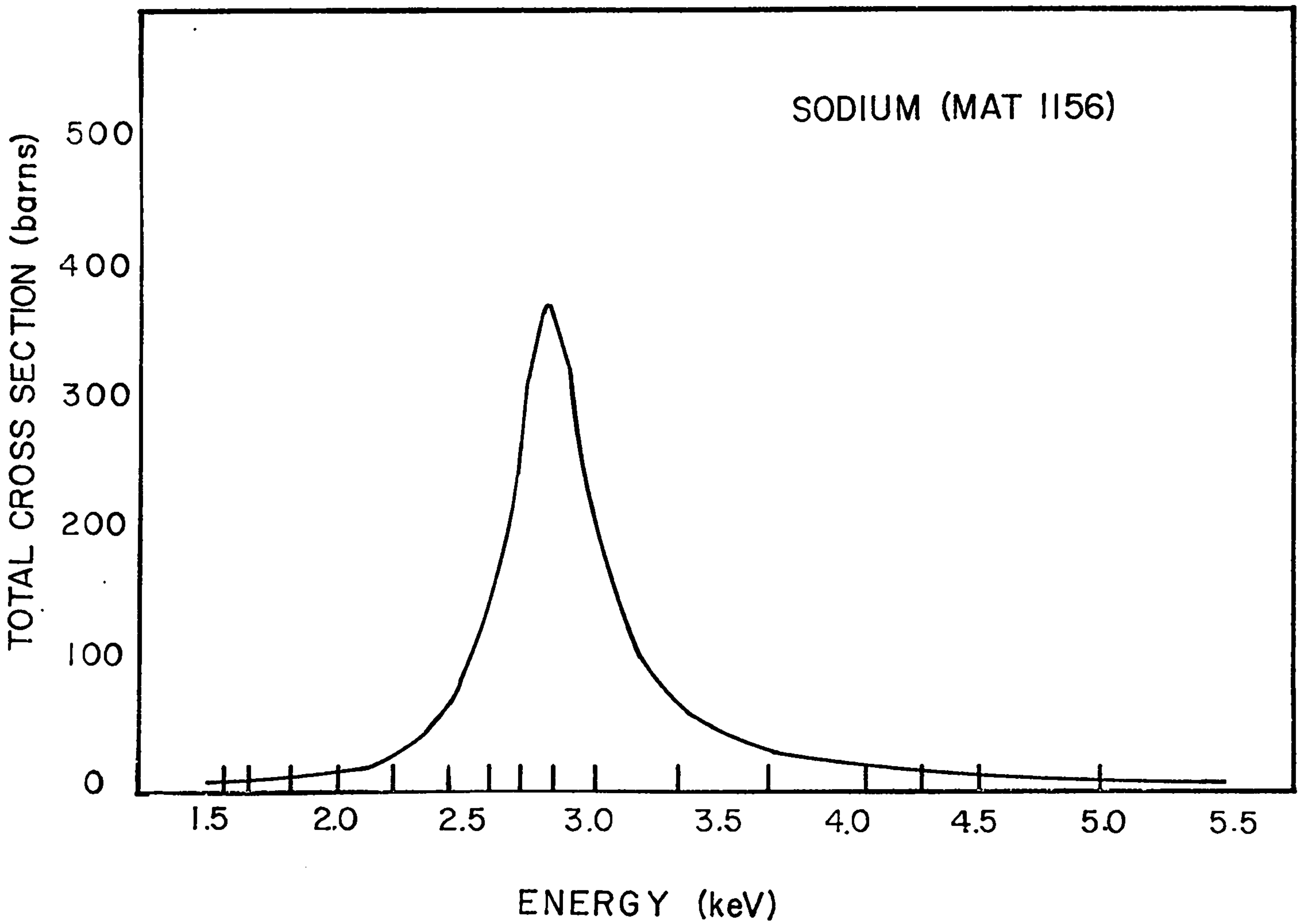

Fig. 2. Proposed CSEWG Standard Structure in the Vicinity of the 2.85 keV Sodium Resonance (Group Boundaries Indicated by Tick Marks on Abscissa).

TABLE I

PROPOSED ENERGY BOUNDS FOR THE STANDARD CSEWG MULTIGROUP FILE

(MAXIMUM ENERGY=19.970 MEV ,MINIMUM LETHARGY= -0.69167)

GROUP	ENERGY(LOWER BOUND) (E.V.)	LETHARGY	LETHARGY DIFFERENCE ROUNDED TO 3 SIGN. FIGURES
1	.19640E+08	-.67500E+00	.017
2	.19155E+08	-.65000E+00	.025
3	.18682E+08	-.62500E+00	.025
4	.18221E+08	-.60000E+00	.025
5	.17771E+08	-.57500E+00	.025
6	.17333E+08	-.55000E+00	.025
7	.16905E+08	-.52500E+00	.025
8	.16487E+08	-.50000E+00	.025
9	.16080E+08	-.47500E+00	.025
10	.15683E+08	-.45000E+00	.025
11	.15296E+08	-.42500E+00	.025
12	.14918E+08	-.40000E+00	.025
13	.14550E+08	-.37500E+00	.025
14	.14191E+08	-.35000E+00	.025
15	.13840E+08	-.32500E+00	.025
16	.13499E+08	-.30000E+00	.025
17	.13165E+08	-.27500E+00	.025
18	.12840E+08	-.25000E+00	.025
19	.12523E+08	-.22500E+00	.025
20	.12214E+08	-.20000E+00	.025
21	.11912E+08	-.17500E+00	.025
22	.11618E+08	-.15000E+00	.025
23	.11331E+08	-.12500E+00	.025
24	.11052E+08	-.10000E+00	.025
25	.10779E+08	-.75000E-01	.025
26	.10513E+08	-.50000E-01	.025
27	.10253E+08	-.25000E-01	.025
28	.10000E+08	0.	.025
29	.97531E+07	.25000E-01	.025
30	.95123E+07	.50000E-01	.025
31	.92774E+07	.75000E-01	.025
32	.90484E+07	.10000E+00	.025
33	.88250E+07	.12500E+00	.025
34	.86071E+07	.15000E+00	.025
35	.83946E+07	.17500E+00	.025
36	.81873E+07	.20000E+00	.025
37	.79852E+07	.22500E+00	.025
38	.77880E+07	.25000E+00	.025
39	.75957E+07	.27500E+00	.025
40	.74082E+07	.30000E+00	.025
41	.72253E+07	.32500E+00	.025
42	.70469E+07	.35000E+00	.025
43	.68729E+07	.37500E+00	.025
44	.67032E+07	.40000E+00	.025
45	.66476E+07	.40833E+00	.008
46	.65924E+07	.41667E+00	.008
47	.65377E+07	.42500E+00	.008
48	.63763E+07	.45000E+00	.025
49	.62189E+07	.47500E+00	.025
50	.60653E+07	.50000E+00	.025
51	.59156E+07	.52500E+00	.025
52	.57695E+07	.55000E+00	.025
53	.54881E+07	.60000E+00	.050
54	.52205E+07	.65000E+00	.050
55	.49659E+07	.70000E+00	.050
56	.48432E+07	.72500E+00	.025
57	.47237E+07	.75000E+00	.025

TABLE I (cont.)

58	.46070E+07	.77500E+00	.025
59	.44933E+07	.80000E+00	.025
60	.42741E+07	.85000E+00	.050
61	.40657E+07	.90000E+00	.050
62	.38674E+07	.95000E+00	.050
63	.36788E+07	.10000E+01	.050
64	.34994E+07	.10500E+01	.050
65	.33287E+07	.11000E+01	.050
66	.32465E+07	.11250E+01	.025
67	.31664E+07	.11500E+01	.025
68	.30882E+07	.11750E+01	.025
69	.30119E+07	.12000E+01	.025
70	.28650E+07	.12500E+01	.050
71	.27253E+07	.13000E+01	.050
72	.25924E+07	.13500E+01	.050
73	.24660E+07	.14000E+01	.050
74	.24251E+07	.14167E+01	.017
75	.23852E+07	.14333E+01	.017
76	.23653E+07	.14417E+01	.008
77	.23457E+07	.14500E+01	.008
78	.23069E+07	.14667E+01	.017
79	.22689E+07	.14833E+01	.017
80	.22313E+07	.15000E+01	.017
81	.21225E+07	.15500E+01	.050
82	.20190E+07	.16000E+01	.050
83	.19691E+07	.16250E+01	.025
84	.19205E+07	.16500E+01	.025
85	.18731E+07	.16750E+01	.025
86	.18268E+07	.17000E+01	.025
87	.17377E+07	.17500E+01	.050
88	.16530E+07	.18000E+01	.050
89	.16122E+07	.18250E+01	.025
90	.15724E+07	.18500E+01	.025
91	.15335E+07	.18750E+01	.025
92	.14957E+07	.19000E+01	.025
93	.14227E+07	.19500E+01	.050
94	.13534E+07	.20000E+01	.050
95	.12873E+07	.20500E+01	.050
96	.12246E+07	.21000E+01	.050
97	.11943E+07	.21250E+01	.025
98	.11648E+07	.21500E+01	.025
99	.11080E+07	.22000E+01	.050
100	.10540E+07	.22500E+01	.050
101	.10026E+07	.23000E+01	.050
102	.97783E+06	.23250E+01	.025
103	.96164E+06	.23417E+01	.017
104	.95369E+06	.23500E+01	.008
105	.90718E+06	.24000E+01	.050
106	.86294E+06	.24500E+01	.050
107	.82085E+06	.25000E+01	.050
108	.78082E+06	.25500E+01	.050
109	.74274E+06	.26000E+01	.050
110	.70651E+06	.26500E+01	.050
111	.67206E+06	.27000E+01	.050
112	.63928E+06	.27500E+01	.050
113	.60810E+06	.28000E+01	.050
114	.57844E+06	.28500E+01	.050
115	.55023E+06	.29000E+01	.050
116	.53665E+06	.29250E+01	.025
117	.52340E+06	.29500E+01	.025
118	.51047E+06	.29750E+01	.025

TABLE I (cont.)

119	.49787E+06	.30000E+01	.025
120	.47359E+06	.30500E+01	.050
121	.45049E+06	.31000E+01	.050
122	.42852E+06	.31500E+01	.050
123	.40762E+06	.32000E+01	.050
124	.38774E+06	.32500E+01	.050
125	.36883E+06	.33000E+01	.050
126	.35084E+06	.33500E+01	.050
127	.33373E+06	.34000E+01	.050
128	.31746E+06	.34500E+01	.050
129	.30962E+06	.34750E+01	.025
130	.30197E+06	.35000E+01	.025
131	.29452E+06	.35250E+01	.025
132	.28725E+06	.35500E+01	.025
133	.28015E+06	.35750E+01	.025
134	.27324E+06	.36000E+01	.025
135	.25991E+06	.36500E+01	.050
136	.24724E+06	.37000E+01	.050
137	.23518E+06	.37500E+01	.050
138	.22371E+06	.38000E+01	.050
139	.21280E+06	.38500E+01	.050
140	.20242E+06	.39000E+01	.050
141	.19255E+06	.39500E+01	.050
142	.18316E+06	.40000E+01	.050
143	.17422E+06	.40500E+01	.050
144	.16992E+06	.40750E+01	.025
145	.16573E+06	.41000E+01	.025
146	.16163E+06	.41250E+01	.025
147	.15764E+06	.41500E+01	.025
148	.14996E+06	.42000E+01	.050
149	.14264E+06	.42500E+01	.050
150	.13569E+06	.43000E+01	.050
151	.12907E+06	.43500E+01	.050
152	.12277E+06	.44000E+01	.050
153	.11679E+06	.44500E+01	.050
154	.11109E+06	.45000E+01	.050
155	.98037E+05	.46250E+01	.125
156	.86517E+05	.47500E+01	.125
157	.76351E+05	.48750E+01	.125
158	.67379E+05	.50000E+01	.125
159	.62511E+05	.50750E+01	.075
160	.59462E+05	.51250E+01	.050
161	.56562E+05	.51750E+01	.050
162	.52475E+05	.52500E+01	.075
163	.46309E+05	.53750E+01	.125
164	.40868E+05	.55000E+01	.125
165	.36066E+05	.56250E+01	.125
166	.35175E+05	.56500E+01	.025
167	.34307E+05	.56750E+01	.025
168	.31828E+05	.57500E+01	.075
169	.28088E+05	.58750E+01	.125
170	.26058E+05	.59500E+01	.075
171	.24788E+05	.60000E+01	.050
172	.24176E+05	.60250E+01	.025
173	.23579E+05	.60500E+01	.025
174	.21875E+05	.61250E+01	.075
175	.21335E+05	.61500E+01	.025
176	.19305E+05	.62500E+01	.100
177	.17036E+05	.63750E+01	.125
178	.15034E+05	.65000E+01	.125
179	.13268E+05	.66250E+01	.125

TABLE I (cont.)

180	.11709E+05	.67500E+01	.125
181	.10333E+05	.68750E+01	.125
182	.91188E+04	.70000E+01	.125
183	.80473E+04	.71250E+01	.125
184	.71017E+04	.72500E+01	.125
185	.62673E+04	.73750E+01	.125
186	.55308E+04	.75000E+01	.125
187	.50045E+04	.76000E+01	.100
188	.45283E+04	.77000E+01	.100
189	.43074E+04	.77500E+01	.050
190	.40973E+04	.78000E+01	.050
191	.37074E+04	.79000E+01	.100
192	.33546E+04	.80000E+01	.100
193	.30354E+04	.81000E+01	.100
194	.28635E+04	.81583E+01	.058
195	.27465E+04	.82000E+01	.042
196	.26126E+04	.82500E+01	.050
197	.24852E+04	.83000E+01	.050
198	.22487E+04	.84000E+01	.100
199	.20347E+04	.85000E+01	.100
200	.18411E+04	.86000E+01	.100
201	.16659E+04	.87000E+01	.100
202	.15846E+04	.87500E+01	.050
203	.15073E+04	.88000E+01	.050
204	.13639E+04	.89000E+01	.100
205	.12341E+04	.90000E+01	.100
206	.96112E+03	.92500E+01	.250
207	.74852E+03	.95000E+01	.250
208	.58295E+03	.97500E+01	.250
209	.45400E+03	.10000E+02	.250
210	.35358E+03	.10250E+02	.250
211	.27536E+03	.10500E+02	.250
212	.21445E+03	.10750E+02	.250
213	.16702E+03	.11000E+02	.250
214	.13007E+03	.11250E+02	.250
215	.10130E+03	.11500E+02	.250
216	.78893E+02	.11750E+02	.250
217	.61442E+02	.12000E+02	.250
218	.47851E+02	.12250E+02	.250
219	.37267E+02	.12500E+02	.250
220	.29023E+02	.12750E+02	.250
221	.22603E+02	.13000E+02	.250
222	.17603E+02	.13250E+02	.250
223	.13710E+02	.13500E+02	.250
224	.10677E+02	.13750E+02	.250
225	.83153E+01	.14000E+02	.250
226	.64760E+01	.14250E+02	.250
227	.50435E+01	.14500E+02	.250
228	.39279E+01	.14750E+02	.250
229	.30590E+01	.15000E+02	.250
230	.23824E+01	.15250E+02	.250
231	.18554E+01	.15500E+02	.250
232	.14450E+01	.15750E+02	.250
233	.11254E+01	.16000E+02	.250
234	.87642E+00	.16250E+02	.250
235	.83368E+00	.16300E+02	.050
236	.68256E+00	.16500E+02	.200
237	.62506E+00	.16588E+02	.088
238	.53158E+00	.16750E+02	.162
239	.41399E+00	.17000E+02	.250

APPENDIX A

SPECIFIC CROSS SECTION PHENOMENA CONSIDERED

Material	Minima	Resonance	Other
Li^{6}		250 keV	
Be^{9}			(n,2n) threshold at ~2 MeV
C^{12}	6.6 MeV		discrete inelastic threshold at 4.8 MeV
N^{14}	4.86 MeV		
O^{16}	2.35 MeV	.44 MeV 1. 1.31	effective threshold at ~10 MeV for $O^{17}(n,p)N^{17} \rightarrow$ delayed neutron
Na^{23}	.297 MeV .52 1.52 1.88 3.08	2.85 keV	
Al^{27}	25 keV	35.2 keV	
Si^{28}	.13 MeV		
Fe^{56}	24 keV .165 MeV .308 .955 1.195		
Ni^{58}	60 keV	17 keV	
U^{238}			effective fission threshold at ~1 MeV
Pu^{239}			inelastic scattering threshold at 8 keV

APPENDIX B

GENERAL ENERGY BOUNDARY CONSIDERATIONS

1. Extension to 20 MeV - current evaluations provide data extending to 20 MeV.
2. (n,2n), (n,3n) and (n,4n) thresholds - particularly for Na, Fe, O, C, Al, D, ^{3}H, Li, U, and Pu.
3. Provision for ample structure in describing (D,T) source.
4. Absolute delayed neutron yield curve generally changes markedly between 5 and 7 MeV.
5. Other group structures in widespread use.