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FCXSEC: Multigroup Cross-Section Libraries for Nuclear Fuel Cycle Shielding Calculations

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FCXSEC: MULTIGROUP CROSS-SECTION LIBRARIES
FOR NUCLEAR FUEL CYCLE SHIELDING CALCULATIONS*

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* Composition-dependent libraries derived from the VITAMIN-C Library
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ABSTRACT

Starting with the pseudo-composition-independent VITAMIN-C cross-section library, composition-dependent fine- $(171n-36\gamma)$ and broad-group $(22n-21\gamma)$ self-shielded AMPX master, broad-group microscopic ANISN-formatted, and broad-group macroscopic ANISN-formatted cross-section libraries were generated to be used for nuclear fuel cycle shielding calculations. The specifications for the data and the procedure used to prepare the libraries are described.

1. INTRODUCTION

The ORNL Chemical Technology Division is involved in a wide variety of nuclear fuel cycle activities that involve the processing and handling of radioactive materials with significant radioactivity. To properly design fuel cycle facilities and equipment it is often necessary to calculate the amount of shielding material that would be required to reduce the radiation dose rate to some specified level. The approach most often used in making this calculation is to use the computer code ANISM¹ to calculate the radiation transport through a one-dimensional radiation shield and to convert the resulting radiation source into dose rates. Occasionally, a more complex problem will require a two- or three-dimensional shielding calculation using DOT² or MORSE,³ respectively. In all of these cases,

three principal types of input are required: the radiation source strength (neutrons and/or gamma rays), a description of the physical problem (dimensions, nuclide concentrations), and cross sections which characterize the interaction of the radiation with matter.

This report is concerned with the generation of cross-section libraries for use in the shielding calculations. The library used in the past for ANISN calculations for nuclear fuel cycle activities was an in-house, coupled 27-neutron-20-gamma-ray group, microscopic cross-section library. This library suffered from two major deficiencies: (1) the source of the cross-section data and the methods by which the library was produced were unknown, and (2) some of the cross-section data for key materials were apparently erroneous.⁴ To alleviate these problems, the ORNL Chemical Technology Division sponsored work in the UCC-ND Computer Sciences Division involving the processing and documentation of AMPX master⁵ and ANISN-formatted microscopic and macroscopic cross-section libraries -- hereinafter referred to as the FCXSEC libraries. These libraries were to have the following attributes:

1. be based on "accepted," currently available, pseudo-problem-independent, cross-section data;
2. include a wide variety of nuclides in a variety of specified materials and concentrations;
3. have neutron and gamma-ray energy structures compatible with a broad class of radiation transport calculations required in nuclear fuel cycle studies;
4. be available as fine-group and broad-group microscopic libraries in AMPX master format as well as broad-group microscopic and macroscopic libraries in ANISN format;

5. be tested for accuracy by checking for internal data consistency;
and
6. be documented with respect to the sources of the basic cross-section data, the processing of the data, and the results of the first order check of the cross sections.

This report fulfills the sixth of the desired attributes of the FCXSEC libraries--that they be well documented. Section 2 describes the sources of the basic cross-section data used in this work. Section 3 describes the processing of these data into microscopic and macroscopic broad-group AMPX master and ANISN-formatted cross-section libraries and the first-order checks of the fine- and broad-group master libraries.

Foreknowledge of the third attribute (above) enabled a separate project to develop an updated photon library⁶ for the ORIGEN⁷ computer code that has an energy group structure that is compatible with the broad-group photon energy structure described herein. This library will allow ORIGEN to be used to predict the photon energy distribution for input to ANISN with a minimum of adjustment.

2. SOURCE OF THE BASIC CROSS-SECTION DATA USED TO GENERATE THE FCXSEC CROSS-SECTION LIBRARIES

Starting point for the generation of the FCXSEC cross-section libraries was the pseudo-problem-independent VITAMIN-C neutron, photon-production, and photon-interaction cross-section libraries in AMPX master format.^{8,9} The VITAMIN-C library contains 171 neutron (171n) and 36 gamma-ray (36 γ) groups and utilizes Bondarenko factors for interpolation to provide problem-dependent resonance self-shielding and temperature corrections. The VITAMIN-C neutron and gamma-ray group structures are listed in Tables 1 and 2, respectively.

Principal source of evaluated data from which the VITAMIN-C data were derived was ENDF/B-IV evaluations.¹⁰ For material not found in ENDF/B-IV, evaluated data from the ENDL library were used.¹¹ The multigroup neutron cross sections and Bondarenko factors were generated with MINX,¹² while the gamma-ray production and interaction cross sections were generated with the LAPHNGAS and SMUG modules, respectively, of the AMPX system.⁵

A detailed discussion of the characteristics of the VITAMIN-C library is given in Ref. 8. The library is distributed by the Radiation Shielding Information Center (RSIC)^{*} in a package identified as DLC-41/VITAMIN-C.

*Radiation Shielding Information Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Table 1. VITAMIN-C 171-Group Neutron Energy Structure

Group No.	Upper Energy (eV)	Group No.	Upper Energy (eV)	Group No.	Upper Energy (eV)
1	1.7333+7	58	1.1648+6	115	2.8500+4
2	1.6487+7	59	1.1080+6	116	2.7000+4
3	1.5683+7	60	1.0026+6	117	2.6058+4
4	1.4918+7	61	9.6164+5	118	2.4788+4
5	1.4550+7	62	9.0718+5	119	2.4176+4
6	1.4191+7	63	8.6294+5	120	2.3579+4
7	1.3840+7	64	8.2085+5	121	2.1875+4
8	1.3499+7	65	7.8082+5	122	1.9305+4
9	1.2840+7	66	7.4274+5	123	1.5034+4
10	1.2214+7	67	7.0651+5	124	1.1709+4
11	1.1618+7	68	6.7206+5	125	9.1188+3
12	1.1052+7	69	6.3928+5	126	7.1017+3
13	1.0513+7	70	6.0810+5	127	5.5308+3
14	1.0000+7	71	5.7844+5	128	4.3074+3
15	9.5123+6	72	5.5023+5	129	3.7074+3
16	9.0484+6	73	5.2340+5	130	3.3546+3
17	8.6071+6	74	4.9787+5	131	3.0354+3
18	8.1873+6	75	4.5049+5	132	2.7465+4
19	7.7880+6	76	4.0762+5	133	2.6126+3
20	7.4082+6	77	3.8774+5	134	2.4852+3
21	7.0469+6	78	3.6883+5	135	2.2487+3
22	6.7032+6	79	3.3373+5	136	2.0347+3
23	6.5924+6	80	3.0197+5	137	1.5846+3
24	6.3763+6	81	2.9850+5	138	1.2341+3
25	6.0653+6	82	2.9720+5	139	9.6112+2
26	5.7695+6	83	2.9452+5	140	7.4852+2
27	5.4881+6	84	2.8725+5	141	5.8295+2
28	5.2205+6	85	2.7324+5	142	4.5400+2
29	4.9659+6	86	2.4724+5	143	3.5358+2
30	4.7237+6	87	2.3518+5	144	2.7536+2
31	4.4933+6	88	2.2371+5	145	2.1445+2
32	4.0657+6	89	2.1280+5	146	1.6702+2
33	3.6788+6	90	2.0242+5	147	1.3007+2
34	3.3287+6	91	1.9255+5	148	1.0130+2
35	3.1664+6	92	1.8316+5	149	7.8892+1
36	3.0119+6	93	1.7422+5	150	6.1442+1
37	2.8650+6	94	1.6573+5	151	4.7851+1
38	2.7253+6	95	1.5764+5	152	3.7267+1
39	2.5924+6	96	1.4996+5	153	2.9203+1
40	2.4660+6	97	1.4264+5	154	2.2603+1
41	2.3852+6	98	1.3569+5	155	1.7603+1
42	2.3653+6	99	1.2907+5	156	1.3710+1
43	2.3457+6	100	1.2277+5	157	1.0677+1
44	2.3069+6	101	1.1679+5	158	8.3152+0
45	2.2313+6	102	1.1109+5	159	6.4760+0
46	2.1225+6	103	9.8037+4	160	5.0435+0
47	2.0190+6	104	8.6517+4	161	3.9279+0
48	1.9205+6	105	8.2500+4	162	3.0590+0
49	1.8268+6	106	7.9500+4	163	2.3724+0
50	1.7377+6	107	7.2000+4	164	1.8554+0
51	1.6530+6	108	6.7379+4	165	1.4450+0
52	1.5724+6	109	5.6562+4	166	1.1254+0
53	1.4957+6	110	5.2475+4	167	8.7642-1
54	1.4227+6	111	4.6309+4	168	6.8256-1
55	1.3534+6	112	4.0868+4	169	5.3158-1
56	1.2873+6	113	3.4307+4	170	4.1399-1
57	1.2246+6	114	3.1828+4	171 ^a	1.0000-1

^aBottom energy of group 171 is 1.0000-5 eV.

Table 2. VITAMIN-C 36-Group Gamma-Ray Energy Structure

Group No.	Upper Energy (eV)	Group No.	Upper Energy (eV)
1	1.40+7	19	1.33+6
2	1.20+7	20	1.00+6
3	1.00+7	21	8.00+5
4	8.00+6	22	7.00+5
5	7.50+6	23	6.00+5
6	7.00+6	24	5.12+5
7	6.50+6	25	5.10+5
8	6.00+6	26	4.50+5
9	5.50+6	27	4.00+5
10	5.00+6	28	3.00+5
11	4.50+6	29	2.00+5
12	4.00+6	30	1.50+5
13	3.50+6	31	1.00+5
14	3.00+6	32	7.50+4
15	2.50+6	33	6.00+4
16	2.00+6	34	4.50+4
17	1.66+6	35	3.00+4
18	1.50+6	36 ^a	2.00+4

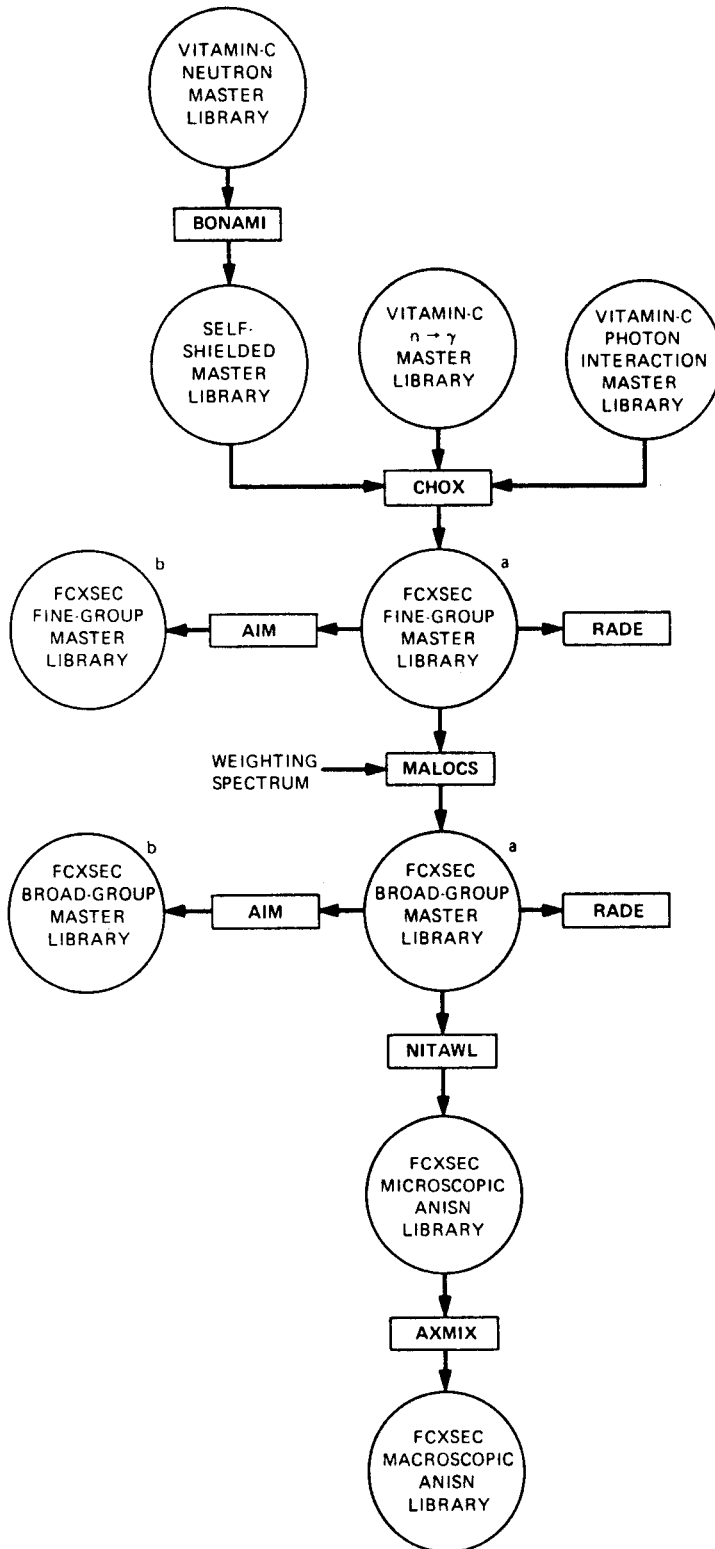
^aBottom energy of the lowest group is 1.00+4 eV.

3. GENERATION OF THE FCXSEC CROSS-SECTION LIBRARIES

Starting with the VITAMIN-C library as distributed by the Radiation Shielding Information Center,⁹ the objectives of the FCXSEC project were as follows:

1. To generate a coupled fine-group ($171n-36\gamma$) microscopic AMPX master library of composition-dependent (self-shielded) cross sections for mixture components and of cross sections for selected materials processed for various values of potential scattering cross sections. (Hereinafter, this library is denoted as the FCXSEC fine-group master library.)
2. Using a specified weighting function, to collapse the FCXSEC fine-group master library data into a broad-group ($22n-21\gamma$) microscopic AMPX master library. (Hereinafter, this library is denoted as the FCXSEC broad-group master library.)
3. To generate an ANISN-formatted microscopic cross-section library from selected data in the FCXSEC broad-group master library. (Hereinafter, this library is denoted as the FCXSEC microscopic ANISN library.)
4. To mix data from the FCXSEC microscopic ANISN library to generate a macroscopic ANISN-formatted library. (Hereinafter, this library is denoted as the FCXSEC macroscopic ANISN library.)

A flowchart showing the calculational procedure to generate the various FCXSEC libraries is shown in Fig. 1. The steps required to produce each FCXSEC library are described below. Results of a first-order check of the fine- and broad-group master libraries are described at the conclusion of this section.



a. BINARY MASTER LIBRARY.
 b. BCD-FORMATTED MASTER LIBRARY.

Fig. 1. Calculational Sequence for Generating the FCXSEC Cross-Section Libraries.

The FCXSEC Fine-Group (171n-36 γ) Master Library

Using materials from the VITAMIN-C neutron cross-section library, the homogeneous option was used in the BONAMI module of the AMPX system to produce self-shielded 171-group master cross sections for components of the mixtures listed in Table 3. Again using the VITAMIN-C library and the BONAMI module, 171-group master cross sections for the individual materials listed in Table 4 were processed for three values of the potential scattering cross sections -- 0.1, 1000, and 10^8 barns/atom. All materials were processed at a temperature of 300°K.

The CHOX module of the AMPX system was used to combine the fine-group self-shielded neutron data described above with gamma-ray production and gamma-ray interaction data from the VITAMIN-C library.^{8,9} The data were combined into coupled fine-group (171n-36 γ) AMPX master data sets -- the FCXSEC fine-group master library. The data set identification numbers for the mixture-dependent and individual materials in the library are listed in Tables 3 and 4, respectively.

Although cross-section libraries in AMPX master format are not used directly by any transport code (i.e., master formatted data must be further processed into formats required by transport codes), the generality of the format has proven to be both comprehensive and efficient for storing multi-group data. Particulars of a master library are described in Section 11.3 of Refs. 5 and 13. Processed multigroup reaction cross sections (1-D cross sections) and data for scattering processes (2-D data) are identified in a master data set by intergers -- MT numbers. ENDF MT numbers¹⁴ are used, where possible, to identify the appropriate cross-section data. A summary

Table 3. FCXSEC Fine (171n-36 γ)- and Broad (22n-21 γ)-Group
Master Cross-Section Libraries – Mixture Components

Mixture	Isotope	Number Density (atoms/bn-cm)	FCXSEC Master Data Set ID No. ^a	Remarks
H ₂ O	¹ H	6.693-02	126901	
	¹⁶ O	3.347-02	127601	
Borated Water	¹ H	6.543-02	126902	
	¹⁶ O	3.473-02	127602	
	¹⁰ B	2.682-04	127302	
	¹¹ B	1.073-03	116002	No SGRPXS ^b
Concrete	¹ H	1.271-02	126903	
	¹⁶ O	2.948-02	127603	
	Mg	1.983-04	128003	
	²⁷ Al	4.756-04	119303	
	Si	1.263-03	119403	
	³² S	6.576-05	712203	
	Ca	3.893-03	119503	
	Fe	3.295-02	119203	
	K	6.625-05	115003	
Ba	8.334-04	715103		
D ₂ O	D	6.645-02	112004	No SGRPXS
	¹⁶ O	3.332-02	127604	
Lithium Hydride	¹ H	6.215-02	126905	
	⁶ Li	4.661-03	127105	
	⁷ Li	5.749-02	127205	
Boral	¹⁰ B	8.054-04	127306	
	¹¹ B	3.222-03	116006	No SGRPXS
	¹² C	1.007-02	127406	
	²⁷ Al	3.831-02	119306	
Dry Air	¹⁴ N	3.875-05	127507	
	¹⁶ O	1.071-05	127607	
Nitric Acid	¹ H	1.437-02	126908	
	¹⁴ N	1.437-02	127508	
	¹⁶ O	4.310-02	127608	
Uranium Dioxide	²³⁸ U	2.445-02	126209	
	¹⁶ O	4.890-02	127609	
	²³⁵ U	2.445-04	126109	
Stainless Steel 304	Ni	7.406-03	119010	
	Cr	1.765-02	119110	
	Fe	5.860-02	119210	

Table 3. (continued)

Mixture	Isotope	Number Density (atoms/bn-cm)	FCXSEC Master Data Set ID No. ^a	Remarks
UF ₆	²³⁸ U	8.009-03	126211	
	²³⁵ U	8.009-05	126111	
	F	4.805-02	127711	
TBP in Dodecane	¹ H	6.644-02	126912	
	¹² C	3.036-02	127412	
	¹⁶ O	2.644-03	127612	
	³¹ P	6.611-04	712112	
Sm ₂ O ₃	¹⁴⁹ Sm	6.013-03	102713	No SGRPXS
	¹⁶ O	2.884-02	127613	
Eu ₂ O ₃	¹⁵¹ Eu	1.174-02	129014	
	¹⁵³ Eu	1.276-02	129114	
	¹⁶ O	3.675-02	127614	
Gd ₂ O ₃	Gd	2.462-02	103015 ^e	No SGRPXS
	¹⁶ O	3.698-02	127615	
Gd(NO ₃) ₃ in Water	¹ H	6.996-02	126916 ^d	
	¹⁶ O	4.479-02	127616	
	¹⁴ N	3.271-03	127516	
	Gd	1.090-03	103016	No SGRPXS
WB ₂	¹⁰ B	1.263-02	127317	
	¹¹ B	5.053-02	116017	No SGRPXS
	¹⁸² W	8.337-03	458217	
	¹⁸³ W	4.548-02	458317	
	¹⁸⁴ W	9.663-03	458417	
	¹⁸⁶ W	8.969-03	458617	
Spent Fuel Oxide	¹⁶ O	4890-02	127618	
	²³⁸ U	2.620-02	126218	
	²³⁴ U	5.082-06	104318	No SGRPXS
	²³⁵ U	2.236-04	126118	
	²³⁶ U	1.108-04	116318	No SGTPXS
	²³⁷ Np	1.233-05	126318	
	²³⁸ Pu	3.736-06	105018	No SGRPXS
	²³⁹ Pu	1.391-04	126418	
	²⁴⁰ Pu	6.350-05	126518	
	²⁴¹ Pu	3.274-05	126618	No SGRPXS
	²⁴² Pu	1.256-05	116118	No SGRPXS
	²⁴¹ Am	1.602-06	105618	No SGRPXS
	²⁴³ Am	2.326-06	105718	No SGRPXS
²⁴⁴ Cm	5.007-07	116218	No SGRPXS	
Thorium Oxide	²³² Th	2.886-02	129619 ^e	
	²³³ U	1.519-03	126019 ^e	
	¹⁶ O	4.890-02	127619 ^e	

Table 3. (continued)

Mixture	Isotope	Number Density (atoms/bn-cm)	FCXSEC Master Data Set ID No. ^a	Remarks
Uranium Metal	²³⁸ U	4.826-02	126220	
	²³⁵ U	9.652-05	126120	
Silver Zeolite	¹⁰⁷ Ag	1.836-03	113821 ^e	No SGRPXS
	¹⁰⁹ Ag	1.707-03	113921 ^e	No SGRPXS
	²⁷ Al	7.086-03	119321	
	Si	1.772-02	119421	
	¹⁶ O	4.606-02	127621 ^e	

^aThe identification numbers for data sets in the mixtures consist of the ENDF MAT number for the materials processed for the VITAMIN-C library and a two-digit suffix associated with the mixtures as follows:

Suffix	Mixture	Suffix	Mixture	Suffix	Mixture
01	H ₂ O	08	Nitric Acid	15	Gd ₂ O ₃
02	Borated Water	09	Uranium Dioxide	16	Gd(NO ₃) ₃ in water
03	Concrete	10	SS304	17	WB ₂
04	D ₂ O	11	UF ₆	18	Spent Fuel Oxide
05	Lithium Hydride	12	TBP in Dodecane	19	Thorium Oxide
06	Boral	13	Sm ₂ O ₃	20	Uranium Metal
07	Dry Air	14	Eu ₂ O ₃	21	Silver Zeolite

^bThe ENDF evaluation used to produce the VITAMIN-C data did not contain photon-production data. Consequently, there are no secondary gamma-ray production cross sections (SGRPXS) in the FCXSEC data set.

^cGd data set for Gd₂O₃ (mixture 15) in the broad-group master library has ID No. 715315. The broad-group data were derived from fine-group master data set 103015.

^dGd data set for Gd(NO₃)₃ (mixture 16) in the broad-group master library has ID No. 715316. The broad-group data were derived from the fine-group master data set 103016.

^eSubsequent to the generation of the FCXSEC broad-group master library and prior to the time that materials in the FCXSEC fine-group master library were collected onto one tape, an intermediate project tape containing data sets 129619, 126019, 127619, 113821, 113921, and 127621 was damaged. The decision was made not to regenerate the "lost" data sets for the final fine-group library.

Table 4. FCXSEC Fine (171n-36γ)- and Broad (22n-21γ)-Group
 Master Cross-Section Library -- Individual Materials

Material	Potential Scattering Cross Section (bn/atom)	FCXSEC Master Data Set ID No. ^a	Remarks	Material	Potential Scattering Cross Section (bn/atom)	FCXSEC Master Data Set ID No. ^a	Remarks
¹² C	10 ⁻¹	127497		Be	10 ⁻¹	128997	
¹² C	10 ³	127498		Be	10 ³	128998	
¹² C	10 ⁸	127499		Be	10 ⁸	128999	
Na	10 ⁻¹	115697		Ti	10 ⁻¹	128697	
Na	10 ³	115698		Ti	10 ³	128698	
Na	10 ⁸	115699		Ti	10 ⁸	128699	
²⁷ Al	10 ⁻¹	119397		V	10 ⁻¹	119697	
²⁷ Al	10 ³	119398		V	10 ³	119698	
²⁷ Al	10 ⁸	119399		V	10 ⁸	119699	
Fe	10 ⁻¹	119297		⁵⁵ Mn	10 ⁻¹	119797	
Fe	10 ³	119298		⁵⁵ Mn	10 ³	119798	
Fe	10 ⁸	119299		⁵⁵ Mn	10 ⁸	119799	
Zrly ^c	10 ⁻¹	128497	No SGRPXS ^b	⁵⁹ Co	10 ⁻¹	119997	
Zrly	10 ³	128498	No SGRPXS	⁵⁹ Co	10 ³	119998	
Zrly	10 ⁸	128499	No SGRPXS	⁵⁹ Co	10 ⁸	119999	
Cd	10 ⁻¹	128197	No SGRPXS	Cu	10 ⁻¹	129597	
Cd	10 ³	128198	No SGRPXS	Cu	10 ³	129598	
Cd	10 ⁸	128199	No SGRPXS	Cu	10 ⁸	129599	
⁹³ Nb	10 ⁻¹	118997		Sn	10 ⁻¹	715097	
⁹³ Nb	10 ³	118998		Sn	10 ³	715098	
⁹³ Nb	10 ⁸	118999		Sn	10 ⁸	715099	
Mo	10 ⁻¹	128797		¹⁸¹ Ta	10 ⁻¹	128597	
Mo	10 ³	128798		¹⁸¹ Ta	10 ³	128598	
Mo	10 ⁸	128799		¹⁸¹ Ta	10 ⁸	128599	
Pb	10 ⁻¹	128897					
Pb	10 ³	128898					
Pb	10 ⁸	128899					

^aData set ID numbers consist of the ENDF MAT number for the material processed for the VITAMIN-C library and a two-digit suffix of 97, 98, or 99 denoting σ_0 's of 10⁻¹, 10³, or 10⁸, respectively.

^bThe ENDF evaluation used to produce the VITAMIN-C data did not contain photon-production data. Consequently there are no secondary gamma-ray production cross sections (SGRPXS) in the FCXSEC data set.

^cZrly = Zircaloy.

of the 1-D and 2-D multigroup data present in processed master data sets in the FCXSEC fine-group (and the subsequently described broad-group) master library is identified by material in Table 5. The definitions of the MT numbers are given in Appendix A.

To facilitate "reading" of the master library at various computer facilities, the AIM module was used to convert the CHOX-produced binary master library to BCD-format -- the format of the library for distribution. Modules are available in the AMPX system for utilizing the FCXSEC master library by converting the BCD-formatted library to binary format, by spectral collapsing, by spacially weighting the cross sections, by further format conversions, and by performing various service operations such as listing and punching data. The AMPX system is distributed by the Radiation Shielding Information Center.

The FCXSEC Broad-Group (22n-21γ) Master Library

After considering various neutron spectra which would be representative of the spectra encountered in nuclear fuel cycle transport calculations, a fine-group (171n) ^{239}Pu thermal fission-1/E-Maxwellian spectrum was selected to collapse the fine-group neutron cross sections to the broad-group structure (22n) listed in Table 6. Characteristics of the spectrum, which was produced with a fake XLACS-2⁵ case, are as follows:

<u>Spectrum Component</u>	<u>Neutron Energy Range (eV)</u>	<u>Remarks</u>
$^{239}\text{Pu}_{\text{th}}$ fission	$1.1109+5 < E_n \leq 1.7333+7$	Fission spectrum temperature, $1.33+6$ eV
1/E	$4.1399-1 < E_n \leq 1.1109+5$	
Maxwellian	$1.0000-5 \leq E_n \leq 4.1399-1$	Maxwellian spectrum temperature, 300°K .

Table 5. Reaction Cross-Section Data Available in Processed FCXSEC Master Data Sets

Material	Neutron Cross-Section Data		SGRP Data (Process) ^a		Gamma-Ray Interaction Cross-Section Data	
	1-D Processes		2-D Processes		1-D Processes	
	1-D Processes	2-D Processes	1-D Processes	2-D Processes	1-D Processes	2-D Processes
¹ H	1,2,27,101,102,251,252,254,1001,1033,2001	2	102(0)		501,504,516,527,602,1527	504,516
D	1,2,16,27,101,102,251,252,254,285,1001,1033,2001	2,16			501,504,516,527,602,1527	504,516
⁶ Li	1,2,4,24,27,52,91,101,102,103,107,251,252,254,285,1001,1033,2001	2,24,52,91	52(1),102(0)		501,504,516,527,602,1527	504,516
⁷ Li	1,2,4,16,24,27,51,91,101,102,104,251,252,254,285,1001,1033,2001	2,16,24,51,91	51(1),102(0)		501,504,516,527,602,1527	504,516
Be	1,2,6-9,27,46-49,101-107,251,252,254,285,740,741,1001,1033,2001	2,6-9,46-49	102(0),741(1)		501,504,516,527,602,1527	504,516
¹⁰ B	1,2,4,27,51-80,101,103,104,107,113,251,252,254,285,1001,1033,2001	2,51-80	4(1),103(1),781(1)		501,504,516,527,602,1527	504,516
¹¹ B	1,2,4,16,27,51-53,91,101,102,103,105,107,251,252,254,1001,1033,2001	2,16,51-53			501,504,516,527,602,1527	504,516
¹² C	1-4,27,51,91,101,102,107,251,252,254,1001,1033,2001	2,51,91	51(1),102(0)		501,504,516,527,602,1527	504,516
¹⁴ N	1,2,4,16,27,51-77,101-105,107,108,251,252,254,285,1001,1033,2001	2,16,51-77	4(1),102(0),103-105(1),107(1)		501,504,516,527,602,1527	504,516
¹⁶ O	1,2,4,27,51-81,101,102,103,104,107,251,252,254,1001,1033,2001	2,51-81	4(1),22(1),102(0),103(1),107(1)		501,504,516,527,602,1527	504,516
F	1-4,16,22,27,28,51-71,91,101-105,107,251,252,254,285,1001,1033,2001	2,16,22,28,51-71,91	3(1),4(1),102(0),107(1)		501,504,516,527,602,527	504,516
²³ Na	1-4,16,27,51-68,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,51-68,91	51-68(1),102(0)		501,504,516,527,602,1527	504,516
Hg	1,2,3,4,16,22,27,28,51-91,101-103,107,251,252,254,285,1001,1033,2001	2,16,22,28,51-91	4(1),16(1),102(0)		501,504,516,527,602,1527	504,516
²⁷ Al	1,2,4,16,27,51-86,101-105,107,251,252,254,1001,1033,2001	2,16,51-86	4(1),28(1),102(0),103(1)		501,504,516,527,602,1527	504,516
Si	1-4,16,22,27,28,51-72,91,101-104,107,251,252,254,1001,1033,2001	2,16,22,28,51-72,91	4(1),22(1),28(1),102(0),103(1),107(1)		501,504,516,527,602,1527	504,516
³¹ P	1,2,4,16,27,28,91,101,102,103,105,107,251,252,254,285,1001,1033,2001	2,16,28,91	3(1),102(0)		501,504,516,527,602,1527	504,516
³² S	1-4,16,22,27,28,51-73,91,101-108,111,112,251,252,254,285,1001,1033,2001	2,16,22,28,51-73,91	4(1),22(1),28(1),102(0),103(1),107(1)		501,504,516,527,602,1527	504,516

Table 5. (Continued)

Material	Neutron Cross-Section Data		Gamma-Ray Interaction Cross-Section Data		
	1-D Processes	2-D Processes	SGRP Data (Process) ^c	1-D Processes	2-D Processes
K	1,2,4,16,22,27,28,51-67,91,101,102,103,107,251,252,254,1001,1033,2001	2,16,22,28,51-67,91	51(1),52(1),53(1),54(1),55(1),56(1),91(1),102(0),103(1),107(1)	501,504,516,527,602,1527	504,516
Ca	1-4,16,22,27,28,51-73,91,101-108,111,112,251,252,254,285,1001,1033,2001	2,16,22,28,51-73,91	4(1),22(1),28(1),102(0),103(1),107(1)	501,504,516,527,602,1527	504,516
Ti	1-4,16,27,51,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,51,91	3(1),102(0)	501,504,516,527,602,1527	504,516
V	1-4,16,22,27,28,51-54,91,101-105,107,251,252,254,285,1001,1033,2001	2,16,22,28,51-54,91	3(1),16(1),22(1),28(1),102(0)	501,504,516,527,602,1527	504,516
Cr	1-4,16,22,27,28,51-91,101-107,251,252,254,1001,1033,2001	2,16,22,28,51-91	3(1),102(0)	501,504,516,527,602,1527	504,516
⁵⁸ Mn	1-4,16,22,27,28,51-55,91,101-104,106,107,251,252,254,1001,1033,2001	2,16,22,28,51-55,91	3(1),51-55(1),102(0)	501,504,516,527,602,1527	504,516
Fe	1-4,16,22,27,28,51-76,91,101-107,251,252,254,285,1001,1033,2001	2,16,22,28,51-76,91	3(1),51(1),52(1),102(0)	501,504,516,527,602,1527	504,516
⁵⁹ Co	1,2,4,16,27,51-59,91,101-105,107,251,252,254,285,1001,1033,2001	2,16,51-59,91	3(1)	501,504,516,527,602,1527	504,516
Ni	1,2,4,16,27,28,51-65,101-103,107,251,252,254,1001,1033,2001	2,16,28,51-65,91	3(1),102(0)	501,504,516,527,602,1527	504,516
Cu	1-4,16,22,27,28,51-61,91,101-104,106,107,251,252,254,285,1001,1033,2001	2,16,22,28,51-61,91	3(1),102(0)	501,504,516,527,602,1527	504,516
Zr ^{1y}	1,2,4,16,27,51-65,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,51-65,91	none	none	none
⁹³ Nb	1,2,4,16,17,22,27,51-62,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,17,22,51-62,91	3(1),102(0)	501,514,516,527,602,1527	504,516
Mo	1,2,4,16,17,27,91,101,102,251,252,254,285,1001,1033,2001	2,16,17,91	3(1),102(0)	501,504,516,527,602,1527	504,516
¹⁰⁷ Ag	1,2,4,16,27,51-56,91,101-105,107,251,252,254,285,1001,1033,2001	2,16,51-56,91	none	501,504,516,527,602,1527	504,516
¹⁰⁹ Ag	1,2,4,16,27,51-55,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,51-55,91	none	501,504,516,527,602,1527	504,516
Cd	1-4,16,27,51-54,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,51-54,91	none	501,504,516,527,602,1527	504,516

Table 5. (Continued)

Material	Neutron Cross-Section Data			Gamma-Ray Interaction Cross-Section Data		
	1-D Processes	2-D Processes	SGRP Data (Process) ^a	1-D Processes	2-D Processes	2-D Processes
Sn	1,2,4,16,17,27,91,101,102,251,252,254,285,1001,1033,2001	2,16,17,91	3(1),102(0)	501,504,516,527,602,1527		504,516
Ba	1,2,4,16,17,27,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,17,91	3(1),102(0)	501,504,516,527,602,1527		504,516
¹⁴⁷ Sm	1,2,4,16,17,27,51-60,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,17,51-60,91	none	none		none
¹⁵¹ Cu	1-4,16,17,22,27,28,51-59,91,101-107,251,252,254,285,1001,1033,2001	2,16,17,22,28,51-59,91	3(1),51(1),52(1),53(1),54(1),55(1),56(1),57(1),58(1),59(1),102(0)	501,504,516,527,602,1527		504,516
¹⁵³ Eu	1-4,16,17,22,27,28,51-61,91,101-107,251,252,254,285,1001,1033,2001	2,16,17,22,28,51-61,91	3(1),51(1),52(1),53(1),54(1),55(1),56(1),57(1),58(1),59(1),60(1),61(1)	501,504,516,527,602,1527		504,516
Gd	1,2,4,16,17,27,91,101,102,251,252,254,285,1001,1033,2001	2,16,17,91	none	none		none
¹⁸¹ Ta	1,2,4,16,17,27,51-60,91,101,102,103,251,252,254,285,1001,1033,2001	2,16,17,51-60,91	3(1),102(0)	501,504,516,527,602,1527		504,516
¹⁸² W	1,2,4,16,17,27,28,51-58,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,17,28,51-58,91	4(1),102(0)	501,504,516,527,602,1527		504,516
¹⁸³ W	1,2,4,16,17,27,28,51-59,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,17,28,51-59,91	4(1),102(0)	501,504,516,527,602,1527		504,516
¹⁸⁴ W	1,2,4,16,17,27,28,51-59,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,17,28,51-59,91	4(1),103(0)	501,504,516,527,602,1527		504,516
¹⁸⁶ W	1,2,4,16,17,27,28,51-59,91,101-103,107,251,252,254,285,1001,1033,2001	2,16,17,28,51-59,91	4(1),102(0)	501,504,516,527,602,1527		504,516
Pb	1-4,16,17,27,51-85,91,101,102,251,252,254,285,1001,1033,2001	2,16,17,51-85,91	3(1)	501,504,516,527,602,1527		504,516
²³² Th	1,2,4,16,17,18,27,51-58,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-58,91	none	501,504,516,527,602,1527		504,516
²³³ U	1,2,4,16,17,18,27,51-57,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-57,91	none	501,504,516,527,602,1527		504,516
²³⁴ U	1,2,4,16,17,18,27,51-56,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-56,91	none	501,504,516,527,602,1527		504,516
²³⁵ U	1-4,16-21,27,51-66,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-66,91	3(1),4(1),18(0),102(0)	501,504,516,527,602,1527		504,516

Table 5. (continued)

Material	Neutron Cross-Section Data		Gamma-Ray Interaction Cross-Section Data			
	1-D Processes	2-D Processes	SGRP Data (Process) ^a	1-D Processes	2-D Processes	
²³⁸ U	1,2,4,16,17,18,27,51-56,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-56,91	none	501,504,516,527,602,1527	504,516	
²³⁹ U	1-4,16-18,20,21,27,51-76,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-76,91	3(1),18(0),102(0)	501,504,516,527,602,1527	504,516	
²³⁷ Np	1,2,4,16,17,18,27,51-61,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-61,91	none	none	none	
²³⁹ Pu	1-4,16-21,27,51-66,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-66,91	3(1),4(1),18(0),102(0)	501,504,516,527,602,1527	504,516	
²³⁹ Pu	1,2,4,16-21,27,51-76,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-76,91	3(1),4(1),18(0),102(0)	501,504,516,527,602,1527	504,516	
²⁴⁰ Pu	1,2,4,16-21,27,51-62,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-62,91	3(1),4(1),10(0),102(0)	501,504,516,527,602,1527	504,516	
²⁴¹ Pu	1,2,4,16-18,27,51-65,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-65,91	none	501,504,516,527,602,1527	504,516	
²⁴² Pu	1,2,4,16,17,18,27,51-60,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-60,91	none	501,504,516,517,602,1527	504,516	
²⁴¹ Am	1,2,4,18,27,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,91	none	none	none	
²⁴² Am	1,2,4,18,27,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-60,91	none	none	none	
²⁴⁴ Cm	1,2,4,16-18,27,51-60,91,101,102,251,252,254,285,452,1001,1018,1033,2001	2,16,17,51-60,91	none	none	none	

^aSecondary gamma-ray production data are either multiplicities (number of gamma rays produced per neutron induced reaction) or SGRPXS. The "Process" identifies the form of the SGRP data as follows:

Process	Data Form
0	Multiplicities
1	SGRPXS

Table 6. Broad-Group (22n) Neutron Energy Structure

Broad-Group Number	Upper Energy (eV)	Contains Fine Groups ^a
1	1.7333+7	1-9
2	1.2214+7	10-13
3	1.0000+7	14-17
4	8.1873+6	18-23
5	6.3763+6	24-28
6	4.9659+6	29-31
7	4.0657+6	32-35
8	3.0119+6	36-39
9	2.4660+6	40-42
10	2.3457+6	43-48
11	1.8268+6	49-58
12	1.1080+6	59-71
13	5.5023+5	72-101
14	1.1109+5	102-129
15	3.3546+3	130-140
16	5.8295+2	141-147
17	1.0130+2	148-152
18	2.9023+1	153-156
19	1.0677+1	157-161
20	3.0590	162-168
21	5.3156-1	169
22 ^b	4.1399-1	170-171

^aSee Table 1 for a listing of the 171-group structure.

^bBottom energy is 1.0000×10^{-5} eV.

A plot of the neutron spectrum (weighting function) is shown in Fig. 2; the multigroup spectrum is listed in Table 7.

A constant weighting function was selected to collapse the fine-group gamma-ray cross sections to the broad-group (21γ) structure listed in Table 8.

Using the neutron and gamma-ray weighting spectra described above, MALOCS was used to collapse FCXSEC fine-group master library data into the broad-group structure -- the FCXSEC broad-group master library. The data set identification numbers for the mixture-dependent and individual materials in the library are listed in Tables 3 and 4 above, respectively.

The FCXSEC Microscopic ANISN Library

NITAWL was used to produce a broad-group ($22n-21\gamma$) microscopic ANISN-formatted library from data in the broad-group master library. The table of contents for the library is given in Table 9. The library is a "standard" ANISN library, i.e., σ_a is in table position one, σ_T is in position three, σ_{gg} is in position four, and the table length is 46. The library consists of neutron data through Legendre order P_3 and gamma-ray interaction data through Legendre order P_5 . Due to limited data in ENDF evaluations, very few materials have photon production data for order greater than P_0 .

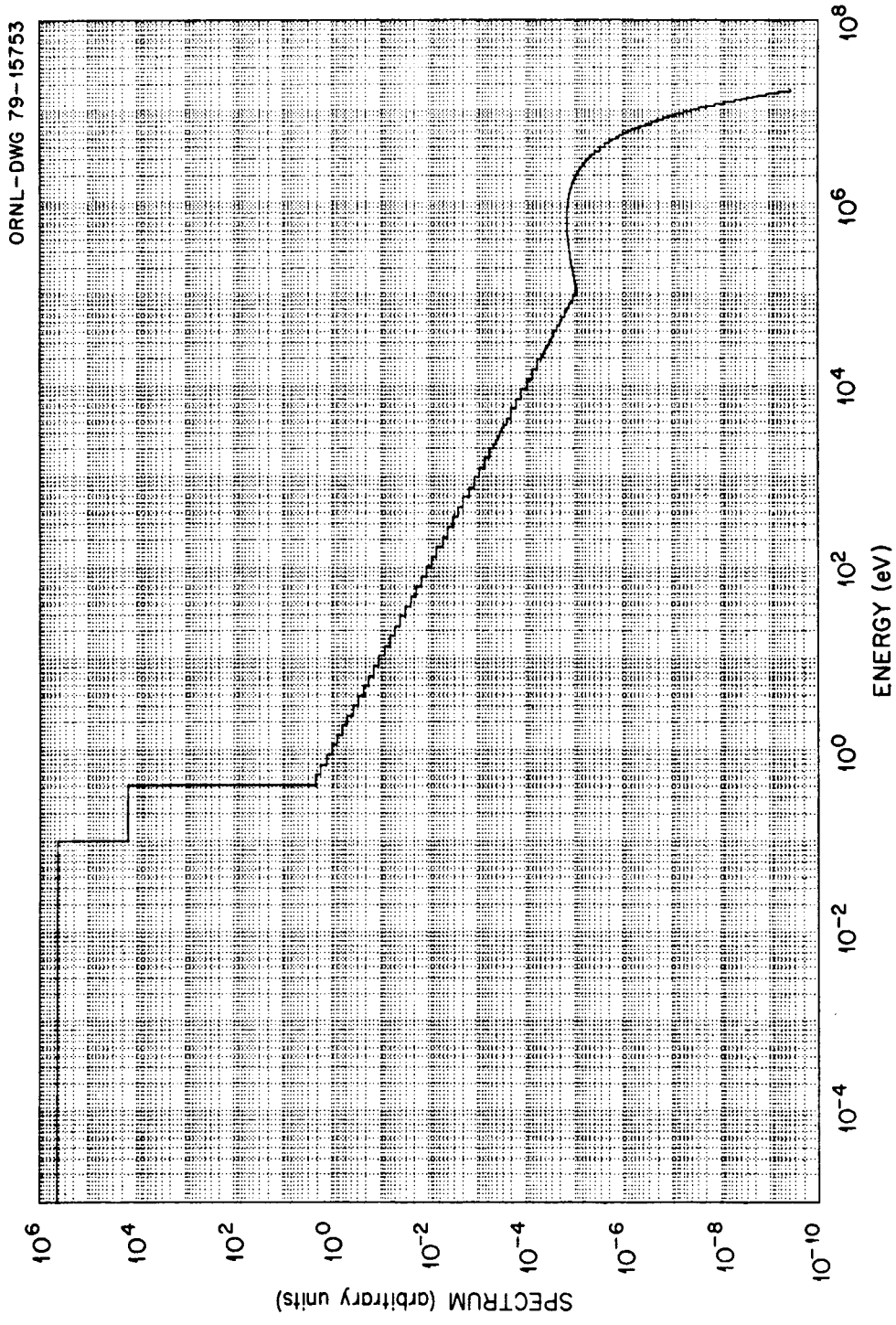


Fig. 2. ²³⁹Pu Thermal Fission-1/E-Maxwellian Spectrum.

Table 7. Fine-Group ^{239}Pu Thermal Fission-
1/E-Maxwellian Weighting Function

Group	Flux	Group	Flux	Group	Flux
1	3.118669E-04	58	7.557980E-01	115	5.406720E-02
2	5.367969E-04	59	1.436780E-00	116	3.551200E-02
3	8.968399E-04	60	5.689900E-01	117	4.996510E-02
4	6.419530E-04	61	7.651670E-01	118	2.499920E-02
5	8.130718E-04	62	6.277140E-01	119	2.500390E-02
6	1.025270E-03	63	6.016590E-01	120	7.501197E-02
7	1.275290E-03	64	5.757490E-01	121	1.249800E-01
8	3.546910E-03	65	5.499250E-01	122	2.500499E-01
9	5.322549E-03	66	5.249280E-01	123	2.499560E-01
10	7.814970E-03	67	4.996750E-01	124	2.500200E-01
11	1.120080E-02	68	4.758170E-01	125	2.500040E-01
12	1.574490E-02	69	4.519530E-01	126	2.500020E-01
13	2.169990E-02	70	4.289930E-01	127	2.499980E-01
14	2.928030E-02	71	4.069260E-01	128	1.500030E-01
15	3.883520E-02	72	3.852050E-01	129	9.999818E-02
16	5.062090E-02	73	3.647280E-01	130	9.998918E-02
17	6.488466E-02	74	6.700889E-01	131	1.000160E-01
18	8.188015E-02	75	5.967500E-01	132	4.998150E-02
19	1.017330E-01	76	2.727240E-01	133	4.999270E-02
20	1.247420E-01	77	2.568550E-01	134	1.000010E-01
21	1.507670E-01	78	4.686180E-01	135	1.000040E-01
22	5.659390E-02	79	4.136950E-01	136	2.500160E-01
23	1.233860E-01	80	4.453090E-02	137	2.499900E-01
24	2.121150E-01	81	1.664490E-02	138	2.499980E-01
25	2.471720E-01	82	3.424810E-02	139	2.500010E-01
26	2.849180E-01	83	9.245056E-02	140	2.499959E-01
27	3.247200E-01	84	1.762379E-01	141	2.500040E-01
28	3.667040E-01	85	3.199580E-01	142	2.499880E-01
29	4.098549E-01	86	1.450370E-01	143	2.500300E-01
30	4.543909E-01	87	1.357009E-01	144	2.500020E-01
31	1.042600E-00	88	1.269290E-01	145	2.499630E-01
32	1.217779E-00	89	1.187200E-01	146	2.500409E-01
33	1.382400E-00	90	1.109450E-01	147	2.499860E-01
34	7.471810E-01	91	1.037019E-01	148	2.499940E-01
35	7.810180E-01	92	9.697247E-02	149	2.499990E-01
36	8.115230E-01	93	9.042078E-02	150	2.500010E-01
37	8.391670E-01	94	8.456880E-02	151	2.499840E-01
38	8.627090E-01	95	7.877707E-02	152	2.438370E-01
39	8.817530E-01	96	7.366955E-02	153	2.561880E-01
40	5.963579E-01	97	6.860459E-02	154	2.500130E-01
41	1.509120E-01	98	6.406987E-02	155	2.499440E-01
42	1.502230E-01	99	5.975620E-02	156	2.500330E-01
43	3.020750E-01	100	5.556710E-02	157	2.499940E-01
44	6.068439E-01	101	5.186550E-02	158	2.499940E-01
45	9.170859E-01	102	1.249959E-01	159	2.500030E-01
46	9.210960E-01	103	1.250040E-01	160	2.499950E-01
47	9.223930E-01	104	4.754260E-02	161	2.500170E-01
48	9.207420E-01	105	3.704120E-02	162	2.541860E-01
49	9.150640E-01	106	9.909075E-02	163	2.458020E-01
50	9.055930E-01	107	6.633258E-02	164	2.499910E-01
51	8.940820E-01	108	1.749960E-01	165	2.499710E-01
52	8.800930E-01	109	7.500035E-02	166	2.500480E-01
53	8.641520E-01	110	1.250000E-01	167	2.499950E-01
54	8.440180E-01	111	1.249890E-01	168	2.499970E-01
55	8.257419E-01	112	1.749980E-01	169	2.538700E-01
56	8.018900E-01	113	7.500285E-02	170	4.890668E-03
57	7.813450E-01	114	1.104420E-01	171	4.320500E-04

Table 8. Broad-Group (21γ) Gamma-Ray Energy Structure

Broad-Group Number	Upper Energy (MeV)	Contains Fine Groups ^a
1	14.0	1-2
2	10.0	3
3	8.0	4-5
4	7.0	6-7
5	6.0	8-9
6	5.0	10-11
7	4.0	12-13
8	3.0	14
9	2.5	15
10	2.0	16-17
11	1.5	18-19
12	1.0	20-21
13	0.7	22-25
14	0.45	26-27
15	0.30	28-29
16	0.15	30
17	0.10	31
18	0.075	32-33
19	0.045	34
20	0.030	35
21	0.020 ^b	36

^aSee Table 2 for a listing of the 36-group structure.

^bBottom energy is 0.010 MeV.

Table 9. FCXSEC Microscopic ANISN Library

Data Set ID No. ^a	Material	Remarks ^b	Data Set ID No. ^c	Material	Remarks ^b
1-6	¹ H	For H ₂ O mixture	139-144	¹² C	For TBP in dodecane mixture
7-12	¹⁶ O	For H ₂ O mixture	145-150	¹⁶ O	For TBP in dodecane mixture
13-18	¹ H	For borated water mixture	431-436 ^d	³¹ P	For TBP in dodecane mixture
19-24	¹⁶ O	For borated water mixture	169-172 ^d	¹⁴⁹ Sm	For Sm ₂ O ₃ mixture, no SGRPX
25-30	¹⁰⁸ B	For borated water mixture	173-178	¹⁶⁰	For Sm ₂ O ₃ mixture
31-36	¹¹⁸ B	For borated water mixture, no SGRPX ^c	151-156	¹⁶⁰	For Eu ₂ O ₃ mixture
37-42	¹ H	For concrete mixture	437-442	¹⁵¹ Eu	For Eu ₂ O ₃ mixture
43-48	¹⁶⁰	For concrete mixture	443-448 ^d	¹⁵³ Eu	For Eu ₂ O ₃ mixture
335-340	Mg	For concrete mixture	179-182 ^d	Gd	For Gd ₂ O ₃ mixture, no SGRPX
341-346	²⁷ Al	For concrete mixture	183-188	¹⁶⁰	For Gd ₂ O ₃ mixture
347-352	³¹ S	For concrete mixture	189-194	¹ H	For Gd(NO ₃) ₃ in water
353-358	³² S	For concrete mixture	195-200	¹⁶⁰	For Gd(NO ₃) ₃ in water
359-364	Ca	For concrete mixture	201-206 ^d	¹⁴ N	For Gd(NO ₃) ₃ in water
365-370	Fe	For concrete mixture	207-210 ^d	Gd	For Gd(NO ₃) ₃ in water, no SGRPX
371-376	K	For concrete mixture	157-162	¹⁰ B	For MB ₂ mixture
377-382	Ba	For concrete mixture	163-168	¹¹ B	For MB ₂ mixture, no SGRPX
49-54	D	For D ₂ O mixture, no SGRPX	449-454	¹⁰ B	For MB ₂ mixture
55-60	O	For D ₂ O mixture, no SGRPX	455-460	¹⁰ W	For MB ₂ mixture
61-66	¹ H	For lithium hydride	461-466	¹⁸⁴ W	For MB ₂ mixture
67-72	⁶ Li	For lithium hydride	467-472	¹⁸⁶ W	For MB ₂ mixture
73-78	⁷ Li	For lithium hydride	211-216	²³⁴ U	For spent fuel oxide mixture, no SGRPX
79-84	¹⁰⁸ B	For boral mixture	217-222	²³⁶ U	For spent fuel oxide mixture, no SGRPX
85-90	¹¹⁸ B	For boral mixture, no SGRPX	223-226 ^d	²³⁷ Np	For spent fuel oxide mixture
91-96	¹² C	For boral mixture	227-232	²³⁹ Pu	For spent fuel oxide mixture
383-388	²⁷ Al	For boral mixture	233-238	²⁴¹ Pu	For spent fuel oxide mixture, no SGRPX
97-102	¹⁴ N	For dry air mixture	239-244	²⁴² Pu	For spent fuel oxide mixture, no SGRPX
103-108	¹⁶ O	For dry air mixture	245-248 ^d	²⁴¹ Am	For spent fuel oxide mixture, no SGRPX
109-114	¹ H	For nitric acid mixture	249-252 ^d	²⁴³ Am	For spent fuel oxide mixture, no SGRPX
115-120	¹⁴ N	For nitric acid mixture	253-256 ^d	²⁴⁴ Am	For spent fuel oxide mixture, no SGRPX
121-126	¹⁶ O	For nitric acid mixture	257-262	¹⁶⁰	For spent fuel oxide mixture, no SGRPX
127-132	¹⁶⁰	For uranium oxide mixture	473-478	²³⁸ U	For spent fuel oxide mixture
389-394	²³⁸ U	For uranium oxide mixture	479-484	²³⁵ U	For spent fuel oxide mixture
395-400	²³⁵ U	For uranium oxide mixture	485-490	²³⁹ Pu	For spent fuel oxide mixture
401-406	Ni	For stainless steel-304 mixture	491-496	²⁴⁰ Pu	For spent fuel oxide mixture
407-412	Cr	For stainless steel-304 mixture	263-268	²³² Th	For thorium oxide mixture, no SGRPX
413-418	Fe	For stainless steel-304 mixture	269-274	²³³ U	For thorium oxide mixture, no SGRPX
419-424	²³⁸ U	For UF ₆ mixture	275-280	¹⁶⁰	For thorium oxide mixture
425-430	²³⁵ U	For UF ₆ mixture	497-502	²³⁸ U	For uranium metal mixture
299-304	F	For UF ₆ mixture	503-508	²³⁵ U	For uranium metal mixture
133-138	¹ H	For TBP in dodecane mixture	281-286	¹⁰⁷ Ag	For silver zeolite mixture, no SGRPX
			287-292	¹⁰⁹ Ag	For silver zeolite mixture, no SGRPX

Table 9. (Continued)

Data Set ID No. ^a	Material	Remarks ^b	Data Set ID No. ^a	Material	Remarks ^b
293-298	¹⁶ O	For silver zeolite mixture	629-634	Pb	$\sigma_0 = 10^{-1}$
509-514	Al	For silver zeolite mixture	635-640	Pb	$\sigma_0 = 10^3$
515-520	Si	For silver zeolite mixture	641-646	Pb	$\sigma_0 = 10^8$
305-310	¹² C	For silver zeolite mixture	647-652	Be	$\sigma_0 = 10^{-1}$
311-316	¹² C	$\sigma_0 = 10^3$	653-658	Be	$\sigma_0 = 10^3$
317-322	¹² C	$\sigma_0 = 10^8$	659-664	Be	$\sigma_0 = 10^8$
323-326 ^d	Zrly	$\sigma_0 = 10^{-1}$, no SGRPXS	665-670	Ti	$\sigma_0 = 10^{-1}$
327-330 ^d	Zrly	$\sigma_0 = 10^3$, no SGRPXS	671-676	Ti	$\sigma_0 = 10^3$
331-334 ^d	Zrly	$\sigma_0 = 10^8$, no SGRPXS	677-682	Ti	$\sigma_0 = 10^8$
521-526	Na	$\sigma_0 = 10^{-1}$	683-688	V	$\sigma_0 = 10^{-1}$
527-532	Na	$\sigma_0 = 10^3$	689-694	V	$\sigma_0 = 10^3$
533-538	Na	$\sigma_0 = 10^8$	695-700	V	$\sigma_0 = 10^8$
539-544	²⁷ Al	$\sigma_0 = 10^{-1}$	701-706	⁵⁵ Mn	$\sigma_0 = 10^{-1}$
545-550	²⁷ Al	$\sigma_0 = 10^3$	707-712	⁵⁵ Mn	$\sigma_0 = 10^3$
551-556	²⁷ Al	$\sigma_0 = 10^8$	713-718	⁵⁵ Mn	$\sigma_0 = 10^8$
557-562	Fe	$\sigma_0 = 10^{-1}$	719-724	⁵⁹ Co	$\sigma_0 = 10^{-1}$
563-568	Fe	$\sigma_0 = 10^3$	725-730	⁵⁹ Co	$\sigma_0 = 10^3$
569-574	Fe	$\sigma_0 = 10^8$	731-736	⁵⁹ Co	$\sigma_0 = 10^8$
575-580	Cd	$\sigma_0 = 10^{-1}$, no SGRPXS	737-742	Cu	$\sigma_0 = 10^{-1}$
581-586	Cd	$\sigma_0 = 10^3$, no SGRPXS	743-748	Cu	$\sigma_0 = 10^3$
587-592	Cd	$\sigma_0 = 10^8$, no SGRPXS	749-754	Cu	$\sigma_0 = 10^8$
593-598	⁹³ Nb	$\sigma_0 = 10^{-1}$	755-760	Sn	$\sigma_0 = 10^{-1}$
599-604	⁹³ Nb	$\sigma_0 = 10^3$	761-766	Sn	$\sigma_0 = 10^3$
605-610	⁹³ Nb	$\sigma_0 = 10^8$	767-772	Sn	$\sigma_0 = 10^8$
611-616	Mo	$\sigma_0 = 10^{-1}$	773-778	¹⁸¹ Ta	$\sigma_0 = 10^{-1}$
617-622	Mo	$\sigma_0 = 10^3$	779-784	¹⁸¹ Ta	$\sigma_0 = 10^3$
623-628	Mo	$\sigma_0 = 10^8$	785-790	¹⁸¹ Ta	$\sigma_0 = 10^8$

^aIdentification numbers are for P₀-P₅ components, respectively, unless otherwise noted.

^bSee Table 3 for isotopic concentrations of the mixtures used in the self-shielding step.

^cThe ENDF evaluation used to produce the VITAMIN-C data did not contain photon-production data. Consequently, there are no secondary gamma-ray production cross sections (SGRPXS) in the FCXSEC data set.

^dIdentification numbers for P₀-P₃ components, respectively.

The FCXSEC Macroscopic ANISN Library

Various mixtures are used repeatedly in transport calculations for nuclear fuel cycle activities. Thus, a macroscopic ANISN-formatted library of the frequently used mixtures was generated by using the AXMIX module to mix data from the FCXSEC microscopic ANISN library. In addition to the mixtures, there are a group of individual materials which are frequently used in nuclear fuel cycle calculations. For convenience, the microscopic data sets for the materials were copied from the FCXSEC microscopic ANISN library onto the "macroscopic" library. The mixtures, the library data sets for the mixtures and the individual materials, and the table of contents for the macroscopic library are given in Table 10. The "P₃" library is a "standard" ANISN library, i.e., Σ_a is in table position one, Σ_T is in position three, Σ_{gg} is in position four, and the table length is 46.

First-Order Checks of the FCXSEC Fine- and Broad-Group Master Libraries

RADE (Rancid AMPX Data Exorcist) was used to check the fine- and broad-group master libraries for internal constancies in the data. Specifically, RADE checks for the following cross-section relationships:

1. $\sigma_T \stackrel{?}{=} \sigma_a + \sigma_s$
2. $\sigma_{in} \stackrel{?}{=} \sum \sigma_{in}^{partial}$
3. $\sigma_a \stackrel{?}{=} \sigma_c + \sigma_f$
4. $\sigma_c \stackrel{?}{=} \sigma_{n\gamma} + \sigma_{n\alpha} + \sigma_{np} + \sigma_{nd} + \dots$
5. $\sigma_e^g \stackrel{?}{=} \sum_{g'} \sigma_{e\ell,0} (g \rightarrow g')$
6. $\sigma_0(g \rightarrow g') \stackrel{?}{>} 0$
7. $\sigma_T, \sigma_a, \sigma_f, \sigma_{n\gamma}, \sigma_{np}, \dots \stackrel{?}{>} 0$

Table 10. FCXSEC "Macroscopic" ANISN Library

Data Set ID No. ^a	Mixture	Material in Mixture	Number Density (atoms/bn-cm)	ID's of FCXSEC Micro Library Data Sets Used in Mix ^b	Remarks
101-104	H ₂ O	¹ H ¹⁶ O	6.693-02 3.347-02	1-4 7-10	
201-204	Stainless Steel 304	Ni Cr Fe	7.406-03 1.765-02 5.860-02	401-404 407-410 413-417	
301-304	Spent U-Fuel	²³⁸ U ²³⁴ U ²³⁵ U ²³⁶ U ²³⁷ Np ²³⁸ Pu ²³⁹ Pu ²⁴⁰ Pu ²⁴¹ Pu ²⁴² Pu ²⁴¹ Am ²⁴³ Am ²⁴⁴ Cm ¹⁶ O	2.620-02 5.082-06 2.236-04 1.108-04 1.233-05 3.736-06 1.391-04 6.350-05 3.274-05 1.256-05 1.602-06 2.326-06 5.007-07 4.890-02	473-476 211-214 479-482 217-220 223-236 227-230 485-488 491-494 233-236 239-242 245-248 249-252 253-256 257-260	No SGRPXS No SGRPXS No SGRPXS No SGRPXS No SGRPXS No SGRPXS No SGRPXS No SGRPXS No SGRPXS No SGRPXS No SGRPXS No SGRPXS No SGRPXS
401-404	Air	N ¹⁶ O	3.875-05 1.071-05	97-100 103-106	
501-504	Spent Th-Fuel	²³² Th ²³³ U ¹⁶ O	2.886-02 1.519-03 4.890-02	263-266 269-272 275-278	No SGRPXS No SGRPXS
601-604	Gd ₂ O ₃	Gd ¹⁵ O	2.462-02 3.698-02	179-182 183-186	No SGRPXS
701-704	Limonite Concrete	H O Mg Al Si S Ca Fe K Ba	1.271-02 2.948-02 1.983-04 4.756-04 1.263-03 6.576-05 3.893-03 3.295-02 6.625-05 8.334-04	37-40 43-46 335-338 341-344 347-350 353-356 359-362 365-368 371-374 377-380	
801-804	Type 2a Concrete	H O C Mg Al Si K Ca Fe Na	1.385-02 4.593-02 1.154-04 1.255-04 1.740-03 1.667-02 4.618-04 1.506-03 3.442-04 9.637-04	37-40 43-46 317-320 335-338 341-344 347-350 371-374 359-362 365-368 527-530	$\sigma_0 = 10^8$ $\sigma_0 = 10^3$

Table 10. (Continued)

Data Set ID No. ^a	Mixture	Material in Mixture	Number Density (atoms/bn-cm)	ID's of FCXSEC Micro Library Data Sets Used in Mix ^b	Remarks
901-904	Natural Boron In Water	¹⁰ B ¹¹ B	2.682-04 1.073-03	25-28 31-34	No SGRPXS
1001-1004	Natural Lithium	⁶ Li ⁷ Li	4.661-03 5.749-02	67-70 73-76	
1101-1104	Plutonium Oxide	²³⁸ Pu ²³⁹ Pu ²⁴⁰ Pu ²⁴¹ Pu ²⁴² Pu ¹⁶ O	3.736-06 1.391-04 6.350-05 3.274-05 1.256-05 5.033-04	227-230 485-488 491-494 233-236 239-242 257-260	No SGRPXS No SGRPXS No SGRPXS
1201-1204	Europium	¹⁵¹ Eu ¹⁵² Eu	1.174-02 1.276-02	437-440 443-446	
1301-1304	Natural B in Boral	¹⁰ B ¹¹ B	8.054-04 3.222-03	25-28 31-34	No SGRPXS
10001-10004	Gd		1.0	207-210	No SGRPXS, microscopic data
10101-10104	²³⁸ U		1.0	497-500	Microscopic Data
10201-10204	²³⁵ U		1.0	503-506	Microscopic Data
10301-10304	¹⁶ O		1.0	127-130	Microscopic Data
10401-10404	¹ H		1.0	1-4	Microscopic Data
10501-10504	Al		1.0	383-386	Microscopic Data
10601-10604	W	¹⁸² W ¹⁸³ W ¹⁸⁴ W ¹⁸⁶ W	8.337-03 4.548-03 9.663-03 8.969-03	449-452 455-458 461-464 467-470	
10701-10704	²³² Th		1.0	263-266	No SGRPXS, microscopic data
10801-10804	²³³ U		1.0	269-272	Microscopic data
10901-10904	C		1.0	305-308	$\sigma_0 = 10^{-1}$, microscopic data
11001-11004	Na		1.0	521-524	$\sigma_0 = 10^{-1}$, microscopic data
11101-11104	Fe		1.0	557-560	$\sigma_0 = 10^{-1}$, microscopic data
11201-11204	Zrly		1.0	323-326	$\sigma_0 = 10^{-1}$, microscopic data
11301-11304	Pb		1.0	629-632	$\sigma_0 = 10^{-1}$, microscopic data
11401-11404	Co		1.0	731-734	$\sigma_0 = 10^8$, microscopic data
11501-11504	K		1.0	371-374	Microscopic data

^aIdentification numbers for the P₀-P₃ components of the mixture cross section set, e.g., 101, 102, and 104 are the ID numbers of the P₀, P₁, P₂, and P₃ components of the water macroscopic cross section set.

^bSee Table 9.

$$8. \quad -1 \leq \bar{\mu}(g \rightarrow g') = \frac{\sigma_1(g \rightarrow g')}{3\sigma_0(g \rightarrow g')} \leq 1$$

The library data were checked to insure that the above relationships were met within a checking tolerance of 1.00×10^{-2} percent. Inconsistencies in both libraries were either very small (~ 0.0001) or were also found on the VITAMIN-C library.

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APPENDIX A:

DEFINITION OF REACTION TYPES IN
FCXSEC MASTER LIBRARIES

Reaction types in ENDF data are identified by integers – MT numbers. The ENDF MT numbers are used in AMPX master libraries, where possible, to identify the appropriate cross-section data. Where processed data are available that are not defined by an ENDF MT number, the data are identified by integers outside the range of the ENDF MT numbers. The following definition of reaction types is taken from Appendix B of the ENDF manual¹⁴ – being augmented where necessary to describe identifiers assigned to processed data in the FCXSEC master libraries.

The MT number generally refers to a specific neutron-nucleus interaction mechanism, but occasionally it indicates that a particular type of information is given. The general ENDF rules for assignment of MT numbers are as follows:

<u>MT (Range)</u>	<u>Description of Class of Reactions</u>
1-100	Reaction types in which secondary particles of the same type as the incident particles are emitted
101-150	Reaction types in which no secondary particles of the same type as the incident particles are emitted
151-200	Resonance region information
201-450	Quantities derived from the basic data
451-699	Miscellaneous quantities
700-799	Excitation cross sections for reactions that emit charged particles
800-999	(not assigned)
1000-2000	AMPX special identifiers

Within systems which process data into AMPX master format, different modules can assign the same MT number to a more or less inclusive set of data pertaining to the implied reaction. Specific MT assignments are given in the following table:

<u>MT</u>	<u>Description</u>
1	Total cross section (redundant, equal to the sum of all partial cross sections)
2	Elastic scattering cross section
3	Nonelastic cross section (redundant, equal to the sum of all partial cross sections except elastic scattering)
4	Total inelastic cross section (redundant, equal to the sum of MT = 51, 52, 53, ..., 90, 91)
5	(to be assigned)
6	(n,2n) cross section for first excited state (describes first neutron)
7	(n,2n) cross section for second excited state (describes first neutron)
8	(n,2n) cross section for third excited state (describes first neutron)
9	(n,2n) cross section for fourth excited state (describes first neutron)
10-15	(to be assigned)
16	direct (n,2n) cross section [total (n,2n) cross section is sum of MT = 6, 7, 8, 9, and 16]
17	(n,3n) cross section
18	Total fission cross section (sum of MT = 19, 20, 21, 38).
19	(n,f) cross section (first-chance fission)
20	(n,n'f) cross section (second-chance fission)
21	(n,2nf) cross sections (third-chance fission)
22	(n,n ^α) cross section

MT	Description
23	(n,n ³ α) cross section
24	(n,2nα) cross section
25	(n,3nα) cross section
26	(n,2n) isomeric-state cross section
27	Absorption cross section (sum of MT = 18 and 101)(includes particle reactions)
28	(n,n ¹ p) cross section
29	(n,n ² α) cross section
30	(n,2n2α) cross section
31	Used only in ENDF/B data as an LR flag to indicate that γ-emission is the mode of decay of the residual nucleus formed in the primary reaction. ^a
32	(n,n ¹ d) cross section
33	(n,n ¹ t) cross section
34	(n,n ¹ ³ He)
35	(n,n ¹ d2α) cross section
36	(n,n ¹ t2α) cross section
37	(n,4n) cross section
38	(n,3nf) cross section (fourth-chance fission)
39	Used only in ENDF/B data to indicate that internal conversion is the mode of decay of the residual nucleus formed in the primary reaction. ^a
40	Used only in ENDF/B data to indicate that electron-positron pair formation is the mode of decay of the residual nucleus formed in the primary reaction.

^aThe "primary" reaction could be, for example, an (n,n'), (n,p), (n,α), (n,np), etc., reaction.

MT	Description
41-45	(to be assigned)
46	cross section for describing the second neutron from (n,2n) reaction for first excited state
47	cross section for describing the second neutron from (n,2n) reaction for second excited state
48	cross section for describing the second neutron from (n,2n) reaction for third excited state
49	cross section for describing the second neutron from (n,2n) reaction for fourth excited state [Note: MT = 46, 47, 48, and 49 should not be included in the sum for the total (n,2n) cross section]
50	(to be assigned)
51	(n,n') to the first excited state
52	(n,n') to the second excited state
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90	(n,n') to the 40th excited state
91	(n,n') to the continuum
92-100	(to be assigned)
101	neutron disappearance (sum of all cross sections in which a neutron is not in the exit channel), i.e.,
	$MT = 101 \text{ is } \sum_{i=2}^{14} (MT=100+i)$
102	(n, γ) radiative capture cross section
103	(n,p) cross section
104	(n,d) cross section

MT	Description
105	(n,t) cross section
106	(n, ³ He) cross section
107	(n,α) cross section
108	(n,2α) cross section
109	(n,3α) cross section
110	(to be assigned)
111	(n,2p) cross section
112	(n,pα) cross section
113	(n,t2α) cross section
114	(n,d2α) cross section
115-119	(to be assigned)
120	Target destruction = nonelastic less total (n,n'γ)
121-150	(to be assigned)
151	General designation for resonance information
152-200	(to be assigned for specific resonance information)
201-202	(to be assigned)
203	Total hydrogen production
204	Total deuterium production
205	Total tritium production
206	Total ³ He production
207	Total ⁴ He production
208-250	(to be assigned)
251	$\bar{\mu}_L$; the average cosine of the scattering angle (laboratory system) for elastic scattering
252	ξ , the average logarithmic energy decrement for elastic scattering

MT	Description
253	γ , the average of the square of the logarithmic energy decrement for elastic scattering, divided by twice the average logarithmic decrement for elastic scattering
254	MINX-produced transport cross section according to $\sigma_{tr} = \sigma_t - \mu \sigma_s$, where σ_t is a current-weighted total cross section and σ_s is MT 2
255-284	(to be assigned)
285	Potential scattering cross section
286-300	(to be assigned)
301-450	Energy release rate parameters, $\overline{E^* \sigma}$, for total and partial cross sections. Subtract 300 from this number to obtain the specific reaction type identification. For example, MT = 302 = (300 + 2) denotes elastic scattering
451	Heading or title information (given only in File 1)
452	$\bar{\nu}$, average total (prompt plus delayed) number of neutrons released per fission event
453	Radioactive nuclide production
454	Fission product yield data
455	Delayed neutrons from fission
456	Prompt neutrons from fission
457	Radioactive decay data
458	Energy release in fission
459-500	(to be assigned)
501	Total photon interaction cross section
502	Photon coherent scattering
503	(to be assigned)
504	Photon incoherent scattering
505-514	(to be assigned)

MT	Description
515	Pair production, electron field
516	Pair production, nuclear and electron field (i.e., pair plus triplet production)
517	Pair production, nuclear field
518	Photofission (γ, f)
519-526	(to be assigned)
527	Sum of all gamma-ray absorption processes
528-531	(to be assigned)
532	Photoneutron (γ, n)
533	Total photonuclear
534-601	(to be assigned)
602	Photoelectric
603-699	(to be assigned)
700	(n, p_0) cross section (cross section for leaving the residual nucleus in the ground state)
701	(n, p_1) cross section for first excited state
702	(n, p_2) cross section for second excited state
703	(n, p_3) cross section for third excited state
704	(n, p_4) cross section for fourth excited state
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718	(n, p_C) cross section for continuum excited state
719	(n, p_C') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing photon)

MT	Description
720	(n,d ₀) cross section for ground state
721	(n,d ₁) cross section for first excited state
722	(n,d ₂) cross section for second excited state
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738	(n,d _C) cross section for continuum excited state
739	(n,d _C ') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing deuteron)
740	(n,t ₀) cross section for ground state
741	(n,t ₁) cross section for first excited state
742	(n,t ₂) cross section for second excited state
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750	(n,t _C) cross section for continuum excited state
759	(n,t _C ') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing triton)
760	(n, ³ He ₀) cross section for ground state
761	(n, He ₁) cross section for first excited state
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778	(n, ³ He _C) cross section for continuum
779	(n, ³ He _C ') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing ³ He)

MT	Description
800-999	(to be assigned)
1000	XSDRNPM-produced transport cross section based on the outscatter approximation, i.e., $\sigma_{tr} \equiv \sigma_a + (1 - \bar{\mu})\sigma_s$ (Note: σ_a is MT 27; σ_s is MT 2.)
1001	XSDRNPM-produced transport cross section based on the inscatter approximation, i.e., $\sigma_{tr} \equiv \sigma_t - \frac{\int_0^\infty \sigma_1(E' \rightarrow E)j(E')dE'}{3j(E)}$
1007	Thermal scattering matrix
1018	Chi (χ) distribution of neutrons from the fission reaction. Chi is represented in ENDF File 5 data as a function of neutron energy. XLACS and XLACS-2 calculate energy-dependent χ 's by group and weight the χ 's over the fission rate ($\nu\Sigma_f\phi$) to produce a single vector.
1033	Not meaningful at this time
1099	Group integral of the weight function triggered by IW (1\$\$ array) in XLACS or XLACS-2.
1452	Product of ν times the fission cross section
1500-1501	Same as 1000, 1001 except for gamma-ray cross sections
1527	Gamma-ray energy absorption coefficients. These data are also called kerma factors. These are calculated in SMUG and are the product of the gamma energy and the MT = 527 absorption cross section.
2001	Not meaningful at this time

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