Decay Chain Data Library for Radioactivity Calculations

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Abstract

Decay Chain Data Library (DCDLIB) is a concise nuclear data library containing all the necessary nuclear information for use in fusion reactor radioactivity studies. Reaction cross sections obtained from ENDF/B-IV and Calculated BNL Cross Sections were processed into 46 group cross sections using MACK program. BNL-325 was referred to when no reaction cross section was available elsewhere. The radioactive decay data was picked up from ENDF/B-IV, or the Table of Isotopes when materials were not covered in ENDF/B-IV.

The computer program, PREP, processes punched-format group cross sections from MACK and radioactive decay data into DCDLIB under the coupled transmutation type number designated as KT. DCDLIB is an essential data library for the DKR, a computer program which calculates radioactivity, afterheat, biological hazard potential, and dose rate due to decay in fusion reactors and can also be used as a reaction cross section library.

Table of Contents

1. Introduction

A computational method to calculate the radioactivity using radioactive decay chains was developed at the University of Wisconsin[1] and DKR[2], a program to calculate the radioactivity in fusion reactors has been written based on this method. Decay chain data library (DCDLIB) was primarily designed to provide a self-contained nuclear data set for the DKR program. The fusion reactor materials whose cross sections are available from ENDF/B-IV[3] have been compiled in DCDLIB. ENDF/B library has been used because it is the best nuclear data library at present, and it provides a unified data format flexible enough to calculate neutron and gamma-ray interactions accurately. The nuclear data in ENDF/B is continuously revised and expanded, and newest version ENDF/B-IV contains dosimetry data for numerous radioisotopes, mostly fission products, compiled in radioactive decay format.[4]

Materials in ENDF/B are either isotopes or elements, sometimes compounds. Since the transmutations must be calculated for each isotope, it is unavoidable to look for another data source if the element consists of more than one isotope and ENDF/B does not supply the data for those isotopes. For example, iron data in ENDF/B-IV are for natural iron, not for the individual isotopes of iron. The Calculated BNL cross sections from THRESH code[5] are good compliments in this case because all the data in it is for individual isotopes. Several cross section sets were taken from BNL-325[6], and when no data for radiative capture cross sections was available from any source, group cross sections were derived for the estimation of epithermal groups from thermal capture cross section using a 1/E weighting function. It was assumed that the light or medium nuclei follow 1/v behavior.

For radioisotopes which were not compiled in ENDF/B-IV, decay data has been taken from the Table of Isotopes.[7]

2. Description of DCDLIB

The data in the DCDLIB are provided in BCD card image format, and a consistent set of units is used for all materials. A material is defined as an isotope and is identified by a number KZA which is a (Z,A) designation of a nuclide. KZA is given by

$$KZA = 1000\ Z + A$$

where Z is the atomic number and A is the mass number of a nuclide.

The data set for each material is divided into the following parts:

(1) HEAD - always needed

(2) Nuclide Information - always needed

(3) Radioactive Decay Data - for radioisotopes only

(4) Cross Section Data - for stable nuclides or radioistopes with cross section only

(5) MEND - always needed

Each data part is described and FORTRAN statements used to read these records are shown below.

The HEAD record consists of one card, and contains information for nuclide identification.

```
READ (IN,100) ESYM, KZA, NUM
100 FORMAT (A4, 68X, I5, I3)
```

where ESYM is the chemical symbol for the element, and NUM is the card numbering foe each card;

NUM = 1 for HEAD record,

0 for MEND record.

The nuclide information record reads as follows:

```
      READ (IN,20) LIS, KZA, LXN, NKT NWD
   20 FORMAT (6I6)
```

where LIS is the energy state of nuclide;

LIS = 0 for ground state,

LIS = 1 for isomeric state,

and LSR is the flag for radioisotope;

LSR = 0 for stable isotope,

LSR = 1 for radioisotopes.

LXN is the flag for the presence of cross section data;

LXN = 0 means no cross section data,

LXN = 1 cross section data.

NKT is the total number of transmutation types and is the sum of the radioactive decay types and the number of reactor cross section sets. The nuclide information needs exactly NWD+1 records, where NWD is the number of comment cards.

Comment cards should be read as follows:

```
      DO 20 I=1, NWD
      IF (NWD. EQ.0) Go to 22
   20 READ (IN,210) (A(J), J=1,18)
  210 FORMAT (18A4)
   22 CONTINUE
```

where A array contains the comment words.

The radioactivity decay data record is read only when LSR = 1.

```
      READ (IN, 300) NDK, NSP, ABTE, AGME, ALPE, EMPC
      IF (NDK. EQ. 0) Go to 33
   30 READ (IN, 310) DCON, QV, KZA
   33 If (NSP. EQ.0) Go to 38
      DO 35 J=1, NSP
      READ (IN, 320) MDKY, NTR, FNBG
      IF (NTR, EQ. 0) Go to 35
      DO 35 K=1, NTR
```

```
      READ (IN, 330) ETR, PTR, CCI
   35 CONTINUE
   38 CONTINUE
  300 FORMAT (2I6, 4E12.3)
  310 FORMAT (12X, 2E12.3, 36X, I5)
  320 FORMAT (2I6, E12.3)
  330 FORMAT (12X, 3E12.3)
```

where NDK is the number of decay modes, NSP is the number of decay energy spectra, ABTE, AGME and ALPE are the energies of beta-, gamma-, and alpha-particle respectively, EMPC is the value of MPCa for public, DCON is decay constant, QV is the Q value for the decay, MDKY is the mode of decay, NTR is the total number of transitions, FNBG is the normalization factor for transition intensities, ETR, PTR are energy and intensity of the transition respectively, and CCI is the internal conversion coefficient, which is ignored if MDKY is other than gamma decay. The cross section data record is given only when LXN = 1. The 46 group neutron cross sections are stored in ANSIN-format.[8] The total reaction cross section is the sum of all transmutation cross sections. Scattering cross sections are not included except when inelastic scattering leaves the target nuclide in an isomeric state. This is done because our main concern is with the transmutation of nuclides. The MEND record must be placed at the end of data:

```
      READ (IN, 500) KZA, NUM
  500 FORMAT (72X, I5, I3)
```

where NUM is the flag for the end of nuclide data, and the value of NUM is always 0 for MEND.

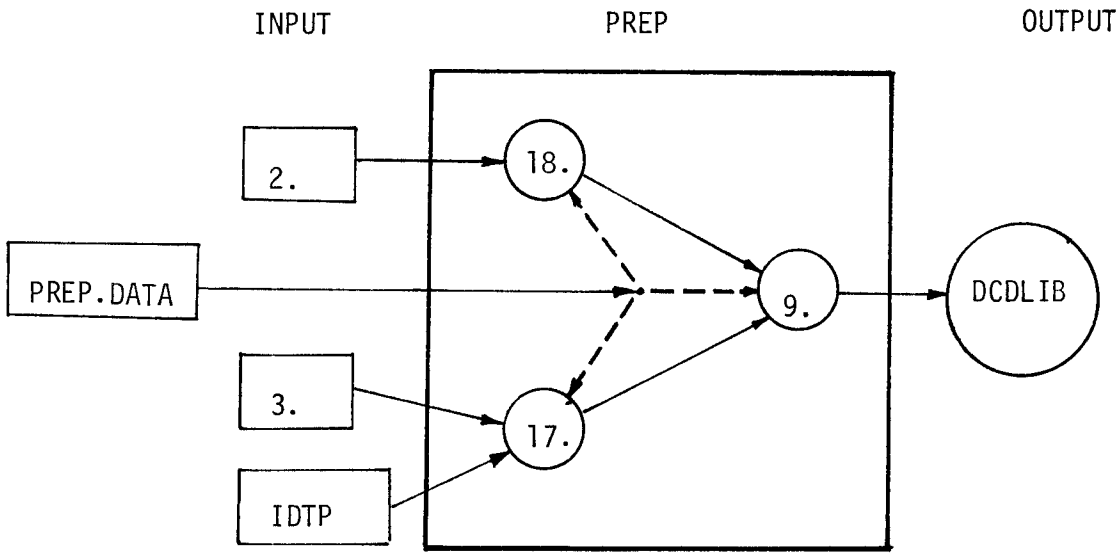
3. Description of PREP Program

The computer program PREP is designed to process neutron reaction cross sections and radioactive decay data into decay chain data library. In PREP, aggregated group cross sections which are punched output of MACK program[9] are used as cross section inputs, and are regrouped under transmutation type number.

Radioactive decay data from either ENDF/B-IV or user-supplied decay data set-PRERAD, are used to construct a radioactive decay data table. Processed cross section tables and radioactive decay data tables are finally mixed to set DCDLIB in the order of increasing KZA number.

The data processing in PREP is shown in Fig. 1.

Fig. 1. Schematic Diagram of PREP



		Logical Unit
*	Reaction Cross sections Data	2.
	PRERAD Radioactive Decay Data	3.
	ENDF/B-4 Radioactive Decay Data	10. (=IDTP)
	Reaction Cross Sections Table	18.
	Radioactive Decay Data Table	17.
	Mixed Table	9.

Acknowledgement

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References

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4. C. W. Reich, R. G. Helmer and N. H. Putnam, "Radioactive Nuclide Decay Data," ANCR-1157 (August, 1974).

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8. W. W. Engle, Jr., "A User's Manual for ANISN," K-1693 (March, 1967).

9. M. A. Abdou, C. W. Maynard and R. Q. Wright, "MACK: A Computer Program to Calculate Neutron Energy Release Parameters (Fluence-to-Kerma Factors) and Multigroup Neutron Reaction Cross Section from Nuclear Data in ENDF Format," ORNL-TM-3994 (January, 1973).

Appendix A. Definition of Transmutation Types

Transmutation types identified by an integer KT

KT	REACTION TYPE†	CHANGE IN KZA,	CHANGE IN LIS	ENDF/B-IV
1	Total Reaction			
2	(n,γ)	+ 1		MT = 102
3	(n,p)	-1000		103
4	(n,2n)	- 1		16
5	(n,d),(n,n')p	-1001		28,104
6	(n,t)	-1002		32,105
7	(n,He^3)	-2002		106
8	(n,α)	-2003		107
9	(n,n)α	-2004		22
10	(n,2n)α	-2005		24
11	(n,2α)	-4007		108
12	(n,2α)t	-5010		113
13	(n,3α)	-6011		109
14	(n,3α)n	-6012		23
15	(n,n')*		+ 1	
16	(n,γ)*	+ 1	+ 1	
17	(n,2n)*	- 1	+ 1	26
18	(n,p)*	-1000	+ 1	
19	(n,d)*,(n,np)*	-1001	+ 1	
20	(to be assigned)			
21	Total Decay			
22	β^-	+1000		RTYP=1.0
23	β^+, EC (=3)	-1000		2.0
24	α (=9)	-2004		4.0
25	γ		- 1	3.0
26	(β^-)*	+1000	+ 1	
27	(β^+)*, (EC)* (=18)	-1000	+ 1	
28	n (=4)	- 1		

† the reaction type with * leads to the isomeric state

Appendix B

Neutron 46 Multigroup Structure in eV

Group Limits

Group	E(Top)	E(Low)	E(Mid-Point)
1	1.4918 (+7)	1.3499 (+7)	1.4208 (+7)
2	1.3499 (+7)	1.2214 (+7)	1.2856 (+7)
3	1.2214 (+7)	1.1052 (+7)	1.1633 (+7)
4	1.1052 (+7)	1.0000 (+7)	1.0526 (+7)
5	1.0000 (+7)	9.0484 (+6)	9.5242 (+6)
6	9.0484 (+6)	8.1873 (+6)	8.6178 (+6)
7	8.1873 (+6)	7.4082 (+6)	7.7977 (+6)
8	7.4082 (+6)	6.7032 (+6)	7.0557 (+6)
9	6.7032 (+6)	6.0653 (+6)	6.3843 (+6)
10	6.0653 (+6)	5.4881 (+6)	5.7767 (+6)
11	5.4881 (+6)	4.9659 (+6)	5.2270 (+6)
12	4.9659 (+6)	4.4933 (+6)	4.7296 (+6)
13	4.4933 (+6)	4.0657 (+6)	4.2795 (+6)
14	4.0657 (+6)	3.6788 (+6)	3.8722 (+6)
15	3.6788 (+6)	3.3287 (+6)	3.5038 (+6)
16	3.3287 (+6)	3.0119 (+6)	3.1703 (+6)
17	3.0119 (+6)	2.7253 (+6)	2.8686 (+6)
18	2.7253 (+6)	2.4660 (+6)	2.5956 (+6)
19	2.4660 (+6)	1.8268 (+6)	2.1464 (+6)
20	1.8268 (+6)	1.3534 (+6)	1.5901 (+6)
21	1.3534 (+6)	1.0026 (+6)	1.1700 (+6)
22	1.0026 (+6)	7.4274 (+5)	3.726 (+5)
23	7.4274 (+5)	5.5023 (+5)	6.4648 (+5)
24	5.5023 (+5)	4.0762 (+5)	4.7892 (+5)
25	4.0762 (+5)	3.0197 (+5)	3.5480 (+5)
26	3.0197 (+5)	2.2371 (+5)	2.6284 (+5)
27	2.2371 (+5)	1.6573 (+5)	1.9472 (+5)
28	1.6573 (+5)	1.2277 (+5)	1.4425 (+5)
29	1.2277 (+5)	6.7379 (+4)	9.508 (+4)
30	6.7379 (+4)	3.1828 (+4)	4.9604 (+4)
31	3.1828 (+4)	1.5034 (+4)	2.3431 (+4)
32	1.5034 (+4)	7.1017 (+3)	1.1068 (+4)
33	7.1017 (+3)	3.3546 (+3)	5.2281 (+3)
34	3.3546 (+3)	1.5846 (+3)	2.4696 (+3)
35	1.5846 (+3)	7.4852 (+2)	1.1666 (+3)
36	7.4852 (+2)	3.5358 (+2)	5.5105 (+2)
37	3.5358 (+2)	1.6702 (+2)	2.6030 (+2)
38	1.6702 (+2)	7.8893 (+1)	1.2296 (+2)
39	7.8893 (+1)	3.7267 (+1)	5.8080 (+1)
40	3.7267 (+1)	1.7603 (+1)	2.7435 (+1)
41	1.7603 (+1)	8.3152 (+0)	1.2959 (+1)
42	8.3153 (+0)	3.9279 (+0)	6.1216 (+0)
43	3.9379 (+0)	1.8554 (+0)	2.8917 (+0)
44	1.8554 (+0)	8.7643 (-1)	1.3659 (+0)
45	8.7643 (-1)	4.1399 (-1)	6.4521 (-1)
46	4.1399 (-1)	2.2000 (-2)	2.1800 (-1)

Appendix C. Content of DCDLIB

* : Isomeric state nuclide
NKT: Total number of transmutation type
R: Radioisotope
S: Stable nuclide
KT: Transmutation type number
1 ~ 19 Reaction type designated by symbol 'X'
21 ~ 29 Radioactive decay type designated by symbol 'O'

NUCLIDE	NKT	KT=	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
			21	22	23	24	25	26	27	28	29										
6 HE	2	R	O	O																	
8 HE	2	R	O	O																	
6 LI	5	S	X	X	X					X		X									
7 LI	6	S	X	X		X	X				X	X									
8 LI	2	R	O	O																	
9 LI	2	R	O	O																	
9 BE	5	S	X	X	X			X		X											
10 BE	2	R	O	O																	
10 B	5	S	X		X		X			X			X								
11 B	6	S	X	X	X	X		X		X											
12 C	4	S	X	X						X					X						
13 C	2	S	X	X																	
14 C	2	R	O	O																	
14 N	8	S	X	X	X	X	X	X		X			X								
16 N	2	R	O	O																	
16 O	5	S	X	X	X		X			X											
19 O	2	R	O	O																	
18 F	2	R	O		O																
19 F	8	S	X	X	X	X	X	X		X	X										
20 F	2	R	O	O																	
23 NE	2	R	O	O																	
24 NA	2	R	O	O																	
25 NA	2	R	O	O																	
26 NA	2	R	O	O																	
24 MG	3	S	X	X	X																
25 MG	3	S	X	X	X																
26 MG	4	S	X	X	X					X											
27 MG	2	R	O	O																	
26 AL	2	R	O		O																
27 AL	8	S	X	X	X	X	X	X		X									X		
28 AL	2	R	O	O																	
29 AL	2	R	O	O																	
30 AL	2	R	O	O																	
30*AL	2	R	O				O														

Appendix C (continued)

NUCLIDE	NKT	KT=	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
			21	22	23	24	25	26	27	28	29										
28 SI	4	S	X	X	X					X											
29 SI	4	S	X	X	X					X											
30 SI	4	S	X	X	X					X											
31 SI	2	R	0	0																	
36 CL	3	R	0	0	0																
38 CL	2	R	0	0																	
39 AR	2	R	0	0																	
41 AR	2	R	0	0																	
38 K	2	R	0		0																
39 K	7	S	X	X	X	X	X			X	X										
40*K	3	R	0	0	0																
41 K	3	S	X		X					X											
45 CA	2	R	0	0																	
47 CA	2	R	0	0																	
45 SC	7	S	X		X	X	X	X		X	X										
46 SC	2	R	0	0																	
46*SC	2	R	0				0														
47 SC	2	R	0	0																	
48 SC	2	R	0	0																	
49 SC	2	R	0	0																	
50 SC	2	R	0	0																	
45 TI	2	R	0		0																
46 TI	6	S	X		X	X	X			X	X										
47 TI	7	S	X		X	X	X	X		X	X										
48 TI	6	S	X		X	X	X			X	X										
49 TI	7	S	X		X	X	X	X		X	X										
50 TI	6	S	X		X	X	X			X	X										
51 TI	2	R	0	0																	
48 V	2	R	0		0																
49 V	8	R	X		X	X	X			X	X										
			0		0																
50 V	7	S	X		X	X	X	X		X	X										
51 V	8	S	X	X	X	X	X	X		X	X										
52 V	2	R	0	0																	
49 CR	2	R	0		0																
50 CR	8	S	X	X	X	X	X		X	X	X										
51 CR	8	R	X		X	X	X			X	X										
			0		0																
52 CR	7	S	X	X	X	X	X			X	X										
53 CR	8	S	X	X	X	X	X	X		X	X										
54 CR	7	S	X	X	X	X	X			X	X										
55 CR	2	R	0	0																	
53 MN	8	R	X		X	X	X			X	X										
			0		0																
54 MN	9	R	X		X	X	X	X		X	X										
			0		0																
55 MN	8	S	X	X	X	X	X		X	X	X										
56 MN	2	R	0	0																	
57 MN	2	R	0	0																	

Appendix C (continued)

NUCLIDE	NKT	KT= 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
		21	22	23	24	25	26	27	28	29										
53 FE	2 R	0		0																
54 FE	8 S	X	X	X	X	X		X	X	X										
55 FE	8 R	X		X	X	X			X	X										
		0		0																
56 FE	8 S	X	X	X	X	X	X		X	X										
57 FE	8 S	X	X	X	X	X	X		X	X										
58 FE	8 S	X	X	X	X	X	X		X	X										
59 FE	2 R	0	0																	
57 CO	8 R	X		X	X	X			X	X										
		0		0																
58 CO	2 R	0		0																
58*CO	2 R	0				0														
59 CO	7 S	X	X	X	X	X	X		X											
60 CO	9 R	X		X	X	X	X		X	X										
		0	0																	
60*CO	2 R	0				0														
61 CO	2 R	0	0																	
57 NI	2 R	0		0																
58 NI	9 S	X	X	X	X	X	X	X	X	X										
59 NI	8 R	X		X	X	X			X	X										
		0		0																
60 NI	9 S	X	X	X	X	X	X		X	X										
61 NI	8 S	X	X	X	X	X	X		X	X									X	
62 NI	8 S	X	X	X	X	X	X		X	X										
63 NI	9 R	X		X	X	X	X		X	X										
		0	0																	
64 NI	7 S	X	X	X	X	X			X	X										
65 NI	2 R	0	0																	
67 NI	2 R	0	0																	
62 CU	2 R	0		0																
63 CU	3 S	X	X						X											
64 CU	3 R	0	0	0																
65 CU	3 S	X	X		X															
66 CU	2 R	0	0																	
67 CU	2 R	0	0																	
68 CU	2 R	0	0																	
63 ZN	2 R	0		0																
64 ZN	4 S	X	X	X	X															
65 ZN	2 R	0		0																
66 ZN	3 S	X	X		X															
67 ZN	3 S	X	X	X																
68 ZN	5 S	X	X	X					X								X			
69 ZN	2 R	0	0																	
69*ZN	2 R	0				0														
70 ZN	4 S	X	X						X								X			
71 ZN	2 R	0	0																	
71*ZN	2 R	0	0																	

Appendix C (continued)

NUCLIDE	NKT	KT=	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
			21	22	23	24	25	26	27	28	29										
88 RB	2	R	0	0																	
89 RB	2	R	0	0																	
90 RB	2	R	0	0																	
88 SR	5	S	X		X	X	X			X											
89 SR	7	R	X		X	X	X			X											
			0	0																	
90 SR	7	R	X		X	X	X			X											
			0	0																	
91 SR	2	R	0	0																	
92 SR	2	R	0	0																	
89 Y	8	S	X	X	X	X	X	X		X	X										
90 Y	9	R	X		X	X	X	X		X	X										
			0	0																	
90*Y	2	R	0				0														
91 Y	9	R	X		X	X	X	X		X	X										
			0	0																	
91*Y	2	R	0				0														
92 Y	2	R	0	0																	
93 Y	2	R	0	0																	
94 Y	2	R	0	0																	
95 Y	2	R	0	0																	
96 Y	2	R	0	0																	
88 ZR	2	R	0		0																
89 ZR	2	R	0		0																
89*ZR	2	R	0				0														
90 ZR	8	S	X		X	X	X			X	X								X	X	
91 ZR	8	S	X		X	X	X	X		X	X									X	
92 ZR	7	S	X		X	X	X	X		X	X										
93 ZR	7	S	X		X	X	X	X		X	X										
94 ZR	7	S	X		X	X	X	X		X	X										
95 ZR	9	R	X		X	X	X	X		X	X										
			0	0																	
96 ZR	7	S	X		X	X	X	X		X	X										
97 ZR	2	R	0	0																	
92 NB	7	S	X		X	X	X	X		X	X										
92*NB	2	R	0		0																
93 NB	9	S	X	X	X	X				X	X						X	X	X		
93*NB	2	R	0				0														
94 NB	11	R	X	X	X	X	X	X		X	X							X			
			0	0																	
94*NB	2	R	0				0														
95 NB	2	R	0	0																	
95*NB	2	R	0				0														
96 NB	2	R	0	0																	
97 NB	2	R	0	0																	
97*NB	2	R	0				0														
98 NB	2	R	0	0																	
100 NB	2	R	0	0																	

Appendix C (continued)

NUCLIDE	NKT	KT=	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
			21	22	23	24	25	26	27	28	29										
91 MO	2	R	0		0																
91*MO	3	R	0		0		0														
92 MO	8	S	X	X		X	X		X	X	X									X	
93 MO	11	R	X		X	X	X	X	X	X	X										
			0		0				0												
93*MO	2	R	0				0														
94 MO	7	S	X		X	X	X	X		X	X										
95 MO	9	S	X	X	X	X	X	X		X	X									X	
96 MO	8	S	X	X	X	X	X	X		X	X										
97 MO	9	S	X	X	X	X	X	X		X	X									X	
98 MO	8	S	X	X	X	X	X	X		X	X										
99 MO	9	R	X		X	X	X	X		X	X										
			0					0													
100 MO	8	S	X	X	X	X	X	X		X	X										
101 MO	2	R	0	0																	
97 TC	7	S	X		X	X	X	X		X	X										
98 TC	7	S	X		X	X	X	X		X	X										
99 TC	9	R	X		X	X	X	X		X	X										
			0	0																	
99*TC	2	R	0				0														
100 TC	2	R	0	0																	
101 TC	2	R	0	0																	
181 HF	2	R	0	0																	
183 HF	2	R	0	0																	
181 TA	4	S	X	X	X	X															
182 TA	2	R	0	0																	
182*TA	2	R	0				0														
183 TA	2	R	0	0																	
184 TA	2	R	0	0																	
185 TA	2	R	0	0																	
186 TA	2	R	0	0																	
181 W	2	R	0		0																
182 W	6	S	X	X	X	X	X			X											
183 W	6	S	X	X	X	X	X			X											
184 W	6	S	X	X	X	X	X			X											
185 W	2	R	0	0																	
186 W	6	S	X	X	X	X	X			X											
187 W	2	R	0	0																	
203 HG	2	R	0	0																	
205 HG	2	R	0	0																	
204 TL	2	R	0	0																	
203 PB	2	R	0		0																
204 PB	7	S	X		X	X	X	X		X	X										
205 PB	2	R	0		0																
206 PB	7	S	X		X	X	X	X		X	X										
207 PB	7	S	X		X	X	X	X		X	X										
208 PB	7	S	X		X	X	X	X		X	X										

Appendix D. Sample of DCDLIB

```
C   Element name
C     LIS   KZA      LSR     LXN     NKT     NWD
          0  6013        0       1       2       0
36R 0.0         0  0.850-05 0  0.130-04 0  0.180-04 0  0.260-04 0  0.400-04
 0  0.580-04 0  0.940-04 0  0.112-03 0  0.169-03 0  0.468-03
36R 0.0         0  0.850-05 0  0.130-04 0  0.180-04 0  0.260-04 0  0.400-04
 0  0.580-04 0  0.940-04 0  0.112-03 0  0.169-03 0  0.468-03
C
C
          0  6014        1       0       2       0
          1       1  4.700-02        .000        .000  1.000-07
                     3.833-12  0.000
                     3.833-12  1.560-01
          1       1  1.000+00
                     1.561-01  1.000+00
C
```

(σT)g=1,46 in ANISN Format

(σi)g=1,46 in ANISN Format

NOK, NSP, $\bar{E}_\beta$, $\bar{E}_\gamma$, $\bar{E}_\alpha$, (MPC)air, λ_T, λ_i, Q_v, MOKY, NTR, FNBG, ETR, PTR

```
KZA   NUM
6013    1
6013    2
   1    1
KT 1    2
   2    1
   2    2
6013    0
6014    1
6014    2
6014    3
  21    1
  22    1
6014    4
6014    5
6014    0
```

Appendix E. PROGRAM PREP ABSTRACT

1. Name of Program

   PREP: Radioactive Decay Chain Data Preparation Program

2. Coding Language and Computer

   FORTRAN IV; UNIVAC 1110

3. Nature of Program

   PREP reads the cross section data in MACK[1] punched output format, and radioactive decay data either from ENDF/B-4[2] or from PRERAD, user-compiled radioactive decay for PREP, and generates the Decay Chain Data Library for radioactivity calculations in fusion reactor design.

   PREP may be used as an auxilliary routine of DKR[3], the radioactivity calculation program, or run independently to provide the Decay Chain Data Library. It is also possible to use PREP to revise the Decay Chain Data Library.

4. Computer Requirement

   PREP can be run in less than 65 K words of core memory with overlay structure. Since PREP is written in most common FORTRAN-IV, it can be operable on any standard FORTRAN compiler. Standard input, output and several logical units are required.

5. References

(1) M. A. Abdou, C. W. Maynard and R. Q. Wright "MACK: A Computer Program to Calculate Neutron Energy Release Parameters (Fluence-to-Kerma Factors) and Multigroup Neutron Reaction Cross Sections from Nuclear Data in ENDF Format," ORNL-TM-3994 (January, 1973)

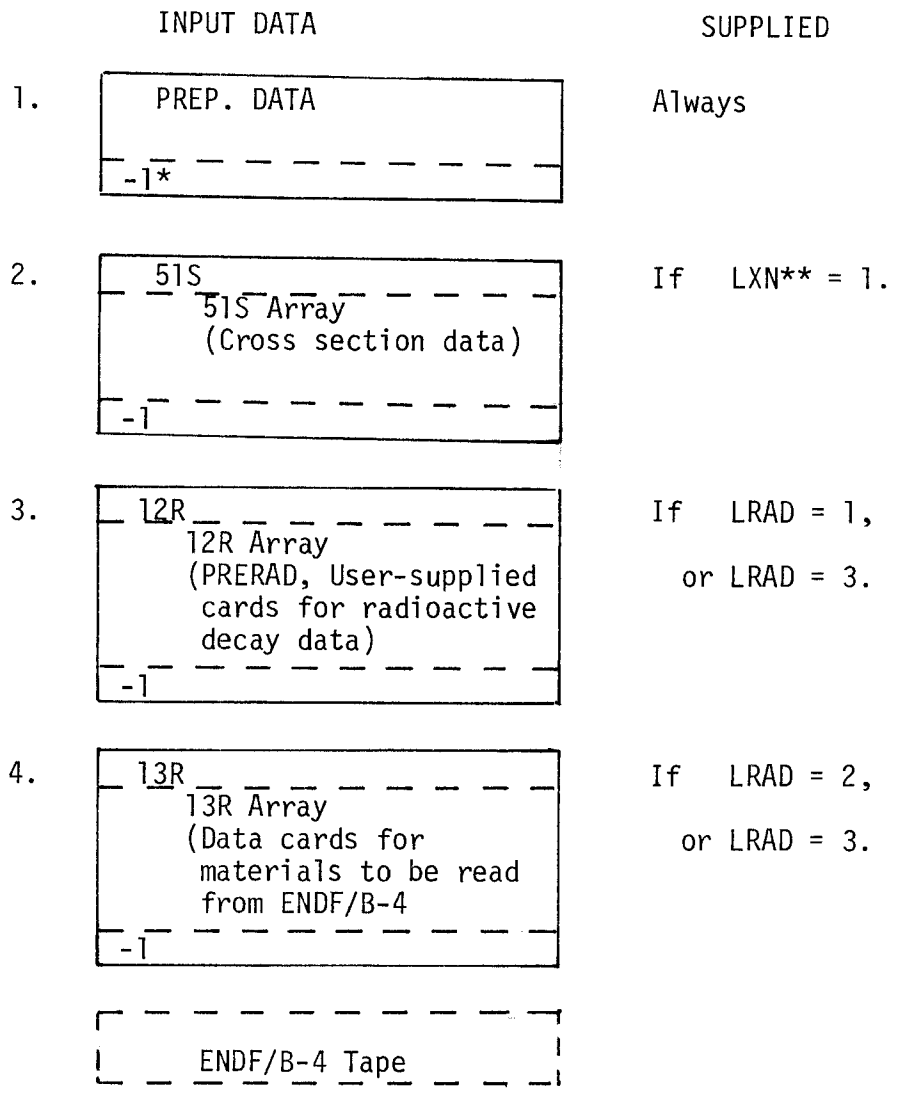
(2) M. K. Drake, Editor, "Data Formats and Procedures for the ENDF Neutron Cross Section Library," BNL-50274 (October, 1970)

(3) T. Y. Sung and W. F. Vogelsang, "DKR - A Radioactivity Calculation Code For Fusion Reactors," UWFDM-170 (September, 1976), University of Wisconsin

Appendix F. Description of PREP Input Data

Input data for PREP is described briefly. Data format is characterized by the standard FORTRAN convention.

Essentially, the input data consists of four parts as shown below. The description of input data for each part is given on the next pages.



* Flag for end of each data part

** See next page or Appendix G

1. PREP. DATA

Card No. 1 (16A4)

Item	Cols.	Name	Description
1	1-64	TITLE	

Card No. 2 (3I6)

1	1-6	LXN	0 = no effect 1 = process cross sections
2	7-12	LRAD	0 = no effect 1 = process PRERAD 2 = process ENDF/B-4 3 = process PRERAD and ENDF/B-4
3	13-18	LMIX	0 = no effect 1 = generate mixed table

Card No. 3 (3I6)

1	1-6	LPRT1	0 = no effect 1 = print cross section table 2 = punch cross section table
2	7-12	LPRT2	0 = no effect 1 = print radioactive decay data table 2 = punch radioactive decay data table
3	13-18	LPRT3	0 = no effect 1 = print mixed table 2 = punch mixed table

2. Cross Section Data

Each material needs opening card (Card No. 1) and closing card (Card No. 6) in addition to the MACK output for group Cross Section Data. The cards, Card No. 2 through Card No. 5, represent each reaction data and are repeated as many times as reaction types for this material in ENDF/B-4.

Card No. 1 (2I6, A4)

Item	Cols.	Name	Description
1	1-6	NZA	(Z,A) Number
2	7-12	NMT	MAT Number in ENDF/B-4
3	13-16	FLGI	Signal for the beginning of new material (= 'OPEN')

Card No. 2 (18A4)

1	1-72	TITLE	Title card for reaction cross section data

Card No. 3 (18A4)

2	1-72	CMENT	Comment for reaction type

Card No. 4 (A3)

1	1-3	SIGNAL	54* = signal for cross section

Card No. 5 (6(I2,A1,F9.0),2I4)

The field which consists of subfields (1), (2),and (3), is repeated six times in a card until data are depleted.

(1)	1-2	IN	Index subfield either 0 or 1 to 99
(2)	3	K	Operation subfield blank, R, or T
(3)	4-12	V	Data subfield cross section in barns
4	73-76	MT	Reaction Type in ENDF/B-4
5	77-80	NUM	Numbering in certain type of cross section

Card No. 6 (2I6,A4)

Item	Cols.	Name	Description
1	1-6	NZA	(Z,A) Number (= 1000 Z + A)
2	7-12	NMT	MAT Number in ENDF/B-4
3	13-16	FLGO	Signal for the end of material data (= 'SHUT')

3. PRERAD

For each radioisotope the following set of cards is required.

Card No. 1 (A4,I2,2I6)

1	1-4	NAME	Chemical symbol for element
2	5-6	LIS	Isomeric state 0 = ground state 1 = 1st excited state, etc.
3	7-12	KZA	(Z,A) Number (= 1000 Z + A)
4	13-18	NWD	Number of comment cards

Card No. 2 (18A4)

1	1-72	CMMT	Comment for radioisotope

Card No. 3 (F9.0,2X,A1,2I6,3E12.3,I6)

1	1-9	THL	Half-life
2	12	UNIT	Unit of time for half life S, M, H, D or Y
3	13-18	NDK	Total Number of Decay Modes
4	19-24	NSP	Total Number of Energy Spectra
5	25-36	ABTE	Average Beta Energy
6	37-48	AGME	Average Gamma Energy
7	49-60	ALPE	Average Alpha Energy
8	61-66	LD3	Flag for the Uncertainties 0 = no effect 1 = read Card No. 3A

Card No. 3A (F9.0,15X,3E12.3)

This card is provided only when LD3 = 1 in Card No. 3

Item	Cols.	Name	Description
1	1-9	THLU	Uncertainty in Half-life
2	25-36	ABTU	Uncertainty in $\bar{E}_{\beta}$
3	37-48	AGMU	Uncertainty in $\bar{E}_{\gamma}$
4	49-60	ALPU	Uncertainty in $\bar{E}_{\alpha}$

Card No. 4 (F6.1,I6,4E12.3,I6)

As many cards as NDK (Total Number of Decay Modes)

1	1-6	RTYP	Decay Type 1.0 = β^- 2.0 = β^+, EC 3.0 = Isomeric Transition 4.0 = α 5.0 = Delayed Neutrons
2	7-12	ISOM	Isomeric state of daughter nuclide 0 = ground state 1 = 1st isomeric state 2 = 2nd isomeric state, etc.
3	13-24	QV	Q value of decay
4	25-36	BR	Branching Ratio
5	37-48	QVU	Uncertainty in Q value
6	49-60	BRU	Uncertainty in Branching Ratio
7	61-66	LD4	Flag for the Uncertainties 0 = no effect 1 = read QVU and BRU

Card No. 5 (F6.1,I6,2E12.3)

As many cards as NSP (Total Number of Energy Spectra)

For transitions other than γ

Item	Cols.	Name	Description
1	1-6	MDAB	Decay Mode of Transition same as RTYP
2	7-12	NTR	Total Number of Transitions
3	13-24	FNB	Normalization Factor for transition intensity
4	25-36	FNBU	Uncertainty in Normalization Factor

For γ transition

1	1-6	MDGM	γ - transition mode (= 0.0)
2	7-12	NGM	Number of γ Transition
3	13-24	FGM	Normalization Factor
4	25-36	FGMU	Uncertainty in Normalization Factor

Card No. 6 (12X,2(F12.3,F6.2,F6.3))

As many cards as NTR and NGM

For transitions other than γ

Item	Cols.	Name	Description
1	13-24	ETR	Energy of Transition
2	25-30	PTR	Intensity of Transition
3	37-48	ETRU	Uncertainty in ETR
4	49-54	PTRU	Uncertainty in PTR

For γ transition

1	13-24	EGM	Energy of γ transition
2	25-30	PGM	Intensity of γ transition
3	31-36	CCI	Internal Conversion Coeff.
4	37-48	EGMU	Uncertainty in EGM
5	49-54	PGMU	Uncertainty in PGM
6	55-60	CCIU	Uncertainty in CCI

4. Data for ENDF/B-4 Materials

Card No. 1 (2I6)

Item	Cols.	Name	Description
1	1-6	IDTP	ENDF/B-4 Tape No.
2	7-12	NN	Total Number of Nuclides Wanted in IDTP

Card No. 2 (6(2I6))

NN fields are specified. Each field consists of subfields (1) and (2) with six fields in a card.

(1)	1-6	NZA	(Z,A) Designation of Nuclide
(2)	7-12	MAT	MAT Number of Nuclide in ENDF/B-4

Appendix G. Identification of Symbols

ABTE	Average beta energy
AGME	Average gamma energy
ALPE	Average alpha energy
BR	Branching ratio
CCI	Internal conversion factor
ETR	Energy of transition other than gamma
EGM	Energy of gamma transition
FGM	Normalization factor for intensity of gamma decay
FNB	Normalization factor for decay spectra other than gamma
IDTP	ENDF/B-4 tape number
ISOM	Isomeric state of radioactive decay daughter
KT	Transmutation type number
KZA	(Z,A) number of a nuclide
LIS	Isomeric state of a nuclide
LMIX	Flag for generating mixed table
LPRT1	Flag for punching cross section table
LPRT2	Flag for punching radioactive decay data table
LPRT3	Flag for punching mixed table
LRAD	Flag for processing radioactive decay data table
LSR	Flag for radioactive isotope
LXN	Flag for processing cross section table

MAT	Material identification number of a nuclide in ENDF/B-4
MDAB	Decay mode of transition
MDGB	Gamma transition mode
MT	Reaction type number in ENDF/B-4
NAME	Chemical symbol for element
NDK	Total number of decay modes
NGM	Total number of gamma transitions
NMT	Same as MAT
NN	Total number of nuclides wanted from IDTP
NSP	Total number of energy spectra
NTR	Total number of transitions other than gamma
NUM	Card numbering
NWD	Number of comment cards
NZA	Same as KZA
PGM	Intensity of gamma transition
PTR	Intensity of transition other than gamma
QV	Q value of radioactive decay
RTYP	Decay type
THL	Half-life
UNIT	Unit of time