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LIBRARIES OF DECAY DATA AND FISSION PRODUCT YIELDS IN THE ABBN-93 CONSTANT SET

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LIBRARIES OF DECAY DATA AND FISSION PRODUCT YIELDS IN THE ABBN-93 CONSTANT SET. This paper describes three new libraries in the ABBN constant set which are essential for calculating radioactivity: basic decay data, radioactive decay photon spectra and fission product yields.

1. Basic decay data

Decay data for radionuclides are needed in the ABBN-93 constant set primarily so that it can be used to calculate the nuclide composition and radiative characteristics of irradiated fuel and other reactor materials. Decay data are also needed to calculate delayed energy release components and photon formation in neutron reactions.

At this point in time there are several quite extensive compilations of decay data which are fairly comprehensively covered in the ENDF/B-6, JENDL-3.2 and JEF-2.2 evaluated nuclear data libraries. We should also mention the decay data libraries included in programs for calculating the nuclide composition of irradiated fuel and reactor materials - such as ORIGEN, Ref. [1], and FISPACT, Ref. [2]. One of the most extensive sources of information on decay data is the ENSDF (Evaluated Nuclear Structure Data File) international library, which contains both recommended and initial experimental data. There are several handbooks which are important sources of evaluated decay data: in particular, Ref. [3], which gives the spectra of photons irradiated by radionuclides taking into account internal conversion and other processes connected with the electron orbit of the atomic nucleus; and Ref. [4], which contains the branching ratios that lead, in particular, to the emission of delayed neutrons.

It is difficult to choose which data to use in practical calculations owing to the variety of information sources, their incompleteness and their evaluation inconsistency. Thus, choosing a standard set of decay data was in fact of the utmost importance in devising a set of constants laying claim to universality and standardization. It should be pointed out that the decay data compiled for ABBN-93 were not evaluated independently on the basis of initial experimental information. The main focus was on making the information provided as complete as possible, internally consistent and user-friendly in performing calculations in conjunction with ABBN-93 neutron and photon data.

The formats for the basic decay data are described in detail in Ref. [5]. The tables contain data for all the isotopes of a specific element, the symbol for which is indicated in the first line (see example below). At least one line is given to each isotope; a whole number identifier is given in the first column.

The first real parameter in the header line is the atomic number Z.

1st column -	four-digit isotope identifier: the three leftmost digits are the mass number; the rightmost digit is the isomer and stability identifier.
2nd column -	a letter indicating the nature of the content of the data given: a hyphen signifies that the isotope is radioactive and its values are given in the subsequent columns as listed below:
"A" signifies,	that the isotope is stable and, instead of the isomeric transition (IT) probability, the isotopic abundance in its natural mixture is given;
"B" signifies,	that as a result of at least one of the possible modes of decay, the product-nucleus may be formed not only in the ground state but also in a metastable state (in that case the data for this isotope are entered on two lines: whereas the decay probability is given, as for all radioactive isotopes, in the first line, the probability of a metastable state forming for the corresponding decay path is given in the second line);
"C" signifies,	that two isomeric states may form during decay, and three lines of data are given for the isotope under consideration; the probability of a first metastable state forming is given in the second line, and the probability of a second metastable state forming is given in the third line.
3rd column -	the unit of time for the half-life: s = seconds; m = minutes; d = days; y = years.
4th column -	the half-life in the unit indicated.
5th column -	"BETA+" is the (β^{+}+ε) decay probability.
6th column -	"BETA-" is the β^{-} decay probability.
7th column -	"IT" is the isomeric transition probability.
8th column -	"ALFA" is the alpha decay probability.
9th column -	"SF" is the spontaneous fission probability.
10th column -	"E-GAM " is the energy removed by photons.
11th column -	"E-BET " is the energy removed by electrons.
12th column -	"E-ALF" is the energy removed by alpha-particles and other heavy charged decay products (for example, fragments during spontaneous fission, protons emitted in several cases following beta-decay, etc.).
13th column -	indicates that there is a 15-group representation of the photon spectrum in the ABBN library of photon spectra for radioactive nuclei.

The MF=90 with MT=0 tables contain data on the energies released directly during decay. In addition, MF=90, MT=1 tables have been drawn up using a special program and have exactly the same format, except that the "E-GAM", "E-BET" and "E-ALF" columns contain the total energy releases in the whole radioactive decay chain right up to decay into a stable nucleus or a nucleus with a half-life of more than 3 years.

The tables give the corresponding branching ratios (in fractions and not in percentages) for those nuclei whereby, during decay, daughter nuclei may form not only in the ground state but also in the metastable states.

The tables also give data for stable isotopes: the abundance of each isotope in its natural mixture. The library of basic decay data now contains information on 2361 nuclides. By way of example, Table 1 gives decay data for Po.

2. Radioactive decay photon spectra

Multiplicities and photon energy spectra emitted during radioactive decay are given in an MF=91 table in a 15-group representation from 0 to 11 MeV. The main data sources for this library were the International Commission on Radiological Protection handbook, Ref. [3], and the JEF-2 library. As in the case of the basic decay data, decay photon spectra for all isotopes were collated in one consolidated MF=91 table named after the chemical symbol of the element to which these isotopes relate. Photon spectra are not necessarily given for all the isotopes for which decay data are given. The decay data library has a sign which indicates whether photon spectra data exist for a given radioactive nucleus. At present, the photon spectra library contains data for 819 radionuclides.

Apart from the 15-group photon spectra, the table gives the energies and yields of several (up to four) of the strongest gamma lines. It should be pointed out that the contributions of these lines to the 15-group spectra given were also taken into account. If the lines identified are considered separately in calculating radioactive decay photon propagation in a medium, their contribution should be subtracted from the 15-group spectra given.

Table 1. Decay data for Po

NAM=PO BIB=FOND MF= 90 MT= 0 Z=84.

LT = 26 LC= 12 LS= 12 LF= (I4,a2,e6.0,a1,5e7.0,3e8.0)

* A		T1/2	BETA+	BETA-	IT	ALFA	SF	E-GAM	E-LOC	E-ALF
2020	-	44.7m	98.0			2.0		8.40-1	1.58-1	1.11-1
2030	-	36.7m	99.89			0.11		1.63+0	1.47-1	5.90-3
2031	-	1.2m	4.5		95.5			1.60+0	2.36-1	
2040	-	3.53h	99.34			0.66		1.15+0	1.50-1	3.55-2
2050	-	1.8h	99.96			0.04		1.59+0	5.32-2	2.10-3
2060	B	8.8d	94.55			5.45		1.19+0	1.41-1	2.84-1
	M					0.0				
2070	-	350.m	99.97			0.03		1.29+0	4.22-2	1.10-3
2071	-	2.8s			100.			1.088	2.88-1	
2080	B	2.898y	2.2-3			100.		1.90-5	1.13-7	5.115
	M					0.0				
2090	-	102.y	0.26			99.74		5.15-3	4.40-4	4.97+0
2100	-	138.4d				100.		8.50-6	8.18-8	5.40+0
2110	B	0.516s				100.		7.70-3	2.00-4	7.59+0
	M					1.0				
2111	B	25.2s				100.		1.49+0	1.00-2	7.55+0
	M					1.0				
2120	-	3.-7s				100.		0.0	0.0	8.95+0
2121		1.42-8s			87.	13.		1.12+0	1.23-1	1.34+0
2122	-	45.1s				100.		9.10-2	3.70-4	8.95+0
2130	-	4.2-6s				100.		0.0	0.0	8.54+0
2140	-	1.64-4s				100.		8.33-5	8.19-7	7.83+0
2150	-	1.78-3s		.04		99.96		1.76-4	6.30-6	7.52+0
2160	-	0.15s				100.		1.69-5	1.61-7	6.91+0
2170	-	9.s		5.		95.		0.	0.	6.329
2180	-	3.05m		0.02		99.98		9.12-6	1.42-5	6.11+0

*

When the 15-group spectra were being plotted, the yields were corrected in such a way as to conserve in the group approximation the total energy of the photons in each energy group. Since the same (average group) energy is ascribed in this approximation to all photons in a given group, the group multiplicity for energy conservation is calculated according to the formula:

$$\Lambda_j = \sum_n \lambda_n \times E_{\gamma,n} / \bar{E}_j + \int_{\Delta E_j} \lambda(E_\gamma) \times (E_\gamma / \bar{E}_j) dE_\gamma \qquad (1)$$

Here λ_n and $E_{\gamma n}$ are the yield and energy of the n-th line in the energy group under consideration, $\lambda(E_\gamma)$ is the continuous spectrum of the multiplicity of decay photons, and $\bar{E}_j$ is the average energy of the photons in the group.

The format of the MF=99 tables, containing data on radioactive decay photon spectra, is described in Ref. [5] and illustrated in Table 2 by the example of tungsten isotopes

Table 2. Photon spectra emitted during the decay of W isotopes

```
NAM=W        BIB=BN93  MF= 99  MT=  0   Z = 74.         DAT=0312.92
LV = 10      LT =  24  LC=  8  LS=  8  LF = (I4,9E7.0)
*            Radioactive decay photon yields.
*               15 groups and the 4 strongest lines
       1769   1779   1789   1799   1819   1859   1879   1889
*
   1
   2
   3
   4
   5
   6
   7
   8         .0109
   9         .3575                              .0386
  10         .4667                              .7249
  11         .2536                .0004         .0     .0068
  12  .7174  .6026         .0017  .0     2.32-4  .1104  .0
  13 1.5050 1.5750  .2117  .7617  .6417 3.38-4  .4167  .0033
  14  .0     .0     .0     .3667  .0     0.0     .0     .0
  15  .2933  .2867  .1133  .2000  .1200 8.39-5  .2200  .0
*
 101        1.0360                      2.13-4  .6858
 201         .1020                      0.1254  .2930
 102         .1156                              .4795
 202         .4980                              .2340
 103         .4270
 203         .1310
 104
 204
*
```

Specialized programs were written to verify the compiled libraries. The first of these was for all the nuclides for which a photon spectrum is given; the energy removed by the photons was calculated on the basis of the group yields given. This value was then compared with the value given in the EGAM column of the decay data library. The causes of discrepancies were established and eliminated. The second program was written with the aim of verifying data for the strong lines that had been identified. The verification procedure consisted of determining the energy remaining once the contribution from the strong lines to each energy group had been subtracted. The remaining value should be zero or positive.

Apart from the aforementioned verification programs, the SUBGAM program was written to calculate the activity and total photon spectrum for a sample of a given composition. The input file includes information on the nuclide composition (nuclear densities) and the user-defined group representation (boundaries of the photon groups). The first calculation is activity, and beta and gamma energy release in the nuclides, using data on the half-lives and energy release on decay from the decay data library. The full photon spectrum is then calculated for a given sample, either in the basic 15-group representation or in another, user-defined, grouping. The SUBGAM program was used to create the MF=91, MT=1 tables which contain data on the spectra of all the photons in the decay chain. SUBGAM is now sometimes used as an independent program.

3. Fission product yields

At the start of the 1970s several evaluations of fission product yields appeared which had been carried out in various laboratories around the world for the basic fissile nuclei. The results of the fission product yield evaluations differed because of the lack of available experimental data. The most comprehensive experimental information available is for thermal neutron fission of ^{235}U, although even in this case it is not possible to measure the independent yields of many short-lived products. There is less experimental information for thermal neutron fission of ^{239}Pu and "fast" neutron fission of ^{235}U (i.e. induced by neutrons with a spectrum close to the part of the fission neutron spectrum that is higher than 1 MeV), although the quality is the same as for ^{235}U. Various semi-empirical methods are being used to evaluate the unmeasured low yields for these nuclei. Of course, there is at times extensive scatter of the evaluated data for these kinds of fission products but, in practical terms, low yield products (which are also, as a rule, very short-lived) do not have a high value and these discrepancies are not significant.

The situation regarding the energy dependence of fission product yields still leaves something to be desired. Even for basic fuel nuclides, detailed energy dependences of yields have not been measured - not even for maximum yield products. The experimental data obtained are for thermal neutrons, "fast" neutrons or neutrons with an energy of the order of 14 MeV - (D-T) neutrons. Here, the "fast" neutron spectrum is usually not particularly well known: it is a fast reactor spectrum, similar to a fission spectrum only in its "hard" part. Accordingly, evaluated data are also given at three "points": for thermal, fast and 14 MeV neutrons. The user may of course wonder how such scant data on yield energy dependence are to be used, but the evaluators have no clear answer.

There are considerably fewer data on the fission product yields for thorium and ^{233}U, and the available evaluations for minor actinides are based only on semi-empirical methods. The data in these cases are clearly not highly reliable.

The main evaluations of recent years are included in the ENDF/B-6, JENDL3 and JEF2 libraries. We had access only to data from the ENDF/B-6 and JENDL-3.2 libraries. The contents of these libraries is given in Table 3.

Table 3. Content of the ENDF/B-6 and JENDL-3 libraries with respect to independent fission product yields

Actinide	**ENDF/B-6**					**JENDL-3**				
	MAT	N	T	F	H	MAT	N	T	F	H
90-Th-227	9025	1175	+							
90-Th-229	9031	1196	+							
90-Th-232	9040	1300,1303		+	+	3905	1230		+	+
91-Pa-231	9131	1223		+						
92-U-232	9219	1195	+							
92-U-233	9222	1223.1215,1207	+	+	+	3922	1230	+	+	+
92-U-234	9225	1228.1211		+	+					
92-U-235	9228	1248.1252,1226	+	+	+	3924	1230	+	+	+
92-U-236	9231	1275.1243		+	+	3925	1230	+		
92-U-237	9234	1286		+						
92-U-238	9237	1303.1276		+	+	3926	1230		+	+
93-Np-237	9347	1239.1232		+	+	3931	1230		+	
93-Np-238	9349	1260		+						
94-Pu-238	9434	1222		+						
94-Pu-239	9437	1228.1224,1204	+	+	+	3943	1230	+	+	+
94-Pu-240	9440	1236.1219		+	+					
94-Pu-241	9443	1258.1257	+	+						
94-Pu-242	9446	1265		+		3946	1230	+		
95-Am-241	9543	1218.1215,1198	+	+	+	3951	61	+		
95-Am-242m	9547	1231	+							
95-Am-243	9549	1231		+		3954	61	+		
96-Cm-242	9631	1186		+						
96-Cm-245	9640	1236	+							
98-Cm-249	9852	1207	+							
98-Cm-251	9858	1237	+							

The ENDF/B-6 library contains the evaluation by England and Rider (T.R. England and B.F. Rider, 1992). It includes 60 sets of independent and correspondingly cumulative fission product yields for 36 fissile nuclei. These yields are given for one or more fission neutron energies per nucleus, and in some cases data are also given for spontaneous fission. The number of products in each set varies, but the average number of fission products is roughly 1200. This evaluation included more than 3000 new experimental values.

The JENDL-3 library includes the earlier evaluation by Rider and Meek (B.F. Rider and M.F. Meek, 1989). Although it has much fewer evaluated sets compared with ENDF/B-6, it does have data on all the main actinides. The yields for some fissile nuclei are given in the energy dependence: for thermal neutrons (0.0253 eV), fast neutrons and neutrons with an energy of 14 MeV. The yield sets for all the nuclei contain the same number of fission products - 1230.

Both libraries use the ENDF/B format, and they are not used to their full extent in calculation programs either in the Russian Federation or abroad. It is common practice to establish program sublibraries of fission product yields on the basis of these data or any other evaluations for use in solving specific tasks and with their own program formats. Therefore, when calculating, analyzing and comparing the results obtained from the various programs, the differences in the fission product yields in the libraries used must always be identified and taken into account. An attempt to overcome this problem was the decision to establish a library of independent fission product yields in the constant set for a wide number of users, i.e. with general purpose comprehensive data.

Analysis of the data from the ENDF/B-6 and JENDL-3.2 libraries showed that there was no reason to give preference to either. It was decided to adopt the data from the ENDF/B-6 library as a basis, since they were more comprehensive, but to standardize the number of products in each set, i.e. 1234. This number includes all the fission products for which data is also given in JENDL-3.2 and several isomers indicated only in ENDF/B-6.

Differences in the fission product sets, for which data are given for various actinides in these libraries, are attributable to products with very small yields and lifetimes. Products not included in the ABBN-93 set, but which figure in the ENDF/B-6 data, were discarded and their yields added to the independent yields of the nearest members of the isomeric chains. Where the nuclide set included in ENDF/B-6 was smaller than that adopted in ABBN-93, the set was supplemented on the basis of data from JENDL-3.2, so that the cumulative yield of the first member of the isomeric chain adopted in ENDF/B-6 (but not the first for the longer chain adopted in ABBN-93) remained the same as in the original ENDF/B-6 library. As regards the fission product radioactive decay schemes, they are practically the same in ABBN-93 as in JENDL-3.2 except for minor corrections made to take the formation of the newly introduced isomers into account, and corrections to several errors detected in the branching ratios.

Fission product yields - $y_{i,p}^{d}$ - are given for all the main fuel nuclides, i, for all the significant fission products, p, in the three energy ranges, d. Independent fission product yields are given in the ABBN MF=72 table. The first energy range comprises groups 26 to 8. In this range it is recommended to use the yield values measured at the thermal energy of the neutrons inducing fission. Exceptions are fuel nuclides which are non-fissile or not easily fissile when exposed to thermal neutrons. For these nuclides in the first energy range, it is recommended to use the yields measured on the fission spectrum or spectra close to it. Data for the first range are given in the table with MT=1.

The second range comprises the groups 7 to 2 and yields are given only if they differ from those given for the first range. Data for the second range are given in the table with MT=2.

The third range comprises groups 1. 0 and -1 (i.e. the region above the (n,n'f) reaction threshold). In this range it is recommended to use the yields measured at an energy of 14-15 MeV. If yields in the third range are given for any nuclide, then yields in the first range are intentionally given.

Data for the third range are given in the table with MT=3. The following default rules are recommended:

- if there are no data for the second range for a given nuclide, data for the first range should be used;

- if there are no data for the third range, data for the second range should be used; and

- if these data are not available either, data for the first range should be used.

In thermal neutron reactor calculations, fission product yields may be calculated on the basis of data only for the first range: the correction for the difference in yields in the second range in that event is, at most, a few per cent for the yield values even in the minimum region when A=110-120. In the same way (and with even greater justification), data only for the first two ranges can be used in fast neutron reactor calculations. Independent yields are normalized to 2.

Data for the ranges are presented in three files called yield1.tab, yield2.tab and yield3.tab respectively for the fission-inducing neutron energy. Table 4 is a fragment from the start of a file showing thermal neutron yields.

Table 4. Fragment of fission product yield

NAM=FP BIB=END6 MF= 72 MT= 1 DAT= .95

LV =10 LT =1235 LC= 20 LS= 7 LF = (I6,6E11.0)

* Independent fission product yields normalized to 2.

*IDENT	lamda	TH-227	TH-229	U-232	U-233	U-235
902270	902290	922320	922330	922350		
* A=66						
230660	1.8734+02	1.3182-18	1.2852-18	1.0474-14	4.1407-19	2.1450-19
240660	2.5941+00	2.5799-14	4.9596-14	2.0499-10	1.6100-14	2.1500-14
250660	3.9496+00	1.1100-11	6.1397-12	2.1100-7	8.7300-12	7.5102-12
260660	1.8908-01	2.6900-10	1.7499-10	1.1620-5	6.7600-10	3.3401-10
270660	2.4889-01	4.9000-10	1.0100-10	4.3990-5	1.2700- 9	2.9301-10
280660	3.5071-06	7.4000-11	1.8299-11	1.4010- 5	5.3900-10	5.1501-11
290660	2.2652-03	7.2100-13	5.1897-14	3.1400- 7	5.3900-12	1.4900-13
300660	0.0000+0	0.0000+0	0.0000+0	3.8100-10	0.0000+0	0.0000+0
* A=67						
240670	6.1449+00	4.0744-15	5.0204-15	7.6896-12	6.0662-15	4.0488-15

The vast majority of practical applications require calculation of the concentrations of the fission products contained in fuel after the fairly considerable time needed to remove the fuel from the reactor core once irradiation is over. Thus, in calculating fission product concentrations it is expedient to start the chains from the isobar with the maximum Z, for which the decay constant, λ, does not exceed the given λ_{max}. This isobar becomes, consequently, the "lowest order" member of the chain. It is assumed that before the start of the calculation the program accessing the ABBN tables for data on decay schemes and fission product yields, using the given λ_{max}, reduces the isobar chains and the independent yield tables, leaving in them only those fission products which are essential for resolving the task (for example, those that may have an influence on the gamma activity of the irradiated fuel after its removal from the reactor core). At the same time, the independent yields of the "lowest order" members of the isobar chains should be replaced with the cumulative yields calculated on the basis of the complete decay schemes given in the MF=71 table.

The data from these three libraries have so far been used in an international test, Ref. [6] to determine the radioactive properties of fresh and spent uranium and MOX fuel. The library of yields has been used for theoretical analysis of the composition of actinide samples after long-term irradiation in the core of a BN-350 reactor, Ref. [7]. All calculations were carried out with the help of the SKALA software package, Ref. [8], using the ABBN-93 libraries as the constant basis, including the decay data and fission product yield libraries described above.

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