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Informal Report

PEFPYD - A Library of Aggregate Fission-Product Decay Data Derived from ENDF/B-IV

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by

R. J. LaBauve and D. C. George

ABSTRACT

Results from summation calculations by the CINDER-10 and peripheral codes and fission-product decay, cross section and yield data from the ENDF/B-IV have been incorporated into a processed ENDF/B fission-product and energy-yield data (PEFPYD) library. The organization and content of this basic fine-group source-term library is described. The library contains aggregate beta and gamma spectra produced by neutrons of one or more energies incident upon six important nuclides. Although the PEFPYD library is described in other Los Alamos Scientific Laboratory reports, it is the purpose here to provide concise documentation for the library alone.

I. INTRODUCTION

The ENDF/B-IV fission-product files contain neutron cross sections, decay constants, decay energies, and other decay data for 824 important fission products. They also contain fission yields for these fission products produced by one or more fission-neutron energies (14 MeV, fast, and thermal fission) of six important nuclides: ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu. Also, spectral data (i.e., beta end-point energies and intensities, gamma-line energies and intensities) exist for the most important decay-heat contributors among the 824 nuclides. In ENDF/B-IV, beta-spectral data exist for 163 fission products, and gamma-spectral data exist for 172 nuclides (nuclides emitting both beta and gamma radiation are included separately in both types of radiation counts). The contents of the ENDF/B-IV fission-product file are detailed in Refs. 1-3 and summarized in Table I.

In recent years, great emphasis has been placed on obtaining experimental and computational information on delayed energy release at short cooling times for nuclear reactor safety studies of the hypothetical loss-of-coolant-accident (LOCA). There is, however, also interest in long cooling times. A computer code system[4,5] has been developed at the Los Alamos Scientific Laboratory (LASL) that uses the ENDF/B-IV fission-product data to calculate cumulative delayed beta and gamma spectra on arbitrary energy grids for arbitrary irradiation histories and cooling times. This code system is shown in Fig. 1.

It can be noted in the figure that the basic ENDF/B-IV fission-product data library is accessed along three paths. The center path, after the preparation of an input library, proceeds via the CINDER-10 code. CINDER-10 is the latest and most versatile version of CINDER, a well-known fission-product and depletion code. The most recent documentation on CINDER is Ref. 4 (for Version 7), but the additional features of Version 10 are discussed in Ref. 6. CINDER-10 calculates fission-product and actinide concentrations, activities, gaseous contents, energy releases, effective group absorption cross sections, etc. for any fissionable nuclide mixture irradiated in arbitrary neutron fluxes for arbitrary intervals of time followed by arbitrary cooling times. The neutron cross sections[7,8] used in CINDER-10 are generated by spectrum collapse of multigroup data generated with the NJOY code.[9] This input path to CINDER-10 is the lower path shown in the figure. Spectrum collapse is achieved with the TOAFEW[8] code.

The ENDF/B-IV data is also accessed by the FPDCYS code along the upper processing path shown in Fig. 1. This code is used to generate multigroup beta and gamma spectra for individual nuclides for which spectral data exist on the ENDF/B-IV file. FPDCYS incorporates four options for calculating beta spectra and two options for calculating gamma spectra. The differences among the four beta-spectrum options are mainly in the ways in which the Fermi function F(Z,W) is represented and calculated. The first of the two gamma-spectrum options consists of incorporating the unbroadened lines weighted by their intensities into an arbitrary number of energy groups. Alternatively, gamma lines are broadened according to detector resolutions before multigrouping in the second option.

The output of FPDCYS and the output of CINDER-10 are input to the FPSPEC code. Actually, only a small portion of the CINDER-10 output is utilized, namely, fission-product activities and total decay energies at the instant of time when corresponding spectra are sought. FPSPEC combines the individual

TABLE I

SUMMARY OF ENDF/B-IV FISSION-PRODUCT DATA FILE CONTENT

824	Nuclides (total)
181	Have differential cross sections
180	Have individual β and γ "lines" (spectral data consisting of energies and intensities)
712	Are unstable and each has an average β, γ, and α energy and branching fraction
10	Yield sets for 6 fissionable nuclides (∿10 000 yields)

(∿310 000 Data entries required in ENDF/B-IV)

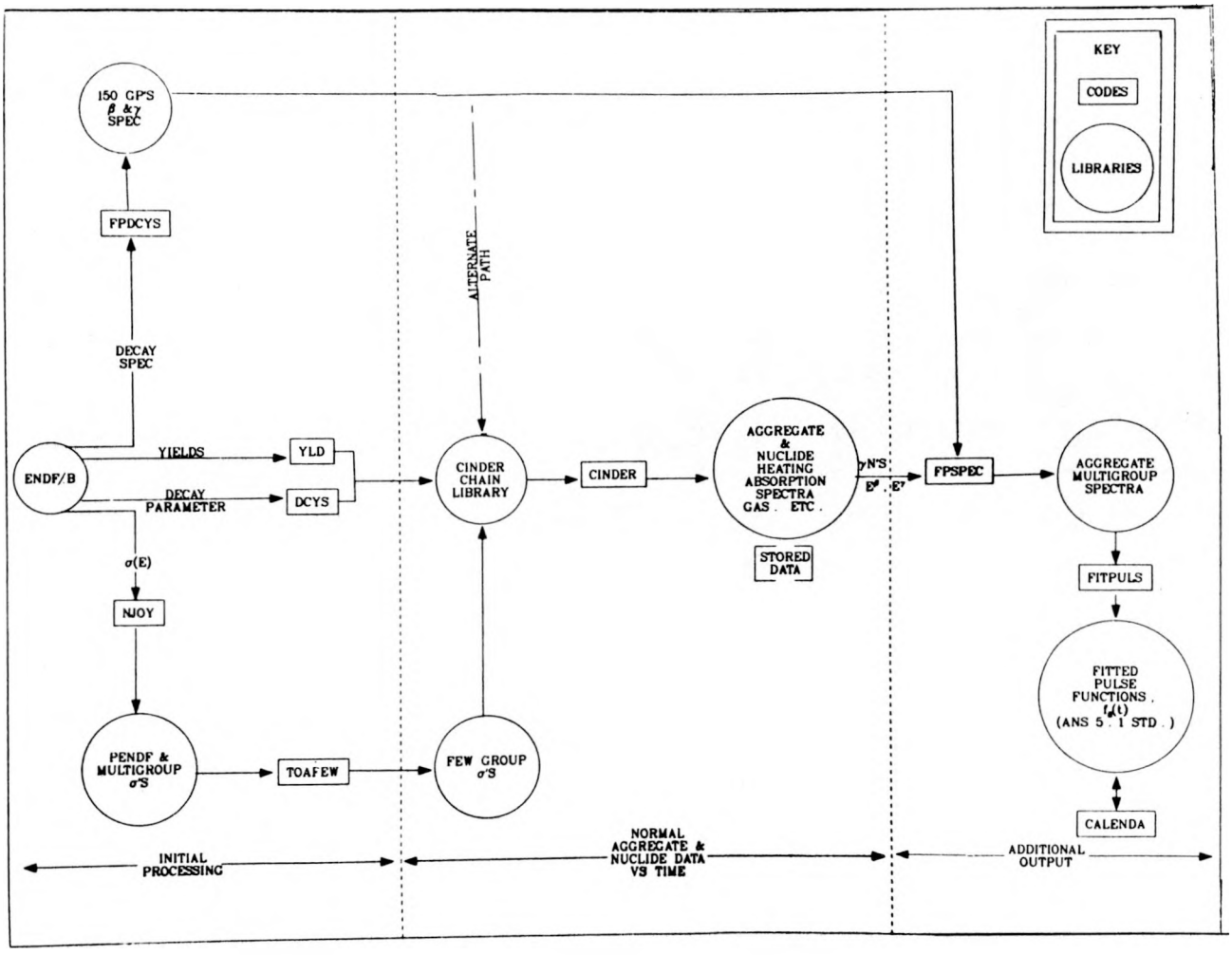

Fig. 1.
LASL nuclide processing codes and libraries.

spectra from FPDCYS and the nuclide activities from CINDER-10 to generate aggregate fission-product spectra for each irradiation and shutdown time. Note that CINDER-10 also incorporates a spectral subroutine capable of utilizing the multigroup data produced by the FPDCYS code. Plots of sample output from FPSPEC are shown in Figs. 2-5. In these illustrations, the calculated spectra are compared with the LASL experiment cited in Ref. 10.

As indicated above, spectral data are not available for all 824 fission products in ENDF/B-IV, and missing spectra must be approximately constructed. This is done for a particular nuclide by assuming that the shape of the beta (or gamma) spectrum for the nuclide is approximated by the spectrum shape of the aggregate 181 nuclides from a pulse after a cooling time approximately equal to the half-life of the nuclide in question. This shape is then normalized to the average beta- (gamma-) decay energy of the nuclide. Figures 6 and 7, respectively, compare the gamma spectra of ^{139}Cs with those constructed for a hypothetical nuclide having the same half-life and average gamma- and beta-decay energies as ^{139}Cs. The nuclide ^{139}Cs is a relatively important nuclide in the 0.1-s cooling time bin for 20 000-h thermal irradiation of ^{235}U. *However, it should be noted that such constructed individual spectra are used only in the aggregate.*

The libraries used in the CINDER-10 and auxiliary codes FPDCYS and FPSPEC are extensive and the codes are designed to use the libraries for any specified irradiation history. However, for many users the scope of application is unnecessary and aggregate results, rather than the detailed nuclide-by-nuclide output, are needed. The purpose of this report and the codes described in Ref. 11 is to eliminate the need for extensive summation code calculations for a wide range of problems. The summation codes and libraries have been used to produce multigroup beta and gamma spectra vs time following fission pulses, including the components of the spectra due to halogens and noble gases for a wide range of applications.

We have used the summation codes and libraries to produce secondary aggregate libraries and pulse functions shown as "additional output" in Fig. 1, which can be used directly or incorporated into neutronics codes. In particular, we have

- Used the summation codes to produce beta- and gamma-temporal spectra in 150 groups following fission pulses for each fuel and fission neutron energy in ENDF/B-IV and stored the results in formats similar to ENDF/B. These files delineate the noble gas and halogen spectra. Users can readily collapse the results to other multigroup spectra.

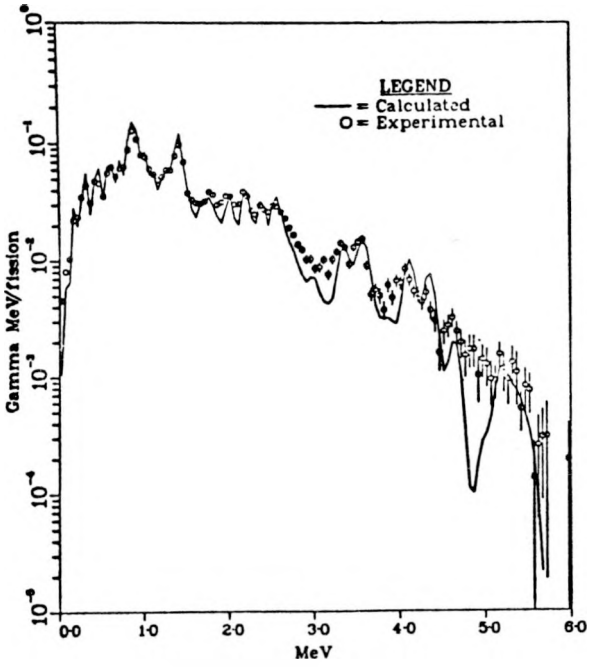

Fig. 2.
Gamma spectrum 5.56-h irradiation of ^{235}U, 70-s cooling.

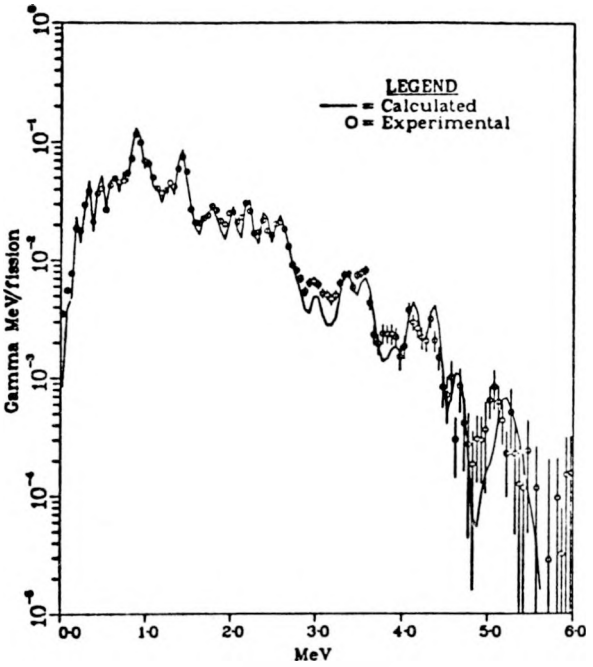

Fig. 3.
Gamma spectrum, 5.56-h irradiation of ^{235}U, 199-s cooling.

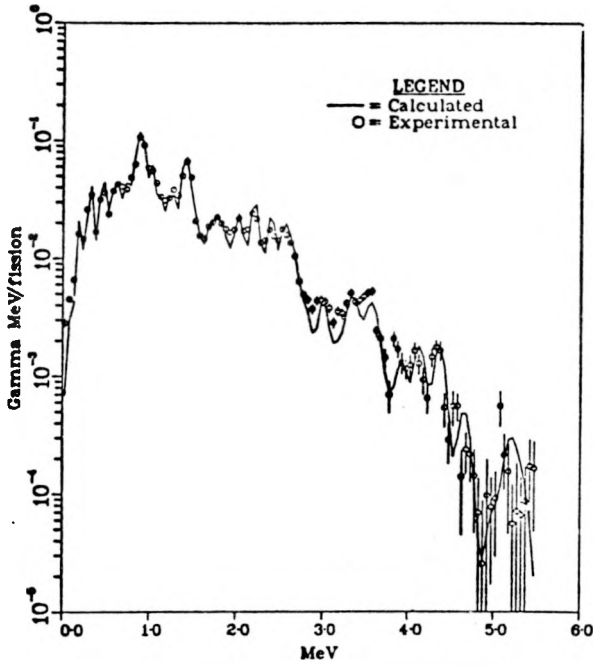

Fig. 4.
Gamma spectrum, 5.56-h irradiation of ^{235}U, 388-s cooling.

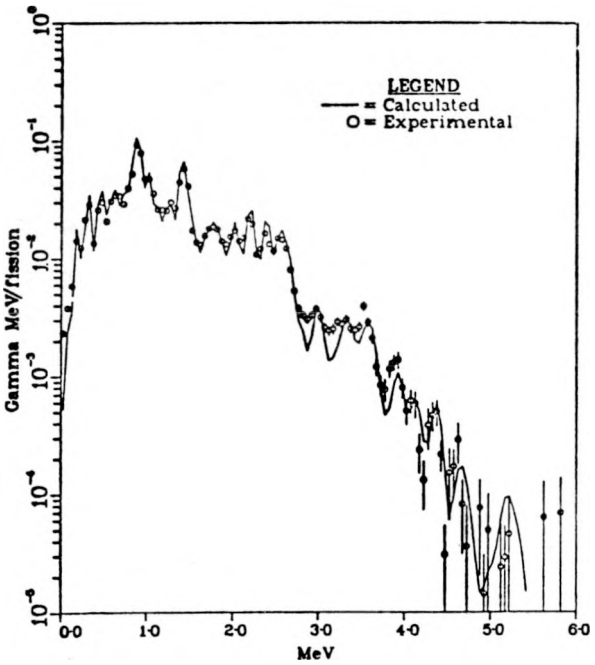

Fig. 5
Gamma spectrum, 5.56-h irradiation of ^{235}U, 660-s cooling.

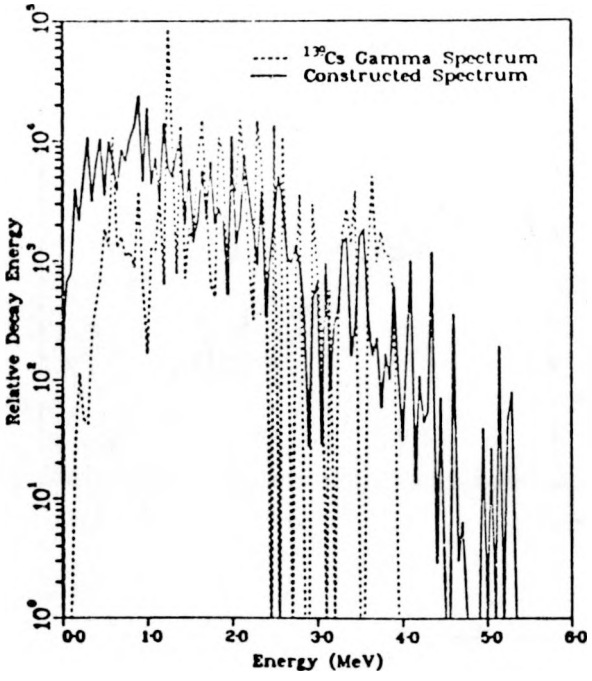

Fig. 6.
^{139}Cs gamma spectrum compared with constructed spectrum.

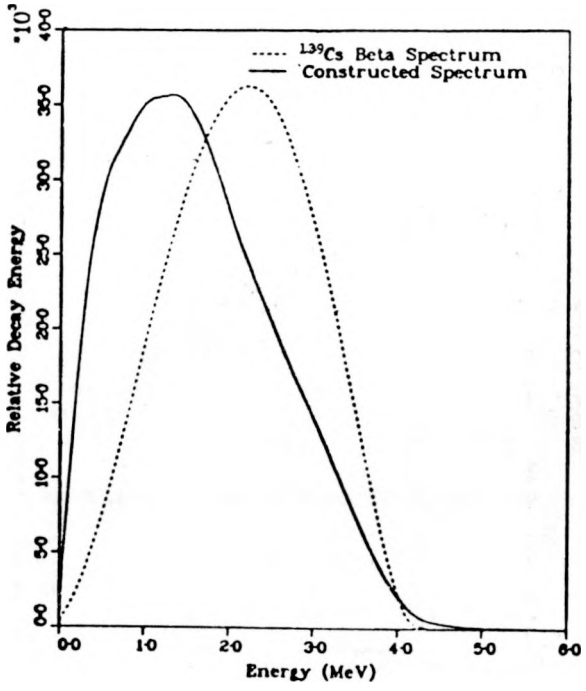

Fig. 7.
^{139}Cs beta spectrum compared with constructed spectrum.

- Collapsing and exponential fitting and folding codes have been developed, the latter being useful for generation of spectra following finite power histories.[11,12]
- For immediate use, exponential fits to a particular few-group spectra have been made available.[11,12]

Because the spectra are based on fission pulses, the libraries have a general utility. The exponential fits, for example, can be folded into any power (fission) history that can be described analytically or by a histogram representation. The effects of neutron absorption are also treated and approximately accounted for in the methodology.[11]

II. LIBRARY FOR PROCESSED ENDF/B AGGREGATE FISSION PRODUCT SPECTRA

Of particular interest is the application of the LASL code system to produce delayed beta- and gamma-spectral data on a fine energy grid (150 groups in 0.05 MeV steps from 0 to 7.5 MeV) for irradiation of the ENDF/B-IV fissionable nuclides with very short pulses (typically 10^{-4}-s irradiation time; shorter pulses do not alter the calculated spectra) of thermal, fast, and 14-MeV neutrons. The results can then be further processed into broad groups and fit with

functions of the type $f_c(t) = \sum_{i=1}^{n} \alpha_i e^{-\lambda_i t}$, as described in Refs. 11 and 12.

The fine-group results from the LASL code system are assembled into a single library in an ENDF-like format.[13] Definitions for the format for this processed ENDF/B fission-product and energy-yield data (PEFPYD) library are as follows.

MAT: Mat-No. of target nucleus, same as in ENDF/B.

MF: File No., used to identify energy type of incident neutron, defined as follows:

MF=80 - fission induced by thermal neutrons

MF=81 - fission induced by fast neutrons

MF=82 - fission induced by high-energy (14-MeV) neutrons.

Fission nuclide and energy combinations available in ENDF/B-IV are given in Table II.

MT: Section number used to describe data contents of the section. MT numbers are as follows:

MT=801 - delayed energy/fission for β^- + γ summed over all fission products

MT=802 - delayed energy/fission for β^- summed over all fission products

MT=803 - delayed energy/fission for γ summed over all fission products

MT=811 - delayed energy/fission for β^- + γ summed over all gaseous fission products (halogens plus noble gases)

MT=812 - delayed energy/fission for β^- summed over all gaseous fission products

MT=813 - delayed energy/fission for γ summed over all gaseous fission products

MT=821 - delayed energy/fission for γ + β^- summed over the noble gas fission products

MT=822 - delayed energy/fission for β^- summed over noble gas fission products

MT=823 - delayed energy/fission for γ summed over noble gas fission products

MT=831 - delayed energy/fission for β^- + γ summed over halogen fission products

MT=832 - delayed energy/fission for β^- summed over halogen fission products

MT=833 - delayed energy/fission for γ summed over halogen fission products

Other MT-numbers can be defined as needed; for example, MT-numbers could be assigned to any of the above spectra summed over energy.

TABLE II

FISSION YIELD DATA IN ENDF/B-IV

	Incident Neutron Energy Type		
Nuclide	Thermal	Fast	High Energy (14 MeV)
^{232}Th	--	Yes	No
^{233}U	Yes	No	No
^{235}U	Yes	Yes	Yes
^{238}U	--	Yes	Yes
^{239}Pu	Yes	Yes	No
^{241}Pu	Yes	No	No

The data are given in a TAB2 record with tables of spectra (decay energy/fission vs energy) given for a number of cooling times. Standard ENDF/B interpolation schemes between cooling times (TAB2 interpolation) are not recommended and, in any case, would be of interest only for fission pulses. However, when the pulse data are placed on a broad-group mesh and fitted with parameters as described in Refs. 11 and 12, calculations for any irradiation-cooling time combinations are possible, precluding the need for interpolation on the fine grid. Histogram interpolation is assigned for TAB1 interpolations.

File 1 (MF=1) information is also included, giving some processing information and a "dictionary" of the data to follow. The structure of MF=1 is as described in ENDF-102.[13] The structure of a section containing the processed data is

[MAT,MF,MT/ZA,AWR,0,0,0,0] HEAD
[MAT,MF,MT/0.0,0.0,0,0,1,NTS/TS_{int}] TAB2
[MAT,MF,MT/0.0,TS_1,0,0,1,NP/E'_{int}/DE(E',TS_1)] TAB1
[MAT,MF,MT/0.0,TS_2,0,0,1,NP/E'_{int}/DE(E',TS_2)] TAB1
- -
- -
[MAT,MF,MT/0.0,TD_{NFS},0,0,1,NP/E'_{int}/DE(E',TS_{NTS})] TAB1
[MAT,MF,MT/0.0,0.0,0,0,0,0] SEND

where

TS = cooling time step in seconds

DE = decay energy in MeV/fission (MeV/s)/(fiss/s)

E' = energy of particle (β^-) [photon (γ)] in MeV

NTS = number of cooling time steps given for a particular MT

NP = number of DE,E' pairs given in a particular TAB1 record.

Other quantities are defined in ENDF-102. Note that interpolation along cooling-time steps (the TAB2 records) is always set to zero, meaning that interpolation is not recommended, and that interpolation is always set to one (histogram) for the TAB1 records. A sample PEFPYD listing is given in Appendix A.

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13. D. Garber, C. Dunford, and S. Pearlstein, Eds., "ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF," Brookhaven National Laboratory report BNL-NCS-50496 (ENDF-102) (General Reactor Technology TID-4500) (October 1975).

LASL Identification
No. LP-2083

APPENDIX A

SAMPLE PEFPYD-LIB LISTING

```
U-233 (MAT 1260) THERMAL                                                    850
9.2233E+04 2.3104E+02          0          0          0          01260 1451     1
         0          0          0          0          0          01260 1451     2
         0          0          0          0          6         131260 1451     3
92 U 233 LASL PROCESSED MARCH 78, R.J. LABAUVE, D.C. GEORGE       1260 1451     4
THERMAL BURST                                                     1260 1451     5
                                                                  1260 1451     6
U-233  FISSION PRODUCT DECAY SPECTRA PROCESSED FROM ENDF/B-IV     1260 1451     7
IN 150 ENERGY GROUPS                                              1260 1451     8
                                                                  1260 1451     9
                                     1        451         22      1260 1451    10
                                    80        801       1202      1260 1451    11
                                    80        802       1208      1260 1451    12
                                    80        803       1029      1260 1451    13
                                    80        811        866      1260 1451    14
                                    80        812        858      1260 1451    15
                                    80        813        750      1260 1451    16
                                    80        821        793      1260 1451    17
                                    80        822        725      1260 1451    18
                                    80        823        705      1260 1451    19
                                    80        831        816      1260 1451    20
                                    80        832        817      1260 1451    21
                                    80        833        711      1260 1451    22
                                                                  1260 1   0    23
                                                                  1260 0   0    24
9.2233E+04 2.3104E+02          0          0          0          0126080801    25
0.         0.                  0          0          1         24126080801    26
        24         0           0          0          0          0126080801    27
0.         0.                  0          0          1        151126080801    28
       151         1           0          0          0          0126080801    29
0.00000+ 0 3.52841- 9 5.00000- 2 3.22830- 8 1.00000- 1 1.59743- 6126080801    30
1.50000- 1 1.29132- 7 2.00000- 1 2.00277- 7 2.50000- 1 5.24900- 7126080801    31
3.00000- 1 1.46303- 7 3.50000- 1 5.16394- 7 4.00000- 1 4.57273- 7126080801    32
4.50000- 1 1.79141- 6 5.00000- 1 3.13850- 6 5.50000- 1 2.24957- 6126080801    33
6.00000- 1 1.02391- 6 6.50000- 1 2.94562- 7 7.00000- 1 5.01967- 7126080801    34
7.50000- 1 4.02570- 7 8.00000- 1 8.84510- 6 8.50000- 1 3.83292- 7126080801    35
9.00000- 1 4.63775- 7 9.50000- 1 7.17263- 7 1.00000+ 0 4.42816- 7126080801    36
1.05000+ 0 5.85547- 7 1.10000+ 0 1.16917- 6 1.15000+ 0 4.29634- 7126080801    37
1.20000+ 0 1.46699- 6 1.25000+ 0 9.80709- 7 1.30000+ 0 1.04599- 6126080801    38
1.35000+ 0 6.24308- 7 1.40000+ 0 1.37299- 6 1.45000+ 0 7.48766- 7126080801    39
1.50000+ 0 8.40361- 7 1.55000+ 0 7.56328- 7 1.60000+ 0 6.60622- 7126080801    40
1.65000+ 0 6.75008- 7 1.70000+ 0 7.09880- 7 1.75000+ 0 8.13122- 7126080801    41
1.80000+ 0 6.81674- 7 1.85000+ 0 7.67507- 7 1.90000+ 0 7.07847- 7126080801    42
1.95000+ 0 8.24278- 7 2.00000+ 0 7.69455- 7 2.05000+ 0 7.30857- 7126080801    43
2.10000+ 0 7.91940- 7 2.15000+ 0 7.33980- 7 2.20000+ 0 7.74519- 7126080801    44
2.25000+ 0 7.99570- 7 2.30000+ 0 8.16737- 7 2.35000+ 0 7.56370- 7126080801    45
2.40000+ 0 8.13900- 7 2.45000+ 0 1.01530- 6 2.50000+ 0 8.09945- 7126080801    46
2.55000+ 0 9.88650- 7 2.60000+ 0 8.04170- 7 2.65000+ 0 7.30580- 7126080801    47
2.70000+ 0 9.72319- 7 2.75000+ 0 8.17771- 7 2.80000+ 0 7.95744- 7126080801    48
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4.35000+ 0 2.50161- 7 4.40000+ 0 2.34331- 7 4.45000+ 0 2.08048- 7126080801    59
4.50000+ 0 2.02252- 7 4.55000+ 0 1.78017- 7 4.60000+ 0 2.25345- 7126080801    60
4.65000+ 0 1.62566- 7 4.70000+ 0 1.56367- 7 4.75000+ 0 1.51789- 7126080801    61
4.80000+ 0 1.93194- 7 4.85000+ 0 1.43603- 7 4.90000+ 0 1.64057- 7126080801    62
4.95000+ 0 1.37519- 7 5.00000+ 0 1.32088- 7 5.05000+ 0 1.48632- 7126080801    63
5.10000+ 0 1.24321- 7 5.15000+ 0 1.83454- 7 5.20000+ 0 1.68122- 7126080801    64
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5.70000+ 0 9.90772- 8 5.75000+ 0 7.79808- 8 5.80000+ 0 7.49872- 8126080801    68
5.85000+ 0 9.05274- 8 5.90000+ 0 9.39758- 8 5.95000+ 0 6.67026- 8126080801    69
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6.75000+ 0 2.63316- 8 6.80000+ 0 2.40447- 8 6.85000+ 0 2.18150- 812608080175
6.90000+ 0 1.96579- 8 6.95000+ 0 1.75811- 8 7.00000+ 0 1.55985- 812608080176
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7.35000+ 0 4.97810- 9 7.40000+ 0 4.04345- 9 7.45000+ 0 3.28865- 912608080179
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1.80000+ 0 4.39172- 7 1.85000+ 0 4.93761- 7 1.90000+ 0 4.54248- 7126080801   148
1.95000+ 0 5.38394- 7 2.00000+ 0 4.92727- 7 2.05000+ 0 4.61637- 7126080801   149
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2.40000+ 0 5.13710- 7 2.45000+ 0 6.32814- 7 2.50000+ 0 5.15984- 7126080801   152
2.55000+ 0 6.51948- 7 2.60000+ 0 5.09995- 7 2.65000+ 0 4.53874- 7126080801   153
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3.15000+ 0 3.74443- 7 3.20000+ 0 3.57603- 7 3.25000+ 0 3.44476- 7126080801   157
3.30000+ 0 3.46412- 7 3.35000+ 0 3.55180- 7 3.40000+ 0 3.41514- 7126080801   158
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3.45000+ 0 2.26613- 7 3.50000+ 0 2.35814- 7 3.55000+ 0 3.53666- 7126080801   212
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4.20000+ 0 1.22564- 7 4.25000+ 0 1.50287- 7 4.30000+ 0 1.08897- 7126080801   217
4.35000+ 0 1.27949- 7 4.40000+ 0 1.11911- 7 4.45000+ 0 1.02566- 7126080801   218
4.50000+ 0 9.85953- 8 4.55000+ 0 8.71000- 8 4.60000+ 0 1.13265- 7126080801   219
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CARDS 241 THROUGH 2614 HAVE BEEN DELETED

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 1.50000- 1 1.48846-19 2.00000- 1 1.64537-19 2.50000- 1 1.63824-19126080802 2394
 3.00000- 1 1.47501-19 3.50000- 1 1.19179-19 4.00000- 1 8.56247-20126080802 2395
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 9.00000- 1 7.94316-20 9.50000- 1 8.20473-20 1.00000+ 0 8.41913-20126080802 2399
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 4.65000+ 0 1.43080-23 4.70000+ 0 1.22887-23 4.75000+ 0 1.04063-23126080802 2424
 4.80000+ 0 8.68122-24 4.85000+ 0 7.12864-24 4.90000+ 0 5.70799-24126080802 2425
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 6.30000+ 0 1.35725-33 6.35000+ 0 0.00000+ 0 0.00000+ 0 0.00000+ 0126080802 2435
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 9.2233E+04 2.3104E+02          0           0           0           0126080803 2437
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9.00000- 1 1.92402- 7 9.50000- 1 4.23937- 7 1.00000+ 0 1.27350- 7126080803 2448
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1.20000+ 0 1.06273- 6 1.25000+ 0 5.54597- 7 1.30000+ 0 5.98311- 7126080803 2450
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