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LAWRENCE LIVERMORE LABORATORY

University of California/Livermore, California

The Lawrence Livermore Laboratory Evaluated Nuclear Data Library

(ENDL) Translated into the ENDF/B Format

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The Lawrence Livermore Laboratory Evaluated Nuclear Data Library
(ENDL) Translated into the ENDF/B Format

ABSTRACT

The LLL Evaluated Nuclear Data Library (ENDL) has been translated into the ENDF/B Format. This translation is for the convenience of those people who wish to use the ENDL data but whose main familiarity is with the ENDF/B formats and procedures. Only the portion of ENDL which deals with neutron-induced interactions (including photon production from neutron-induced reactions) has been translated. Those parts of the ENDL library which deal with charged-particle-induced reactions have not been translated since they cannot be accommodated within the ENDF/B system. In order to provide a basis for judging the validity of the ENDL data, calculations were made of the output neutron time spectra from the LLL pulsed-sphere experiments, using for the calculations both the ENDL cross sections and the ENDF/B-III cross sections. Comparisons between these two sets of calculations and the experimental output neutron time spectra provide a basis for judging the relative merits of the ENDL and ENDF/B-III data sets in the 5 to 20 MeV neutron-energy regime.

Introduction

The Lawrence Livermore Laboratory Evaluated Nuclear Data Library (ENDL) has existed in one form or another since 1958. During these fifteen years it has undergone numerous changes in form, format, and, of course, content. The changes in form and format have come about because of changing laboratory needs and because newer and more powerful computational facilities allow for a more detailed representation of the physics. Experience has shown that the lifetime of a system for representing the data, the associated formats, and the concomitant processing code is about three to five years. The current system^{1,2} is now due for a change, and it is anticipated that a new system³ and processing code⁴ will be operational in mid-1974. The reason that it is possible to make such relatively frequent changes in the system, formats, and processing code follows from the magnitude and convenience of the LLL computational facility, and, even more important, from the fact that the activities of the Physical Data Group are primarily directed toward the task of supplying the data needs for only one laboratory, LLL.

During the course of the past fifteen years, requests for the ENDL data have come from many places outside of the laboratory: other AEC laboratories, DOD laboratories, other U.S. Government agencies and contractors, and universities. To comply with both the letter and the spirit of the law, the ENDL data have been made readily available, but often in a form that is unfamiliar to the requestor (and therefore inconvenient to use). While the ENDF/B system^{5,6} does not contain provisions for some of the data representations used in ENDL, it is a relatively stable system, has been well publicized, is generally well-known, and will accommodate almost all of the data forms for neutron-induced reactions, including photon production, used in

ENDL. It should be noted that the ENDF/B system will accommodate some data representations which are not currently available in the ENDL system.

In order to accommodate persons outside of LLL who request the ENDL data, the ENDL library has now been translated into the ENDF/B format. The translated data are available from the Radiation Shielding Information Center (RSIC), Oak Ridge National Laboratory, P. O. Box X, Oak Ridge, Tennessee 37830.

Philosophy and Contents of ENDL

The primary responsibility of the LLL Physical Data Group is to supply the best available calculational constants for the laboratory's needs. To this end, several activities are carried out by the group: a library of experimental neutron-induced reaction data^{7,8,9,10,11,12,13} (ECSIL) is maintained; a library of evaluated data (ENDL¹) for reactions induced by neutrons and charged particles is maintained; a processing code² is maintained which manipulates the ENDL data into the forms required for the laboratory's various neutronics, photonics, and linked neutronics-photonics codes; advanced Monte-Carlo neutronics, photonics, and linked neutronics-photonics computer programs¹⁴ are developed and maintained; finally, a file of evaluated integral neutron experiments¹⁵ is maintained for data-testing purposes.

The emphasis in this section is on the philosophy and contents of the ENDL data collection, and in particular on the portion of ENDL that pertains to neutron-induced reactions, including photon production. Historically, the original ENDL data were all produced at LLL and were in that sense a private collection. However, during the past five or so years excellent evaluations that were done elsewhere have become available, especially for the light isotopes and for neutron energies less than about 1 keV. Many

of these data have been incorporated into ENDL, usually with some modifications, especially for neutron energies greater than about five MeV. The bulk of the ENDL data have been produced at LLL, but whenever a new evaluation from another source has become available, it has been inspected, tested (if possible), and, if judged superior to existing ENDL data, adopted in part or in toto. Current plans are to continue to adopt as much useful informative as possible from extra-laboratory evaluations, with the ultimate objection of finally adopting a complete version of ENDF/B for the neutron files (realistically, this will likely be ENDF/B-V or ENDF/B-VI).

Many of the evaluations contained in ENDL have not been documented in any formal way. This is a recognized deficiency in the library. The seriousness of this deficiency must be judged by the user. This lack of documentation is primarily due to lack of available time for producing the reports, but it is also connected to the fact that the ENDL library is dynamic, with changes made as they are needed. The process of attaching addenda to reports so as to keep them up-to-date creates severe problems of logistics. To aid in the overall assessment of the evaluated data, particularly in the absence of formal documentation, reports have been written which contain the results of testing the most important materials against measured parameters of integral neutron experiments.

Table I is a table of contents for the five magnetic tapes which contain the ENDL data in the ENDF/B format. In Table I, 64 materials are listed for which complete evaluations are provided. In addition, eight isotopes are listed for which only one activation reaction in each case has been evaluated. Finally, a pseudo-material labeled "Crude Fission Product" is included. This pseudo-material is complete in form, but it represents only a zero-order

approximation to an average fission-product. The Crude Fission-Product material is not to be taken too seriously, but for some applications it has proved to be a convenient construct.

Translation Procedures from ENDL to ENDF/B

A computer code (LTOE) was written for the CDC 7600 to translate from the ENDL to the ENDF/B form. The size of LTOE is 1,377,767₈ or 393,207₁₀ computer words. The complete translated library contains 88,072 card image records, and it required slightly less than two minutes of CDC 7600 time to produce from the ENDL form. As mentioned above, there are some quantities and some representations in ENDL for which there are no equivalent representations in the ENDF/B system. As a result of this circumstance, local and total energy deposits were not translated, and the Legendre representations of energy-angle distributions, $\pi_{\ell}(E \rightarrow E')$, were truncated at the $\ell = 0$ term. The Legendre truncation affects only the secondary-neutron distribution from the (n,2n) reaction of the deuteron. The only other reaction represented by the Legendre energy-angle formalism in ENDL is the Be⁹ (n,2n) reaction, and an alternate formalism for that reaction is available. In working with Be⁹ in the ENDF/B format, care should be exercised, since the recently-approved MT numbers 6, 7, 8, 9, 46, 47, 48 and 49 are used to describe the (n,2n) reaction.

Testing the ENDL Data

Figures 1 through 16 show a comparison of calculated secondary neutron time spectra with experimental data from the 14 MeV LLL Pulsed Sphere Program.¹⁶ The calculations were done using the TART¹⁴ Monte Carlo code

and the ENDL library. Although the experiments and the theoretical calculations were carried out for several sphere thicknesses and two scattering angles, we show here for illustrative purposes only one material thickness and one detector angle for each material.

As a check on the TART code, the MCN Monte Carlo code¹⁷ was run at LASL by E. D. Cashwell in a calculation of some of the same pulsed spheres as those calculated by TART, with both codes using the same version of ENDL. Within Monte Carlo statistics, the results of the TART and MCN calculations were essentially identical. The handling of the evaluated data and the method of calculation are different in the two codes: specifically, the MCN code uses evaluated cross sections in a pointwise mode as presented in the evaluation, whereas TART averages the pointwise cross sections into 175 pre-selected groups; also, in the calculation of spectra MCN does an expectation calculation while TART does an analog calculation. Thus the agreement between the TART and MCN calculations constitutes a good (integral) check on the reliability of the two calculations. An inadvertent test of the sensitivity of the calculations to the exact form of the ENDL cross sections occurred in the following manner. Because of an error in communications, the first MCN calculation was done with an incorrect energy distribution for the $(n,2n)$ neutrons from iron: the peak of the energy distribution was shifted by 500 keV. The MCN results clearly differed from the TART results. After locating and correcting the error, the calculations then agreed. Our final conclusions are that the TART and MCN codes are sensitive to the input ENDL data, and that the calculations agree when the same input is used.

In studying the results of Figures 1-16, it should be noted that 100 nanoseconds must be added to the flight times as labeled on the abscissae of the plots. Thus the values labeled $2.4E + 02$ nanoseconds on the plots

are at 340 ($3.4E + 02$) nanoseconds. The experimental data for times greater than 340 nanoseconds are not to be taken seriously, according to J. D. Anderson of E-Division, since the detection efficiencies fall off drastically at these late times.

For some of the earlier experiments in the pulsed sphere program, the location of the experimental elastic peak is shifted in time from the calculated value (note for example the plot for water in Figure 1, which is the extreme example of this apparent disagreement). As another difficulty, the experimental time resolution cannot be determined accurately, which leads to a problem in matching the height of the elastic peak, since the full width at half maximum is an input value for the calculations which affects both the height and the width of the elastic peak. In the present calculations, the values shown in Reference 16 were used. By changing the values of Ref. 16 within their uncertainties, the elastic peak values can be matched. However, the ground rules established for the TART sphere calculations preclude making changes either in the evaluated data or in the method of calculation solely in order to obtain agreement between experiment and calculation. A more meaningful comparison between calculation and experiment in this respect is that of the integral under the elastic peak. The integrals were obtained over the time interval from zero to 160 nanoseconds. After 160 nanoseconds, the measured and calculated spectra have fallen to values that are at least one order of magnitude less, and, for heavy materials, as much as two and one-half orders of magnitude less, than the elastic peak values. Table II presents the results of the comparison between calculated and experimental integrals under the elastic peak

The LLL pulsed spheres comprise the only integral neutron experiments for 14 MeV neutrons which span the mass range from the lightest elements

to the heaviest. There is a gap from iron to lead (from mass ~ 56 to mass ~ 208) which should be filled-in if the set is to be complete. Since the LLL pulsed spheres include only a few of the total number of elements and isotopes, neutron emission spectra for incident 14 MeV neutrons have not been measured for the majority of the isotopes. Enough emission spectra have been measured, however, so that when these are considered together with the many measurements of neutron emission spectra obtained from charged-particle-induced reactions, it is possible to use systematics to deduce a recipe¹⁸ for the emission spectra, especially for the non-equilibrium (high energy) portion of the spectrum.

Although it is possible to fit any or all of the pulsed spheres by a process of successive approximations, in which the cross sections and spectra are adjusted until the degree of fit is as desired, we have chosen instead to use the pulsed sphere calculations simply as tests of existing evaluated data, and in particular to test the recipes used for the fission spectra and for the high energy portion of the emission spectra from inelastic scattering. Perhaps the most important use of these comparisons between spectral calculations and measurements is as a diagnostic tool, to direct attention to elements that apparently have poor-quality evaluations. Once we have identified such a material, the evaluation is examined for obvious errors. Experimental microscopic data are checked for new or overlooked data, and changes are made in the evaluation if there is a reason for such a change based on experimental data, reliable theoretical calculations, or an established recipe. If there is no reason to change the data based on one of these three considerations, then no change is made.

We have also made calculations of the LLL pulsed spheres using the ENDF/B-III evaluation library. The results of these calculations are presented

in Figures 17 to 28, which should be compared to the corresponding figures among Figures 1-16.

This work reported in this section is the result of the efforts of many people. A code for editing the TART calculation and magnetic tapes containing the pulsed sphere experimental data were supplied by J. Kammerdiener and C. Logan. E. Plechaty, in addition to his efforts in developing and running the TART code, converted the pulsed-sphere experimental data into a form that is convenient for retrieval from the photo-store, modified the edit code for teletype operation, and wrote a code for displaying the combined results of the calculations and the experiments on the television monitor. H. Barschall participated on a daily basis in discussing the representation of the physics in the data evaluations, suggesting auxiliary calculations which would check TART usage of the data, and arranging for E. Cashwell of LASL to make the MCN calculations. J. Anderson has made valuable suggestions (for the past many years) with respect to the physics of the emission spectra used in the evaluations, and has also provided advice as to the regions of greatest validity of the pulsed sphere measurements. S. Grimes calculated emission spectra from nuclear models which were then compared with the same quantities estimated from nuclear systematics.

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Table I. A listing of the magnetic tapes that contain the LLL ENDL data translated into the ENDF/B format.

LLL ENDL Data in ENDF/B Format			
Tape Number 1			
<u>ZA</u>	<u>Material</u>	<u>MAT Number</u>	<u>Nxy Included</u>
0001	Neutron	7000	--
1001	Hydrogen	7001	Yes
1002	Deuteron	7002*	Yes
1003	Triton	7003	--
2003	He ³	7004	Yes
2004	He ⁴	7005	--
3006	Li ⁶	7006	Yes
3007	Li ⁷	7007	Yes
4009	Be ⁹	7008	Yes
5010	B ¹⁰	7009	Yes
5011	B ¹¹	7010	Yes
6012	C ¹²	7011	Yes
7014	N ¹⁴	7012	Yes
8016	O ¹⁶	7013	Yes
9019	F ¹⁹	7014	Yes
11023	Na ²³	7015	Yes
12000	Mg ^{Nat}	7016	Yes
13027	Al ²⁷	7017	Yes
14000	Si ^{Nat}	7018	Yes
15031	P ³¹	7019	Yes
16032	S ³²	7020	Yes
17000	Cl ^{Nat}	7021	Yes
18000	Ar ^{Nat}	7022	Yes

* The energy-angle distribution of secondary neutrons from the n,2n reaction for D is represented by an energy-angle Legendre expansion in the ENDL system. No equivalent representation exists in the ENDF/B system. Consequently, the representation in the translated form is deficient.

Table I (continued).

LLL ENDL Data in ENDF/B Format

Tape Number 2

<u>ZA</u>	<u>Material</u>	<u>MAT Number</u>	<u>Nxγ Included</u>
19000	K ^{Nat}	7023	Yes
20000	Ca ^{Nat}	7024	Yes
22000	Ti ^{Nat}	7025	Yes
23051	V ⁵¹	7026	No (Planned)
24000	Cr ^{Nat}	7027	No (Planned)
25055	Mn ⁵⁵	7028	Yes
26000	Fe ^{Nat}	7029	Yes
28058	Ni ⁵⁸	7030	Yes
29000	Cu ^{Nat}	7031	Yes
31000	Ga ^{Nat}	7032	Yes
40000	Zr ^{Nat}	7033	No (Planned)
41093	Nb ⁹³	7034	Yes
42000	Mo ^{Nat}	7035	Yes
47107	Ag ¹⁰⁷	7036	No (Planned)
47109	Ag ¹⁰⁹	7037	No (Planned)
48000	Cd ^{Nat}	7038	Yes
50000	Sn ^{Nat}	7039	Yes
56138	Ba ^{Nat}	7040	Yes

Table I (continued).

LLL ENDL Data in ENDF/B Format

Tape Number 3

<u>ZA</u>	<u>Material</u>	<u>MAT Number</u>	<u>Nxy Included</u>
63000	EuNat	7041	Yes
64000	GdNat	7042	Yes
67165	Ho ¹⁶⁵	7043	Yes
73181	Ta ¹⁸¹	7044	Yes
74000	WNat	7045	Yes
78000	PtNat	7046	Yes
79197	Au ¹⁹⁷	7047	Yes
82000	PbNat	7048	Yes
90232	Th ²³²	7049	Yes
92233	U ²³³	7050	Yes

Tape Number 4

92234	U ²³⁴	7051	Yes
92235	U ²³⁵	7052	Yes
92236	U ²³⁶	7053	Yes
92237	U ²³⁷	7054	Yes
92238	U ²³⁸	7055	Yes
92239	U ²³⁹	7056	Yes
92240	U ²⁴⁰	7057	Yes
93237	Np ²³⁷	7058	Yes
94238	Pu ²³⁸	7059	Yes
94239	Pu ²³⁹	7060	Yes
94240	Pu ²⁴⁰	7061	Yes
94241	Pu ²⁴¹	7062	Yes
95242	Am ²⁴²	7063	Yes

Table I (continued).

LLL ENDL Data in ENDF/B Format

Tape Number 5

<u>ZA</u>	<u>Material</u>	<u>MAT Number</u>	<u>Nxy Included</u>
21045	Sc ⁴⁵ (Partial)	7064	No
26054	Fe ⁵⁴ (Partial)	7065	No
26056	Fe ⁵⁶ (Partial)	7066	No
26058	Fe ⁵⁸ (Partial)	7067	No
75185	Re ¹⁸⁵ (Partial)	7068	No
75187	Re ¹⁸⁷ (Partial)	7069	No
77191	Ir ¹⁹¹ (Partial)	7070	No
77193	Ir ¹⁹³ (Partial)	7071	No
99120	Crude Fission Product	7072	No

Table II. Integrals of the Time Spectra Under the Elastic Peak

Material	Sphere Thickness (mean free paths)	Angle (degrees)	Experimental Integral	Calculated Integral	Calc.-Exp. Exp.
H ₂ O	1.9	30	.309	.274	-.113
H ₂ O	1.9	120	.336	.297	-.116
D ₂ O	2.1	30	.302	.269	-.109
Li ⁶	0.5	30	.815	.799	-.020
Li ⁶	0.5	120	.831	.817	-.017
Li ⁷	0.5	30	.815	.813	-.002
Li ⁷	0.5	120	.835	.831	-.005
Be ⁹	0.8	30	.718	.670	-.067
C	0.5	30	.757	.736	-.027
C	0.5	120	.840	.837	-.003
N	1.1	30	.668	.612	-.084
Mg	0.7	30	.664	.721	+.086
Mg	0.7	120	.742	.794	+.070
Al	0.9	30	.590	.583	-.012
Al	0.9	120	.647	.646	-.002
Ti	1.2	30	.521	.549	+.054
Fe	0.9	30	.615	.615	+.000
Fe	0.9	120	.674	.683	+.013
Fe	4.8	30	.073	.058	-.205
Fe	4.8	120	.078	.070	-.102
Pb	1.4	30	.545	.483	-.114
Pb	1.4	120	.508	.533	+.049
U ²³⁵	0.7	30	.645	.686	+.061
U ²³⁵	0.7	120	.732	.789	+.078

Table II (continued).

Material	Sphere Thickness (mean free paths)	Angle (degrees)	Experimental Integral	Calculated Integral	Calc.-Exp. Exp.
U^{238}	0.8	30	.643	.653	+.015
U^{238}	0.8	120	.708	.749	+.058
Pu^{239}	0.7	30	.646	.706	+.093
Pu^{239}	0.7	120	.723	.790	+.093

Figure 1. Comparison of TART calculations with LLL pulsed sphere data for water, using the ENDL evaluated library.

Figure 2. Comparison of TART calculations with LLL pulsed sphere data for heavy water, using the ENDL evaluated library.

Figure 3. Comparison of TART calculations with LLL pulsed sphere data for teflon, using the ENDL evaluated library.

Figure 4. Comparison of TART calculations with LLL pulsed sphere data for lithium 6, using the ENDL evaluated library.

Figure 5. Comparison of TART calculations with LLL pulsed sphere data for lithium 7, using the ENDL evaluated library.

Figure 6. Comparison of TART calculations with LLL pulsed sphere data from carbon, using the ENDL evaluated library.

Figure 7. Comparison of TART calculations with LLL pulsed sphere data for nitrogen, using the ENDL evaluated library.

Figure 8. Comparison of TART calculations with LLL pulsed sphere data for oxygen, using the ENDL evaluated library.

Figure 9. Comparison of TART calculations with LLL pulsed sphere data for magnesium, using the ENDL evaluated library.

Figure 10. Comparison of TART calculations with LLL pulsed sphere data for aluminum, using the ENDL evaluated library.

Figure 11. Comparison of TART calculations with LLL pulsed sphere data for titanium, using the LNDL evaluated library.

Figure 12. Comparison of TART calculations with LLL pulsed sphere data for iron, using the ENDL evaluated library.

Figure 13. Comparison of TART calculations with LLL pulsed sphere data for lead, using the ENDL evaluated library.

Figure 14. Comparison of TART calculations with LLL pulsed sphere data for uranium 235, using the ENDL evaluated library.

Figure 15. Comparison of TART calculations with LLL pulsed sphere data for uranium 238, using the ENDL evaluated library.

Figure 16. Comparison of TART calculations with LLL pulsed sphere data for plutonium, using the ENDL evaluated library.

Figure 17. Comparison of TART calculations with LLL pulsed sphere data for lithium 6, using the ENDF/B-III evaluated library.

Figure 18. Comparison of TART calculations with LLL pulsed sphere data for lithium 7, using the ENDF/B-III evaluated library.

Figure 19. Comparison of TART calculations with LLL pulsed sphere data for carbon, using the ENDF/B-III evaluated library.

Figure 20. Comparison of TART calculations with LLL pulsed sphere data for nitrogen, using the ENDF/B-III evaluated library.

Figure 21. Comparison of TART calculations with LLL pulsed sphere data for oxygen, using the ENDF/B-III evaluated library.

Figure 22. Comparison of TART calculations with LLL pulsed sphere data for magnesium, using the ENDF/B-III evaluated library.

Figure 23. Comparison of TART calculations with LLL pulsed sphere data for aluminum, using the ENDF/B-III evaluated library.

Figure 24. Comparison of TART calculations with LLL pulsed sphere data for iron, using the ENDF/B-III evaluated library.

Figure 25. Comparison of TART calculations with LLL pulsed sphere data for lead, using the ENDF/B-III evaluated library.

Figure 26. Comparison of TART calculations with LLL pulsed sphere data for uranium 235, using the ENDF/B-III evaluated library.

Figure 27. Comparison of TART calculations with LLL pulsed sphere data for uranium 238, using the ENDF/B-III evaluated library.

Figure 28. Comparison of TART calculations with LLL pulsed sphere data for plutonium, using the ENDF/B-III evaluated library.

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