ENDL Type Formats for the Livermore Evaluated Photon Data Library, EPDL

I. Contents

This report describes the input formats for the Lawrence Livermore Evaluated Photon Data Library, EPDL. Tables and graphs of these data have been reported in ref. (1) and (2) and the evaluation process is discussed in ref. (3). These formats are an extension of the ENDL concepts which form the basis for Lawrence Livermore National Laboratory's evaluated data libraries.⁴

This library contains complete information for particle transport for Z=1-100 and for incident photons energies from 10 eV, or threshold, to 100 GeV. Units are barns and MeV (millions of electron volts). The specific data are the following:

- 1) Coherent scattering,
 - a) integrated cross section (b),
 - b) form factor,
 - c) real and imaginary anomalous scattering factors,
 - d) average energy of the scattered photon (MeV),
- 2) Incoherent scattering
 - a) integrated cross section (b),
 - b) scattering function,
 - c) average energy of the scattered photon and recoil electron (MeV).
- 3a) Total photoelectric reaction
 - a) integrated cross section (b),
 - b) average energy to the residual atom, i.e., local deposition (MeV),
 - c) average energy of the secondary photons and electrons (MeV).
- 3b) Photoelectric reaction, by subshell
 - a) integrated cross section (b),
 - o) average energy to the residual atom, i.e., local deposition (MeV),
 - c) average energy of the secondary photons and electrons $(\mbox{MeV})\,.$
- 4) Pair production reaction
 - a) integrated cross section (b),
 - b) average energy of the secondary electron and positron (MeV).
- 5) Triplet production reaction
 - a) integrated cross section (b),
 - b) average energy of the secondary electron and positron (MeV).

In the context of particle transport, the EPDL file only contains data for photon transport. In order to perform coupled photon-electron transport calculations, two additional libraries are required. These are the Livermore Evaluated Electron Data Library (EEDL)⁵, which describes

the interaction of electrons with matter and the Livermore Evaluated Atomic Data Library (EADL) 6 , which describes atomic relaxation.

In Section II, formats and definitions for the EPDL parameters are given. This is followed in Section III by the definitions, formats, and sorting order for the data in the EPDL file. In Section IV, the subshell designators are defined. Finally in Section V, several examples are given.

II. Formats and Definitions for the EPDL Parameters

All data are in the Livermore ENDL (Evaluated Nuclear Data Library) format⁴. Although the ENDL format is much more detailed, in this report only the definitions pertinent to the EPDL file are given. The data are in a series of character tables. Each table starts with two header lines that contain the parameters that physically describe the data that follow. The two header lines are followed by a series of data lines, one data point per line. Each table is terminated by an end of table line which is blank except for a 1 in column 72 (column 72 is blank on all other lines in the table). A table may be followed by another table or an end of file.

The two header lines in general in the ENDL format contain a great deal of information. However, as applied to the EPDL photon data the only fields of interest are as shown in Table I.

TABLE I. Header Line Formats for the EPDL Character File

Line	Columns	Format	Definition
1 1	1-3 4-6	I3 I3	<pre>Z - atomic number A - mass number (in all cases=0, for elemental data)</pre>
1	8-9	I2	<pre>Yi - incident particle designator (see Table II)</pre>
1	11-12	12	Yo - outgoing particle designator (see Table II)
1	14-24	E11.4	AW - atomic mass (amu)
1	26-31	I 6	Date - date of evaluation (YYMMDD)
1	32	I1	<pre>Iflag - interpolation flag</pre>
2	1-2	12	<pre>C - reaction descriptor (see Table II)</pre>
2	3-5	13	I - reaction property (see Table II)
2	6-8	13	S - reaction modifier (see Table II)
2	22-32	E11.4	X1 - subshell designator (see Table VI)

Table II defines the ENDL parameters that are on the header lines. The actual values for these parameters are what classifies the data in the EPDL file.

TABLE II. Definition of the EPDL Parameters

Yi - incident particle designator =7, photon (in all cases) C - reaction descriptor =71, coherent scattering =72, incoherent scattering =73, photoelectric effect =74, pair production =75, triplet production S - reaction modifier =0, no X1 field data required =91, X1 field data required X1 - value depends upon the value of S if S=0, X1=0. if S=91, X1=subshell designator (see Table VI) Yo - secondary particle designator =0, no outgoing particle =7, photon =8, positron =9, electron I - reaction property =0, integrated cross section =10, average energy of the secondary particle, Yo =11, average energy to the residual atom =941, form factor =942, scattering function

In Table III, a summary of the contents of the EPDL file is given in terms of the EPDL parameters.

=943, imaginary anomalous scattering factor =944, real anomalous scattering factor

Table III. Summary of the EPDL Data Base

Yi	С	S	X1	Yo	I	Data Types
				Co	oherent	scattering
7	71	0	0.	0	0	integrated coherent cross section
7	71	0	0.	0	941	form factor
7	71	0	0.	0	943	imaginary anomalous scattering factor
7	71	0	0.	0	944	real anomalous scattering factor
7	71	0	0.	7	10	average energy of the scattered photon

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Incoherent scattering										
7	72	0	0.	0	0	integrated incoherent cross section				
7	72	0	0.	0	942	scattering function				
7	72	0	0.	7	10	average energy of the scattered				
				_		photon				
7	72	0	0.	9	10	average energy of the recoil				
						electron				
Photoelectric										
7	73	0	0.	0	0	<pre>integrated photoelectric cross section</pre>				
7	77	0	0.	0	11	average energy to the residual atom				
7	73 73	0	0.	7	10	average energy of the secondary				
7	13	U	0.	,	10	photons				
7	73	0	0.	9	10	average energy of the secondary				
,	13	Ü	٠.	,		electrons				
Photoelectric (by subshell)										
		01	- *		0	integrated photoelectric cross				
7	73	91	^	0	U	section				
7	73	91	*	0	11	average energy to the residual atom				
7	73 73	91	*	7	10	average energy of the secondary				
•	75	J_		•	-+	photons				
7	73	91	*	9	10	average energy of the secondary				
·						electrons				
					Pair p	production				
7	 74	0	0.	0	0	integrated pair production cross				
,	12	U	٠.	Ŭ	•	section				
7	74	0	0.	8	10	average energy of the secondary				
,		_				positron				
7	74	0	0.	9	10	average energy of the secondary				
						electron				
Triplet production										
7	7 5	0	0.	0	0	integrated triplet production cross section				
7	75	0	0.	8	10	average energy of the secondary				
	. •	-				positron				
7	75	0	0.	9	10	average energy of the secondary				
						electron				

^{*}Subshell designator (see Table VI).

III. Definitions and Formats for the EPDL Data Lines and Sorting Order

The definitions for the data lines are described in Table IV, followed by their formats in Table V. This is followed by the sorting order of all of the data in the file.

The general ENDL data format defines some 35 types of reaction properties and is used to describe neutron, charged particle, photon, electron, positron, and atomic relaxation processes. The EPDL data definitions are but a small subset of this, as shown here.

TABLE IV. Definitions of the EPDL Data

E - incident photon energy

 σ - cross section

<E'p> - average energy of the secondary particle

 $\langle E_{loc} \rangle$ - average energy to the residual atom, i.e., local deposition

x - argument for form factor and scattering function^a

F - form factor

S - scattering function

I - imaginary anomalous scattering factor

R - real anomalous scattering factor

By definition for photon scattering, the average energy for the coherently scattered photon is equal to the energy of the incident photon. These values are carried in the data files so as not to make any special unique cases. For the photoelectric effect, photons and electrons are released from the atom. These are accounted for in energy deposition through the atom relaxation data from ref. (6). The average energy to the residual atom insures energy conservation and is deposited locally.

The format for the full ENDL data line is 6E11.4. However, the actual number of fields used (up to 6 maximum) depends explicitly upon the reaction property designator, I. Following each set of data is an end of table line with a 1 in column 72, i.e., format of 71X, II.

TABLE V. Actual formats for the EPDL Data Lines in Terms of the Reaction Property, I (see Table IV for definitions)

I	Fiel	d Number	(6E11.4	format)	
	1	2	3 4	5	6
0	E	σ			
10	E	<e 'd=""></e>			
11	E	<e'<sub>p> <e<sub>loc></e<sub></e'<sub>			
941	×	F			
942	x	S			
943	E	I			
944	E	R			

^a the parameter x (cm⁻¹) is defined by x=sin($\theta/2$)/ λ , where θ is the photon scattering angle and λ is its wave length (cm).

The EPDL data is sorted in the following order for the character file:

The data is sorted into ascending order by Z (Z=1-100). Within each Z, data is sorted by increasing C number (C=71-75). Within each C number, data is sorted by increasing S number (S=0 or 91). Within each S number, data is sorted by increasing X1 field (X1=1.-61.). Within each X1 field, data is sorted by increasing Yo number (Yo=0-9). Within each Yo number, data is sorted by increasing I number (I=0-944).

Within each data block, data is sorted by increasing field number (see Table V) over all independent variables, i.e., the number of fields required for the data minus one. Field 1 is the slowest varying variable, field 2 the next slowest varying, etc.. For any variable, the sort is by increasing value, e.g., by increasing incident photon energy.

IV. Atomic Subshell Designators

Atomic subshells in the ENDL format are specified by prescribed floating point designators. Although this description can specify shells, partial shells, and subshells, only the latter are used in the EPDL file. The designators are given in Table VI.

TABLE VI. Atomic Subshell Designators

Desig- nator	Subshell		Desig- nator	Subshell		Desig- nator	- S	Subshell	
1.	K	(1s1/2)	21.	N4	(4d3/2)	41.	P1	(6s1/2)	
2.	L	(2)	22.	N5	(4d5/2)	42.	P23	(6p)	
3.	L1	(2s1/2)	23.	N67	(4f)	43.	P2	(6p1/2)	
4.	L23	(2p)	24.	И6	(4f5/2)	44.	Р3	(6p3/2)	
5.	L2	(2p1/2)	25.	N7	(4f7/2)	45.	P45	(6d)	
6.	L3	(2p3/2)	26.	0	(5)	46.	P4	(6d3/2)	
7.	М	(3)	27.	01	(5s1/2)	47.	P5	(6d5/2)	
8.	M1	(3s1/2)	28.	023	(5p)	48.	P67	(6f)	
9.	M23	(3p)	29.	02	(5p1/2)	49.	Р6	(6f5/2)	
10.	M 2	(3p1/2)	30.	03	(5p3/2)	50.	P7	(6f7/2)	
11.	м3	(3p3/2)	31.	045	(5d)	51.	P89	(6g)	
12.	M45	(3d)	32.	04	(d3/2)	52.	P8	(6g7/2)	
13.	M4	(3d3/2)	33.	05	(5d5/2)	53.	Р9	(6g9/2)	
14.	M5	(3d5/2)	34.	067	(5f)	54.	P1011	(6h)	
15.	N	(4)	35.	06	(5f5/2)	55.	P10	(6h9/2)	
16.	N1	(4s1/2)	36.	07	(5f7/2)	56.	P11	(6h11/2)	
17.	N 23	(4p)	37.	089	(5g)	57.	Q	(7)	
18.	N2	(4p1/2)	38.	08	(5g7/2)	58.	Q1	(7s1/2)	
19.	N 3	(4p3/2)	39.	09	(5g9/2)	59.	Q23	(7p)	
20.	N4 5	(4d)	40.	Ρ	(6)	60.	Q2	(7p1/2)	
						61.	Q3	(7p3/2)	

V. Examples

In this section, several examples of EPDL data are given. These may not coincide with the data in the existing file as improvements are continually being made. As described earlier, the data is in an Ell.4 format, with the exception of machine independent modifications made to give more significant figures within the eleven columns. Note also that some of the data lines may have been deleted in order to condense the table to an acceptable size.

The first example is for incoherent scattering. There are two tables included here. The first is for the average energy to the scattered photon and the second is for the average energy to the recoil electron.

```
10000 7 7 2.01790+ 1 891031 2 0.00000+ 0 0.00000+00 0.00000+ 0
72 10 0 0.00000+ 0 0.00000+ 0 0.00000+ 0 0.00000+ 0 0.00000+ 0
1.0000000-5 9.99973- 6
1.3335200-5 1.33347- 5
1.7154400-5 1.71536- 5
5.1628600-5 5.16212- 5
1.0000000-4 9.99722- 5
1.3335200-4 1.33303- 4
2.2067300-4 2.20540- 4
1.0000000-3 9.97285- 4
1.5124700-3 1.50632- 3
1.9152500-3 1.90544- 3
 3.03991+ 0 1.28051+ 0
 5.51354+ 0 2.00305+ 0
 1.00000+ 1 3.16457+ 0
 1.77828+ 1 4.97924+ 0
 4.21697+ 1 1.00257+ 1
 1.00000+ 2 2.06173+ 1
 3.16228+ 2 5.53470+ 1
 1.00000+ 3 1.52030+ 2
 5.62341+ 3 7.14193+ 2
 1.00000+ 4 1.20394+ 3
 1.00000+ 5 9.95532+ 3
10000 7 9 2.01790+ 1 891031 2 0.00000+ 0 0.00000+00 0.00000+ 0
72 10 0 0.00000+ 0 0.00000+ 0 0.00000+ 0 0.00000+ 0 0.00000+ 0
1.0000000-5 2.74017-10
1.3335200-5 4.87716-10
1.7154400-5 8.11753-10
5.1628600-5 7.40653- 9
1.0000000-4 2.78343- 8
1.3335200-4 4.93021- 8
2.2067300-4 1.33607- 7
5.6742200-4 8.78699- 7
1.0000000-3 2.71464- 6
1.5124700-3 6.15721- 6
1.9152500-3 9.81358- 6
2.3547700-3 1.46577- 5
2.8213400-3 2.08466- 5
3.5579900-3 3.25158- 5
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```
4.2839800-3 4.63741- 5
5.0042900-3 6.22147- 5
5.9498600-3 8.59610- 5
1.00000+ 1 6.83543+ 0
1.77828+ 1 1.28036+ 1
4.21697+ 1 3.21440+ 1
1.00000+ 2 7.93827+ 1
3.16228+ 2 2.60881+ 2
1.00000+ 3 8.47970+ 2
 5.62341+ 3 4.90922+ 3
1.00000+ 4 8.79606+ 3
1.00000+ 5 9.00447+ 4
      The second example is for the photoelectric cross section of the K
shell in neon (Z=10).
10000 7 0 2.01790+ 1 8910315 2 0.00000+ 0 0.00000+00 0.00000+ 0
73 0 91 0.00000+ 0 1.00000+ 0 0.00000+ 0 0.00000+ 0 0.00000+ 0
8.5818000-4 3.00531+ 5
8.7884100-4 2.98840+ 5
8.9466300-4 2.95665+ 5
9.0000000-4 2.93990+ 5
9.1199600-4 2.88968+ 5
9.2731100-4 2.80552+ 5
9.4032700-4 2.72220+ 5
9.6141200-4 2.57631+ 5
1.0005600-3 2.31342+ 5
1.0211800-3 2.19483+ 5
1.0582800-3 2.01377+ 5
1.1778800-3 1.58025+ 5
1.2140200-3 1.47004+ 5
1.2799500-3 1.28637+ 5
1.3317300-3 1.15882+ 5
 8.00000+ 3 1.28280- 8
 1.00000+ 4 1.02586- 8
 1.50000+ 4 6.83907- 9
 2.00000+ 4 5.12930- 9
 3.00000+ 4 3.41953- 9
 4.00000+ 4 2.56465- 9
 5.00000+ 4 2.05172- 9
 6.00000+ 4 1.70977- 9
 8.00000+ 4 1.28185- 9
 1.00000+ 5 1.02586- 9
                                                                        1
```

References

- 1) D. E. Cullen, et. al., <u>Tables and Graphs of Photon-Interaction Cross Sections Derived from the LLNL Evaluated Photon Data Library (EPDL)</u>, <u>Z = 1 50)</u>, Lawrence Livermore National Laboratory, Livermore, CA, Vol. 6, Part A, Rev. 4 (1991).
- 2) D. E. Cullen, et. al., <u>Tables and Graphs of Photon-Interaction Cross Sections Derived from the LLNL Evaluated Photon Data Library (EPDL)</u>, <u>Z = 51 100</u>), Lawrence Livermore National Laboratory, Livermore, CA, Vol. 6, Part B, Rev. 4 (1991).
- 3) D. E. Cullen, S. T. Perkins, and J. A. Rathkopf, <u>The 1989 Livermore Photon Data Library (EPDL)</u>, <u>Lawrence Livermore National Laboratory</u>, Livermore, CA, UCRL-ID-103424 (1990).
- 4) R. J. Howerton, et. al., <u>OMEGA, A CRAY 1 Executive Code for LLNL Nuclear Data Libraries</u>, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-50400, Vol. 25 (1983). See specifically Ch. I and II.
- 5) S. T. Perkins, D. E. Cullen, and S. M. Seltzer, <u>Tables and Graphs of Electron-Interaction Cross Sections Derived from the LLNL Evaluated Electron Data Library (EEDL), Z = 1 100), Lawrence Livermore National Laboratory, Livermore, CA, Vol. 31 (1991).</u>
- 6) S. T. Perkins, et. al., <u>Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library (EADL)</u>, Z = 1 100, Lawrence Livermore National Laboratory, Livermore, CA, Vol. 30 (1991).