ENDL Type Formats for the Livermore Evaluated Electron Data Library, EEDL

I. Contents

This report describes the input formats for the Lawrence Livermore Evaluated Electron Data Library, EEDL. Tables and graphs of these data have been reported in ref. (1). These formats are an extension of the ENDL concepts which form the basis for Lawrence Livermore National Laboratory's evaluated data libraries[2].

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

1) Elastic transport
   a) transport cross section, $\sigma_{el}(1-\overline{\cos\theta},)$ (b).

2) Large angle elastic scattering (over cosθ=-1. to 0.999999)
   a) integrated large angle scattering cross section (b),
   b) average energy of the scattered electron (MeV),
   c) average energy to the residual atom, i.e., local deposition (MeV),
   d) angular distribution of the scattered electron.

3) Elastic scattering
   a) integrated scattering cross section (b).

2) Ionization (by subshell, over the recoil electron energy range down to 0.1 eV),
   a) integrated cross section (b),
   b) average energy of the scattered and recoil electron (MeV),
   c) spectra of the recoil electron (MeV^{-1}).

3) Bremsstrahlung (over the photon energy range down to 0.1 eV),
   a) integrated cross section (b),
   b) average energy of the secondary electron and photon (MeV),
   c) spectra of the secondary photon (MeV^{-1}).

4) Excitation
   a) integrated cross section (b),
   b) average energy to the residual atom, i.e., local deposition (MeV).

In the context of particle transport, the EEDL file only contains data for electron transport. In order to perform coupled photon-electron transport calculations, two additional libraries are required. These are the Livermore Evaluated Photon Data Library (EPDL)[3,4,5], which

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

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

II. Formats and Definitions for the EEDL Parameters

All data are in the Livermore ENDL (Evaluated Nuclear Data Library) format[2]. Although the ENDL format is much more detailed, in this report only the definitions pertinent to the EEDL 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 EEDL electron data the only fields of interest are as shown in Table I.

TABLE I. Header Line Formats for the EEDL Character File

Line	Columns	Format	Definition
1	1-3	I3	Z - atomic number
1	4-6	I3	A - mass number (in all cases=0, for elemental data)
1	8-9	I2	Yi - incident particle designator (see Table II)
1	11-12	I2	Yo - outgoing particle designator (see Table II)
1	14-24	E11.4	AW - atomic mass (amu)
1	26-31	I6	Date - date of evaluation (YYMMDD)
1	32	I1	Iflag - interpolation flag =0 or 2, linear in x and y =3, logarithmic in x, linear in y =4, linear in x, logarithmic in y =5, logarithmic in x and y
2	1-2	I2	C - reaction descriptor (see Table II)
2	3-5	I3	I - reaction property (see Table II)
2	6-8	I3	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 EEDL file. In what follows, the scattered electron is the incident electron after the reaction. By ENDL convention, this is the one of highest energy. The recoil electron is the other electron involved in the reaction. By definition, this is the one of lowest energy. Both of these, along with the photon, are defined as outgoing particles.

TABLE II. Definition of the EEDL Parameters

Yi - incident particle designator
=9, electron (in all cases)

C - reaction descriptor
=7, elastic transport
=8, large angle elastic scattering
=10, elastic scattering
=81, ionization
=82, bremsstrahlung
=83, excitation

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 - outgoing particle designator
=0, no outgoing particle
=7, photon
=9, electron
=19, electron as recoil

I - reaction property
=0, integrated cross section
=10, average energy of the secondary particle, Yo
=11, average energy to the residual atom
=21, spectra of recoil particle
=22, angular distribution

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

Table III. Summary of the EEDL Data Base

Yi	C	S	X1	Yo	I	Data Types
				Elastic transport		
9	7	0	0.	0	0	transport cross section
				Large angle elastic scattering		
9	8	0	0.	0	0	integrated large angle scattering cross section
9	8	0	0.	0	11	average energy to the residual atom
9	8	0	0.	9	10	average energy of the scattered electron
9	8	0	0.	9	22	angular distribution of the scattered electron
				Elastic scattering		
9	10	0	0.	0	0	integrated scattering cross section
				Ionization (by subshell)		
9	81	91	*	0	0	integrated ionization cross section
9	81	91	*	9	10	average energy of the scattered electron
9	81	91	*	19	10	average energy of the recoil electron
9	81	91	*	19	21	spectra of the recoil electron
				Bremsstrahlung		
9	82	0	0.	0	0	integrated bremsstrahlung cross section
9	82	0	0.	7	10	average energy of the secondary photon
9	82	0	0.	7	21	spectra of the secondary photon
9	82	0	0.	9	10	average energy of the secondary electron
				Excitation		
9	83	0	0.	0	0	integrated excitation cross section
9	83	0	0.	0	11	average energy to the residual atom

*Subshell designator (see Table VI).

III. Definitions and Formats for the EEDL 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 EEDL data definitions are but a small subset of this, as shown here.

TABLE IV. Definitions of the EEDL Data

E - incident electron energy
σ - cross section
$\langle E'_p \rangle$ - average energy of the secondary particle
$\langle E_{loc} \rangle$ - average energy to the residual atom, i.e., local deposition
E' - energy of the secondary particle
p - particle spectra, unit normalized
x - angular variable, $x=1-\cos\theta$, where θ is the scattering angle
f - angular distribution, unit normalized, over the range x=0.000001 to 2. ($\cos\theta$=-1. to 0.999999)

By definition for electron scattering, local energy deposition is zero and the average energy to the scattered electron is equal to the energy of the incident electron. These values are carried in the data files so as not to make any special unique cases.

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,I1.

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

I	Field Number (6E11.4 format) 1	2	3	4	5	6
0	E	σ				
10	E	$\langle E'_p \rangle$				
11	E	$\langle E_{loc} \rangle$				
21	E	E'	p			
22	E	x	f			

The EEDL 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=7-83).
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=0-19).
Within each Yo number, data is sorted by increasing I number (I=0-22).

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 electron 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 EEDL file. The designators are given in Table VI.

TABLE VI. Atomic Subshell Designators

Designator	Subshell		Designator	Subshell		Designator	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.	N6	(4f5/2)	44.	P3	(6p3/2)
5.	L2	(2p1/2)	25.	N7	(4f7/2)	45.	P45	(6d)
6.	L3	(2p3/2)	26.	O	(5)	46.	P4	(6d3/2)
7.	M	(3)	27.	O1	(5s1/2)	47.	P5	(6d5/2)
8.	M1	(3s1/2)	28.	O23	(5p)	48.	P67	(6f)
9.	M23	(3p)	29.	O2	(5p1/2)	49.	P6	(6f5/2)
10.	M2	(3p1/2)	30.	O3	(5p3/2)	50.	P7	(6f7/2)
11.	M3	(3p3/2)	31.	O45	(5d)	51.	P89	(6g)
12.	M45	(3d)	32.	O4	(d3/2)	52.	P8	(6g7/2)
13.	M4	(3d3/2)	33.	O5	(5d5/2)	53.	P9	(6g9/2)
14.	M5	(3d5/2)	34.	O67	(5f)	54.	P1011	(6h)
15.	N	(4)	35.	O6	(5f5/2)	55.	P10	(6h9/2)
16.	N1	(4s1/2)	36.	O7	(5f7/2)	56.	P11	(6h11/2)
17.	N23	(4p)	37.	O89	(5g)	57.	Q	(7)
18.	N2	(4p1/2)	38.	O8	(5g7/2)	58.	Q1	(7s1/2)
19.	N3	(4p3/2)	39.	O9	(5g9/2)	59.	Q23	(7p)
20.	N45	(4d)	40.	P	(6)	60.	Q2	(7p1/2)
						61.	Q3	(7p3/2)

V. Examples

In this section, several examples of EEDL 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 E11.4 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 ionization of the K shell of neon (Z=10). There are three tables included here. The first is for the cross section, the second is for the average energy to the scattered electron, and the last is for the average energy to the recoil electron.

```
 10000  9  0  2.01790+ 1 890224  2  0.00000+ 0  0.00000+00  0.00000+ 0
81  0 91  0.00000+ 0  1.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
8.5818000-4 0.00000+ 0
8.9363500-4 3.23634+ 3
9.4681700-4 7.77731+ 3
1.0000000-3 1.18614+ 4
1.1294600-3 1.99954+ 4
1.4219100-3 3.17379+ 4
1.5848900-3 3.56965+ 4
     .           .
     .           .
     .           .
     .           .
 2.51189- 1 4.19030+ 3
 6.30957- 1 3.34578+ 3
 1.25893+ 0 3.25903+ 3
 6.30957+ 0 3.85697+ 3
 1.58489+ 1 4.35886+ 3
 3.98107+ 1 4.77751+ 3
 1.00000+ 5 5.02661+ 3
                                                                        1
 10000  9  9  2.01790+ 1 890224  2  0.00000+ 0  0.00000+00  0.00000+ 0
81 10 91  0.00000+ 0  1.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
8.5818000-4 0.00000+ 0
1.0000000-3 1.07274- 4
1.5848900-3 5.75419- 4
3.1622800-3 1.95536- 3
1.5848900-2 1.42187- 2
 1.00000+ 5 1.00000+ 5
                                                                        1
 10000  9 19  2.01790+ 1 890224  2  0.00000+ 0  0.00000+00  0.00000+ 0
81 10 91  0.00000+ 0  1.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
8.5818000-4 0.00000+ 0
9.4681700-4 2.19068- 5
1.1294600-3 6.36649- 5
1.4219100-3 1.22281- 4
     .           .
     .           .
     .           .
     .           .

 1.58489+ 1 1.45968- 3
 2.51189+ 2 1.64901- 3
 1.25893+ 3 1.81370- 3
```

```
 6.30957+ 3 1.97748- 3
 1.00000+ 5 2.25772- 3
                                                                    1
```

The second example is for bremsstrahlung in neon (Z=10). Specifically it is for the spectra of emerging photons.

```
 10000  9  7  2.01790+ 1 890125  2  0.00000+ 0  0.00000+00  0.00000+ 0
82 21  0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
1.0000000-5 1.00000- 7 2.13421+ 6
1.0000000-5 1.33352- 7 1.60043+ 6
1.0000000-5 1.65482- 7 1.28970+ 6
1.0000000-5 2.28757- 7 9.32963+ 5
     .          .          .
     .          .          .
     .          .          .
     .          .          .

1.0000000-5 8.00000- 6 2.67332+ 4
1.0000000-5 9.90000- 6 2.16081+ 4
1.0000000-5 1.00000- 5 2.13918+ 4
 1.00000+ 1 1.00000- 7 5.78550+ 5
 1.00000+ 1 1.28640- 7 4.49744+ 5
 1.00000+ 1 1.62897- 7 3.55162+ 5
     .          .          .
     .          .          .
     .          .          .
     .          .          .
 1.00000+ 1 9.79949+ 0 4.12884- 4
 1.00000+ 1 9.90000+ 0 3.02337- 4
 1.00000+ 1 9.94987+ 0 2.08154- 4
 1.00000+ 1 1.00000+ 1 1.43310- 4
 1.00000+ 5 1.00000- 7 3.64819+ 5
 1.00000+ 5 1.48551- 7 2.45585+ 5
 1.00000+ 5 2.15282- 7 1.69461+ 5
 1.00000+ 5 3.04838- 7 1.19676+ 5
 1.00000+ 5 4.22367- 7 8.63748+ 4
     .          .          .
     .          .          .
     .          .          .
     .          .          .
 1.00000+ 5 9.93290+ 4 8.71995- 8
 1.00000+ 5 9.94963+ 4 5.03059- 8
 1.00000+ 5 9.96220+ 4 3.33003- 8
 1.00000+ 5 9.97164+ 4 2.44382- 8
 1.00000+ 5 9.98581+ 4 1.53639- 8
 1.00000+ 5 1.00000+ 5 9.65906- 9
                                                                    1
```

References

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2) R. J. Howerton, et. al., OMEGA, A CRAY 1 Executive Code for LLNL Nuclear Data Libraries, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-50400, Vol. 25 (1983). See specifically Ch. I and II.

3) D. E. Cullen, et. al., Tables and Graphs of Photon-Interaction Cross Sections Derived from the LLNL Evaluated Photon Data Library (EPDL), Z = 1 - 50), Lawrence Livermore National Laboratory, Livermore, CA, Vol. 6, Part A, Rev. 4 (1991).

4) D. E. Cullen, et. al., Tables and Graphs of Photon-Interaction Cross Sections Derived from the LLNL Evaluated Photon Data Library (EPDL), Z = 51 - 100), Lawrence Livermore National Laboratory, Livermore, CA, Vol. 6, Part B, Rev. 4 (1991).

5) D. E. Cullen, S. T. Perkins, and J. A. Rathkopf, The 1989 Livermore Photon Data Library (EPDL), Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-103424 (1990).

6) S. T. Perkins, et. al., Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library (EADL), Z = 1 - 100), Lawrence Livermore National Laboratory, Livermore, CA, Vol. 30 (1991).