ENDL Type Formats for the Livermore Evaluated Atomic Data Library, EADL

I. Contents

This report describes the input formats for the Lawrence Livermore Evaluated Atomic Data Library, EADL. 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 atomic relaxation information for use in particle transport analysis for Z =1-100 and for each subshell. Units are cm and MeV (millions of electron volts). The specific data are the following:

1) Subshell data,
   a) number of electrons,
   b) binding and kinetic energy (MeV),
   c) average radius (cm),
   d) radiative and nonradiative level widths (MeV),
   e) average number of released electrons and x-rays,
   f) average energy of released electrons and x-rays (MeV),
   g) average energy to the residual atom, i.e., local deposition (MeV).

2) Transition probability data
   a) radiation transition probabilities,
   b) nonradiative transition probabilities.

3) Whole atom data,
   a) form factor and scattering function,
   b) real and imaginary anomalous scattering factors.

In the context of particle transport, the EADL file only contains data for atomic relaxation. 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 Electron Data Library (EEDL)[6], which describes the interaction of electrons with matter.

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

II. Formats and Definitions for the EADL 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 EADL 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 EADL atomic data the only fields of interest are as shown in Table I.

TABLE I. Header Line Formats for the EADL 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)
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 EADL file.

TABLE II. Definition of the EADL Parameters

Yi - incident particle designator
=0, no incident particle (in all cases)

C - reaction descriptor
=91, subshell parameters
=92, transition probabilities
=93, whole atom parameters

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

I - reaction property
=912, number of electrons
=913, binding energy
=914, kinetic energy
=915, average radius
=921, radiative level width
=922, nonradiative level width
=931, radiative transition probability
=932, nonradiative transition probability
=933, particles per initial vacancy
=934, energy of particles per initial vacancy
=935, average energy to the residual atom, i.e., local deposition, per initial vacancy
=941, form factor
=942, scattering function
=943, imaginary anomalous scattering factor
=944, real anomalous scattering factor

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

Table III. Summary of the EADL Data Base

Yi	C	S	X1	Yo	I	Data Types
			Subshell parameters			
0	91	0	0.	0	912	number of electrons
0	91	0	0.	0	913	binding energy
0	91	0	0.	0	914	kinetic energy
0	91	0	0.	0	915	average radius
0	91	0	0.	0	921	radiative level width
0	91	0	0.	0	922	nonradiative level width
			Transition probabilities			
0	92	0	0.	0	935	average energy to the residual atom, i.e., local deposition, per initial vacancy
0	92	0	0.	7 or 9	933	average number of particles per initial vacancy
0	92	0	0.	7 or 9	934	average energy of particles per initial vacancy
0	92	91	*	7	931	radiative transition probability
0	92	91	*	9	932	nonradiative transition probability

			Whole atom parameters			
0	93	0	0.	0	941	form factor
0	93	0	0.	0	942	scattering function
0	93	0	0.	0	943	imaginary anomalous scattering factor
0	93	0	0.	0	944	real anomalous scattering factor

*See Table VI.

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

TABLE IV. Definitions of the EADL Data

i - subshell designator
j - secondary subshell designator
k - tertiary subshell designator
N - number of electrons
E_{be} - binding energy
E_{ke} - kinetic energy
<r> - average radius
Γ_r - radiative level width
Γ_{nr} - nonradiative level width
f_r - radiative transition probability[a]
E_r - energy of radiative transition
f_{nr} - nonradiative transition probability[b]
E_{nr} - energy of nonradiative transition
N_p - average number of particles per initial vacancy
E_p - average energy of particles per initial vacancy
$\langle E_{loc} \rangle$ - average energy to the residual atom, i.e., local deposition, per initial vacancy
x - argument for form factor and scattering function[c]
F - form factor
S - scattering function
I - imaginary anomalous scattering factor
R - real anomalous scattering factor

[a] radiative transition; given a vacancy in subshell i being filled by an electron from subshell j resulting in the emission of an x-ray, E_r being the x-ray's energy.

[b] nonradiative transition; given a vacancy in subshell i moving to subshell j resulting in the emission of an electron from subshell k, E_{nr} being the electron's energy.

[c] the parameter x (cm^{-1}) is defined by $x=\sin(\theta/2)/\lambda$, where θ is the photon scattering angle and λ is its wave length.

For a given initial subshell vacancy, the transition probabilities are normalized such that the summation over all radiative transitions, f_r, and all nonradiative transitions, f_{nr}, is unity. Likewise, for a given initial subshell vacancy, energy conservation insures that the average energy into the free x-rays and electrons, E_p, plus the average local energy deposition, $\langle E_{loc} \rangle$, equals the subshell binding energy, E_{be}.

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 EADL 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
912	i	N				
913	i	E_{be}				
914	i	E_{ke}				
915	i	$\langle r \rangle$				
921	i	Γ_r				
922	i	Γ_{nr}				
931	j	f_r	E_r			
932	j	k	f_{nr}	E_{nr}		
933	i	N_p				
934	i	E_p				
935	i	$\langle E_{loc} \rangle$				
941	x	F				
942	x	S				
943	E	I				
944	E	R				

The EADL 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=91-93).
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=912-944).

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 subshell number.

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 EADL 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 EADL 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 subshell parameters for neon (Z=10). There are four tables here. The first table is the number of electrons, the second table is the binding energy, the third table is the kinetic energy, and the last table is the average radius.

```
 10000  0  0  2.01790+ 1 901205  2  0.00000+ 0  0.00000+00  0.00000+ 0
91912  0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
 1.00000+ 0 2.00000+ 0
 3.00000+ 0 2.00000+ 0
 5.00000+ 0 2.00000+ 0
 6.00000+ 0 4.00000+ 0
                                                                     1
 10000  0  0  2.01790+ 1 901205  2  0.00000+ 0  0.00000+00  0.00000+ 0
91913  0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
 1.00000+ 0 8.58180- 4
 3.00000+ 0 4.32300- 5
 5.00000+ 0 2.00800- 5
 6.00000+ 0 1.99600- 5
                                                                     1
 10000  0  0  2.01790+ 1 880712  2  0.00000+ 0  0.00000+00  0.00000+ 0
91914  0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
 1.00000+ 0 1.27900- 3
 3.00000+ 0 1.50970- 4
 5.00000+ 0 1.28010- 4
 6.00000+ 0 1.27250- 4
                                                                     1
 10000  0  0  2.01790+ 1 880712  2  0.00000+ 0  0.00000+00  0.00000+ 0
91915  0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
 1.00000+ 0 8.28310-10
 3.00000+ 0 4.63000- 9
 5.00000+ 0 4.92350- 9
 6.00000+ 0 4.93900- 9
                                                                     1
```

The second example are the radiative and nonradiative transition probabilities from the K shell of neon (Z=10).

```
 10000  0  7  2.01790+ 1 901205  2  0.00000+ 0  0.00000+00  0.00000+ 0
92931 91  0.00000+ 0  1.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
 5.00000+ 0 4.64329- 3 8.38100- 4
 6.00000+ 0 9.22967- 3 8.38220- 4
                                                                     1
  10000  0  9  2.01790+ 1 901205  2  0.00000+ 0  0.00000+00  0.00000+ 0
92932 91  0.00000+ 0  1.00000+ 0  0.00000+ 0  0.00000+ 0  0.00000+ 0
 3.00000+ 0 3.00000+ 0 9.30584- 2 7.71720- 4
 3.00000+ 0 5.00000+ 0 9.21024- 2 7.94870- 4
 3.00000+ 0 6.00000+ 0 1.81578- 1 7.94990- 4
 5.00000+ 0 5.00000+ 0 1.45681- 2 8.18020- 4
 5.00000+ 0 6.00000+ 0 3.85131- 1 8.18140- 4
 6.00000+ 0 6.00000+ 0 2.19689- 1 8.18260- 4
                                                                     1
```

References

1) 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).

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, D. E. Cullen, and S. M. Seltzer, 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).