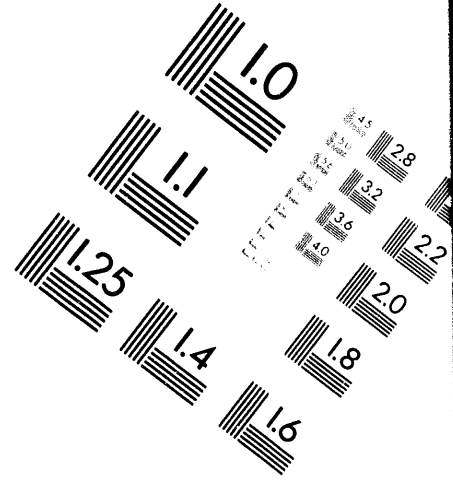
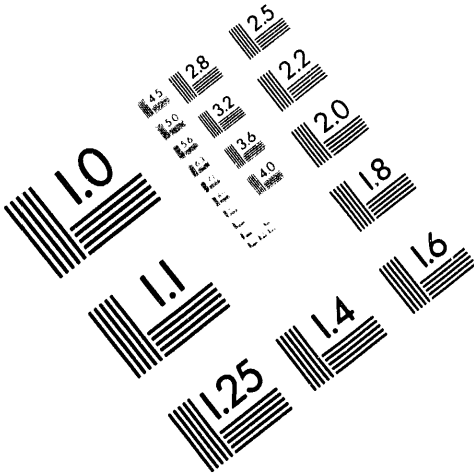




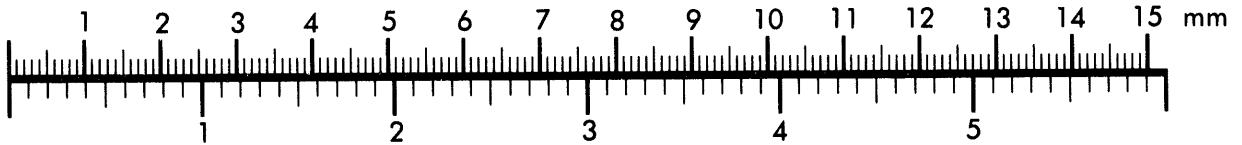
AIM

Association for Information and Image Management

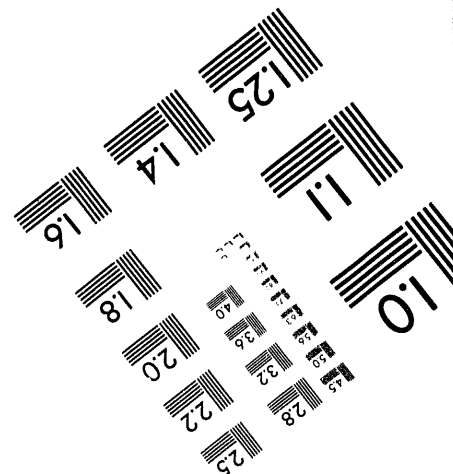
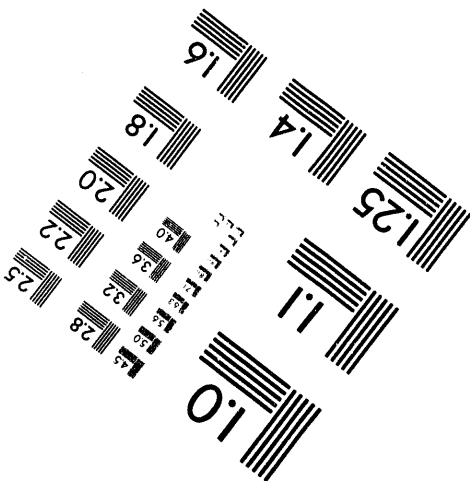
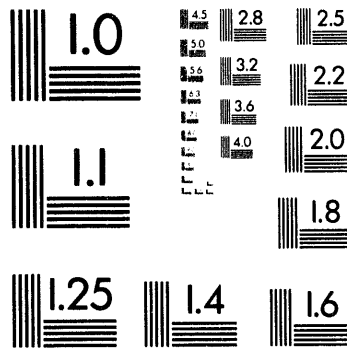
1100 Wayne Avenue, Suite 1100
Silver Spring, Maryland 20910
301/587-8202



Centimeter



Inches



MANUFACTURED TO AIM STANDARDS
BY APPLIED IMAGE, INC.

1 of 1

**ENDL Type Formats for the LLNL Evaluated Atomic
Data Library, EADL, for the Evaluated Electron Data
Library, EEDL, and for the Evaluated Photon Data
Library, EPDL**

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July 4, 1994

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MASTER

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ENDL Type Formats for the LLNL Evaluated Atomic Data Library, EADL, for the Evaluated Electron Data Library, EEDL, and for the Evaluated Photon Data Library, EPDL

ABSTRACT

The character file formats for the Lawrence Livermore National Laboratory evaluated atomic relaxation library (EADL), the electron library (EEDL), and the photon library (EPDL) are given in this report.

INTRODUCTION

Over the past five years, Lawrence Livermore National Laboratory has published extensive compilations derived from three of its main atomic data libraries. These are specifically the evaluated atomic relaxation data library, EADL, the evaluated electron interaction data library, EEDL, and the evaluated photon interaction data library, EPDL. All of these libraries span atomic numbers, Z , from 1 to 100. Additionally the particle interaction libraries cover the incident particle energy range from 10 eV to 100 GeV.

The purpose of these libraries is to furnish data for particle transport calculations. Thus the files have been released for external distribution in a machine independent character format. In a complete coupled electron-photon transport analysis, results from all three of the data files are required. Therefore it is reasonable to discuss the formats for all three libraries in the same work; that is the approach taken here. This report is composed of three sections, each section describing one of the libraries. For ease of reading, each section is separate and unique unto itself, including its own table numbers and references. This report will accompany any request for copies of these evaluated data libraries.

This report and these three data libraries are available from the data centers at Brookhaven National Laboratory, RSIC (Oak Ridge National Laboratory), OECD/NEA Data Bank (France) and IAEA (Vienna).

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 libraries².

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) format². 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)

Y_o - 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

Y _i	C	S	X _l	Y _o	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
$\langle r \rangle$	- 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,11.

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

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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 libraries².

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, $\overline{\sigma_{e1}(1-\cos\theta)}$ (b).
- 2) Large angle elastic scattering (over $\cos\theta=-1$. 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 (EPDLA)^{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) format². 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	Xl	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,11.

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

```

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.
.
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.
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

```

```

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

```

```

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

```

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.
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.
.
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

. . .
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. . .
. . .

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

. . .
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. . .

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

1) 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).

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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).

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),
 - b) average energy to the residual atom, i.e., local deposition (MeV),
 - c) average energy of the secondary photons and electrons (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	1-3	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 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
 =943, imaginary anomalous scattering factor
 =944, real anomalous scattering factor

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

Table III. Summary of the EPDL Data Base

Yi	C	S	X1	Yo	I	Data Types
Coherent 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

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	integrated photoelectric cross section
7	73	0	0.	0	11	average energy to the residual atom
7	73	0	0.	7	10	average energy of the secondary photons
7	73	0	0.	9	10	average energy of the secondary electrons
Photoelectric (by subshell)						
7	73	91	*	0	0	integrated photoelectric cross section
7	73	91	*	0	11	average energy to the residual atom
7	73	91	*	7	10	average energy of the secondary photons
7	73	91	*	9	10	average energy of the secondary electrons
Pair production						
7	74	0	0.	0	0	integrated pair production cross 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	75	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
<Eloc>	- 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

^a 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 (cm).

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,11.

TABLE V. Actual formats for the EPDL 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	<E'p>				
11	E	<Eloc>				
941	x	F				
942	x	S				
943	E	I				
944	E	R				

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

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 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 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 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

```

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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

```

4.2839800-3 4.63741- 5
 5.0042900-3 6.22147- 5
 5.9498600-3 8.59610- 5

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 .
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 .
 .
 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

1

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

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 .
 .
 .
 .
 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

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