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EPICS2014:
Electron Photon Interaction Cross Sections
(Version 2014)

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Abstract: EPICS2014 is the Electron Photon Interaction Cross Section library that provides the atomic data needed to perform coupled Electron-Photon transport calculations, to produce accurate macroscopic results, such as energy deposition and dose. Atomic data is provided for elements, Z = 1 to 100, over the energy range 10 eV to 100 GeV; nuclear data, such as photo-nuclear, and data for compounds, are not included. All of the data are in a simple computer independent text format that is standard and presented to a high precision that can be easily read by computer codes written in any computer language, e.g., C, C++, and FORTRAN. EPICS include four separate data bases that are designed to be used in combination. These include the Electron Data Library (EEDL), Evaluated Photon Data Library (EPDL), Evaluated Atomic Data Library (EADL) and Excitation Data Library (EXDL). All four are given in the Extended ENDL format (ENDLX). The first three only are also given in the ENDF-6 format because the format for the Excitation Data is not defined in ENDF-6.

The report is available on-line on https://www-nds.iaea.org/publications/nds/iaea-nds-218/

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Vienna, September 2014

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Overview

Photon interaction data has been used at Lawrence Livermore National Laboratory (LLNL) for well over 50 years. Roughly 25 years ago this photon data library was greatly expanded in detail to define EPDL [1, 2], by including: photoelectric Subshell data, anomalous scattering factors, excitation, etc. Soon after this expansion electron interaction data, EEDL [3], was added, to allow completely coupled electron photon transport calculation to accuracy determine macroscopic quantities, such as energy deposit and dose. At that time the LLNL data libraries were adopted as the standard ENDF/B data for photon and electron transport calculations, and today they still are the standard data included in ENDF/B-VII.1 library [4].

I have now modernized these data libraries by reviewing recently published data and making changes where I felt they were necessary. I also corrected some electron interaction data that was incorrectly translated from the ENDL to the ENDF format, namely MF/MT=26/527, **which is defined in ENDF as the average energy loss by an electron due to Bremsstrahlung; it is now correct in EPICS2014. Earlier in EEDL in the ENDF format it was the average secondary energy of an electron, not the average energy loss. The RED text shown here is the only change in this document from the original to rev.1.**

I also took this opportunity to update the data in ENDL [9] and ENDF [5] formats to a standard, high precision format that can be easily read by computer codes written using current computer languages, such as C, C++, and FORTRAN; for details see [6, 7]. This standard, high precision format has been used by me with the Extended ENDL format (ENDLX) for many years to prepare input data for use with my TART Monte Carlo transport code [11]. It has also been used for many years (since circa 2000) with the ENDF format in my PREPRO codes [12].

What is EPICS

The Electron Photon Interaction Cross Sections, EPICS, provides the atomic data needed to perform coupled Electron-Photon transport calculations, to produce accurate macroscopic results, such as energy deposit and dose. Atomic data is provided for elements, Z = 1 to 100, over the energy range 10 eV to 100 GeV; note that nuclear data, such as photo-nuclear, and data for compounds, are not included. All of the data are in a simple computer independent text format that is standard and presented to a high precision that can be easily read by computer codes written in any computer language, e.g., C, C++, and FORTRAN. EPICS include four separate data bases that are designed to be used in combination, these include,

1) **The Evaluated Electron Data Library (EEDL),** to describe the interaction of electrons with matter [3].
2) **The Evaluated Photon Data Library (EPDL)**, to describe the interaction of photons with matter [1, 2].
3) **The Evaluated Atomic Data Library (EADL)**, to describe the emission of electrons and photons back to neutrality following an ionizing event, caused by either electron or photon interactions [8]
4) **The Evaluated Excitation Data Library (EXDL)**, to describe the excitation of atoms due to photon interaction [2]

All of these are available in the Extended ENDL [9] format (ENDLX) in which the evaluations were originally performed. The first three are also available in the ENDF format [4]; as yet ENDF does not include formats to handle excitation data (EXDL).

ENDF Format

The ENDF format is documented in ENDF-102 [5], and as such will not be described here. Here I will only suggest that you read refs. [6, 7]; these address standardizing and precision of data in the ENDF format, and how to guarantee that the data you use meets these criteria. **You can be assured that ALL of the EPICS2014 in the ENDF format meet these criteria.**

Extended ENDL Format (ENDLX)

Generally the two header lines in the ENDL format contain a great deal of information. However, as applied to the EPICS atomic data the only fields of interest are as shown in the below table. For the definition of these quantities see ref. [9].

Header Line Formats for the EPICS Data Files

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
1	11-12	I2	Yo - outgoing particle designator
1	14-24	D11.4	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
2	3-5	I3	I - reaction property
2	6-8	I3	S - reaction modifier
2	22-32	D11.4	X1 - subshell designator

The only differences between the standard and Extended ENDL format (ENDLX) are the header information is now in standard format and the data table uses D16.9, rather than D11.4 format; the objective is to assure the data is in a standard, high precision format that can easily be read using any computer language. **You can be assured that ALL of the EPICS2014 in the Extended ENDL format (ENDLX) meet these criteria.**

Example of the Same Data in Original and Extended ENDL Formatted (ENDLX) Data

Original

```
  1000  7  0  1.007970+0 9707045 2  0.0         0.0
0.0
71  0  0  0.0         0.0         0.0         0.0         0.0
 1.000000-6 9.887553-6
 1.059784-6 1.235246-5
 1.126020-6 1.538627-5
 1.196396-6 1.933495-5
 1.271171-6 2.449127-5
 1.350619-6 3.121326-5
 1.392826-6 3.537646-5
 1.481238-6 4.569015-5
 1.575262-6 5.929956-5
 1.727606-6 8.834929-5
 1.894683-6 1.326150-4
```

Extended

```
  1000  7  0  1.00797    9707045 2  0.0         0.0
0.0
71  0  0  0.0         0.0         0.0         0.0         0.0
 1.000000000D-06 9.887553000D-06
 1.059784000D-06 1.235246000D-05
 1.126020000D-06 1.538627000D-05
 1.196396000D-06 1.933495000D-05
 1.271171000D-06 2.449127000D-05
 1.350619000D-06 3.121326000D-05
 1.392826000D-06 3.537646000D-05
 1.481238000D-06 4.569015000D-05
 1.575262000D-06 5.929956000D-05
 1.727606000D-06 8.834929000D-05
 1.894683000D-06 1.326150000D-04
```

Note that the "E-less" floating point form (e.g. **`1.007970+0`**) is not used in the Extended ENDL format (ENDLX). This means that ALL of the Extended ENDL (ENDLX) data is in a standard format that can easily be read by C, C++, and FORMAT codes.

Comparison to Similar Data

In modernizing this data I searched for comparable data published from other sources. There is a multitude of comparable results available, but here I will present only one comparison to illustrate differences in one set of very important data. One thing that is common to all four EPICS data libraries are the atomic binding energies, and therefore transition energies for all elements of the periodic table, for Z = 1 through 100. Only if these are consistent between electron, photon, and relaxation data will our calculated results by reliable.

More recent atomic transition energies were published in the Review of Modern Physics [10]; below I will refer to this data as RMP. My initial comparison between my EADL data and the RMP results appear to show rather large differences of over 6% for a few elements; these results are shown below in figures 1 and 2.

But by examining the tabulated data shown below in table 1 it is obvious that the RMP data contain simple typographical errors, where their data for Z = 33 and 34 is actually the data for Z = 34 and 35. Similar there data for Z = 60 is actually the data for Z = 61. When I made these corrections to the RMP data, the results in figures 3 and 4 showed excellent agreement, well within our needs to calculate macroscopic results such as energy deposition and dose.

From figures 3 and 4 we can see that both sets of data show a very simple Z^2 dependence, and differ only slightly in the slope of this dependence. Compared to EADL the RMP data is about 1% higher for low Z, and 1/2 % lower for high Z. In an attempt to put this in perspective note that the binding energy of hydrogen (Z=1) is about 13.6 eV, but this does not exist in nature, and for the H2 radical is it about 16.4 eV, over 20% higher. There are similar large differences for low energy edges for compounds, compared to the elemental data included in EPICS, but these differences are at very low energies and do not significantly affect the macroscopic quantities that EPICS is designed to accurately calculate. Hopefully this can aid the reader to appreciate that the up to 1% difference we see between EADL and RMP is well within the accuracy we need in our applications to calculate macroscopic results.

The bottom line on this comparison is that later does not necessarily mean better. In this case I found that the more recent data had errors in it, and when I corrected the errors, the two sets of transition energies (EPICS and RMP) agree to well within acceptable limits; they are virtually indistinguishable for use in our applications. These transition energies are a necessary component of EPICS, but only a tiny component, and for our applications the small differences between the two sets are really negligible. In order to change the EPICS transition energies I would have had to completely replace the energy dependent electron and photon cross section, as well as the anomalous scattering factors. I estimate that this would be about a two man-year effort, and the result would be at least a two year delay in making this data available, and very little change in the macroscopic quantities that we are interested in, e.g., energy deposit and dose. **Therefore I have decided not to change the EPICS transition energies.**

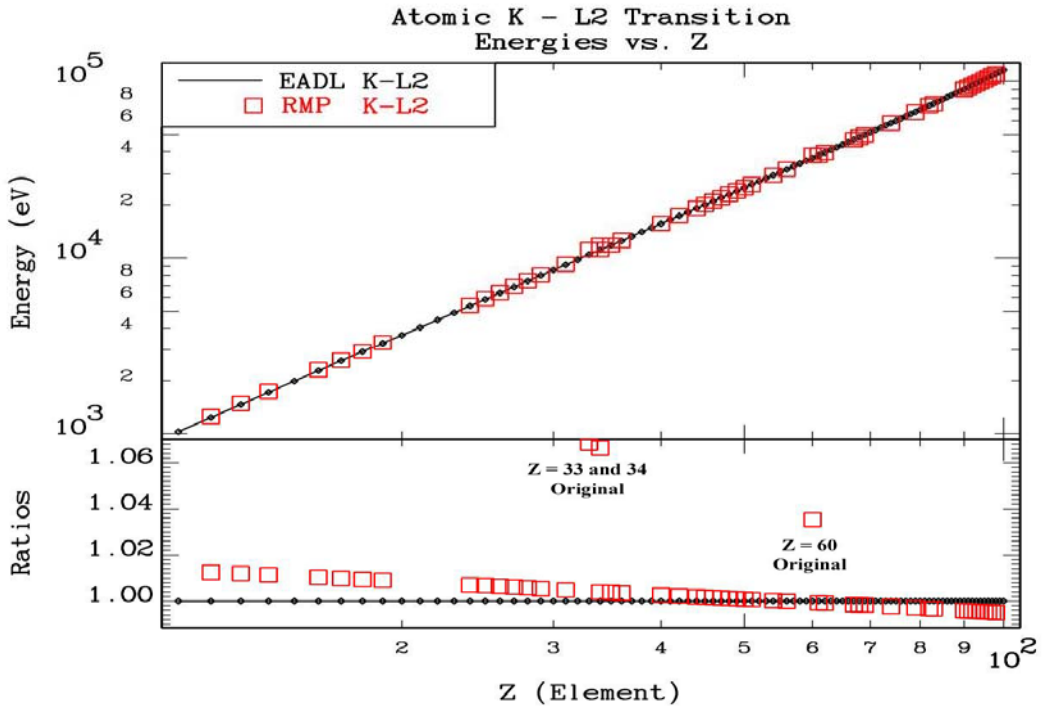

Fig. 1: Comparison of Original K – L2 Transition Energies

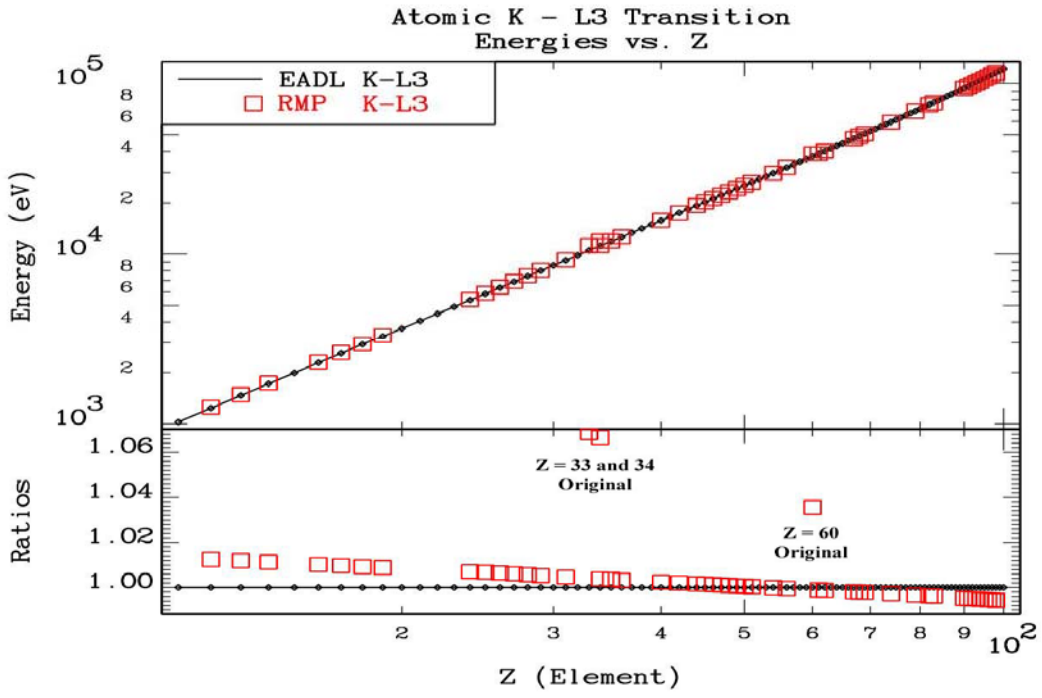

Fig. 2: Comparison of Original K – L3 Transition Energies

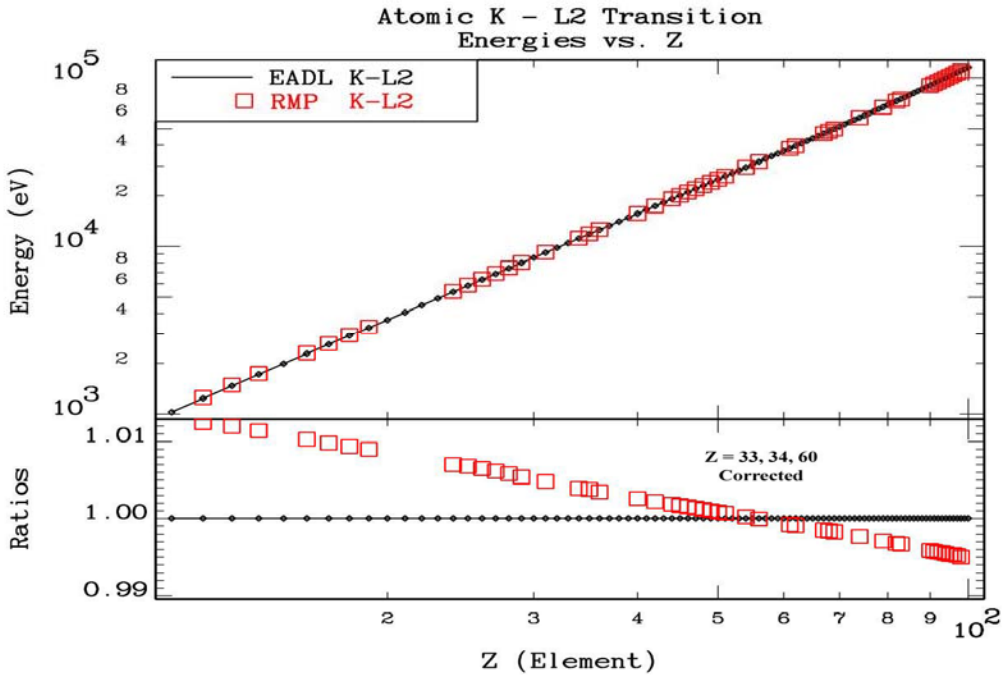

Fig. 3: Comparison of Corrected K – L2 Transition Energies

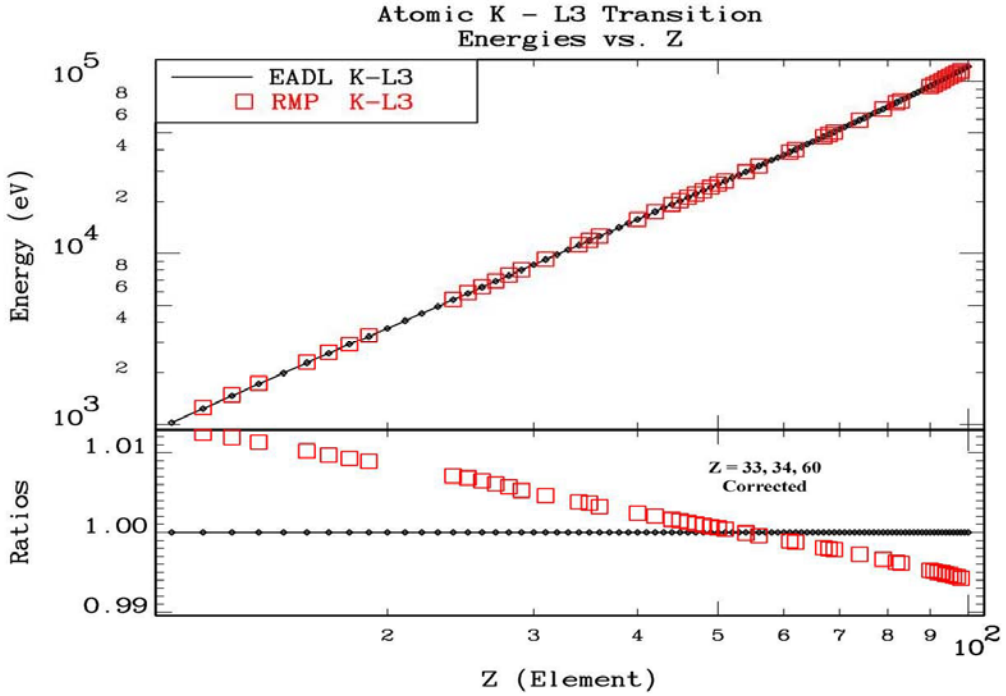

Fig. 4: Comparison of Corrected K – L3 Transition Energies

Table 1: Comparison of Transition Energies (eV)

EADL = Evaluation Atomic Data Library
RMP = Review of Modern Physics
Diff. = 100%(RMP – EADL)/EADL

Z	K – L2			*	K – L3		
	EADL	RMP	Diff.	*	EADL	RMP	Diff.
11	1027.600			*	1027.800		
12	1238.000	1253.437	1.25%	*	1238.300	1253.688	1.24%
13	1468.700	1486.295	1.20%	*	1469.200	1486.708	1.19%
14	1719.800	1739.394	1.14%	*	1720.500	1739.985	1.13%
15	1991.300			*	1992.200		
16	2283.200	2306.700	1.03%	*	2284.500	2307.885	1.02%
17	2595.400	2620.846	0.98%	*	2597.200	2622.440	0.97%
18	2928.200	2955.566	0.93%	*	2930.500	2957.682	0.93%
19	3281.700	3311.196	0.90%	*	3284.700	3313.948	0.89%
20	3656.000			*	3659.800		
21	4052.100			*	4056.900		
22	4469.400			*	4475.400		
23	4907.700			*	4915.100		
24	5367.900	5405.538	0.70%	*	5376.800	5414.805	0.71%
25	5847.900	5887.686	0.68%	*	5858.700	5898.801	0.68%
26	6349.800	6391.026	0.65%	*	6362.700	6404.006	0.65%
27	6873.200	6915.538	0.62%	*	6888.400	6930.378	0.61%
28	7417.800	7461.034	0.58%	*	7435.800	7478.252	0.57%
29	7984.700	8027.842	0.54%	*	8005.700	8047.823	0.53%
30	8571.900			*	8596.400		
31	9180.600	9224.835	0.48%	*	9209.000	9251.674	0.46%
32	9811.600			*	9844.200		
33	**10463.000**	**11181.530**	**6.87%**	*	**10501.000**	**11222.520**	**6.87%**
34	**11138.000**	**11877.750**	**6.64%**	*	**11180.000**	**11924.360**	**6.66%**
35	**11833.000**			*	**11881.000**		
33	**10463.000**			*	**10501.000**		
34	**11138.000**	**11181.530**	**0.39%**	*	**11180.000**	**11222.520**	**0.38%**
35	**11833.000**	**11877.750**	**0.38%**	*	**11881.000**	**11924.360**	**0.36%**
36	12552.000	12595.424	0.35%	*	12607.000	12648.002	0.33%
37	13292.000			*	13354.000		
38	14055.000			*	14125.000		
39	14840.000			*	14919.000		
40	15650.000	15690.645	0.26%	*	15737.000	15774.914	0.24%
41	16481.000			*	16579.000		
42	17336.000	17374.290	0.22%	*	17444.000	17479.372	0.20%
43	18214.000			*	18334.000		
44	19115.000	19150.490	0.19%	*	19248.000	19279.160	0.16%
45	20040.000	20073.670	0.17%	*	20186.000	20216.120	0.15%
46	20988.000	21020.150	0.15%	*	21150.000	21177.080	0.13%
47	21961.000	21990.300	0.13%	*	22139.000	22162.917	0.11%
48	22957.000	22984.050	0.12%	*	23153.000	23173.980	0.09%
49	23978.000	24002.030	0.10%	*	24193.000	24209.750	0.07%
50	25023.000	25044.040	0.08%	*	25257.000	25271.360	0.06%
51	26093.000	26110.780	0.07%	*	26349.000	26358.860	0.04%
52	27187.000			*	27465.000		
53	28306.000			*	28609.000		
54	29452.000	29458.250	0.02%	*	29781.000	29778.780	-0.01%
55	30622.000			*	30979.000		
56	31819.000	31816.615	-0.01%	*	32206.000	32193.262	-0.04%

57	33041.000			*	33459.000		
58	34291.000			*	34743.000		
59	35567.000			*	36056.000		
60	**36870.000**	**38171.550**	**3.53%**	*	**37396.000**	**38725.110**	**3.55%**
61	**38200.000**			*	**38767.000**		
60	**36870.000**			*	**37396.000**		
61	**38200.000**	**38171.550**	**-0.07%**	*	**38767.000**	**38725.110**	**-0.11%**
62	39558.000	39523.390	-0.09%	*	40168.000	40118.481	-0.12%
63	40943.000			*	41599.000		
64	42356.000			*	43060.000		
65	43799.000			*	44555.000		
66	45270.000			*	46080.000		
67	46770.000	46699.980	-0.15%	*	47637.000	47547.100	-0.19%
68	48299.000	48221.610	-0.16%	*	49227.000	49127.240	-0.20%
69	49859.000	49772.670	-0.17%	*	50850.000	50741.475	-0.21%
70	51448.000			*	52507.000		
71	53069.000			*	54199.000		
72	54719.000			*	55924.000		
73	56402.000			*	57686.000		
74	58116.000	57982.670	-0.23%	*	59483.000	59318.847	-0.28%
75	59863.000			*	61318.000		
76	61642.000			*	63189.000		
77	63455.000			*	65100.000		
78	65302.000			*	67048.000		
79	67184.000	66990.730	-0.29%	*	69038.000	68804.600	-0.34%
80	69099.000			*	71066.000		
81	71052.000			*	73138.000		
82	73039.000	72805.420	-0.32%	*	75250.000	74970.110	-0.37%
83	75064.000	74816.210	-0.33%	*	77407.000	77109.200	-0.38%
84	77127.000			*	79607.000		
85	79228.000			*	81853.000		
86	81368.000			*	84145.000		
87	83549.000			*	86486.000		
88	85760.000			*	88864.000		
89	88027.000			*	91307.000		
90	90330.000	89957.040	-0.41%	*	93795.000	93347.380	-0.48%
91	92678.000	92283.400	-0.43%	*	96337.000	95866.400	-0.49%
92	95066.000	94650.840	-0.44%	*	98928.000	98431.580	-0.50%
93	97498.000	97068.400	-0.44%	*	101570.000	101056.300	-0.51%
94	99979.000	99523.200	-0.46%	*	104280.000	103734.050	-0.52%
95	102510.000	102031.300	-0.47%	*	107040.000	106473.300	-0.53%
96	105080.000	104590.300	-0.47%	*	109870.000	109272.300	-0.54%
97	107710.000	107194.300	-0.48%	*	112750.000	112127.300	-0.55%
98	110390.000	109837.300	-0.50%	*	115700.000	115035.300	-0.57%
99	113100.000			*	118700.000		
100	115890.000			*	121790.000		

Utility Codes

Two utility codes that use the EPICS2014 data in the Extended ENDL (ENDLX) Format are provided; these include,

RELAX [13] to calculate relaxation electron or photon induced ionization of an atom.

SCATMAN [14] to calculate anomalous scattering factors.

Both provide output results in the **PLOTTAB** [15] format, so that you can easily create plots to "see" the results.

Acknowledgments

I thank **Morgan White** (LANL) for initially pointing out that the "E- less" format used for many years in ENDF is not compatible for simple use in C and C ++ codes, and is indeed not even s standard officially approved format for use with FORTRAN. I also thank **Morgan White** for encouraging me to review recently published data. I thank **Grady Hughes** (LANL) for pointing out the error in the EEDL data in the ENDF format (as described above). I thank **Mark Baird** (RSICC, ORNL) for promptly providing the RELAX and SCATMAN codes, documentation and input data files from the RSICC collection. I thank **Bojan Zefran** (IJS), for providing the LINUX executables, and **Jean-Christophe Sublet** (UKAEA), for providing the MAC executables, for the RELAX and SCATMAN codes.

I especially thank **Andrej Trkov** (NDS, IAEA, Vienna), for reviewing/correcting a preliminary version of the EPICS2014 data and this report. Andrej contributed an incredible amount of time, energy and expertize, and has added enormously to making the EPICS2014 package what it is today; **thank you Andrej, I could not have done this without you.**

Primary References

Today's EPICS2014 data is derived from my earlier electron and photon data libraries, and the primary references remain,

The ENDL Format: [9] D.E. Cullen, "ENDL Type Formats for the LLNL Evaluated Atomic Data Library (**EADL**), Evaluated Electron Data Library (**EEDL**), and Evaluated Photon Data Library (**EPDL**)", Lawrence Livermore National Laboratory, UCRL-ID-117796, Rev. 1, May 2002.

The Photon Data: [2] D.E. Cullen, "EPDL97: the Evaluated Photon Data Library, '97 Version," Lawrence Livermore National Laboratory, UCRL--50400, Vol. 6, Rev. 5, September 1997.

The Electron Data: [3] D.E. Cullen, S.T. Perkins and S.M. Seltzer, "Tables and Graphs of Electron Interaction Cross 10 eV to 100 GeV Derived from the LLNL Evaluated Electron Data Library (**EEDL**), Z = 1 - 100", Lawrence Livermore National Laboratory, UCRL-50400, Vol. 31, November 1991.

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