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A Survey of Atomic Binding Energies for use in EPICS2017

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Abstract: I have presented here my Survey of Atomic Binding Energies for use in EPICS2017. There are few original results of my own in this report; all the original work was done by others in putting together the three compilations that I used. All I did was use existing compilations of atomic binding energies and transition energies, I added a few tests for the expected systematic, and I put the final results into the ENDF/B format [2], so that they can be easily used by as many computer codes as possible. I also used graphics to compare the sources to give the reader a realistic estimate of the uncertainty in this data.

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Vienna, September 2017

Acknowledgements

I should like to start by thanking Thomas Carlson and Gwyn P. Williams for providing their excellent compilations of atomic binding energies, and NIST for providing their compilation of transition energies. These were the three sources of data that I used to produce what I judge to be the BEST binding energies to use in EPICS2017 [to be published]. I must also thank Francesc Salvat (U. Barcelona), Gwyn P. Williams (Jefferson Lab), Cedric Powell (NIST), and Yuri Ralchenko (NIST), for their contributions toward this report and their extremely useful feedback in reviewing preliminary versions of this paper; I feel that the final paper is much improved by their constructive criticism.

Furthermore, I also thank the many users of the EPICS data (EADL, EEDL and/or EPDL) for their feedback both informally, in contacting me, and more formally in published reports; both pro and con feedback are extremely useful. Lastly, I will mention that today it is this feedback from users that is the primary source leading to improvements in this data. So, I STRONGLY RECOMMEND that if you use this data, PLEASE be sure to send me a copy of your results. I don't read minds, so if you do not inform me of problems it is unlikely that they will be corrected.

Contents

1. What is EPICS?

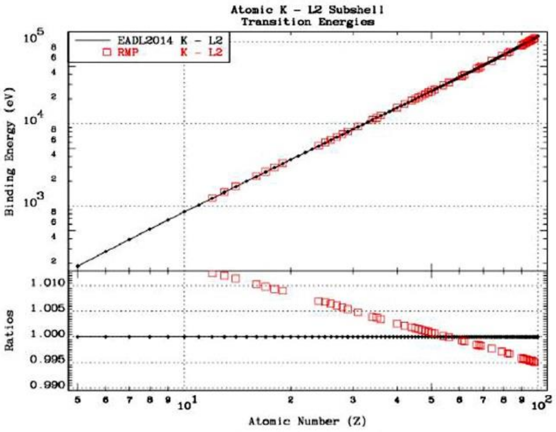
The Electron-Photon Interaction Cross Sections (EPICS) [1] is part of the ENDF/B system [2], to compliment the ENDF/B neutron data, and allow coupled calculations in engineering applications. I should stress that EPICS is not intended as the cutting edge of science. Rather it is intended as a simple computer based interface for engineering applications primarily designed for use to calculate integral results, such as: energy deposit, DOSE, damage, etc.

To a large extend the success of the ENDF system is that it uses a simple text based computer format that today, and into the future, can be read and used on any computer using almost any computer language. It is extensively documented in ENDF-102 [2], ENDF Bible, that everyone (data producers and users) agree to use and follow the ENDF rules. These data files are so small that there has never been any need to try to optimize its format. As such the ENDF/B format has not changed in fifty years and by today it has been almost uniformly adopted throughout the World. Allowing everyone to use the same data in this simple format, has contributed greatly to the amount of user feedback that we receive from ENDF formatted data users; **pro or con, this feedback is what drives improvements to our data**.

The electron and photon data used in EPICS are limited to elemental, cold, neutral, isolated atoms; this is in line with its intent for use in engineering applications. This limits the data to be used ONLY at higher energies. I recommend that it not be used in applications below 100 eV; F. Salvat recommends not below 1 keV [3]. Users should be aware that the EPICS data extends to low energy ONLY to allow data such as anomalous scattering factors to be calculated (this involves an integral over the entire range of the photoelectric cross sections). At lower energies atomic effects become progressively more important and invalidate the designed features, again: **EPICS data are limited to elemental, cold, neutral, isolated atoms. WARNING: CAVEAT EMPTOR: Do not try to use this data at lower energies – if you do, your results can be very inaccurate and you will have nobody to blame except yourself.**

2. Overview

First a brief overview: Based on other currently available data the EPICS2014 [1] data showed a distinct bias in the atomic binding energies, and therefore transition energies (**the transition energy between any two subshells is the difference between the binding energies of the two subshells; this is what an observer would see/measure as emitted by the atom. For example, the K-L2 transition energy is the difference between the K and L2 subshell binding energies**). In the EPICS2014 report I showed a comparison of the EPICS2014 KL2 and KL3 transition energies to the data of Deslattes [4], which clearly illustrated this bias. One of the objectives of EPICS2017 is to eliminate this bias, by updating it to include recent atomic data that has been shown to produce better agreement with measured and theoretical results. As a quick introduction, the below two figures illustrate results again compared to Deslattes [4] results using EPICS2014 and EPICS2017; here the Deslattes data is referred to as RMP (Review of Modern Physics). On the left we see results for the KL2 transition and on the right for the KL3 transition. In each case the upper half of the plot shows a bias in the transition energy versus Z for EPICS2014, of up to about 1/2 % for high Z and over 1 % for low Z. The bottom half of each plot shows that EPICS2017 has eliminated this bias and now produces excellent agreement across the entire periodic table. There will be much more discussion of uncertainties below, but for now suffice it to say as an introduction that with EPICS2017 this bias has been eliminated.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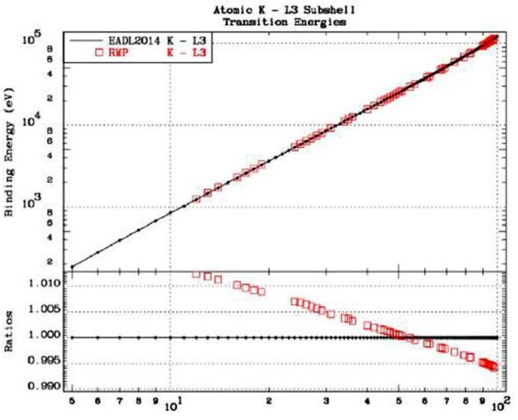
Transition Energies
EADL2014 K - L2
RMP K - L2
Binding Energy (eV)
Ratios
Atomic Number (Z)
10^5
10^4
10^3
1.010
1.005
1.000
0.995
0.990
5 6 7 8 9 10^1 2 3 4 5 6 7 8 9 10^2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Transition Energies
EADL2014 K - L3
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Binding Energy (eV)
Ratios
Atomic Number (Z)
10^5
10^4
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1.010
1.005
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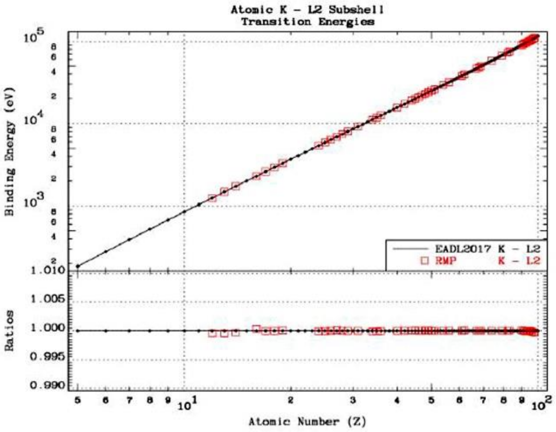
5 6 7 8 9 10^1 2 3 4 5 6 7 8 9 10^2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Transition Energies
EADL2017 K - L2
RMP K - L2
Binding Energy (eV)
Ratios
Atomic Number (Z)
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1.010
1.005
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0.995
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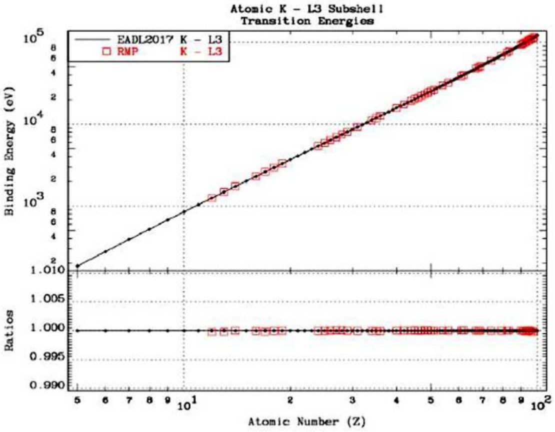
5 6 7 8 9 10^1 2 3 4 5 6 7 8 9 10^2


Atomic K - L3 Subshell
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Binding Energy (eV)
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10^5
10^4
10^3
1.010
1.005
1.000
0.995
0.990
5 6 7 8 9 10^1 2 3 4 5 6 7 8 9 10^2

3. Sources of Binding and Transition Energies

In updating EPICS our approach was to avoid any long research project and to instead use the existing published data that has already proven it worth in applications. The available data that we used includes,

1) **Deslattes** [4]. In this report it has only been used for EPICS2014 to EPICS2017 LK2 and KL3 transitions comparisons shown above.
2) **Carlson** [5]. Theoretical results suited for EPICS needs (elemental, cold, neutral, isolated atom). This is the most complete data set that I have, but it is from 1975.
3) **Williams** [6]. This is for solids, so it is closer to reality, and of more general use than EPICS is designed for. Compared to Carlson's theoretical results, Williams' data may seem incomplete, but this is only because the valence electrons are not included in this data set.
4) **NIST** [7] For Z>10 for transition energies this includes both theoretical and measured values and uncertainties. In principle, this is the same as Deslattes' data [4], but as I documented in EPICS2014 [1] Deslattes' published report has errors in it, whereas the original NIST data available on-line does not. So that in this report I have used the original on-line data and referenced it as NIST.

One problem we must address is the uncertainty in the data. It seems to be human nature that the producers of data are overly optimistic as to the magnitude of the uncertainty in their results. This often results in data being reported that are not physically realistic. Over the last 50 years any number of times I have been faced with multiple sets of measured and/or theoretical results that all claim to be accurate to within say 1 %, but all differ from one another by much more than 1%. They are all trying to estimate the same physical quantity, so obviously they cannot all be correct. As but one example, from the NIST [7] we have the theoretical and measured results for the 10-Ne K edge: theory 870.73 +/- 0.16 eV (+/- 0.018 %), and measured 866.9001 +/- 0.0090 (+/- 0.001 %). People complain to us, the producers/users of this data, when their applications cannot reproduce these results, when in fact this data appears to be inconsistent. In this example case, the theoretical and measured results differ by 3.83 (0.44 %), which is many times the estimated uncertainty of +/-0.16 or +/-0.009. If we assume a normal distribution 3.83 is 20 or more times sigma, meaning that there is virtually zero probability of the data and assigned uncertainties being consistent.

From a theoretical viewpoint, this would seem to present an insurmountable obstacle, but from a practical viewpoint it isn't a real problem. My 50 years of experience has been that rather than rely solely on the author's estimate of uncertainty (let's admit it, a somewhat biased observer; this is like asking the author of a Broadway show to write the review of his own show), it is better to have two or more "experts" independently evaluate the data, and then use the difference between their estimates as a real world estimate of uncertainties. Fortunately, in this case we have independent estimates from a number of sources, e.g., Carlson and Williams. By comparing their results, we can estimate real world, instead of Disneyland uncertainties. In this case Carlson and Williams closely agree on their estimates of the 10-N K edge as 870.1 and 870.2 eV, respectively. This is in close agreement with the NIST theoretical value 870.73, but still well outside the 870.73 +/- 0.16 eV (+/- 0.018 %), range, and far from the measured, 866.9001 +/- 0.0090 (+/- 0.001 %) range. Below we will have a chance to closely examine the values and differences between the Carlson and Williams results, as well as the Deslattes and NIST results (in principle what I refer to here as Deslattes and NIST are identical; see the references for details).

All our sources include high quality results that we judge to be reliable. But these sources are not necessarily complete, which presents a problem for use in our applications. In pure science it is perfectly acceptable to say we do not know or cannot estimate something. But in our application as a simple engineering interface within the ENDF/B system, that is not acceptable. For better or worse we must supply our best estimate, or in the worst cases our best guess. Below we will see that the uncertainty in the atomic subshell binding energies is strongly Z, and therefore energy dependent. Fortunately for our use we are primarily interested in macroscopic quantities, such as energy deposit, DOSE, and damage, so we will be interested in higher electron and photon energies. Again, I will remind the reader that I recommend that the EPICS2017 data not be used for transport below 100 eV; or 1 keV, F. Salvat [1]. Below these energies there can be enormous uncertainties in the data, due to effects that are not included in our simple engineering data base for use as part of the ENDF/B system. Again, let us stress that our data is strictly designed for: elemental, cold, neutral, isolated atoms; no molecular or other combined effects are included. As but one example, consider that our data includes the generally accepted value of 13.6 eV as the H K shell binding energy, but H does not exist in nature. For H2, that does exist in nature, the binding energy is 16.4 eV, over 20% higher than 13.6 eV. Let me repeat: based on our objective of elemental, cold, neutral, isolated atoms we use 13.6 eV, which agrees with the evaluated values from both Carlson and Williams. This is but the simplest example; difference in binding for compounds, etc., can be enormous. Fortunately, these differences have little or no effect on the macroscopic quantities we are interested in when transporting well above the binding energy, e.g., when transporting a photon that has 1 keV energy, macroscopic quantities such as energy deposit, DOSE or damage will be little affected by whether we use 13.6 or 16.4 eV as the binding energy of H.

One last point before we start comparing our various sets of data. You will see that decreasing Z (atomic number), and therefore decreasing energy (binding or transition) results in increasing differences between our sources of data. At higher Z and energy all the sources closely agree (usually to within a small fraction of 1%). With decreasing Z and energy, we will see increasing differences (often well in excess of 1 %). Be aware that these differences are merely the tip-of-the-iceberg. Here all our sources are trying to predict the same quantities, but not necessarily what EPICS is designed to model (elemental, cold, neutral, isolated atoms), so that the 1 % differences we see can be small compared to real world differences due to compounds, etc. But as long as users follow our suggestions and do not misuse our data, they should be able to accurately calculate the macroscopic quantities this data is designed to produce.

But **CAVEAT EMPTOR** (**let the user beware**) if you ignore our WARNINGS and transport electrons and/or photons to lower energies your results can become progressive worse, and you will have nobody to blame but yourself.

4. Expected Electrons per Shell and EADL data

Below I list the electron configurations that we expect for elemental, cold, neutral, isolated atoms, for the elements Z = 1 through 100. For all elements, this is exactly the configurations used by EADL, so I need not repeat the list here. For each element, Z = 1 through 100, there obviously must be exactly Z electrons, and the only question asked here is what shell they are in – let me repeat that: What SHELL, not SUBSHELL.

For each Z, I have started from the correct configuration for element Z-1, and then tried to define which shell the next – and only the next – electron is assigned by each author. So that in the below tables no configuration can be incorrect by more than one electron. For any Z in which no additional information is provided, merely for the matter of completeness the tables assign the next electron to the last subshell used; see more details on this point included below for the Williams data.

Z-Ele	K	L	M	N	O	P	Q
1-H	1	0	0	0	0	0	0
2-He	2	0	0	0	0	0	0
3-Li	2	1	0	0	0	0	0
4-Be	2	2	0	0	0	0	0
5-B	2	3	0	0	0	0	0
6-C	2	4	0	0	0	0	0
7-N	2	5	0	0	0	0	0
8-O	2	6	0	0	0	0	0
9-F	2	7	0	0	0	0	0
10-Ne	2	8	0	0	0	0	0
11-Na	2	8	1	0	0	0	0
12-Mg	2	8	2	0	0	0	0
13-Al	2	8	3	0	0	0	0
14-Si	2	8	4	0	0	0	0
15-P	2	8	5	0	0	0	0
16-S	2	8	6	0	0	0	0
17-Cl	2	8	7	0	0	0	0
18-Ar	2	8	8	0	0	0	0
19-K	2	8	8	1	0	0	0
20-Ca	2	8	8	2	0	0	0
21-Sc	2	8	9	2	0	0	0
22-Ti	2	8	10	2	0	0	0
23-V	2	8	11	2	0	0	0
24-Cr	2	8	13	1	0	0	0
25-Mn	2	8	13	2	0	0	0
26-Fe	2	8	14	2	0	0	0
27-Co	2	8	15	2	0	0	0
28-Ni	2	8	16	2	0	0	0
29-Cu	2	8	18	1	0	0	0
30-Zn	2	8	18	2	0	0	0
31-Ga	2	8	18	3	0	0	0
32-Ge	2	8	18	4	0	0	0
33-As	2	8	18	5	0	0	0
34-Se	2	8	18	6	0	0	0
35-Br	2	8	18	7	0	0	0
36-Kr	2	8	18	8	0	0	0
37-Rb	2	8	18	8	1	0	0
38-Sr	2	8	18	8	2	0	0
39-Y	2	8	18	9	2	0	0
40-Zr	2	8	18	10	2	0	0
41-Nb	2	8	18	12	1	0	0
42-Mo	2	8	18	13	1	0	0
43-Tc	2	8	18	13	2	0	0
44-Ru	2	8	18	15	1	0	0
45-Rh	2	8	18	16	1	0	0
46-Pd	2	8	18	18	0	0	0
47-Ag	2	8	18	18	1	0	0
48-Cd	2	8	18	18	2	0	0
49-In	2	8	18	18	3	0	0
50-Sn	2	8	18	18	4	0	0
51-Sb	2	8	18	18	5	0	0
52-Te	2	8	18	18	6	0	0
53-I	2	8	18	18	7	0	0
54-Xe	2	8	18	18	8	0	0
55-Cs	2	8	18	18	8	1	0
56-Ba	2	8	18	18	8	2	0
57-La	2	8	18	18	9	2	0
58-Ce	2	8	18	19	9	2	0
59-Pr	2	8	18	21	8	2	0
60-Nd	2	8	18	22	8	2	0
61-Pm	2	8	18	23	8	2	0
62-Sm	2	8	18	24	8	2	0
63-Eu	2	8	18	25	8	2	0
64-Gd	2	8	18	25	9	2	0
65-Tb	2	8	18	27	8	2	0
66-Dy	2	8	18	28	8	2	0
67-Ho	2	8	18	29	8	2	0
68-Er	2	8	18	30	8	2	0
69-Tm	2	8	18	31	8	2	0
70-Yb	2	8	18	32	8	2	0
71-Lu	2	8	18	32	9	2	0
72-Hf	2	8	18	32	10	2	0
73-Ta	2	8	18	32	11	2	0
74-W	2	8	18	32	12	2	0
75-Re	2	8	18	32	13	2	0
76-Os	2	8	18	32	14	2	0
77-Ir	2	8	18	32	15	2	0
78-Pt	2	8	18	32	17	1	0
79-Au	2	8	18	32	18	1	0
80-Hg	2	8	18	32	18	2	0
81-Tl	2	8	18	32	18	3	0
82-Pb	2	8	18	32	18	4	0
83-Bi	2	8	18	32	18	5	0
84-Po	2	8	18	32	18	6	0
85-At	2	8	18	32	18	7	0
86-Rn	2	8	18	32	18	8	0
87-Fr	2	8	18	32	18	8	1
88-Ra	2	8	18	32	18	8	2
89-Ac	2	8	18	32	18	9	2
90-Th	2	8	18	32	18	10	2
91-Pa	2	8	18	32	20	9	2
92-U	2	8	18	32	21	9	2
93-Np	2	8	18	32	22	9	2
94-Pu	2	8	18	32	24	8	2
95-Am	2	8	18	32	25	8	2
96-Cm	2	8	18	32	25	9	2
97-Bk	2	8	18	32	27	8	2
98-Cf	2	8	18	32	28	8	2
99-Es	2	8	18	32	29	8	2
100-Fm	2	8	18	32	30	8	2

4.1. Carlson Data

Below is the corresponding list for the Carlson data. It is identical to what we expect and show in the above table, except for Pd-46, where Carlson includes 1 electron in the O shell, and we expect none (0). This is a minor difference that will not affect the macroscopic results we are interested in.

Z-Ele	K	L	M	N	O	P	Q	Z-Ele	K	L	M	N	O	P	Q
1-H	1	0	0	0	0	0	0	49-In	2	8	18	18	3	0	0
2-He	2	0	0	0	0	0	0	50-Sn	2	8	18	18	4	0	0
3-Li	2	1	0	0	0	0	0	51-Sb	2	8	18	18	5	0	0
4-Be	2	2	0	0	0	0	0	52-Te	2	8	18	18	6	0	0
5-B	2	3	0	0	0	0	0	53-I	2	8	18	18	7	0	0
6-C	2	4	0	0	0	0	0	54-Xe	2	8	18	18	8	0	0
7-N	2	5	0	0	0	0	0	55-Cs	2	8	18	18	8	1	0
8-O	2	6	0	0	0	0	0	56-Ba	2	8	18	18	8	2	0
9-F	2	7	0	0	0	0	0	57-La	2	8	18	18	9	2	0
10-Ne	2	8	0	0	0	0	0	58-Ce	2	8	18	19	9	2	0
11-Na	2	8	1	0	0	0	0	59-Pr	2	8	18	21	8	2	0
12-Mg	2	8	2	0	0	0	0	60-Nd	2	8	18	22	8	2	0
13-Al	2	8	3	0	0	0	0	61-Pm	2	8	18	23	8	2	0
14-Si	2	8	4	0	0	0	0	62-Sm	2	8	18	24	8	2	0
15-P	2	8	5	0	0	0	0	63-Eu	2	8	18	25	8	2	0
16-S	2	8	6	0	0	0	0	64-Gd	2	8	18	25	9	2	0
17-Cl	2	8	7	0	0	0	0	65-Tb	2	8	18	27	8	2	0
18-Ar	2	8	8	0	0	0	0	66-Dy	2	8	18	28	8	2	0
19-K	2	8	8	1	0	0	0	67-Ho	2	8	18	29	8	2	0
20-Ca	2	8	8	2	0	0	0	68-Er	2	8	18	30	8	2	0
21-Sc	2	8	9	2	0	0	0	69-Tm	2	8	18	31	8	2	0
22-Ti	2	8	10	2	0	0	0	70-Yb	2	8	18	32	8	2	0
23-V	2	8	11	2	0	0	0	71-Lu	2	8	18	32	9	2	0
24-Cr	2	8	13	1	0	0	0	72-Hf	2	8	18	32	10	2	0
25-Mn	2	8	13	2	0	0	0	73-Ta	2	8	18	32	11	2	0
26-Fe	2	8	14	2	0	0	0	74-W	2	8	18	32	12	2	0
27-Co	2	8	15	2	0	0	0	75-Re	2	8	18	32	13	2	0
28-Ni	2	8	16	2	0	0	0	76-Os	2	8	18	32	14	2	0
29-Cu	2	8	18	1	0	0	0	77-Ir	2	8	18	32	15	2	0
30-Zn	2	8	18	2	0	0	0	78-Pt	2	8	18	32	17	1	0
31-Ga	2	8	18	3	0	0	0	79-Au	2	8	18	32	18	1	0
32-Ge	2	8	18	4	0	0	0	80-Hg	2	8	18	32	18	2	0
33-As	2	8	18	5	0	0	0	81-Tl	2	8	18	32	18	3	0
34-Se	2	8	18	6	0	0	0	82-Pb	2	8	18	32	18	4	0
35-Br	2	8	18	7	0	0	0	83-Bi	2	8	18	32	18	5	0
36-Kr	2	8	18	8	0	0	0	84-Po	2	8	18	32	18	6	0
37-Rb	2	8	18	8	1	0	0	85-At	2	8	18	32	18	7	0
38-Sr	2	8	18	8	2	0	0	86-Rn	2	8	18	32	18	8	0
39-Y	2	8	18	9	2	0	0	87-Fr	2	8	18	32	18	8	1
40-Zr	2	8	18	10	2	0	0	88-Ra	2	8	18	32	18	8	2
41-Nb	2	8	18	12	1	0	0	89-Ac	2	8	18	32	18	9	2
42-Mo	2	8	18	13	1	0	0	90-Th	2	8	18	32	18	10	2
43-Tc	2	8	18	13	2	0	0	91-Pa	2	8	18	32	20	9	2
44-Ru	2	8	18	15	1	0	0	92-U	2	8	18	32	21	9	2
45-Rh	2	8	18	16	1	0	0	93-Np	2	8	18	32	22	9	2
46-Pd	2	8	18	17	1	0	0	94-Pu	2	8	18	32	24	8	2
	2	8	18	18	0	0	0	95-Am	2	8	18	32	25	8	2
				**	**	Expect		96-Cm	2	8	18	32	25	9	2
47-Ag	2	8	18	18	1	0	0	97-Bk	2	8	18	32	27	8	2
48-Cd	2	8	18	18	2	0	0	98-Cf	2	8	18	32	28	8	2
								99-Es	2	8	18	32	29	8	2

4.2. Williams data

Below is the corresponding list derived from the Williams data. At first glance, this appears to be quite different, however most of the differences are not because Williams has assigned electrons to the wrong shell, but rather because he hasn't defined some subshell data, in which case the table merely reflected that the shell is not uniquely defined. **Remember that Williams data is primarily for solids, and in each case what is not listed is the valence electron**. For example, for 3-Li Williams does not define any L subshell binding energy, so that as far as the below table there is only an uncertainty as to where the third electron is assigned. Since only K shell data are included the table says 3 electrons are in the K shell, which is nonsense; this should only be read to indicate the value valance, L shell, electron is not defined.

There is a similar problem throughout the Z range, where the outer most electron (valence) binding energies may not be defined. Where subshell values are given they are excellent and can be usefully used to compare to our other sources, but the missing values make it difficult to use this data as a complete standard to convert EPICS to.

```
Z-Ele     K   L   M   N   O   P   Q
 1-H  1   0   0   0   0   0   0
 2-He 2   0   0   0   0   0   0
 3-Li 3   0   0   0   0   0   0
          2   1   0   0   0   0   0 Expect
         **  **
 4-Be     3   1   0   0   0   0   0
          2   2   0   0   0   0   0 Expect
         **  **
 5-B      3   2   0   0   0   0   0
          2   3   0   0   0   0   0 Expect
         **  **
 6-C      3   3   0   0   0   0   0
          2   4   0   0   0   0   0 Expect
         **  **
 7-N      2   5   0   0   0   0   0
 8-O      2   6   0   0   0   0   0
 9-F      3   6   0   0   0   0   0
          2   7   0   0   0   0   0 Expect
         **  **
10-Ne     2   8   0   0   0   0   0
11-Na     2   9   0   0   0   0   0
          2   8   1   0   0   0   0 Expect
             **  **
12-Mg     2   9   1   0   0   0   0
          2   8   2   0   0   0   0 Expect
             **  **
13-Al     2   9   2   0   0   0   0
          2   8   3   0   0   0   0 Expect
             **  **
14-Si     2   9   3   0   0   0   0
          2   8   4   0   0   0   0 Expect
             **  **
15-P      2   9   4   0   0   0   0
          2   8   5   0   0   0   0 Expect
             **  **
16-S      2   9   5   0   0   0   0
          2   8   6   0   0   0   0 Expect
             **  **
17-Cl     2   9   6   0   0   0   0
          2   8   7   0   0   0   0 Expect
             **  **
18-Ar     2   8   8   0   0   0   0
19-K      2   8   9   0   0   0   0
          2   8   8   1   0   0   0 Expect
                 **  **
20-Ca     2   8   9   1   0   0   0
          2   8   8   2   0   0   0 Expect
                 **  **
21-Sc     2   8   9   2   0   0   0
22-Ti     2   8  10   2   0   0   0
23-V      2   8  11   2   0   0   0
```

```
Z-Ele     K   L   M   N   O   P   Q
24-Cr     2   8  13   1   0   0   0
25-Mn     2   8  14   1   0   0   0
          2   8  13   2   0   0   0 Expect
                 **  **
26-Fe     2   8  14   2   0   0   0
27-Co     2   8  15   2   0   0   0
28-Ni     2   8  16   2   0   0   0
29-Cu     2   8  18   1   0   0   0
30-Zn     2   8  19   1   0   0   0
          2   8  18   2   0   0   0 Expect
                 **  **
31-Ga     2   8  19   2   0   0   0
          2   8  18   3   0   0   0 Expect
                 **  **
32-Ge     2   8  19   3   0   0   0
          2   8  18   4   0   0   0 Expect
                 **  **
33-As     2   8  19   4   0   0   0
          2   8  18   5   0   0   0 Expect
                 **  **
34-Se     2   8  19   5   0   0   0
          2   8  18   6   0   0   0 Expect
                 **  **
35-Br     2   8  19   6   0   0   0
          2   8  18   7   0   0   0 Expect
                 **  **
36-Kr     2   8  18   8   0   0   0
37-Rb     2   8  18   9   0   0   0
          2   8  18   8   1   0   0 Expect
                     **  **
38-Sr     2   8  18   9   1   0   0
          2   8  18   8   2   0   0 Expect
                     **  **
39-Y      2   8  18   9   2   0   0
40-Zr     2   8  18  10   2   0   0
41-Nb     2   8  18  12   1   0   0
42-Mo     2   8  18  13   1   0   0
43-Tc     2   8  18  14   1   0   0
          2   8  18  13   2   0   0 Expect
                     **  **
44-Ru     2   8  18  15   1   0   0
45-Rh     2   8  18  16   1   0   0
46-Pd     2   8  18  18   0   0   0
47-Ag     2   8  18  19   0   0   0
          2   8  18  18   1   0   0 Expect
                     **  **
48-Cd     2   8  18  19   1   0   0
          2   8  18  18   2   0   0 Expect
                     **  **
49-In     2   8  18  19   2   0   0
          2   8  18  18   3   0   0 Expect
                     **  **
```

Z-Ele	K	L	M	N	O	P	Q	
50-Sn	2	8	18	19	3	0	0	
	2	8	18	18	4	0	0	Expect
				**	**			
51-Sb	2	8	18	19	4	0	0	
	2	8	18	18	5	0	0	Expect
				**	**			
52-Te	2	8	18	19	5	0	0	
	2	8	18	18	6	0	0	Expect
				**	**			
53-I	2	8	18	19	6	0	0	
	2	8	18	18	7	0	0	Expect
				**	**			
54-Xe	2	8	18	18	8	0	0	
55-Cs	2	8	18	18	9	0	0	
	2	8	18	18	8	1	0	Expect
					**	**		
56-Ba	2	8	18	18	9	1	0	
	2	8	18	18	8	2	0	Expect
					**	**		
57-La	2	8	18	18	9	2	0	
58-Ce	2	8	18	18	10	2	0	
	2	8	18	19	9	2	0	Expect
				**	**			
59-Pr	2	8	18	20	9	2	0	
	2	8	18	21	8	2	0	Expect
				**	**			
60-Nd	2	8	18	21	9	2	0	
	2	8	18	22	8	2	0	Expect
				**	**			
61-Pm	2	8	18	22	9	2	0	
	2	8	18	23	8	2	0	Expect
				**	**			
62-Sm	2	8	18	23	9	2	0	
	2	8	18	24	8	2	0	Expect
				**	**			
63-Eu	2	8	18	24	9	2	0	
	2	8	18	25	8	2	0	Expect
				**	**			
64-Gd	2	8	18	24	10	2	0	
	2	8	18	25	9	2	0	Expect
				**	**			
65-Tb	2	8	18	26	9	2	0	
	2	8	18	27	8	2	0	Expect
				**	**			
66-Dy	2	8	18	27	9	2	0	
	2	8	18	28	8	2	0	Expect
				**	**			
67-Ho	2	8	18	28	9	2	0	
	2	8	18	29	8	2	0	Expect
				**	**			
68-Er	2	8	18	29	9	2	0	
	2	8	18	30	8	2	0	Expect
				**	**			
69-Tm	2	8	18	30	9	2	0	
	2	8	18	31	8	2	0	Expect
				**	**			
70-Yb	2	8	18	31	9	2	0	
	2	8	18	32	8	2	0	Expect
				**	**			
71-Lu	2	8	18	32	9	2	0	
72-Hf	2	8	18	32	10	2	0	
73-Ta	2	8	18	32	11	2	0	
74-W	2	8	18	32	12	2	0	
75-Re	2	8	18	32	13	2	0	
76-Os	2	8	18	32	14	2	0	
77-Ir	2	8	18	32	15	2	0	
78-Pt	2	8	18	32	17	1	0	
79-Au	2	8	18	32	18	1	0	
80-Hg	2	8	18	32	19	1	0	
	2	8	18	32	18	2	0	Expect
					**	**		
81-Tl	2	8	18	32	19	2	0	
	2	8	18	32	18	3	0	Expect
					**	**		
82-Pb	2	8	18	32	19	3	0	
	2	8	18	32	18	4	0	Expect
					**	**		
83-Bi	2	8	18	32	19	4	0	
	2	8	18	32	18	5	0	Expect
					**	**		
84-Po	2	8	18	32	19	5	0	
	2	8	18	32	18	6	0	Expect
					**	**		
85-At	2	8	18	32	19	6	0	
	2	8	18	32	18	7	0	Expect
					**	**		
86-Rn	2	8	18	32	18	8	0	
87-Fr	2	8	18	32	18	9	0	
	2	8	18	32	18	8	1	Expect
						**	**	
88-Ra	2	8	18	32	18	9	1	
	2	8	18	32	18	8	2	Expect
						**	**	
89-Ac	2	8	18	32	18	9	2	
90-Th	2	8	18	32	18	10	2	
91-Pa	2	8	18	32	19	10	2	
	2	8	18	32	20	9	2	Expect
						**	**	
92-U	2	8	18	32	20	10	2	
	2	8	18	32	21	9	2	Expect
						**	**	

4.3. Different Subshells for EADL and Carlson

As seen on the preceding tables, the EADL and Carlson data have an almost identical number of electrons for each atomic **shell**. However, there are quite a few differences in the number of electrons for each **subshell**. The below tables list where they differ. Where EADL has a subshell occupied and Carlson does not, the binding energy of the subshell is listed. Where Carlson has a subshell occupied and EADL does not, the binding energy and the word **Carlson** are listed.

PLEASE note that the below results are based not on the complete Carlson results [5], but rather on the abstracted file "binden.tab"; the complete results include some of these low energy edges.

Fortunately, all the differences are for subshells with very small binding energies, i.e., all are in the eV range, and correspond to the case where the binding energy of adjacent subshells are very similar. For example, 5-B, where the L2 and L3 binding energies are very similar. EADL distributes the electrons between L1, L2 and L3, whereas Carlson only uses L1 and L2. Since the binding energies of L2 and L3 are almost identical, for our purposes the differences are of no consequences. **As such we will in all cases use the subshell configurations defined by EADL.**

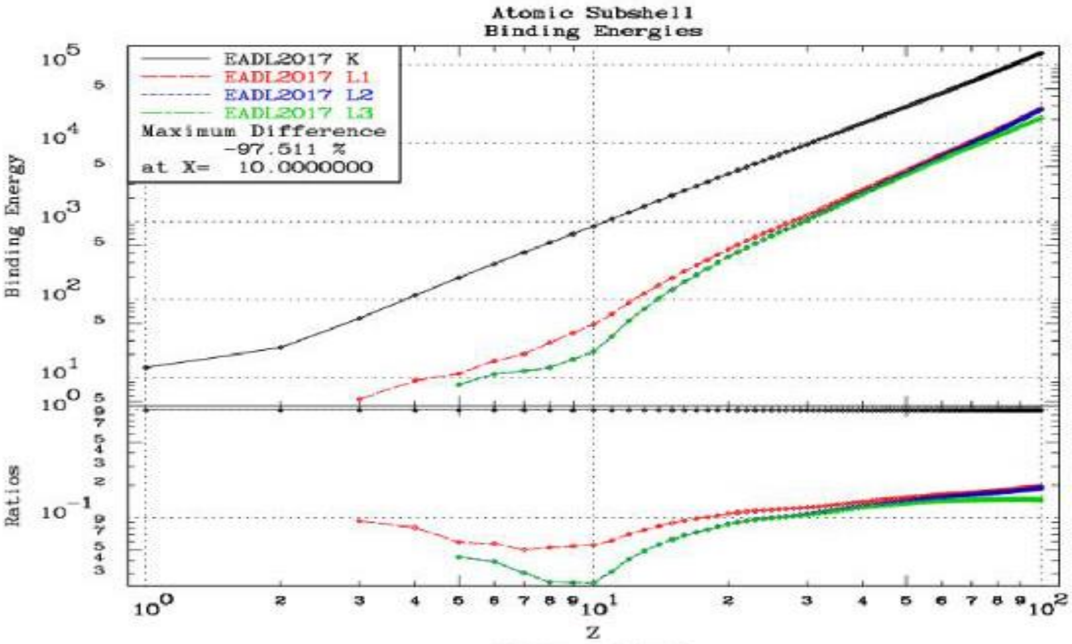
Z-Ele	#	Subshell	Binding Energy (eV)
5-B	4	L3 (2p3/2)	6.66
6-C	4	L3 (2p3/2)	8.98
13-Al	7	M3 (3p3/2)	4.87
14-Si	7	M3 (3p3/2)	6.52
21-Sc	9	M5 (3d5/2)	7.04
22-Ti	9	M5 (3d5/2)	8.34
23-V	9	M5 (3d5/2)	9.53
24-Cr	9	M5 (3d5/2)	6.37
31-Ga	12	N3 (4p3/2)	4.88
32-Ge	12	N3 (4p3/2)	6.29
39-Y	14	N5 (4d5/2)	5.13
40-Zr	14	N5 (4d5/2)	6.52
41-Nb	14	N5 (4d5/2)	5.76
42-Mo	14	N5 (4d5/2)	6.77
46-Pd	17	O1 (5s1/2)	8.34 Carlson
49-In	19	O3 (5p3/2)	4.58
50-Sn	19	O3 (5p3/2)	5.77
57-La	21	O5 (5d5/2)	5.34
58-Ce	16	N7 (4f7/2)	6.51
58-Ce	20	O4 (5d3/2)	5.77 Carlson
59-Pr	16	N7 (4f7/2)	7.24
59-Pr	20	O4 (5d3/2)	5.61 Carlson
60-Nd	16	N7 (4f7/2)	7.85
60-Nd	20	O4 (5d3/2)	5.66 Carlson
61-Pm	16	N7 (4f7/2)	8.35
61-Pm	20	O4 (5d3/2)	5.70 Carlson
62-Sm	16	N7 (4f7/2)	8.75
62-Sm	20	O4 (5d3/2)	5.63 Carlson
63-Eu	16	N7 (4f7/2)	9.08
63-Eu	20	O4 (5d3/2)	5.68 Carlson
64-Gd	21	O5 (5d5/2)	4.85
65-Tb	20	O4 (5d3/2)	5.90 Carlson
66-Dy	20	O4 (5d3/2)	5.95 Carlson
67-Ho	20	O4 (5d3/2)	6.00 Carlson
68-Er	20	O4 (5d3/2)	6.00 Carlson
69-Tm	20	O4 (5d3/2)	6.45 Carlson
71-Lu	21	O5 (5d5/2)	4.03
72-Hf	21	O5 (5d5/2)	5.18
73-Ta	21	O5 (5d5/2)	6.30
74-W	21	O5 (5d5/2)	7.41
77-Ir	26	P1 (6s1/2)	9.27 Carlson
81-Tl	28	P3 (6p3/2)	4.30
82-Pb	28	P3 (6p3/2)	5.29
89-Ac	30	P5 (6d5/2)	4.00
90-Th	22	O6 (5f5/2)	6.00 Carlson
90-Th	30	P5 (6d5/2)	4.98
91-Pa	23	O7 (5f7/2)	6.80
91-Pa	30	P5 (6d5/2)	4.13
92-U	23	O7 (5f7/2)	7.95
92-U	30	P5 (6d5/2)	4.13
93-Np	23	O7 (5f7/2)	9.03
93-Np	30	P5 (6d5/2)	4.11
94-Pu	23	O7 (5f7/2)	6.25
94-Pu	29	P4 (6d3/2)	6.00 Carlson
95-Am	23	O7 (5f7/2)	7.00
95-Am	29	P4 (6d3/2)	6.00 Carlson
96-Cm	30	P5 (6d5/2)	3.93
97-Bk	30	P5 (6d5/2)	3.85
98-Cf	29	P4 (6d3/2)	7.00 Carlson
99-Es	29	P4 (6d3/2)	7.00 Carlson

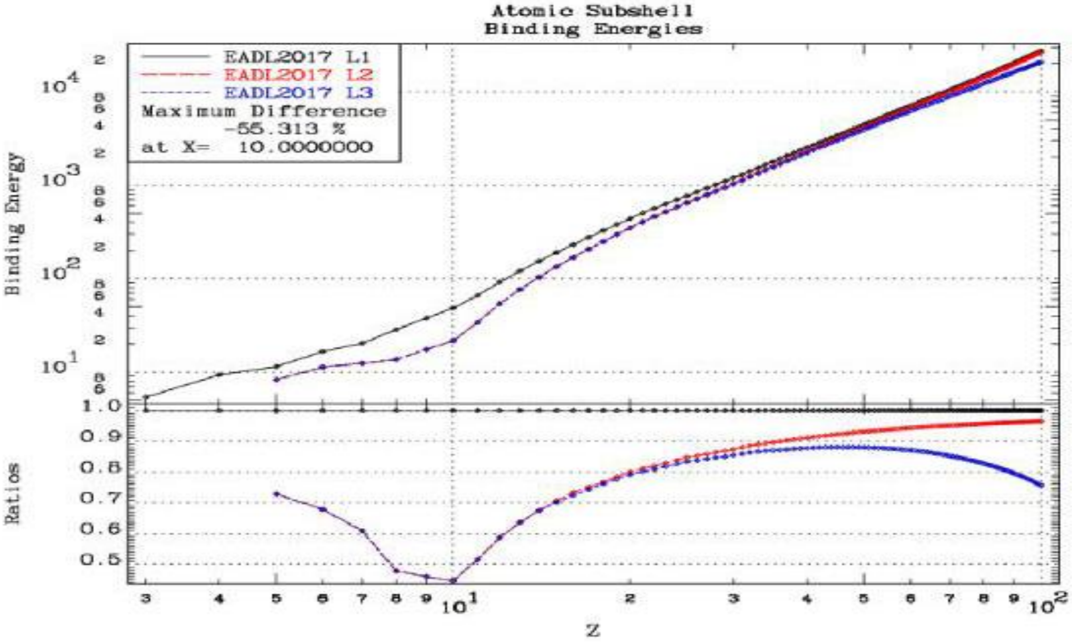
4.4. A quick survey of what the binding energies look like

For those who are not familiar with atomic binding energies and their variation with Z (atomic number) and subshell, here is a quick overview.

4.4.1. K and L edges

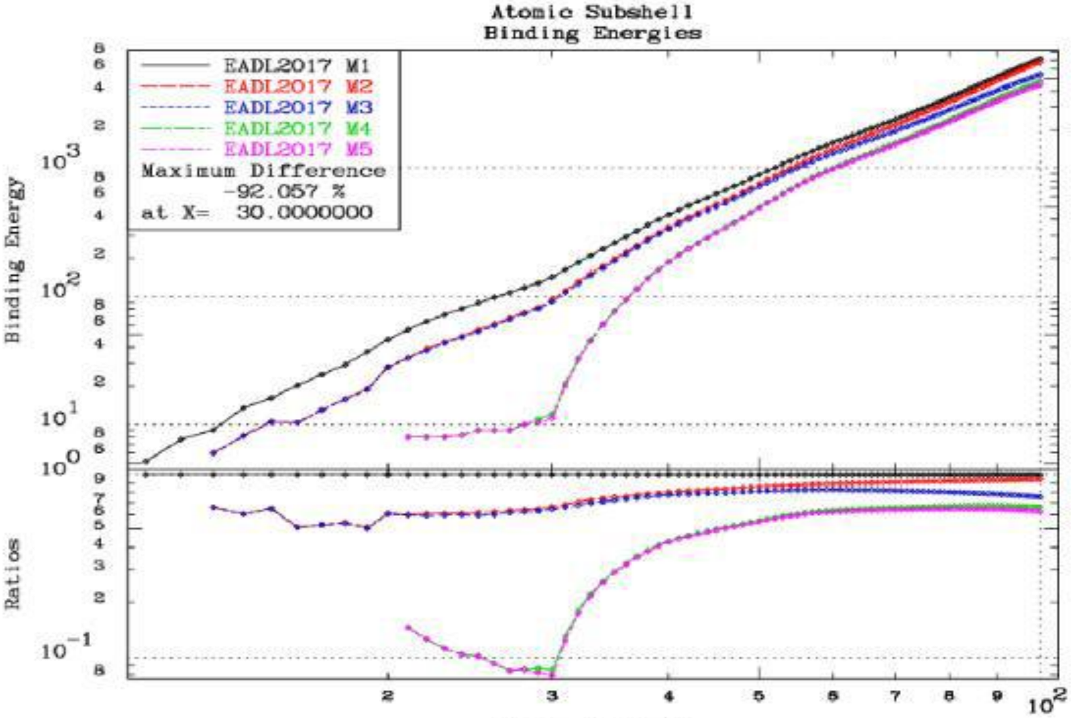
Note the Z dependence of the binding energy: simple Z dependence until the subshell is filled and, then Z^2 dependence across the remainder of the periodic table. For the K edges the energy scale is from 13.6 eV for 1-H to over 150 keV for 100-Fm. Also note that the L2 and L3 binding energies are very similar for low Z, but they do differ at higher Z.

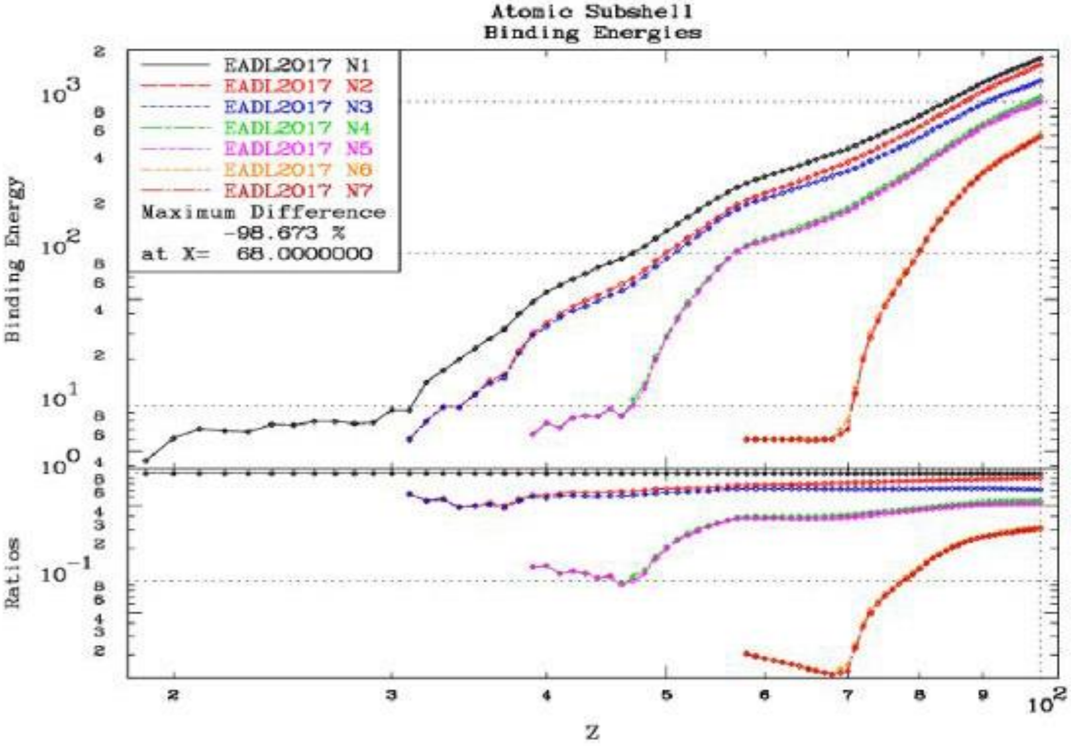




4.4.2. M and N edges

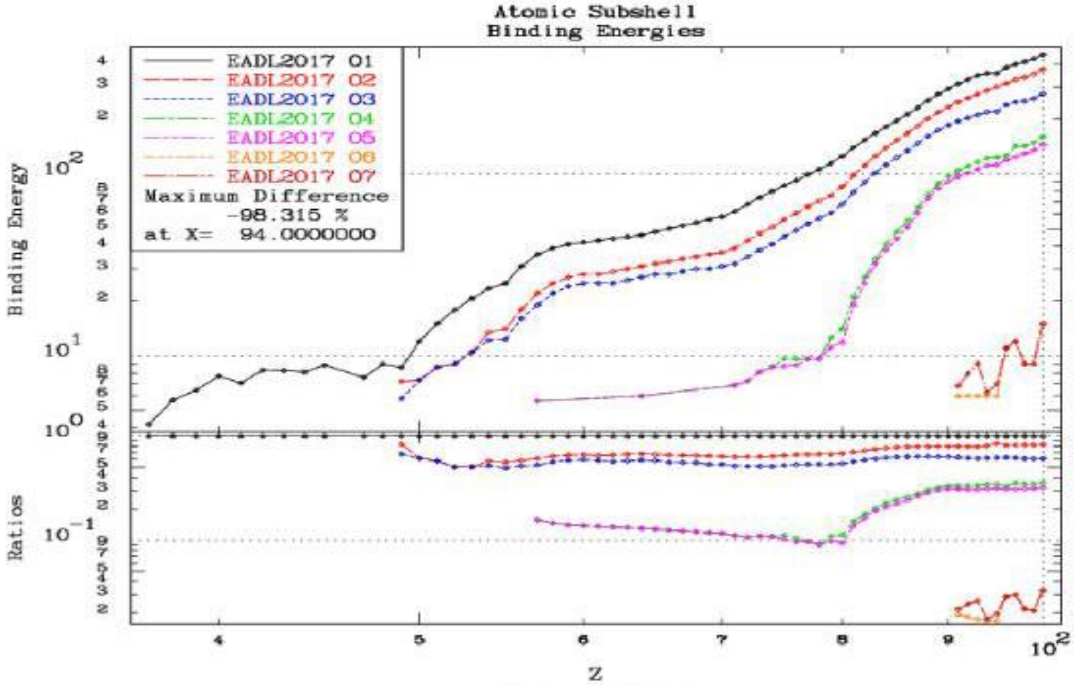
We still see a fairly smooth variation of the binding energy versus Z. Here the energy scale is much lower, only up to less than 8 keV for the M subshells and 2 keV for the N subshells.

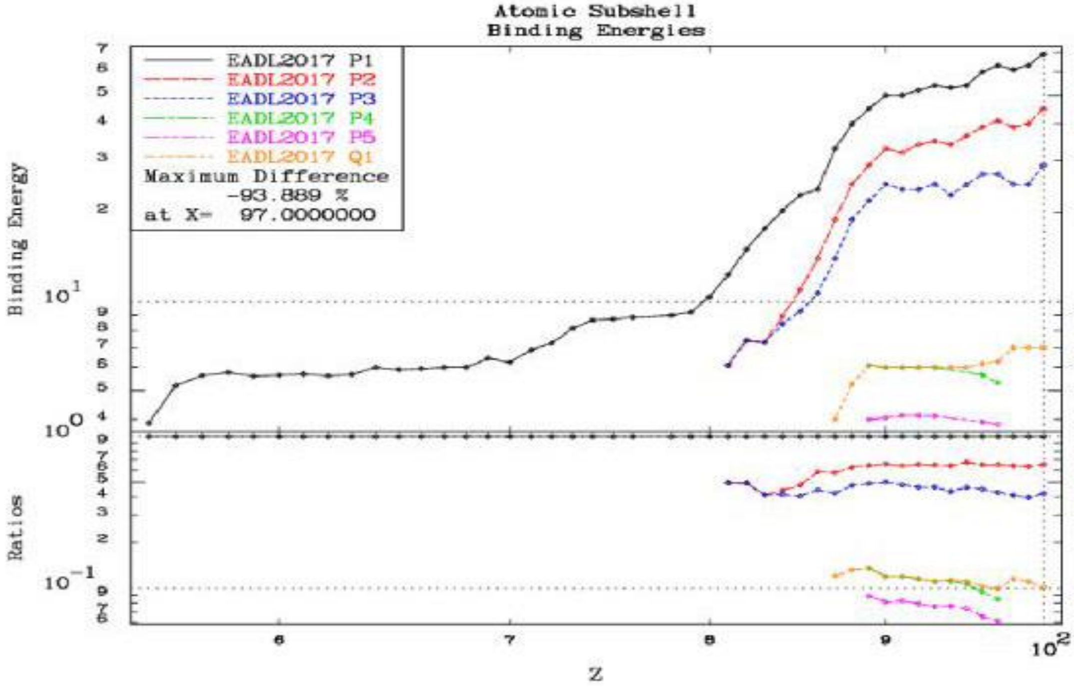




4.4.3. O, P and Q Edges

Here the energy scale is only up to about 400 eV for O subshells and up to 70 eV for P subshells. The P4, P5 and Q1 subshells are all down in the eV range.





4.5. Details

Now comes the heavy lifting part of this report, to compare details from all our sources, show differences and how these compare to the final values adopted for use in EPICS2017. This is “heavy” because it involves many graphic results for both binding energies (29 of them) and transition energies (49 of them).

To help guide you here are the general rules we used for selecting data for use with EPICS2017. Both Carlson and Williams data were used for comparison; we consider both to be comparable in accuracy. Where they differ, preference was given to the Carlson data, only because it is more complete for outer subshells, making it more compatible with EPICS designed use. In some cases, the Carlson data is incomplete for low Z; these are generally low energy cases and we used the older EPICS data and Z dependent systematics to complete the definitions. Lastly, we used Z dependent variation and assumed that some subshell binding energies are identical for low Z, e.g., L2 and L3, N4 and N5, O4 and O5.

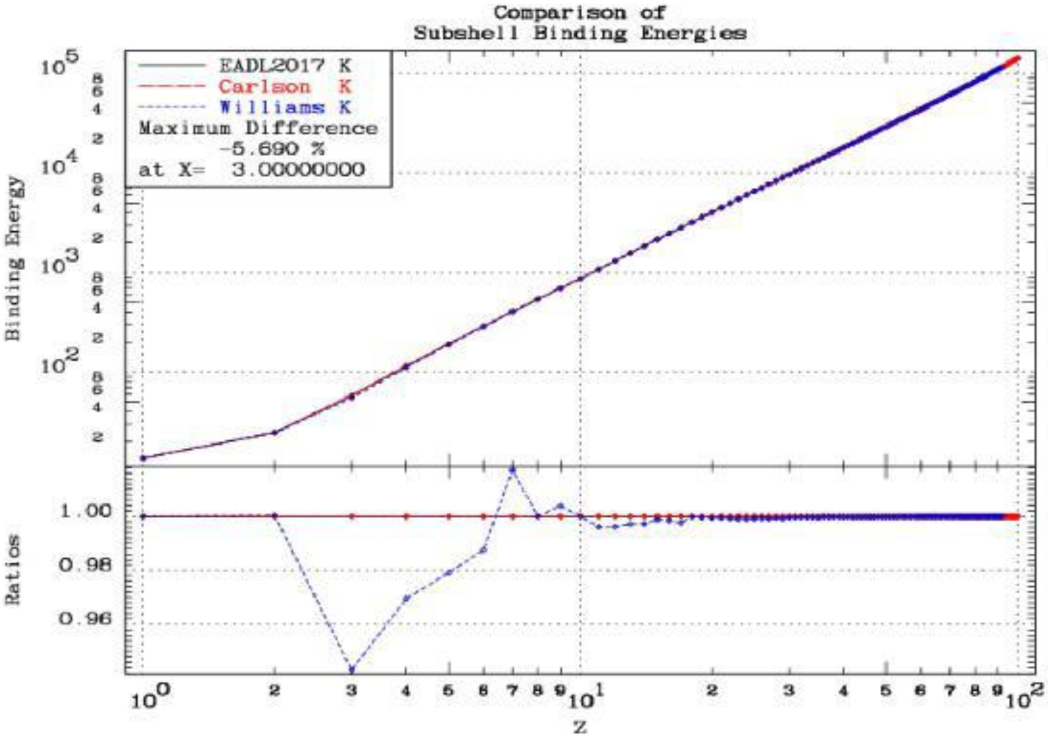
In viewing the below figures of the binding energies please be aware that I consider both Carlson and Williams data to be equally valid and both are high quality results. The Carlson data is closer to what EPICS is designed for: elemental, cold, neutral, isolated atoms, and the Williams data is more closely related to reality; solids, including molecular effects. Generally, for high Z elements these two sources agree. For lower Z elements when they disagree I have given preference to the Carlson data, only because it is closer to EPICS’s intent. But the Williams data is equally valid, indeed maybe even more valid based on its later date of publication. The differences shown in the below figures should be considered the “experts” (Carlson and Williams) estimate of the uncertainty in the data; not an indication that one in better than the other.

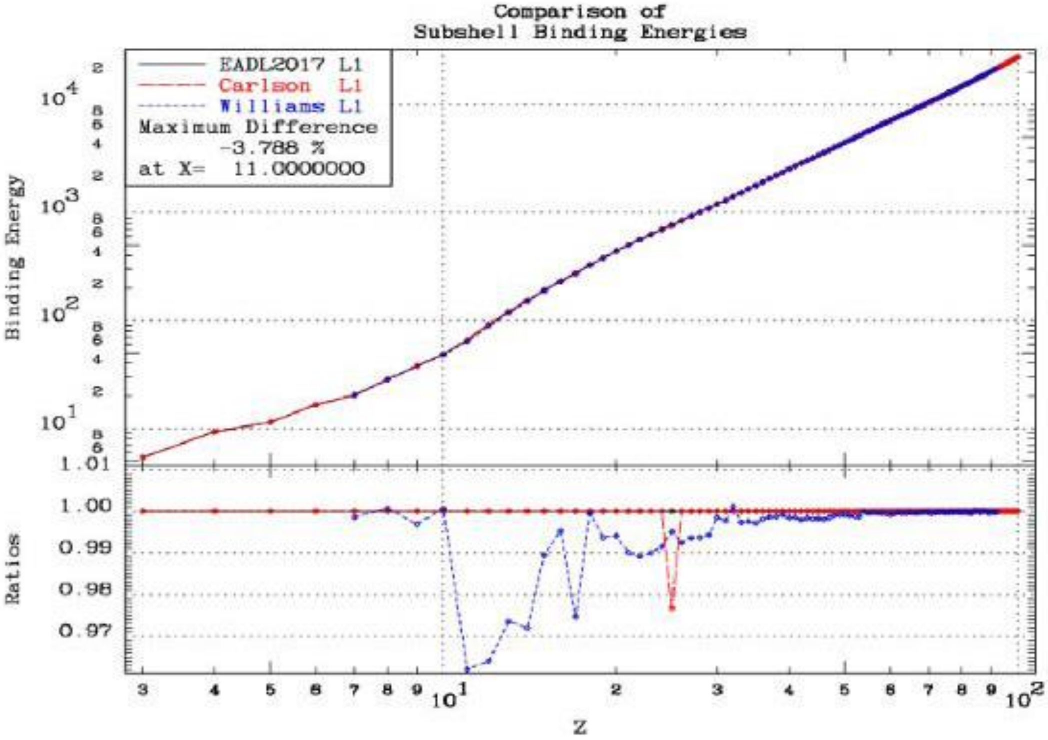
Similarly, for the below figures of the transition energies, where we have three sources of “expert” data, Carlson, Williams and NIST, the spread in the results should be considered an estimate of the uncertainty of the results. NIST data includes both theoretical and measured results. In particular it is interesting here to see the difference between the NIST theoretical and measured results, and to compare the “real” differences to the quoted uncertainties; again, I will merely mention that the quoted uncertainties appear to be, let’s say, extremely optimistic. As with the binding energies, here I judge the spread in the results not to indicate any fault in the data, but rather to be the “experts” estimate of the real World uncertainty.

In all of the below figures, the top 2/3 shows the data and the bottom 1/3 the ratio of all data to the EPICS2017 results. When all data closely agree, the ratio is never scaled to less than +/- 1 %, to avoid exaggerating very small differences. To judge the differences and their importance, I suggest you consider both the per-cent differences, and the energies at which these differences can be seen, e.g., differences at low binding energies (low Z) are not as important as high energy differences.

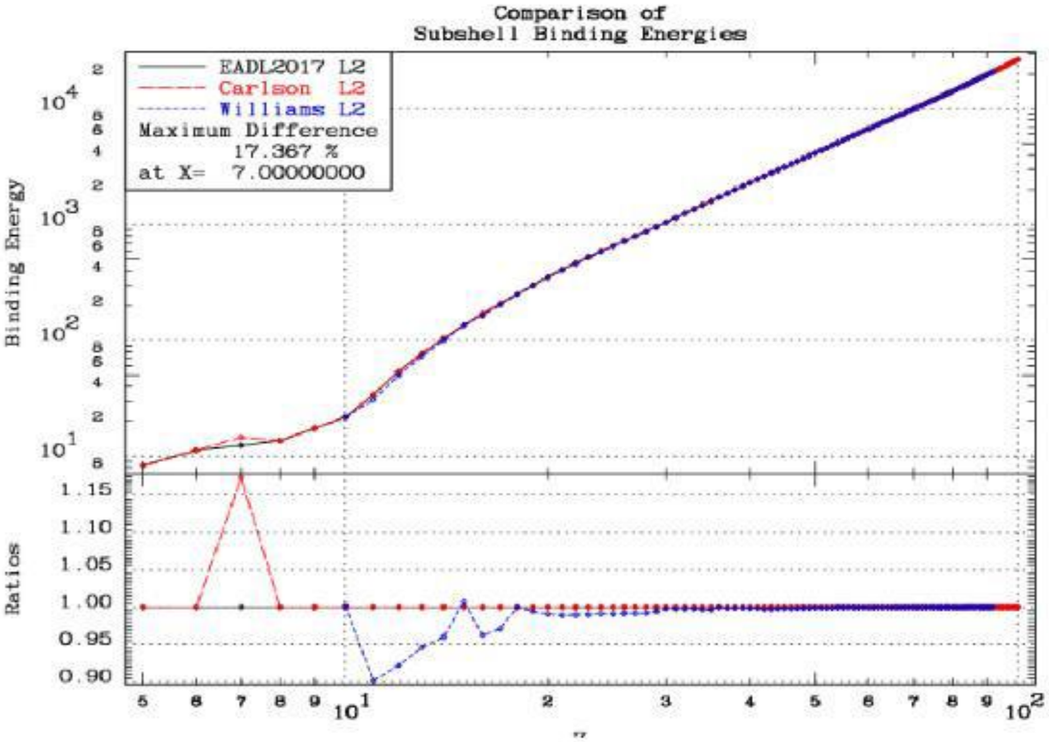
Last point**: “Please do not shoot the messenger”.** In the below figures, I have merely tried to represent the data from the various sources exactly as I found them. The magnitude of the differences shown may come as a shock to some readers, but these only represent the real uncertainties due to the differences between theoretical values for elemental, cold, neutral, isolated atoms (Carlson and EPICS), and reality for solids (Williams). So, again, please do not shoot the messenger (me) for making these differences more obvious in these figures.

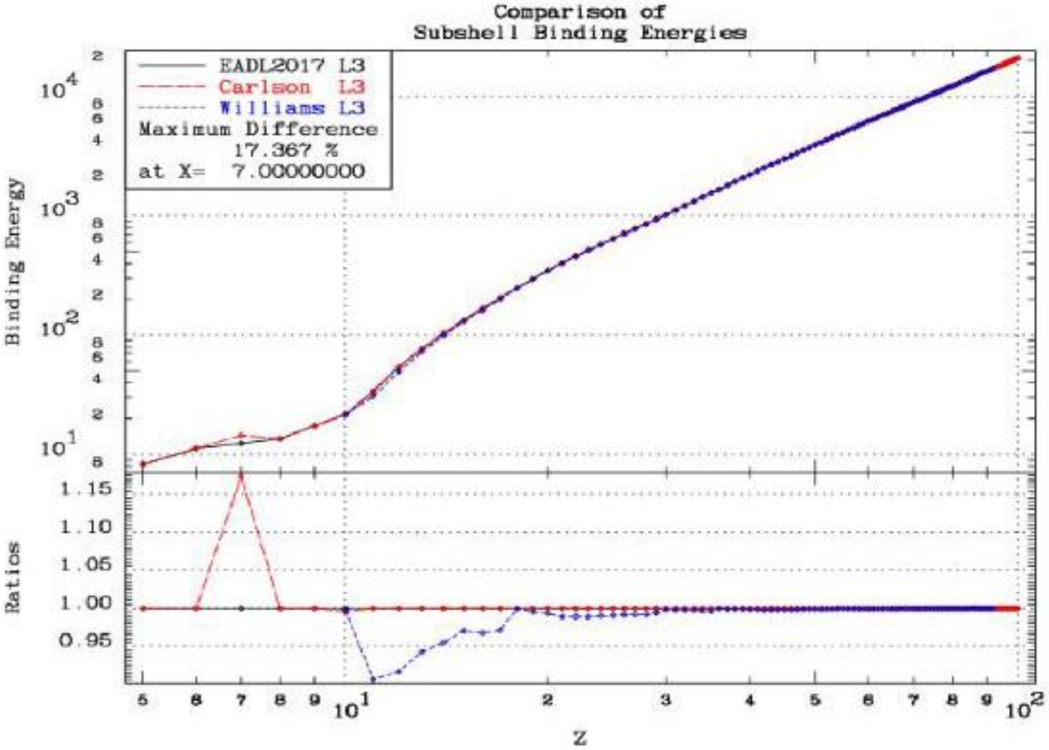
4.5.1. K and L1 Edges



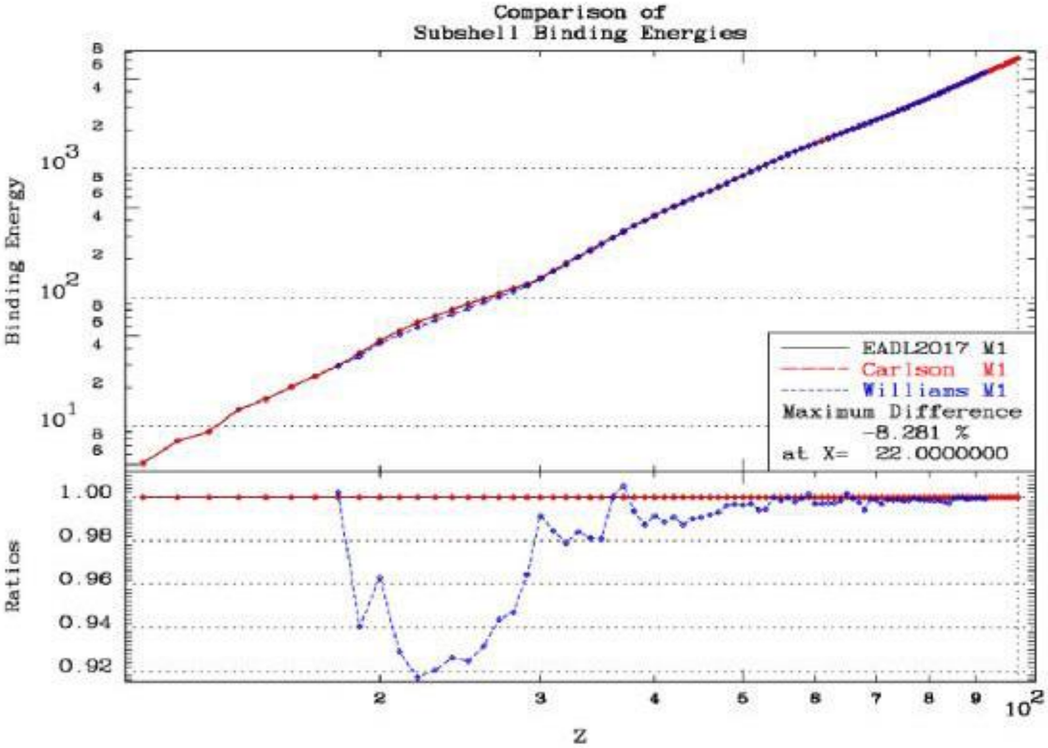


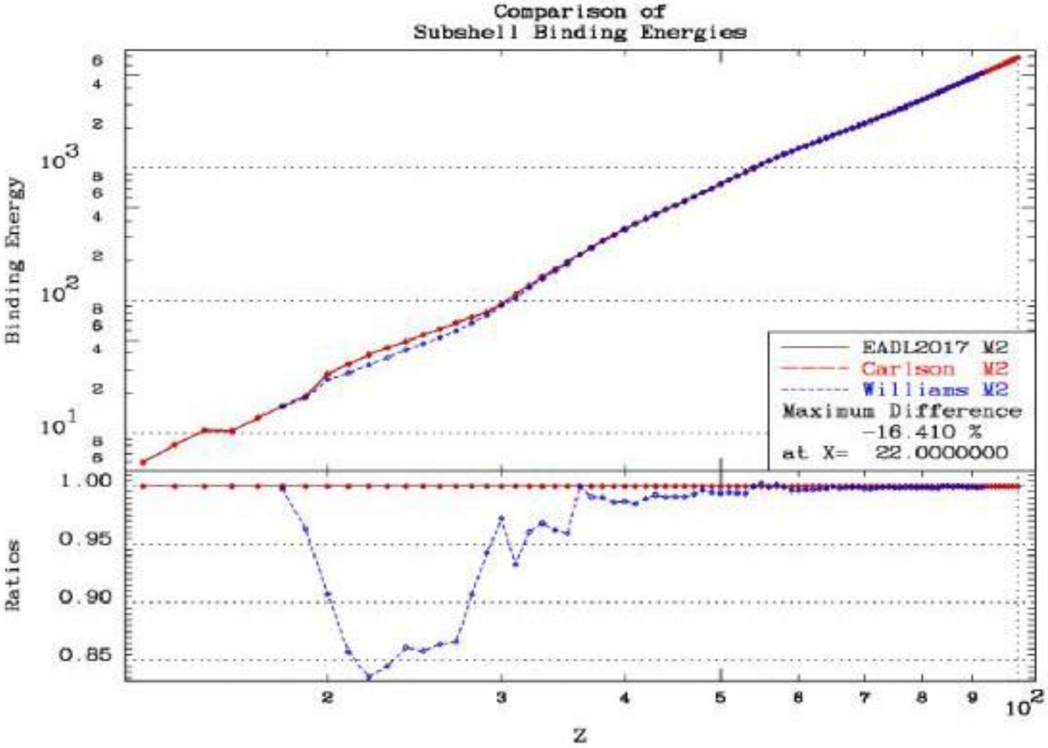
4.5.2. L2 and L3 Edges



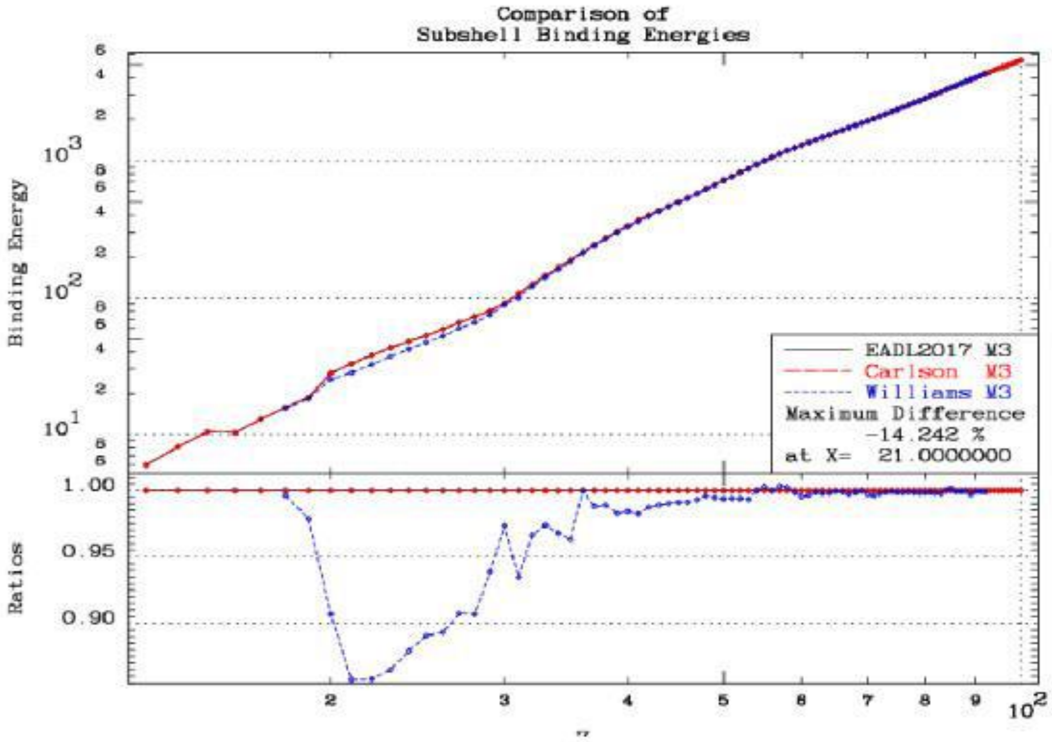


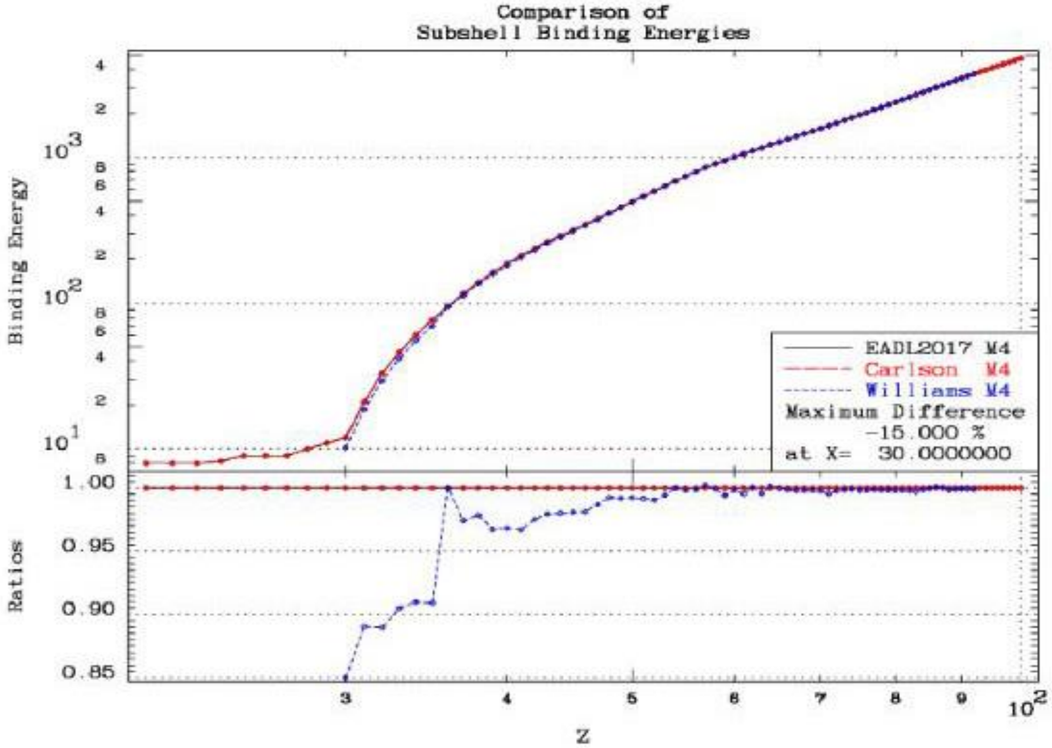
4.5.3. M1 and M2 edges



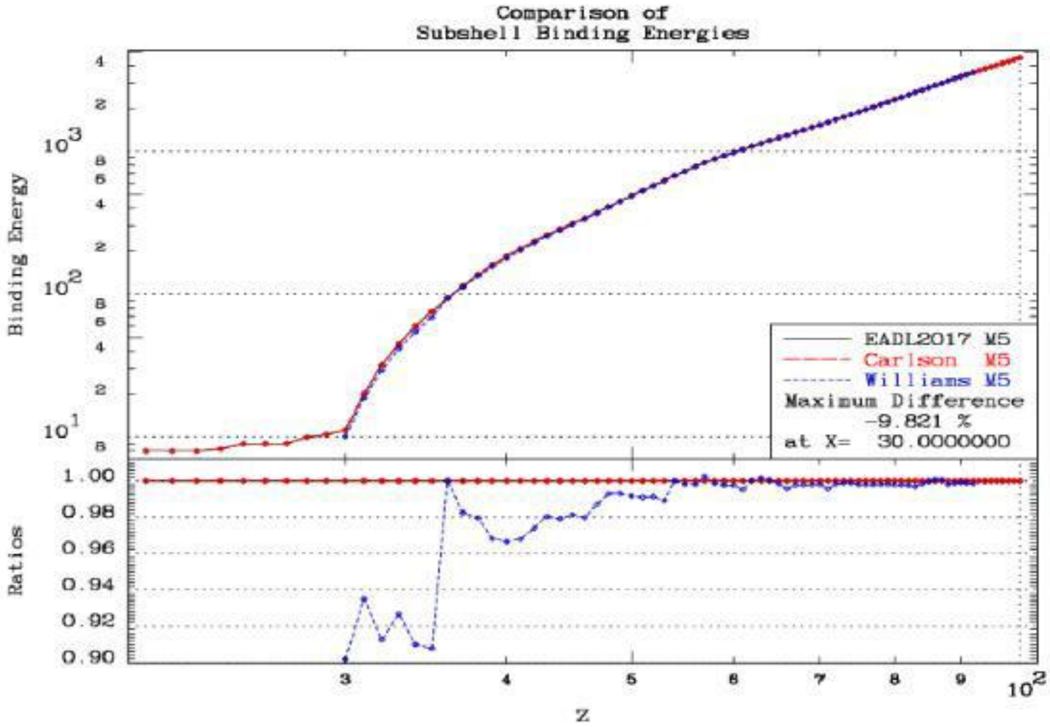


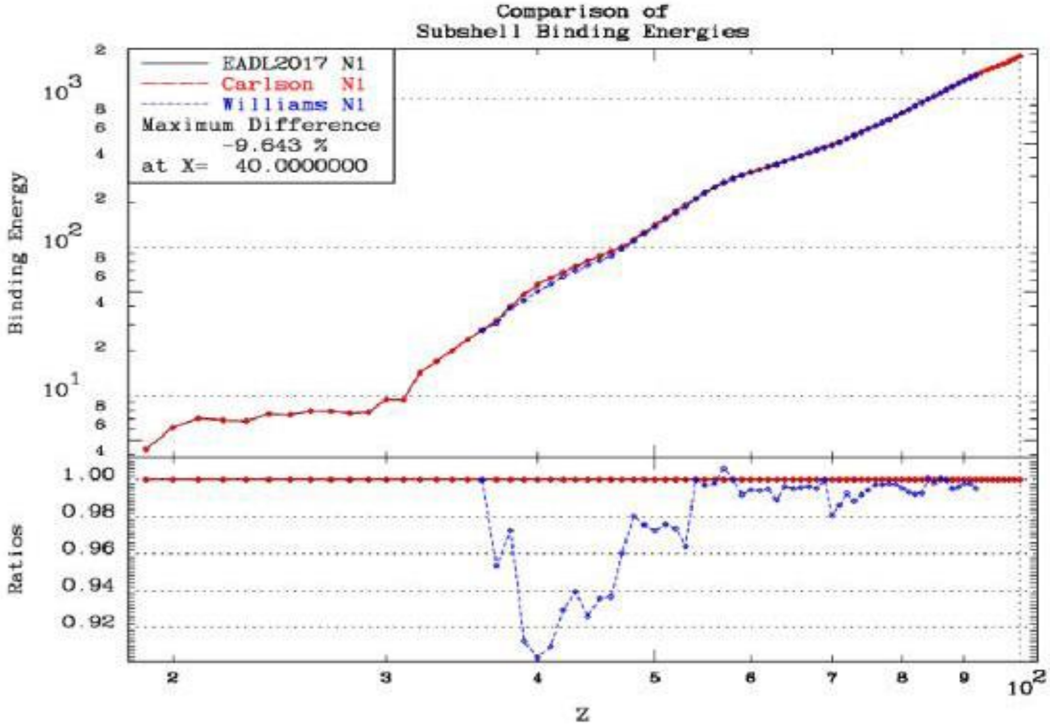
4.5.4. M3 and M4 edges



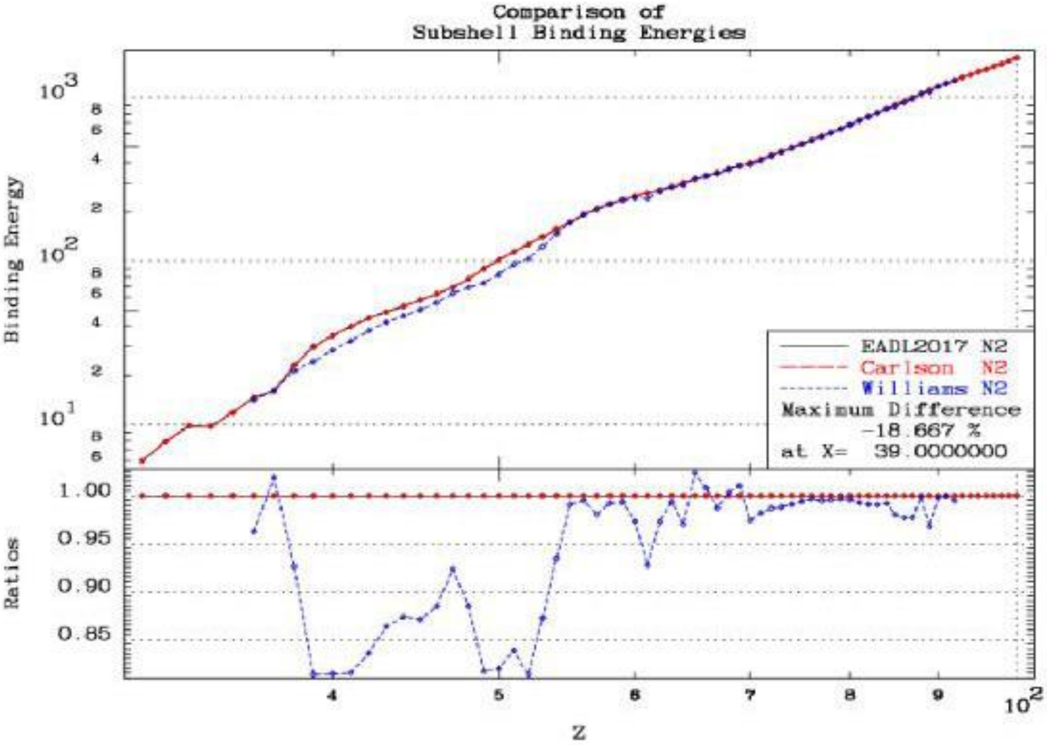


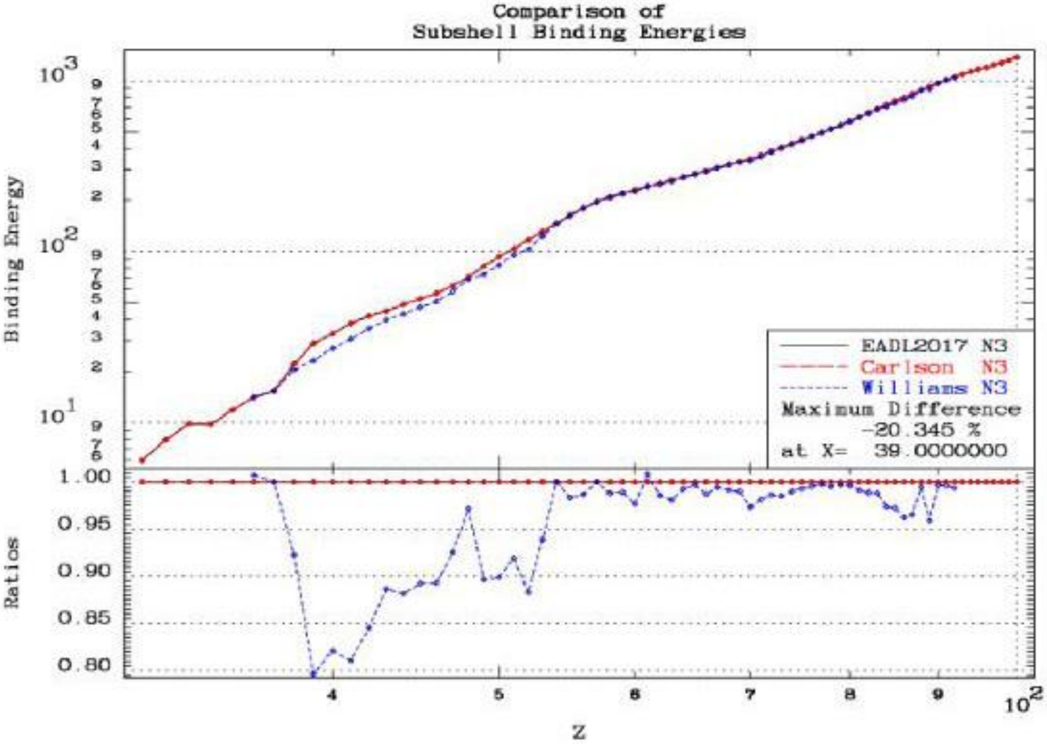
4.5.5. M5 and N1 Edges



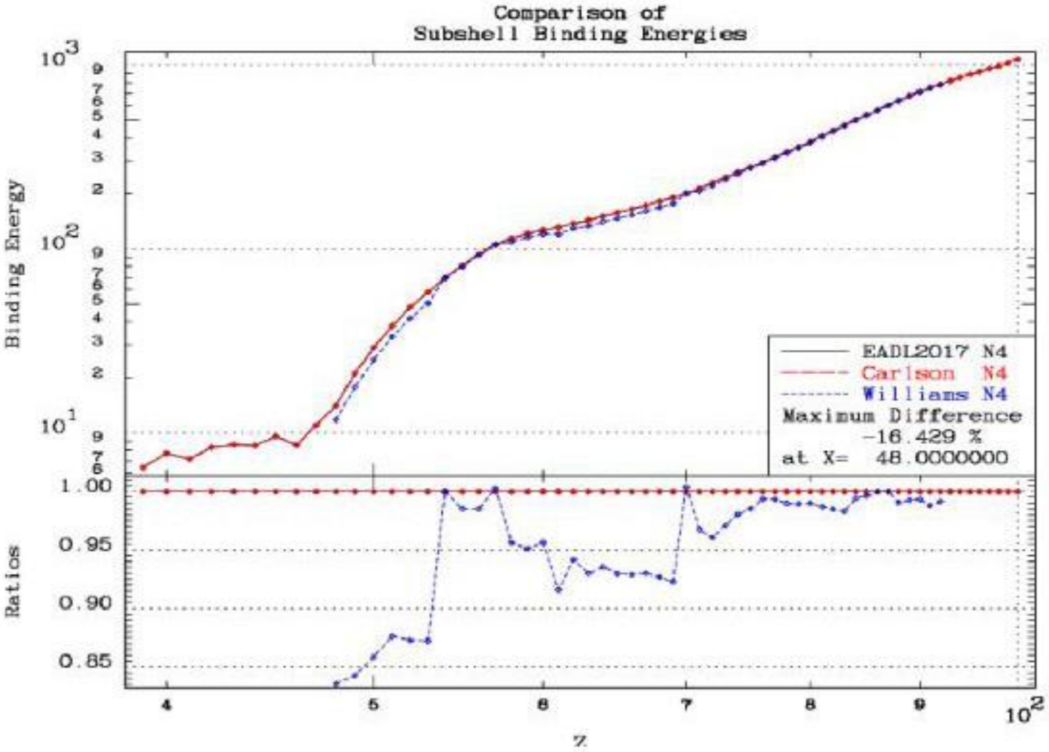


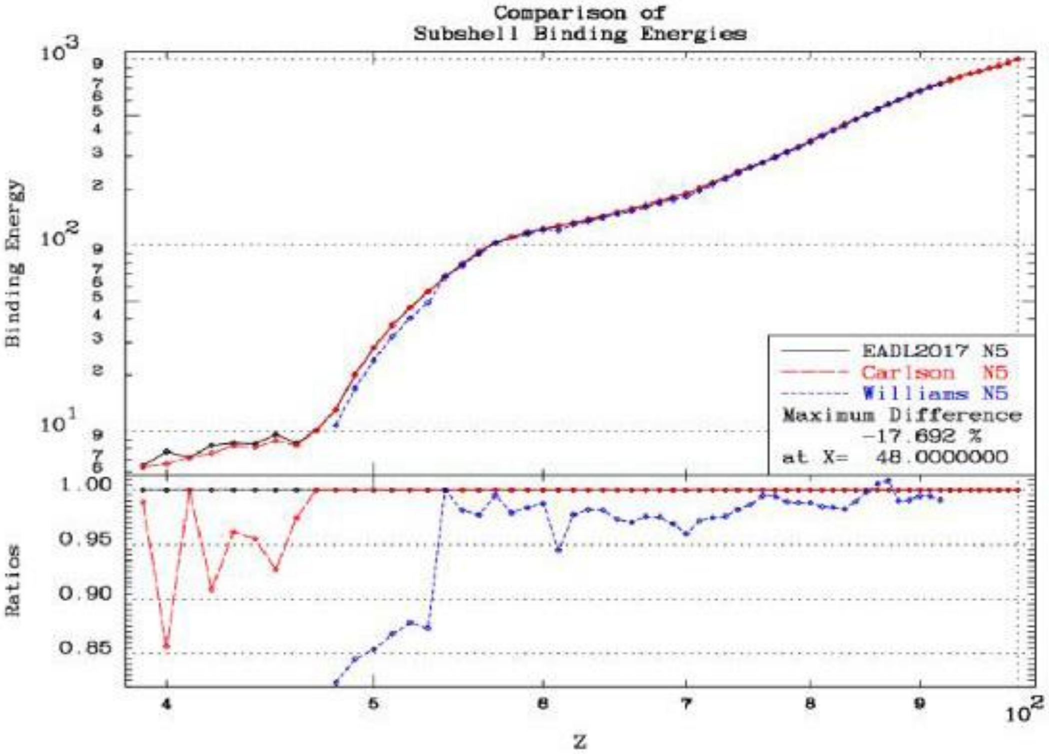
4.5.6. N2 and N3 Edges



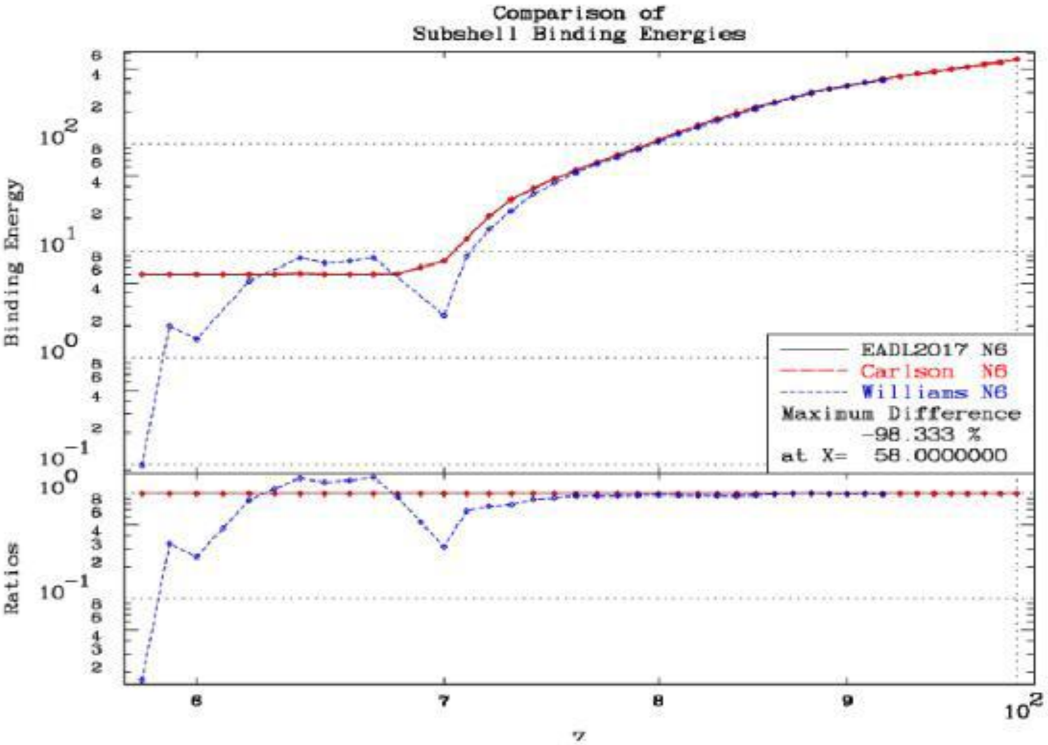


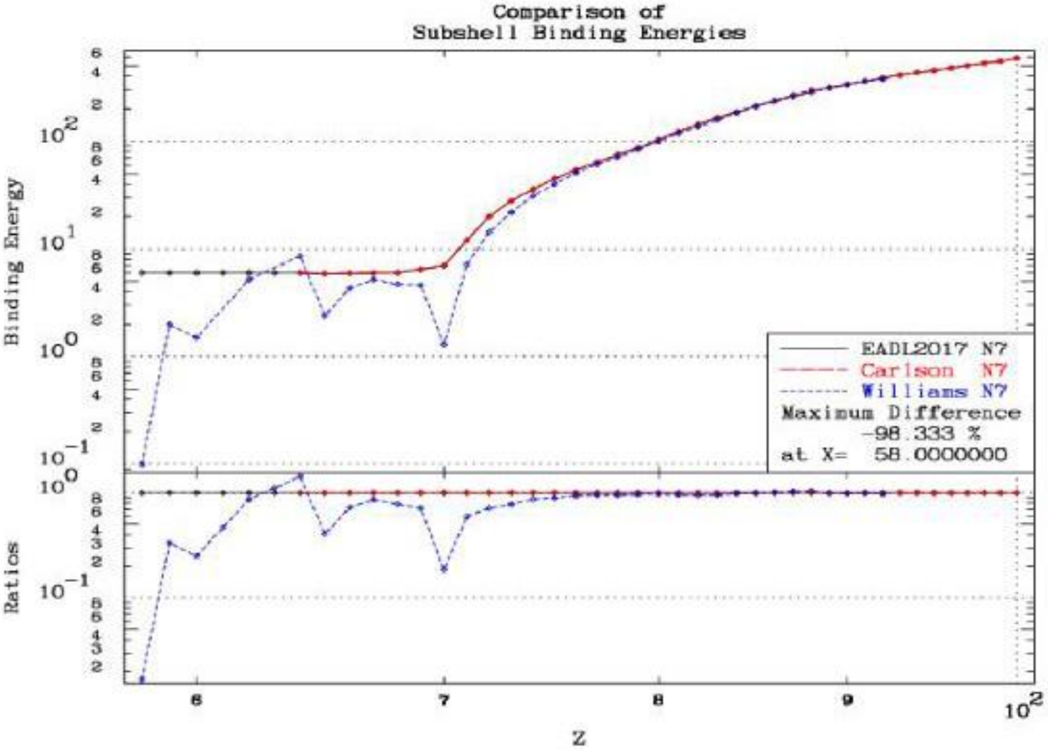
4.5.7. N4 and N5 Edges



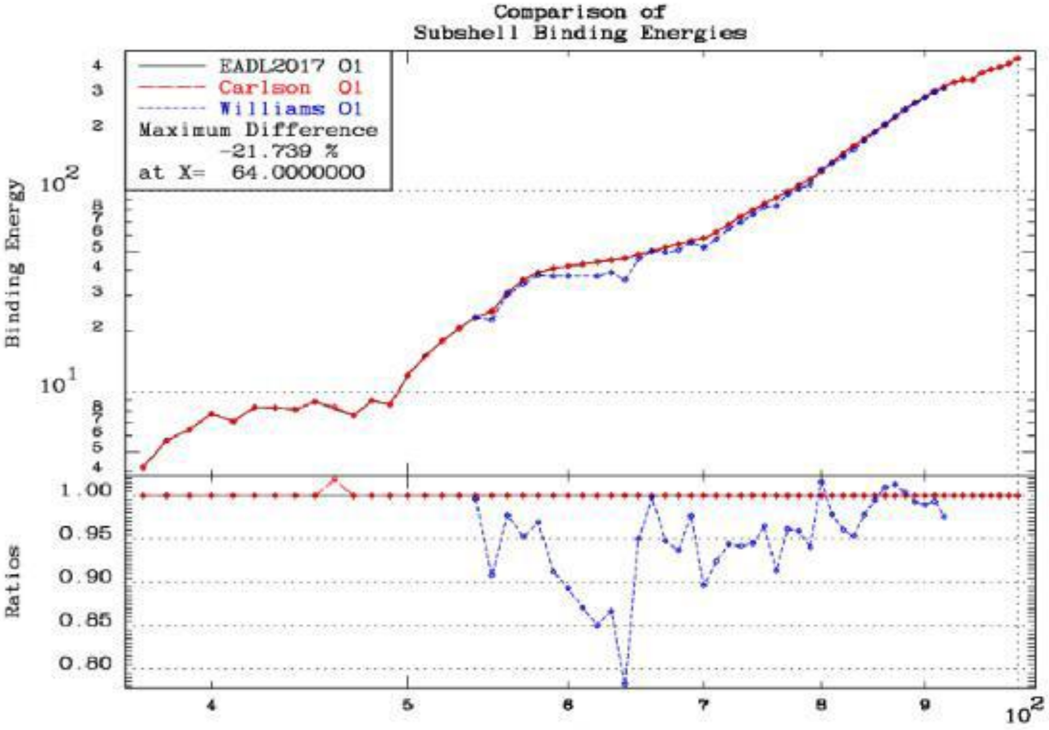


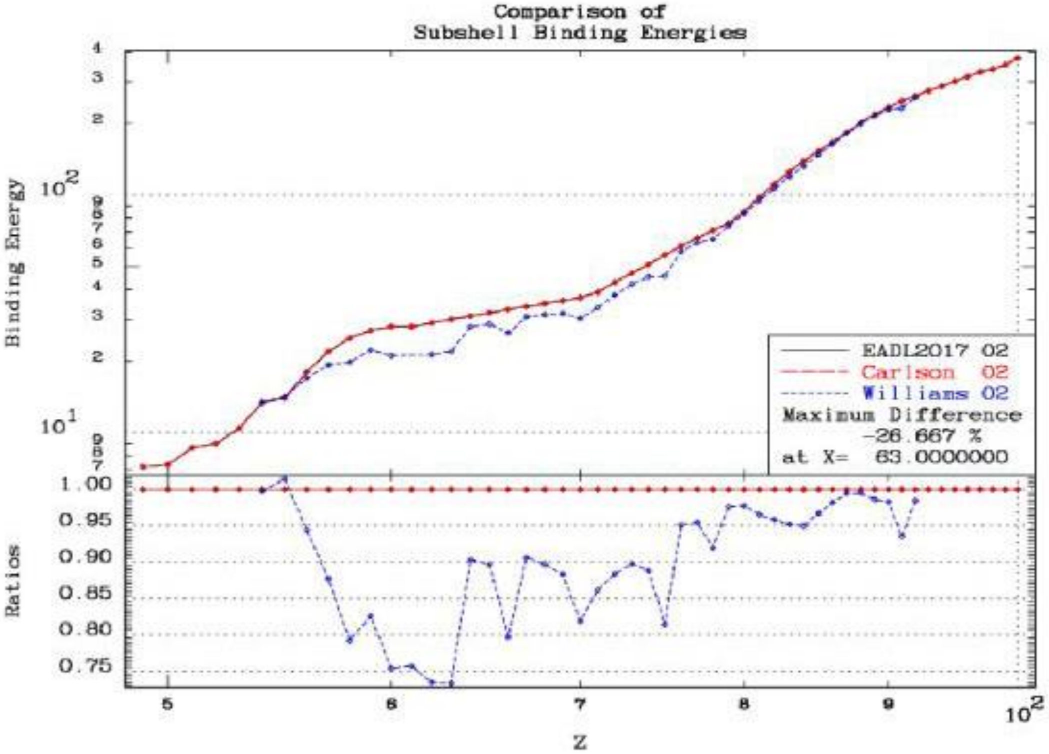
4.5.8. N6 and N7 Edges



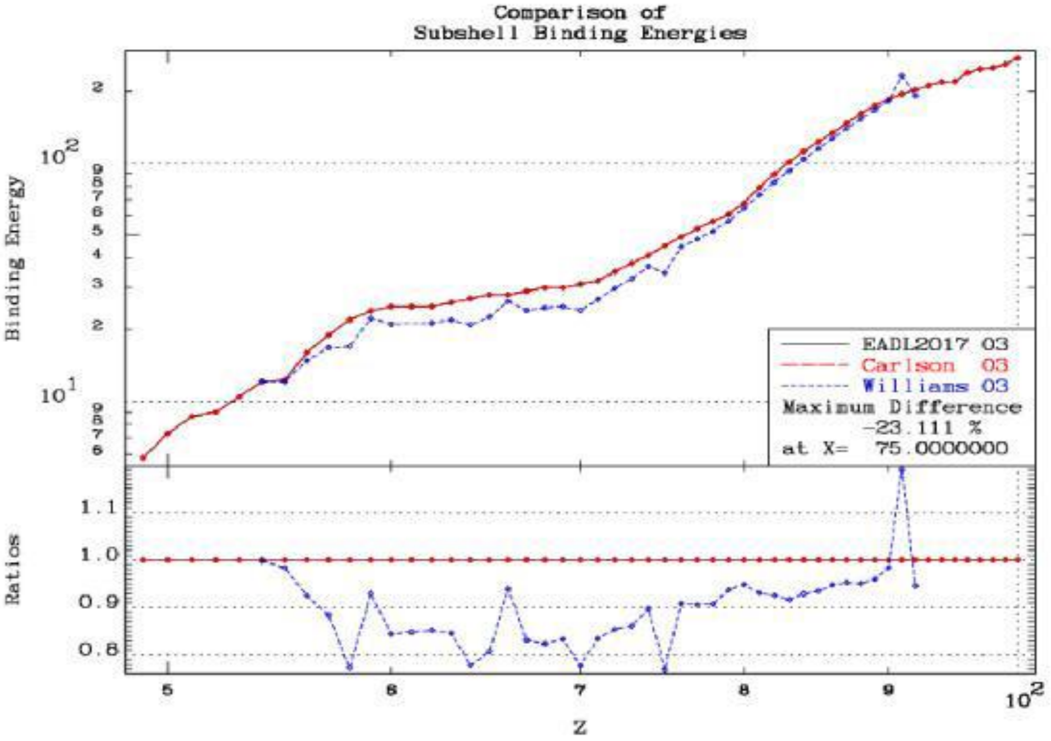


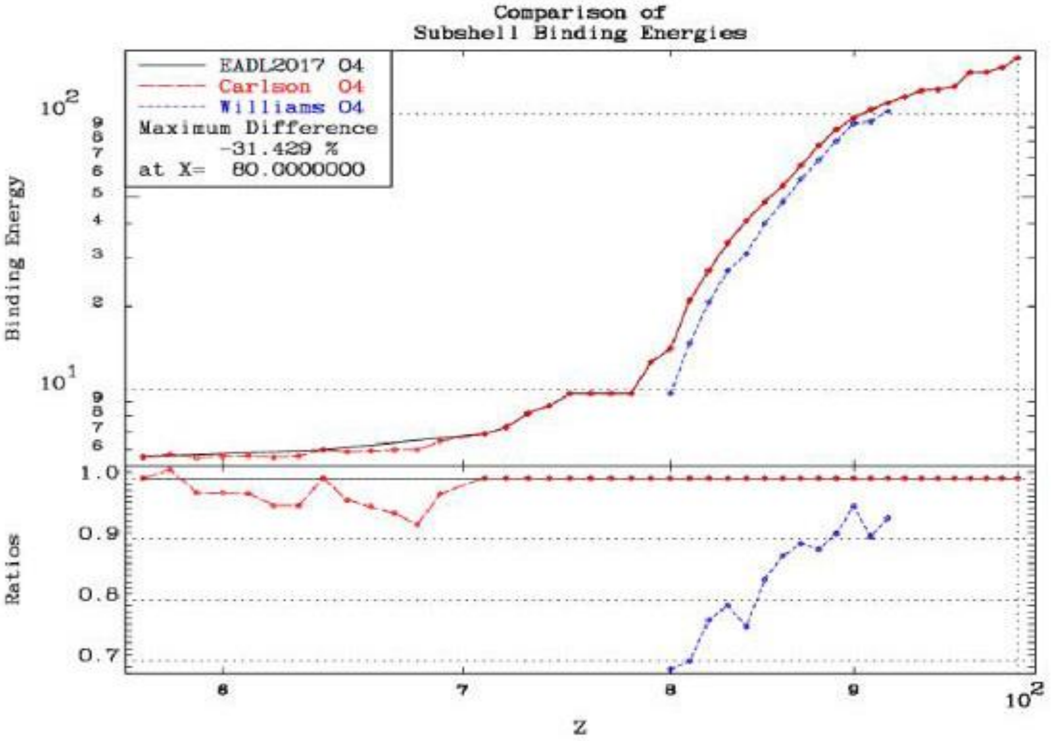
4.5.9. O1 and O2 Edges



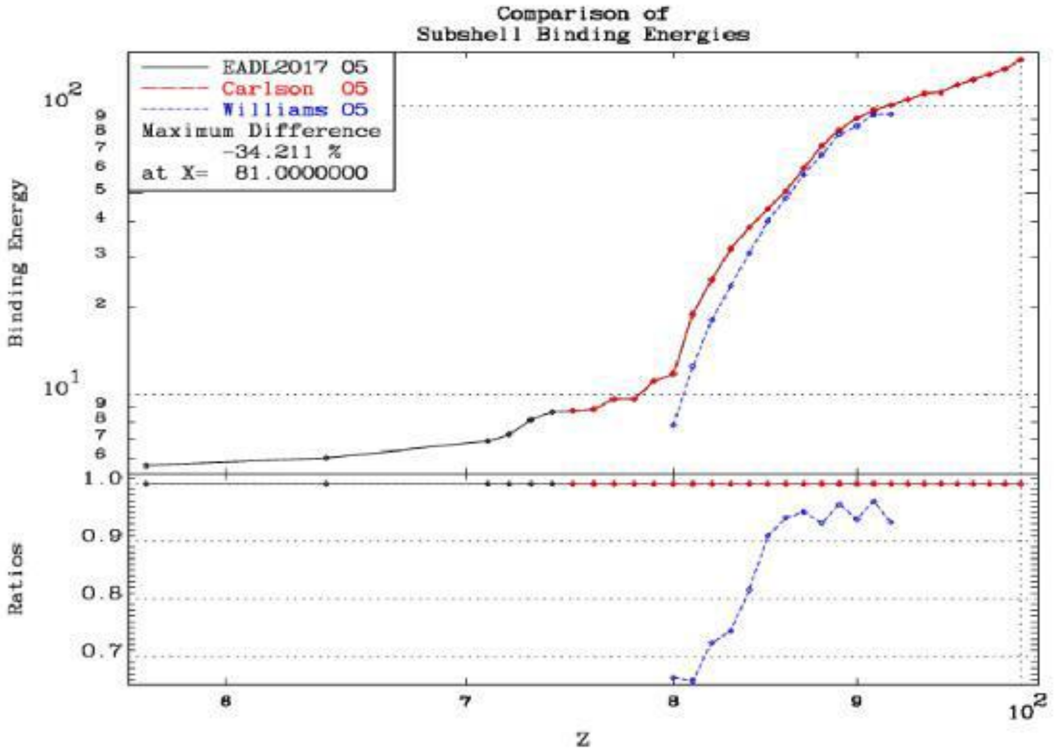


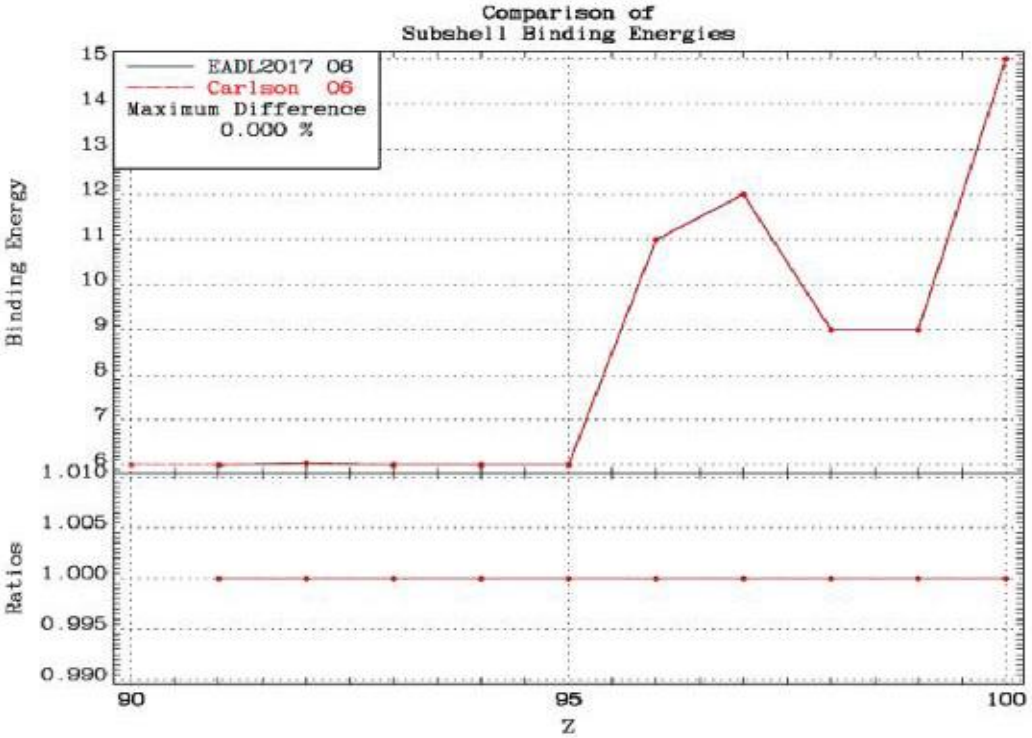
4.5.10. O3 and O4 Edges



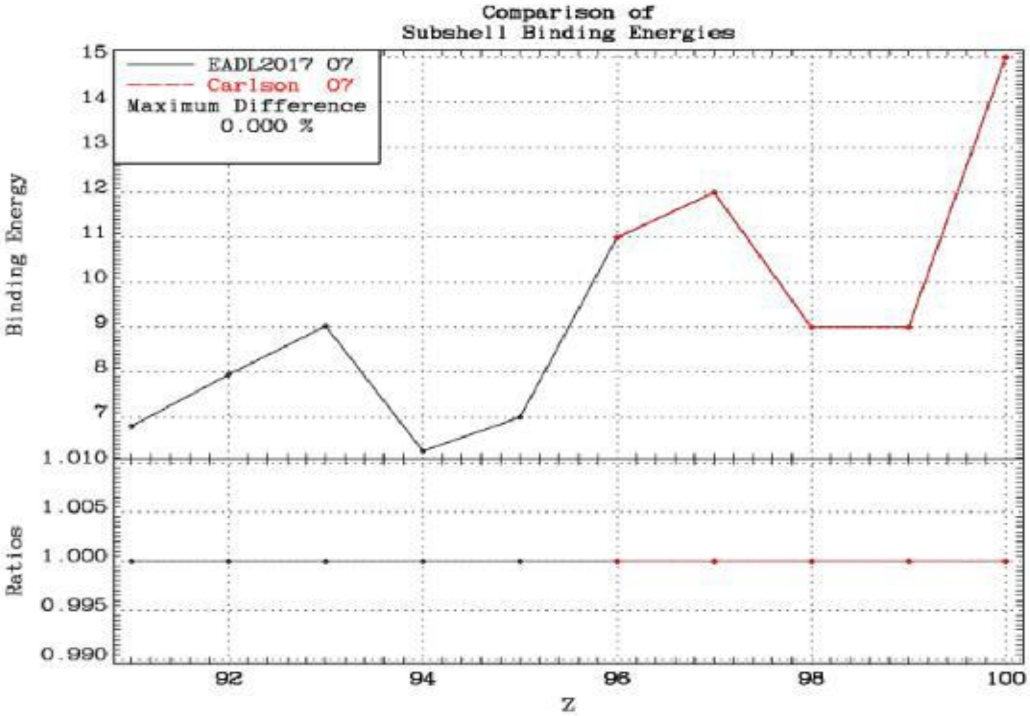


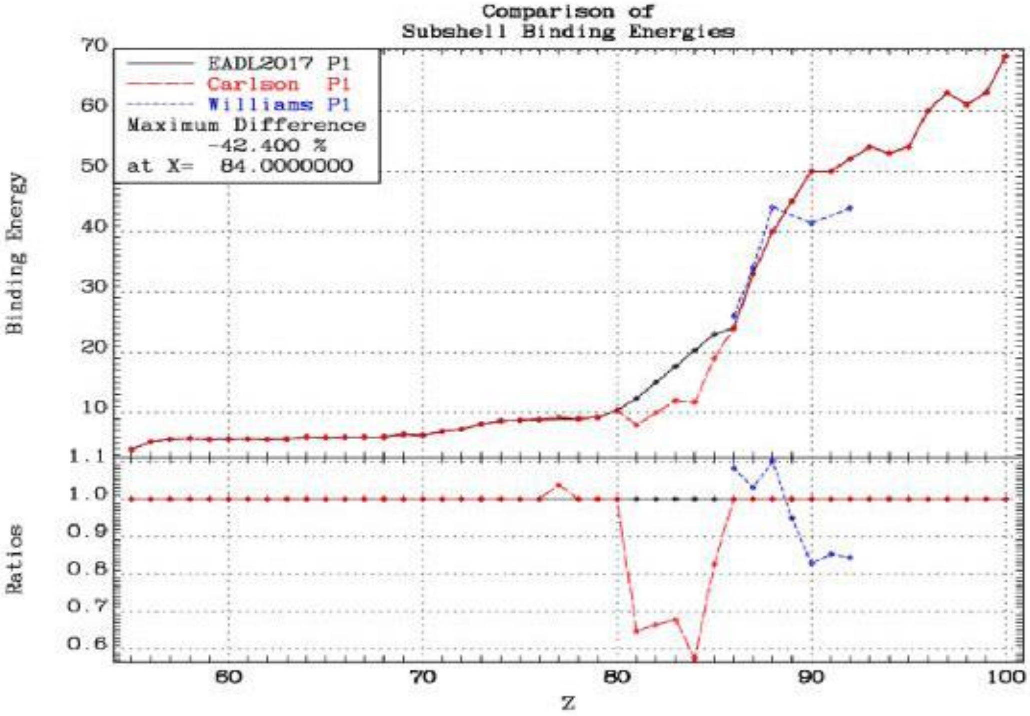
4.5.11. O5 and O6 Edges



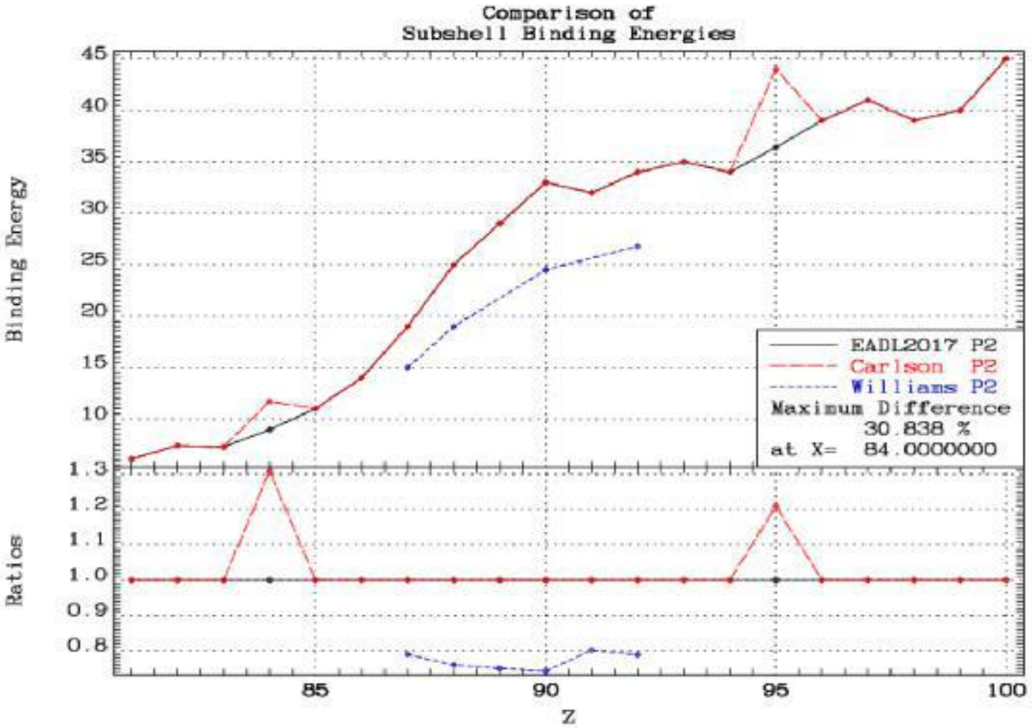


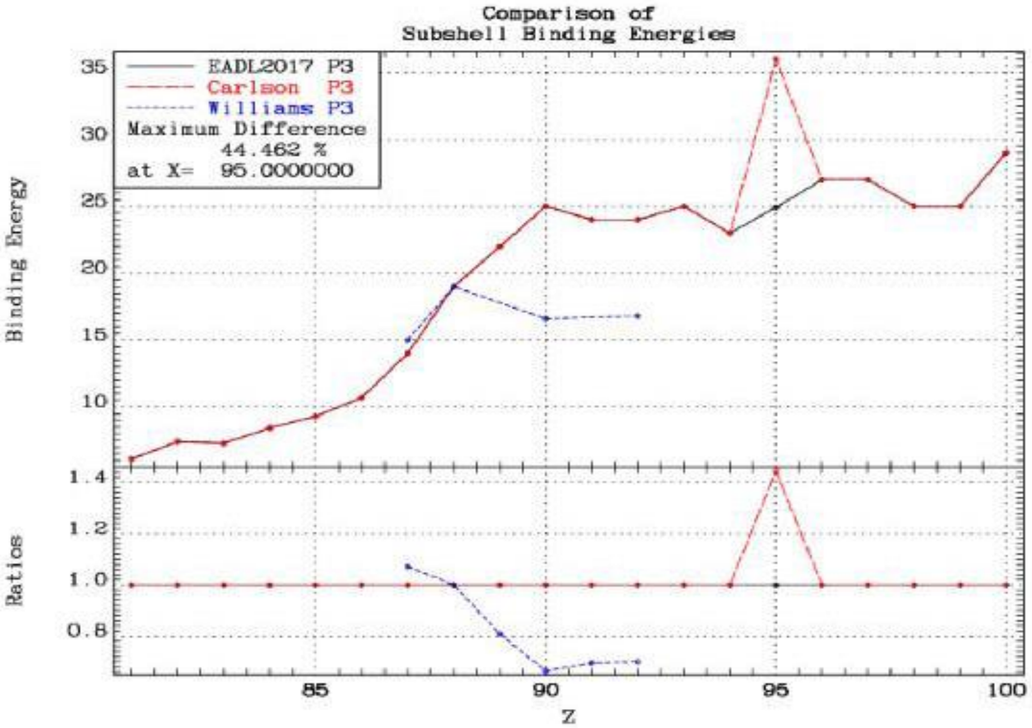
4.5.12. O7 and P1 Edges



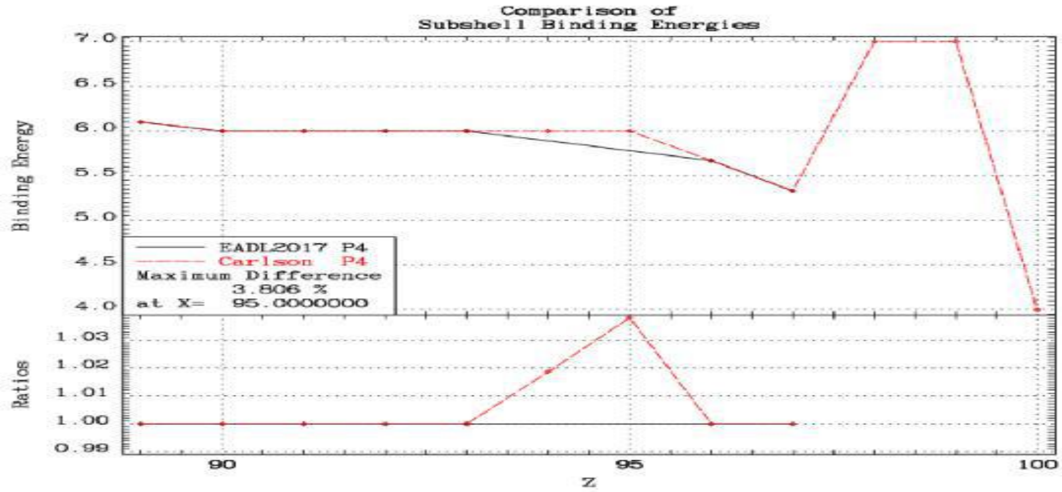


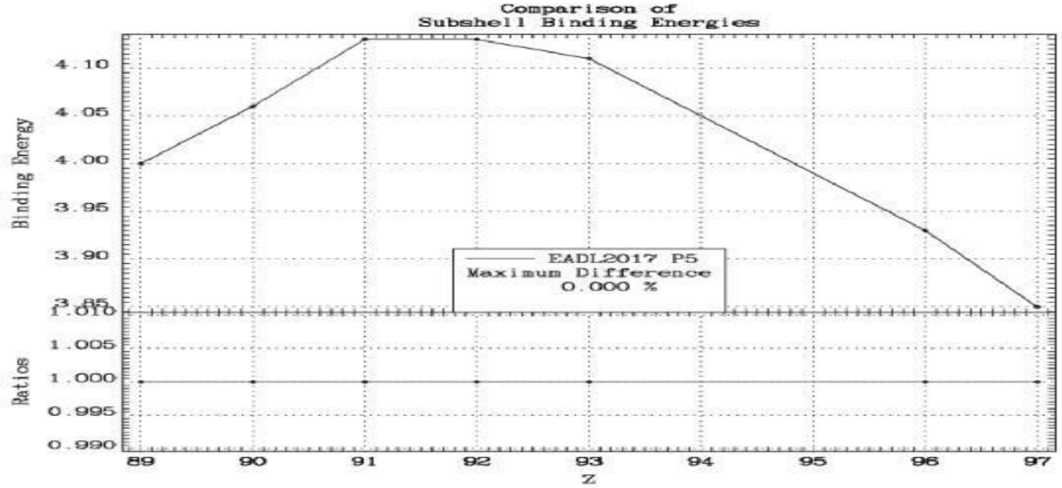
4.5.13. P2 and P3 Edges

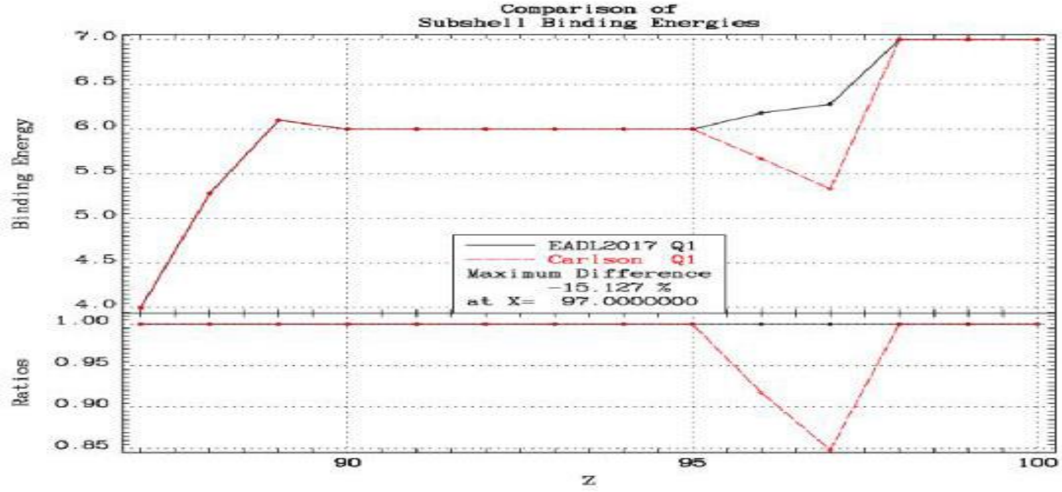




4.5.14. P4, P5 and Q1 Edges





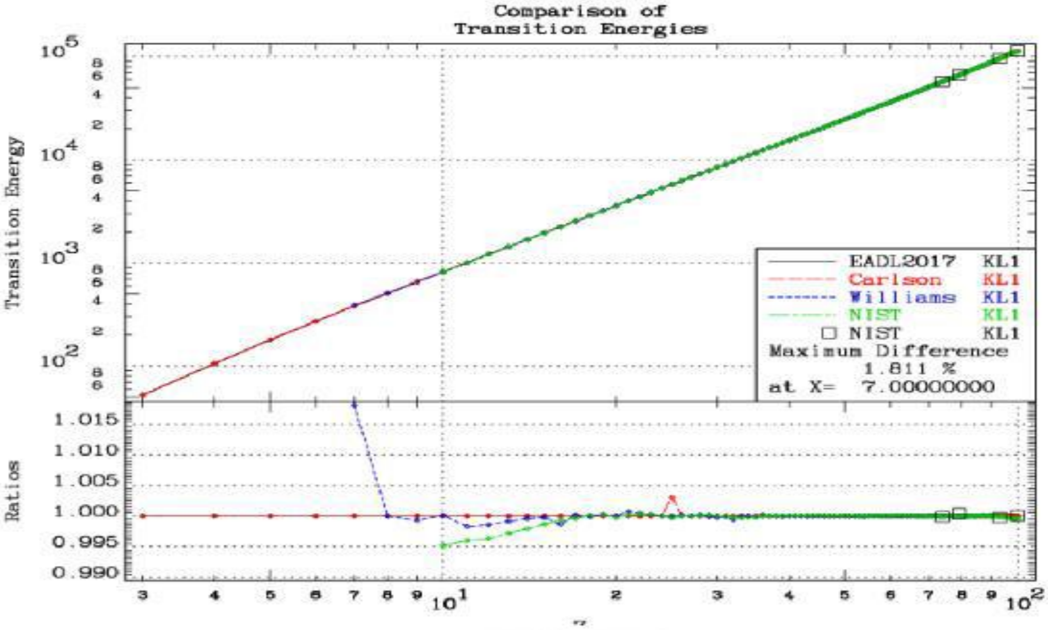


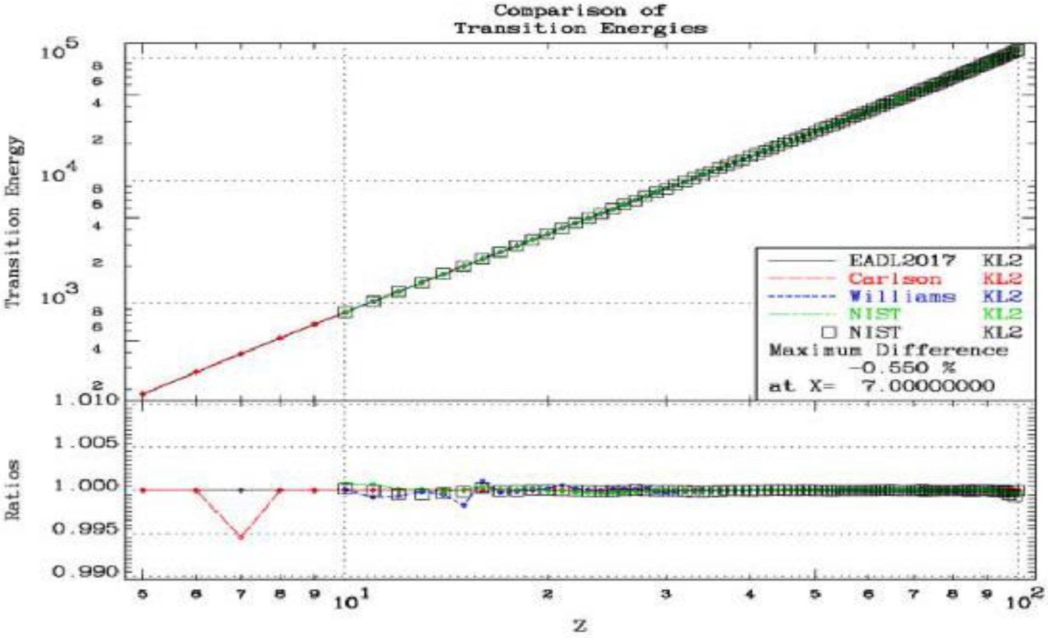
5. Transition Energies

5.1. Details

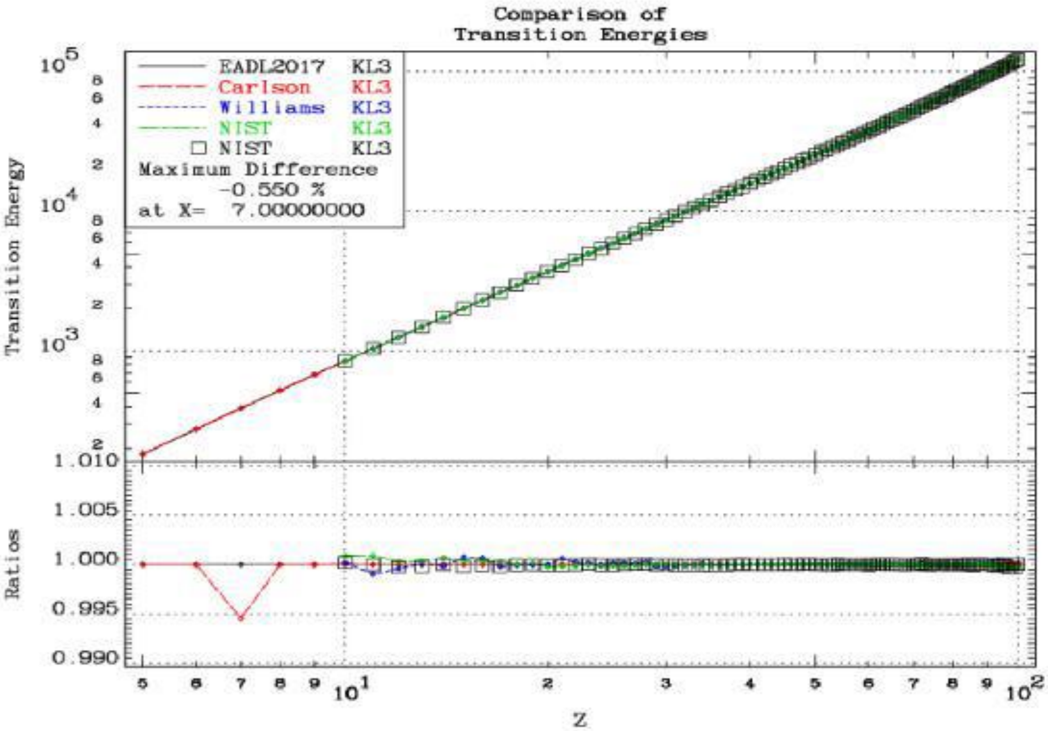
What we refer to as the NIST data is a collection of measured and theoretical results from many sources; see ref. [7]. Here the measured results are shown as squares at discrete values of Z. The theoretical data are shown as continuous curves.

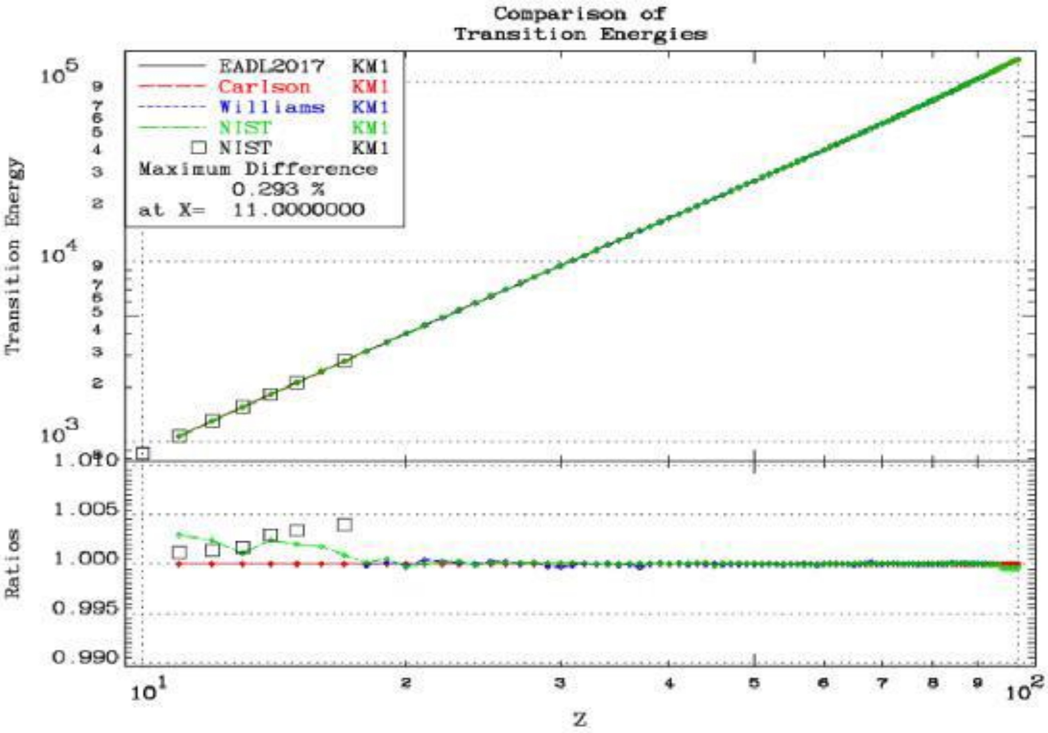
5.1.1. KL1 and KL2 Transitions



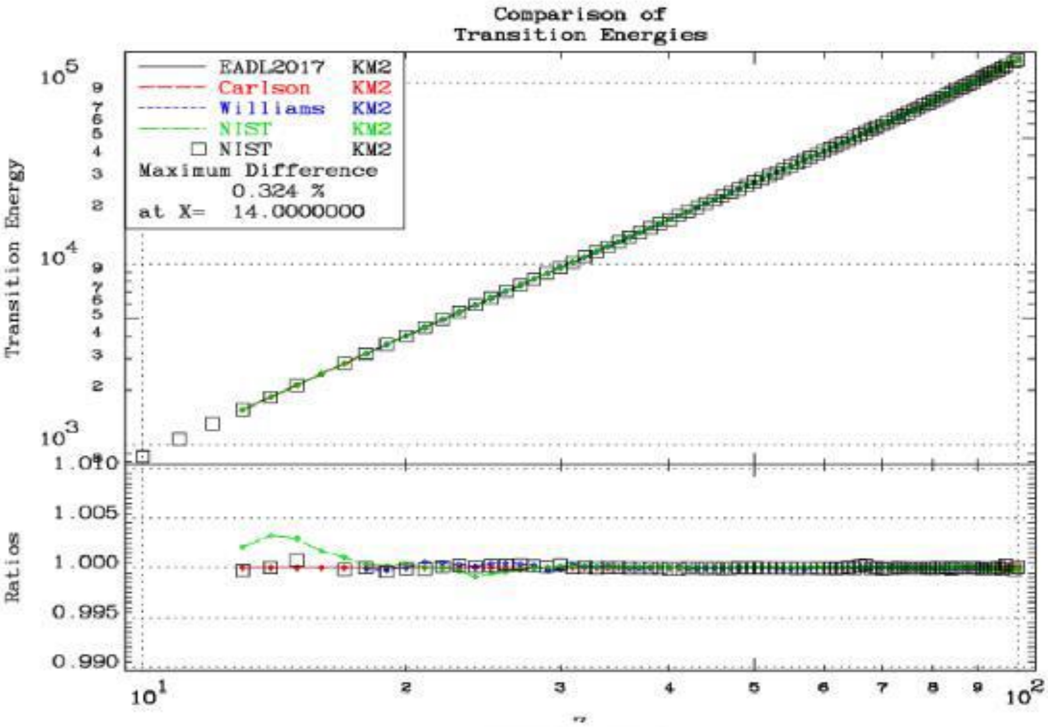


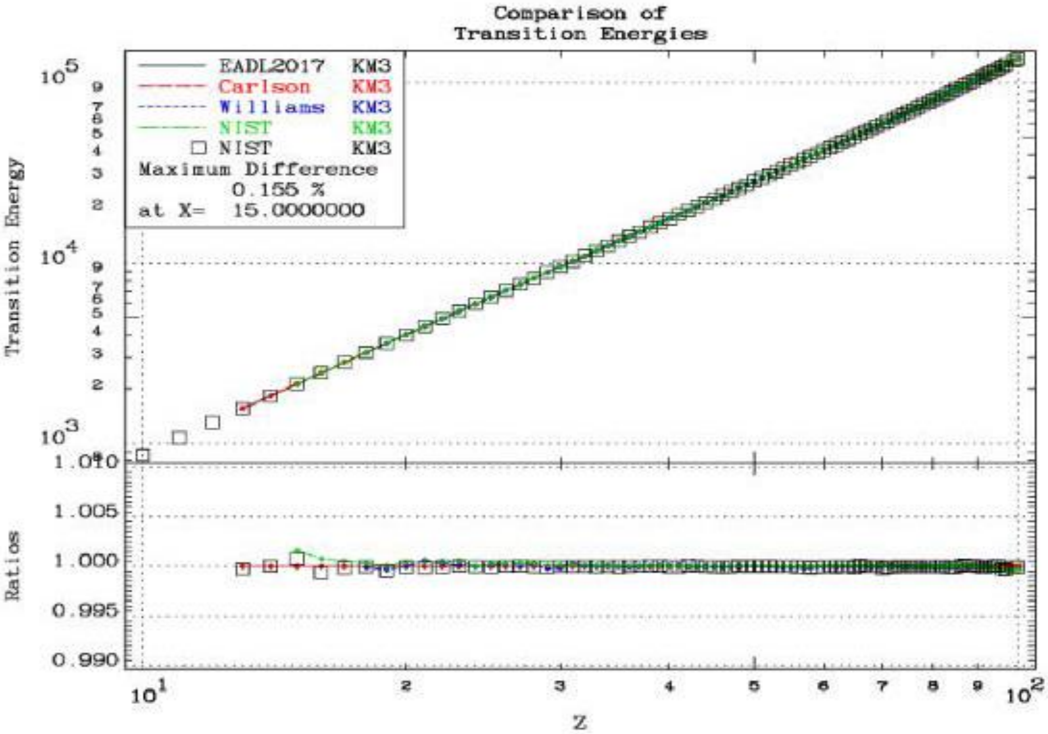
5.1.2. KL3 and KM1 Transitions



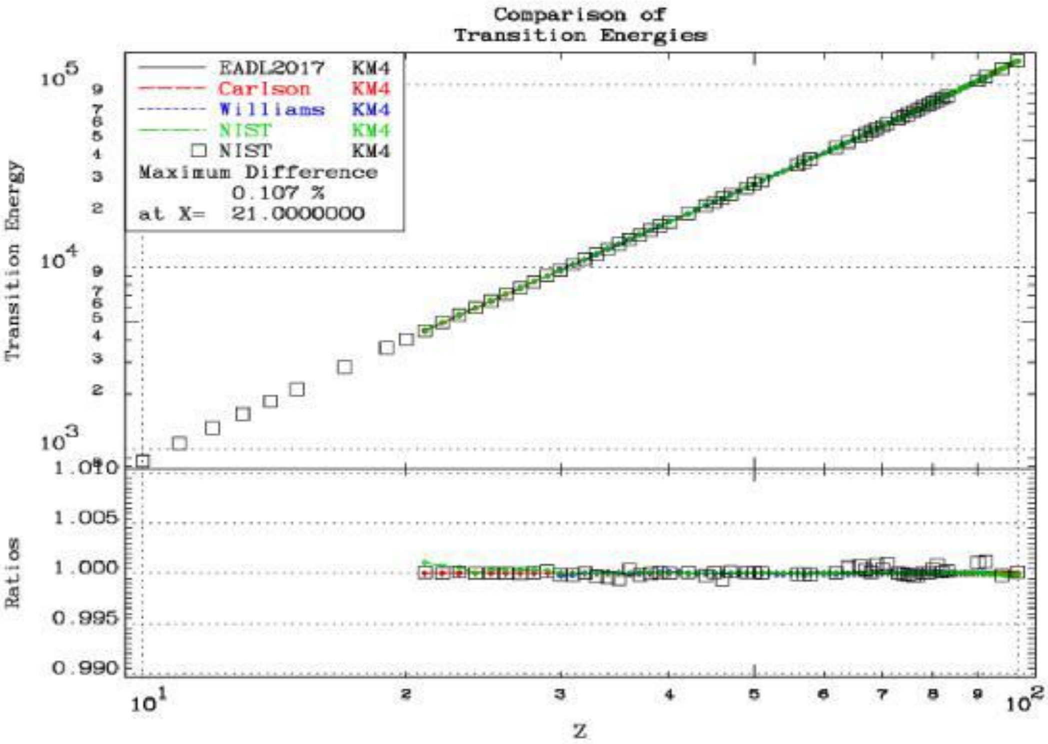


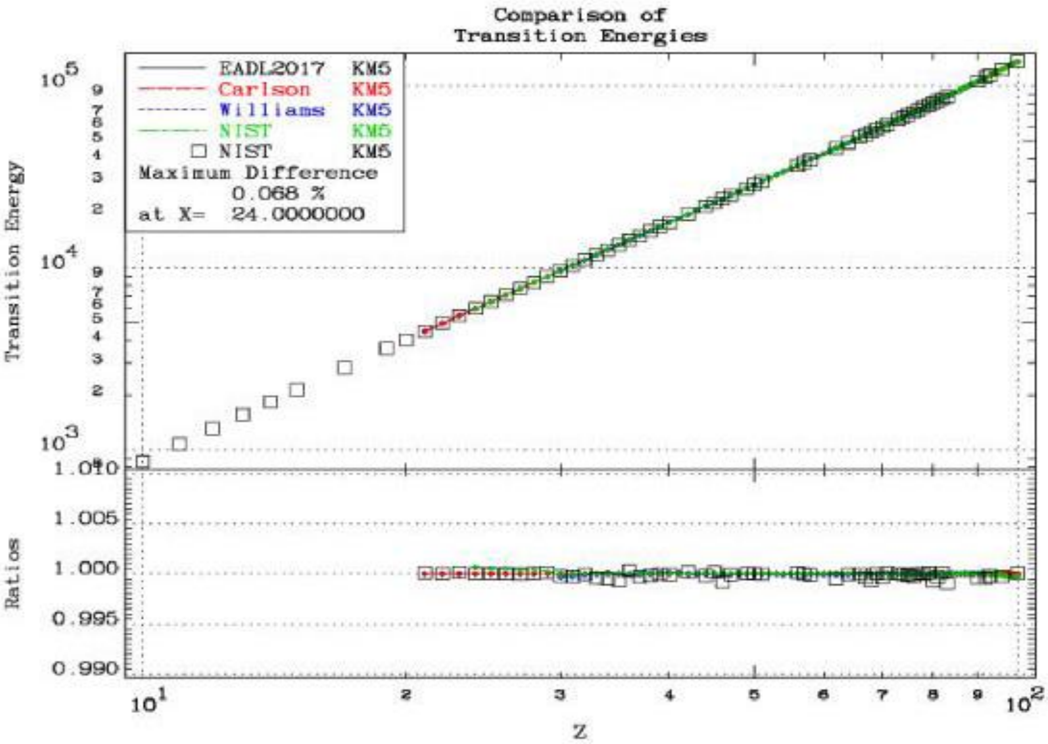
5.1.3. KM2 and KM3 Transitions



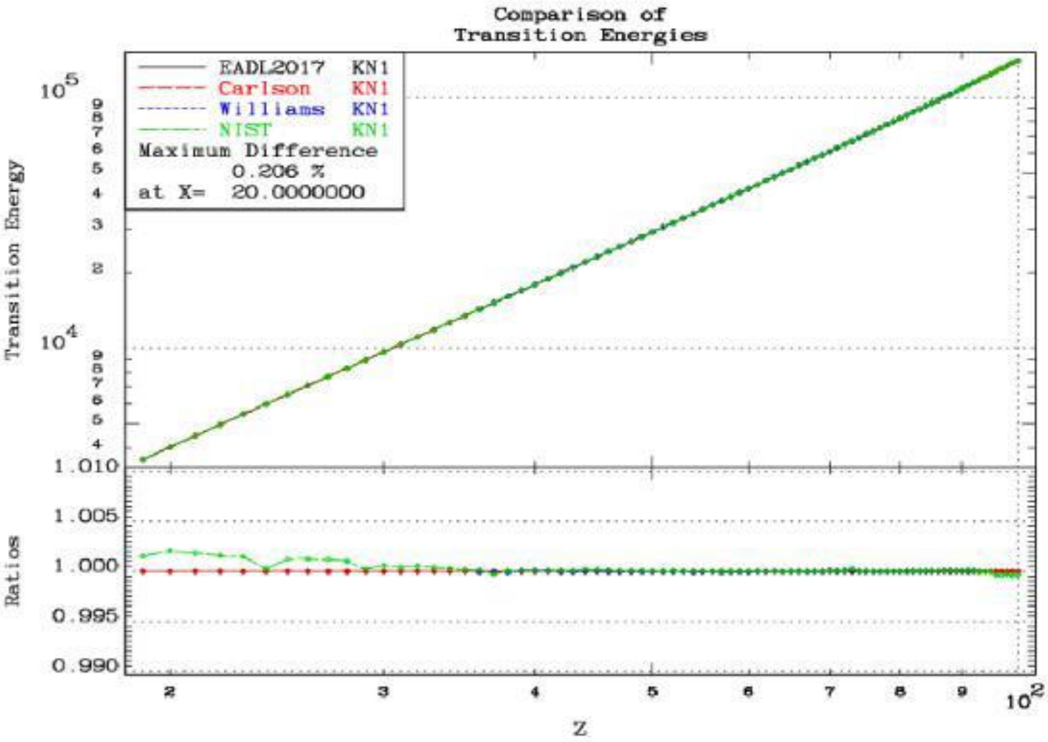


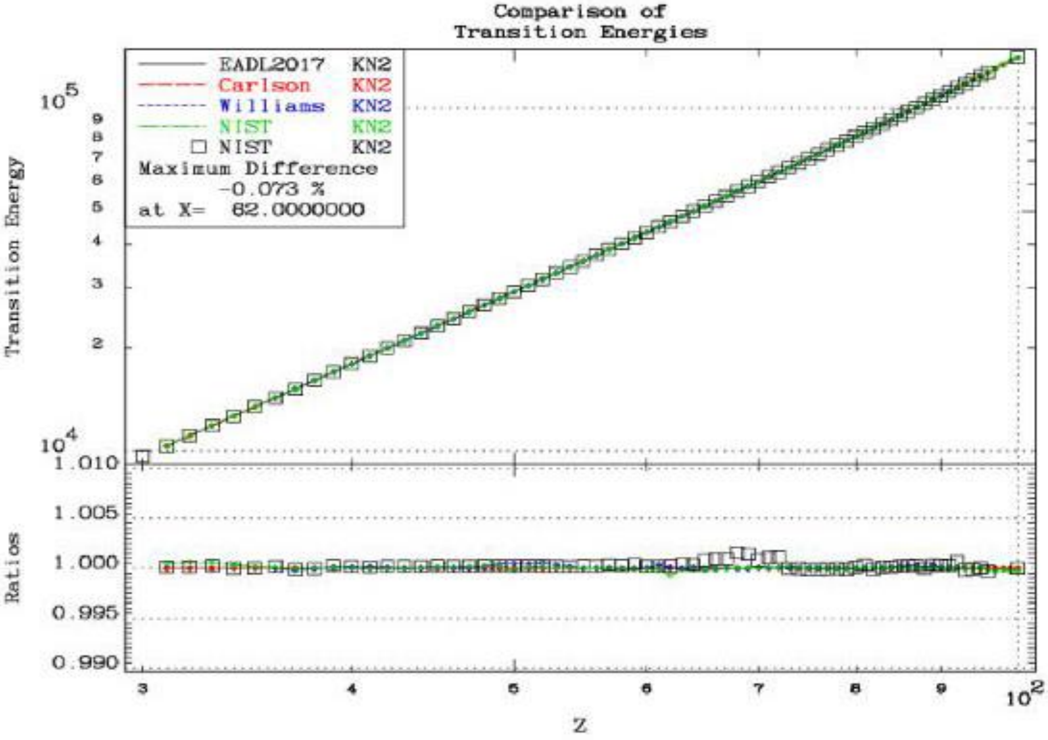
5.1.4. *KM4 and KM5 Transitions*



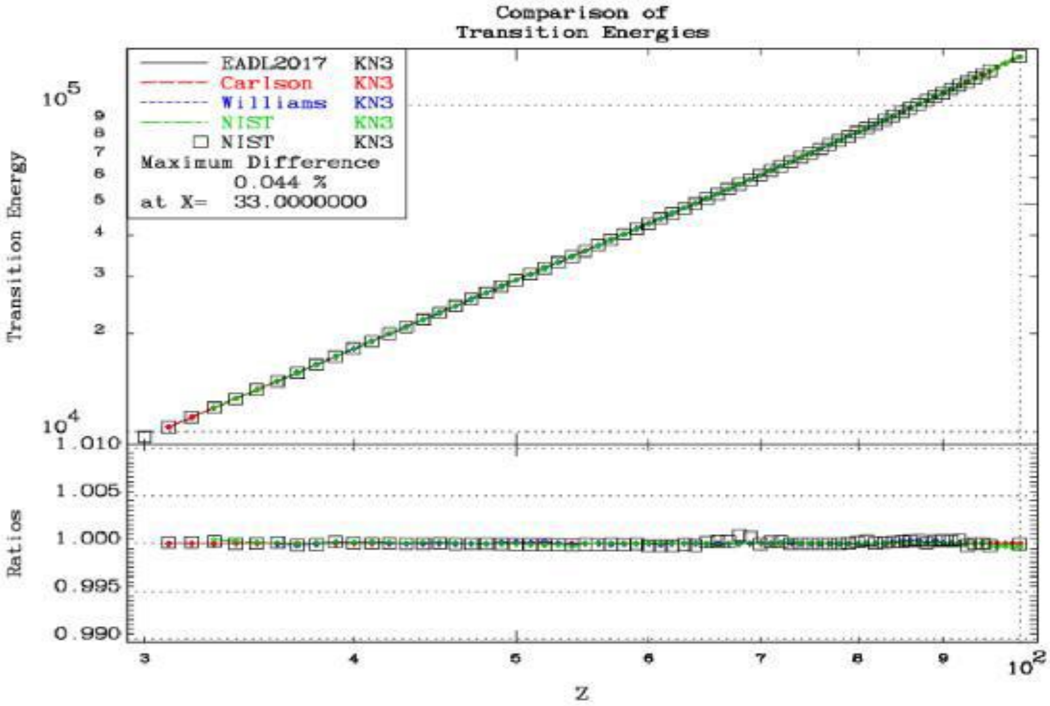


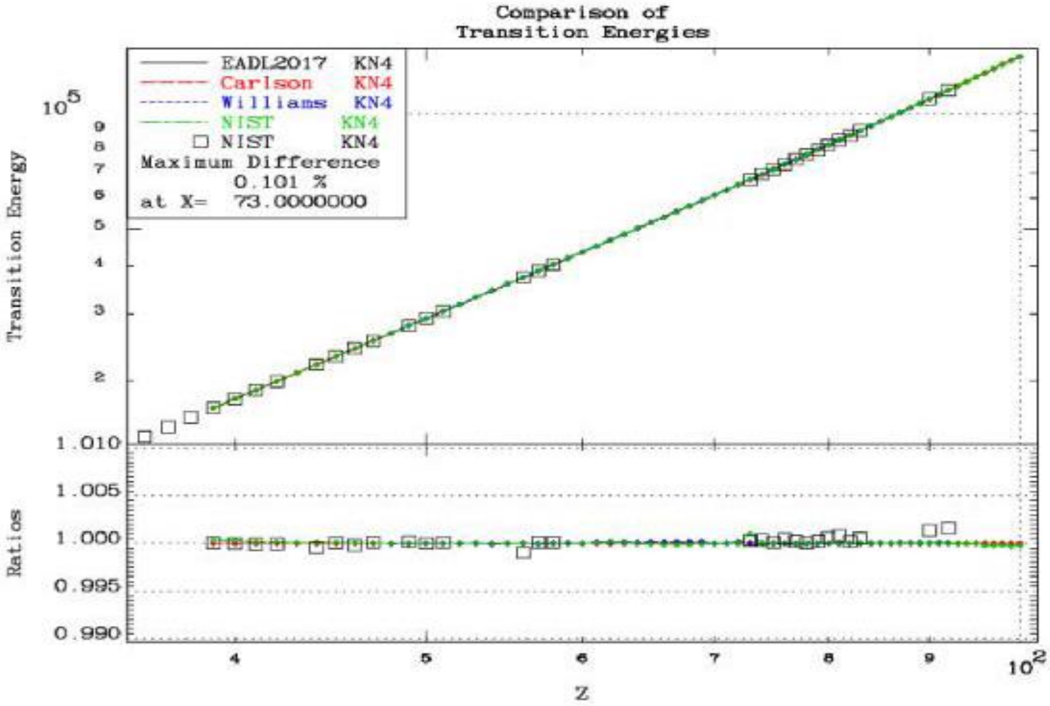
5.1.5. KN1 and KN2 Transitions



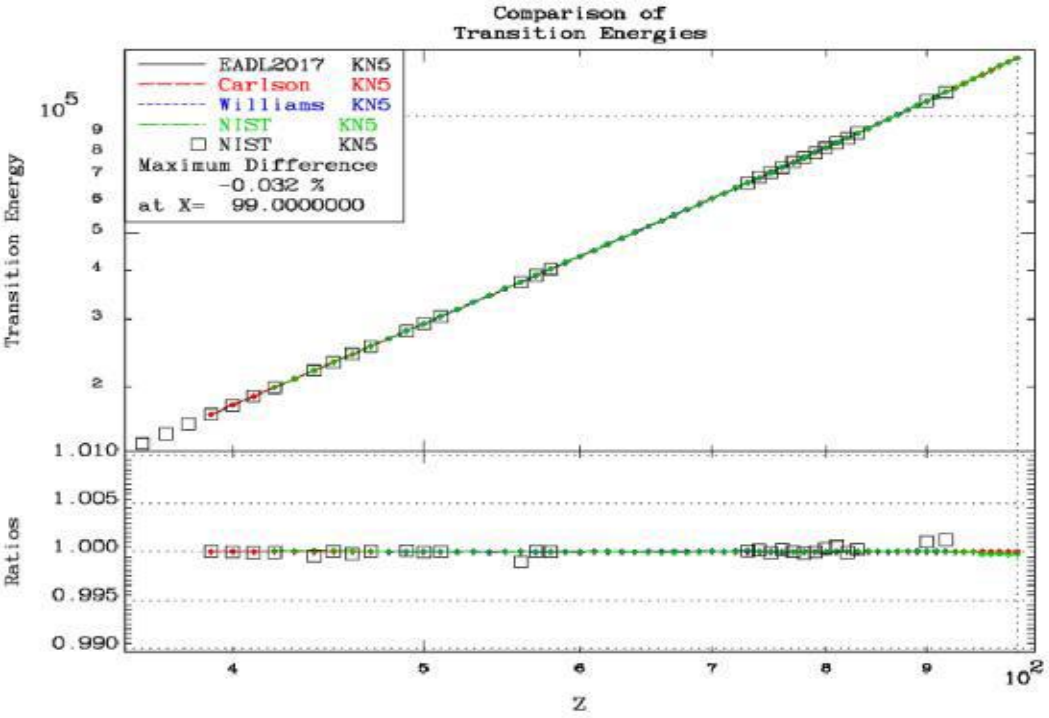


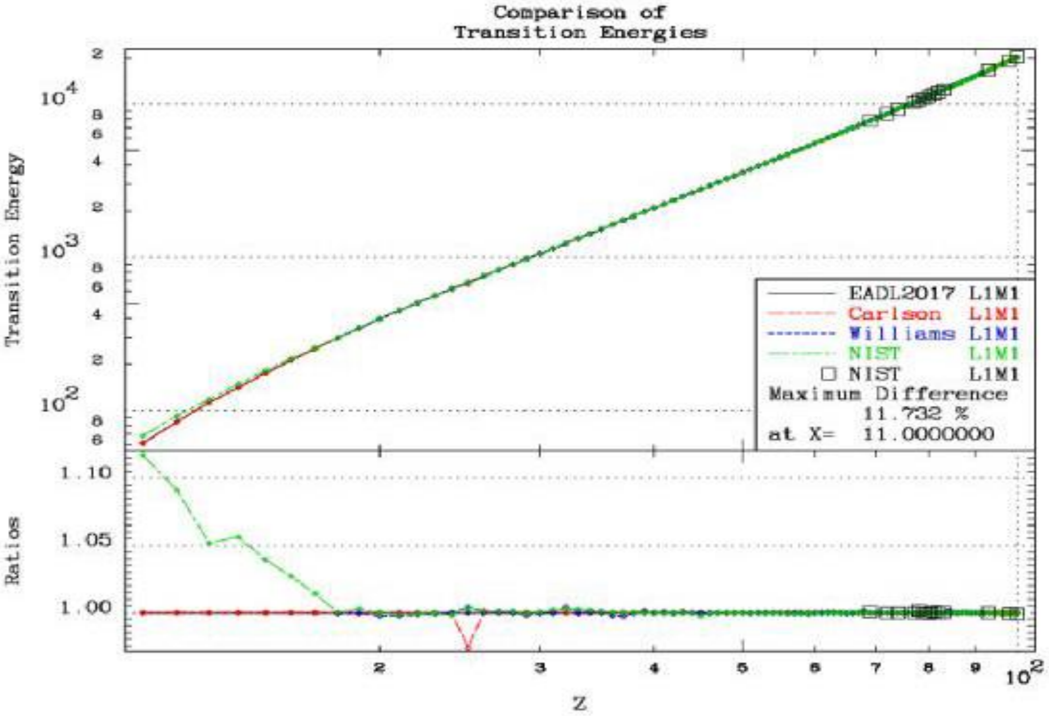
5.1.6. KN3 and KN4 Transitions



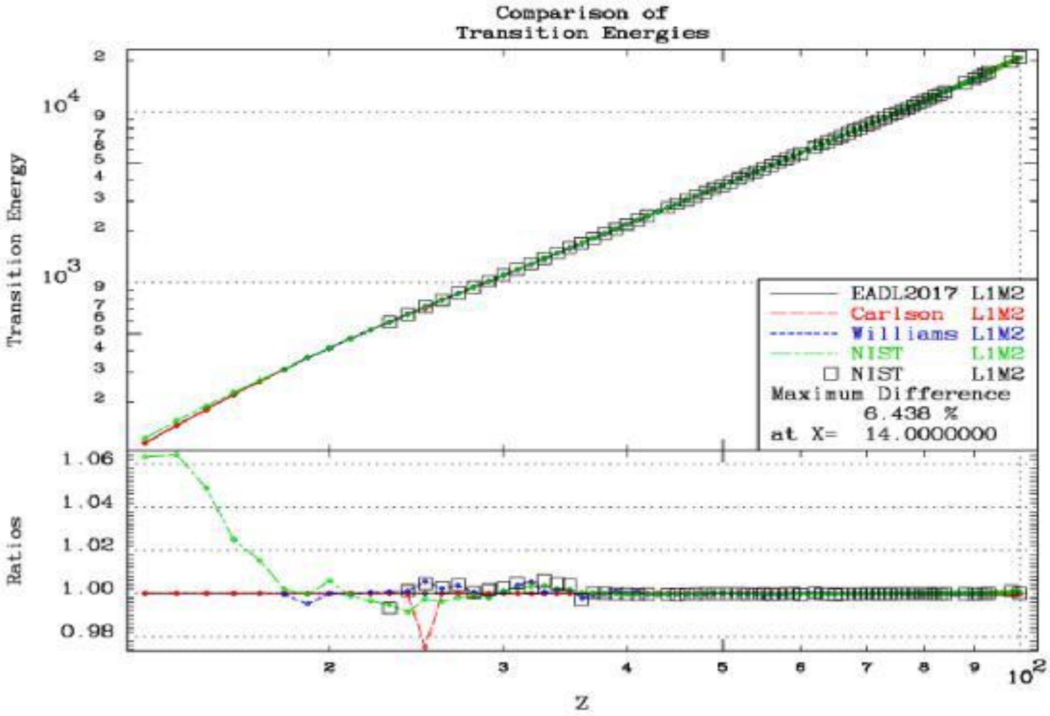


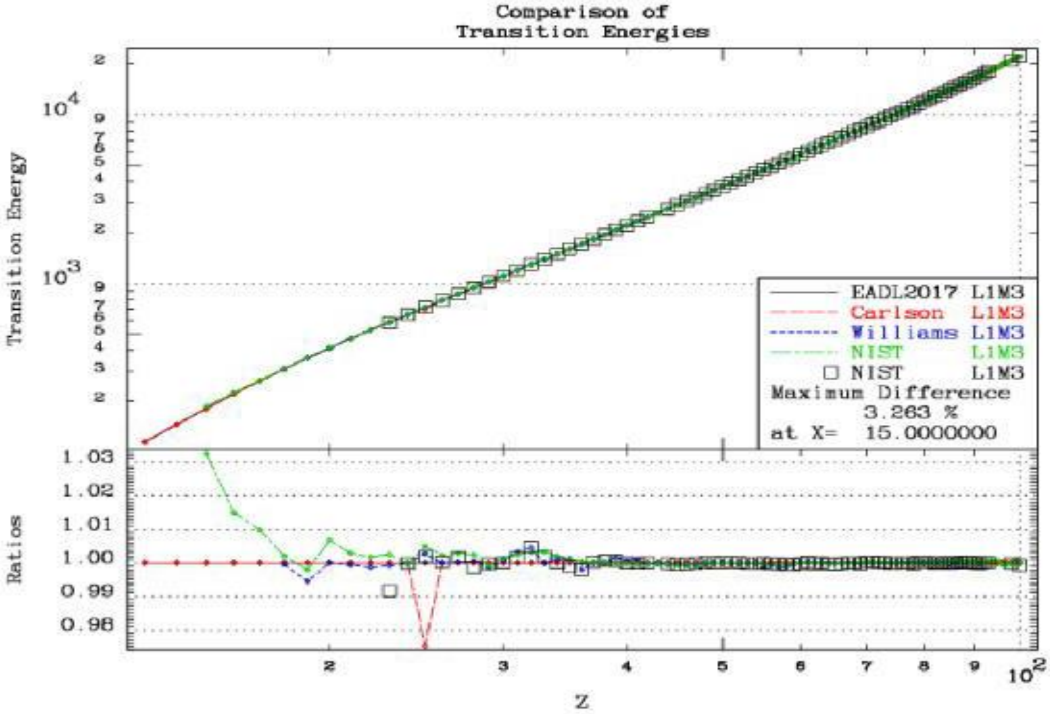
5.1.7. KN5 and L1M1 Transitions



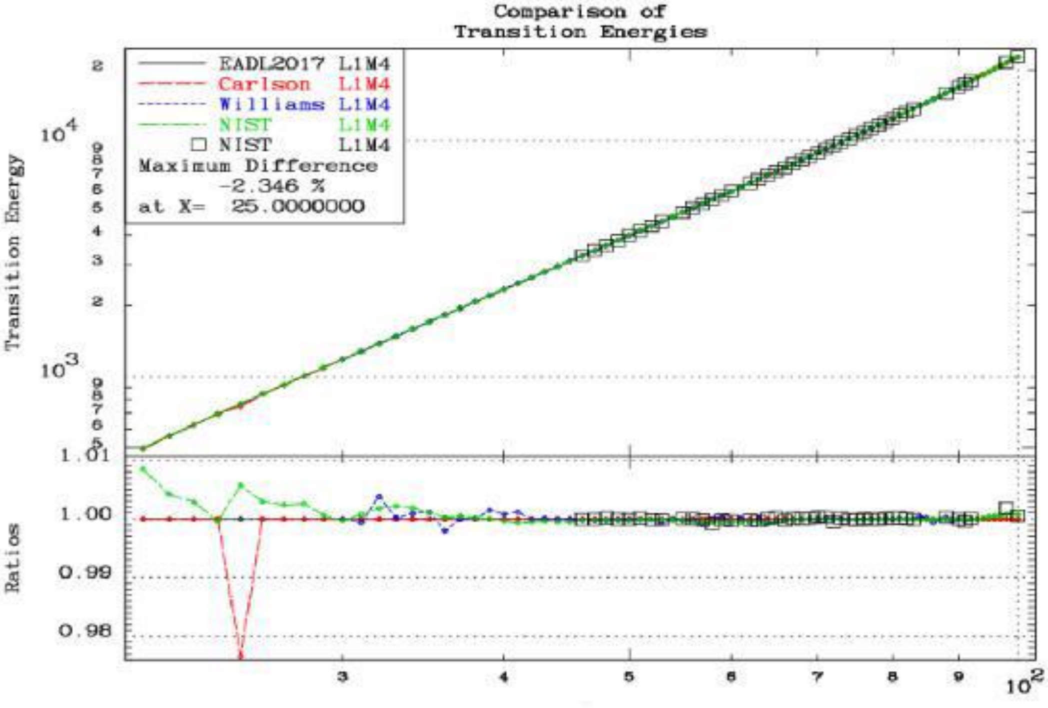


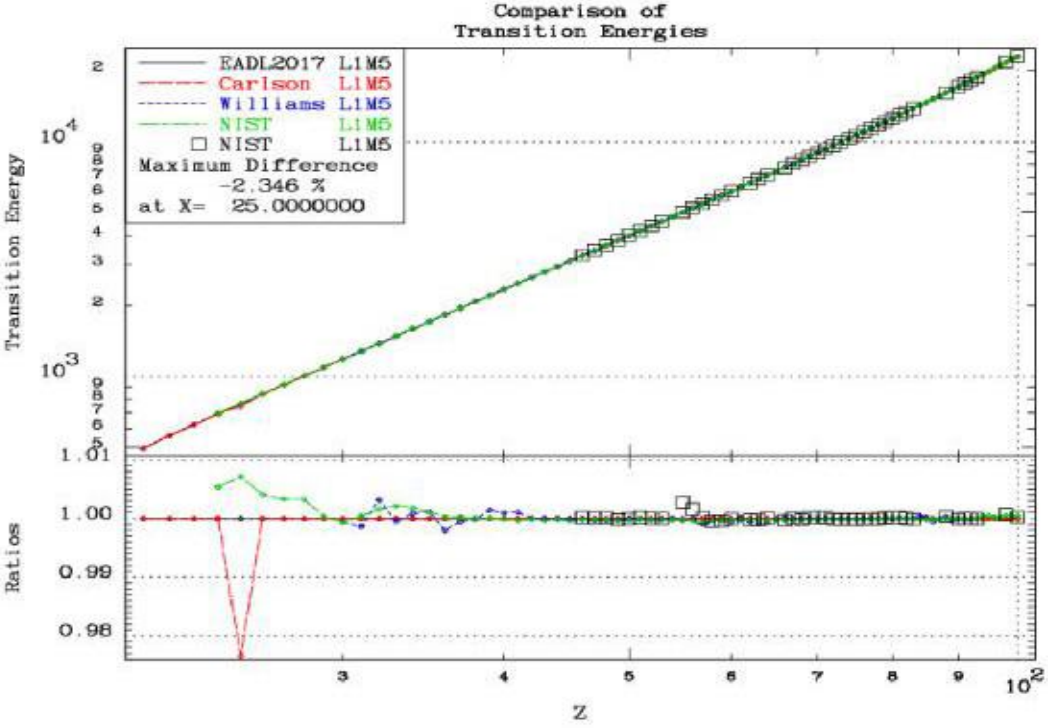
5.1.8. L1M2 and L1M3 Transitions



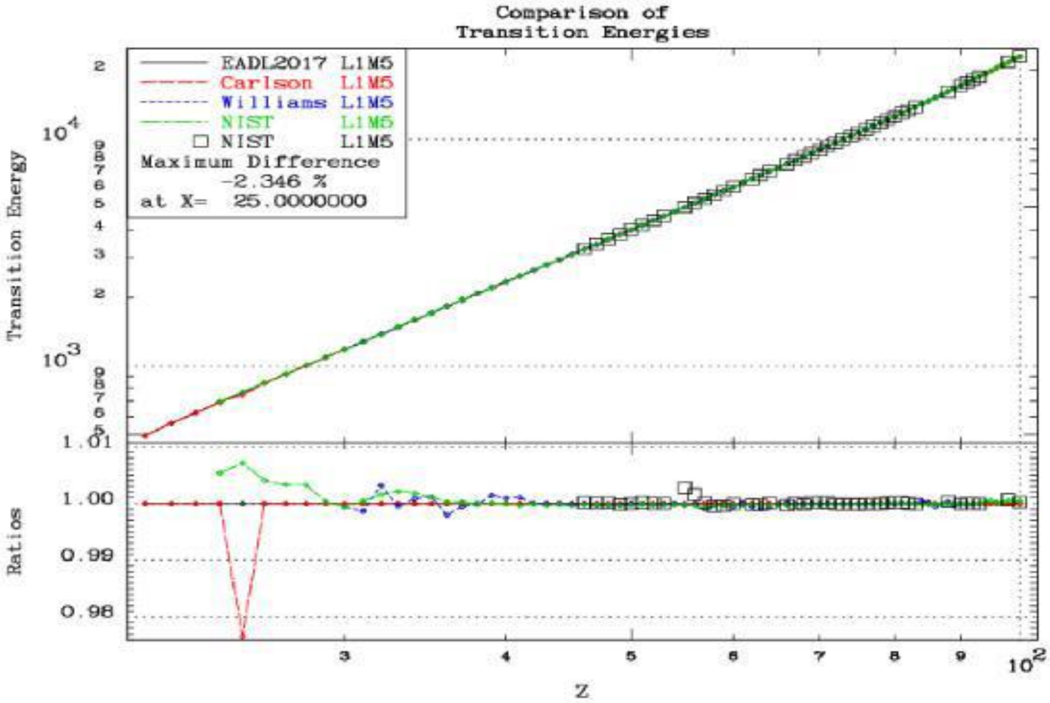


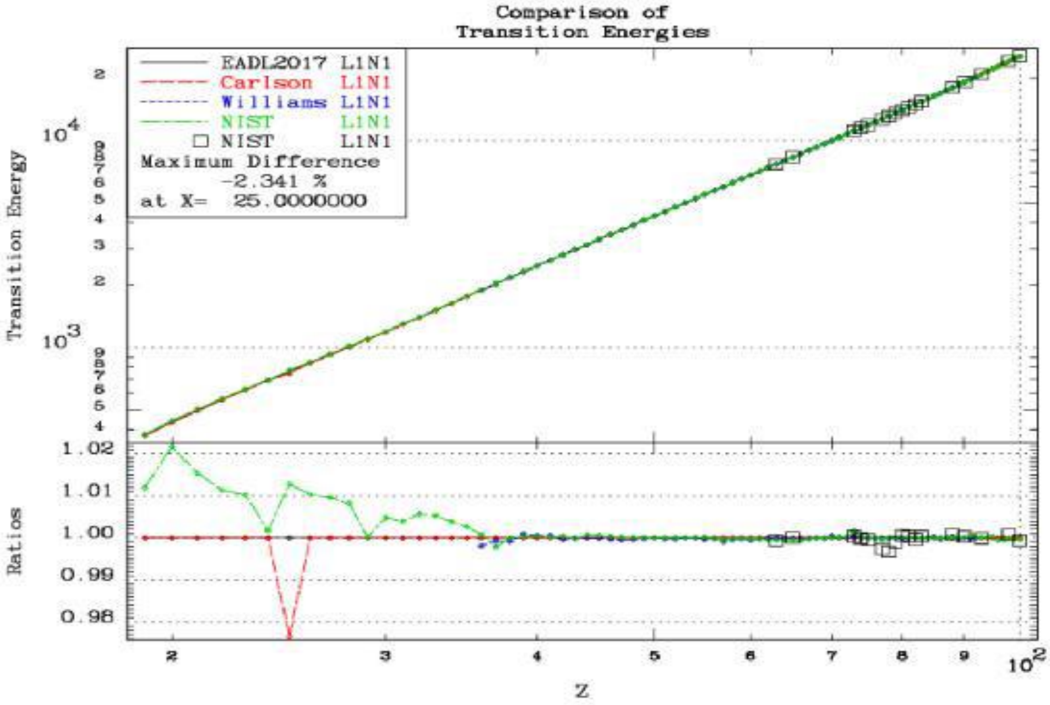
5.1.9. *L1M4 and L1M5 Transitions*



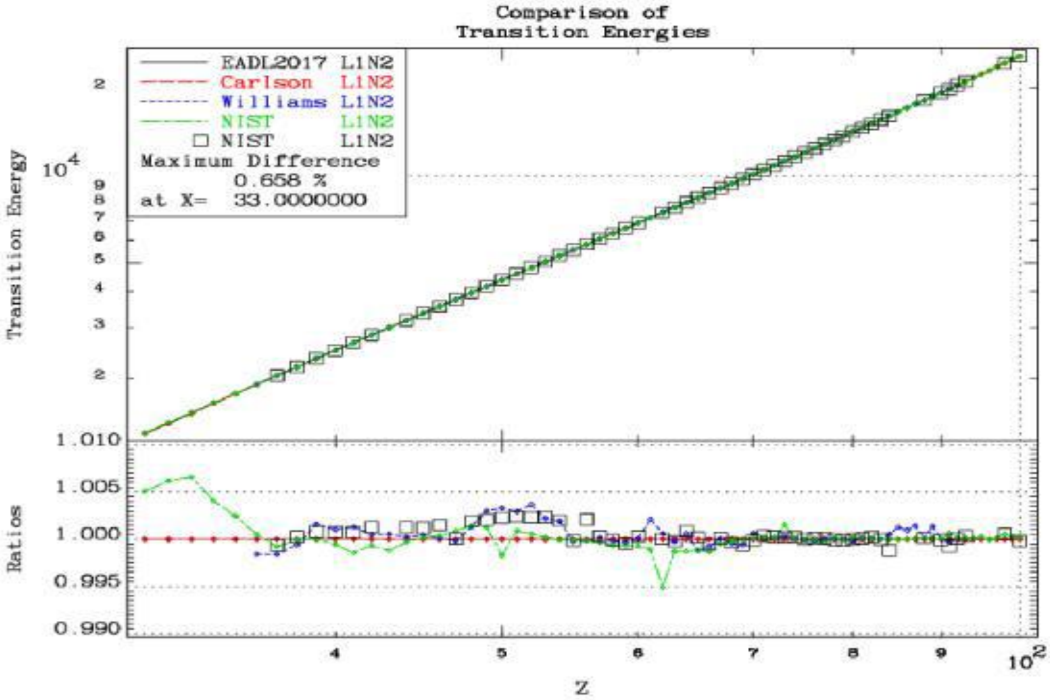


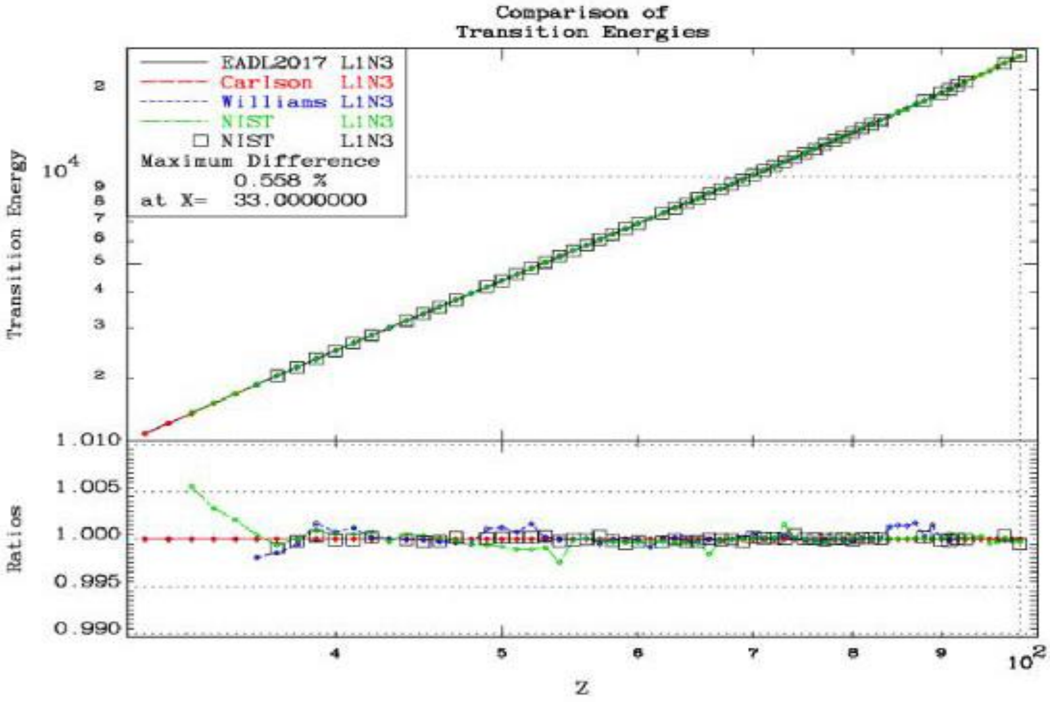
5.1.10. L1M5 (repeat) and L1N1 Transitions



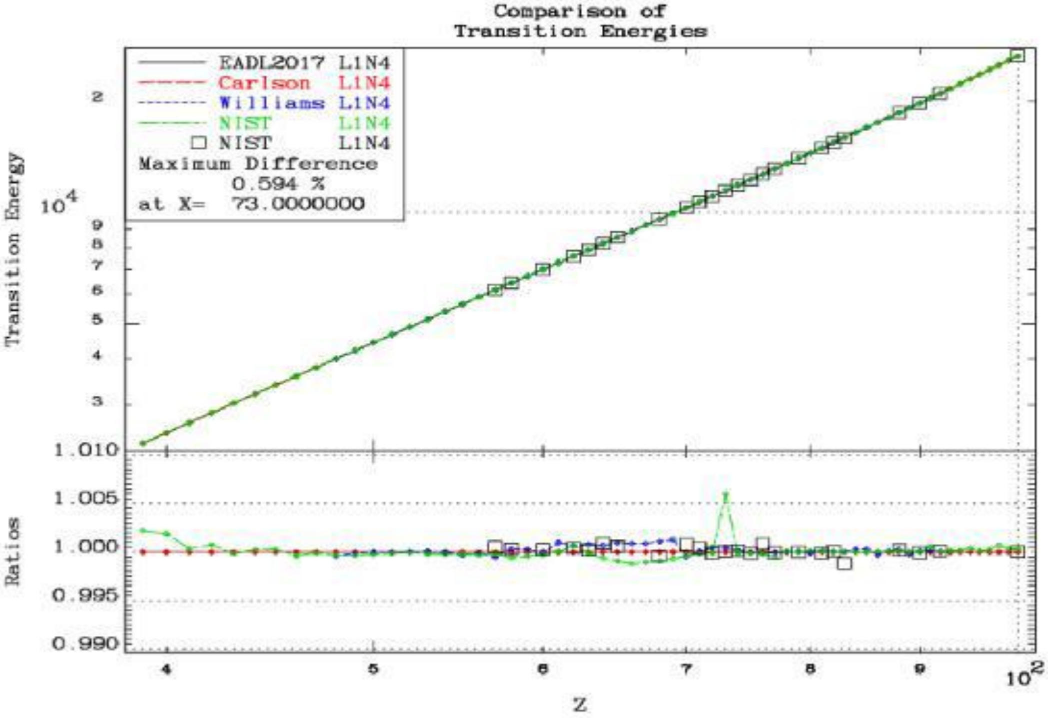


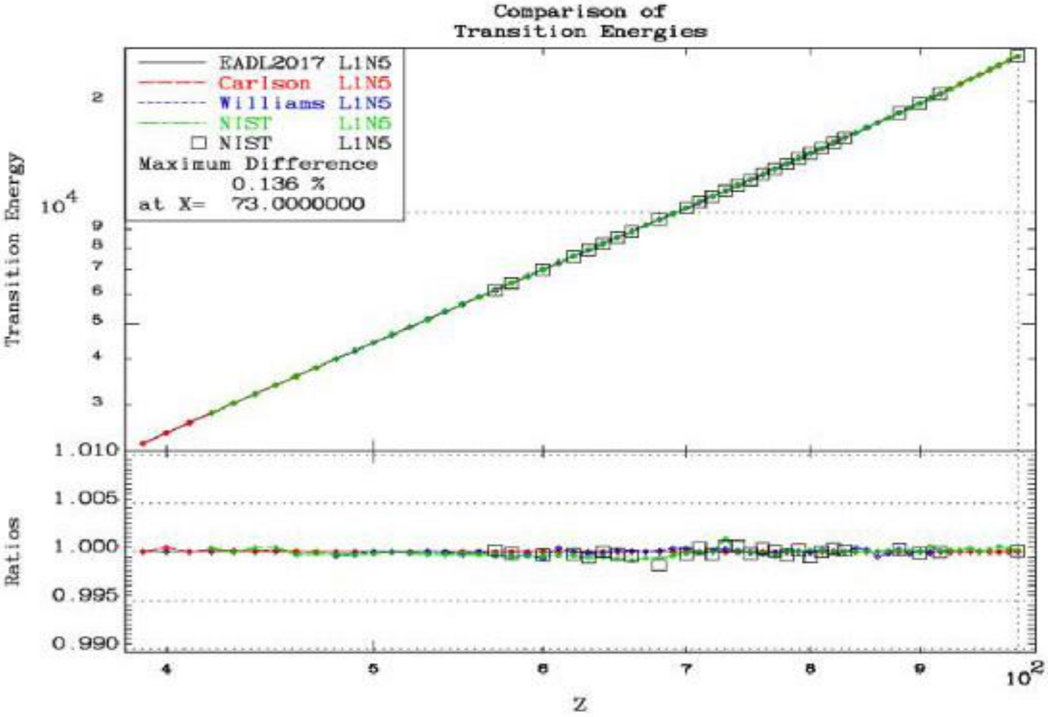
5.1.11. L1N2 and L1N3 Transitions



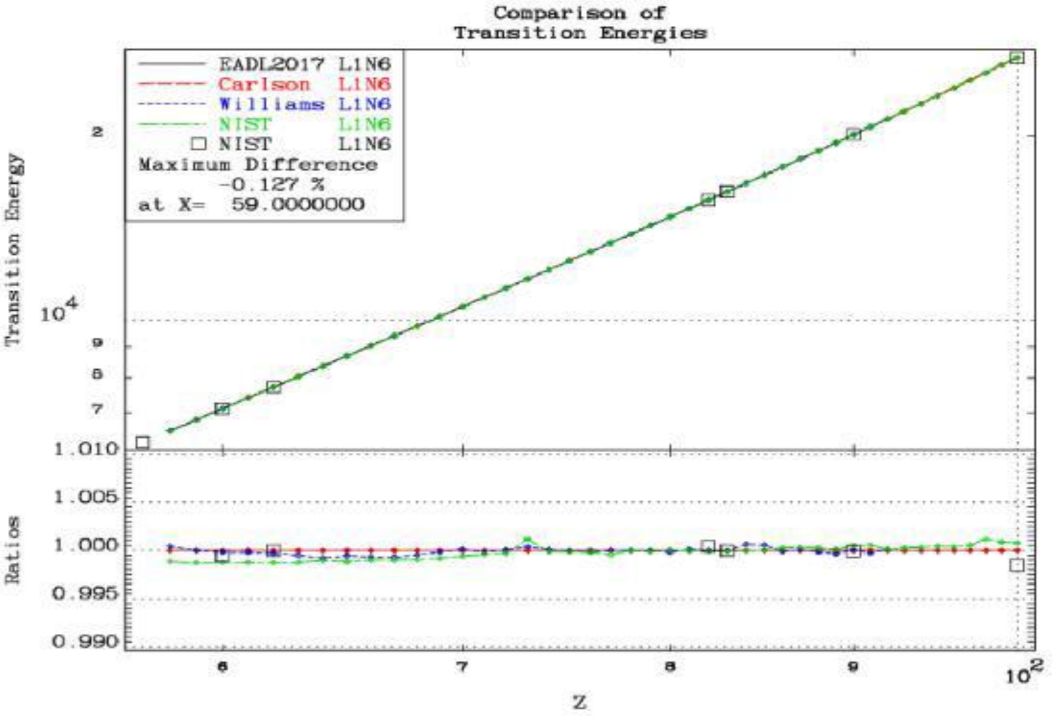


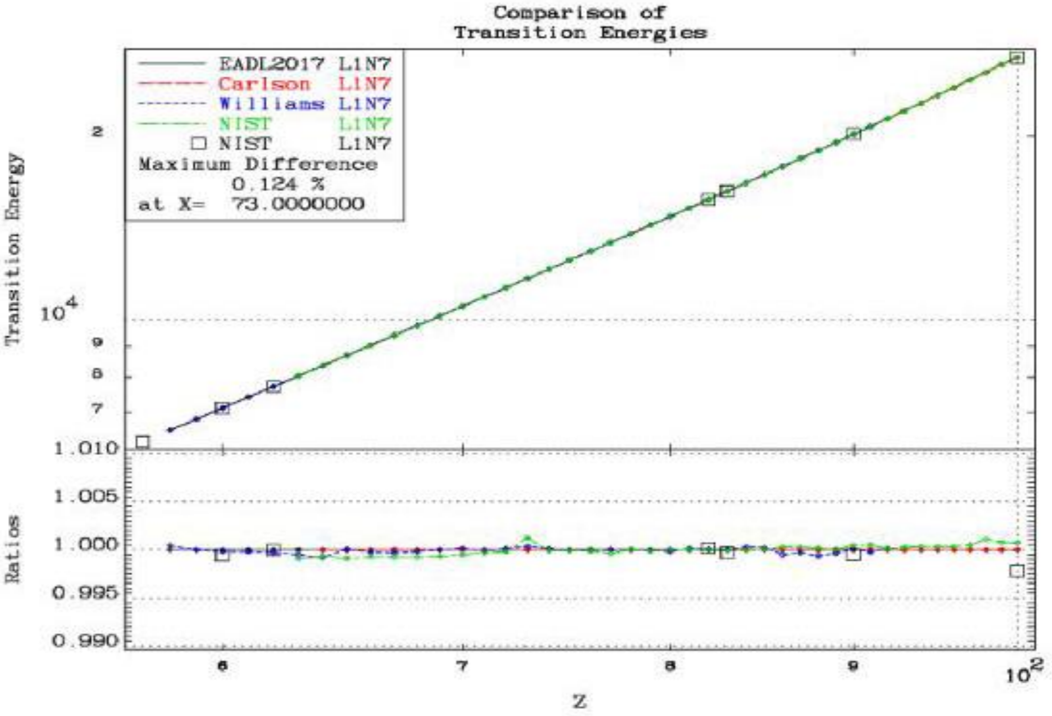
5.1.12. *L1N4 and L1N5 Transitions*



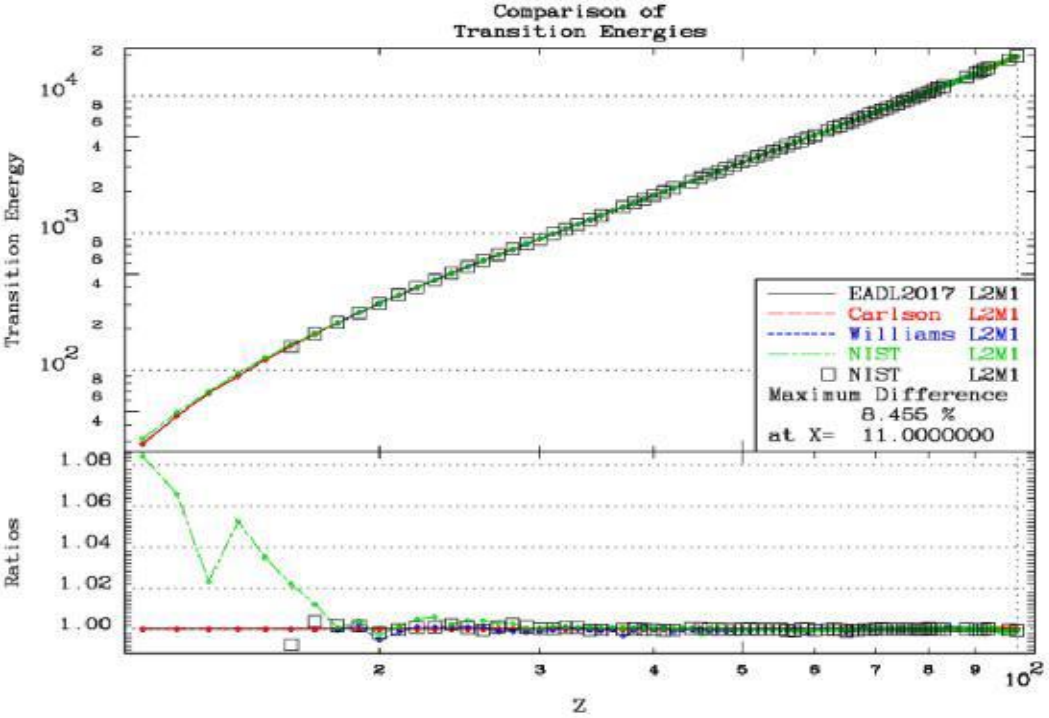


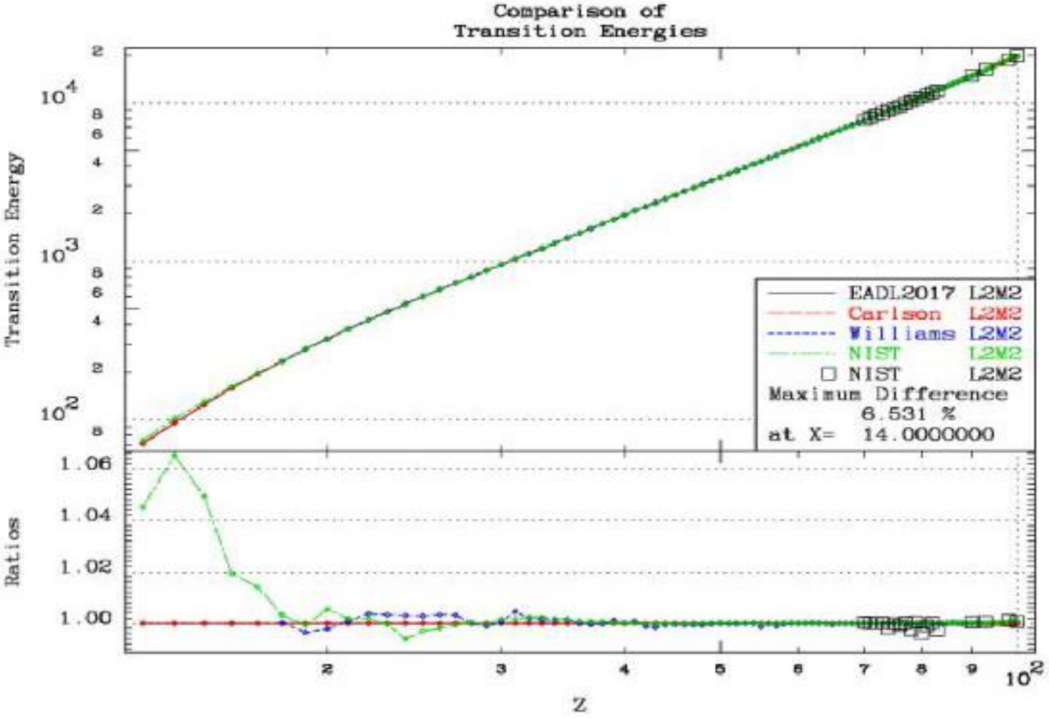
5.1.13. L1N6 and L1N7 Transitions



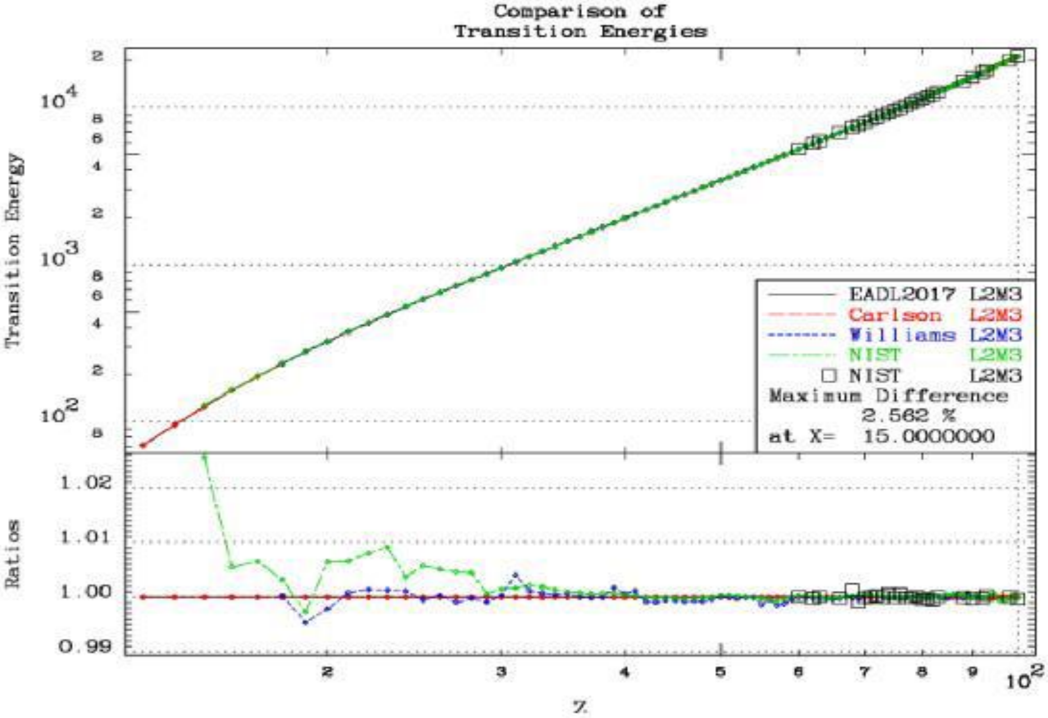


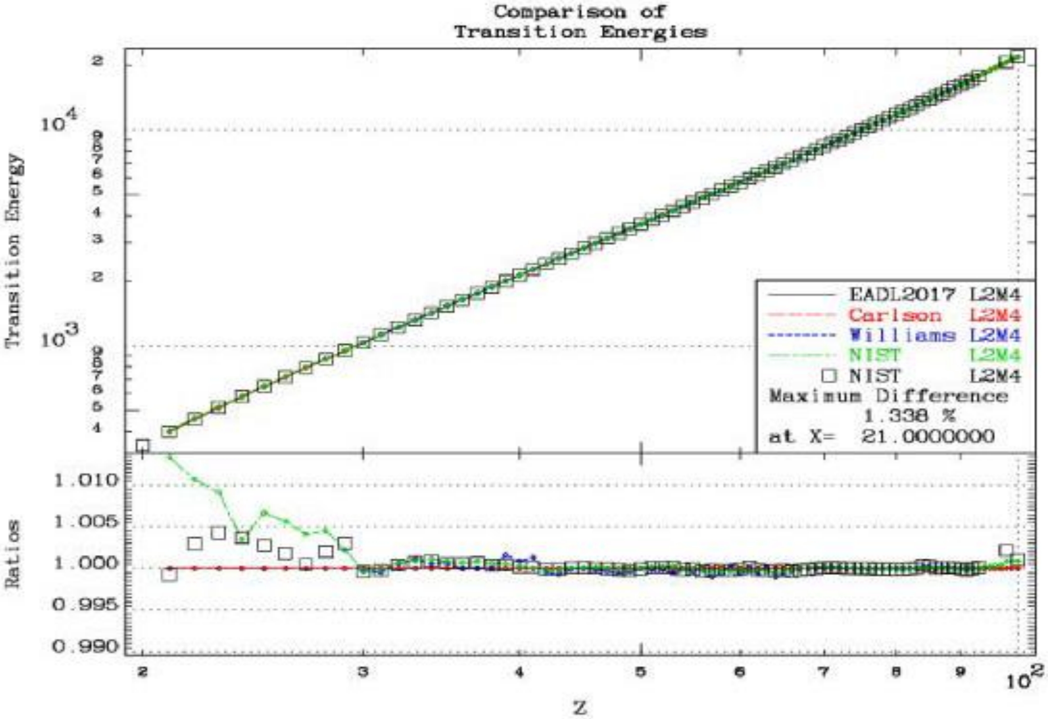
5.1.14. L2M1 and L2M2 Transitions



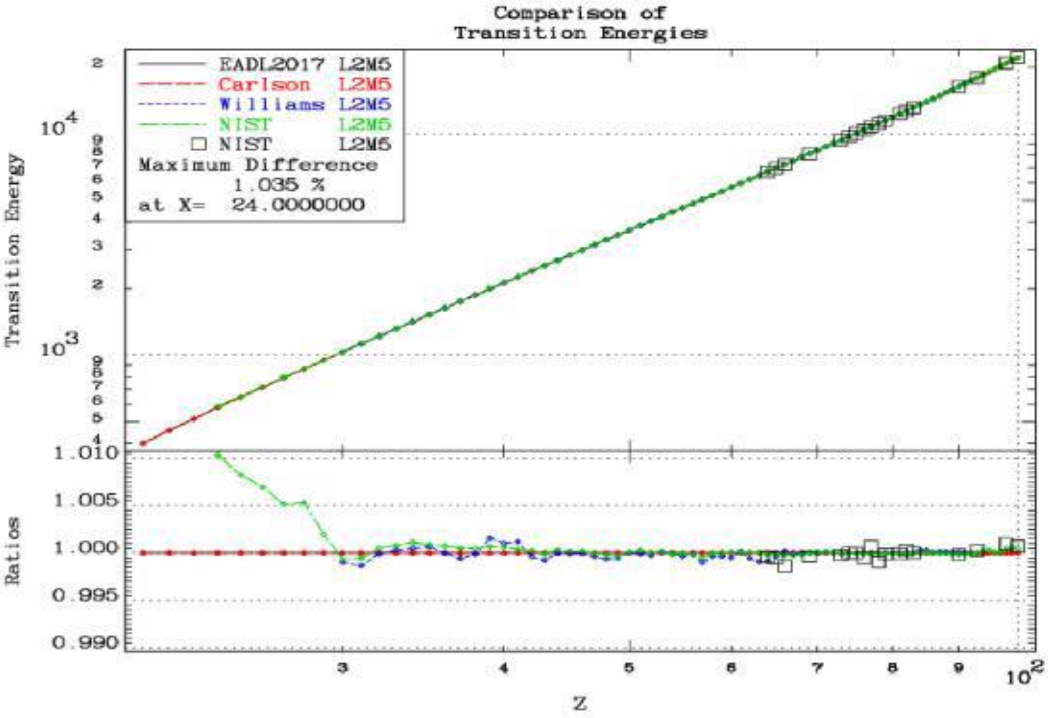


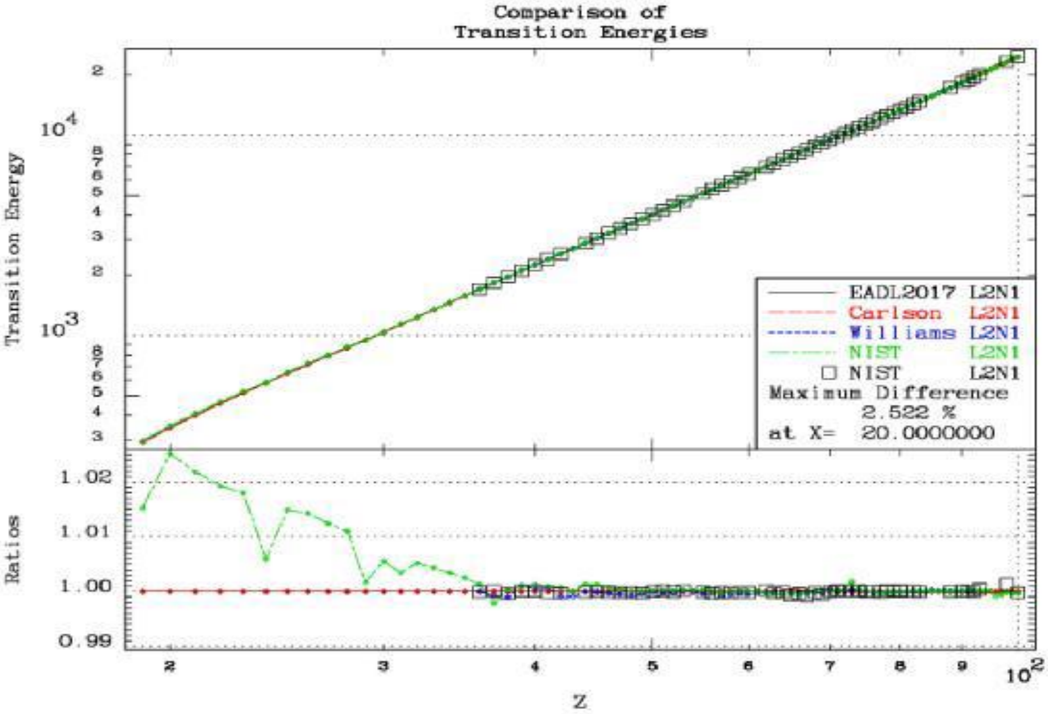
5.1.15. L2M3 and L2M4 Transitions



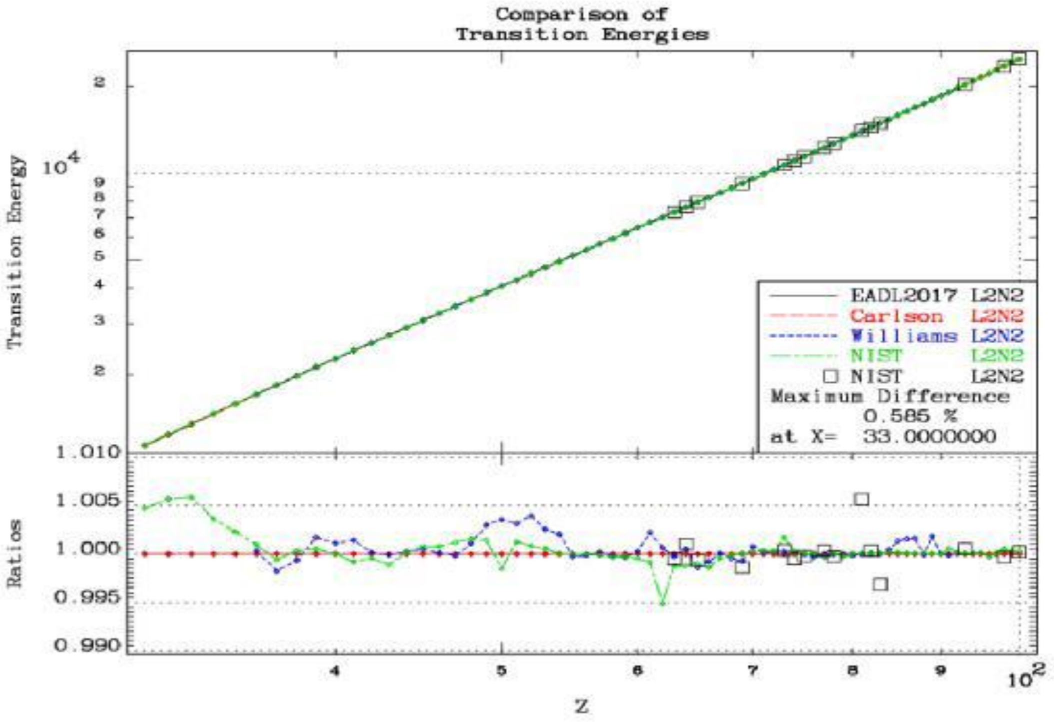


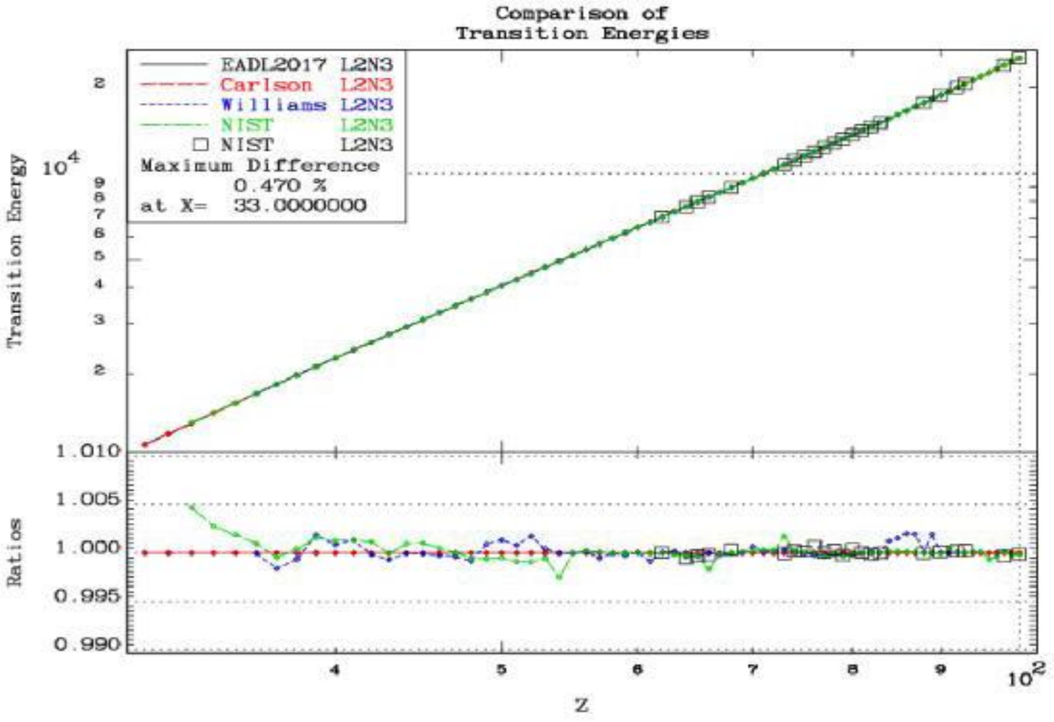
5.1.16. L2M5 and L2N1 Transitions



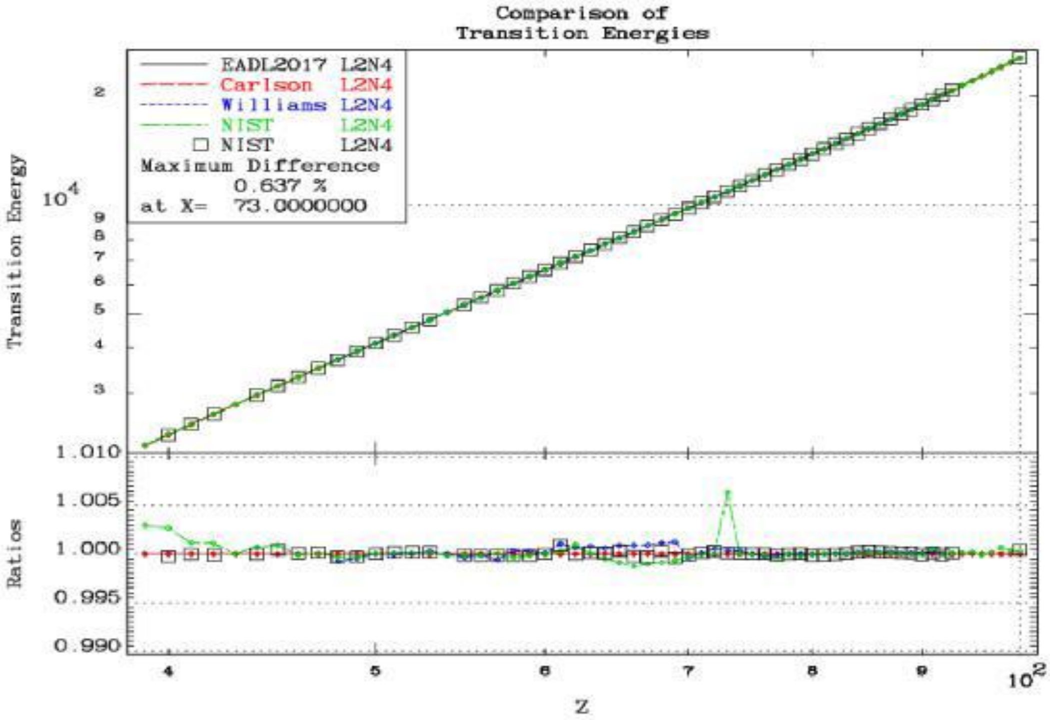


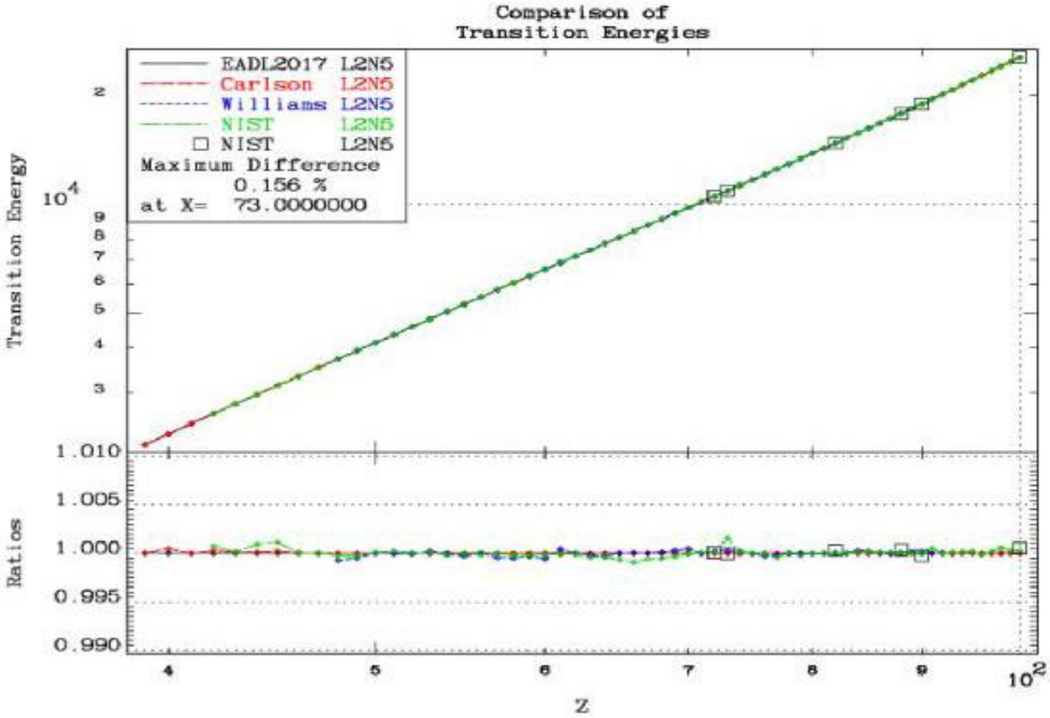
5.1.17. L2N2 and L2N3 Transitions



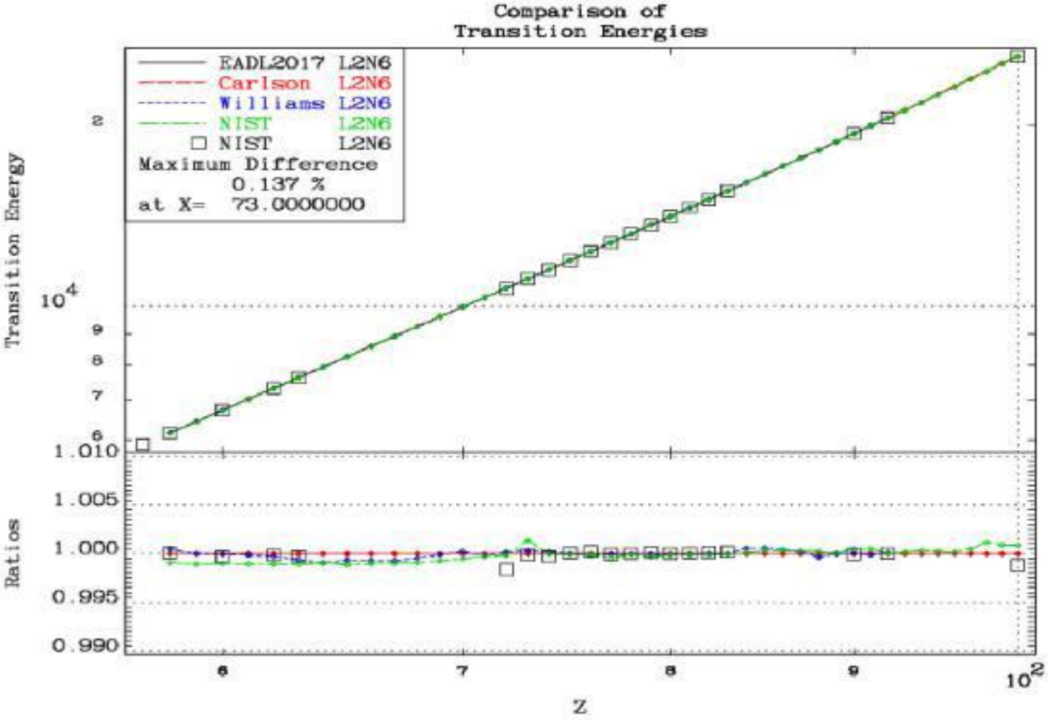


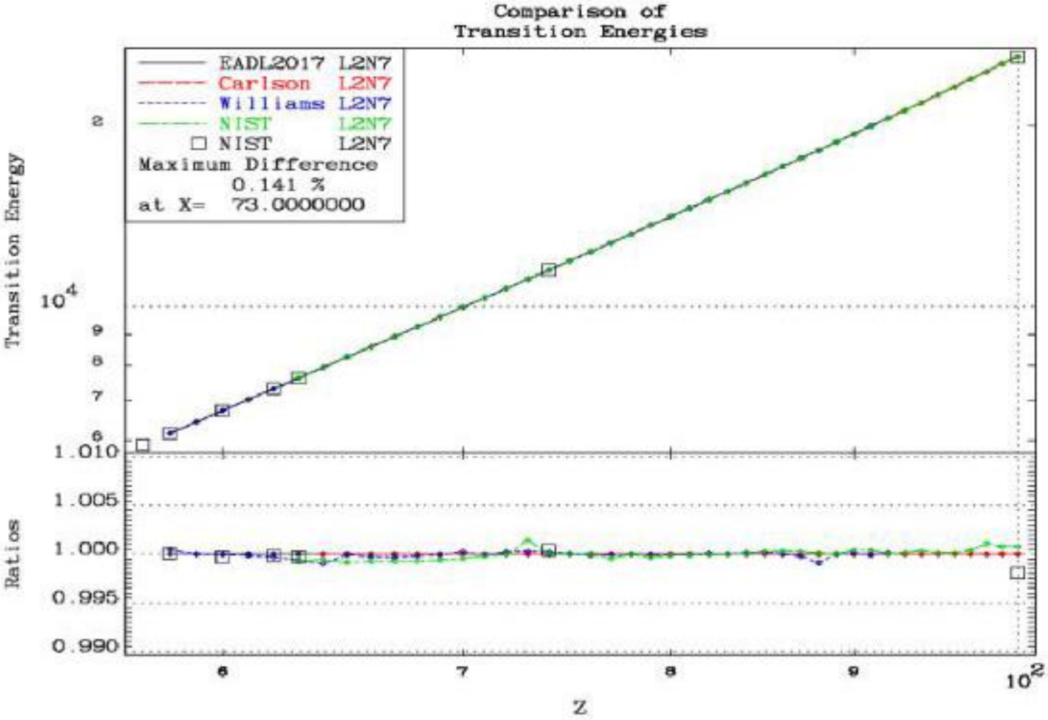
5.1.18. L2N4 and L2N5 Transitions



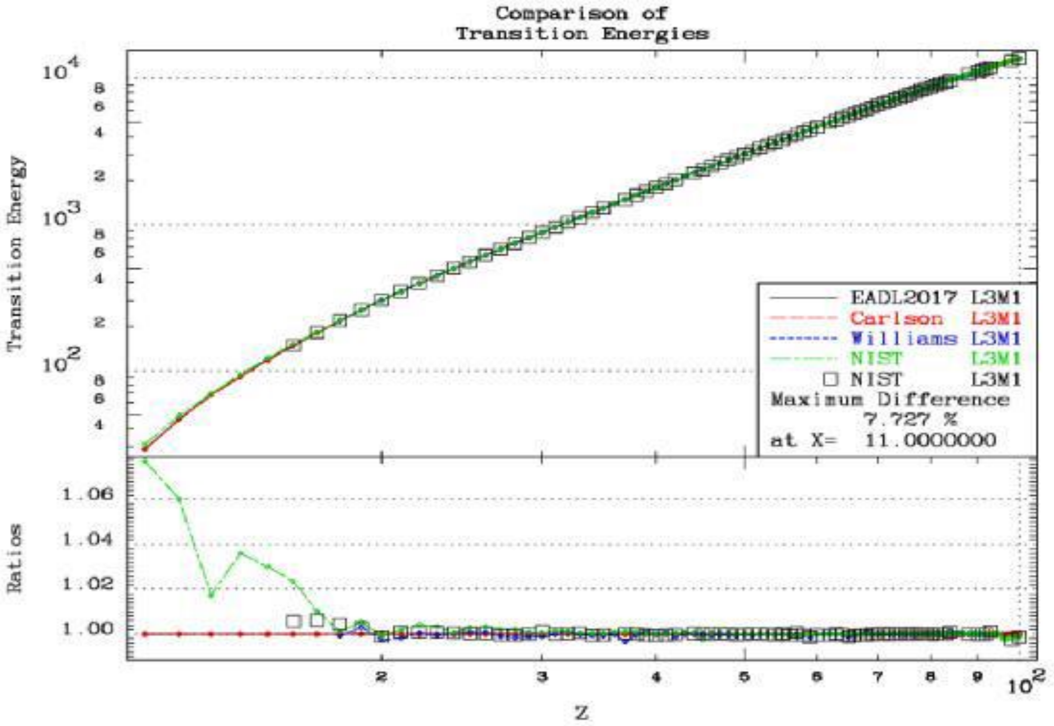


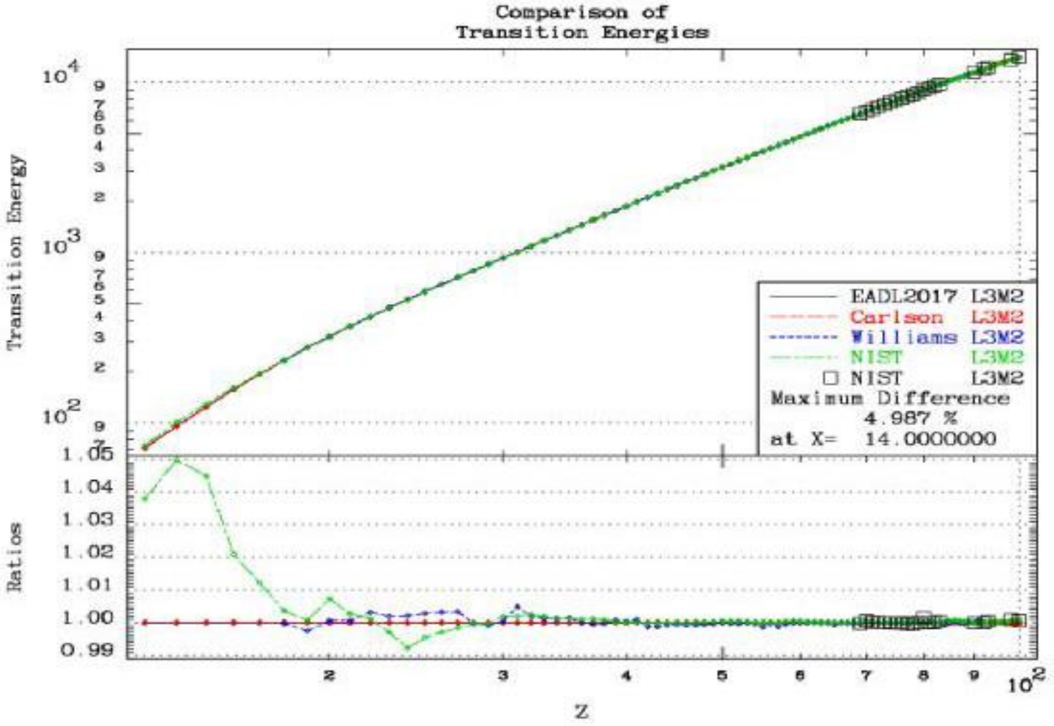
5.1.19. L2N6 and L2N7 Transitions



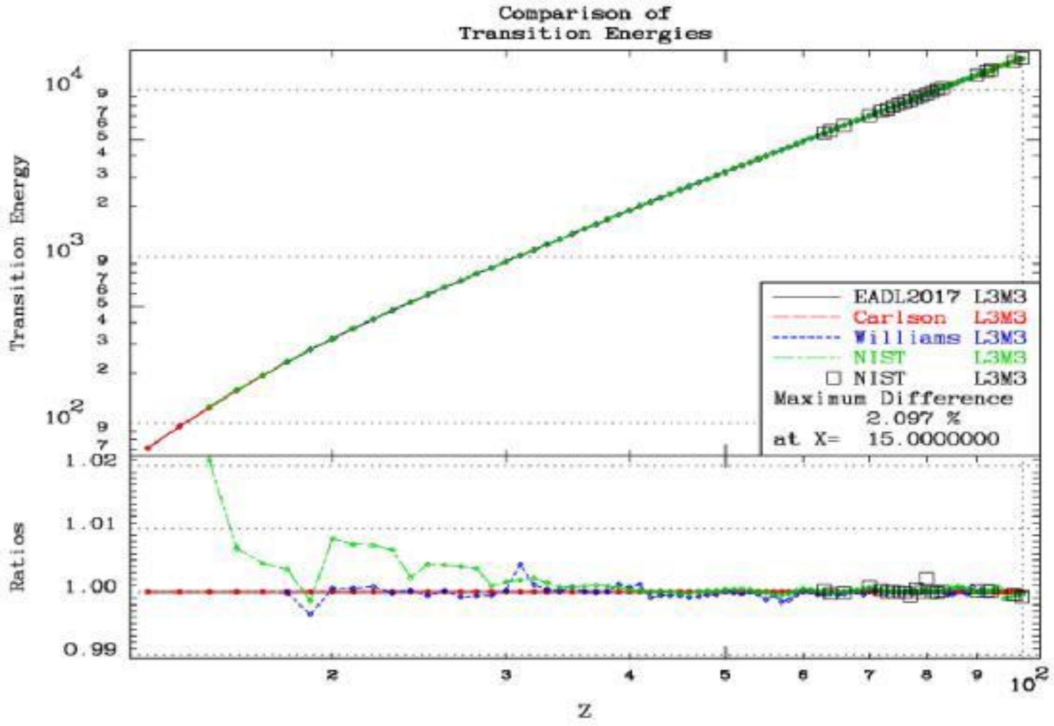


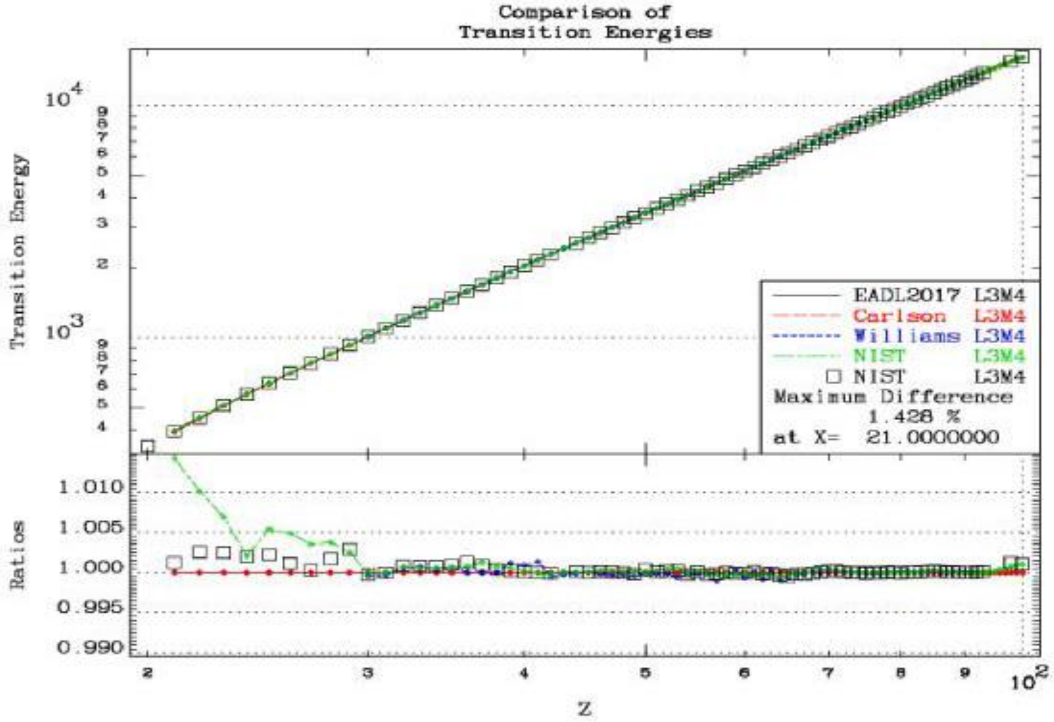
5.1.20. L3M1 and L3M2 Transitions



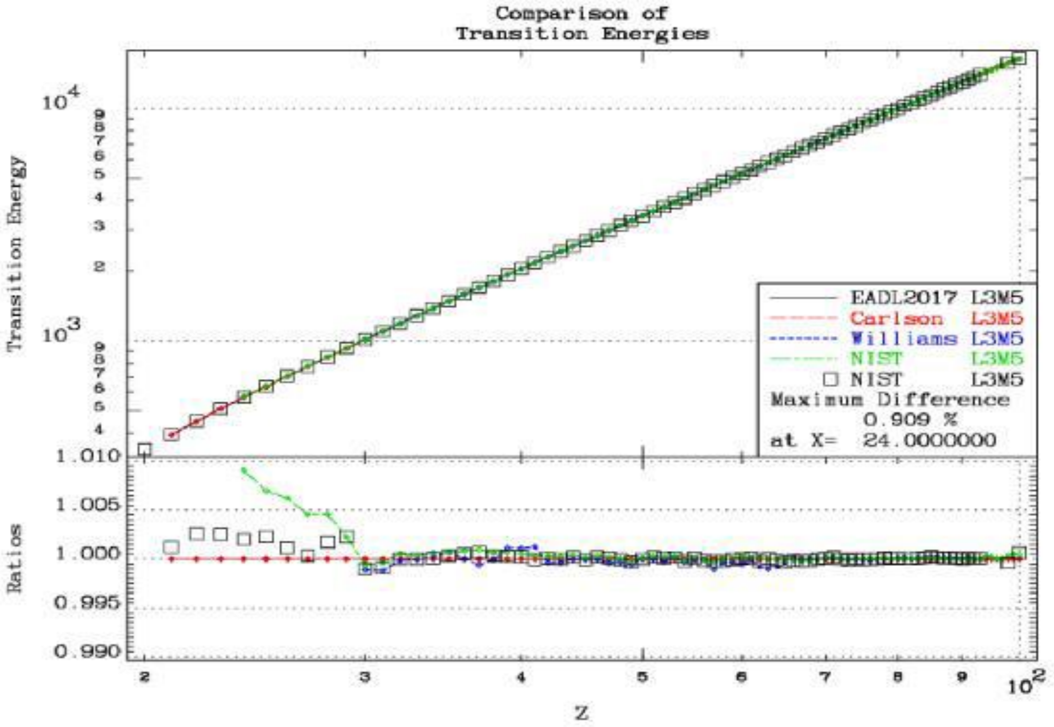


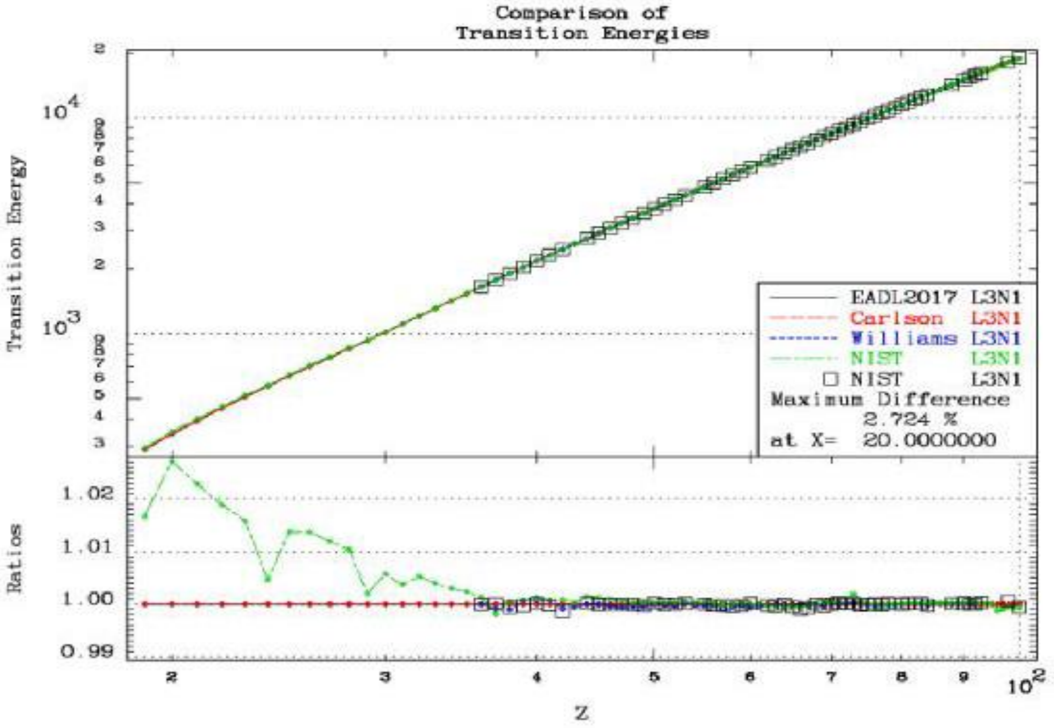
5.1.21. L3M3 and L3M4 Transitions



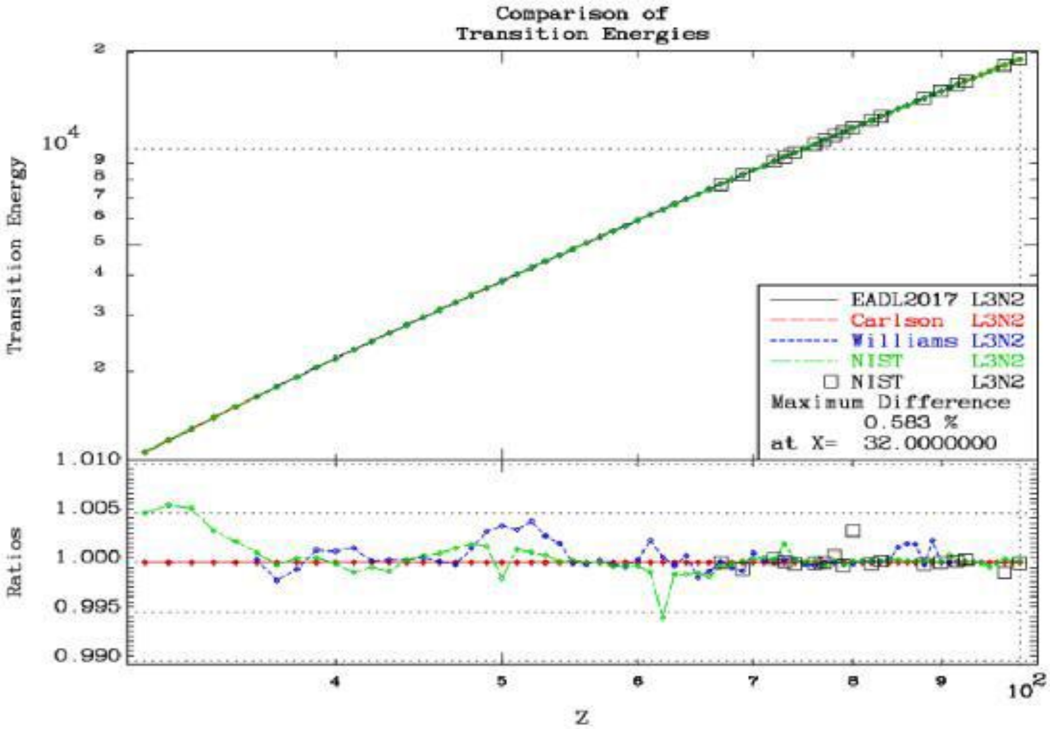


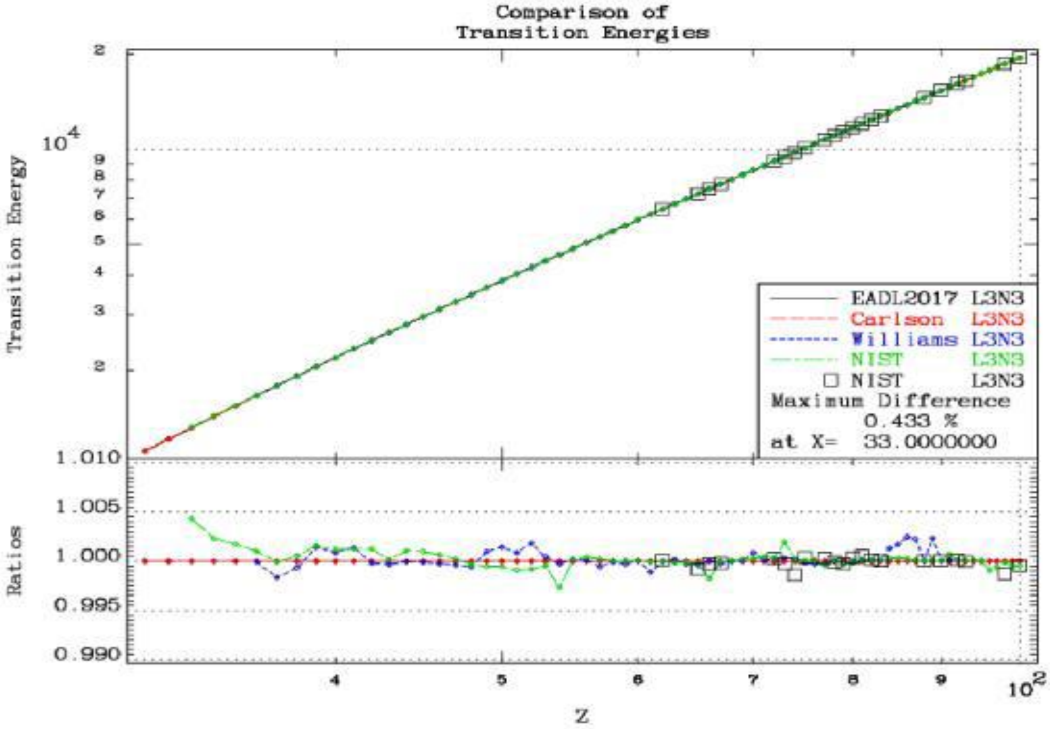
5.1.22. L3M5 and L3N1 Transitions



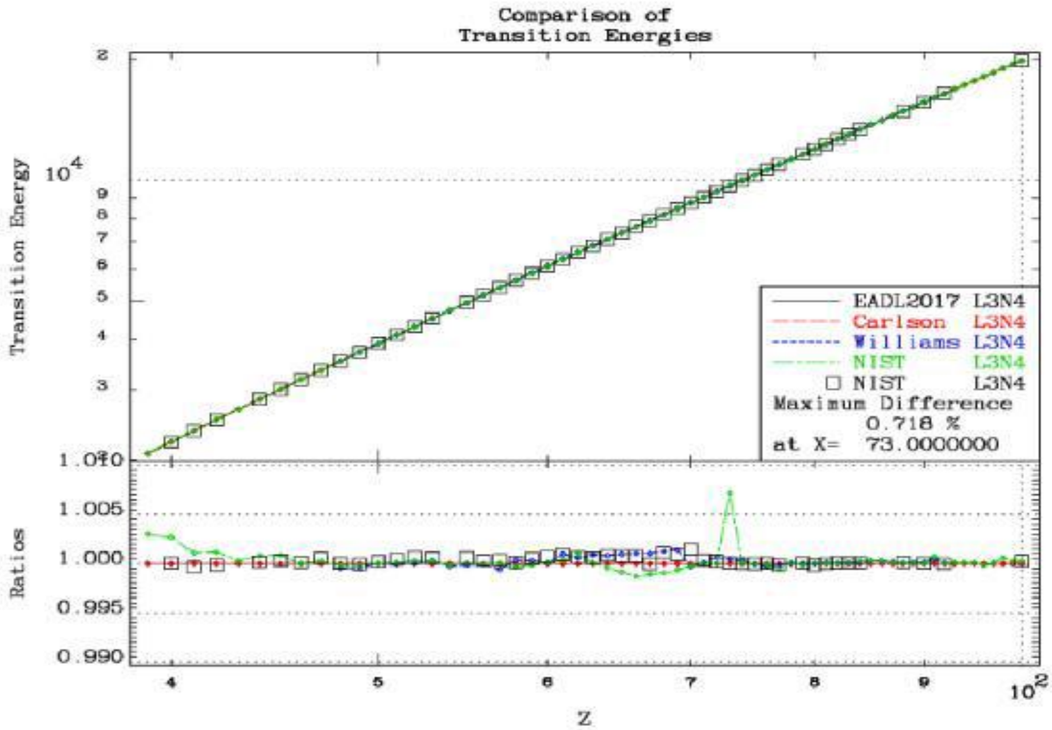


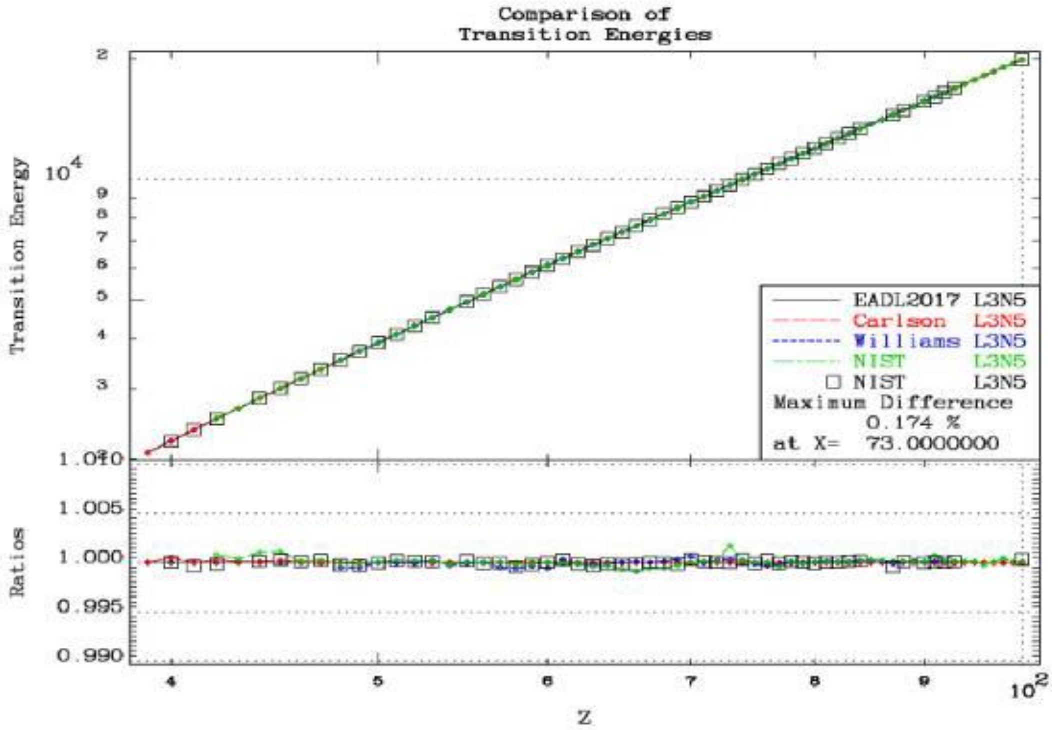
5.1.23. L3N2 and L3N3 Transitions



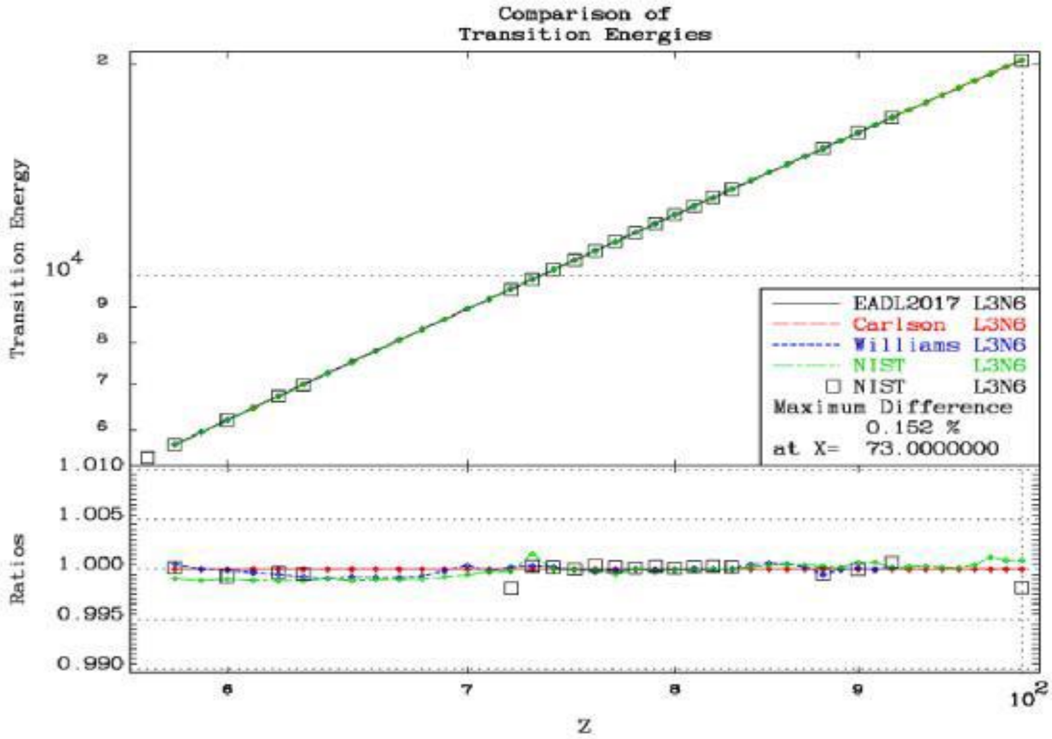


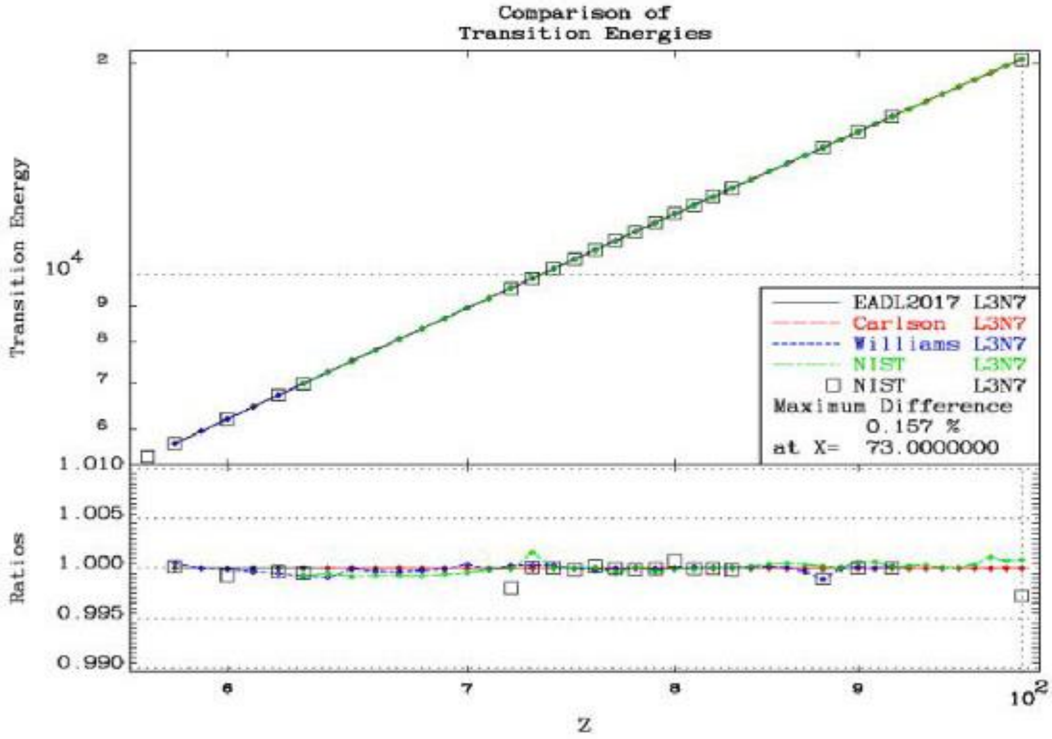
5.1.24. L3N4 and L3N5 Transitions





5.1.25. L3N6 and L3N7 Transitions





6. Release of the EPICS2017

I am hoping to release a complete EPICS (EADL, EEDL, EPDL) by the end of 2017. With this document, the binding energies have been defined (EADL), but what remains to be done is to re-define the cross sections and other parameters to use the new binding energies (EEDL and EPDL). To ensure an energy balance for photon and electron transport calculations it is imperative that all parts of EPICS use the same binding energies. Therefore, the numerical values for the newly adopted binding energies (EADL) will not be released until all parts of EPICS have been updated; again, hopefully by end 2017.

7. Conclusions

I have presented here my Survey of Atomic Binding Energies for use in EPICS2017. There are few original results of my own in this report; all of the original work was done by others in putting together the three compilations that I used. All I did was use existing compilations of atomic binding energies and transition energies, I added a few tests for the expected systematic, and I put the final results into the ENDF/B format [2], so that they can be easily used by as many computer codes as possible. I also used graphics to compare the sources to give the reader a realistic estimate of the uncertainty in this data.

The data I used included compilation of binding energies by Thomas Carlson [5] and Gwyn P. Williams [6] and the transition energies of NIST [7]. These were the three sources of data that I used to produce what I judge to be the BEST binding energies to use in EPICS2017 [to be published].

References

[1] D.E. Cullen, **EPICS2014**: Electron Photon Interaction Cross Sections (Version 2014), IAEA-NDS-218, September 2014.

[2] **ENDF format:** “ENDF-6 Formats Manual: Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII”, CSEWG Document ENDF-102, Eds.: M. Herman and A. Trkov (July 2010). Note, that the ENDF formats and conventions have had a number of updates, latest being the ENDF-6 formats, available on-line at http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf

[3] F. Salvat, Private Communication (2017).

[4] R.D. Deslattes, et al., “X-Ray transition energies: new approach to a comprehensive evaluation”, Reviews of Modern Physics **75** (2003).

[5] T.A. Carlson, “Photoelectron and Auger Spectroscopy” Plenum Press (1975), Appendix 1: “Atomic Binding Energies for Each Subshell for Elements Z = 1-106”. An abstract of this data for Z = 1-99, and omitting some low energy edges for low Z elements is available from a number of sources at a text file named “binden.tab“, e.g. in NIST-164.

[6] G.P. Williams, “Electron Binding Energies of the Elements”, August 2013; available on-line.
Binding Energies of the Elements
This was kindly provided to me as a private Communication (2017) by Gwyn P. Williams; this webpage only contains to numerical values; the numerous references are available at Gwyn P. William website,
http://www.jlab.org/~gwyn

[7] The tabulated transition energies for Z=10 to 100 are available on-line at **NIST**.
https://physics.nist.gov/cgi-bin/XrayTrans/search.pl?sorttype=element&lower=0&upper=1e6&units=eV.
The references that this data is based on can be found at
https://physics.nist.gov/PhysRefData/XrayTrans/Html/refs.html.

These were kindly provided to me as a Private Communication (2017), by Yuri Ralchenko, NIST, Wash. D.C.