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A Survey of Electron Cross Section Data for use in EPICS2017

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Abstract: I have presented here my Survey of Atomic Electron Cross Section Data for use in EPICS2017. There are few original results in this report; most of the original work was done by those who put together the compilations that I used; one being my own EEDL data. I started from my existing compilations of electron cross section data (EEDL), and compared it to PENELOPE data. I added new edge energies to ionization subshells and updated ionization subshell cross sections and energy spectra to correspond to the new edges. I discovered and corrected an error in the ENDF formatted translation, involving the scattering cross sections. I also added sum cross sections for total and ionization, as well as a few tests for the expected systematics. In this report I extensively used graphics to illustrate the energy dependence and simple Z dependence of the cross sections, and to illustrate the important differences between cross section and energy deposition. I put the final results into the ENDF/B format, so that they can be easily used by as many computer codes as possible. **After reviewing all the electron data, I have decided for EPICS2017 that it is sufficient to only change binding energies, to insure they are consistent with the changes already made to EADL and EPDL.**

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Vienna, December 2017

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1. Acknowledgement

I should like to start by thanking **Francesc Salvat** (U Barcelona) for providing the PENELOPE compilations of electron interaction cross sections. These, plus my own EPICS2014 data, were the evaluated sources that I used to produce what I judge to be the BEST electron interaction cross sections for use in EPICS2017. I also thank **Francesc Salvat** for his contributions toward this report and his extremely useful conversations and feedback in reviewing preliminary versions of this paper; I feel that the final paper is much improved by his constructive criticism. I also thank **Steve Seltzer** (NIST), the true father of our Evaluated Electron Data Library (EEDL), going back to our joint original publication in 1991 [1]; at the time Steve had the models and we had the computer power, and this turned out to be the right mix we needed to put this data library together. I thank **Andrej Trkov** and **Kira Nathani** (NDS, IAEA, Vienna) for editing my reports into a form suitable for publication by the Nuclear Data Section, IAEA.

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.**

2. What is EPICS?

The Electron-Photon Interaction Cross Sections (EPICS) [2] is part of the ENDF/B system [3], to compliment the ENDF/B neutron data, and allow coupled calculations in engineering applications. I should like to 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.

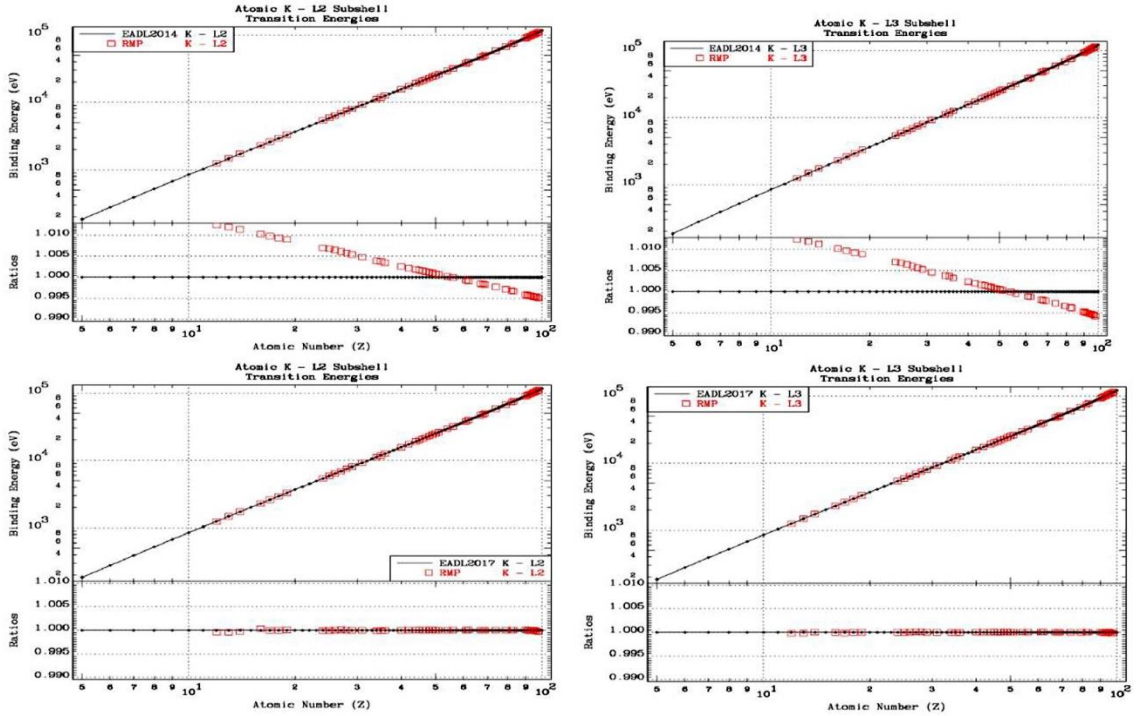
To a large extent the success of the ENDF system is that it uses a simple text based computer format that today, and into the future, can be read and used on any computer using almost any computer language. It is extensively documented in ENDF-102 [3], the ENDF Bible, defining all the rules and conventions that everyone (data producers and users) agree to use. 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 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 **ATOMIC DATA**, 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 should not be used in applications below 100 eV; Francesc Salvat recommends not below 1 keV [4].** Users should be aware that the EPICS data extends to low energy (eV range) ONLY to allow data such as anomalous and coherent scattering factors to be calculated (this involves an integral over the entire energy 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 ATOMIC elemental, cold, neutral, isolated atoms. This does not include NUCLEAR data, which at high energies can be substantial**. **WARNING: CAVEAT EMPTOR: Do not try to use this data at lower energies (eV range) – if you do, your results can be very inaccurate, and you will have nobody to blame except yourself.**

3. Overview: The Quest to Improve Our Data

Based on my earlier survey of binding energies we have improved the 2017 binding energies in our EADL data base [5]. For consistency and to conserve energy, these binding energies have now been incorporated into EPDL, for photons [6], and with the current report into EEDL, for electrons. The new binding energies require an update to the electron ionization cross sections and emission spectra. I have also taken this opportunity to correct an error that was introduced during the translation of the original evaluations from the ENDL to the ENDF formats. Lastly, for convenience, I added sum cross sections for total and ionization. Here I document the results of these updates.

First a brief overview: Based on other currently available data the EPICS2014 [2] 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 KL2 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 [7], 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 [7] results using EPICS2014 and EPICS2017; here the Deslattes data is referred to as RMP (Review of Modern Physics). In the below figures, the top 2/3 shows the data and the bottom 1/3 the ratio of all the data to the EPICS2017 results. 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.



4. Sources of Atomic Photon Cross Section Data

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

1) **EPICS2014** [2]. This was used as a standard for comparison to the other available data sets. In line with the intended use of EPICS, as a simple interface for use in engineering applications, changes are made to these data today only after they are proven to be necessary based on experimental measurements; new, and unproven theory is not sufficient to warrant a major change in EPICS.
2) **PENELOPE** [8]. This is currently widely used electron-photon transport that I consider to be state-of-the-art code and atomic data; as such I judge it to be an excellent source to compare to in my search for new and improved data.

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, realistic uncertainty estimates.

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 several sources, e.g., EPDL2014 and PENELOPE. Moreover, only recently F. Salvat went through a similar study to update the atomic data used by PENELOPE uses multiple sources [8], so we can rely heavily on his earlier study. By comparing their results, we can estimate real world, instead of Disneyland uncertainties.

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. The uncertainty in the available data 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, Francesc Salvat** [4]. 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 (Z=1), 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. This is but the simplest example; differences 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.

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. With

decreasing Z and energy, we see increasing differences. 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 differences we see can be small compared to real world differences due to compounds, etc. If 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.

5. Important Differences between Neutrons, Photons and Electrons

When we transport "particles" there are a few important differences between neutron and photons (addressed elsewhere) and electrons (addressing here), these include,

1) Neutrons and photons have no charge (are neutral), so we are dealing with "particles" having local interactions, on the scale of most problems, we can consider them as "point" interactions with an individual atom or nucleus. This makes it easier to define cross sections as barns/atom, and discrete energy ranges at each collision site.

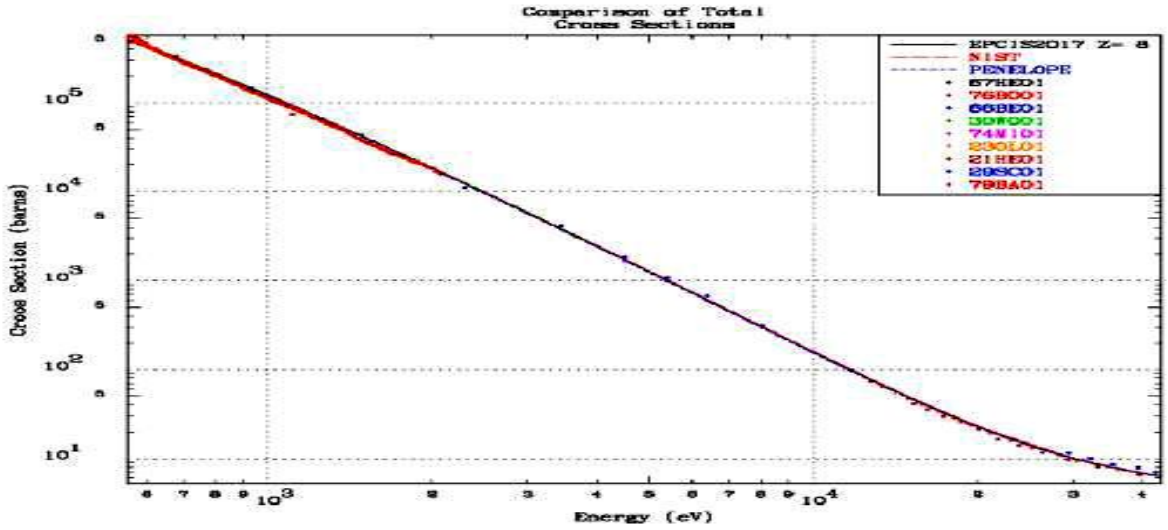
2) In contrast electrons are negatively charged, so we are dealing with "particles" that are continuously interacting with the electromagnetic field in any media. This makes it more difficult to define interactions at a "point", and corresponding cross sections as barns/atom, and energy change. Here cross sections can change due to the density of material, compounds versus elemental data, and other causes. What is important in this situation is **STOPPING POWER**, dE/dx, energy loss per unit of distance travelled, and what I will refer to as **TURNING POWER**. If electrons traveled in a straight line, continuously losing energy, it would be extremely easy to track them, simply using dE/dx. But, electrons also scatter, changing their direction of travel; this is what I refer to as **TURNING POWER**. This change in direction, causing straggling, greatly complicates how we must transport/track electrons.

3) Neutrons and photons in "collisions" tend to lose a fraction or their energy; it doesn't take too many collisions for a MeV energy neutron to thermalize, or for a MeV energy photon to disappear. This makes it practical and indeed relatively easy for us to track neutrons and photons, e.g., any "particle" history only involves a manageable number of "collisions".

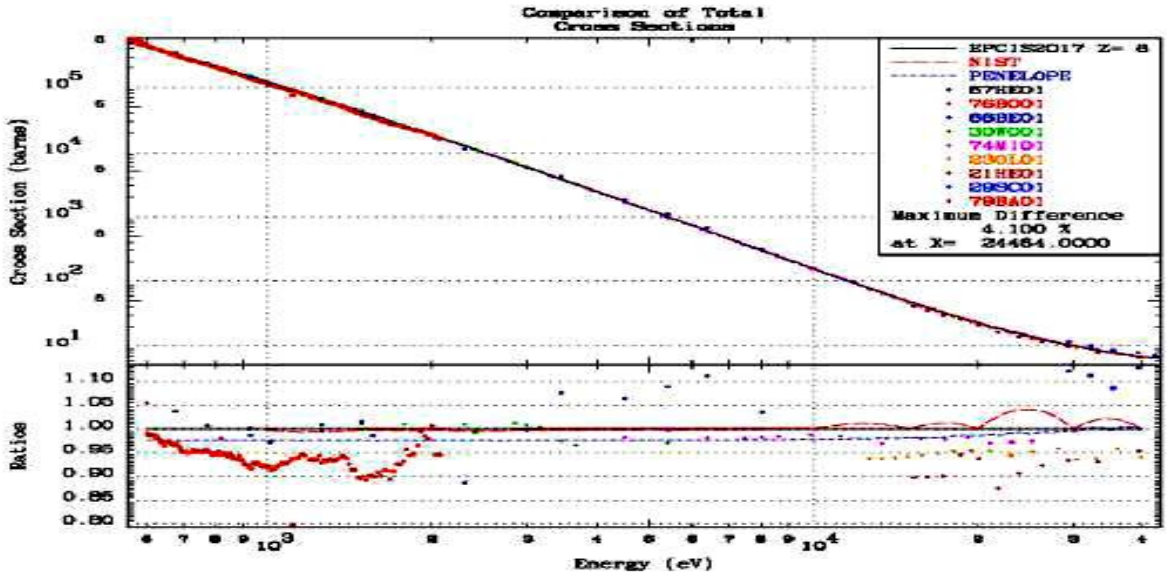
4) In contrast electrons in "collisions" tend to lose the same amount of energy at all incident energies, and this can be a very small amount of their incident energy. For example, if an electron loses only 10 eV per "collision", to slow for 1,000 eV to 100 eV, requires 90 "collisions"; from 10 keV to 1 keV, requires 900 collisions; from 100 keV to10 keV, requires 9,000 "collisions"; from 1 MeV to 100 keV, requires 90,000 collisions. This greatly – make that GREATLY – complicates and makes it very time consuming to perform analogue electron transport. This has led to the development of a number of approximate methods, modeling "pseudo-collisions", to reduce the number of "event" actually modelled to a reasonable/practical number. These approximate models are beyond the scope of this study; we only supply the EEDL data that users can start from to develop and use these approximate methods.

6. The Importance of Ratios

The photon and electron cross sections that we use vary over many orders of magnitude in incident energy and in cross section (barns/atom) values. This makes it very difficult to actually "see" differences on a plot. For example, the below plot compares 8O (Z=8) photon total cross sections, for three evaluated data sets and eight experimental measurements. From this plot, you might think that they all agree.



The problem is we have two decades of energy and five decades of cross section, making it almost impossible to see **differences**. Below is the same plot as above, but I have added the ratio of everything to EPICS2017. Here we can see that the evaluated data sets differ by over 4% and the measured data by up to 20%. My point here is that ratios are VERY IMPORTANT to "see" when we are interested not just in values, but also in differences. Since this a major concern of this paper the figures/plots will mostly include ratios, and **I STRONGLY recommend that you focus on the ratios to "see" differences**.



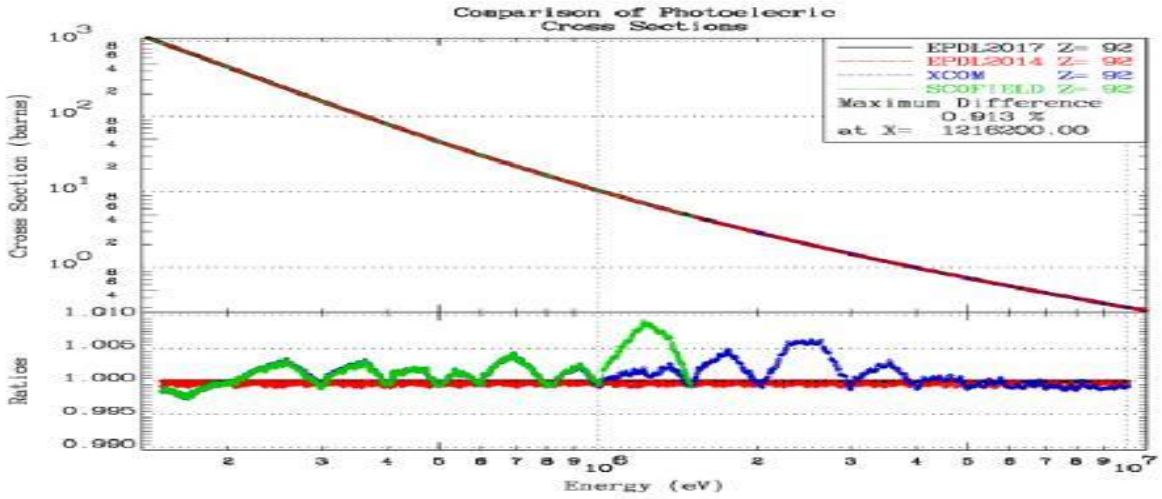
7. The Importance of Interpolation

In our applications, we are interested in the value of the cross sections at ALL energies, not just the energies where they are tabulated; without this we cannot uniquely define integrals. We cannot stress enough the importance of how you interpolate between tabulated values. The ENDF format recognizes the importance of interpolation, as each and every table of data is accompanied by an interpolation law.

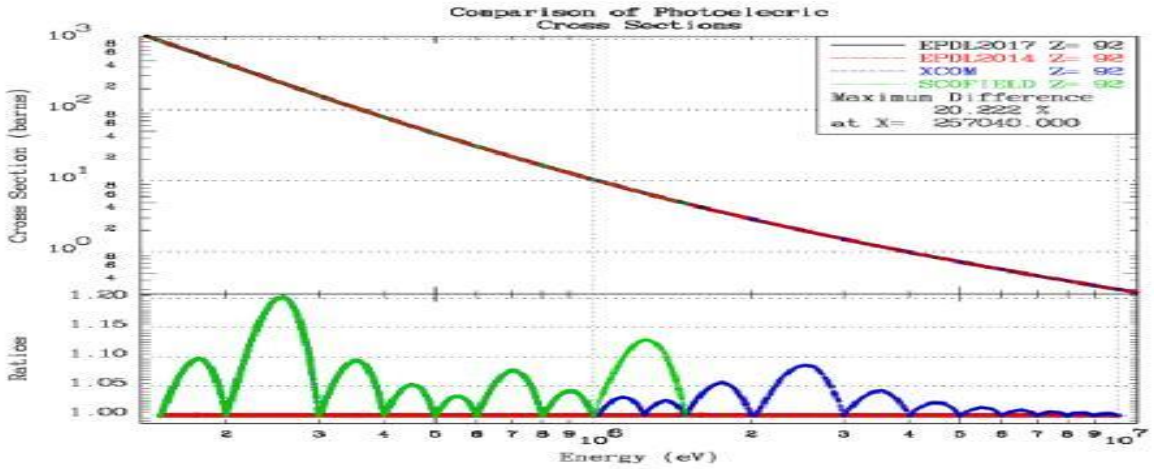
Generally experienced ENDF data users are aware of the importance of correctly interpolating, but for those who are not so aware we present a simply example that we hope will scare the hell out of you, and make you aware of just how much damage you can do to your calculated results by not obeying the intended interpolation laws.

Below are two plots of exactly the same tabulated data. In each case the upper 2/3 of the plot shows the data and the lower 1/3 the ratio of all data to the first set of data (in this case EPDL2017). The only difference between the two plots is that in the first one we used LOG-LOG (log X vs. log Y) interpolation between the tabulated points and in the second one we used LIN-LIN (linear X vs. linear Y) interpolation.

In the first plot, below, we used LOG-LOG interpolation between tabulated values. As a result, we see agreement between all of the data sets at all energies to better than 1%, even though much of the data is tabulated on a sparse energy grid. We see even much better agreement at energies near where more than one set are tabulated. For example, the base of each "cusp", shows close agreement to EPICS2017, i.e., their ratio is very close to 1.0 at these tabulated energy points.



In the second plot, below, the only difference from the above plot is that we used LIN-LIN interpolation between tabulated values. Now we see interpolated values that differ by more than 20%. If these two plots do not convince you of the importance of correctly interpolating nothing will: **CAVEAT EMPTOR!!!!**



In this report I have attempted to give the "BEST" visual interpretation of ALL the data, by using LOG-LOG interpolation between tabulated values, as shown in the first of the above two figures. But be WARNED that it is up to you, the data users, to ensure you interpret the data as intended.

In earlier versions of EPICS (EADL, EEDL, EPDL) in the ENDF format I used the ENDF format's ability to specify that the data should use LOG-LOG interpolated; here I assumed users would be familiar with ENDF conventions to properly interpret the data. Boy was I wrong. Far too many users completely ignored the ENDF conventions, and produced nonsense results. Hopefully I have learned my lesson: **starting with EPICS2017 all the data has been linearized using my PREPRO/LINEAR code [9]. The result is libraries are roughly three (3) times as large (e.g., have about 3 times as many energy points), but it can be accurately interpolated using LIN-LIN interpolation. I judge the increase in size to be worth and gain of avoiding interpolation problems.**

8. Subshells for EPICS and PENELOPE

For EPICS2017 (EEDL) whenever possible I used the PENELOPE ionization subshell data as a guideline. It was not possible to simply adopt the PENELOPE data, because EEDL includes both Ionization and Excitation, whereas PENELOPE includes only Ionization. There is also the complication, that I will remind you, that EEDL is designed for simple engineering applications: elemental, cold, neutral, isolated atoms, and PENELOPE is designed to handle much more general conditions. Part of PENELOPE's more general treatment involves density, compounds and how to deal with valence electrons.

The EPICS and PENELOPE 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 table lists where they differ. Where EPICS has a subshell occupied and PENELOPE does not, the binding energy of the subshell is listed. Where PENELOPE has a subshell occupied and EPICS does not, the binding energy and the word **PENELOPE** are listed.

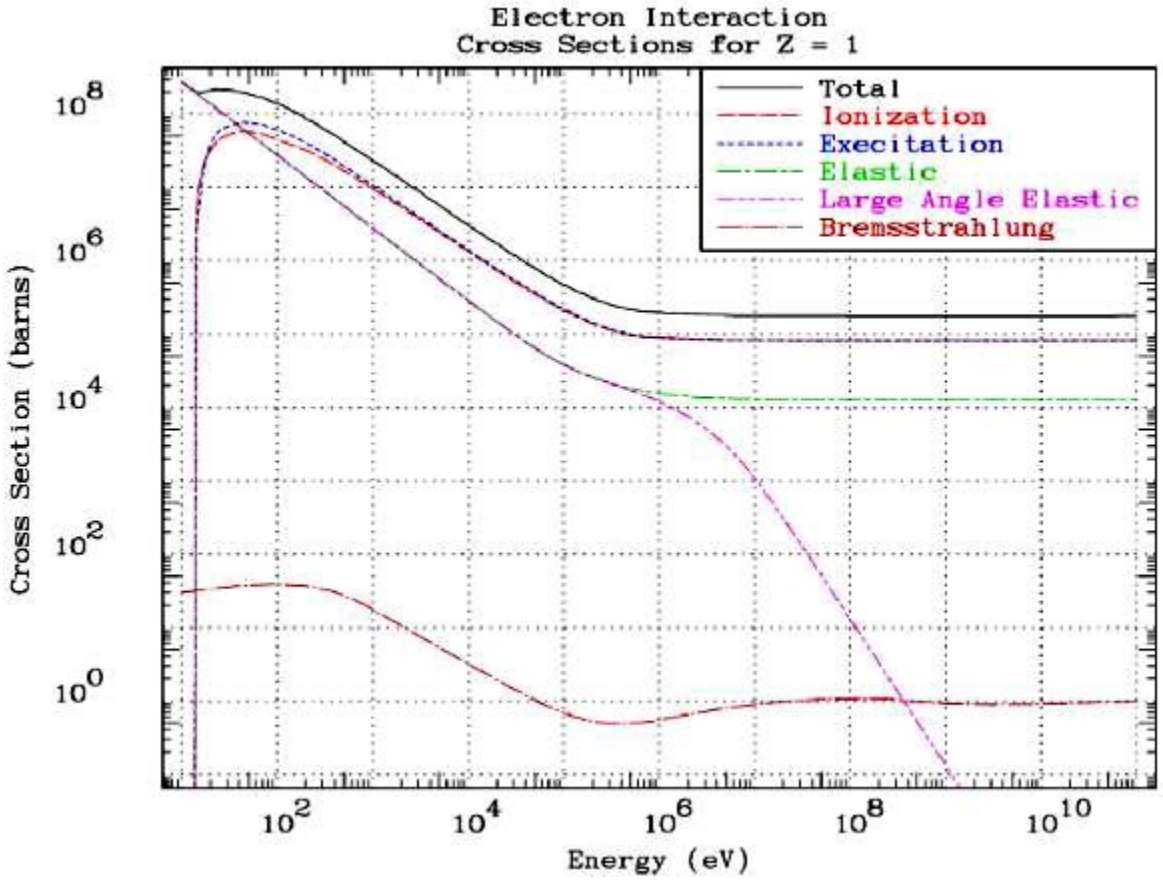
PLEASE note that the below results are based not on the complete PENELOPE results [8], but rather on the abstracted file "binden.tab"; the complete results include some of these low energy edges.

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. EPICS distributes the electrons between L1, L2 and L3, whereas PENELOPE 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 EPICS.**

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

9. History 101: Mea Culpa

We did the original Evaluated Electron Data Library (EEDL) evaluations [1] in the ENDL format. Later someone else translated them to the ENDF format. The original evaluations included data for total electron scatter and in addition so called "large angle" scatter. At higher energies, MeV and above, the angular distributions become extremely forward peaked, i.e., electrons scattered through incredibly small angles. The total scatter cross section includes scattering through the entire cosine range from +1 to -1. At higher energies the angular distribution is so forward peaked that we defined "large angle" scatter as scatter outside the very narrow cosine range +1 to 0.999999. This may sound like nonsense until we look at typical electron scatter cross sections; here is a plot of the Z = 1 data. Above 1 MeV the total scatter approaches a constant, while the large angle scatter rapidly decreases with increasing energy as $1/E^2$. Here we can see that there is virtually no large angle scatter at higher energies.



The history lesson and Mea Culpa comes in because in translating this data from the original ENDL format to the ENDF format, the translator made the mistake of only translating the Large Angle Scatter cross section and identified it in the ENDF format as the Total Scatter. As a result, anyone who tried to use this data starting from the ENDF format would actually be using the large angle scatter cross section and think high energy electrons do not scatter (see the above plot). I only recently discovered this ERROR and I have corrected it in this EEDL 2017; this now includes both total and large angle scatter data. The Mea Culpa comes in because even though someone else performed the translation, the responsibility for these data bases is mine, and I failed to check the translation, so I accept all blame for this ERROR.

10. Contents of EEDL

EEDL2017 includes more data in the ENDF format than earlier versions of this data base, this includes,

MF/MT	Definition
23/501	Total
23/522	Ionization (sum of all subshells)
23/525	Large Angle Scatter
23/526	Scatter (Total)
23/527	Bremsstrahlung
23/528	Excitation
23/534 through 23/572	Ionization Subshells
26/525	Large Angle Scatter Angular Distributions
26/527	Bremsstrahlung Photon Energy Spectra Electron Average Energy Loss
26/528	Excitation Average Energy Loss
26/534 through 26/572	Ionization Subshell Energy Loss

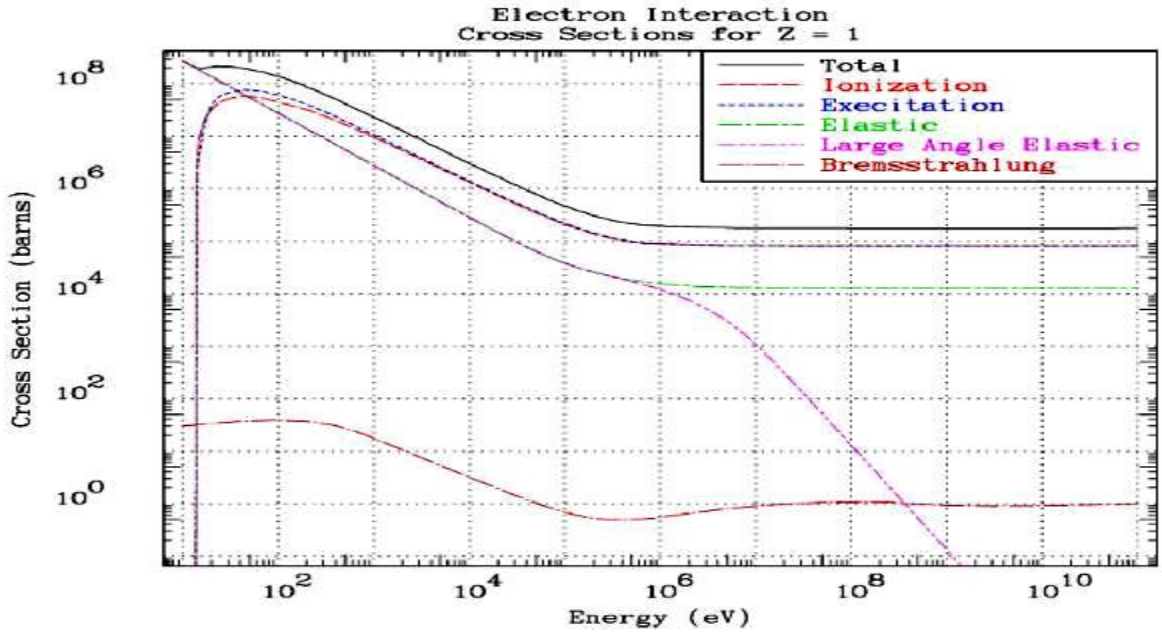
The MF=23 data are cross sections, tabulated as (energy, cross section) pairs. The **Total** (MT=501), **Ionization** (MT=522), and **Large Angle Scatter** (MT=525) are included in EEDL2017; they were not included in earlier versions. The **Scatter** (MT=526) is now the correct Total Scatter (again, in earlier version this was erroneously the large angle scatter). The **Ionization Subshells** (MT=534 through 572) have been updated to include the new binding energies. The **Bremsstrahlung** and **Excitation** are identical to what was included in the earlier EPICS2014 data base.

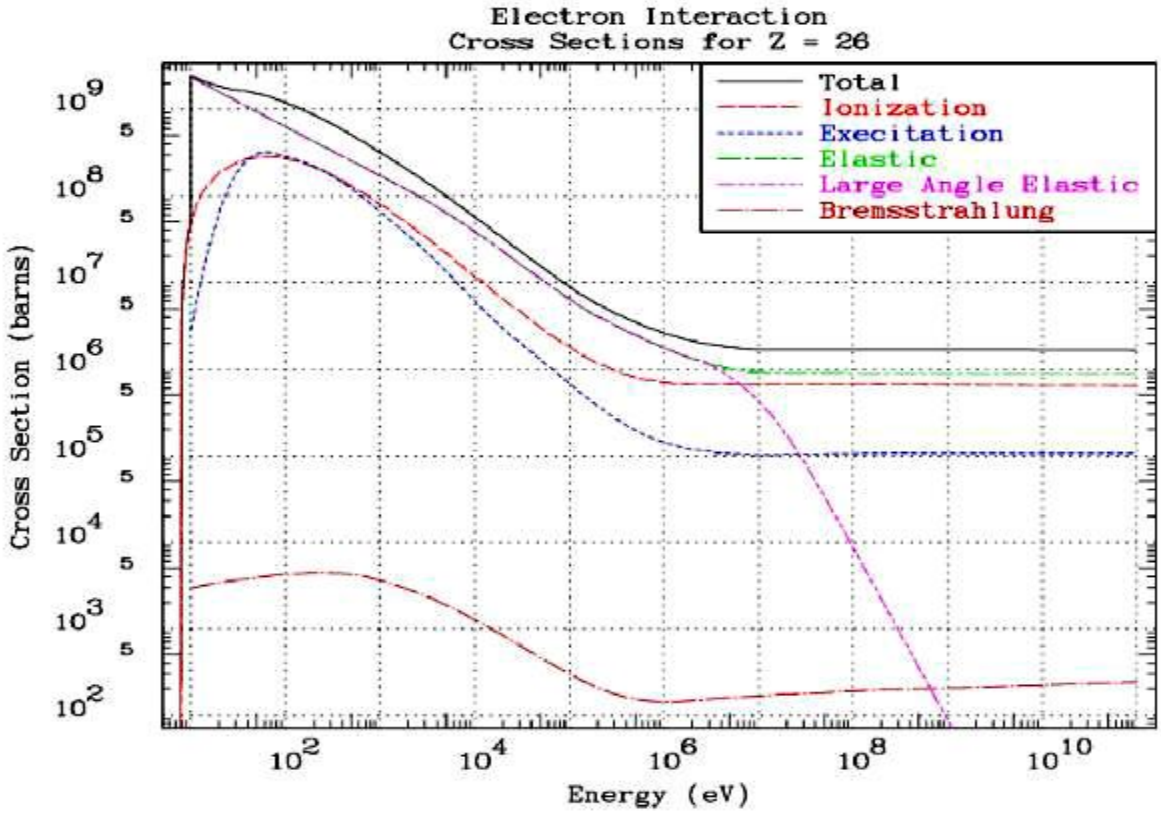
The MF=26 data are angular distributions and energy loss by electrons in a single collision. The **Large Angle Scatter Angular Distributions** describe scatter from cosine 0.999999 to -1.0, i.e., outside the narrow cosine range +1.0 to 0.99999. There are no angular distributions given for **Total Scatter**; scatter to the extremely narrow cosine range +1.0 to 0.999999 can be analytically defined by a small angle Coulomb expression defined by Seltzer [1]. The **Excitation** and **Ionization** Subshell data all define the energy loss by the electron; no information is provided to describe photons. For Excitation and Ionization; there are models available to define the relaxation of ionized atoms [11]. For **Bremsstrahlung** photon production spectra and electron average loss are both given; Bremsstrahlung is a three-body process, so there is no simple, unique correlation between the secondary photon and electron.

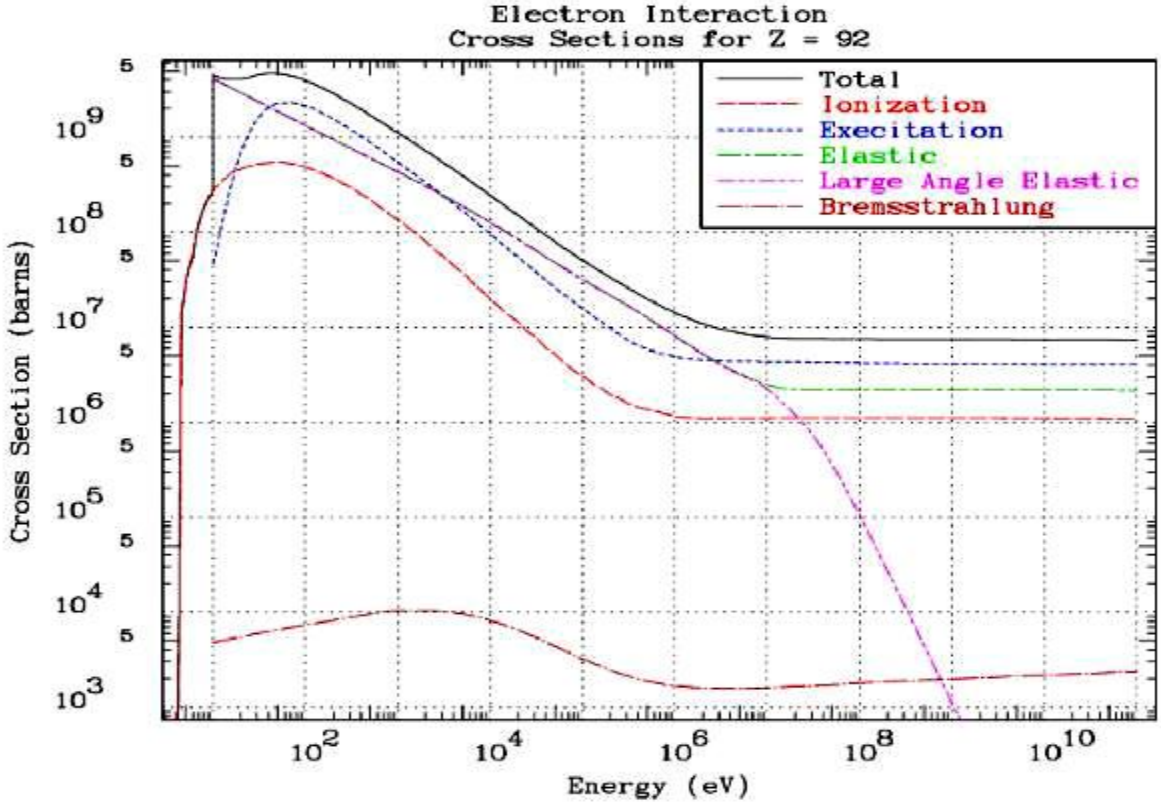
11. Electron Cross Section Overview

In this report, you will see that atomic electron interaction cross sections are simply related to the elemental atomic number, Z, across the entire periodic table; in this report we will present results for Z = 1 through 100. First, we present energy dependent cross sections for three elements: Z = 1, 26, 92, that illustrate the variation of the cross sections with energy across the periodic table, from very low to high Z. What you can learn from the below three plots includes,

1) **Ionization and Excitation** are important at all energies; these are the only processes that continuously lose/deposit energy locally, directly to the surrounding material, e.g., at all energies they are a primary source of **stopping power**, dE/dx,
2) **Bremsstrahlung** (braking radiation) is an important process at high energy; it significantly contributes to electron energy loss (**stopping power**), not by depositing energy to the surrounding material, but rather by creating photons; these photons must also be tracked. In principle, the low energy Bremsstrahlung spectra has a singularity, varying as p(E) ~ dE/E. In practice, this is not a serious problem, because the energy change E*p(E) ~ dE, predicting a simple linear dependence in energy loss. This does present a certain uncertainty in the definition of the Bremsstrahlung cross section, which we eliminate by truncating the spectra at a somewhat arbitrary lower energy; EEDL using 1 eV, whereas PENELOPE uses 10 eV [8]. As a result, we should not expect the EEDL and PENELOPE "cross sections" to be exactly equal, but we do expect the energy loss defined by both codes to be very similar, which is what EEDL is designed to accomplish.
3) **Elastic Scatter** is important at all energies, and is the only process that contributes to **turning power**, by causing electrons to scatter and straggle from their direction of motion. This is particularly important at energies below roughly 1 MeV. At higher energies the electrons still scatter, but through progressively smaller angles, or cosine ranges. We can see this effect on the below plots by comparing the **Elastic** and **Large Angle Elastic**. Here "large angle" means to a cosine outside of the range +1.0 to 0.999999, i.e., almost all of the scatter is in the extremely small cosine range +1.0 to 0.999999. The Elastic and Large Angle Elastic are roughly the same up to about 1 MeV. At higher energies, the Elastic approaches a constant, and the Large Angle Elastic decreases at about $1/E^2$ rate, i.e., at higher energies there is virtually no large angle scatter.



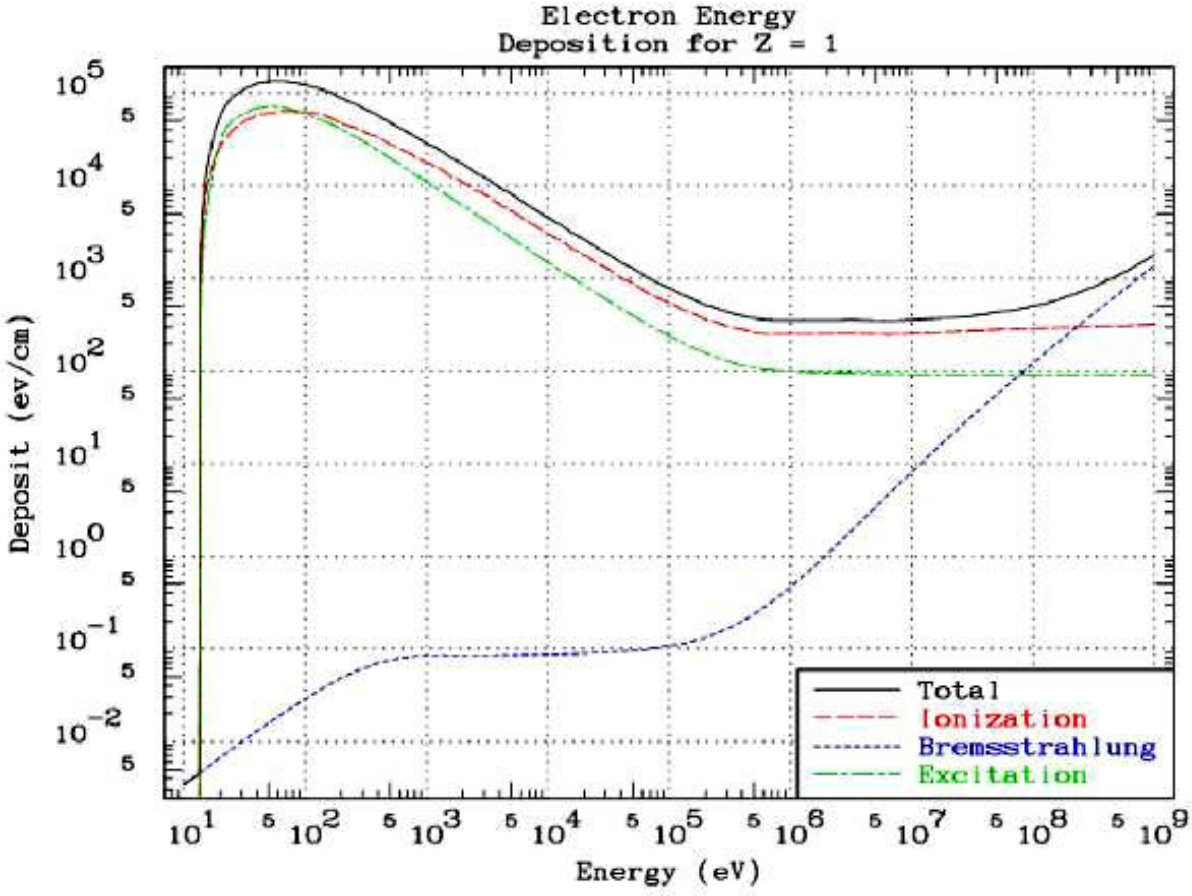

Electron Interaction
Cross Sections for Z = 26
Total
Ionization
Excitation
Elastic
Large Angle Elastic
Bremsstrahlung
Cross Section (barns)
Energy (eV)

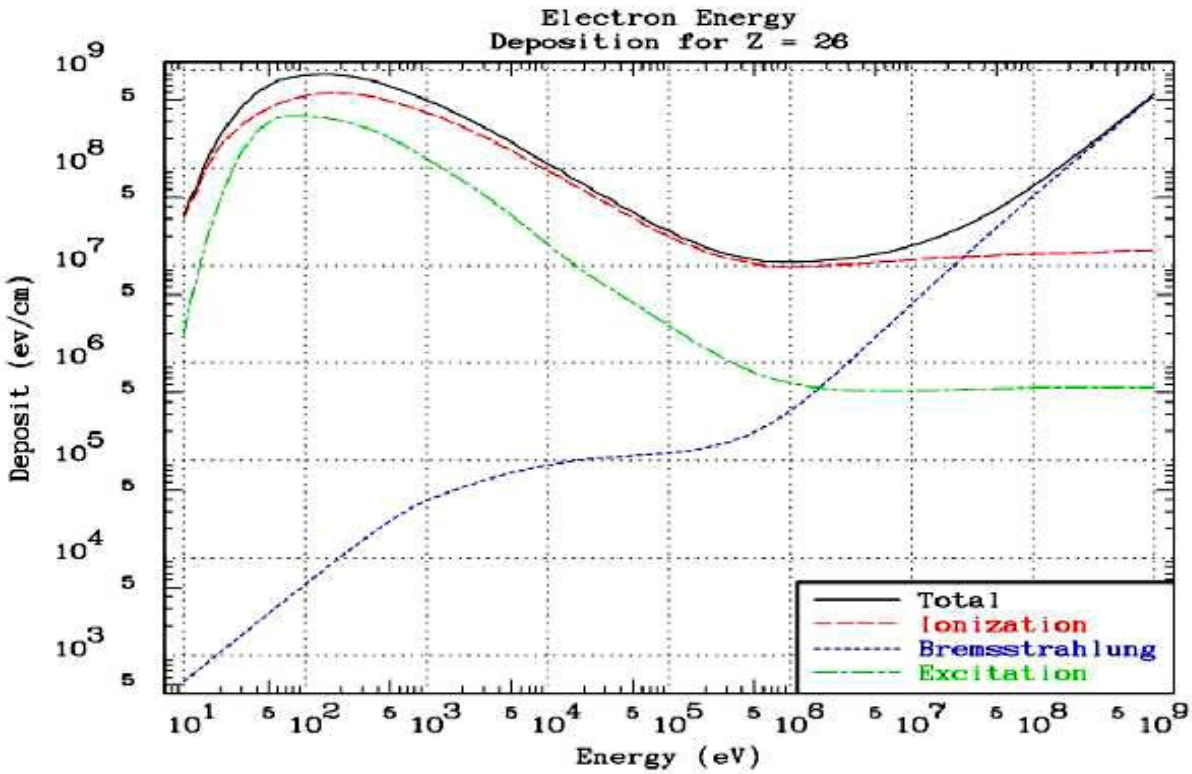

Electron Interaction
Cross Sections for Z = 92
Total
Ionization
Excitation
Elastic
Large Angle Elastic
Bremsstrahlung
Cross Section (barns)
Energy (eV)

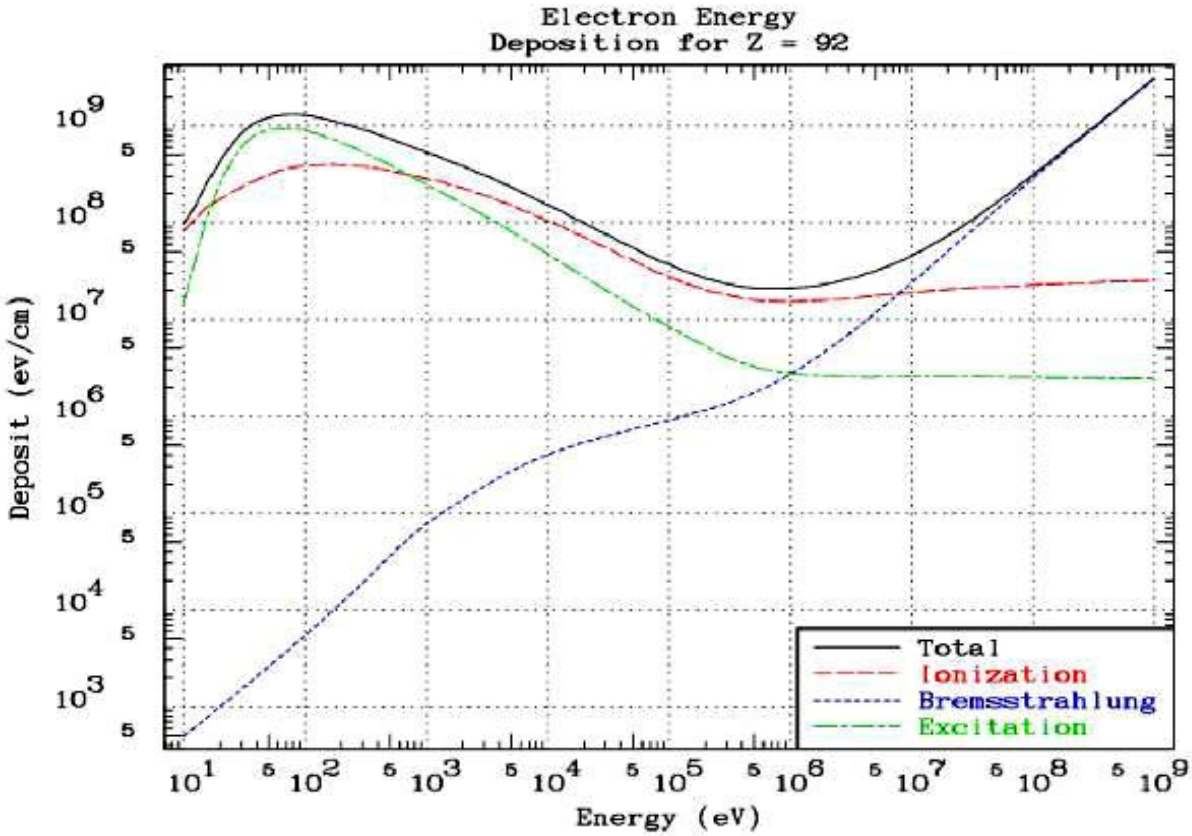
12. Electron Energy Deposition Overview

The above three figures illustrate electron interaction cross sections. But in electron transport what is most important is the **Stopping Power** and **Turning Power**. The below three figures illustrate the **Stopping Power** for the same three elements shown above: Z = 1, 26, 92. The Stopping Power is the product of the cross section times the energy loss per collision. For convenience, the below plots illustrate the Stopping Power at some nominal material density to introduce distance (cm). Here we see a very different picture, and hopefully more clearly the relative importance of each process to the energy loss by electrons.

In terms of cross section **Bremsstrahlung** would seem to be irrelevant, but the below plots of Stopping Power illustrate that at high energies it is THE DOMINANT process by which electrons lose energy; the cross section may be quite small, but the energy loss per collision can be quite large. **Ionization** and **Excitation** are important at all energies. In terms of cross section **Excitation** appears to be comparable to **Ionization**, but in terms of Stopping Power it is considerably less, because Excitation energies are so much lower than Ionization energies. Note that the **Ionization** and **Excitation** are almost constant above the MeV range; as mentioned earlier, electrons tend to lose the same amount of energy per collision, which makes simulation difficult, i.e., they have many collisions.



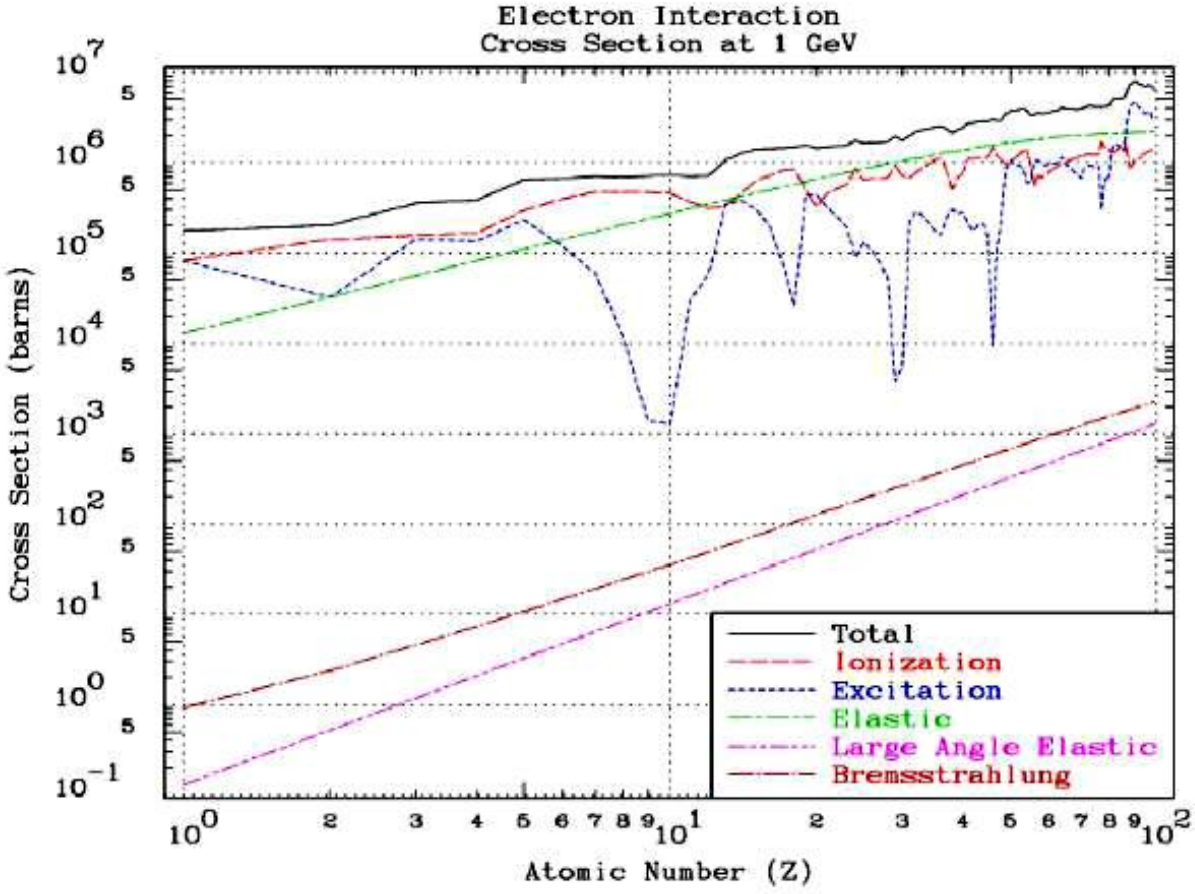

Electron Energy
Deposition for Z = 26
Deposit (ev/cm)
Energy (eV)
Total
Ionization
Bremsstrahlung
Excitation

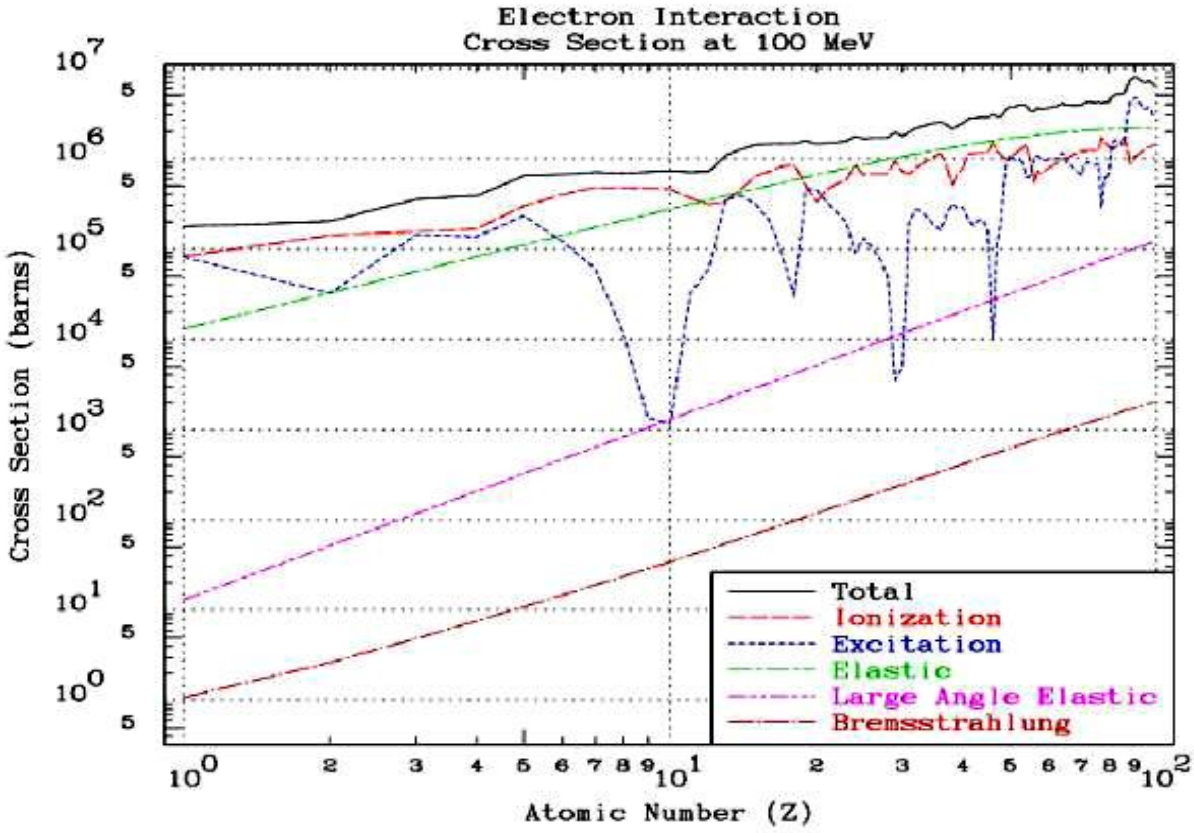

Electron Energy
Deposition for Z = 92
Deposit (ev/cm)
Energy (eV)
Total
Ionization
Bremsstrahlung
Excitation

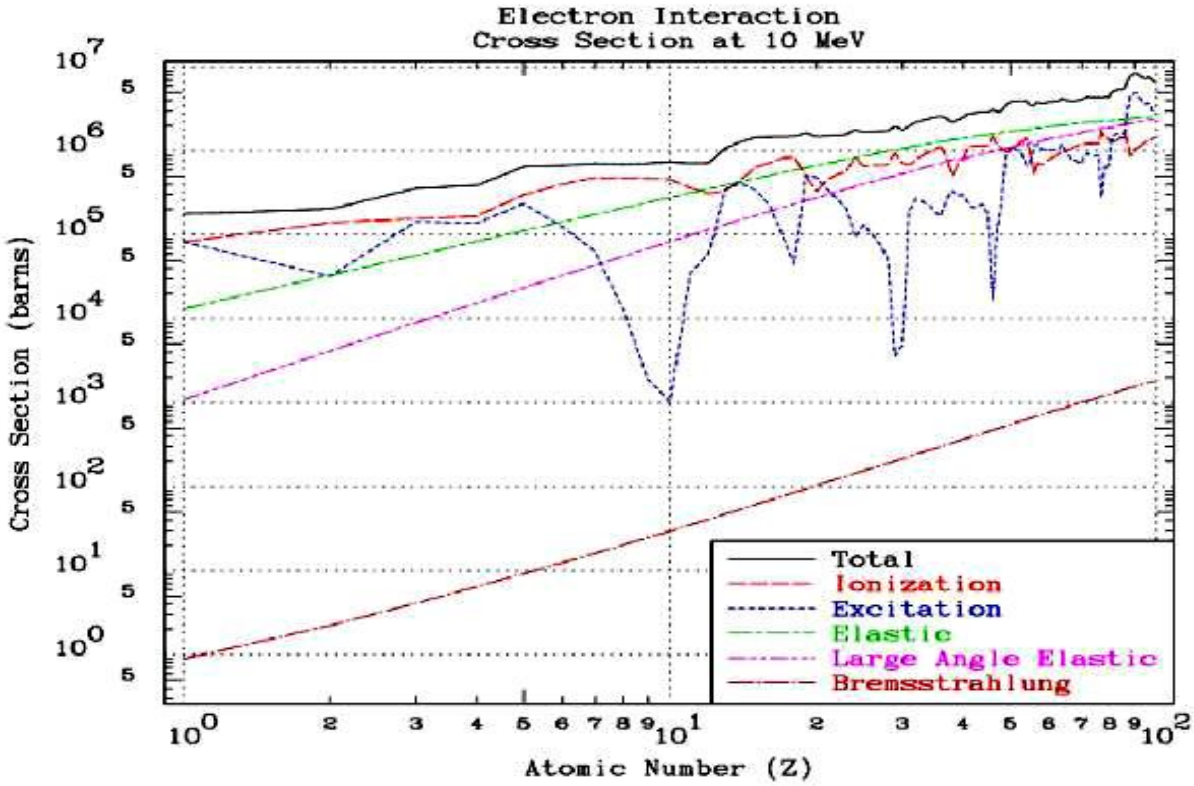
13. Cross Section Systematics versus Atomic Number (Z)

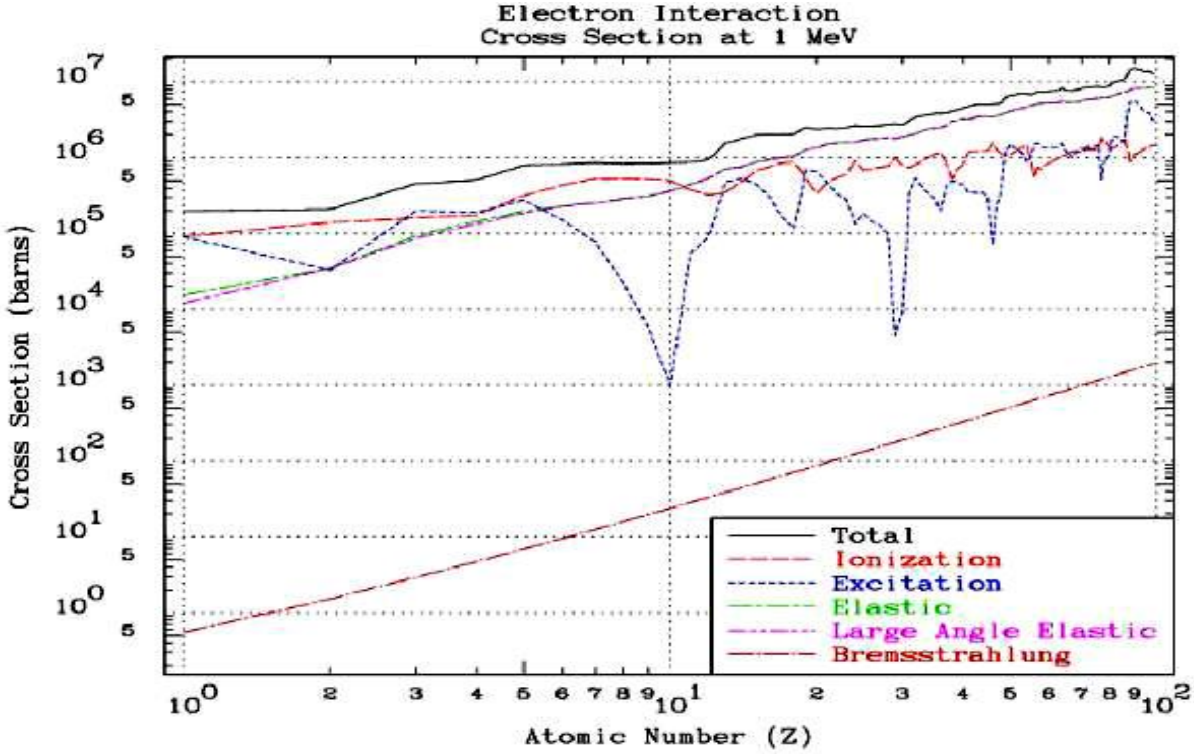
Above figures illustrate **the energy dependence** of the electron cross sections. To illustrate the simply atomic number (Z) dependence, the below figures show the variation of the cross sections for each process versus Z at seven incident photon energies: 1 GeV, 100 MeV, 10 MeV, 1 MeV, 100 keV, 10 keV and 1 keV. We show the results from high energy (1 GeV) to low energy (1 keV) to proceed from very simple variation versus atomic number (Z) to more complicated variations at low energies due to atomic shell effects.

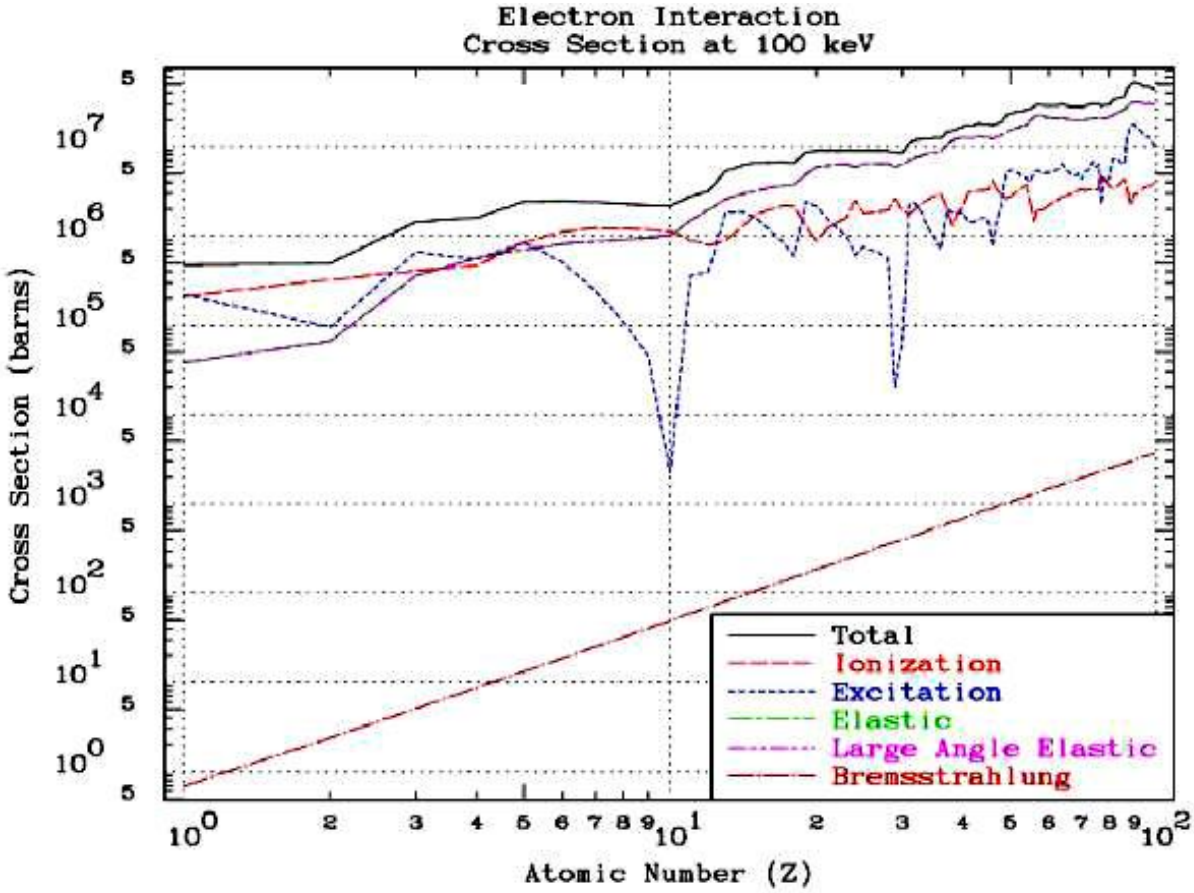
For **Bremsstrahlung** at all incident energies we see the simple variation of cross sections versus Z, i.e., almost straight lines on a log-log plot, showing variations as a power of Z ($Z^{N\backslash}$), see Ref. [10]. At higher energies, we also see simple variation versus Z for both **Elastic** and **Large Angle Elastic** cross sections. Note, that at higher energies the **Large Angle Elastic** is tiny compared to the **Elastic**: at 1 GeV about five decades less; at 100 MeV about three decades less; at 10 MeV still about one decade less; by 1 MeV and lower energies they are comparable. For **Excitation** we see strong shell effects at all incident energies, with sharp dips at and near closed shells.

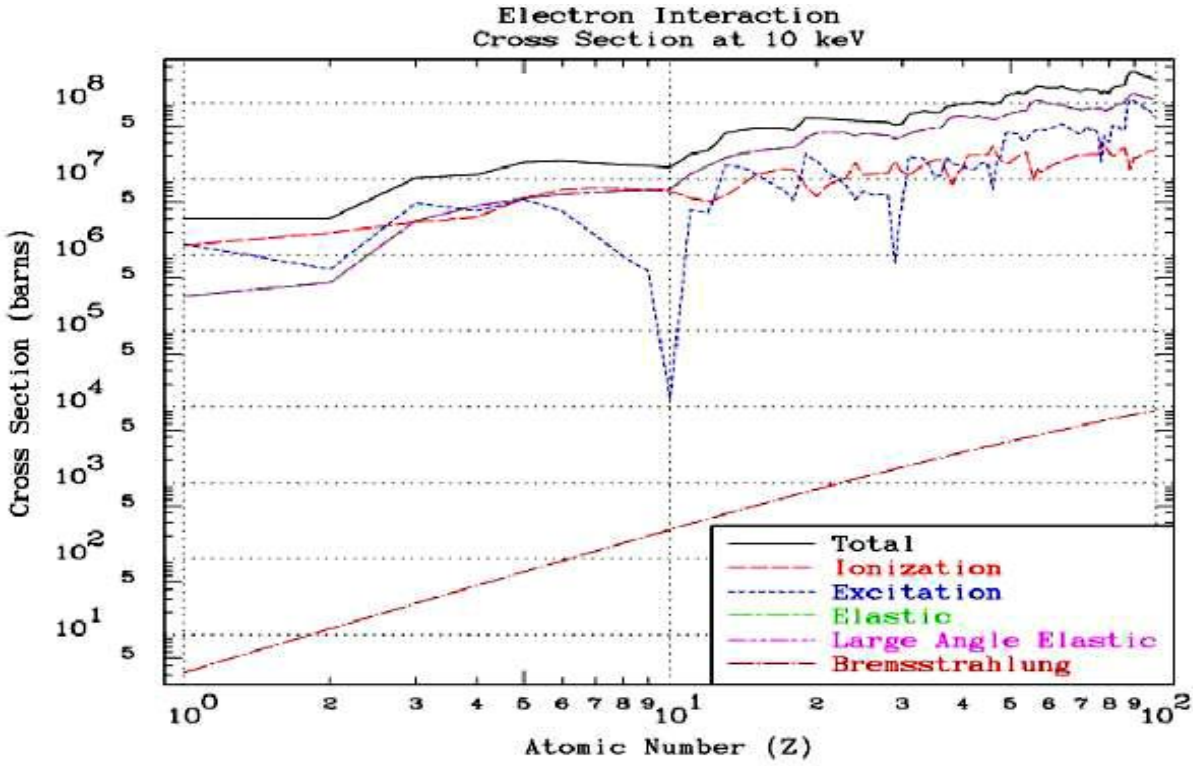


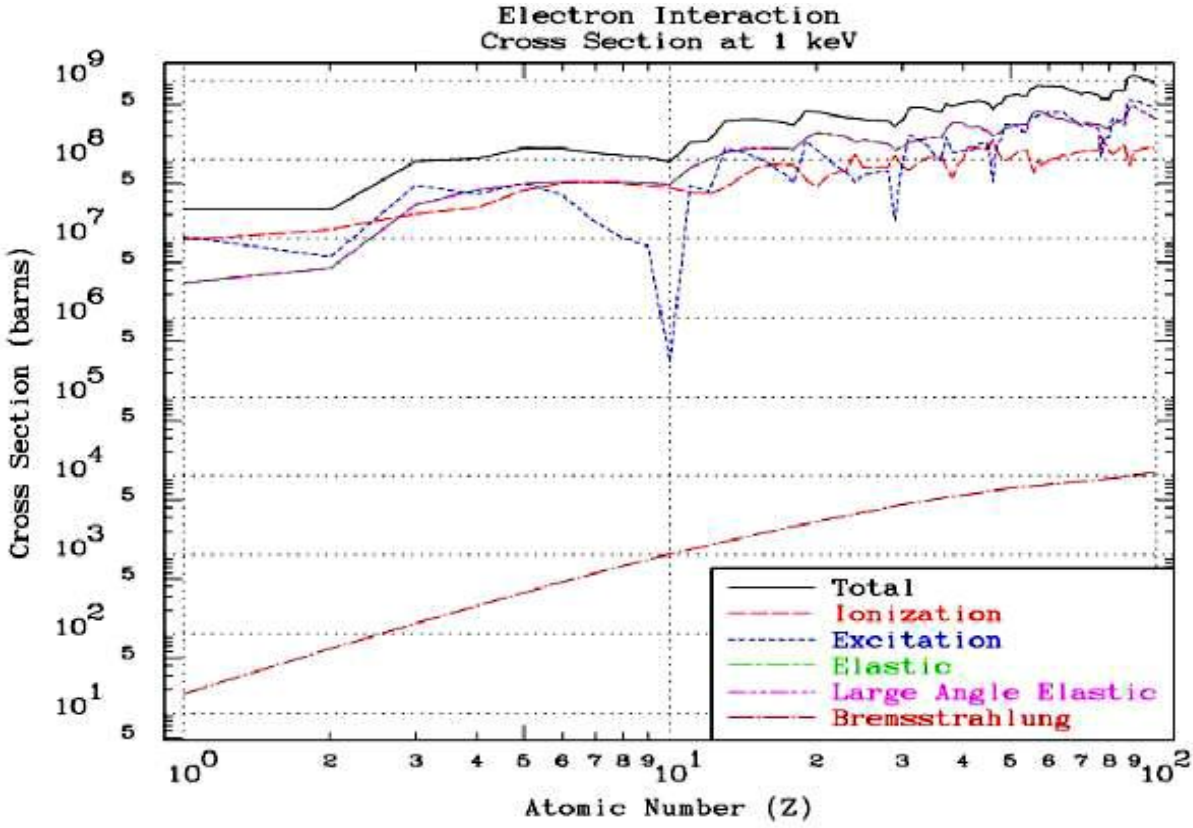

Electron Interaction
Cross Section at 100 MeV
Cross Section (barns)
Atomic Number (Z)
Total
Ionization
Excitation
Elastic
Large Angle Elastic
Bremsstrahlung


Electron Interaction
Cross Section at 10 MeV
Cross Section (barns)
Atomic Number (Z)
Total
Ionization
Excitation
Elastic
Large Angle Elastic
Bremsstrahlung


Electron Interaction
Cross Section at 1 MeV
Cross Section (barns)
Atomic Number (Z)
Total
Ionization
Excitation
Elastic
Large Angle Elastic
Bremsstrahlung


Electron Interaction
Cross Section at 100 keV
Cross Section (barns)
Atomic Number (Z)
Total
Ionization
Excitation
Elastic
Large Angle Elastic
Bremsstrahlung

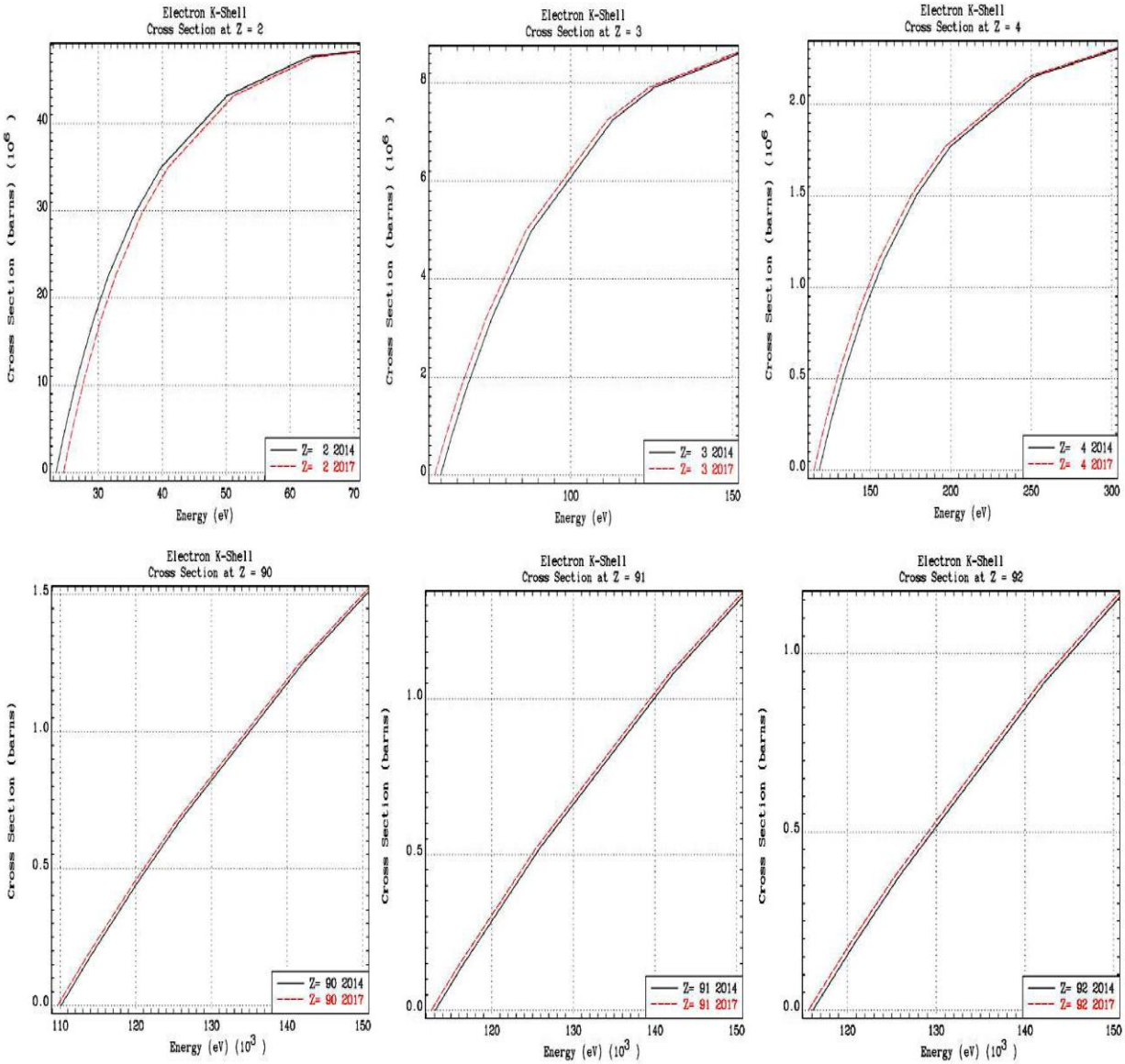

Electron Interaction
Cross Section at 10 keV
Cross Section (barns)
Atomic Number (Z)
Total
Ionization
Excitation
Elastic
Large Angle Elastic
Bremsstrahlung


Electron Interaction
Cross Section at 1 keV
Cross Section (barns)
Atomic Number (Z)
Total
Ionization
Excitation
Elastic
Large Angle Elastic
Bremsstrahlung

14. The Effects of New Binding Energies

The above comparison of EPICS2014 [2] and Deslattes [7] binding energies show that for the EPICS2017 binding energies to agree with the Deslattes data, a shift in the EPICS2017 binding energies by up to 1% for low Z elements and 0.5% for high Z elements is required. The below plots illustrate for K-Shells the differences between the EPICS2014 and EPICS2017 cross sections. First are results for low Z = 2, 3, 4, where the 2017 values are shifted to slightly higher energies, and then for high Z = 90, 91, 92, where the 2017 values are shifted to slightly lower values.

The Important thing that we can learn from these plots is that it is difficult to even see the differences in the K-Shell cross sections. Updating the binding energies is important so that the EPICS2017 data reproduce the well-known characteristic fluorescence x-rays, as shown in Deslattes paper [7], but based on the small shifts in the electron ionization data, shown below, we should not expect much of a change in the transport and slowing down of electrons.



15. Release of EPICS2017

I am hoping to complete EPICS (EADL, EEDL, EPDL) by the end of 2017. Earlier publications documented the completion of the atomic data EADL [5] and photon data EPDL [6]. With this document, the electron data (EEDL) have been completed. To ensure an energy balance for photon and electron transport calculations it is imperative that all parts of EPICS use the same binding energies and corresponding photoelectric edges. Therefore, the numerical values for the newly adopted binding energies (EADL), photon data (EPDL), and electron data (EEDL), will all be released simultaneously. Work on creating these data bases is now completed before the end 2017. All that remains is to package and completely check them before their release to the public, which is planned for early in 2018.

16. Conclusions

I have presented here my Survey of Atomic Electron Cross Section Data for use in EPICS2017. There are few original results in this report; most of the original work was done by those who put together the compilations that I used; one being my own EEDL data. I started from my existing compilations of electron cross section data (EEDL), and compared it to PENELOPE data. I added new edge energies to ionization subshells and updated ionization subshell cross sections and energy spectra to correspond to the new edges. I discovered and corrected an error in the ENDF formatted translation, involving the scattering cross sections. I also added sum cross sections for total and ionization, as well as a few tests for the expected systematics. In this report, I extensively used graphics to illustrate the energy dependence and simple Z dependence of the cross sections, and to illustrate the important differences between cross section and energy deposition. I put the final results into the ENDF/B format, so that they can be easily used by as many computer codes as possible. **After reviewing all the electron data, I have decided for EPICS2017 that it is sufficient to only change binding energies, to insure they are consistent with the changes already made to EADL and EPDL.**

If after reading this paper you are left with the impression that our data are not perfect, good, you get the point. Our data is far from perfect and improving it is an ever-continuing effort. I can only hope that this paper, is some small way, contributes to our efforts toward understanding and improving our data. Most important: I encourage you, the reader, to also contribute to this effort, by reporting your measured and calculated results to me.

17. References

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

[2] D.E. Cullen, **EPICS2014**: Electron Photon Interaction Cross Sections (Version 2014), IAEA-NDS-218, September 2014, Nuclear Data Section (NDS), IAEA, Vienna, Austria.

[3] **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

[4] F. Salvat, Private Communication (2017). Cross sections at lower energies are known to be extremely uncertain, and are not recommended for use in transport calculation.

[5] D.E. Cullen, **EADL2017:** Survey of Atomic Binding Energies for use in EPICS2017, IAEA-NDS-224, September 2017, Nuclear Data Section (NDS), IAEA, Vienna, Austria.

[6] D.E. Cullen, **EPDL2017:** Survey of Atomic Photon Cross Section Data for use in EPICS2017, IAEA-NDS-225, November 2017, Nuclear Data Section (NDS), IAEA, Vienna, Austria.

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

[8] F. Salvat, **PENELOPE**-2014: Code System for Monte Carlo Simulation of Electron and Photon Transport Workshop, Barcelona, Spain, 29 June-3 July 2015.

[9] D.E. Cullen, **PREPRO/LINEAR**, part of PREPRO2017: 2017 ENDF/B Pre-processing Codes, IAEA-NDS-39, Rev. 17, May 2017, Nuclear Data Section (NDS), IAEA, Vienna, Austria.

[10] **LOG-LOG**: On a log-log plot a straight line indicates: log(sigma) ~ N*log(Z), and you can estimate N by noting for each decade change in Z how many decades the cross section (sigma) changes. For example, at 1 GeV, between Z=1 and 10 the total changes by less than two decades (N < 2), and the photoelectric changes by roughly five decades (N ~ 5). We can also see the variations of Pair as Z^2 and Triplet as Z.

[11] D.E. Cullen, PROGRAM **RELAX**: A Code Designed to Calculate X-Ray and Electron Emission Spectra as Singly Charged Atoms Relax Back to Neutrality, Lawrence Livermore National Laboratory, UCRL-ID-110438, March 1992.