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A Survey of Photon Cross Section Data for use in EPICS2017

by

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Abstract: I have presented here my Survey of Atomic Photon Cross Section Data for use in EPICS2017. There are few original results of in this report; most of the original work was done by those who put together the compilations that I used; one being my own EPDL data. I started from my existing compilations of photon cross section data (EPDL), and compared it to PENELOPE, NIST and Scofield data. I added new edge energies to photoelectric and calculated the corresponding anomalous and coherent scattering data. I also added a few tests for the expected systematics. I put the final results into the ENDF/B format, so that they can be easily used by as many computer codes as possible. In this report I extensively used graphics to illustrate the simple Z dependence of the data and to compare sets of data, to give the reader a realistic estimate of the uncertainty in this data. **After reviewing all the data, I have decided for EPICS2017 to only change: binding energies, photoelectric cross sections, anomalous and coherent scatter.**

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Vienna, February 2018

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1. Dedication

I dedicate this paper to **John Hubbell**, my colleague, co-author of papers as far back as 1989, and most important to me, my friend. In many fields people have said: We can see so far because we stand on the shoulders of giants. In photon cross sections John was that giant, and we can still see so far because of his work that we continue to use today, long after he has left us. All of us who had the privilege of knowing you, miss you today John.

2. Acknowledgement

February 2018 Update: This paragraph is the only change in this report for the February 2018 update. I thank **Marilena Bandieramonte** (CERN) for discovering and reporting an ERROR in the ENDL formatted version of EPDL2017. This ERROR only involved the ENDL formatted data for the total ionization cross section, but I took this opportunity to improve the Form Factors and Scattering Functions in the ENDL format to insure they can be accurately interpolated using linear interpolation. There were NO CHANGES to the ENDF formatted data. The remainder of this report are identical to the original November 2017 report.

I should like to start by thanking Francesc Salvat (U Barcelona), Paul Bergstrom (NIST), and Jim Scofield (LLNL) for providing their compilations of photon 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 photon interaction cross sections for use in EPICS2017. I also thank these three individuals 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.

3. 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 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 [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 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.**

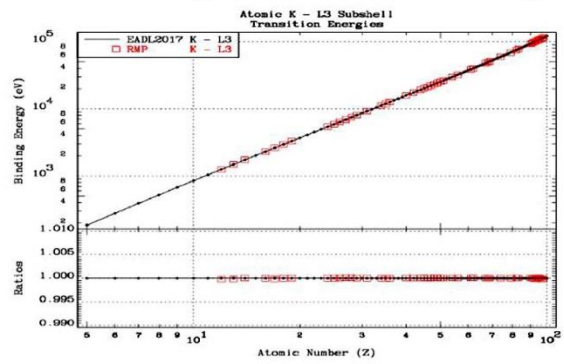
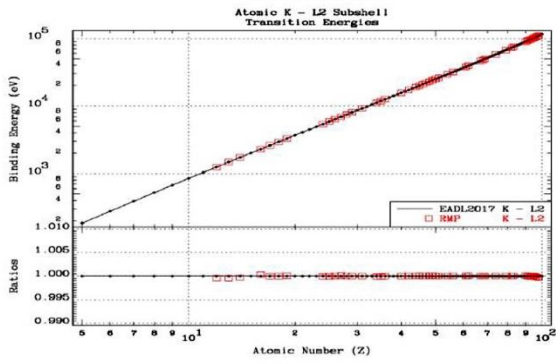
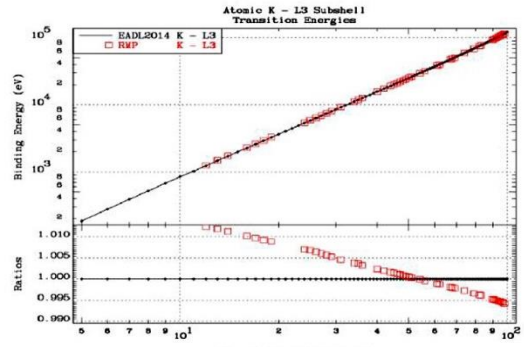
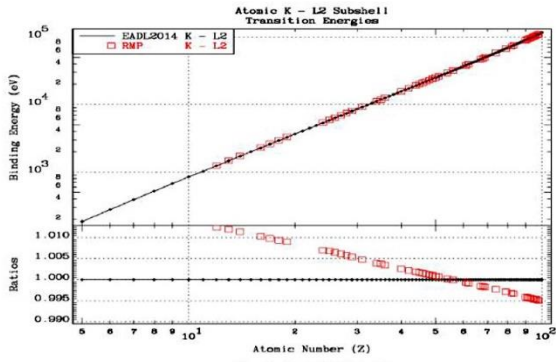
The electron and photon data used in EPICS are limited to **ATOMIC DATA**, elemental, cold, neutral, isolated atoms; this is in line with its intent for use in engineering applications. This limits the data to be used ONLY at higher energies. **I recommend that it should not be used in applications below 100 eV;**

Francesc Salvat recommends not below 1 keV [3]. 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.**

4. 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 [4]. For consistency and to conserve energy, these binding energies must now be incorporated into EPDL, for photons, and EEDL, for electrons. The new binding energies require an update to the photoelectric cross sections as well as anomalous and coherent scattering data (which must be defined as an integral over the new photoelectric data). Here I document the results of these updates, and I also take this opportunity to review all the other photon data for EPDL.

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 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 [5], 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 [5] 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.



5. 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** [1]. 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** [6]. 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.
- 3) **NIST** [7]. This is tabulated data from the XCOM code, provided to me by Paul Bergstrom (NIST), for $Z = 1$ through 100.
- 4) **Scofield** [8]. These are Jim Scofield's photoelectric cross sections tabulated from 1 keV to 1.5 MeV for $Z = 1$ through 101.
- 5) **Hubbell** [9, 10]. These NIST reports document the many experimentally measured data included in John Hubbell's collection. These data and reports were used for comparison to the above mentioned evaluated data sets. In selecting the BEST data for use in EPICS2017 I viewed hundreds of plots comparing evaluated and measured data; far too many to include in this short document, but invaluable in understanding particularly the spread/uncertainty in measured values.

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, PENELOPE, NIST and Scofield. 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. Below we will see that 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 [3].** 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

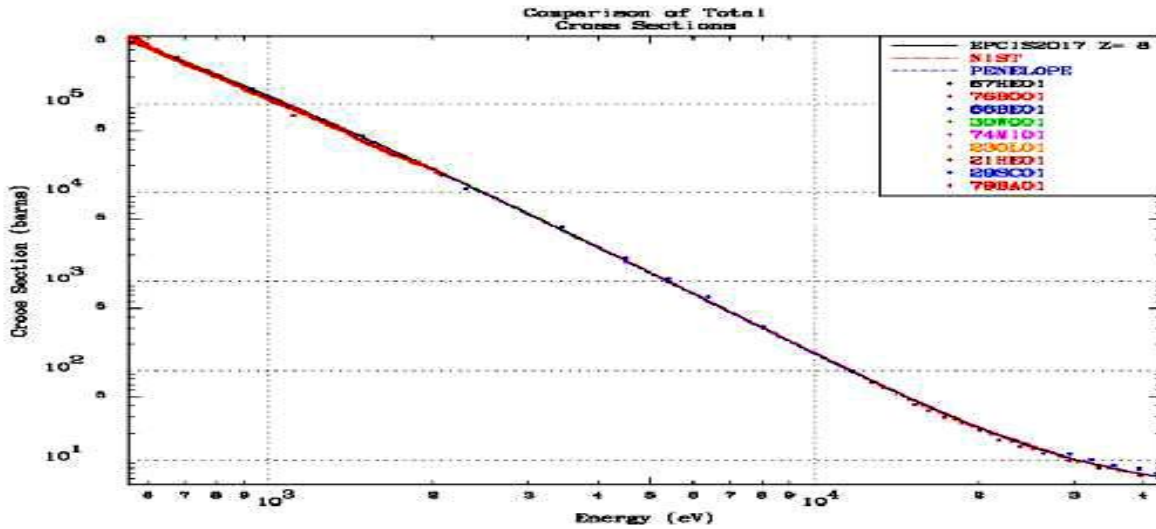
20% higher than 13.6 eV. Let me repeat: based on our objective of elemental, cold, neutral, isolated atoms we use 13.6 eV. This is but the simplest example; differences in binding for compounds, etc., can be enormous. Fortunately, these differences have little or no effect on the macroscopic quantities 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.

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 up to a small fraction of 1%). With decreasing Z and energy, we will see increasing differences (often 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. 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.

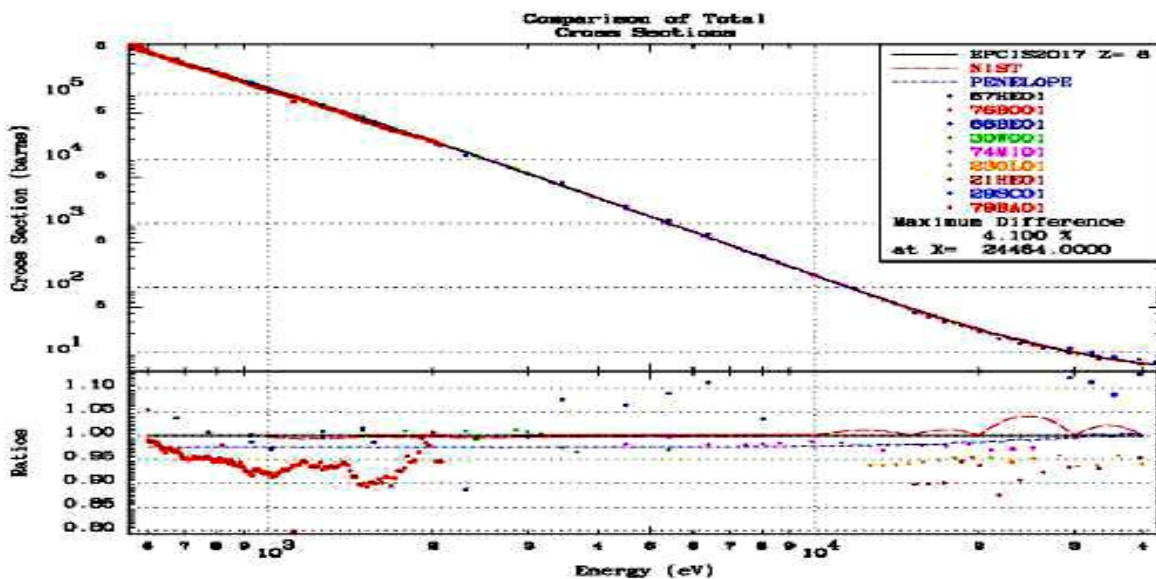
But **CAVEAT EMPTOR (let the user beware)** if you ignore our WARNINGS and transport electrons and/or photons to lower energies your results can become progressive worse, and you will have nobody to blame but yourself.

6. The Importance of Ratios

The photon cross sections that we use vary over many orders of magnitude in incident photon energy and in cross section (barn) values. This makes it very difficult to actually “see” differences on a plot. For example, the below plot compares 8O (Z=8) 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.



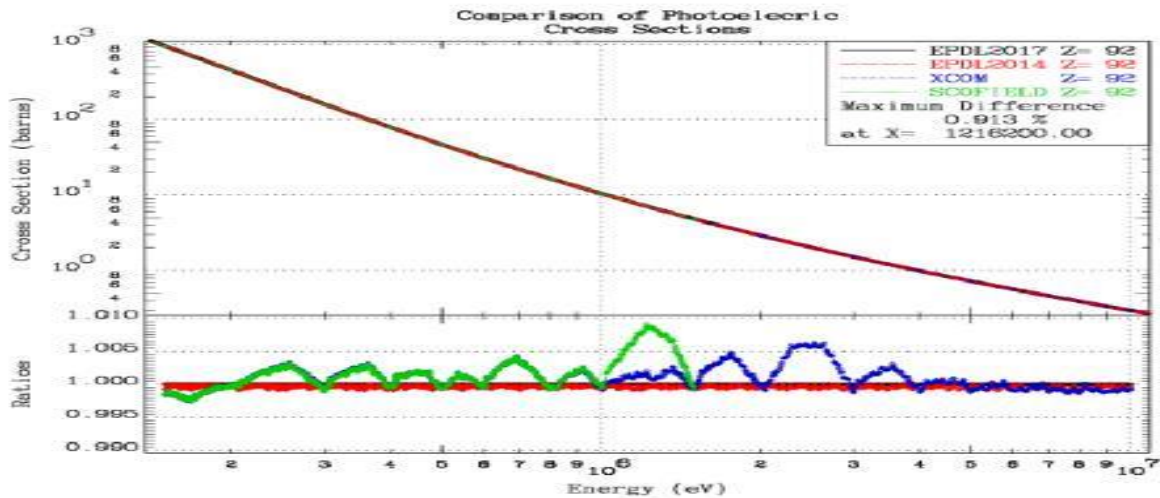
7. The Importance of Interpolation

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.

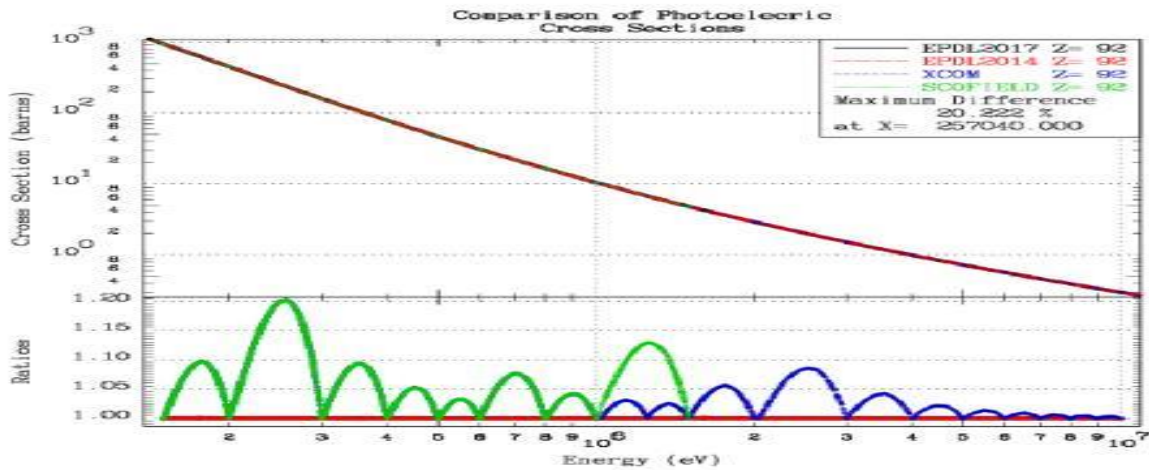
Generally experienced ENDF data users are aware of the importance of correctly interpolating, but for those who are not so aware we present a simply example that we hope will scare the hell out of you, and make you aware of just how much damage you can do to your calculated results by not obeying the 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, The result is that **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” 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 insure 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 [11]. The result is libraries are roughly three (3) times as large (e.g., has 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.**

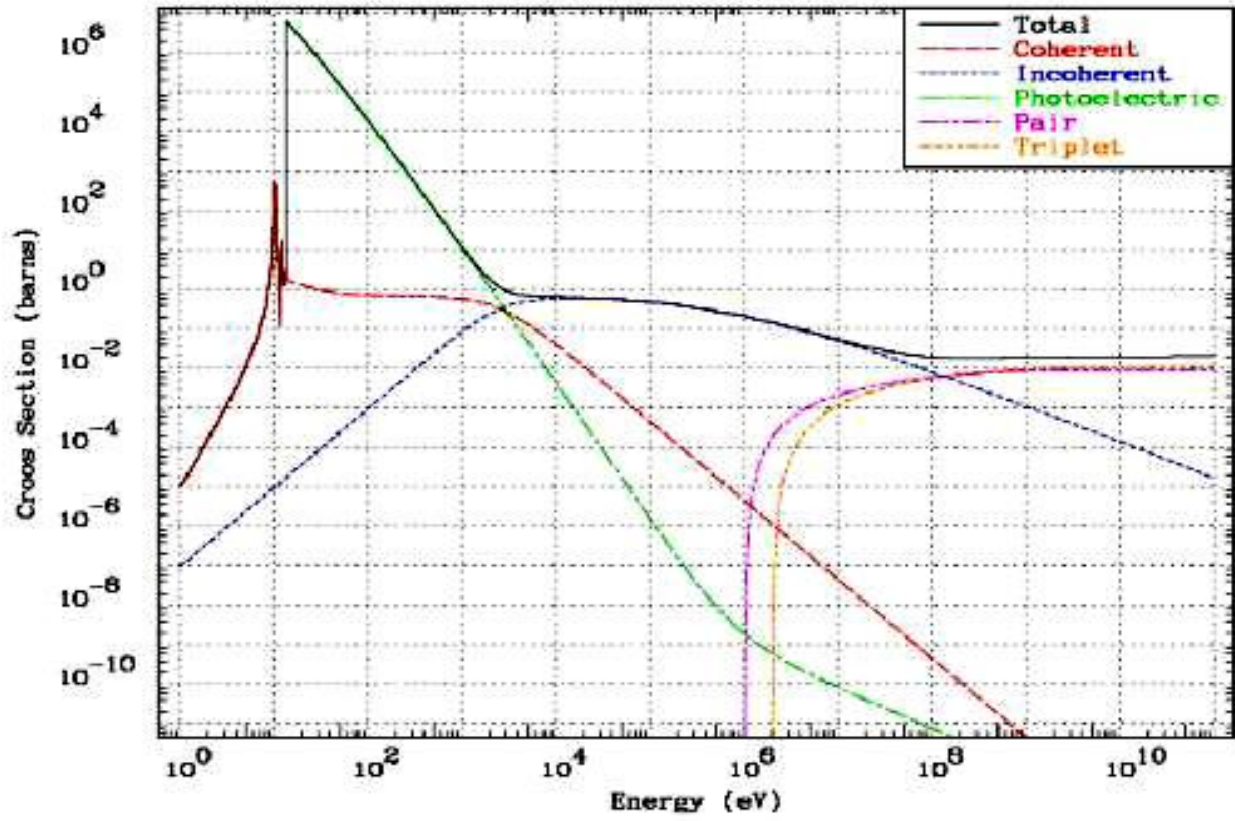
8. Photon Cross Section Overview

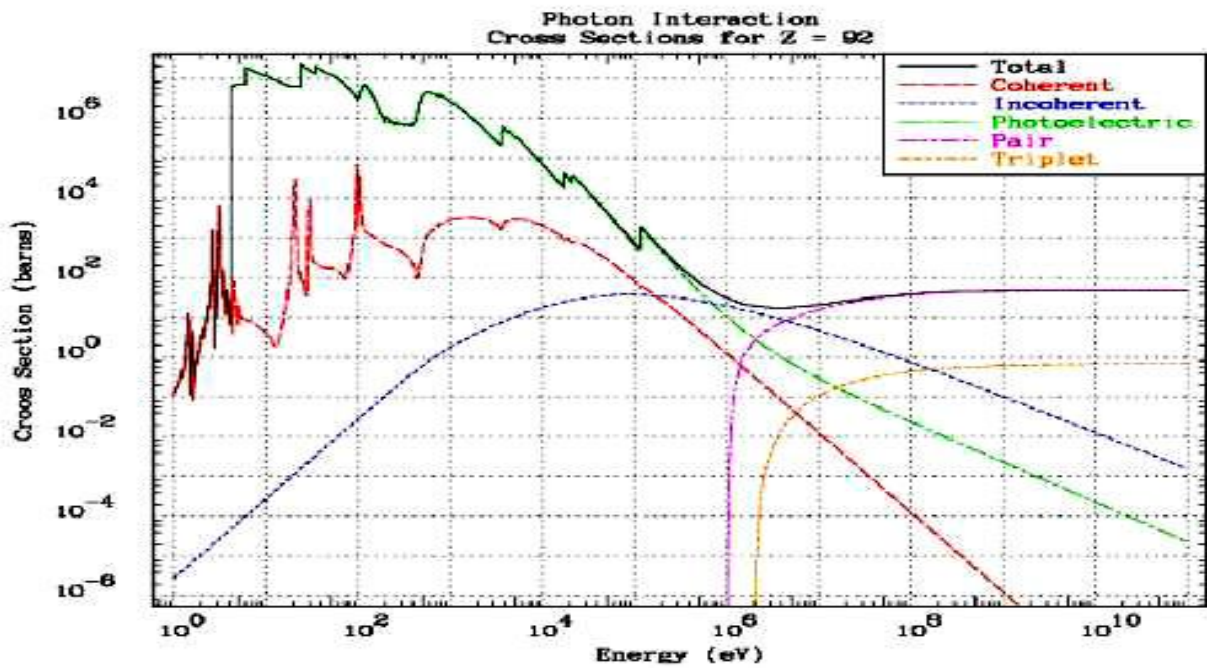
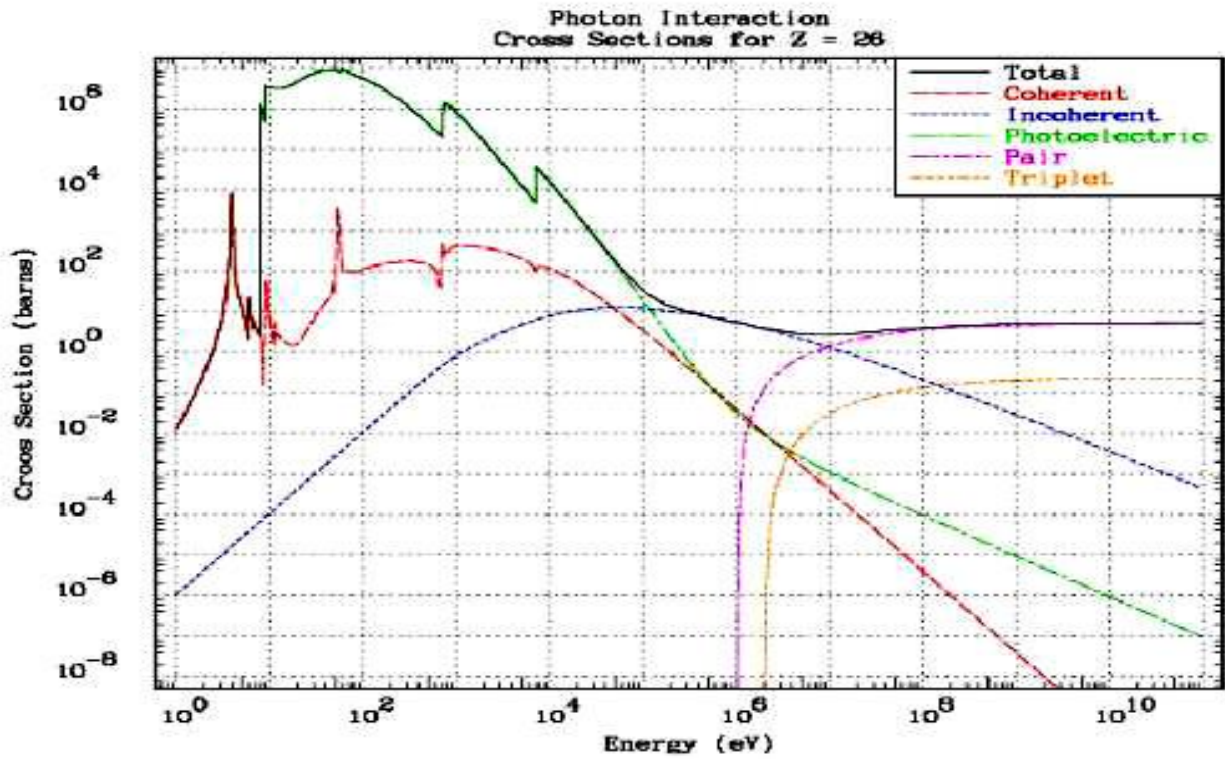
In this report you will see that atomic photon interaction cross sections are simply related to the elemental atomic number, Z , across the entire periodic table; in this report we will present results for $Z = 1$ through 100.

First, we present energy dependent cross sections for three elements: $Z = 1, 26, 92$, that illustrate the variation of the cross sections across the periodic table, from very low to high Z . What you can learn from the below three plots includes,

- 1) At low energies (keV range) **Photoelectric** Absorption is always the dominant process.
- 2) In the MeV range **Incoherent** Scatter becomes an important process, particularly for low Z elements.
- 3) At higher energies (MeV to GeV) **Pair** and **Triplet** Production become the dominant processes.
- 4) Although **Coherent** scatter is important there is no energy range in which it is the dominant process.
- 5) The **Pair** scales as Z^2 , and the **Triplet** as Z , e.g., at high energy for $Z = 1$ they are almost equal, for $Z = 92$, the **Pair** is about 92 times larger than the **Triplet**.

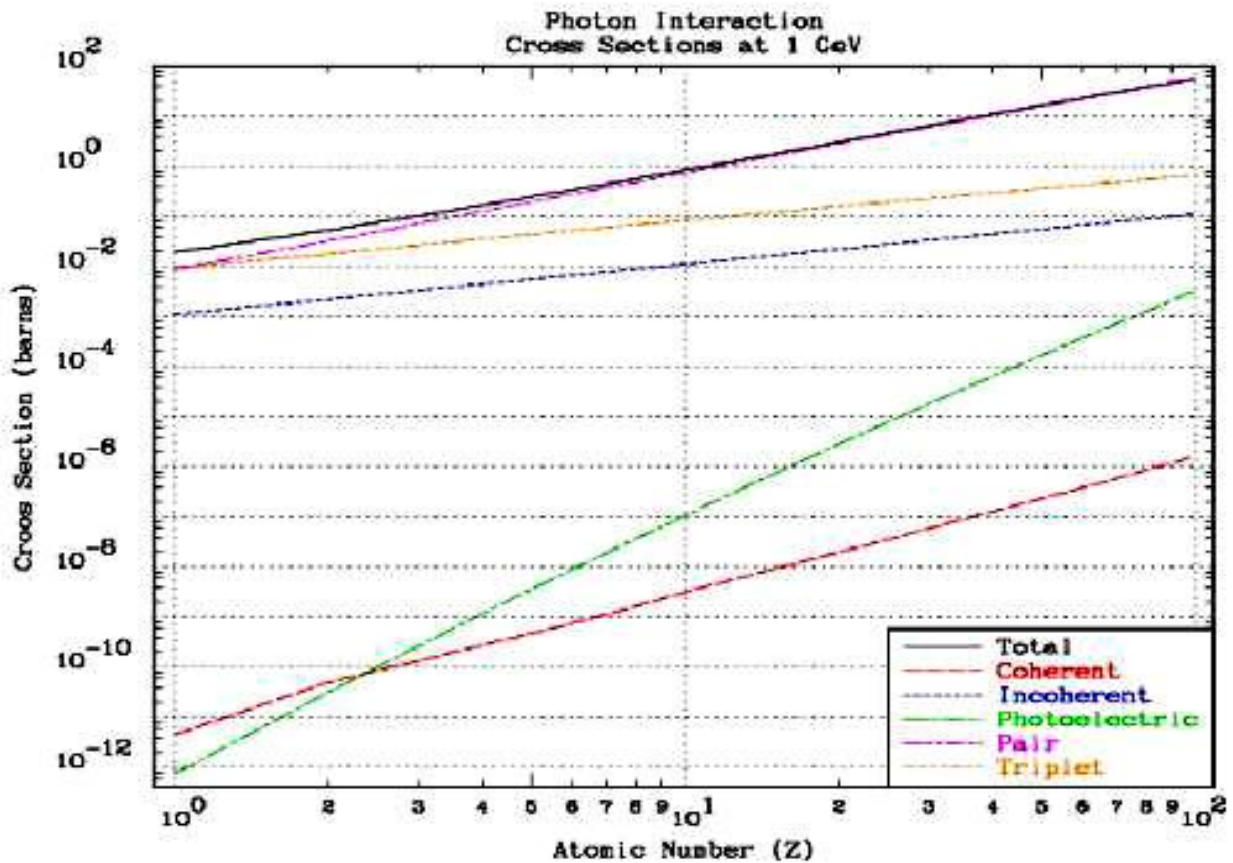
Photon Interaction
Cross Sections for $Z = 1$

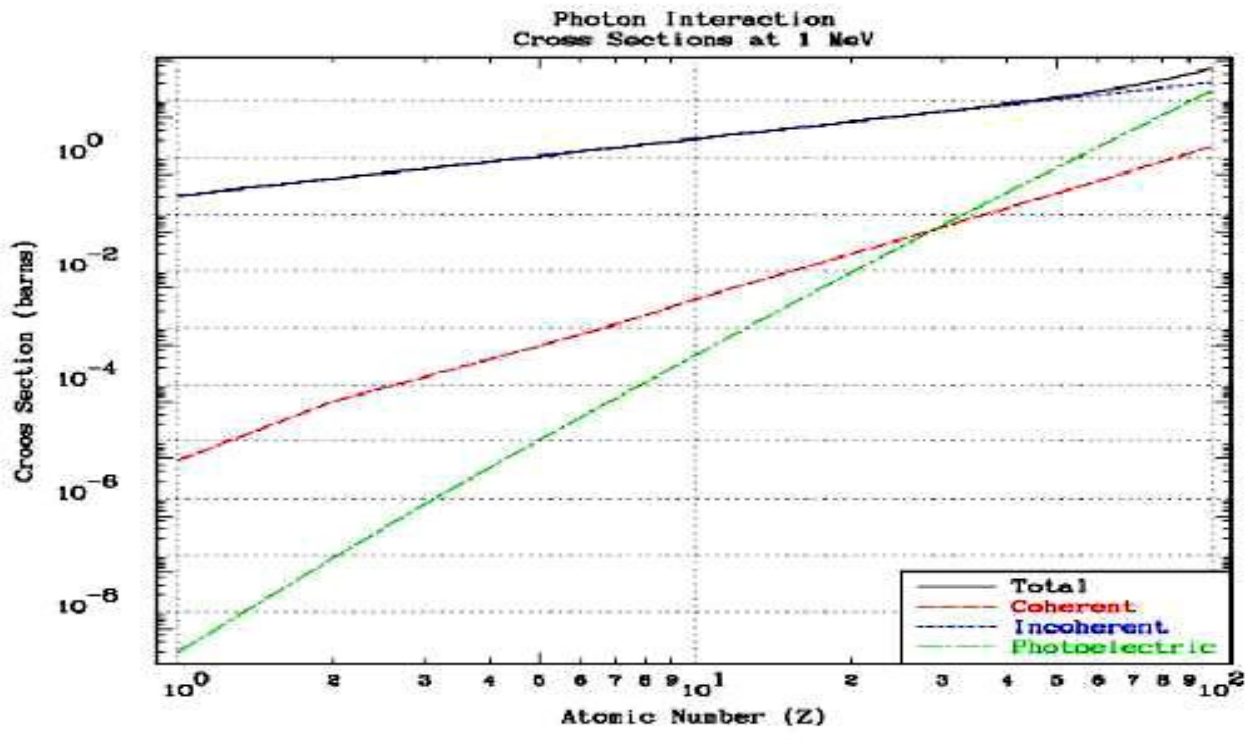
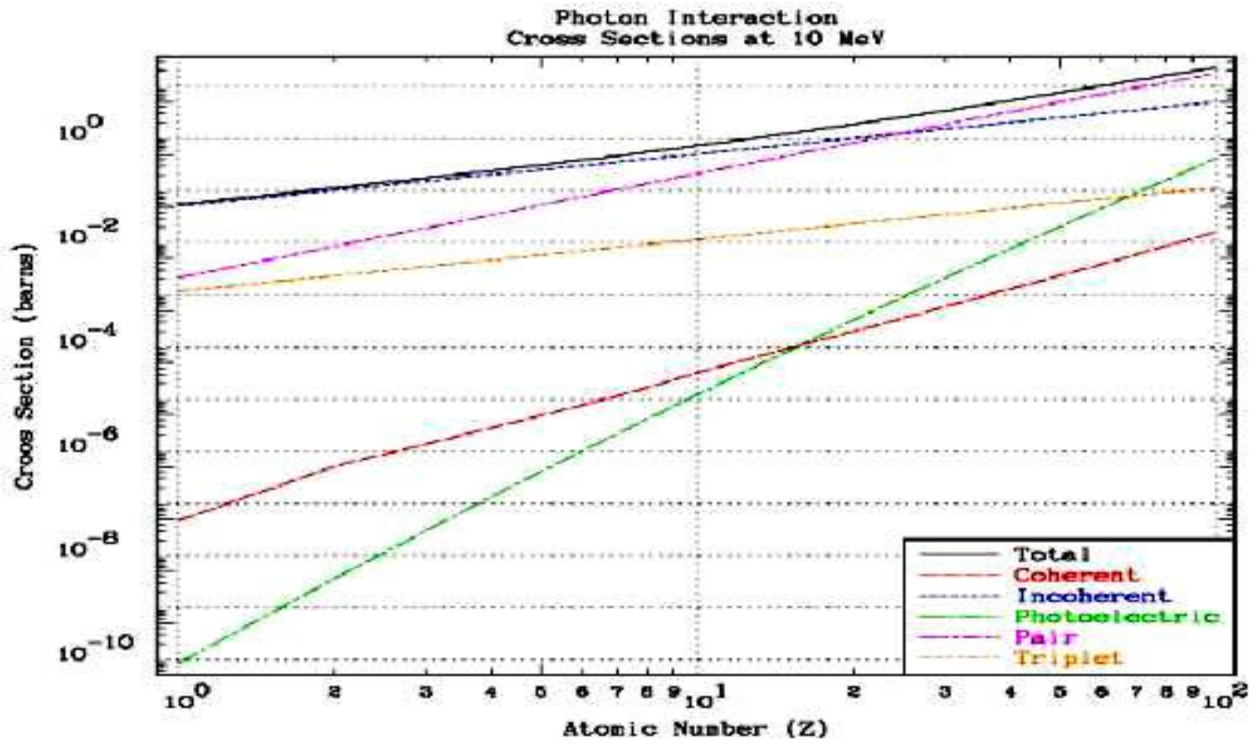


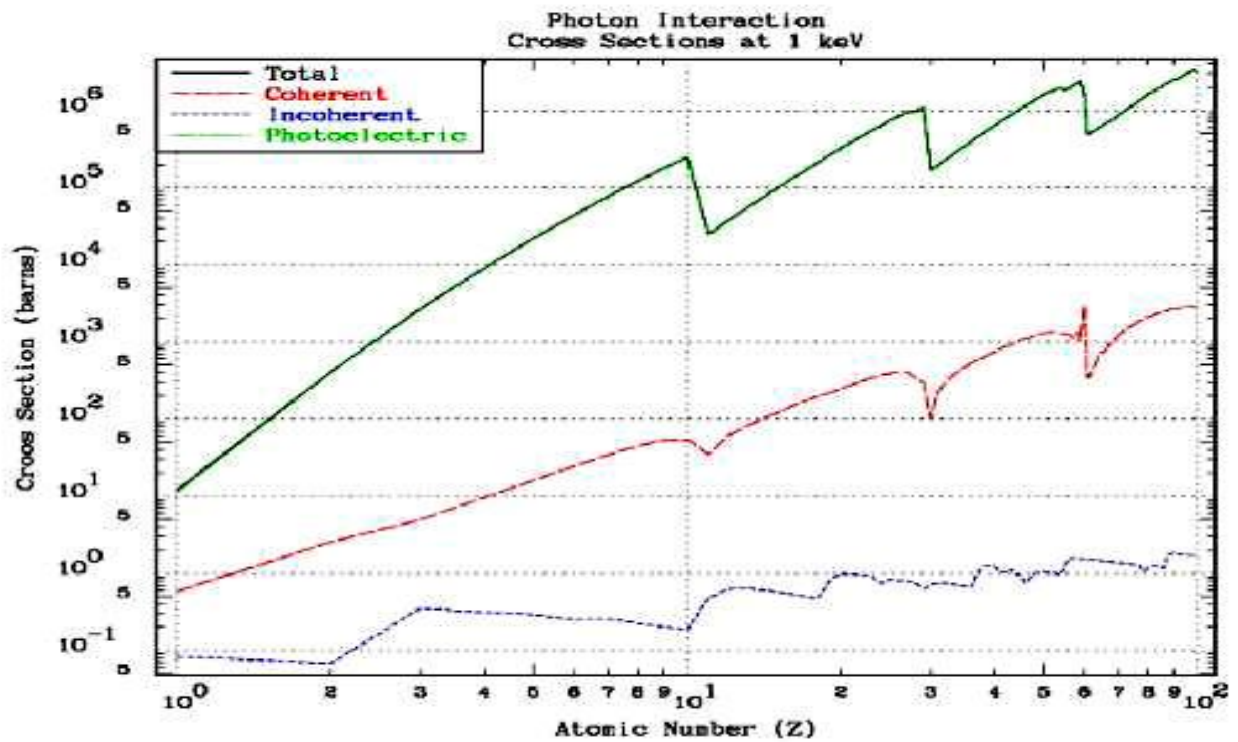
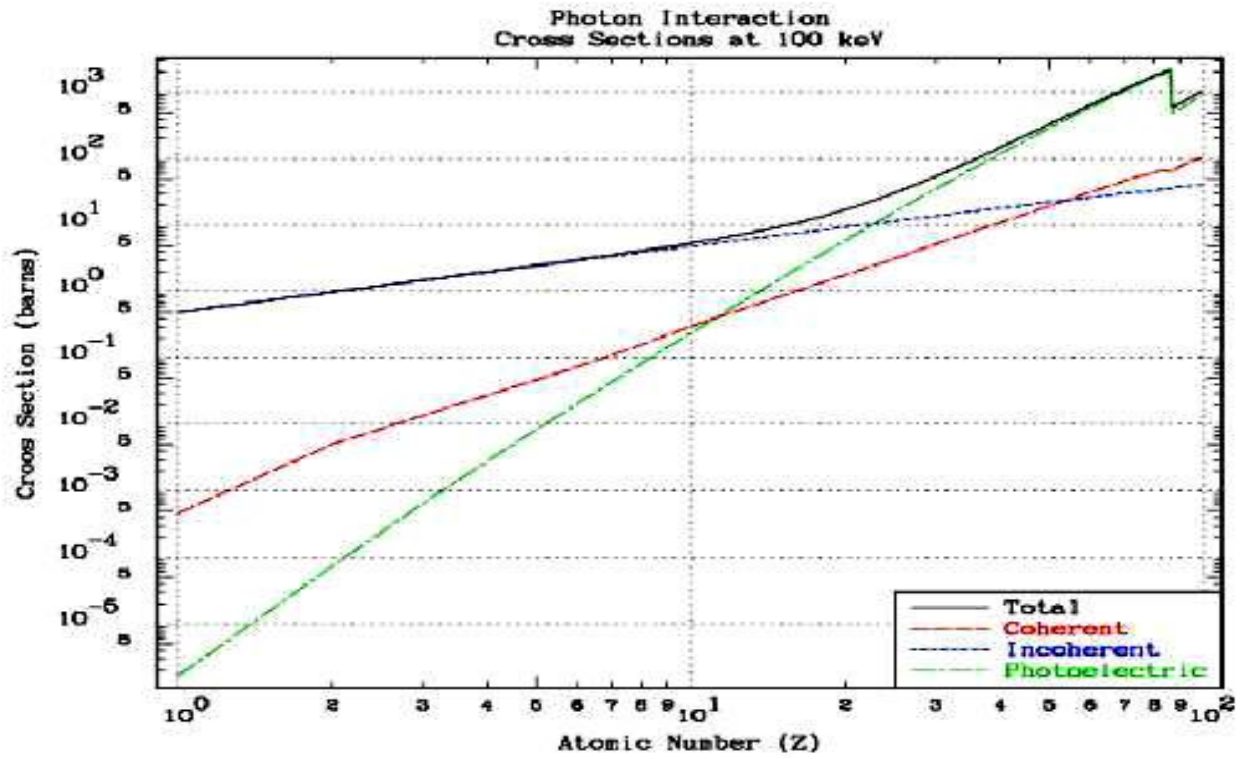


The above three figures illustrate the energy dependence of the photon cross sections. To illustrate the simply atomic number (Z) dependence the below five figures show the variation of the cross sections for each process versus Z at five incident photon energies: 1 GeV, 10 MeV, 1 MeV, 100 keV and 1 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.

At the highest energies (1 GeV and 10 MeV) we can see the simple variation of all five processes versus Z , i.e., almost straight lines on a log-log plot, showing variations as a power of Z (Z^N), see Ref. [12]. By 1 MeV we still see this simple variation, however we are below the pair and triplet thresholds, so we only see three processes. By 100 keV we start to see shell effects for high Z elements whose K shell energy is above 100 keV. Finally, by 1 keV we see shell effects across the periodic table for all three processes.







9. 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.

To help guide you here are the general rules we used for selecting data for use with EPICS2017. I judge all the sources that I used to be high quality and at least potentially all equally qualified candidates for use in EPICS2017. However, let me again stress EPICS is not intended as the cutting edges of science. It is designed for use in engineering applications, whenever possible using data that has been proven to agree with experimental measurements. It is impossible to measure everything, so theory also plays an important role to fill the gaps where we have no measurements. In selecting which theories to use I employ a conservative standard to only use a theory that has been verified to agree with measurements.

The bottom line is that EADL, EEDL, and EPDL data have been used for decades and documented in many reports to produce good, acceptable, results. So, I am not about to throw away this wealth of experience and make drastic changes without “seeing” evidence that the change is needed to improve agreement with practical applications.

In viewing the below figures of the cross sections please be aware that I consider all the sources to be equally valid and all are high quality results. The NIST and Scofield data is closer to what EPICS is designed for: elemental, cold, neutral, isolated atoms, and the PENELOPE data is more closely related to reality; solids, including molecular effects. Generally, for high Z elements these sources agree. The differences shown in the below figures should be considered the “experts” (PENELOPE, NIST and Scofield) estimate of the uncertainty in the data; not an indication that one is better than the other.

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. 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 percent differences, and the energies at which these differences can be seen, e.g., differences at low energies (low Z) are not as important as high energy differences.

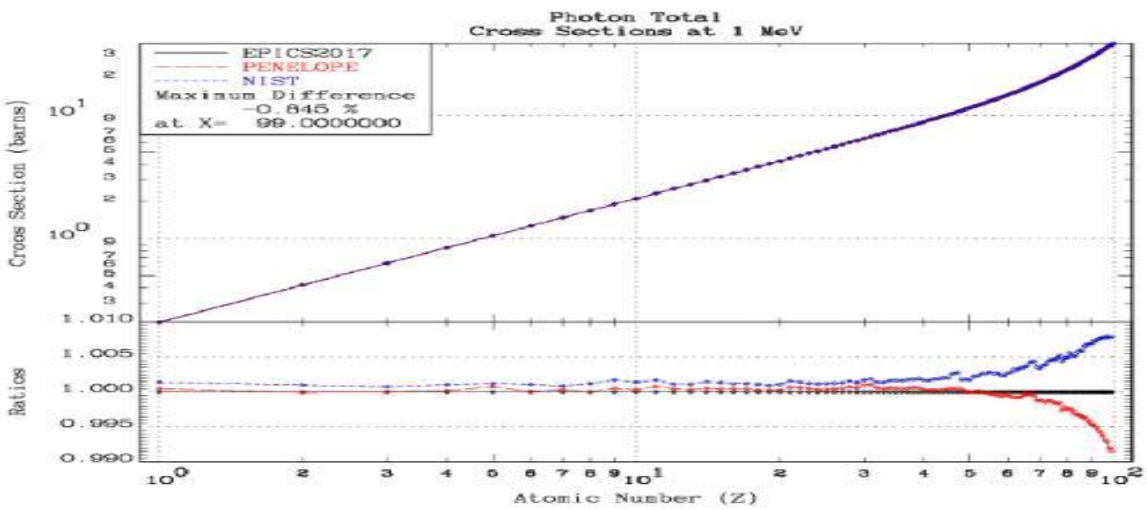
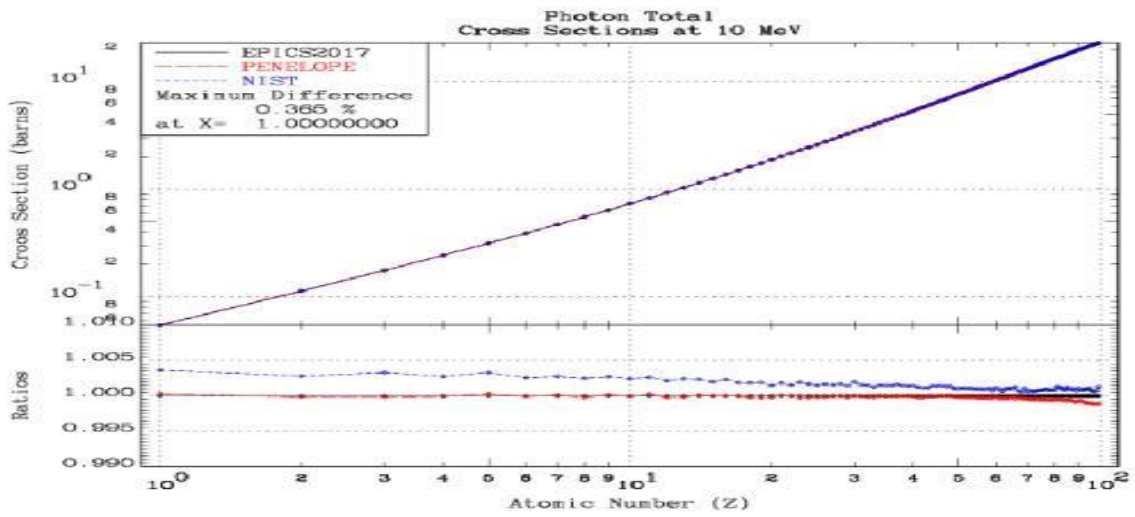
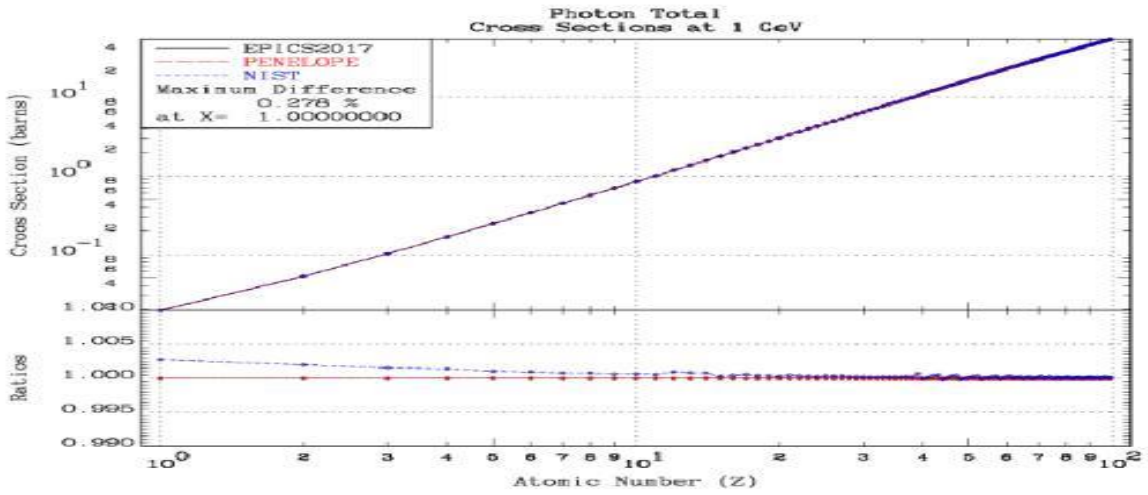
Last point: **“Please do not shoot the messenger”**. In the below figures, I have merely tried to represent the data from the various sources exactly as I found them. The magnitude of the differences shown may come as a shock to some readers, but these only represent the real uncertainties due to the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

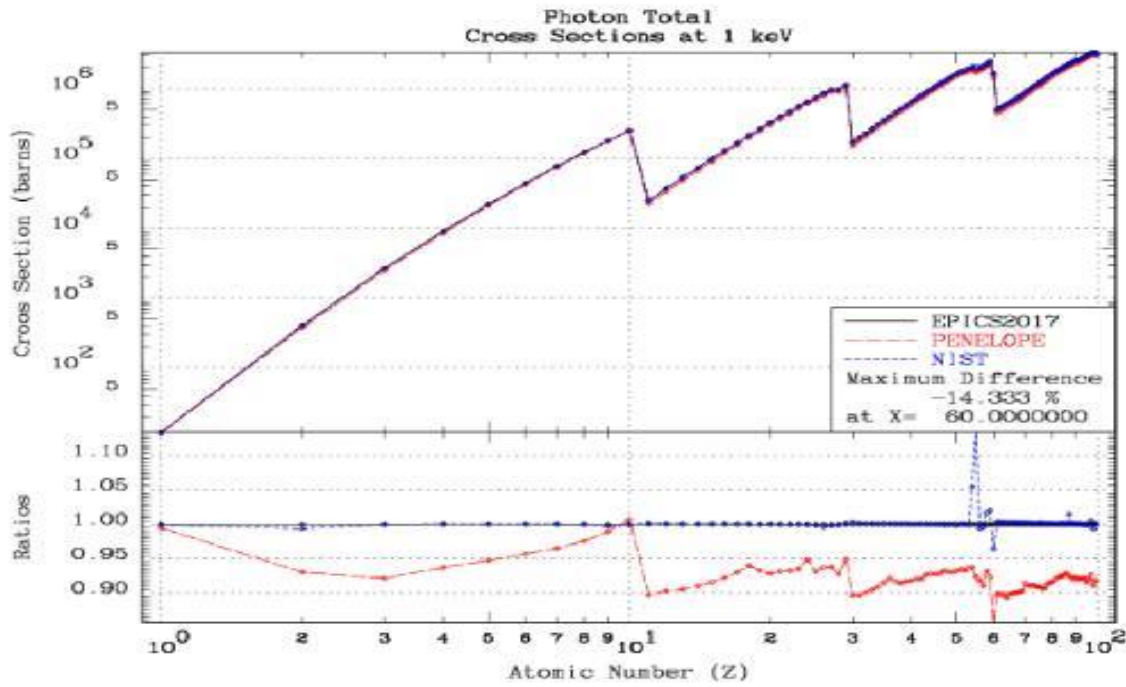
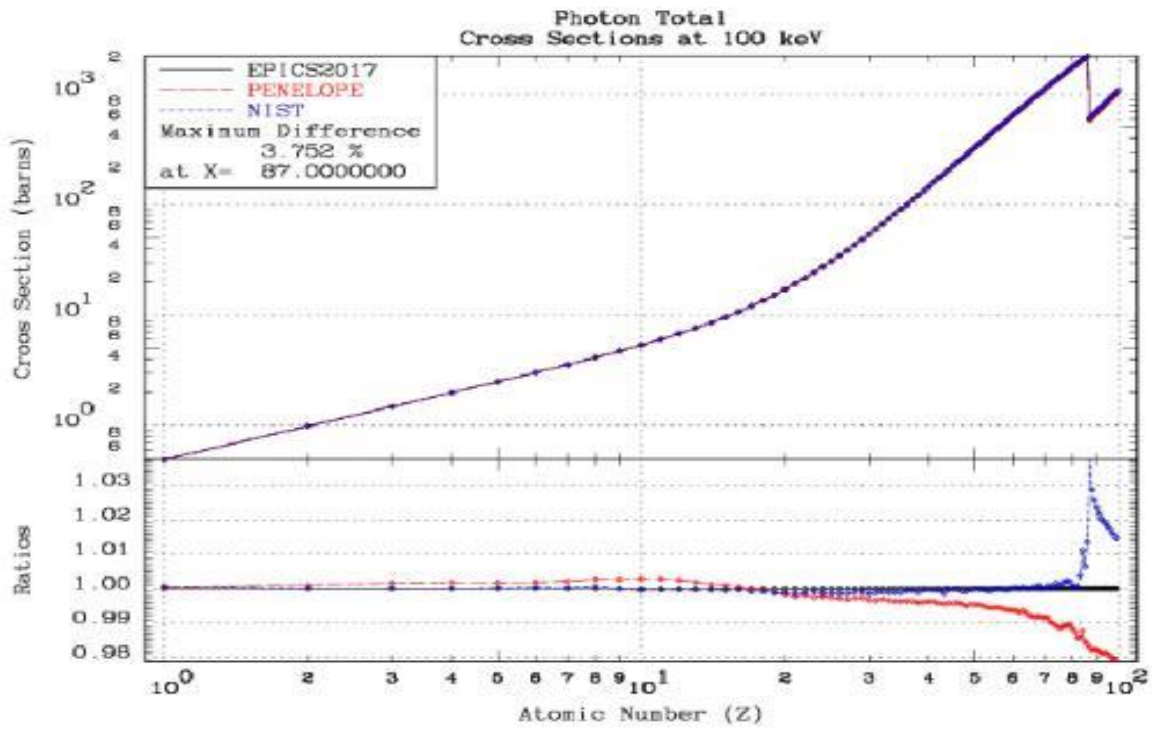
10. Total Cross Section Comparisons

Below I compare the total cross section at five (5) incident photon energies: 1 GeV, 10 MeV, 1 MeV, 100 eV and 1 keV, for Z = 1 through 100; here I compare EPICS2017, PENELOPE, and NIST data. Here’s a quick summary,

- 1) At 1 GeV they are agree to closer than 0.3% across the entire periodic table.
- 2) At 10 MeV they still agree to closer than 0.4%.
- 3) At 1 MeV we see difference of up to 0.8% for high Z.
- 4) At 100 keV we see differences up to a few per-cent, again for high Z
- 5) At 1 keV we see differences between PENELOPE and the others of up to 15%

Here the only MAJOR difference is the BIG one between the PENELOPE and other results at 1 keV. Below I will investigate and try to explain the sources of these differences,

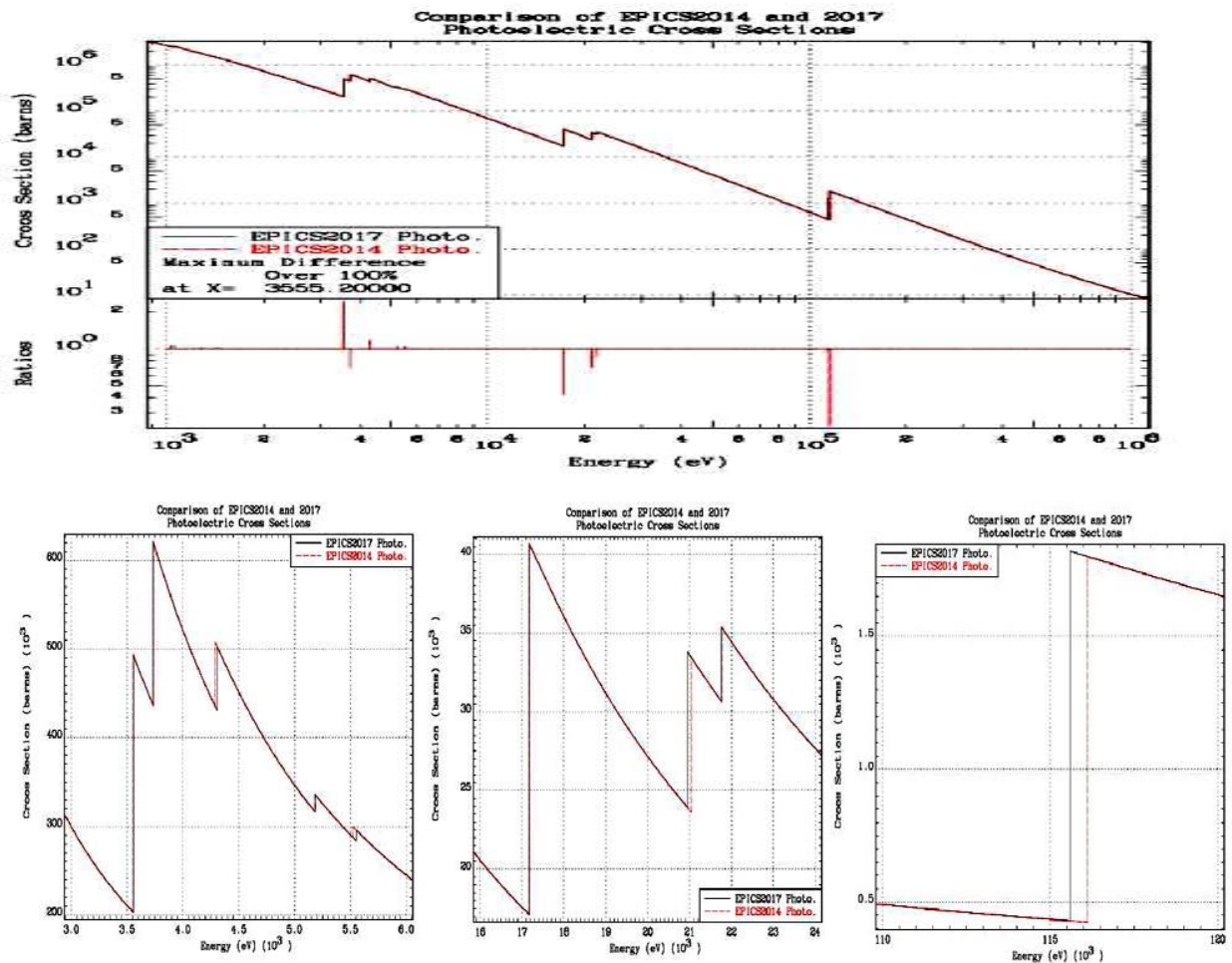




11. The Effect of New Binding Energies

As described above, new binding energies have been adopted for EICS2017, and documented in [4]. The effect of these new binding energies on the photon cross sections is to shift the photoelectric edges, requiring a modification to the photoelectric cross section. For consistency, this change also requires a change in the anomalous and coherent cross sections (which are defined by an integral over the modified photoelectric cross section) [13].

The EPICS2014 has been mentioned in numerous reports as having a total cross section that agrees well with measurements. To maintain this agreement and introduce the new binding energies I have only modified the photoelectric cross sections near edges by smoothly interpolating or extrapolating from old to new edges. Below I show an example for $Z=92$ comparing the EPICS2017 and 2014 photoelectric. The first figure shows agreement over a broad energy range, except for narrow energy ranges near edges. The lower figures show details near the M, K and K edges, illustrating agreement, except over extremely narrow energy intervals near the edges, usually differing over only a fraction of 1% the energy. **If anything, $Z=92$ is an extreme example of the required shifts in the edges (the shifts are largest for high Z elements at high energies), so these figures serve to illustrate the minimum changes in the photoelectric to accommodate the new binding energies**

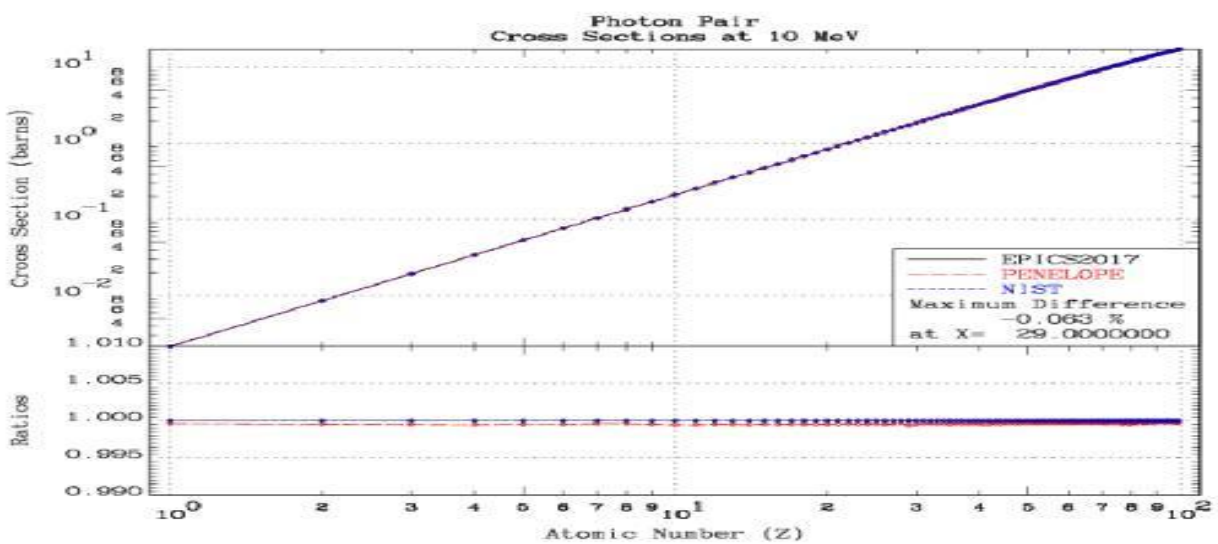
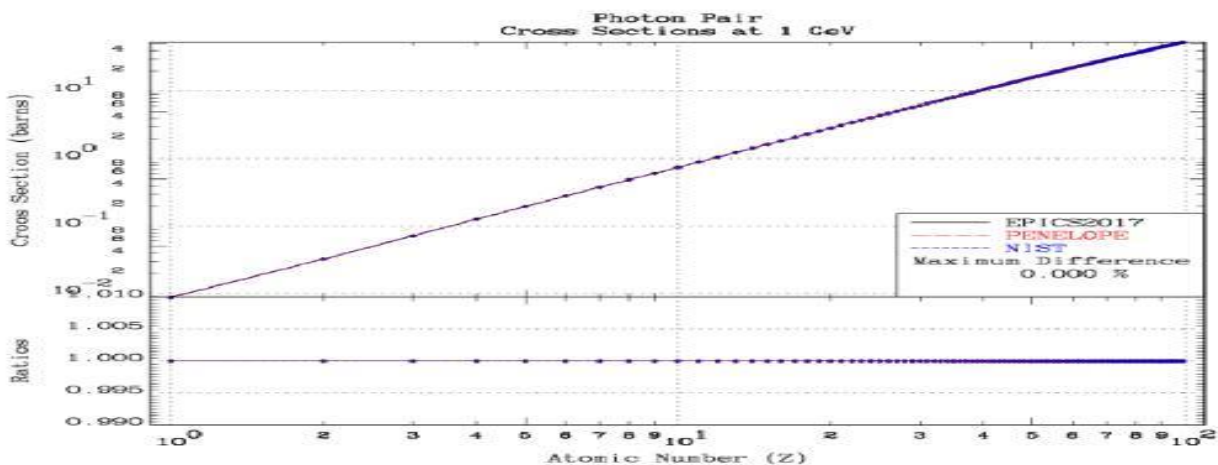


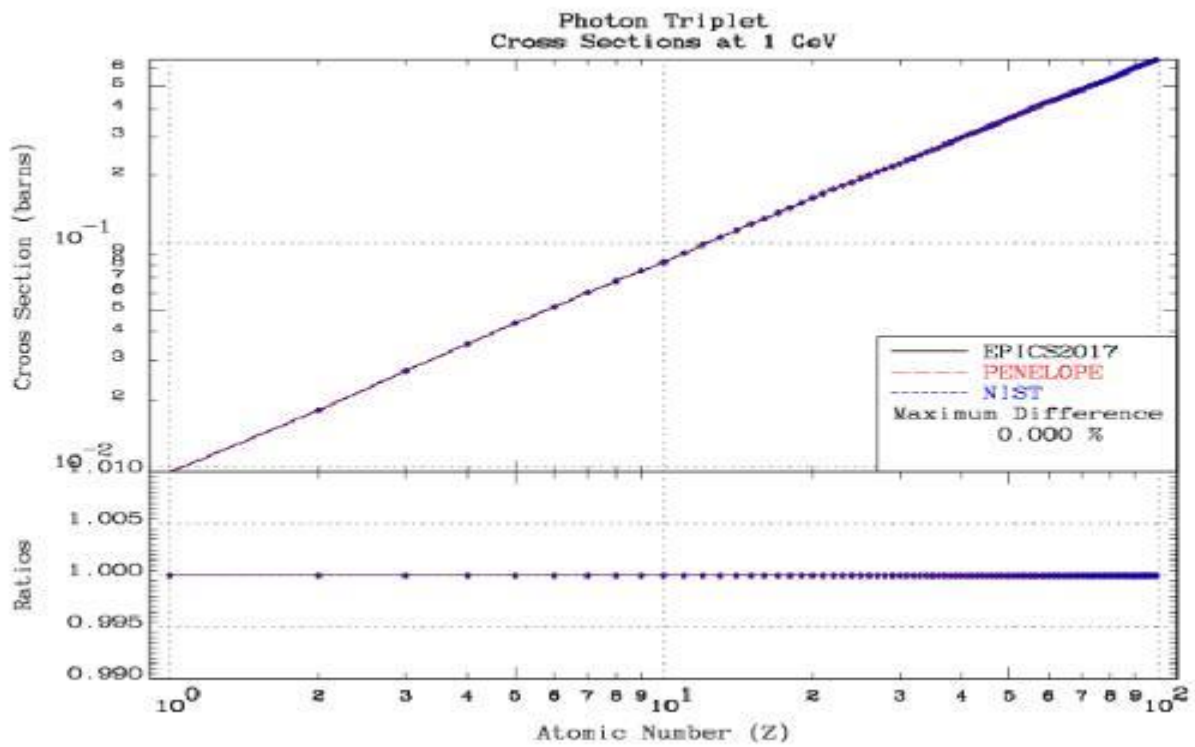
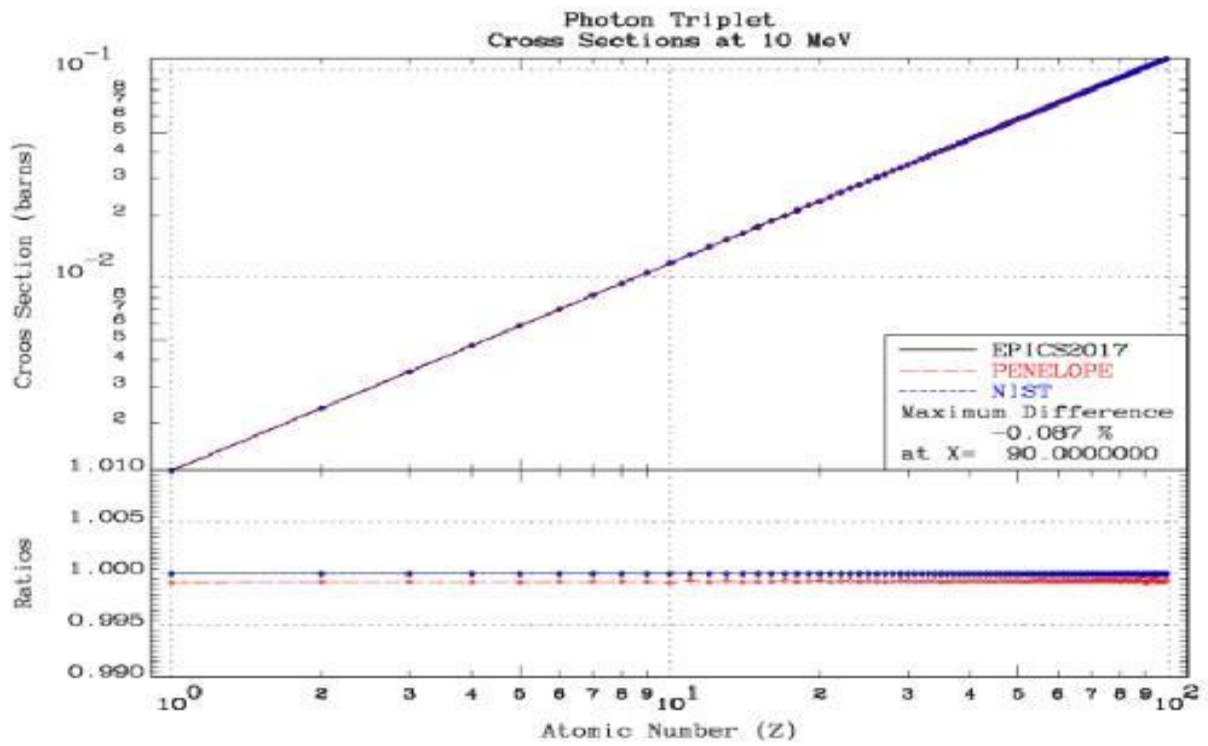
12. Pair and Triplet Production

Pair and Triplet Production are only energetical possible at high energy, with thresholds at: Pair 1.022 MeV, and Triplet 2.044 MeV. At high energies both show very simple atomic number (Z) dependence: Pair varies as Z^2 , and Triplet as Z. For example, for Z = 1 they are roughly of equal magnitude, and by Z = 100 Pair of roughly 100 times larger than Triplet.

Below I show comparisons of Pair and Triplet vs Z, Z = 1 through 100, comparing EPICS2017, PENELOPE and NIST. First, I show Pair to 10 MeV and 1 GeV, and then Triplet at the same two energies.

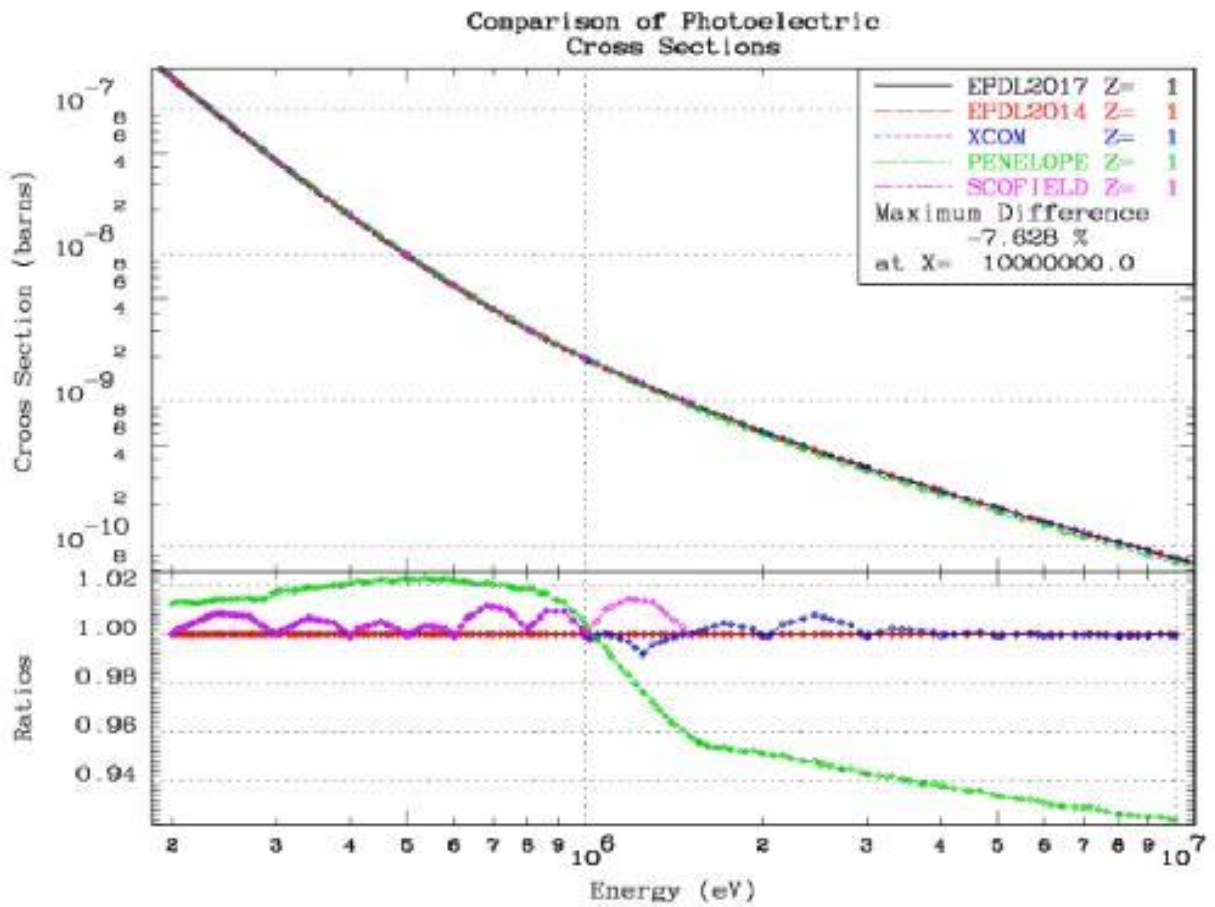
What we see is close agreement between all three sets of data across the entire periodic table, Z = 1 to 100; they all agree to within a small fraction of 1%. **Based on these results I judge there not to be any significant source of uncertainty, and certainly not enough difference to warrant changing EPICS.** As such will not address them further in this report.

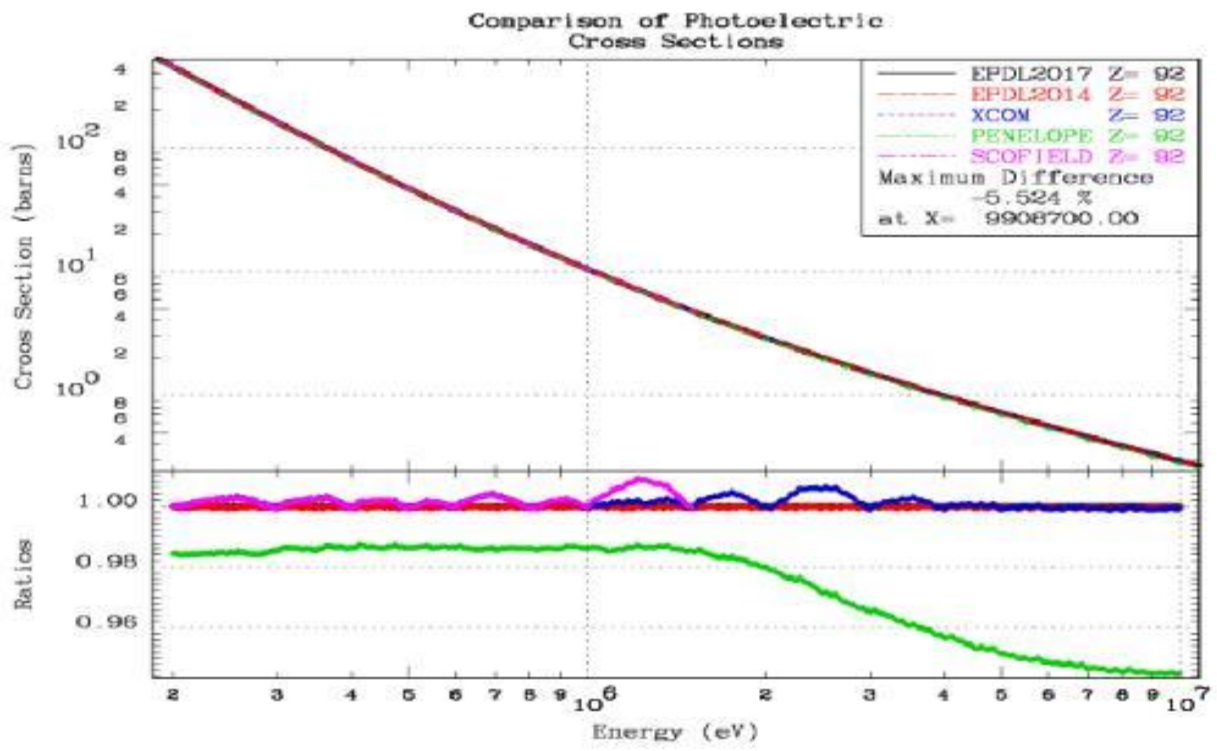
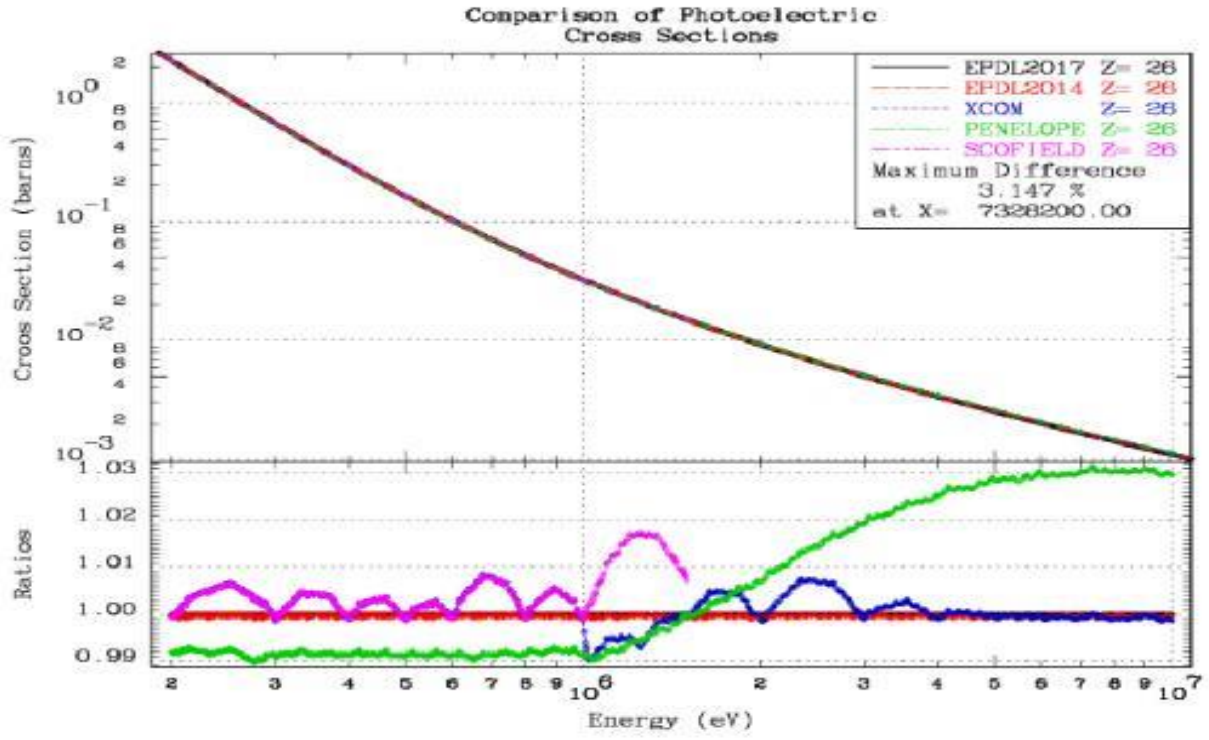




13. Photoelectric at High Energies

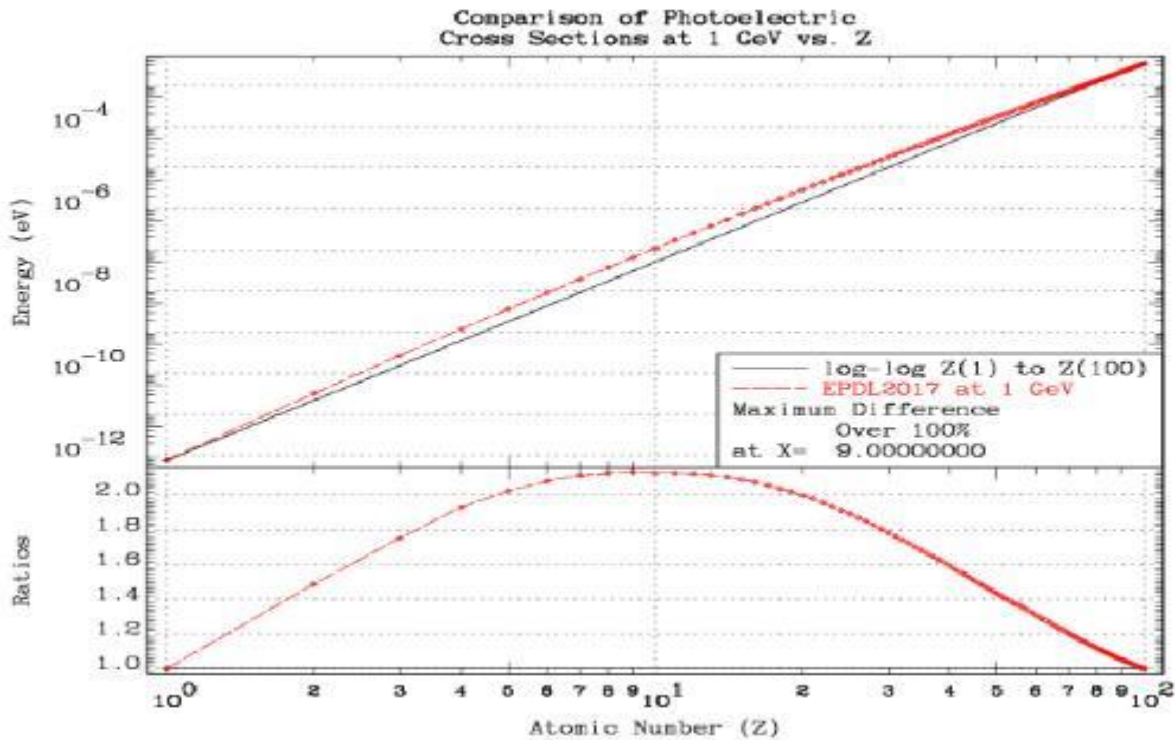
Above roughly a few 100 keV we see differences between the PENELOPE data and all the other data sets (EPDL, NIST, Scofield); here all data sets, including PENELOPE, claim to extrapolate from the Scofield data (only up to 1.5 MeV) to the GeV range. For example, the below figures illustrate the differences for a few elements ($Z = 1, 26, 92$); these differences appear across the entire periodic table (see, the following page).



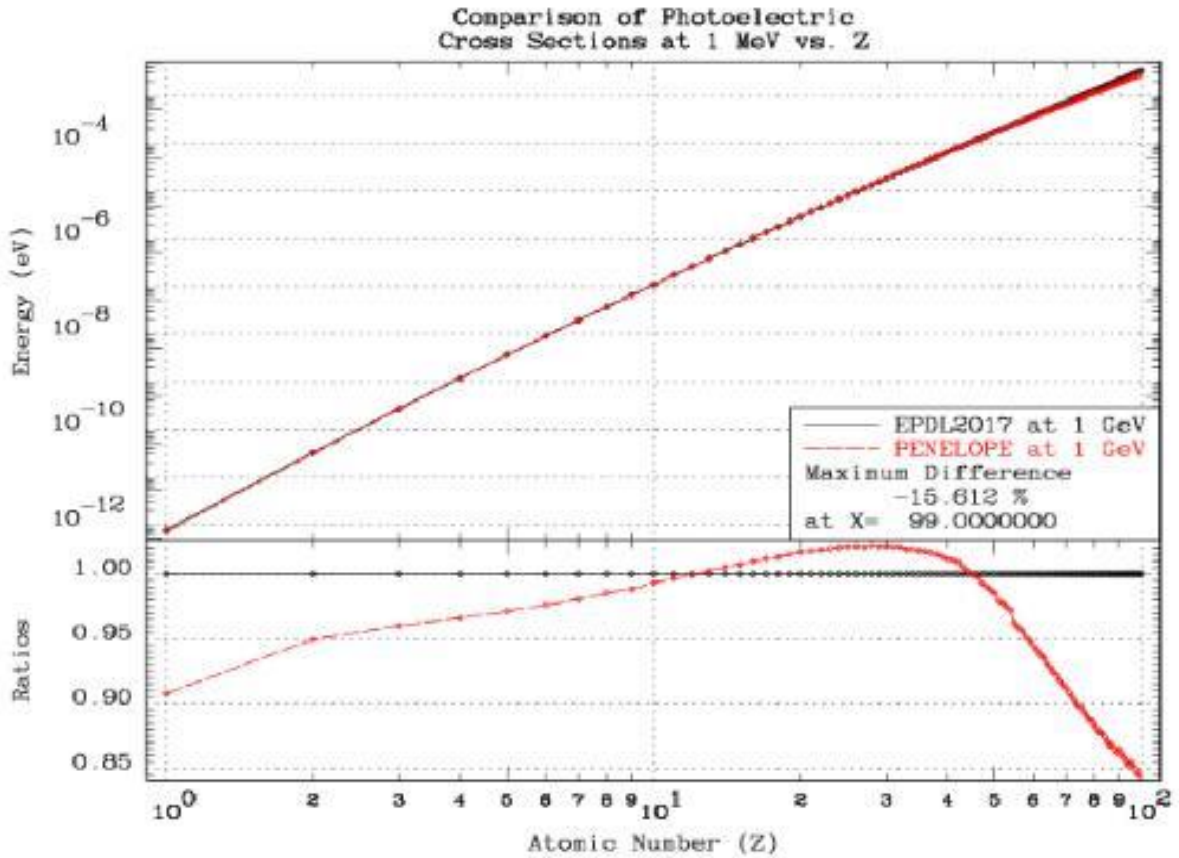


We judge these differences to be due to minor differences in the fitting procedure used by the various codes in attempting to extrapolate from the Scofield data (only up to 1.5 MeV) to high energies (GeV); note, that in the above three examples the PENELOPE data does not agree with the Scofield data that it claims it is extrapolating from. **Above roughly 1 MeV the photoelectric is only a minor part of the total cross section and is increasing as $1/E$, and we judge the difference between the PENELOPE data and all the other data sets to be unimportant and as such we have not changed EPICS, and ignored the PENELOPE high energy extension.**

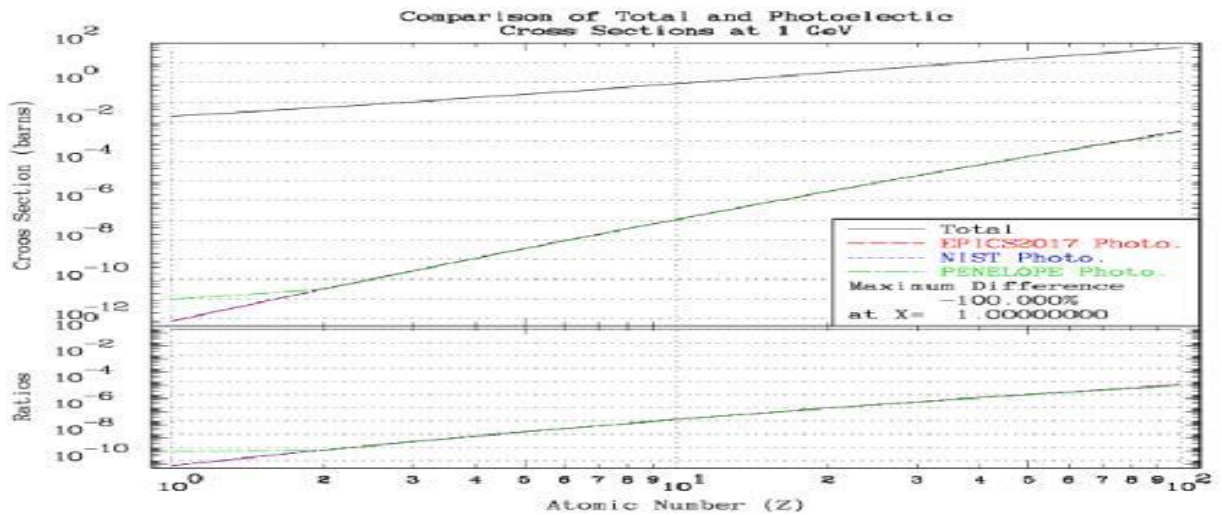
The below figures illustrate the variation of the photoelectric cross section at 1 GeV versus the atomic number (Z). The first figure compares a straight line from the EPDL values at Z = 1 to Z = 100 using log-log interpolation (a straight line on a log-log scaled plot) to the EPDL values at each Z = 1 to 100. Over this range the EPDL values vary from 7.748×10^{-13} at Z = 1 to 3.369×10^{-3} at Z = 100; roughly a change of 1.0×10^{10} in cross section for a change of Z of 100. The difference between the two is roughly a maximum factor of only 2 for a change in cross section of roughly 10 billion; illustrating the simple log-log Z dependence of the cross section.



The below figure compares the EPDL and PENELOPE values at 1 GeV versus the atomic number (Z). Here we see a bias between the two starting at about 10% for Z = 1, disappearing near Z = 10, and then increasing to over 15% for high Z.

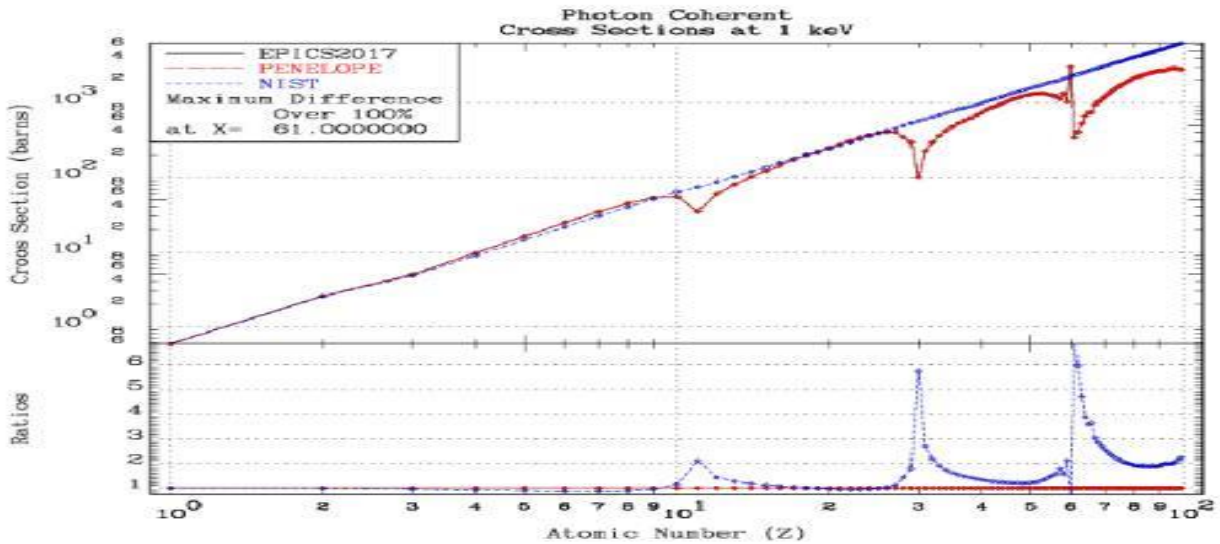


Let me again state our conclusion that although the differences we see here seem relatively large (10% to 15%), at this energy the photoelectric is only a tiny portion of the total (see, the below figure: it is less than 0.01%). **We choose to ignore the differences shown for the PENELOPE data and have adopted the EPDL2017 values as shown; these values agree with the other data sets.**

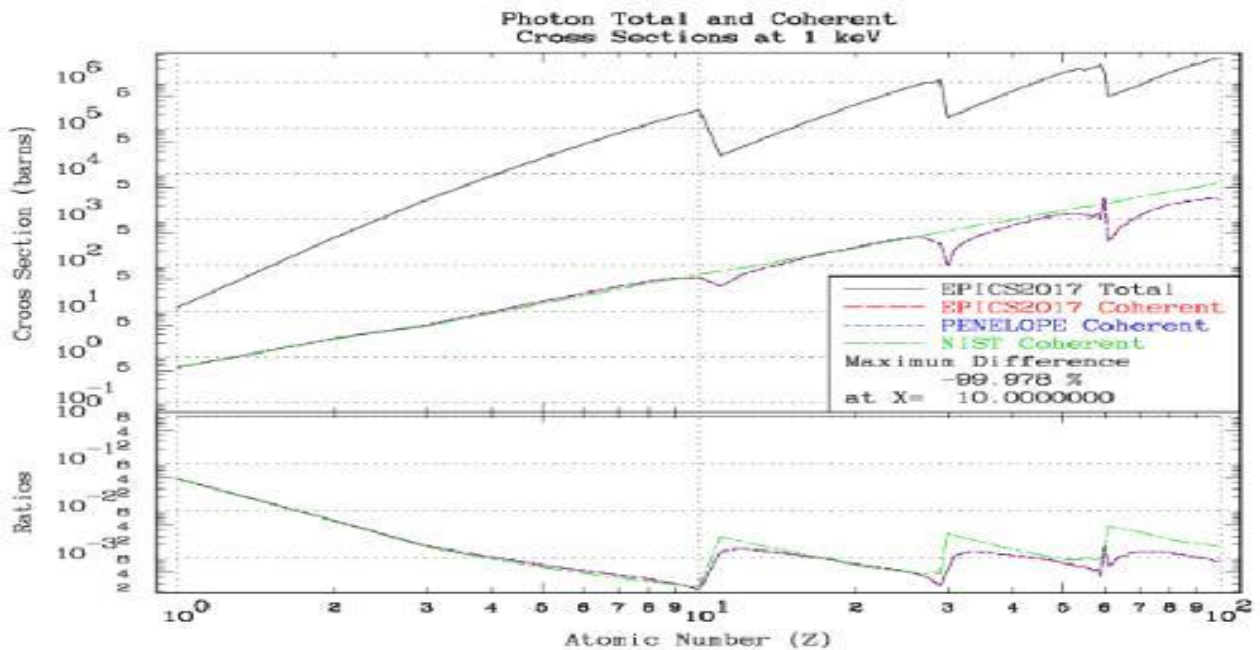


14. Differences at Low Energies

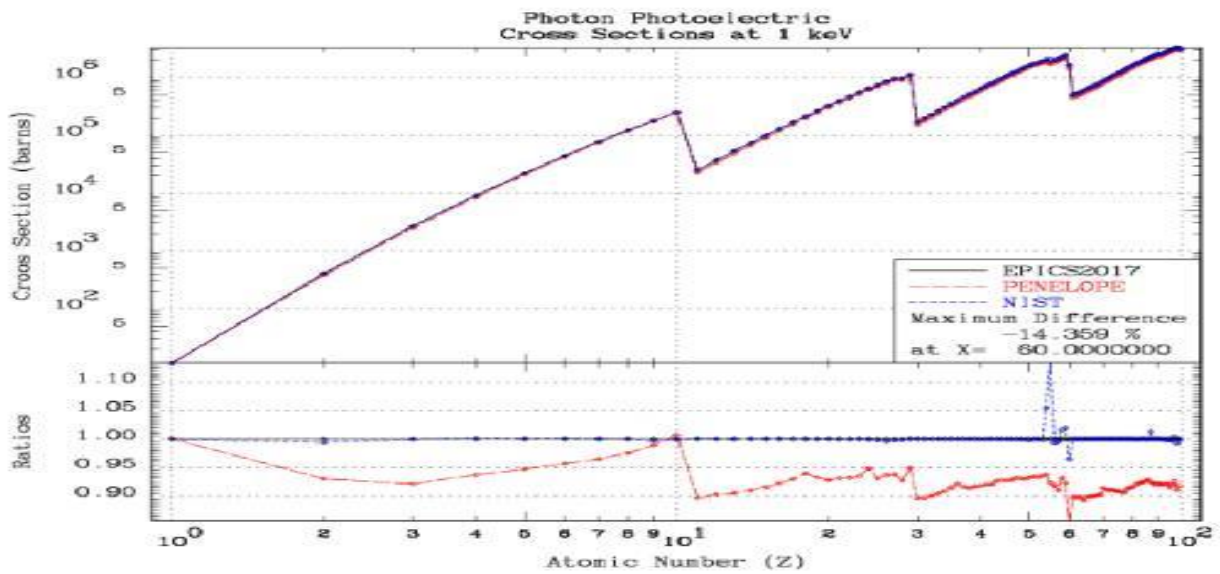
At low energies we see fairly large differences in the NIST Coherent cross section which can easily be explained, since NIST does not include anomalous scattering. Again, let me mention that Coherent scatter is never the dominant process, and where the “dips” due to anomalous scattering are large, it is because the photoelectric is ENORMOUS, overshadowing the Coherent.



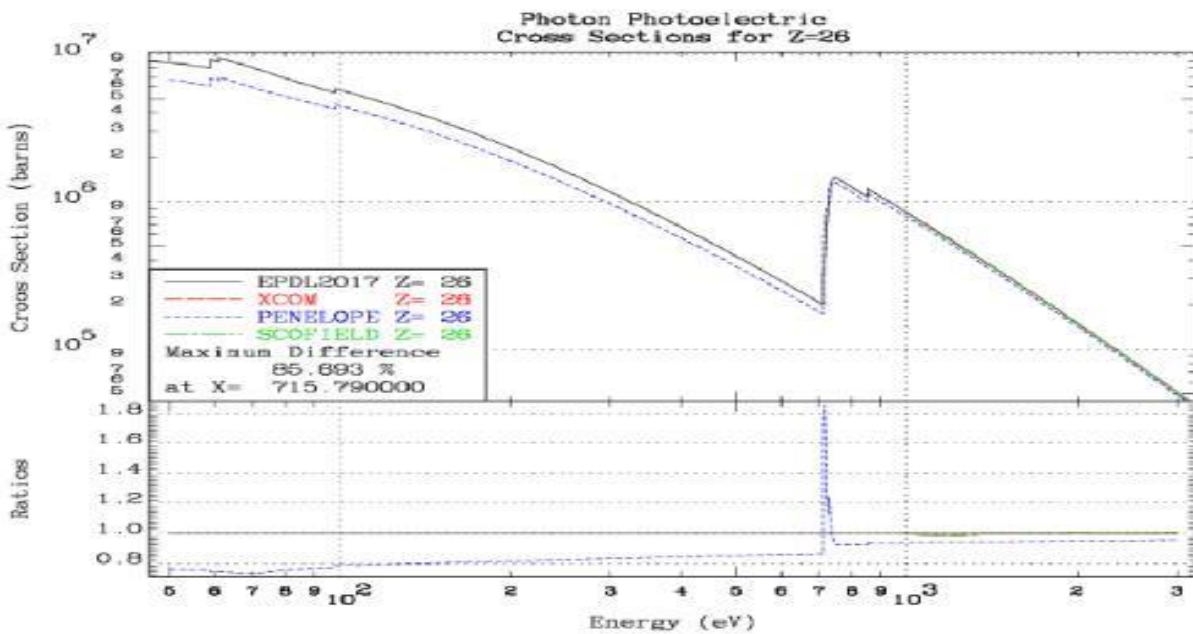
The below figure comparing the total and coherent for Z=1 to 100, illustrates that at 1 keV Coherent is never more than about 5% of the total (at low Z) and usually much less than 1% (closer to 0.1%).

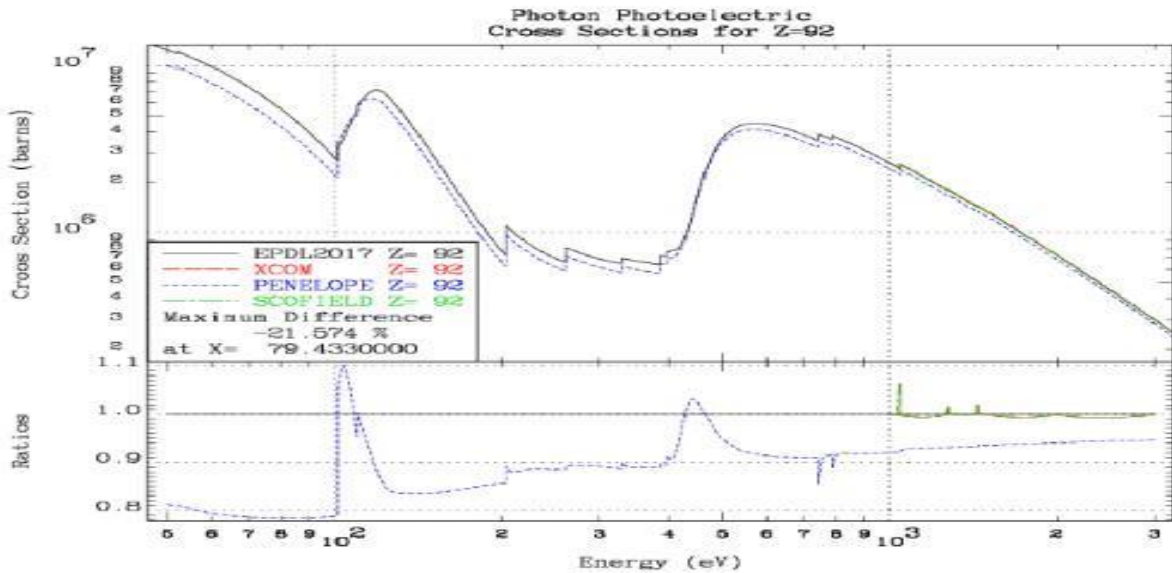


The biggest differences that we see at low energies are in the PENELOPE photoelectric, which can be up to 10% or 20% lower than the other data sets across the periodic table.



The below two figures contain energy dependent results for Z = 26 and 92, showing differences over broad energy ranges of 15% to 20%.





It now appears that these differences are due to an unfortunate misunderstanding as to where and how to apply the “normalization screening correction” [14], and this re-normalization was unfortunately applied to the PENELOPE cross sections at low energies.

Recently **Jim Scofield** clarified the situation when he wrote: “This renormalization should have been at high energies and experimentally it is best not to do it. There are a number of ways to produce better theoretical results, this simple fix is not one of them.” [15]

In response, **Paul Bergstrom** wrote: “I agree with Jim that it is a high-energy result. However, the measured data don’t clearly prefer normalized or unrenormalized.” [16]

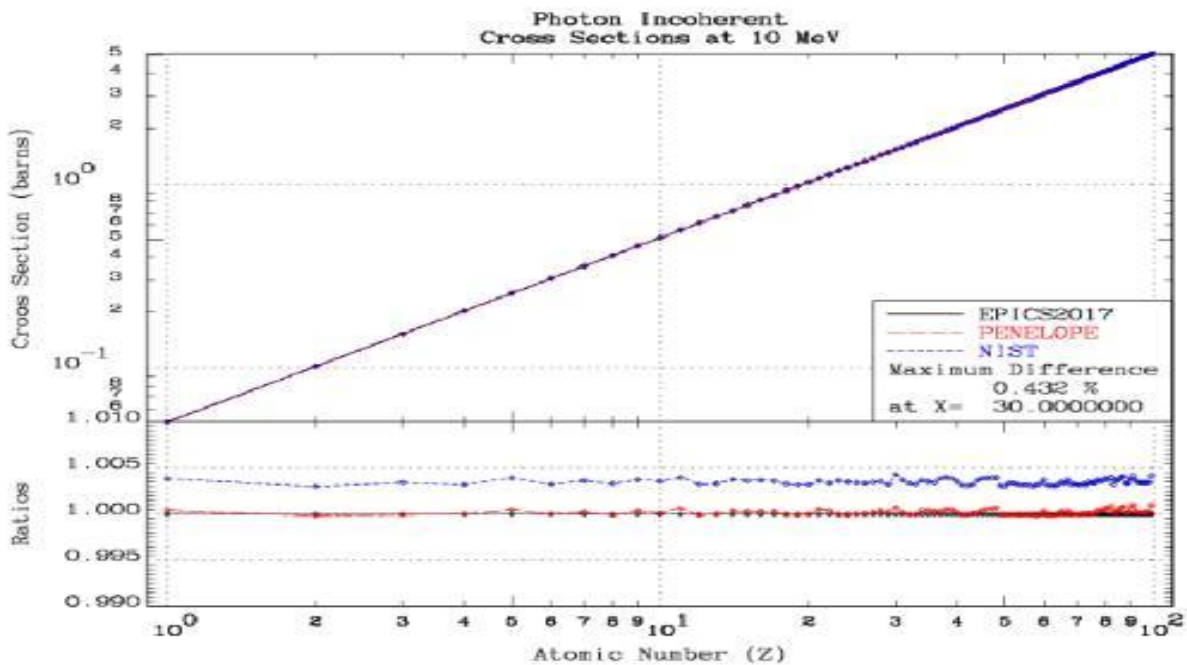
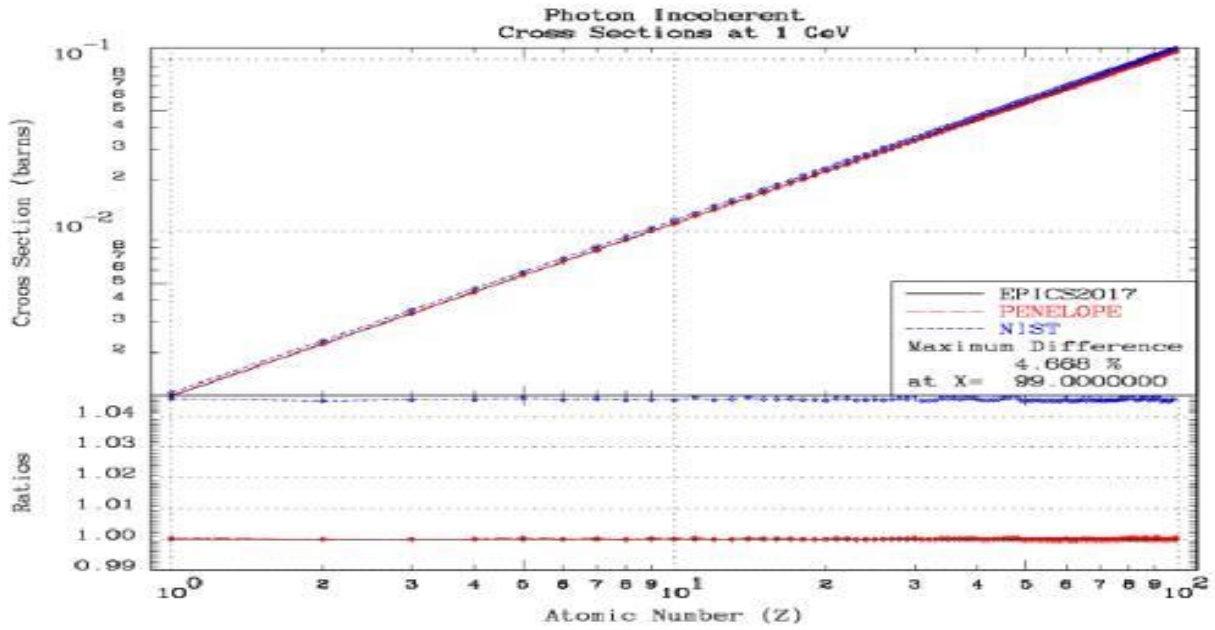
In addition, **Francesc Salvat** summarized the situation when he wrote: “The renormalization of photoabsorption cross sections is under debate, and it will be for a long time because experimental measurements are scarce and apparently contradictory. I prefer including renormalization because it is plausible from a purely theoretical approach. I have nothing to add to the debate.” [17]

The most authoritative comment on “re-normalizing” is in the **Journal of the ICRU**: “Thus, while theoretical considerations might also favor the use of renormalized Scofield photoeffect cross sections, it does not seem prudent to make a formal recommendation in this equivocal situation.” [18]

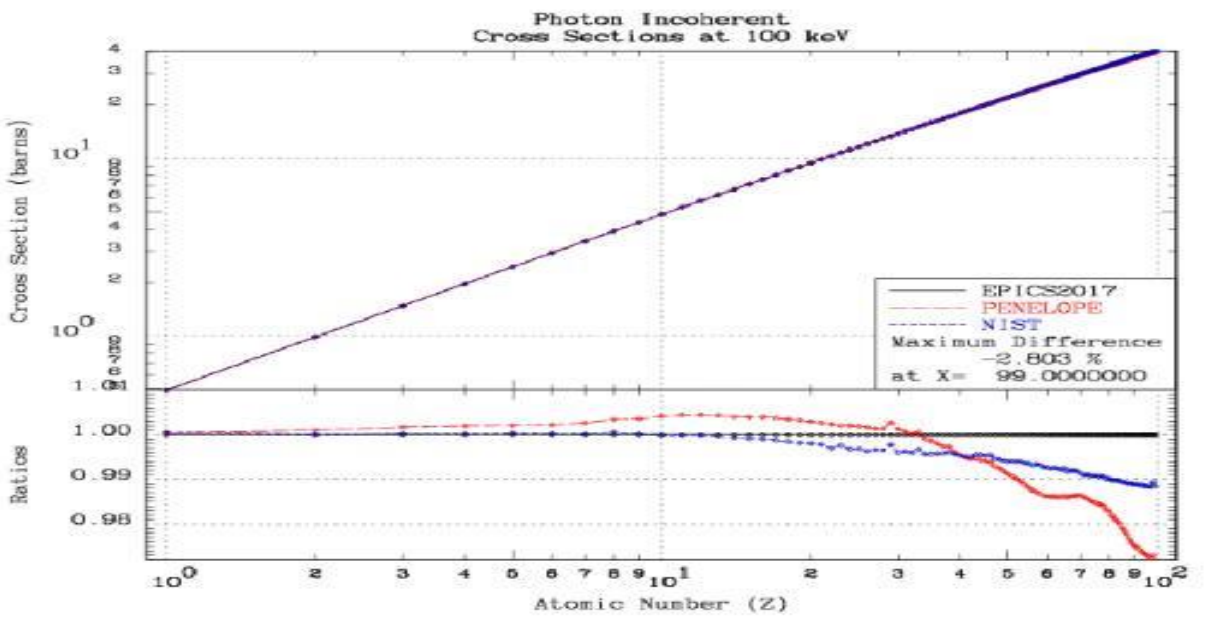
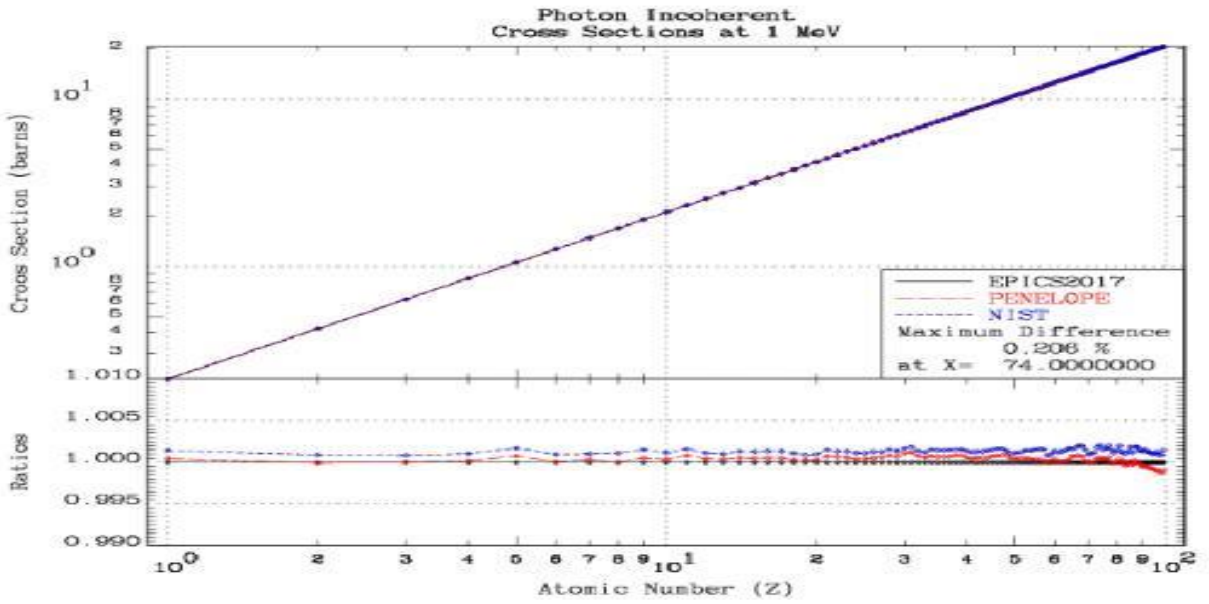
Based on current information the EPICS2017 photoelectric has NOT been renormalized, so our results agree with the NIST and Scofield data, which can be up to 10% or 20% higher than the PENELOPE data.

15. Incoherent

At higher energies, 1 GeV and 10 MeV, the NIST Incoherent is roughly 4% higher than the other data sets.

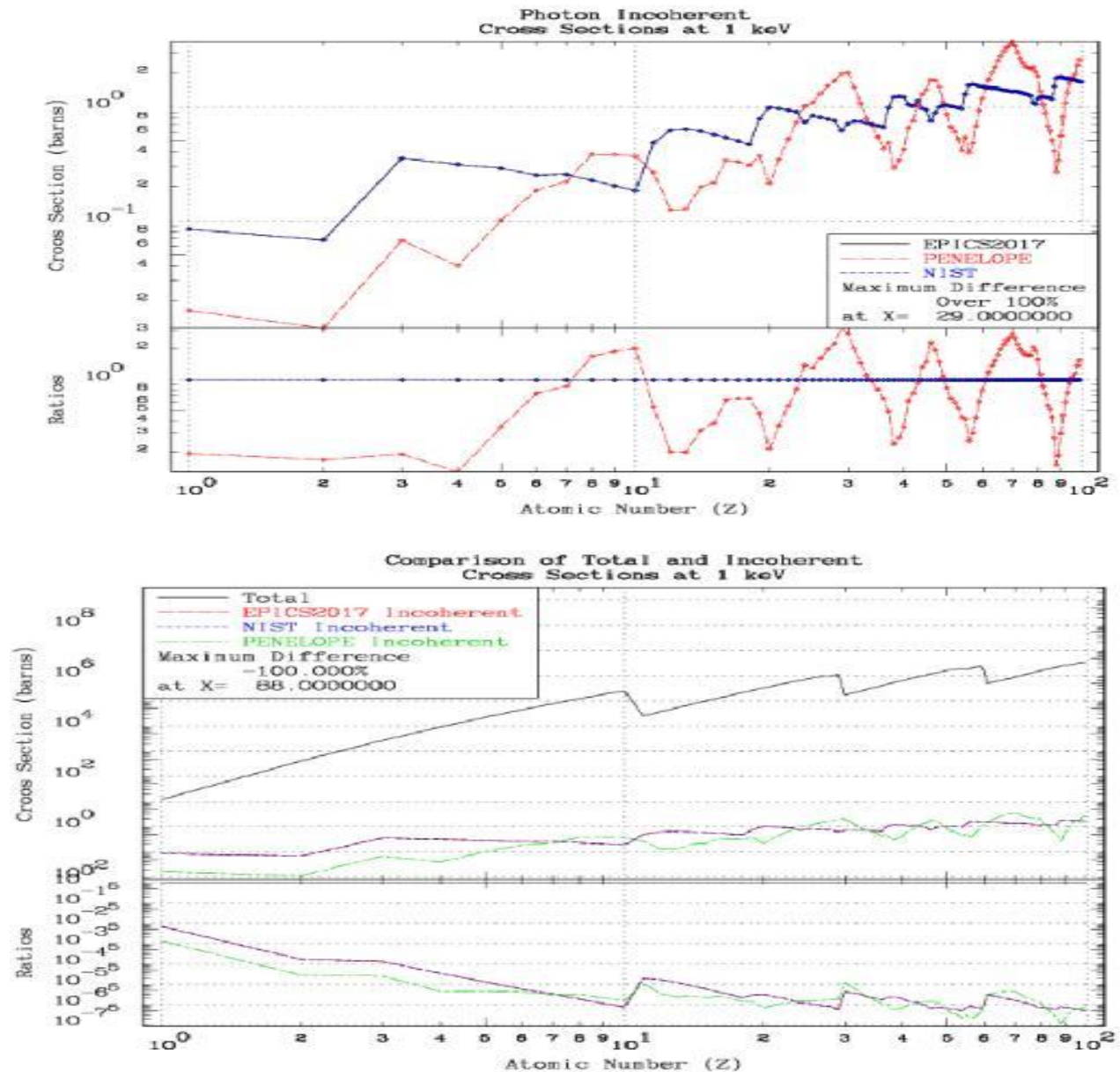


By 1 MeV this difference has disappeared. But as we proceed lower in energy by 100 keV we see a spread of almost 3% between the three data sets.



By the time we reach 1 keV the EPICS2017 and NIST agree, but the PENELOPE results are quite different. The bad news is that as yet I cannot explain this difference. The good news is shown in the below figure comparing the total and incoherent at 1 keV for $Z = 1$ to 100; the incoherent is always less than 1% of the total for low Z elements, and much less for high Z elements.

From these incoherent comparisons we see roughly a 4% difference in the 10 MeV to 1 GeV range, but much larger differences at low energies. One important point that I hope readers learn from these comparisons is that with decreasing energies the uncertainty in the cross sections are growing, so **PLEASE heed the WARNING repeated multiple times in this report: Do not use this data to transport below 100 eV (D.E. Cullen) or 1 keV (F. Salvat); if you do, your results will be unreliable, and you will have nobody to blame but yourself.**



16. Release of EPICS2017

I am hoping to release a complete EPICS (EADL, EEDL, EPDL) by the end of 2017. An earlier publication [4] documented the completion of EADL. With this document, the photon cross sections have been defined (EPDL), but what remains to be done is to re-define the electron cross sections (EEDL). 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) and photon cross sections (EPDL) will not be released until all parts of EPICS have been updated; again, hopefully by end 2017.

17. Conclusions

I have presented here my Survey of Atomic Photon 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 EPDL data. I started from my existing compilations of photon cross section data (EPDL), and compared it to PENELOPE, NIST and Scofield data. I added new edge energies to photoelectric and calculated the corresponding anomalous and coherent scattering data. I also added a few tests for the expected systematics. I put the final results into the ENDF/B format, so that they can be easily used by as many computer codes as possible. In this report I extensively used graphics to illustrate the simple Z dependence of the data and to compare sets of data, to give the reader a realistic estimate of the uncertainty in this data. **After reviewing all the data, I have decided for EPICS2017 to only change: binding energies, photoelectric cross sections, anomalous and coherent scatter.**

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, in some small way, contributes to our efforts toward understanding and improving in our data. Most important: I encourage you the reader to also contribute to this effort, by reporting your measured and calculated results to me.

References

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- [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/endl-manual.pdf>
- [3] 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.
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- [6] F. Salvat, **PENELOPE-2014**: Code System for Monte Carlo Simulation of Electron and Photon Transport Workshop, Barcelona, Spain, 29 June-3 July 2015.
- [7] P. Bergstrom, **NIST**, Private Communication (2017); identified here as NIST are tabulated XCOM data for elements, $Z = 1$ through 100 kindly supplied by Paul Bergstrom
- [8] J.H. Scofield, “Theoretical Photoionization Cross Sections from 1 to 1500 keV”, UCRL-51326 (1973), Lawrence Livermore National Laboratory.
- [9] J. Hubbell, **HUBBELL#1**: Experimentally Measured Total X-Ray Attenuation Coefficients Extracted from Previously Unprocessed Documents Held by the NIST Photon and Charged Particle Data Center **I**, NISTIR 5893 (September 1996).
- [10] J. Hubbell **HUBBELL#2**: Experimentally Measured Total X-Ray Attenuation Coefficients Extracted from Previously Unprocessed Documents Held by the NIST Photon and Charged Particle Data Center **II**, NISTIR 7163 (September 2004).
- [11] D.E. Cullen, **PREPRO/LINEAR**, “PREPRO2017: 2017 ENDF/B Pre-processing Codes”, IAEA-NDS-39, Rev. 17, May 2017.
- [12] **LOG-LOG**: On a log-log plot a straight line indicates: $\log(\sigma) \sim N \cdot \log(Z)$, and you can estimate N by noting for each decade change in Z how many decades the cross section (σ) 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 ($N \sim 5$). We can also see the variations of Pair as Z^2 and Triplet as Z .
- [13] **SCATMAN**, "Program SCATMAN: A Code Designed to Calculate Photon Coherent Scattering Anomalous Scattering Factors and Cross Sections", Lawrence Livermore National Laboratory, UCRL-ID-103422, November 1989.
- [14] L. Sabbatucci and F. Salvat, **PHOTOEFFECT**, “Theory and Calculation of the Atomic Photoeffect”, *Radiation Physics and Chemistry* **121** (2016) 122–140bbatucci and Francesc Salvat.
- [15] J.H. Scofield, Private Communication, 2017.
- [16] P. Bergstrom, Private Communication, 2017.
- [17] F. Salvat, Private Communication, 2017.
- [18] **Journal of the ICRU** Vol 14 No 1 (2014) 75, Report 90 Oxford University Press doi:10.1093/jicru/ndw040

APPENDIX: Comparison of Measured and Evaluated Data

The below figures are a sample of the many hundreds that I viewed in deciding what are the BEST values to use in EPICS2017. Also of high importance was for me to “see” how our evaluated data compare to measured data, also how they differ (as a something rough estimate of certainty).

All the measured data are from John Hubbell’s collection of **Total photon cross sections**, as described in [9, 10]. This collection includes data for 82 elements between Z=1 and 94, and reference/elements for 1,911 sets of measurements of 22,306 data points. Since I am here interested in energy dependent trends I only plotted sets that included 10 or more energy points. This reduced the data I viewed down to 78 elements, for 633 reference/elements, 18,199 data points.

Please note that for each measured data point this collection only includes (energy, cross section) pairs, but no uncertainty information. As a result from the below plots we have no way of estimating measured uncertainty; for more information see [9, 10].

In selecting the following figures, from the many available, I have tried to select those that we can learn the most from, such as,

- 1) Narrow energy ranges between photoelectric edges, where we can “see” how measurements compare to the un-normalized EPICS2017 and NIST data, and the normalized PENELOPE data.
- 2) Broad energy ranges, where we can “see” generally where data has and has not been measured.
- 3) Low energy, below 1 keV, to HOPEFULLY convince readers to NEVER use our data to transport particles to low energy (below 100 eV or 1 keV). Again, let me stress that low energy data is included in EPICS2017 only to allow anomalous scattering factors to be calculated, which involves an integral over the entire energy range of the photoelectric cross section. The below figures show ENORMOUS differences (in some cases over 1000 %) at low energy.
- 4) High energy, particularly to illustrate the giant dipole resonance, that is not included in any of the evaluated data sets shown here.
- 5) Mid energy range, near 1 MeV, where the photoelectric changes shape from $1/E^3$ at lower energy to $1/E$ at higher energy, and the evaluated photoelectric cross sections slightly diverge.

On each plot the element is only defined in the legend box by EPICS2017 Z=?? The plots are in ascending Z order from Z=1 through 94.

With that as background I will leave it to the reader to judge the below figures.

