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**EPICS2023:  
August 2023 Status Report**

by

Dermott E. Cullen

National Nuclear Data Center, BNL, alumnus

Nuclear Data Section, IAEA, Vienna, alumnus

University of California, LLNL, retired

1466 Hudson Way

Livermore, CA 94550

E.Mail: [RedCullen1@comcast.net](mailto:RedCullen1@comcast.net)

Website: <http://redcullen1.net/HOMEPAGE.new/>

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**Abstract:** This report is intended to bring readers up-to-date as to the current (August 2023) status of the Electron-Photon Interaction Cross Sections, version 2023 (EPICS2023). These evaluated data were last released in 2017, and the actual evaluated data have not changed since then. However, there have been significant changes and corrections to how these data actually appear (are coded) in the ENDL and ENDF formats. Herein we document recent corrections to the Evaluated Electron Data Library (EEDL) bremsstrahlung ZAP (particle produced), correcting it to 0 (photon), from 11 (electron), in earlier versions of EEDL in the ENDF format. We also document deleting extraneous duplicate energy points from the Evaluated Photon Data Library (EPDL) data in both ENDL and ENDF formats, and the addition of repeated energies at threshold energies, to ensure all subshell data starts with zero energy in both ENDL and ENDF formats. The first part of this document is new and covers recent changes (since 2019). I recommend you read EPICS2019 document for earlier changes. The bottom line is that these data files have been up-to-date and FREELY available on-line at no cost to users for years and we have no current plans to make any significant changes to the actual data. We stress that changes in the data are driven strictly by feedback from users, so PLEASE ensure that you send any test results and/or suggestions to the author, so that our entire community of users can benefit from your experience.

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Nuclear Data Section  
International Atomic Energy Agency  
P.O. Box 100  
A-1400 Vienna  
Austria

E-mail: [NDS.Contact-Point@iaea.org](mailto:NDS.Contact-Point@iaea.org)  
Fax: (43-1)26007  
Telephone: (43-1)2600-21725  
Web: <http://www-nds.iaea.org>

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Vienna, August 2023

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## 1. August 2023 Status Report

This report is intended to bring readers up-to-date as to the current (August 2023) status of the Electron-Photon Interaction Cross Sections, version 2023 (EPICS2023). These evaluated data were last released in 2017, and the actual evaluated data have not changed since then. However, there have been significant changes and corrections to how these data actually appear (are coded) in the ENDL and ENDF formats. Here we document recent corrections to the Evaluated Electron Data Library (EEDL) bremsstrahlung ZAP (particle produced), correcting it to 0 (photon), from 11 (electron), in earlier versions of EEDL in the ENDF format. We also document deleting extraneous duplicate energy points from the Evaluated Photon Data Library (EPDL) data in both ENDL and ENDF formats, and the addition of repeated energies at threshold energies, to ensure all subshell data starts with zero energy in both ENDL and ENDF formats. The first part of this document is new and covers recent changes (since 2019). I recommend you read EPICS2019 document for earlier changes. The bottom line is that these data files have been up-to-date and FREELY available on-line at no cost to users for years and we have no current plans to make any significant changes to the actual data. **We stress that changes in the data are driven strictly by feedback from users, so PLEASE ensure that you send any test results and/or suggestions to the author, so that our entire community of users can benefit from your experience.**

**Bottom line:** Now that all the reported formatting problems that I am aware of are in place, I am hoping with this document to answer remaining questions and to inform as many potential users as possible, to **ONLY USE THE MOST RECENT** version of data. Failure to do so obviously may lead to erroneous results in your applications. **See my website for the latest EPICS2023 information.**

## 2. What EPICS is and is not?

The Electron-Photon Interaction Cross Sections, 2023 version (EPICS2023) includes **ELEMENTAL, cold, neutral, isolated ATOMIC data, in the absence of electrical or magnetic fields**, and its documentation for: Atomic Data, **EADL** [1], Photon Interaction Data, **EPDL** [2], and Electron Interaction Data, **EEDL** [3]. It is currently FREELY available online at no cost in both the original ENDL format [4], in which it was created, and the ENDF format [5], to which it was subsequently translated. **EPICS is designed to handle traditional ENDL and ENDF applications involving keV and MeV energy** “particles” (photons and electrons), that can be accurately described by simple ELEMENTAL data (atomic number  $Z = 1 - 100$ ). It is important to also understand that **EPICS is not designed** to handle density or molecular and other binding effects that are important at low energies. Nor is it designed to handle **NUCLEAR** effects, that are important at high energy. This limits the use of this data to exactly what it was designed to handle: I will repeat **ATOMIC data in the keV and MeV energy range**. And it is important for users to understand that currently there are no plans to extend this data to handle a wider range of applications, i.e., it currently serves its intended purpose, so we see no reason to #@\$%^ with it.

Important features of all releases of EPICS and its sub-libraries (EADL, EEDL, EPDL), are,

- 1) All elements with atomic number,  $Z = 1 - 100$ , were done at once using the same methods for all to preserve important atomic number ( $Z$ ) dependent parameters, e.g., subshell binding energies.
- 2) All three libraries (EADL, EPDL, EEDL) use the same subshell binding energies, in order to conserve energy when performing coupled electron-photon calculations.

## Differences between EPICS2014 and EPICS2017 and EPICS2023

- 1) EPICS2017 includes updated subshell binding energies, these will affect photons and electrons.
- 2) EPICS2017 all data is **lin-lin interpolable** - to avoid misuse of earlier **log-log interpolable** data.
- 3) EPICS2014 includes **photo-excitation**; EPICS2017 does not - it is judged to be outside the designed purpose and was never previously (before EPIC2014) included in ENDF -102 data.
- 4) EPICS2023 corrects EEDL bremsstrahlung ZAP (particle emitted), to 0 (photons), which is earlier versions was incorrectly defined as 11 (electrons); this caused the bremsstrahlung to appear to emit only electrons and no photons.
- 5) EPICS2023 deletes extraneous repeated energies in earlier versions of the photon data, EPDL.
- 6) EPICS2023 ensures that all thresholds start with a zero cross section, e.g., all photoionization subshells); earlier versions confused users in interpolating or extrapolating data.

### **PLEASE DO NOT ASSUME ANYTHING!**

Of the changes described above by far the BIGGEST problem that we had is that users refused to believe and/or obey the documentation. Specifically, in earlier versions of EPICS the data was **log-log interpolable**. Again, let me stress that we are not interested in results at discrete energies; these are not physically observable. We are interested in results integrated over energy, which are observable; these strongly depends on how we interpolate data and results. Based on feedback from users, who had problems using log-log interpolation, I converted ALL data to be linear-linear interpolable, using my PREPRO/LINEAR code [6] (LINEAR has been used and demonstrated to be accurate over almost 50 years). Generally, this led to an increase in the number of data points required to accurately represent the data, causing our codes to run longer. This is acceptable to us under Howerton's first law[7] **"We are in no rush for the wrong answer"**. Yes, I do listen to user feedback, and I do try to improve how the data is presented for your use.

I assumed that solved the problem. Unfortunately, it did not. Some users refused to believe the documentation and ASSUMED, because some of the data tables were actually smaller, the interpolation must still be log-log. What they overlooked was:

- 1) In going from EPICS2014 to EPICS2017 **photo-excitation was dropped**, and interpolation was changed from log-log to lin-lin. Dropping the excitation allowed some tables to be smaller in EPICS2017 than they were in EPICS2014, even using lin-lin interpolation.
- 2) **MOST IMPORTANT: YOU HAVE MY EMAIL ADDRESS – THERE IS NO REASON TO ASSUME ANYTHING!** If they simply asked I would have explained. Unfortunately, some users did not ask, made the wrong assumption, and published misleading results, e.g., using the wrong interpolation can result in differences of a factor of two or more (**100%**). Even after I explained that their assumption was wrong, some users still refused to admit that there could be errors in their results due to their erroneous assumption.

### 3. It Takes a Village

I do not claim to be an expert in photon or electron interaction data; my expertise is in the ENDL and ENDF formats, and my ability in compiling all the data we need and bringing them together in these formats, so that users can use and test the data. But to make the effort forth while **"It Takes a Village"** = it takes all of us working together, pooling our knowledge to iterate and improve the photon and electron data that we ALL need.

You may do the most brilliant work and discover the most interesting results, which you can be proud of. But if you do not report your result to me, our community of users will not benefit. They cannot benefit if

I am not aware of your results and how they may be used to verify or improve future versions of our data. Basically, until YOU verify this data, we are in a classic “Garbage In = Garbage Out” situation, i.e., bad atomic and nuclear data produces bad results, regardless of how perfect your transport code may be.

In order to ensure that your feedback is useful we must be sure you are using the data EXACTY as it is provided to you, and that you obey ALL the ENDL and ENDF rules, so that you are indeed actually using the same data as the rest of our community. Here, I will again stress the importance of obeying the interpolation law defined by the ENDL and ENDF formats. Refusal of users to follow the rules, I am sorry to say, can invalidate results and as a consequence these results cannot be used to improve the data used by our community (our Village). Indeed, if you do not follow the rules, results may be misleading and appear to show phantom problems with the data, which may not be real, causing us to waste valuable time/energy. The success – or failure – of this effort is entirely in your hands: we can succeed if you follow the rules, use our data exactly as it is defined, and report your result to me – or waste your efforts and we fail. **THE CHOICE IS YOURS.**

#### 4. Acknowledgement

First let me acknowledge the many users of these data who in their tests located data and formatting mistakes and took the time to report these mistakes to me. This allowed me to correct the mistakes, and to make the corrected results available to users. **Almost all the corrections to our data files today are based on feedback from users, and this feedback (pro and con, both help), is much appreciated.** We all (all = our community – our Village – creators and users of the data) gain by pooling this wealth of expertise, ultimately making everyone’s calculated results more accurate and reliable.

I thank **Marilena Bandieramonte** (CERN) for reporting errors that led to the February 2018 update. I thank **Jiri Ulrich** (PSI, CH) for reporting errors that led to the April 2018 update; see the 2019 report for details. I thank **Bret Beck** (LLNL) for finding and correcting the ERROR in the bremsstrahlung ZAP (particle produced); it is now correct, 0 (photon), rather than the ERROR 11 (electron). I thank the many users who reported duplicate (energy, cross section) pairs, which have now been deleted. I thank the users who asked: how is the cross section defined outside of it tabulated range; this has now been improved by adding an extra energy point at thresholds, to ensure each reaction starts with zero cross section.

I thank **Maurice Greene** (AMPX), and **Bob McFarlane** (NJOY), for being part of our Village and agreeing to coordinate improvements in the three U.S. codes: AMPX, NJOY, PREPRO. This cooperative effort extends back over most of the last half century and has led to significant improvements in the results produced by all three codes. We would not be where we are today without this cooperation. I am sorry to say that my good friends Maurice has passed on, and Bob has retired. I can only hope that in the future others step up to take on their roles, **so that our Village can continue to improve our data and codes.**

I thank the many readers who took the time to review the early draft of EPICS status reports, in particular I thank **Andrej Trkov** (IJS), **Cesc Salvat** (U. Barcelona), **Dave Brown** (NNDC. BNL), for their helpful suggestions, which have been incorporated into the final versions. I also thank **Roberto Caputo** and **Kira Nathani** (NDS, IAEA, Vienna), for editing and producing the final version of this paper as an IAEA report.

## 5. The Purpose of ENDF

A primary objective of the ENDF “system” is to provide NUCLEAR and ATOMIC data in a computer independent format, with well-defined/documented definitions for ALL quantities in the format. Over 50 years ago, when ENDF started there were no commonly accepted unique definitions for much of the data, e.g, every lab, school, and textbook had a different definition of the equations for neutron resonance parameters. Therefore, the ENDF “system” included not only data, but of even more importance the ENDF Bible: ENDF-102 [5], that defines ALL formats and conventions. In ENDF-102 no claim is made that the definitions used are always the BEST; what is more important is that: 1) They are unique, and 2) They are used by everyone = **data creators and users, alike, agree to follow these definition and conventions; without these agreements we would have chaos.**

Another objective of ENDF was to allow data testing, which is only possible if everyone agrees to follow the same rules and conventions. Without this agreement it would be IMPOSSIBLE to perform meaningful, useful data testing, i.e., otherwise this would be comparing apples and oranges. Both objectives, used in combination, allow us to pool the wealth of user experience, in the hope that this experience can be used in the future to further improve our data, and to accomplish this as quickly as possible to meet our needs. Over the last 50 years this plan has been highly successful and has, in my personal judgement, led to making today’s data file vastly superior to what we used back then. But, this is an iterative process, and we are not yet finished – this is why **your feedback is so important.**

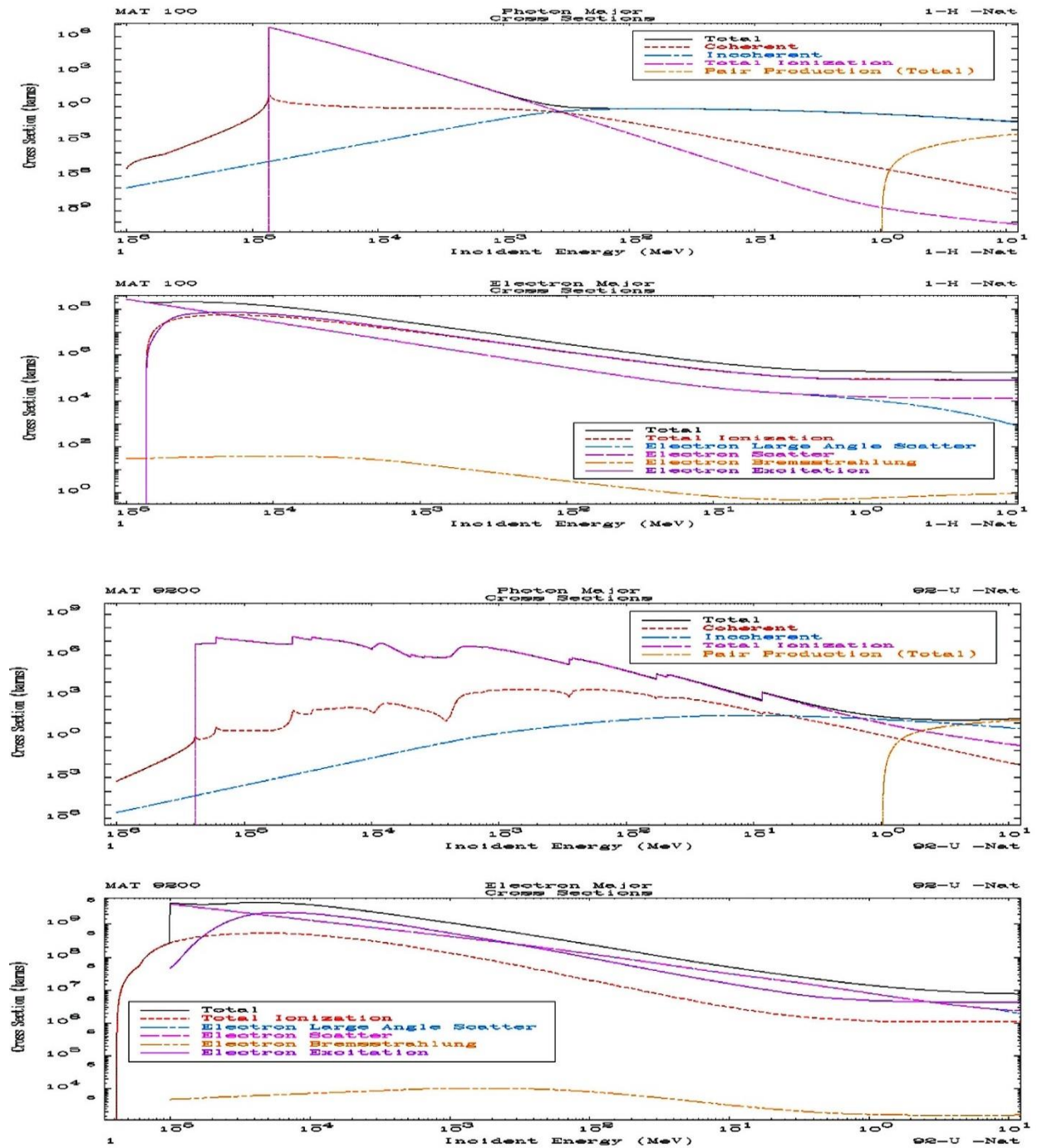
Another advantage of using the ENDF, and to a lesser degree ENDL, is the software provided for data in these formats. For example, for EPICS and this document I used my PREPRO codes [6] to linearize the EPDL photon data using PREPRO/LINEAR, and to create many of the figures shown herein I used PREPRO/COMPLIT. Similarly, for ENDL, I use the utility code RELAX to calculate the photon and electron spectra emitted as an atom relaxes from an ionized state back to neutrality; in particular, I calculate the fluorescence used by the TART Monte Carlo code [8]. I also used the EPICSHOW code [9] to produce two figures used in this report.

The success – or failure – of this plan obviously depends on YOU – the data user. You, and all the other members of our community (our Village) of users, are expected to report the results of your use back to us. We do not read minds, so that without your assistance we cannot improve the data as rapidly as possible, for the good of ALL users including yourself. We strongly urge you to join us in this effort, so that we have: “All for one, and one for all”. **YOU HAVE MY EMAIL ADDRESS – PLEASE SEND ME YOUR RESULTS.**

## 6. What’s Different in EPICS2023: EPICS2023 Overview

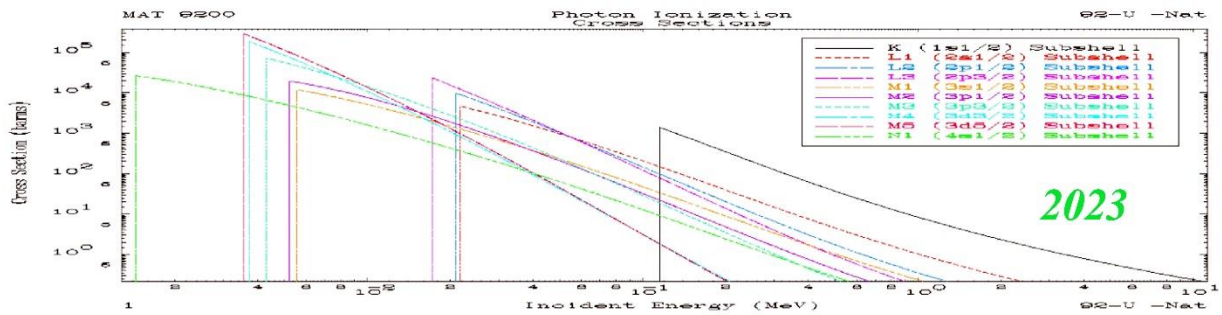
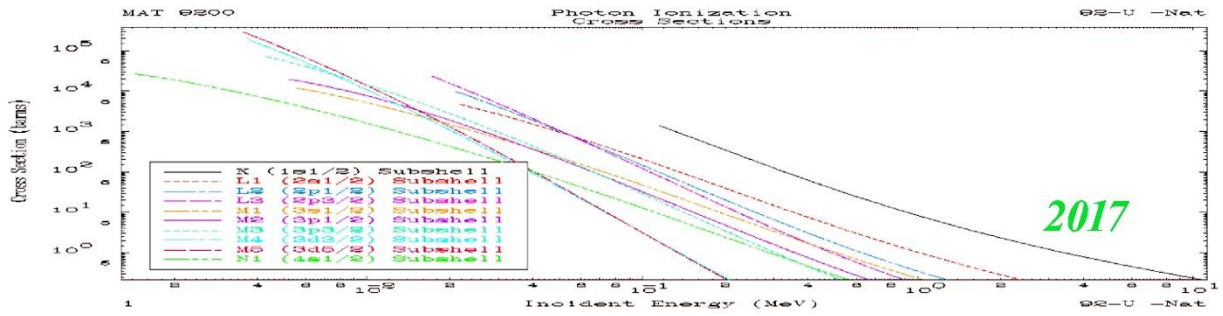
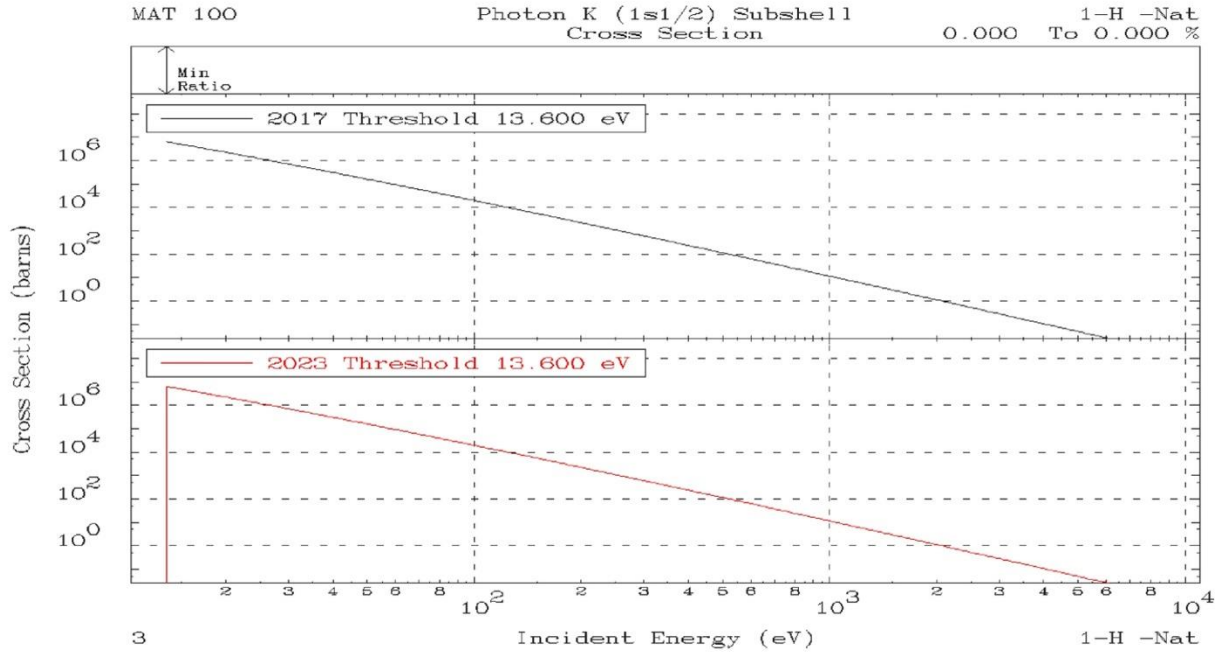
Below are overview pictures of  $Z = 1$  and 92, photon and electron data. Generally, the photon data extends down to 1 eV, and the electron data down to 10 eV; it may abruptly end at these energy limits or extend slightly beyond. **WARNING** – we again remind readers that the data are given over these energy ranges as better than nothing, but we **STRONGLY** recommend that it should only be used for applications in the keV to MeV energy range; outside this range it has large uncertainty and is unreliable = **CAVEAT EMPTOR!**





### Cross Sections Outside Tabulated Range

Many users who were new to the ENDL and ENDF formats asked: How are cross sections defined outside of the energy range they are tabulated; see the below pictures of H and U from EPICS2017, where photoionization start at their edges with a maximum value. In the hope that it clarifies the data. for EPICS2023 I added an additional starting energy point with zero cross section at each edge; see EPICS2023 data below.



## Duplicate Energy Points in EPDL

A number of EPICS users reported duplicate energy points in the EPDL data, i.e., same energy and cross sections. These appear in both the original ENDL format, in which the evaluations were performed, and the ENDF format, to which they were translated. These have now been deleted from both ENDL and ENDF formats. Note, that ENDL does not include SUM cross sections, which are included in ENDF; so that the number and values (cross section) of duplicated points are more numerous in ENDF and naturally sums in ENDF will differ from the parts in ENDL (as we see below). To my knowledge, these duplicate points did not create any numerical problems, as far as calculated physical observable integrals are concerned.

### ENDL format examples of duplicate points (energies in MeV)

```

17000 7 0 35.453 2308032 2 0.0 0.0 0.0
73 0 0 0.0 0.0 0.0 0.0 0.0
2.770000000D-04 3.249675230D+06
2.770000000D-04 3.249675230D+06
19000 7 0 39.102 2308032 2 0.0 0.0 0.0
73 0 0 0.0 0.0 0.0 0.0 0.0
4.340000000D-06 3.495570000D+04
4.340000000D-06 3.495570000D+04
24000 7 0 51.996 2308032 2 0.0 0.0 0.0
73 0 0 0.0 0.0 0.0 0.0 0.0
8.000000000D-05 5.039403760D+06
8.000000000D-05 5.039403760D+06
    
```

### ENDF format examples of duplicate points (energies in eV)

```

277.000000 2924541.91 277.000000 3249831.91 277.000000 3249831.91 MAT-MF- MT-####
1234567890123456789012 1700-23-501- 241
4.34000000 34956.0067 4.34000000 34956.0067 4.35247133 33279.8352 1900-23-501- 36
1234567890123456789012 80.00000000 5039457.02 80.00000000 5039457.02 80.4457625 5011959.88 2400-23-501- 191
1234567890123456789012
    
```

## Bremsstrahlung Data Incorrectly Identified in EEDL ENDF Format

Bret Beck (LLNL) discovered and corrected a serious ERROR in the bremsstrahlung data in the EEDL data in the ENDF format; this ERROR does NOT appear in the original EEDL data in the ENDL format and appeared to be an ERROR introduced in the translation to the ENDF format. **WARNING** – if this data were used in any application assuming electrons, rather than photons were emitted, the results would be complete rubbish!!!! **Many thanks Bret.**

The ERROR is that ZAP (“particle” produced) is erroneously identified as an electron (ZAP=11),

```

1000.00000 .999241400 0 0 2 0 100-26-527- 1
11.00000000 5.438673E-4 0 1 1 2 100-26-527- 2
    
```

This has been corrected to photon (ZAP=0), by changing one number on the second line of each MF/MT = 26/527, for all 100 evaluations, Z – 1 to 100.

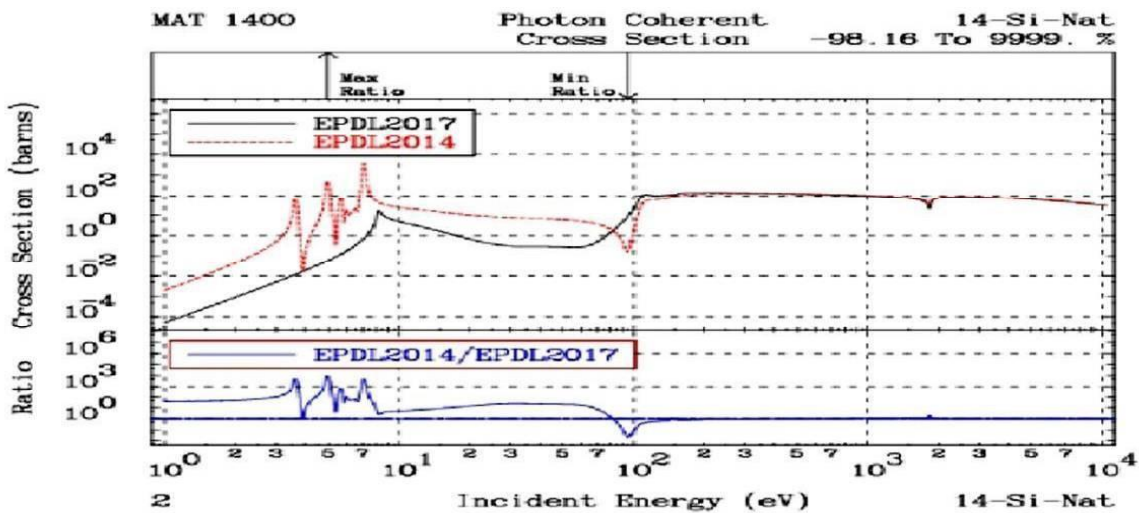
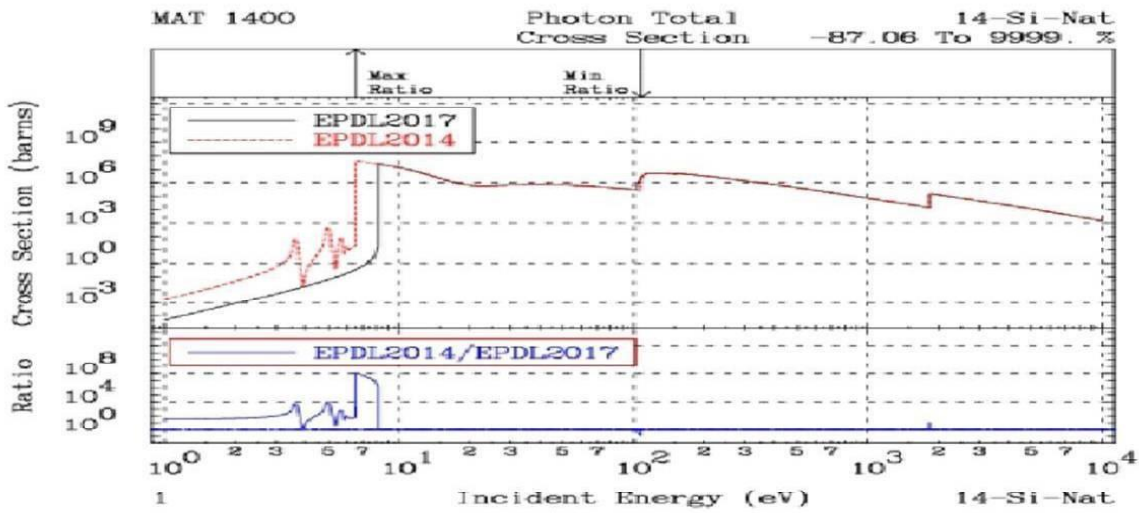
```

1000.00000 .999241400 0 0 2 0 100-26-527- 1
0.0 5.438673E-4 0 1 1 2 100-26-527- 2
    
```

### Reminder: EPDL does not include EXCITATION

Below is but one example showing that as of EPICS2017, EPDL has not included EXCITATION (this figure is a copy of what appears in the earlier EPDL report). Hopefully, this example will illustrate that the combination of changing from log-log to lin-lin interpolation (tends to increase the number of energy points) AND removing excitation (tends to decrease the number of energy points), can result in a net decrease in the number of energy points in EPICS2017. Removing the excitation particularly simplifies the anomalous scattering, which in turn simplifies the coherent scatter, greatly **reducing the number of tabulated energy points required to accurately define the data even using lin-lin interpolation.**

Also, hopefully this example illustrates that **excitation need not be included in EPDL** because it is a lower energy phenomenon, below the keV to MeV energy range that EPICS is designed to accurately model.



### For Coupled Photon-Electron Calculations

The **TART** [8] Monte Carlo code performs coupled neutron-photon calculation, but it does not perform electron transport; all electron energy is deposited at the space point they are produced. If you have applications that really require coupled photon-electron calculations or are outside the designed range of EPICS (keV to MeV), I make the following recommendations.

For **lower energy** applications, or those in which molecular, chemical, density effects are important consider using **PENELOPE** [10], which is designed, and has an excellent reputation, for accurately calculating coupled photon-electron applications.

For **medium energy** applications, in the keV to MeV range, consider using **MCNP** [11], which can now handle coupled photon-electron applications.

For **higher energy** applications, consider using one of the higher energy codes, such as **GEANT** [12] and **FLUKA** [13]. These include PHOTONUCLEAR physics that is not included in EPICS; EPICS only includes ATOMIC, not NUCLEAR data.

**Below the keV energy range** there are atomic binding effects not considered by the EPICS data. For example, the currently BEST estimate of the K shell electron in H is 13.6 eV. The good news is that this is a well-known value and is what is included in EPICS2023. The bad news is that H does not exist in nature; the binding energy for H<sub>2</sub> is 16.4 eV, 21% higher. And for something that might seem like a simple change from H<sub>2</sub> to H<sub>2</sub>O (water) the binding has a completely different value. Let me again, here stress: EPICS only includes ELEMENTAL data (for elements with atomic number,  $Z = 1$  through 100), e.g., there is no data for H<sub>2</sub>, H<sub>2</sub>O, or any other material. The good news is that this has a major effect only at lower energies, below keV energy range where EPICS data should be used, so EPICS meets our current ENDF needs.

**Above the MeV range** that we normally encounter in ENDL and ENDF applications, **photonuclear** events become progressively more important. Again, we stress EPICS2017 included **ATOMIC, no NUCLEAR** data, and there are no plans, or indeed, need to extend it to include photonuclear data. There is no need because ENDF already includes a separate file of photonuclear data, which can be used in conjunction with EPICS atomic data to model particle transport; see the NNDC website for details.

### Use ONLY the Most Recent EPICS Data

The EPICS2023 data will soon be FREELY available ON-LINE at: the National Nuclear Data Center, Brookhaven National Laboratory, the Nuclear Data Section, IAEA, Vienna, Austria, and NEA/DB, Paris, France. But the BEST place to ensure that you have the most recent data is at my website,

<http://redcullen1.net/homepage.new/>

## 7. Conclusions

Usually, my conclusions mostly repeat my introductory remarks, inline with my normal approach: 1) tell them what you are about to explain, 2) explain it, 3) tell them what you have explained. In this case I will present different closing remarks: **a plea for YOU the reader to help in maintaining, verifying, and improving our data and codes.**

First some background. By the time I completed my thesis on integral particle transport, it was obvious to me that regardless of how accurate I designed and implemented any transport code, I was in a “garbage in = garbage out” situation unless I had good nuclear and atomic data. In an attempt to help improve our data, I initially took a post at what later became the National Nuclear Data Center (NNDC), Brookhaven National Laboratory, where the Evaluated National Data File (ENDF) was in its infancy. There I quickly realized that the potential of ENDF could only be fully exploited if it had software to support the effort, so I began to work on what today are the ENDF Pre-Processing Codes, PREPRO2023 [6]. My second position was at the Lawrence Livermore National Laboratory (LLN), where I continued to work on nuclear and atomic data, but also could return to my first true love: particle transport, working on the TART2022 code [8].

Today it is over 56 years since I started working at NNDC, BNL, and over 50 years since I moved to LLNL. As you can see by this report, and the references in this report, I have continued my work on: ENDF support codes, PREPRO2023 [6], and Monte Carlo Transport, TART2022 [8], and Atomic Electron-Photon Interaction Cross Sections, EPICS2023, **even though I retired in 2009, over 14 years ago.** I have carried on this effort without financial or facility support because I felt I could still make an important contribution, and to keep myself mentally active.

Since I am retired now I am more of a spectator, than a participant in any projects at any research facility. In order to keep this effort going I need YOUR support – not financial support – I need support from the READER of this report, and USERS of my codes and data. Specifically, I need feedback from YOU – both PRO and CON feedback help. PRO feedback demonstrating that these data and codes are useful and accurate in your applications and encourage me to carry on. CON feedback demonstrates that we can still make improvements in our applications.

But I do not read minds, and I do not have the time nor the energy to search many publications. What I need is for **YOU TO SEND ME COPIES OF YOUR REPORTS** – plus any additional background information, as to how you judge the quality of our codes and data – or lack thereof. The future of this work is in your hands – **PLEASE BECOME PART OF OUR VILLAGE AND HELP!!!!**

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