INTERNATIONAL ATOMIC ENERGY AGENCY

NUCLEAR DATA SERVICES

DOCUMENTATION SERIES OF THE IAEA NUCLEAR DATA SECTION

IAEA-NDS-228

EPICS2017:
April 2019 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
Website: http://home.comcast.net/~redcullen1

April 2019

Abstract: This report is intended to bring readers up-to-date as to the current (April 2019) status of the Electron-Photon Interaction Cross Sections, version 2017 (EPICS2017). These evaluated data were initially released in 2017, and the evaluations have not changed since then. However, there have been two changes in how these data actually appear (are coded) in the ENDL and ENDF formats; the last being in April 2018. The bottom line is that this data has been up-to-date and FREELY available on-line at no cost to users for a year and we have no current plans to make any changes

Nuclear Data Section International Atomic Energy Agency
A-1400 Vienna
Austria
E-mail: NDS.Contact-Point@iaea.org
Fax: (43-1)26007
Telephone: (43-1)2600-21725
Web: http://www-nds.iaea.org
P.O. Box 100

Disclaimer

Neither the author nor anybody else makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information disclosed, or represents that its use would not infringe privately owned rights.

The IAEA-NDS would appreciate any comment on this report at: NDS.Contact-Point@iaea.org.

The IAEA-NDS-reports should not be considered as formal publications. When a nuclear data library is sent out by the IAEA Nuclear Data Section, it will be accompanied by an IAEA-NDS-report which should give the data user all necessary documentation on contents, format and origin of the data library.

IAEA-NDS-reports are updated whenever there is additional information of relevance to the users of the data library.

For citations care should be taken that credit is given to the author of the data library and/or to the data center which issued the data library. The editor of the IAEA-NDS-report is usually not the author of the data library.

Vienna, April 2019

Contents

1 April 2019 Status Report

This report is intended to bring readers up-to-date as to the current (April 2019) status of the ElectronPhoton Interaction Cross Sections, version 2017 (EPICS2017). These evaluated data were initially released in 2017, and the evaluations have not changed since then. However, there have been two changes in how these data actually appear (are coded) in the ENDL and ENDF formats; the last being in April 2018. **The bottom line is that this data has been up-to-date and FREELY available on-line at no cost to users for a year and we have no current plans to make any changes.**

Following the initial release of EPIC2017 extensive data testing was performed. This testing found no actual errors in the evaluations, but it did find errors in the data as it was coded in the ENDL and the ENDF formats. As soon as our data testers reported these errors to me, I updated the actual data files, and as a result several versions were distributed. I documented these modifications of the coding/format both in earlier reports and in the data files themselves. There have been no changes to the numerical values in the files for almost a year (April 2018). However, recent publications indicate that some users are still using data that was superseded almost a year ago, e.g., see ref. [6].

Bottom line: Now that all the reported formatting problems have been in place for almost a year, 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.

2 What EPICS2017 is and isn't

The Electron-Photon Interaction Cross Sections, 2017 version (EPICS2017) includes **ELEMENTAL, cold, neutral, isolated ATOMIC** data 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** tradition 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

1) EPICS2017 included updated subshell binding energies – affects 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

3 Acknowledgement

First let me acknowledge the users of these data who in their tests located 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 as-soon-as-possible. **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 = the community of creators and users of the data) gain by pooling this wealth of experience, ultimately making everyone's calculated results more accurate and reliable. In particular, I will repeat here the acknowledgement I included earlier in the EPDL and EADL documentation.

The following paragraph is copied from the **EPDL, February 2018** report [2],

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 sections, 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.

The following paragraph is copied from the **EADL, April 2018** report [1],

April 2018 Update: This paragraph is the only change in this report for the April 2018 update. I thank **Jiri Ulrich (PSI, CH)** for discovering and reporting an ERROR in the ENDF formatted version of EADL2017. This ERROR only involved the ENDF formatted data for the transition energies; the binding energies were correct, but the transition energies were the 2014 values; these have now been corrected There were NO CHANGES to the ENDL formatted data. The remainder of this report are identical to the original September 2017 report.

There have been no other changes to EPICS2017 since the above indicated changes to EPDL/ENDL and EADL/ENDF formatted data, and neither of these involved any changes to the actual evaluation; both changes only involved correcting mistakes made in coding data in ENDL and ENDF formats (mea culpa).

I also acknowledge "First Assessment….of EPICS…" [6], but cannot thank the authors, because they never informed me of this work; it was only by chance that I discovered this report earlier in April 2019. Consider the above two acknowledgements leading to improvements in EPDL, February 2018, and EADL, April 2018. Each of these only required one e-mail contact and a few days to correct the coding of the data. Compare this to ref.[6]: Submitted for publication March 2018, Revised June 2018, Published August 2018, essentially the same material presented orally August 2018, I discovered this work only in April 2019; 13 months after it was first submitted for publication, and the latest oral presentation still includes data that was superseded by April 2018, one year ago. As soon as I read ref. [6] I wrote a draft of this status report, to correct the unfortunate assumptions made in ref. [6], and I forwarded this draft to an author of ref. [6] in the hope of correcting these assumptions. She responded [20] that she was too busy to read this status report, and she suggested that I delay release until a meeting planned for next October 2019. I judge this to be an unacceptable

delay in informing the many users who rely on us. In this situation I can only hope that this 13 month delay has not resulted in errors in the results produced by the authors of ref' [6], or in the work of any readers who may have read ref' [6], and I am proceeding with immediate release of this status report. In retrospect this seems like such a shame: this situation could have been avoided by one e.mail contact 13 months ago. This is the only paragraph that has been substantially changed since the initial draft that I sent to the author of ref' [6] for review.

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

4 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 definitions for ALL quantities included in the format. Over 50 years ago when ENDF started there were no commonly accepted definitions for much of the data, e.g., almost every lab, school and textbook had a different definition of the equations for neutron resonance parameters. Therefore, the ENDF "system" includes not only the data, but of even more importance the ENDF Bible, ENDF-102 [4], 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) That everyone – data creators and users, alike, agree to follow these definitions and conventions; without this agreement 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 WAS IMPOSSIBLE, i.e., otherwise this would be comparing apples & oranges. Both objectives, used in combination, allow us to pool the wealth of user's 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 user needs. Over the last 50 years this plan has been highly successful and has, in my personal judgement, led to making today's data files vastly superior to what we were using way back then.

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 [7] to linearize the EPDL photon data using PREPRO/LINEAR, and to create many of the figures shown here I used PREPRO/COMPLOT. Similarly, for ENDL, I use the utility code RELAX to calculate the photon and electron spectra emitted as an atomic 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 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, to 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."

5 What is the most Recent Data?

The authors of ref. [6] expressed concern regarding confusion because of the two versions of EPDL and EADL (as I described above), so obviously they were aware of the superseded data, and yet they continue referencing it (?). When I checked all of the data/code centers are up-to-date and distributing only the latest EPIC2017 data (see, the below list of centers). Since there have been two different versions of EPDL and EADL, let me first cover how you can be sure you are using ONLY the most recent, up-to-date documents and data. The **most recent data and documents** can be obtained from,

Indirectly through my website,
http://redcullen1.net/HOMEPAGE.NEW/index.htm
or, The Nuclear Data Section, IAEA, Vienna, Austria https://www-nds.iaea.org/epics/
or, The National Nuclear Data Center (NNDC), Brookhaven National Laboratory
https://www.nndc.bnl.gov/endf/epics/
or, The Nuclear Energy Agency/Data Base (NEA/DB)
https://www.oecd-nea.org/tools/abstract/detail/iaea1435/
or, The Radiation Shielding Information Code Center(RSICC):
Request DLC-272/EPICS2017

The **most recent documentation** (included with the EPICS2017 distributions), for the data files are,

EEDL – A Survey of Electron Cross Section Data for use in EPICS2017, IAEA-NDS-226, **December 2017** [3]

EPDL – A Survey of Photon Cross Section Data for use in EPICS2017, IAEA-NDS-225, Rev.1, **February 2018** [1]

EADL – A Survey of Atomic Binding Energies for use in EPICS2017, IAEA-NDS-224, Rev. 1, **April 2018** [2]

If **you are currently using any of the EPICS2017 data but are not sure which version you are using**, you can also look inside the data files themselves; both ENDL and ENDF formats are designed to be self documenting, in the sense that they include dates, and in the case of ENDF a history of changes made to the data.

ENDL – The date is included on the first line of each table – below is an example of the EADL C (z=6) data – it is dated 180717 = 2018, July 17. Here I show the binding energies for the subshells of C.

```
  6000  0  0  12.0112    180717  2  0.0         1.0000E+50  0.0
91913  0  0.0         0.0         0.0         0.0         0.0
 1.000000000E+00 2.880000000E-04
 3.000000000E+00 1.659000000E-05
 5.000000000E+00 1.126000000E-05
 6.000000000E+00 1.126000000E-05
```

ENDF – The date is included on the seventh (7) line of each evaluation (element) – below I again show the EADL C (z=6) data – it is data April 2018.

```
  6-C  2017 Evaluated Atomic Data Library (EADL) by D.E. Cullen  2017 0  0    0
6000.00000 11.9078164         -1          0           0          0 600 1451    1
0.0         0.0                0          0           0          6 600 1451    2
0.0         1.0000D+11         0          0           6          6 600 1451    3
0.0         0.0                0          0          67          2 600 1451    4
 6-C -  0 NDS,IAEA   Eval-Dec17 D.E.Cullen                         600 1451    5
NDS-IAEA-224         Dist-Apr18                                    600 1451    6
```

The above tables show the same data in the ENDL and ENDF formats. Note, the difference in the dates, April 2018 in ENDF and July 2018 in ENDL – the difference is explained in the documentation; the ENDF formatted files were re-formatted for compatibility with C, C++, and FORTRAN codes much earlier in September 2014 (see, the below history), whereas the ENDL formatted file was not re-formatted until July 2018. It is important to understand that re-formatting the data in the ENDL format did not change the numerical values; all it did was replace "D" (.o.k., in FORTRAN, but a potential problem is C), by "E" (which is acceptable by both FORTRAN and C).

In the ENDF format the history of any changes to the data are also documented in the history section; this feature of text within the actual data file does not exist in the ENDL format.

```
================================================================ 600 1451   61
  History                                                        600 1451   62
================================================================ 600 1451   63
 (1) November, 1991 - Initial release in the ENDL format.        600 1451   64
 (2) November, 2001 - Initial release in the ENDF-6 format.      600 1451   65
 (3) September,2014 - Insure Standard C, C++, FORTRAN Format     600 1451   66
 (4) September,2014 - Updated based on recently published data   600 1451   67
 (5) September,2017 - New Binding Energies\Same Probabilities    600 1451   68
 (6) April,    2018 - Corrected Transition Energies              600 1451   69
================================================================ 600 1451   70
```

The bottom line is that based on the documentation (reports) and the data files themselves, the numerical values in ENDL and ENDF formats, has not been changed since April 2018 – an entire year ago. Also note that based on the documentation this was the last time any of EPICS2017 data was updated (EEDL, Dec. 2017/EPDL, Feb. 2018, and EADL, April. 2018). Also note that this is the data currently distributed by major code/data centers around the World.

6 What More Can We Do?

We do try to be as responsive as possible to data user needs, by correcting any problems with this data as soon as it is reported to me, superseding earlier data, and updating both documentation and data, as soon as possible. Unfortunately, this puts up into a "Catch-22" situation where we are wrong if we do, and wrong if we don't, correct data as-soon-as-possible. Even with all our efforts to inform users, there are bound to be some users who do not get the word and continue to use superseded data, e.g., ref. [6].

The BEST we can do is ask users to PLEASE, PLEASE, PLEASE tell me directly of any problems you have in using this data, and register with me as a user of this data, so that I can include you on my distribution list to be informed of any updates; send me an e.mail stating you are a user: redcullen1@comcast.net.

7 Examples of Noted Problems

Below I will try to briefly cover as many of the earlier reported problems with the coding of this data, and also address as many misinterpretations of the data as possible. Again, I mention that there have been no other changes to EPICS2017 since the above indicated changes to EPDL and EADL in the ENDF format, and neither of these involved any changes to the actual evaluations.

7.1 Energy Conservation

The primary objective of simultaneously producing evaluations for z = 1 – 100, ELEMENTAL data for ATOMIC parameters, as well as photon and electron interaction data, was to **guarantee energy conservation in coupled photon-electron transport calculations**. This made the above-mentioned April 2018 correction to the EADL2017 transition energies in the ENDF formatted data particularly

important (again, thanks to Jiri Ulrich). Thanks to this update, one year ago, currently all three libraries publicly available **EPICS2017 data files EXACTLY CONSERVE ENERGY**.

Unfortunately, ref. [6] and the related August 2018 oral presentation still refer to the superseded data, so it is worthwhile illustrating here the current correct data. Below is a copy of the current EADL data in the ENDF format, which is the same data as shown above when discussing dates inside the data and referenced in ref. [6]. The current K-shell binding energy (288 eV), and the K-L1 and K-L2 transition energies (276.14 eV) exactly conserve energy.

```
6000.00000 11.9078164          0          0          4          0 60028533    1
1.00000000 0.0                 0          0         54          8 60028533    2
288.000000 2.00000000 0.0        0.0        0.0        0.0        60028533    3
3.00000000 0.0         276.740000 5.61488D-4 0.0        0.0        60028533    4
4.00000000 0.0         276.740000 .001120600 0.0        0.0        60028533    5
2.00000000 2.00000000 254.820000 .413609000 0.0        0.0        60028533    6
```

The above results show the data in the ENDF format is correct. Using the EPICS2017 utility code RELAX (distributed with EPICS2017), one can now easily verify that the data in the ENDL format also **EXACTLY CONSERVES ENERGY**.

The bottom line here is that currently the EADL data EXACTLY CONSERVES ENERGY, but the recently published report [6] indicates that some users may still be using the data that was superseded a year ago.

7.2 Interpolation of Data

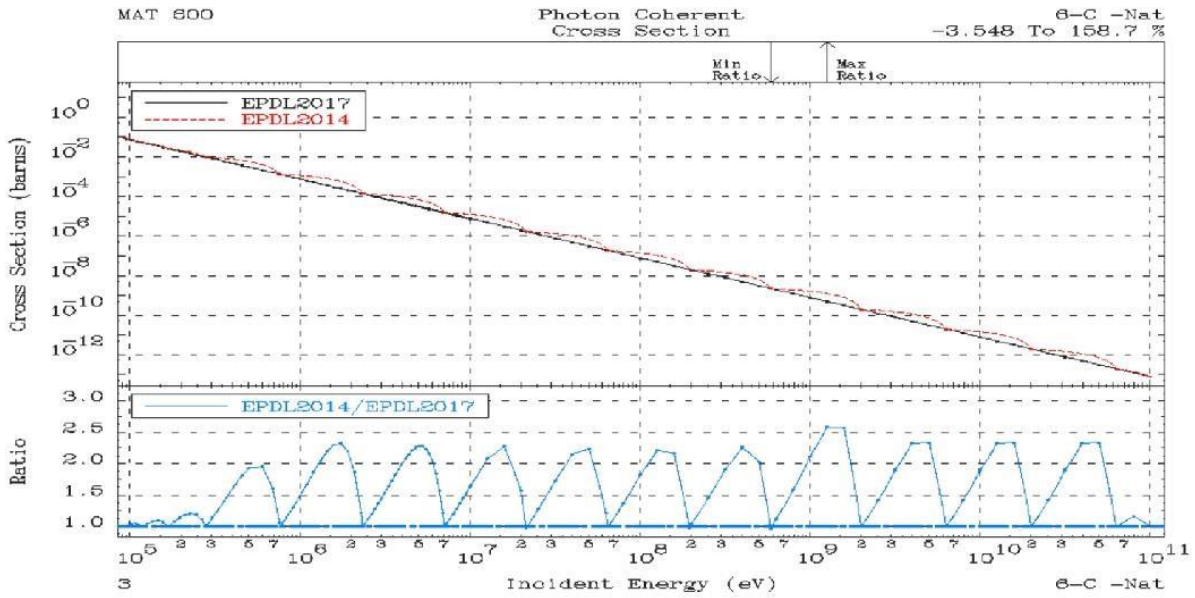
Interpolation is an extremely important point that I have tried to stress for decades throughout each and every version of our released photon and electron data. In our applications we are not interested in results at some arbitrary energy point, or points; these are physically unobservable. We are interested in INTEGRALS, over incident particles energy (and often space); these are observable and cause the effects we are interested in.

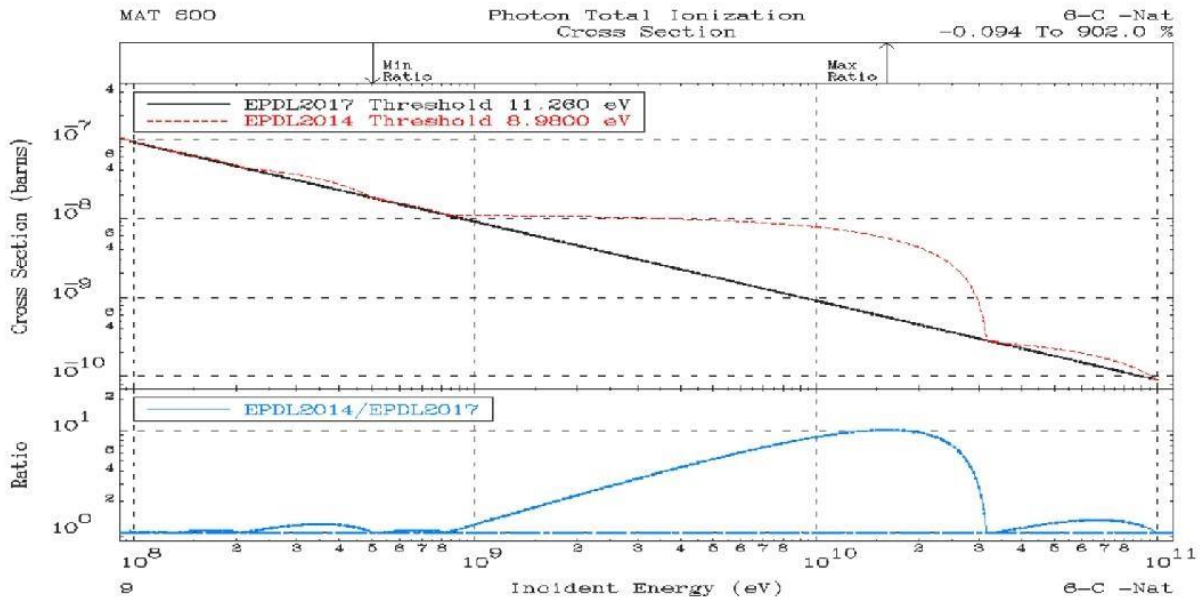
In both ENDF and ENDL formats, we represent our data as tabulated values at discrete incident energies PLUS an interpolation law to **allow us to define the data at ALL incident energies**; not just those at which the data are tabulated. Failure to obey these interpolation laws can result in ENORMOUS errors in the interpolated values and the integrals we are actually interested in.

In all versions of this data, up to and including EPICS2014 [10], photon (EPDL) and electron (EEDL) data within the data files themselves the data were defined to be log-log interpolable between tabulated values. In addition, in the documentation I stressed the importance of users following these interpolation laws if they wanted to obtain reliable results. Even with all these precautions in place, some users refused to follow the rules, often resulting in nonsense results, and blaming their results on poor data, rather than their own stupidity.

As a result, starting with EPICS2017 I tried to avoid this problem by re-calculating the energy dependent photon and electron data, and I supplemented this using PREPRO/LINEAR [7] to convert the EPDL data to be lin-lin interpolable. The results for the photon data was to increase the number of tabulated energy point by roughly a factor of three. Compared to erroneously linearly interpolating the original log-log tabulated values this simplified and improved the interpolated photon data values. The below 2 figures illustrate that for the C (z=6) data failure to obey the defined interpolation law for photon (i.e., using lin-lin interpolation for the EPIC2014 data), results in errors of over a factor of

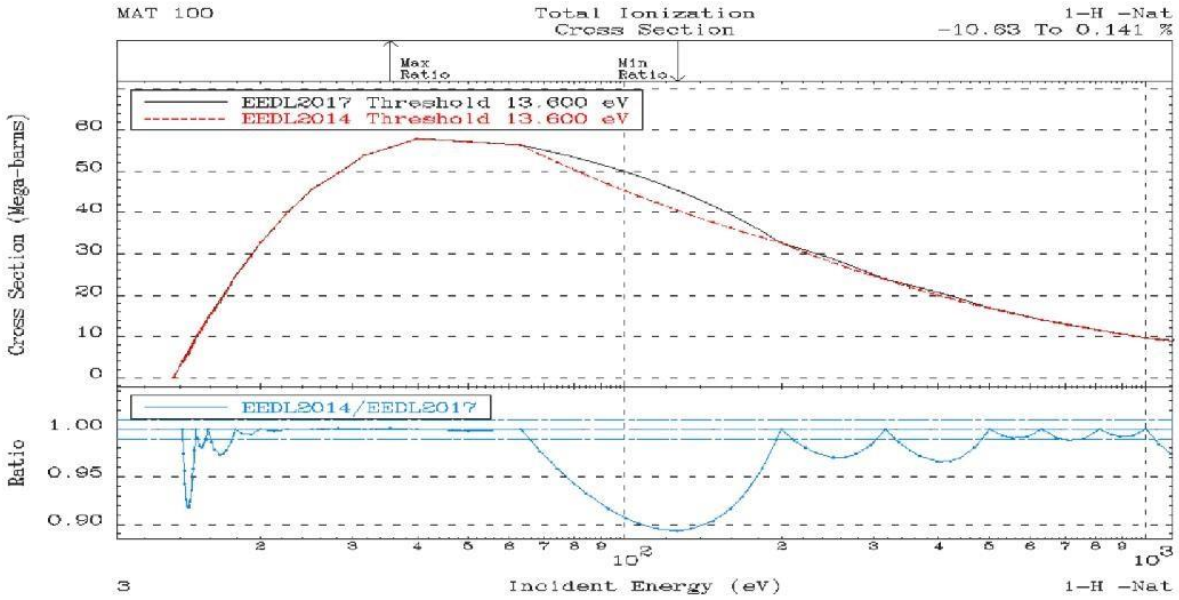
two (over 100%) for the coherent cross section and a factor of nine (900%) for the total photoionization. Here the bottom line is obvious: **for photons the factor of three increase in the number of tabulated photon cross section energy points is necessary, due to the change in the cross sections over many decades of value at high energy.**





In contrast the results for the electron data were quite different. After re-calculating the data and comparing results using lin-lin versus log-log interpolation we found that the lin-lin interpolated data agree better with the physically expected results. For example, the below plot illustrates that the EPICS2017 data for the total ionization using lin-lin interpolation differs from the EPICS2014 data using log-log interpolation by over 10%, and the EPICS2017 using lin-lin interpolation agrees better with what we physically expect. Here the bottom line is: **for electrons we did not have to increase the number of tabulated energies, and yet we can still use the simpler more efficient lin-lin interpolation**. As explained further later in this report, in changing from log-log to lin-lin

interpolation, the major difference between photons and electron cross sections is in the high energy range, requires three times as many points for photons, but no similar increase for electrons.



Bottom line: For EPICS2017 the documentation directs users to use lin-lin interpolation between tabulated values for both photon (EPDL) and electron (EEDL) data, and this is consistent with the interpolation laws within both ENDL and ENDF data formats which also specifies lin-lin interpolation. PLEASE: we beg users to strictly follow our recommendation and use the interpolation laws included in both ENDL and ENDF formats.

You might ask: If all of this is so clearly defined for EPICS2017 in both document and data, why am I spending more time here stating the same thing again. It is because some users still seem to think they know better; earlier there were some users who refused to use log-log interpolation (I did try to address this problem in EPICS2017 by going to lin-lin interpolation), but unfortunately, now there are users who refuse to use lin-lin interpolation. Some users noted the fact that in converting the data from EPICS2014 using log-log, to EPICS2017 using lin-lin interpolation the number of points used for photons increased by a factor of three, but the number of electron data points did not drastically change = **that is correct**. But they interpreted this to mean that the electron data still requires log-log interpolation = **that is incorrect**. The difference in the required number of energy points for photons versus electrons can best to understood by noting that at high energy the photon ionization cross sections are rapidly decreasing as roughly $1/E^k$ (ideal for log-log; but require more points for lin-lin), while for electrons they are roughly constant (ideal for lin-lin, not requiring more points). As the above figure illustrates, for electrons the EEDL data using lin-lin interpolation produces more physically acceptable results, and in the above case failure to follow the proscribed lin-lin interpolation results in up to 10% errors. PLEASE ignore all other assumptions and suggestions and follow our instructions to use **lin-lin interpolation for both EPDL and EEDL**.

8 ENDL, ENDF and Other Formats

No data format is perfect to meet all needs, and most recognize this fact and try to focus on the purpose for which they were designed. For example, Evaluated NUCLEAR Data Library (ENDL) format was designed as an in-house format used primarily by Livermore, and to a lesser degree by Los Alamos; it was designed to meet needs for higher energy neutrons (eV to MeV), e.g., it has no thermal neutron or even resonance region format, and it uses only tabulated energy dependent data. In contrast, the

Evaluated NUCLEAR Data File (ENDF) format was originally designed to meet the need of NUCLEAR reactor designers. Note that here I capitalized NUCLEAR, because this was the primary area of interest for both ENDL and ENDF. From their inception ATOMIC data for photons were included in both ENDL and ENDF because roughly 10% of the energy released in neutron fission is in the form of photons; most in the keV to MeV range. Initially the photon data was quite crude (only a few whole atom cross sections), but adequate to meet the needs for Livermore and Los Alamos high energy needs (ENDL) as well as for reactor design (ENDF).

ENDL and ENDF use different units for energy: ENDL MeV and ENDF eV. In addition, both use the same units for Form Factors and Scattering function; both represent these as a series of tabulated (x, y) pairs and an interpolation law between pairs. Unlike many publications that use wavelength for (x), both ENDL and ENDF use incident photon energy. For example, if you compare EPDL Form Factors in ENDL and ENDF formats you will find exactly the same tabulated (y) values, but (x) values, in either eV (ENDF) or MeV (ENDL). Above I tried to stress the importance of following the definitions used by the ENDF, and ENDL formats. **The decision to include form factors and scattering functions using incident photon energy (rather than wavelength) was not up to us in coding EPICS in these formats, rather it is imposed on us – and you – by these formats – PLEASE follow the rules and interpret this data as defined.**

At Livermore starting in 1989 EPDL [11] extended the photon data to include more information, such as subshell data, and by 1991 EADL [12] and EEDL [13], were created to define electron interaction data; both data files were designed and implemented solely in the ENDL format. Although there was no immediate need for these data within ENDF, based on interest from outside Livermore, we agreed to have these data files converted from the local Livermore ENDL format to the more widely used ENDF format.

EPICS2017 data is currently available in both the original ENDL format in which were developed, and the ENDF format to which they were later translated **However, users should be aware that not all of the data in the ENDL format could be converted to the ENDF format and in addition some quantities were created for inclusion in the ENDF that do not exist in the ENDL format**, (see, the excellent summary in [6]). For example, ENDL does not include "sums", such as total, and total inelastic (sum of levels) , and ENDF does not include average energy deposits, as well as transport cross sections. There are also a variety of atomic parameters in the ENDL format that were used during the evaluation process, that were judged not to be required to use the data, that have not been translated to the ENDF format. Worst of all, many years ago when it was initially translated from ENDL to ENDF, small angle electron scatter, that was added to ENDF to allow the electron data to be translated from ENDL, was erroneously translated to ENDF as the total electron elastic scattering cross section; I only discovered this error and corrected it between EPICS2014 and EPICS2017, so that today this data in the ENDF format is correct.

The bottom line here is to understand that the evaluations were performed and tested in the ENDL format and they are judged to be complete in this format. In comparison the data in the ENDF format is as complete as we could make it based on the limitations of the ENDF format. In addition, "sum" cross sections were added to the ENDF formatted data, e.g., total. Also be aware that the two EPICS2017 updates (one to EADL and one to EEDL), were not to correct any error in the original evaluations, but rather solely due to faulty translation of the data to ENDL and from ENDL to ENDF format. You, the user, are obviously free to use whichever format you are most familiar with and best meets your needs. **But if you have no preference, we recommend that you use the complete evaluations in the ENDL format.**

9 Energy and Space Range of Application

9.1 Energy Range of Application

Throughout the documentation for EPICS, and even earlier individual versions of EADL, EEDL, and EPDL, we stress that this data is designed to meet our needs to follow keV and MeV energy range "particles", and is limited to **ELEMENTAL, cold, neutral, isolated, ATOMIC data**. Currently there are no plans to extend this data to include nuclear, molecular, chemical or density effects. As a result in the documentation I suggest – no, let me make that stronger – **I WARN potential users not to use this data in their application below 100 eV; F. Salvat [14], recommends 1 keV (which today I am inclined to agree with), or above the MeV energy range.**

Below this 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 EPICS2017. The bad news is that H does not exist in nature; the binding energy for H_2 is 16.4 eV, 21% higher. And for something that might seem like a simple change from H_2 to H_2O (water) the binding is 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_2, H_2O, or any other material. The good news is that this has a major effect only at lower energies, below the energy range where EPICS data should be used, so EPICS meets our current 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 file of photonuclear data, that may be used in conjunction with the EPICS ATOMIC data, to model "particle" transport; see the NNDC website for details of photonuclear data.

Let me state once again: the data, particularly, the photon ionization has been extended to lower energies
ONLY TO ALLOW US TO CALCULATE ANOMALOUS SCATTERING FACTORS; this involves integrating over the entire energy range of the **total ionization cross section**. It was never intended – and we strongly advised against using this low energy data for ANY – repeat ANY – other purpose. In distributing the data I could have cut it off and only distributed higher energy data, but frankly I thought his would be insulting to potential data users. Instead I decided to treat all readers as adults who would understand and heed our WARNINGS. Boy was I wrong: it really re-enforced my old saying: **we cannot make our code or data idiot proof, because idiots are so ingenuous.** In this case we have received feedback from users asking about this lower energy data, which we appreciate hearing, because it helps us to better understand user needs and gives us a chance to correct any misinterpretation. To some users the source of the differences in the low energy cross sections between EPICS2014 and EPCS2017 were not apparent, so let me take a moment to explain.

9.2 Changes in Low Energy Photon Coherent Cross Sections

The photon coherent cross section in EPICS is defined as a combination of form factors and anomalous scattering factors. The anomalous scattering factors are defined by an integral over the photon total ionization cross section. So that any change in the ionization will result in a change in the anomalous scatter.

For EPICS2017 the chain of cause and effect is clear,

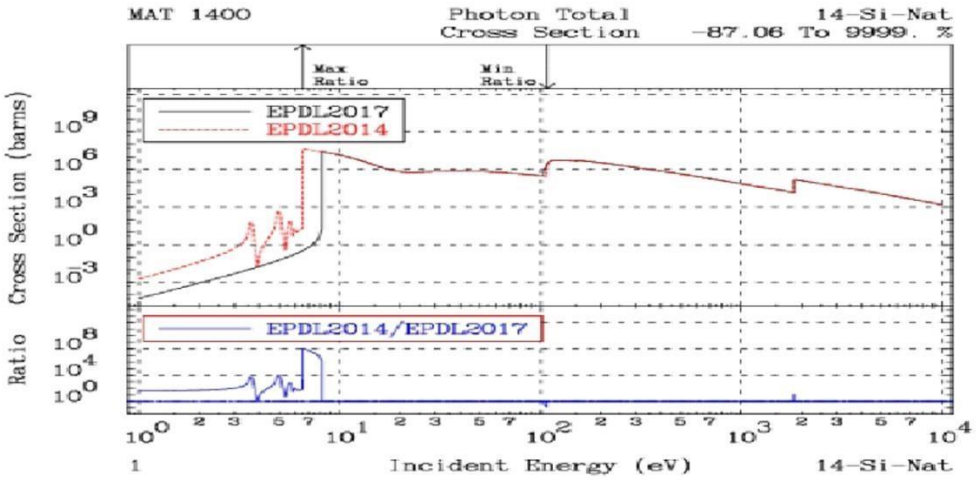
1) EPICS2014 erroneously included excitation; EPIC2017 does not - only ionization is used
2) New binding energies were adopted for EADL.
3) The new binding energies affected the photon ionization cross sections.
4) Which in turn, affected the anomalous scattering factors.
5) Which in turn, affect the coherent scatter.

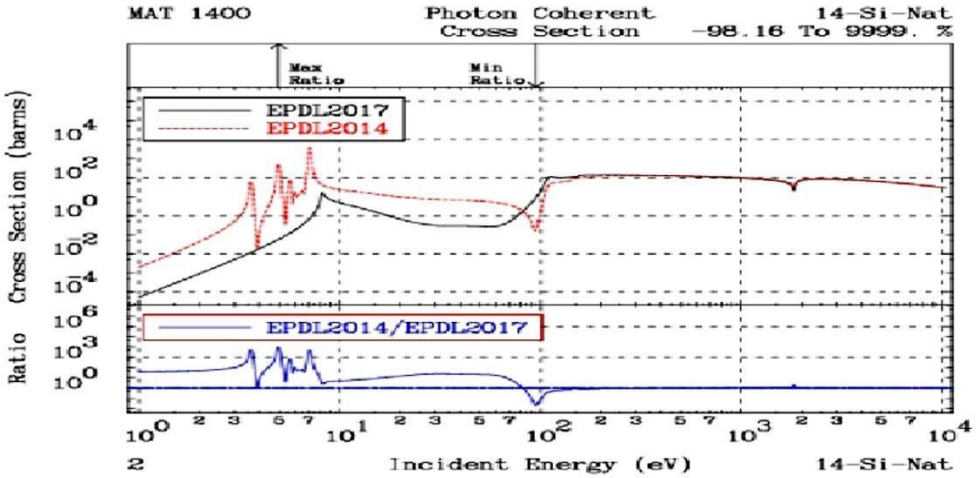
Of these at very low energy the one that any user can easily "see" is the effect of not including excitation in EPICS2017, and only using ionization (not excitation) to calculate anomalous scattering factors.

In the case of Si (z=14) the new, 2017, binding energies differ from the older, 2014, values; in the eV energy range they are slightly higher, explaining the difference in the photon total, and in turn the coherent (through the anomalous scatter); we can see these differences in the below plots of Si (z = 14) ELEMENTAL data. The most obvious difference between the EPICS2014 and EPICS2017 data below roughly 7 eV is because EPICS2014 erroneously included excitation (resulting in the "bumps" below 7 eV), whereas EPICS2017 does not. The anomalous scatter should be defined only in terms of the ionization (it is normalized to the atomic number (z) of each element); excitation must not be included.

Removing excitation from the definition of the anomalous scattering function and coherent scattering greatly reduced the number of tabulated energy points required to accurately represent this data, even after it was converted from log-log to lin-lin interpolation. This was not made clear in earlier documentation resulting in confusion by some users, who erroneously assumed that since the number of tabulated points did not increase it must still be log-log interpolable. This is another example of why we STRONGLY RECOMMEND that you not make any assumptions, you should contact us and ask. When users guess incorrectly (interpolation) this will obviously affect the accuracy of their calculated results.

The point to focus on here is not the difference at very low energy, where we WARN you not to use this data. Rather focus on the agreement above roughly 100 eV, and certainly by 1 keV. You might ask: Which of these agree with reality – unfortunately, **the answer is NEITHER**. Even with the improved 2017 binding energies, and correct definition of anomalous scattering (based only on ionization), the low energy cross sections are still limited in accuracy by the models we are using. When we originally assembled EPDL [11] Jim Scofield stressed the limits of his model, but we convinced him that SOLELY to allow us to calculate anomalous scatter it was better to have any guess, rather than to abruptly end all of the data at some arbitrary energy. Based on our plea Scofield agreed to supply this lower energy data, but again, solely to allow us to calculate anomalous scattering factors. **So PLEASE do not abuse this data; I repeat the WARNING:**
Do no use EPICS data below 100 eV, or 1 keV [14].





Hopefully the above section on limiting the ENERGY RANGE in which you can accurately use EPICS, convinces you as to what you should NOT DO. The question remains: what should you do if you have problems involving "particles" outside the keV to MeV energy range? Again, I will stress that EPICS is designed only to handle a very specific range of applications, and there are no current plans to extend it.

10 For Coupled Photon-Electron Calculations

If you have applications that really require coupled photon-electron calculations, or are outside the designed range of EPICS, I make the following recommendations.

For **lower energy** applications, or those, in which molecular, chemical, density effects are important consider using **PENELOPE** [16], 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** [17], which can now handle coupled photon-electron applications.

For **higher energy** applications, consider using one of the higher energy codes, such as **GEANT** [18] and **FLUKA** [19].

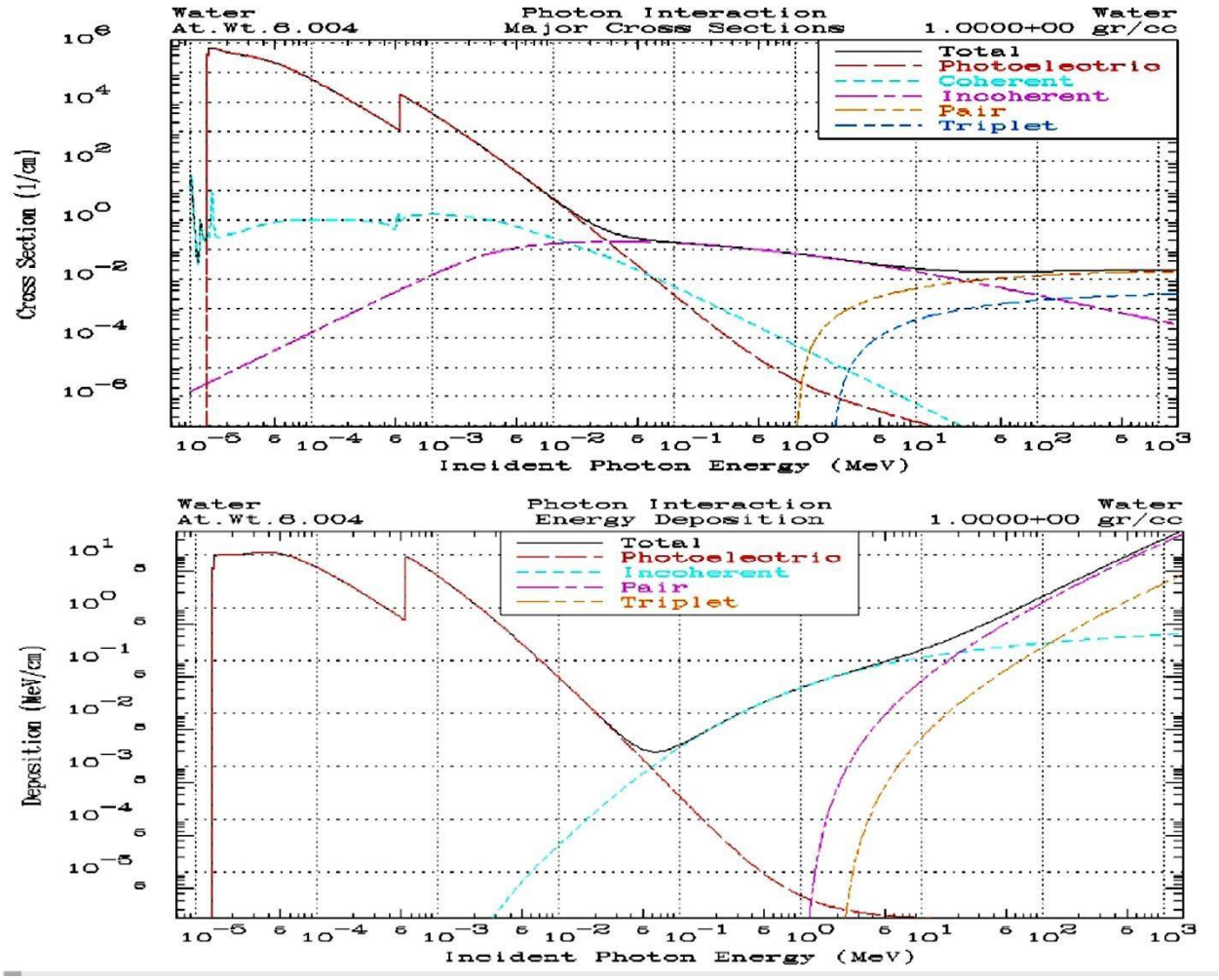
11 Size Matters: Space Range of Applications

If you are stuck with a code that uses EPICS data, such as I am in using the TART [8] Monte Carlo code, I will try to briefly explain what I do, and to show you why; **this is where the SPACE RANGE comes into play**. First, TART is currently limited to an upper neutron energy range of 20 MeV, which limits the upper energy range of induced or source photons to within the upper energy limit of where the EPICS ATOMIC data can be accurately used. Next, TART [8] currently does not track electrons, and it limits photon sources and tracking to a minimum of 100 eV; the minimum photon energy is a user input option. but it cannot be less than 100 eV. While tracking photons that are initially above 100 eV, any photon that due to an "interaction" ends up below 100 eV is assumed to be totally absorbed and its energy is deposited at the spatial point of the "interaction". When/where is this assumption justified?

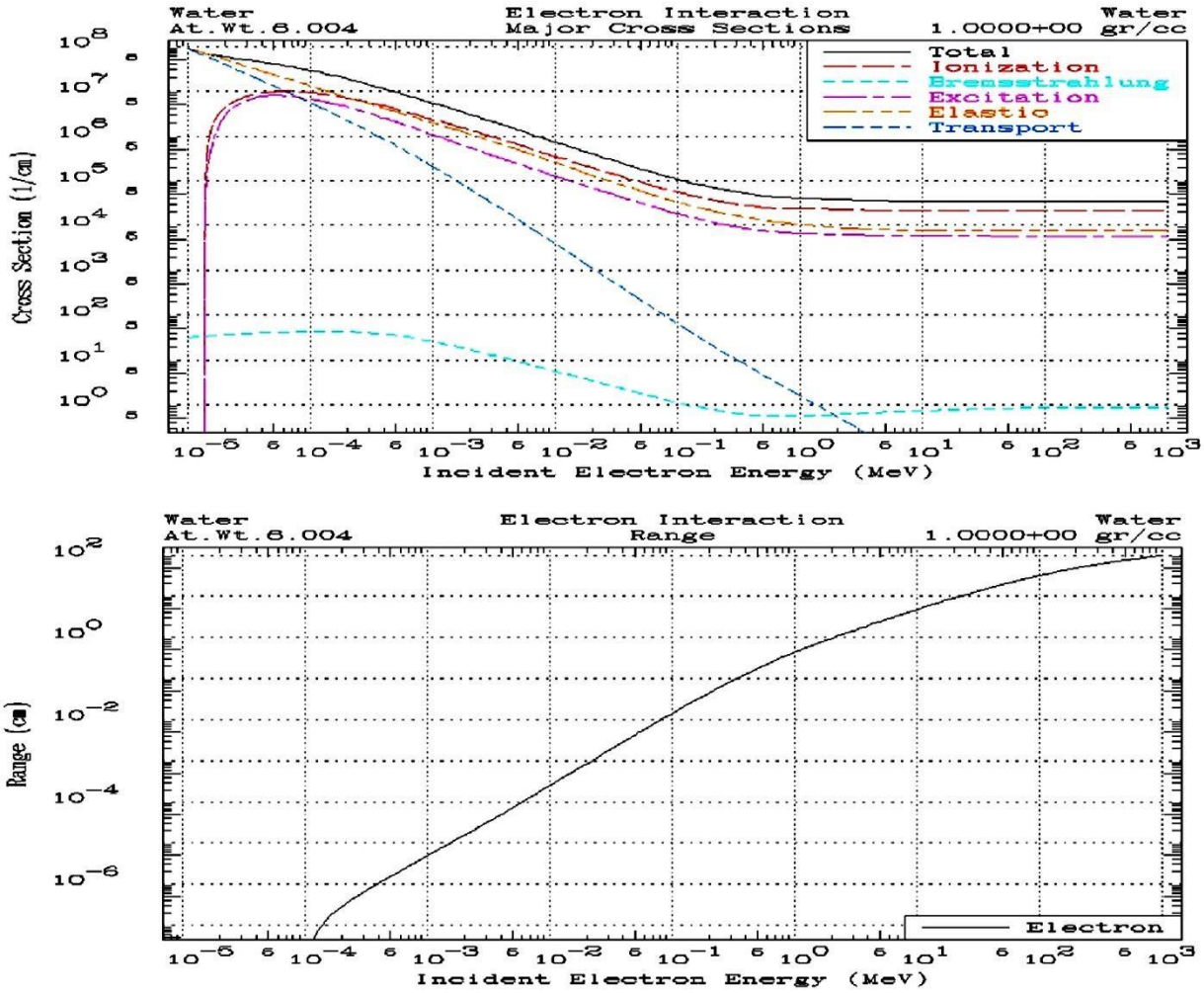
TART, like many Monte Carlo code defines spatial zones, and defines results only averaged over each spatial zone; results such as: flux, material damage and energy deposit. Below I will briefly attempt to explain why I feel we can justify absorbing and depositing low energy photons locally. Basically, if the distance to the boundary of the zone is large compared to the distance to the next photon collision AND the outcome of any collision will be photo-absorption, we know what the outcome of tracking the photon will be; so why bother wasting time tracking it: deposit its energy, end the photon Mont Carlo history, and move on. Below I will attempt to provide you with some idea what this means in terms of physical distance.

First, a WARNING – the below pictures of data are intended merely to illustrate approximate values, and the data itself is from EPICS2014, as shown by EPICSHOW [9] and does not exactly correspond to the current EPICS2017 data; it need not be for this illustrative purpose. The below figures illustrate the approximate photon interaction data for water (H_2O) at 1 gram/cc density; the (Y) axis is in macroscopic units. First, I show the cross sections and next the average energy deposit. From the cross sections we can see that at low energy virtually every "event" is photoelectric (absorbing all the photon's energy), e.g., in the extreme low energy the photoelectric is a millions of times greater than any other process; even at 1 keV it is almost 10,000 times any other process. At 1 keV the distance to collision is less than 0.001 (10^{-3}) cm, i.e., within less than 0.001 cm the photon will be totally photo-absorbed and deposit its energy locally.

Note also the effect of excitation near 10 eV (the blue "wiggles') , a million times less than the ionization. This excitation was erroneously included in EPICS2014/EPDL and mistakenly used to calculate anomalous scatter; as mentioned above, this error was corrected, and excitation is not included in EPICS2017/EPDL. Also, here I will mention an important difference between photons and electrons. With photons, each ionization event is catastrophic, where the photon loses all its energy and disappears in one single event; here relative to ionization, excitation is irrelevant and is not included in EPICS2017/EPDL photon data. In contrast electrons lose energy through many, many events, each individual event causing a small energy loss; here excitation is relevant and is included with the EPICS2017/EEDL, electron data.



The below figures illustrate the EPICSHOW [9] approximate electron interaction data for water (H_2O) at 1 gram/cc density; the (Y) axis is in macroscopic units. First, I show the cross sections and next the "maximum" electron range versus initial electron energy; this is the "maximum", because it ignores straggling and correspond to the total distance travelled by an electron. Unlike low energy photos that can lose all their energy in a single photo-absorption event, electrons lose small amounts of energy and require many "events" to lose/deposit their energy. So that in this case to determine a characteristic dimension we need to use the electron range. From the below figure we can see that in water the range of 1 keV electron is less than 0.00001 (10^{-5}) cm, and a 100 keV electron it is roughly 0.01 (10^{-2}) cm.



Bottom line: Size Matters when you (or the TART Monte Carlo code [8]) decide how to handle photons below some lower cutoff energy (be it 100 eV or 1 keV). The APPROXIMATION to deposit all of the photons energy locally is valid in spatial zones down to sub-cm size, e.g., less than 10^{-2} to 10^{-3} cm in the above example. The current TART assumption not to track electrons is based on the range of electrons generated from photon events (typically up to eV to keV) is valid in spatial zones down to roughly the same sub-cm size as the photon assumption, e.g., in the above example roughly 0.01 cm.

Again, if these energy and spatial dimensions limitations do not meet your needs I suggest you use PENELOPE [16] for complete coupled photon-electron calculation

12 Running Time and Storage Requirements

Neither running time nor storage requirements were considered in creating these evaluations. In all cases we followed Bob Howerton's first law [15]: "**We are in no rush for the wrong answer**". In all cases we included all the data we judged to be necessary to meet our needs, and no more than what we judged we need. We never compromised quality for speed or size; we have followed the same ground rules for over 50 years. During this time, we have seen computer sizes go from kilobytes, to

megabytes, to gigabytes, to terabytes, and speeds from microseconds, to nanoseconds, to picoseconds. Way back when this started kilobyte/microsecond computers costs millions of dollars, and a 20 megabytes storage disk was the size of a washing machine. Today's computers can be purchased for hundreds of dollars and terabyte sized disk drives are the size of a package of cigarettes cost about $100. By today the pendulum of cost has swung, so that computer costs are trivial and the main cost in our projects is **YOUR SALARY**. So, I strongly suggest: **Do not worry about reducing running time or storage requirements; instead worry about not wasting your valuable time.** If reducing running time by a factor of two prevents you have getting an accurate answer, you are not saving half of your time, you are wasting half of your time. If you are still worried about speed/size, see [6], which included an interesting study comparing EPIC2014 and EPICS2017.

13 Conclusions: A plea for Sanity

This report is intended to bring readers up-to-date as to the current (April 2019) status of the Electron-Photon Interaction Cross Sections, version 2017 (EPICS2017). These evaluated data were initially released in 2017, and the evaluations have not changed since then. However, there have been two changes in how these data actually appear (are coded) in the ENDL and ENDF formats; the last being in April 2018. **The bottom line is that this data has been up-to-date and FREELY available on-line at no cost to users for a year and we have no current plans to make any changes; we are now ready to hear feedback from you, the users.**

The primary purpose for making these data publicly FREELY available on-line at no cost to users is to allow us to pool the experience of as many users as possible, in the hope of continuing to improve this data to better and more accurately meet the needs of YOU – the data user. Whether or not this effort succeeds or fails is completely in YOUR HANDS. So PLEASE help us to succeed and send us your feedback – be it pro or con, all constructive criticism is appreciated and HELPS our entire community. Hopefully, you will understand that it would be insane not to accept when we "Make an offer you can't refuse" [private communication, Don Corleone, 1972].

References

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

EADL2017: Survey of Atomic Binding Energies for use in EPICS2017, IAEA-NDS-224, Rev. 1, April, 2018, Nuclear Data Section (NDS), IAEA, Vienna, Austria

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

EPDL2017: Survey of Atomic Photon Cross Section Data for use in EPICS2017, IAEA-NDS-225, Rev. 1, February 2018, Nuclear Data Section (NDS), IAEA, Vienna, Austria.

[3] **EEDL2017**: Survey of Electron Cross Section Data for use in EPICS2017, IAEA-NDS-226, December 2017, Nuclear Data Section (NDS), IAEA, Vienna, Austria.

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

[5] **ENDF Format.** ENDF-6 Formats Manual: Data Formats and Procedures for the Evaluated Nuclear

Data Files ENDF/B-VI, ENDF/B-VI,andENDF/B-VIII, ENDF-102, Brookhaven National Laboratory, ENDF-102, rev. 215, February 2018, edited by A. Trkov, et al.

[6] **First Assessment** of ENDF/B-VIII and EPICS Atomic Data Libraries, IEEE Transactions on Nuclear Science **65**/8, August 2018, by Min Cheol Han, et al.

[7] **PREPRO2017**: 2017 ENDF/B Pre-processing Codes, IAEA-NDS-39, Rev. 17, May 2017.

[8] **TART2016:** An Overview of a Coupled Neutron-Photon, 3-D, Combinatorial Geometry, Time Dependent Monte Carlo Transport Code, Lawrence Livermore National Laboratory**,** LLL-SM704560, Code Release LLNL-CODE-708759, September 2016.

[9] Program **EPICSHOW:** A Computer Code to Allow Interactive viewing of the EPIC Data Libraries (Version 94-1), UCRL-ID-116819, Feb. 1994; latest update 2016.

[10] **EPICS2014**: Electron Photon Interaction Cross Sections", IAEA-NDS-2018, Nuclear Data Section, IAEA, Vienna, Austria, September 2014
EPICS2014: Electron Photon Interaction Cross Sections", IAEA-NDS-2018, rev.1, Nuclear Data Section, IAEA, Vienna, Austria, August 2015

[11] **EPDL:** Tables and Graphs of Photon-Interaction Cross Sections from 10 eV to 100 GeV Derived from the LLNL Evaluated Photon Data Library (EPDL), UCRL-50400, Vol. 6, Rev. 4, Part A: Z = 1 to 50, October 1989
Tables and Graphs of Photon-Interaction Cross Sections from 10 eV to 100 GeV Derived from the
LLNL Evaluated Photon Data Library (EPDL), UCRL-50400, Vol. 6, Rev. 4, Part B: Z = 51 to 100, October 1989

[12] **EADL:** Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library (EADL), Z = 1 - 100, Lawrence Livermore National Laboratory, UCRL-50400, Vol. 30, October 1991.

[13] **EEDL:** Tables and Graphs of Electron Interaction Cross 10 eV to 100 GeV Derived from the LLNL Evaluated Electron Data Library (EEDL), Z = 1 - 100, Lawrence Livermore National Laboratory, UCRL-50400, Vol. 31, November 1991.

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

[15] **R.J. Howerton**, Private Communication, circa 1972.

[16] **PENELOPE:** F. Salvat, "Penelope—A code system for Monte Carlo simulation of electron and photon transport, Boulogne-Billancourt, France, Tech. Rep. NEA/NSC/DOC(2015)3, 2015.

[17] **MCNP:** T. Goorley et al., Initial MCNP6 release overview, Nucl. Technol. **180**/3 (2012) 298–315.

[18] **GEANT4:** J. Allison et al., Recent developments in Geant4, Nucl. Instrum. Methods Phys. Res. Section A **835** (2016) 186–225.

[19] **FLUKA:** T.T. Böhlen et al., The FLUKA code: Developments and challenges for high energy and medical applications, Nucl. Data Sheets **120** (2014) 211–214. [20] **M. Pia**, Private Communication, April 2019.