Technical note 5: Rayleigh scattering process

Zhuxin LI, Claire MICHELET, Sébastien INCERTI

CENBG, Version November 16, 2020

Introduction

This technical note explains the implementation of EPICS2017 database for Rayleigh scattering process, which includes the following parts:

- Section 1: description of Livermore cross section data format for Rayleigh scattering process
- Section 2: format of original EPICS2017 data library
- Section 3: implementation of cross section in Geant4 for the 10.7 version (November, 2020)
- Section 4: cross section data difference between EPICS2017 and Livermore
- Section 5: form factor fit

1. Livermore model for Rayleigh scattering

1.1. G4LivermoreRayleighModel model class

For the Rayleigh scattering process in Geant4, the ***G4LivermoreRayleighModel*** class performs the following tasks:

- read the tabulated cross section data from Geant4 data library
- compute the interpolated cross section for the energy value of the incident gamma
- generate the final state.

1.2. Location of cross section data files

For the 10.7 version of Geant4, the Livermore total cross section data files that the class reads are contained in the directory:

$G4LEDATA/livermore/rayl

The ***G4EMLOW7.9 ($G4LEDATA*)** directory contains the 7.9 version (October 2019) of the data files for low energy electromagnetic processes.

Data files of implementation of EPICS2017 are located in ***$G4LEDATA/epics2017/rayl***

1.3. Format

Cross section files are composed of **two header lines** and **a series of "cross section" data** (energy – "cross section" points[1])

The file name is:

re-cs-Z.dat *("re" is for "Rayleigh effect")*

where *Z* is the atomic number of the element.

Fig. 1 presents an example of a part of total "cross section" data file *re-cs-1.dat* for Hydrogen.

[1] "cross section" refers to energy × energy × cross section in this technical note

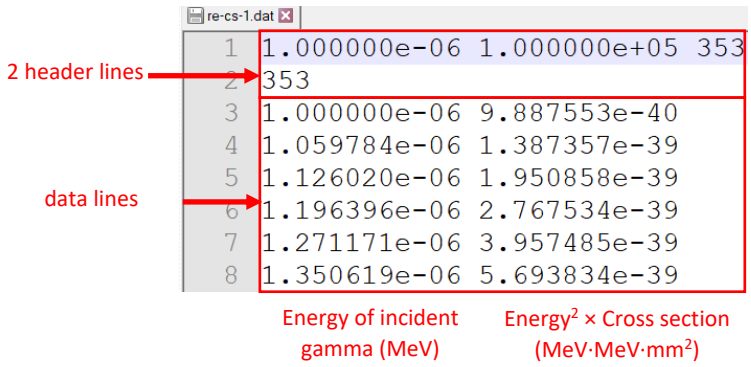

Fig. 1. Example of the beginning of the data file for Hydrogen for Livermore

1.3.1. Information in the header lines

The 3 figures (Fig. 1) in the first header line indicate the lowest and highest energy values in the table (in **MeV**), and the number of energy – "cross section" points.

As we know the coherent scattering is probable in high atomic number materials and with photons of low energy. Thus in Geant4 the energies for cross sections are limited up to 10 MeV, and the cross section files only contain the points below 10 MeV (10 MeV is included meanwhile). However, there was a small inconsistency of the highest energy value in the first header line, which was supposed to be the real highest energy instead of 1.000000e+05 MeV. This small inconsistency appeared systematically in all cross section files. So it has been corrected in the implementation of EPICS2017.

The figure in the second header line repeats the number of energy – "cross section" points.

1.3.2. Information in the data lines

As illustrated in Fig. 1, the first column contains the energy values in **MeV**, from the lowest to highest energy value given in the first header line. The second column contains the corresponding "cross section" data, which is the product of **square of energy and cross section** instead of genuine cross section, in **MeV·MeV·mm²** with 7 **significant digits**.

2. Format of Rayleigh scattering data in EPICS2017

In ***EPDL2017.ALL***, as introduced in Technical note 1, we can simply locate the data lines relevant to the Rayleigh scattering (coherent scattering) process, by choosing ***71*** and ***93 (for whole atom parameters)*** for the reaction descriptor in the second header line (Fig. 2, line 2). In fact, five types of data relevant to Rayleigh scattering process are given for each element:

1) the cross section (Fig. 2)

2) form factor (Fig. 3)

3) real anomalous scattering factor (Fig. 4)

4) imaginary anomalous scattering factor (Fig. 5)

5) average energy of the scattered photon (Fig. 6)

Fig. 2-6 present an example of the **data** tables relevant to the Rayleigh scattering process for Hydrogen. Some of the parameters in the header lines are identical in these three tables (see Technical note 1):

The first header line specifies: Z = 1, A = 000, Yi = 7 (incident particle = photon) (Fig. 2, in red).

The second header line specifies: C =71 (reaction descriptor: Rayleigh scattering) (Fig. 2, in red).

We are only interested in the cross section and form factor data in this technical note (not in real and imaginary anomalous scattering factors nor in the energy of scattered photon) for the purpose of updating the Geant4 database. Nevertheless, we will still present all the available information.

2.1. Cross section

Fig. 2 presents an example of a part of **cross section data table relevant to the Rayleigh scattering** process for Hydrogen.

In this example (Fig. 2, in blue):

- In the first header line: Yo = 0, means that the given information is not about the secondary particles
- In the second header line: I = 0, means that the data lines below are the cross section data

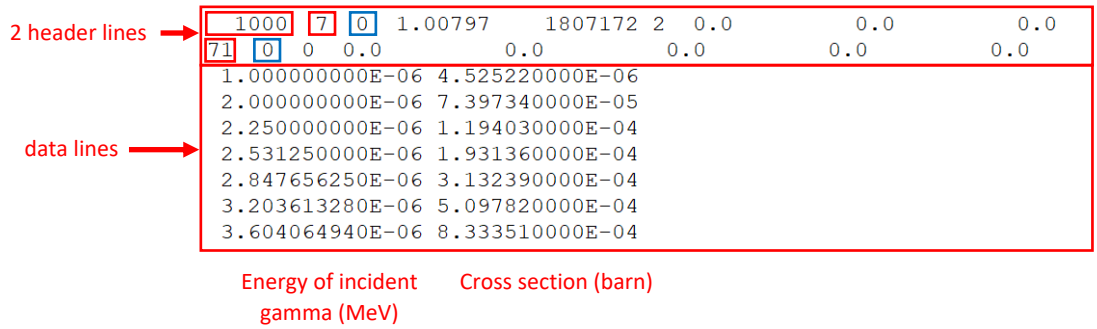

Fig. 2. Example of cross section data table relevant to the Rayleigh scattering process for Hydrogen in EPDL2017.ALL

2.2. Form factor

Fig. 3 presents an example of a part of **form factor data table relevant to the Rayleigh scattering** process for Hydrogen.

In this example (Fig. 3):

- In the first header line (blue): Yo = 0, means that the given information is not about the secondary particles
- In the second header line (red): C = 93, means that the data lines below are whole atom parameters
- In the second header line (blue): I = 941, means that the data lines below are form factor

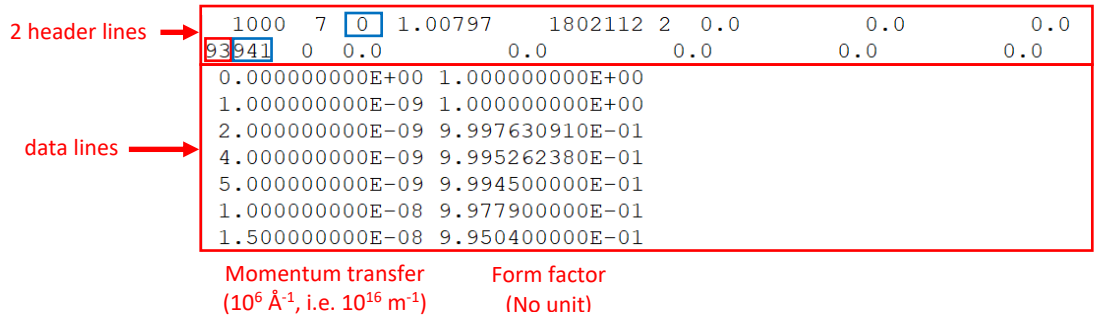

*Fig. 3. Example of form factor data table relevant to the Rayleigh scattering process for Hydrogen in **EPDL2017.ALL***

Note that the unit of momentum transfer in ***EPDL2014.ALL*** is cm^{-1}, which is not the same as in ***EPDL2017.ALL***

2.3. Real anomalous scattering factor

Fig. 4 presents an example of **real anomalous scattering factor** for Hydrogen.

In this example (Fig. 4)

- In the first header line (blue): Yo = 0, means that the given information is not about the secondary particles
- In the second header line (red): C = 93, means that the data lines below are whole atom parameters
- In the second header line (blue): I = 944, means that the data lines below are real anomalous scattering factor

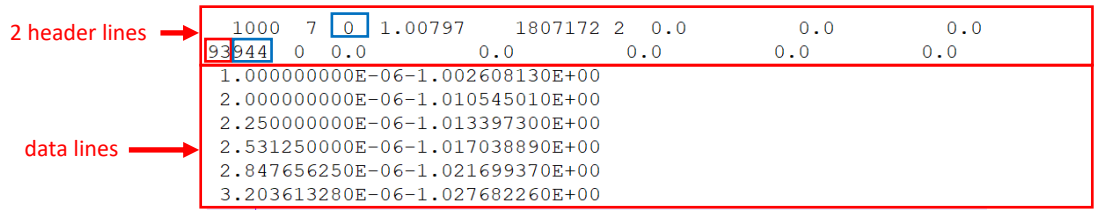

Fig. 4. Example of real anomalous scattering factor data table relevant to the Rayleigh scattering process for Hydrogen in EPDL2017.ALL

2.4. Imaginary anomalous scattering factor

Fig. 5 presents an example of **imaginary anomalous scattering factor** for Hydrogen.

In this example (Fig. 5):

- In the first header line (blue): Yo = 0, means that the given information is not about the secondary particles
- In the second header (red): C = 93, means that the data lines below are whole atom parameters
- In the second header line (blue): I = 943, means that the data lines below are imaginary anomalous scattering factor

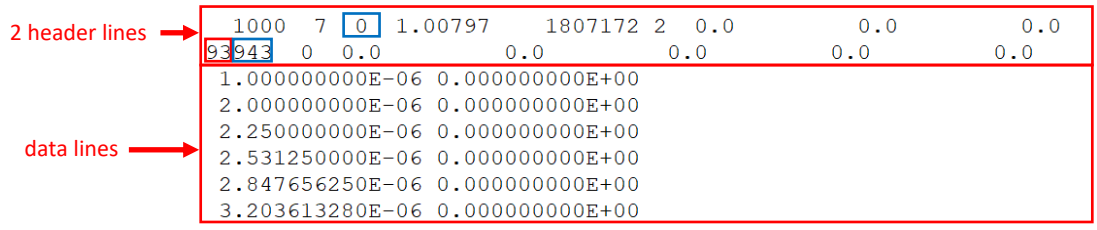

Fig. 5. Example of imaginary anomalous scattering factor data table relevant to the Rayleigh scattering process for Hydrogen in EPDL2017.ALL

2.5 Average energy of the scattered photon

Fig. 6 presents an example of **average energy of the scattered photon** for Hydrogen.

In this example (Fig. 6, in blue):

- In the first header line: Yo = 7, means secondary particles are photon.

- I = 10, means that the data lines indicate the average energy of secondary particles, namely photon in this case.

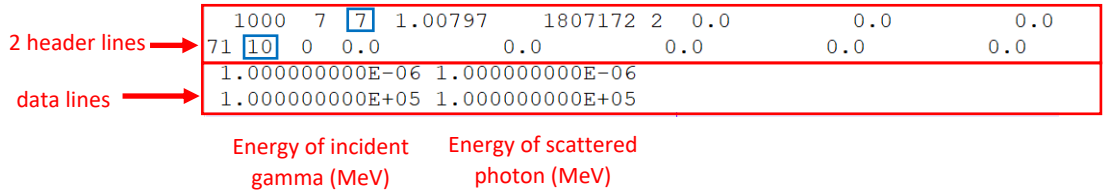

Fig. 6. Example of average energy of the scattered photon for Hydrogen in file EPDL2017.ALL

2.6. Units

Energy used in ***EPDL2017.ALL*** is in **MeV**.

Cross section is in **barn**.

Momentum transfer is in 10^6 $Å^{-1}$, i.e. 10^{16} m^{-1}.

3. Implementation of cross section in Geant4

3.1. *generate_re_csE2_2017.c* macro

generate_re_csE2_2017.c is a ROOT macro, which is used to generate the total "cross section" data (product of energy and cross section) files from ***EPDL2017.ALL*** for elements (Z:1-100), these files will be added to Geant4 data library.

As explained in section 2, Rayleigh scattering cross section data is distinguished by the header line:

```
71 0 0 0.0      0.0      0.0      0.0      0.0
```

This macro produces respectively 100 "cross section" data files (one file for one element), saved in the directory called ***epics2017/rayl***

The output file is named: ***re-cs-Z.dat***

where *Z* is the atomic number of the element.

The units for energy and "cross section" in the generated data files are in **MeV** and in **MeV·MeV·mm²**.

Command

To use the ***generate_re_csE2_2017.c*** macro, firstly you should place this macro and the ***EPDL2017.ALL*** file in the same directory. Secondly, type the following command in the Terminal:

```
root generate_re_csE2_2017.c
```

Note that ***generate_re_csE2_2014.c*** is available to extract "cross section" data from ***EPDL2014.ALL***

3.2. Format

The format of the implemented total cross section data files obtained from ***EPDL2017.ALL*** follows the format of Geant4 Livermore data files contained in the directory ***$G4LEDATA/livermore/rayl*** (as detailed in section 1).

It is composed of **2 header lines** followed by **a series of physical data lines** with 2 columns (energy in **MeV** and "cross section" in **MeV·MeV·mm²**). The cross section, originally given in **barns** in ***EPDL2017.ALL***, is converted to **mm²**. A major difference compared to Livermore data is the number of significant digits. **We kept 10 significant digits for both energy and "cross section" data** *(However, we*

*noticed that not all the significant digits are actually used for Rayleigh scattering cross section data in **EPDL2017.ALL**).*

The format of the total cross section data files is illustrated in Fig. 6.

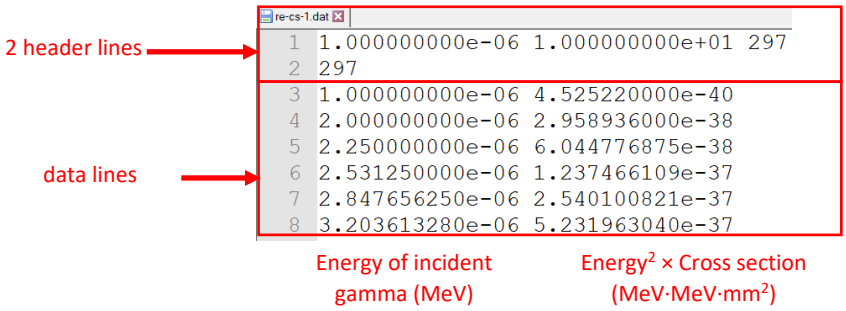

Fig. 6. Example of a part of "cross section" data file for Hydrogen for EPICS2017

3.2.1. Information in the header lines

Just as the data files of Livermore, the three figures in the first header line indicate the lowest and highest energy values in the table (in **MeV**), as well as the number of data points. Note that the energy is still limited up to 10 MeV. The figure in the second header line repeats the number of data points.

3.2.2. Information in the data lines

As illustrated in Fig. 6, the first column contains the energy values of the incident gamma in **MeV** with **10 significant digits**, from the lowest to highest energy value given in the first header line. The second column contains the corresponding "cross section" data in **MeV·MeV·mm²** with **10 significant digits** as well.

4. Comparison of cross section data

Before implementing the new database in Geant4, we have compared cross section data (attention: here, it is genuine cross section data) between EPICS2017 and EPDL2014 (=EPDL97), which was used to generate the Livermore data files of Geant4. This comparison is performed using ***plot_cs.c*** macro.

4.1. plot_cs.c

The ***plot_cs.c*** ROOT macro reads data files in

- ***epics2017/rayCS/re-cs-Z.dat*** extracted from ***EPDL2017.ALL*** by ***generate_re_cs_2017.c***
- ***epics2014/rayCS/re-ce-Z.dat*** extracted from ***EPDL2014.ALL*** by ***generate_re_ce_2014.c***

It then plots the following figures for cross section data. There is one figure per element.

- cross section data of EPICS2017 (Z: 1-100) (example in Fig. 7, for Hydrogen)
- cross section data of EPDL2014 (used to generate Livermore data files) (Z: 1-100) (example in Fig. 8, for Hydrogen)
- comparison of cross section data between EPICS2017 and EPDL2014 (Livermore) (Z: 1-100) (example in Fig. 9, for Hydrogen)

The generated figures are saved in the corresponding directories:

- ***plots/epics2017***
- ***plots/epics2014***
- ***plots/comparison***

Command

To use the ***plot_cs.c*** macro, you should put it in the same directory as the data file directories ***epics2017*** and ***livermore*** are, so that it can read the files contained inside. The ***plots/*** directories above are automatically generated when the macro runs, by the command:

```
root plot_cs.c
```

The figures below (Fig. 7-9) display examples for Hydrogen.

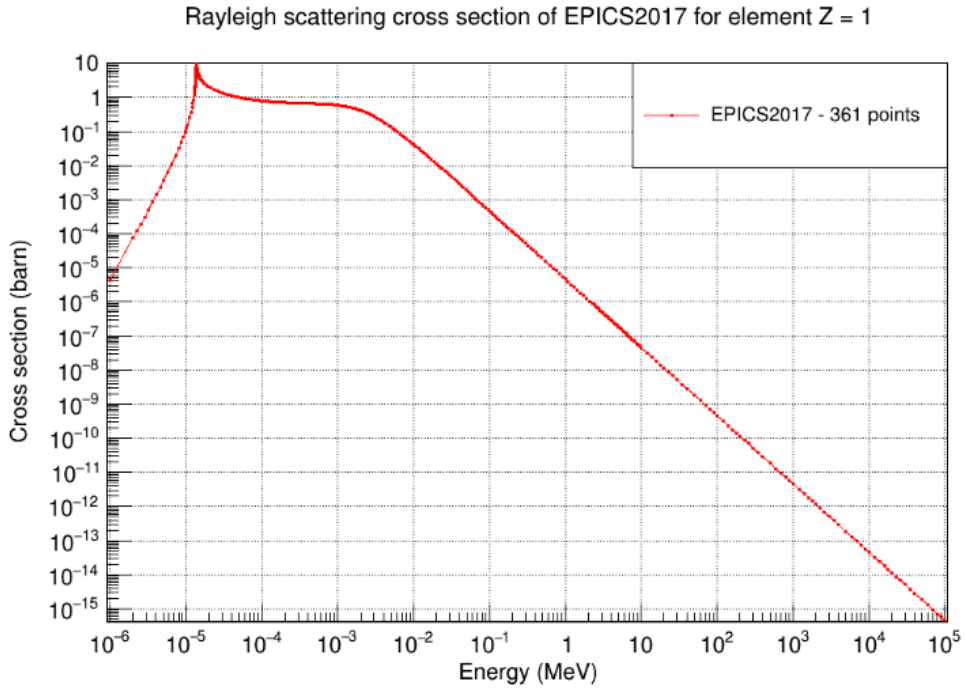

Fig. 7. An example of cross section data of EPICS2017 for Hydrogen

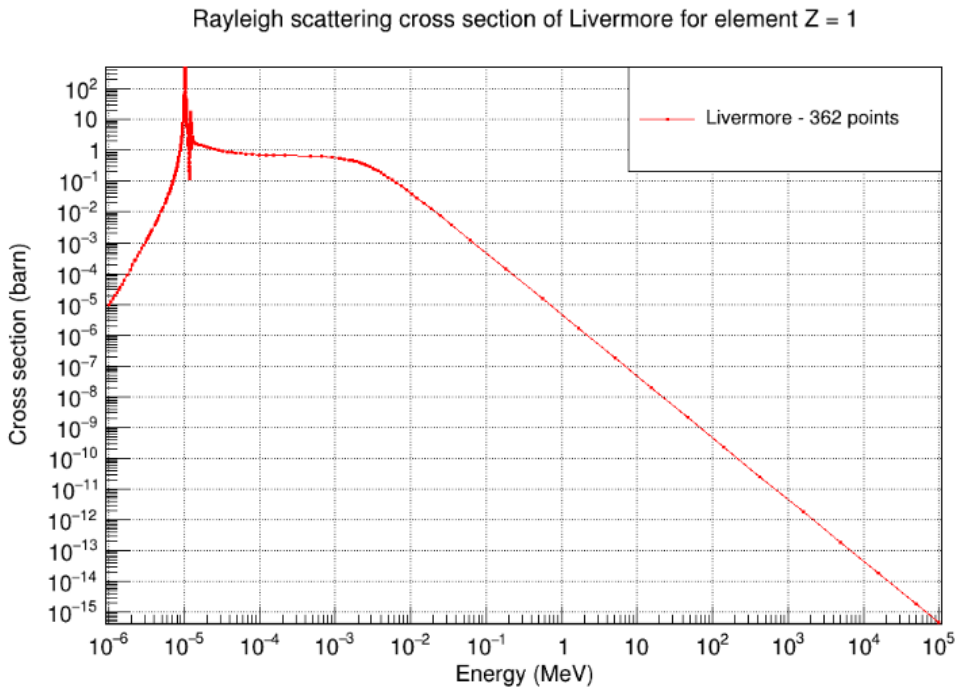

Fig. 8. An example of cross section data of Livermore (EPDL2014) for Hydrogen

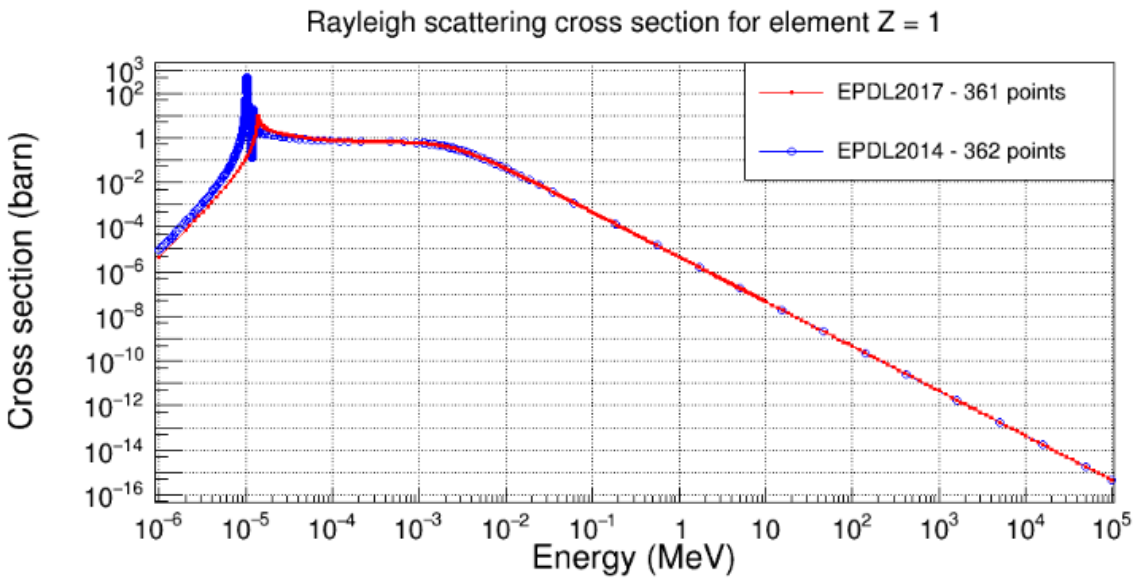

Fig. 9. An example of comparison of cross section data between EPICS2017 and EPDL2014 (Livermore) for Hydrogen

4.2. Discussion

Dermott E. Cullen has modified new edge energies to photoelectric and calculated the corresponding anomalous and coherent scattering data in EPICS2017. Thus, we observed a huge difference between EPICS2017 and Livermore in Fig. 10.

A Survey of Photon Cross Section Data for use in EPICS2017

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

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.**

Besides, unlike what we saw in gamma conversion and Compton effect, the cross section data in EPICS2017 has less points than Livermore and the energies in Livermore are not included in EPICS2017.

Considering those changes, we did not plot the relative difference of cross sections of EPICS2017 compared to Livermore as we usually did for other processes.

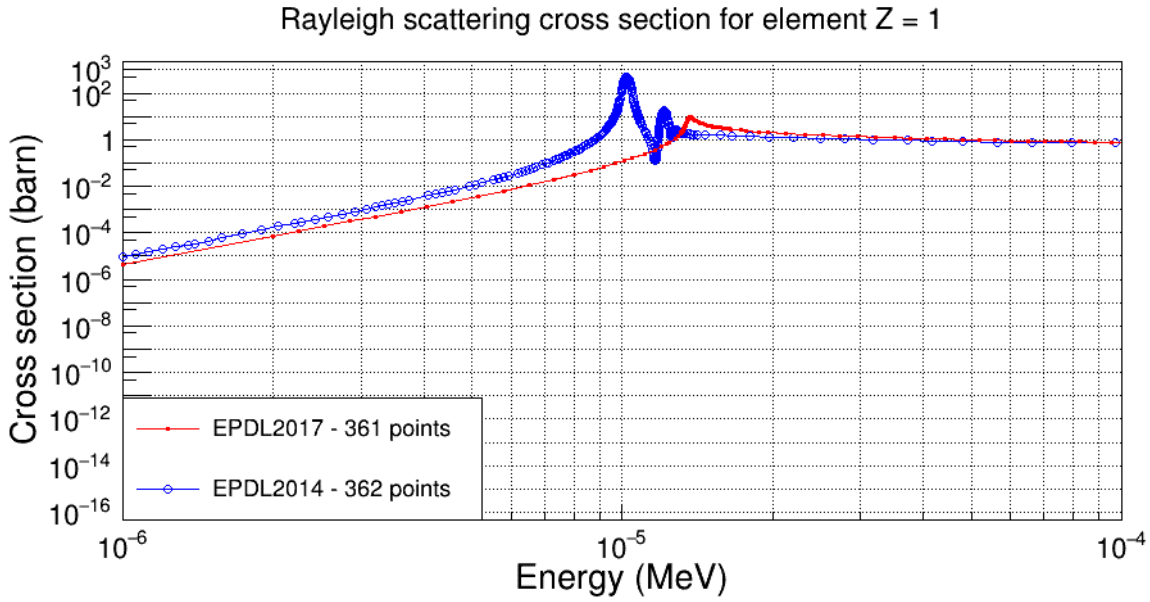

Fig. 10. A zoom over range 10^{-6} – 10^{-4} MeV of cross section data between EPICS2017 and EPDL2014 (Livermore) for Hydrogen

5. Form factor fit

For low energy incident photons, the simulation of the Rayleigh scattering process is performed according to the product of Rayleigh formula and the square of Hubbel's form factor $FF^2(q)$[], where q is the momentum transfer.

Details are given in section 5.3.

5.1. generate_formFactor_2017.c macro

In order to parameterize the new form factor data, we firstly need to extract form factor data files from ***EPDL2017.ALL*** by using ***generate_formFactor_2017.c*** macro for elements (Z:1-100).

Command

To generate form factor from ***EPDL2017.ALL***, make sure you put this macro and ***EPDL2017.ALL*** in the same directory, and then type the following command in the Terminal:

```
root generate_formFactor_2017.c
```

The output files are named: ***re-ff-Z.dat***

where *Z* is the atomic number of the element.

They are saved in ***epics2017/formFactor*** directory.

Note that another macro ***generate_formFactor_2014.c*** is also provided if you want to extract form factors from ***EPDL2014.ALL***.

5.2. *plot_formFactor.c*

plot_formFactor.c is meant to plot the comparison of form factors between EPICS2017 and Livermore (values from EPDL2014 = EPDL97) given that form factor data files have been prepared as described in section 5.1. It generates one figure for each element.

Command

To run this macro, make sure you put it and the form factor data files that you extracted and prepared as explained in section 5.1 in the same directory. Then type the following command in the Terminal:

```
root plot_formFactor.c
```

An example of comparison for Helium is illustrated in Fig. 10.

The figure is composed of two graphs:

1. Comparison of form factors between EPICS2017 and Livermore
2. Relative difference (%) of form factors for EPICS2017 compared to Livermore:

$$RD = \frac{FF_{EPICS2017} - FF_{Livermore}}{FF_{Livermore}} \times 100\%$$

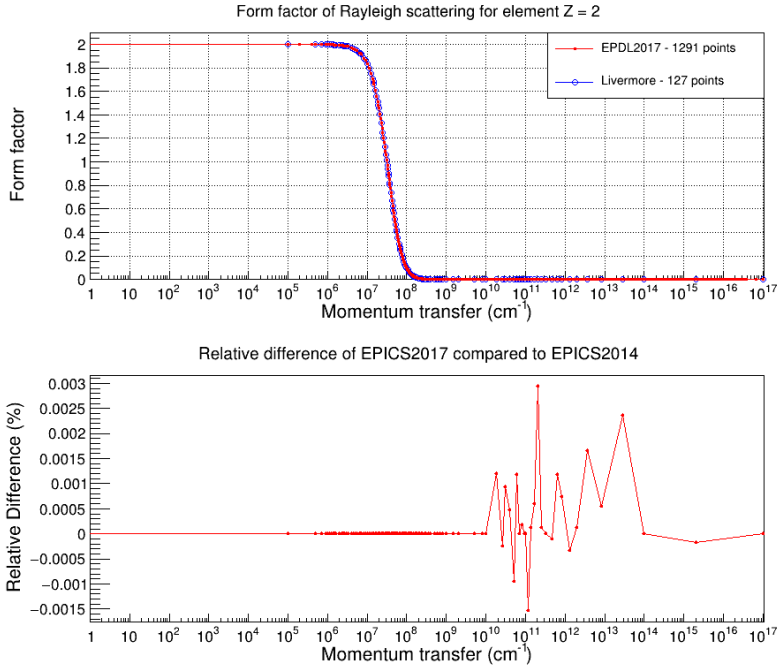

Fig. 10. An example of comparison of form factor data between EPICS2017 and Livermore for Helium

In addition, this macro calculates the maximal difference of form factors of EPICS2017 compared to Livermore for each element. Finally, it gives an output file ***MaximalDifferenceOfFormFactorBetween2014And2017.txt***. This file will be used in section 5.3.

Discussion

1. Number of points

For each element, EPICS2017 contains more momentum transfer – form factor points than Livermore does. For example, Helium has 1291 points for EPICS2017 while only 127 for Livermore, so that we can compare the 127 points with the same energy (Fig. 11, bottom graph).

2. Rounding errors

Besides, all the points of Livermore are included in EPICS2017. However, from the relative comparison graphs (for instance, Fig. 10, bottom graph), we observe that some points display differences between the two databases. These differences are actually negligible (relative difference < $5 \cdot 10^{-5}$). They only come from the way of rounding the cross section values. For instance, for Helium, at q = 2.048600000e+11 cm^{-1}:

- $FF_{EPICS2017}$ = 1.702300000e-14

- $FF_{Livermore}$ = 1.702250000e-14

5.3 *plotMaximalDifferenceOfFormFactorBetween2014And2017WithZ.c* macro

Once you get ***MaximalDifferenceOfFormFactorBetween2014And2017.txt***, you can make use of ***plotMaximalDifferenceOfFormFactorBetween2014And2017WithZ.c*** macro to see the maximal difference of form factors of EPICS2017 compared to Livermore according to Z.

Command

To run this macro, make sure you put it and the ***MaximalDifferenceOfFormFactorBetween2014And2017.txt*** file in the same directory. Then type the following command in the Terminal:

```
root plotMaximalDifferenceOfFormFactorBetween2014And2017WithZ.c
```

Fig. 11 shows the figure generated by this macro.

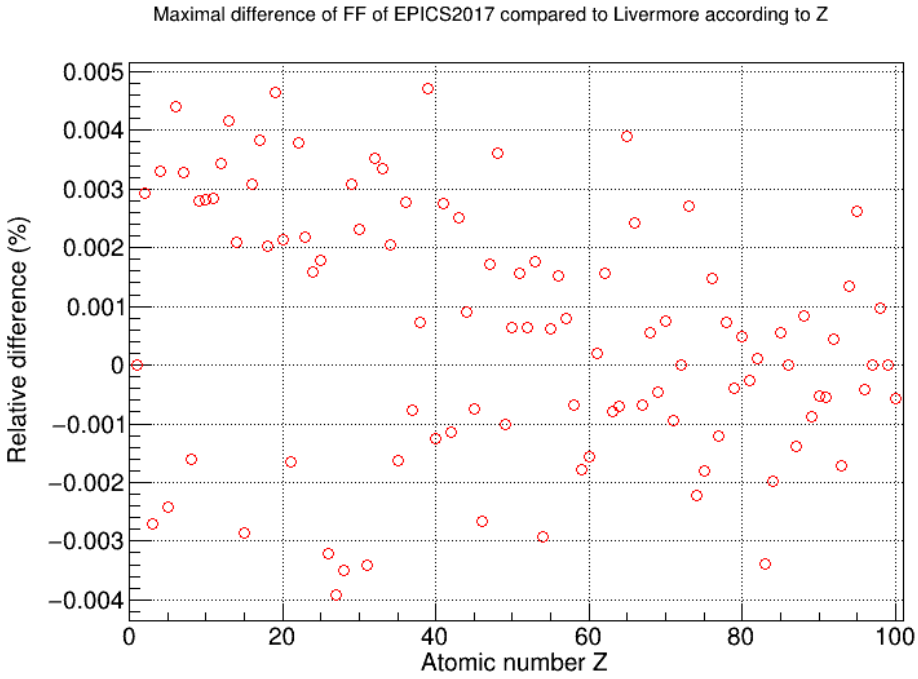

Fig. 11. Maximal difference of FF of EPICS2017 compared to Livermore according Z

5.4. *fit_formFactor_2017.c* macro

In previous ***G4LivermoreRayleighModel***, the form factor data were derived from EPDL97 and fitted according to a method proposed by D.E. Cullen [1]. Eventually, the form factor (**square of form factor**) data was parameterized by a simplified function, as follows:

$$FF^2(q) = \sum_{i=0}^{2} \frac{a_i}{(1 + b_i q^2)^{N_i}}$$

Where a_i, b_i, N_i are fitting parameters.

The fitted parameters are used in ***G4RayleighAngularGenerator*** to generate the final state of the scattered photon after interaction.

Based on the same fitting method, new form factors with just more points in EPICS2017 are fitted by using the macro ***fit_formFactor_2017.c,*** which reads the tabulated fit for form factor data extracted from ***EDPL2017.ALL***

It is important to point out four aspects that play a significant role in the fitting process:

- The fitting function used in the macro is a transformed function of what we introduced above so as to apply the following constraint []:

$$Z^2 = \sum_{i=0}^{2} a_i$$

More precisely in the macro, the a_0 parameter was expressed as:

$$a_0 = Z^2 - a_1 - a_2$$

- Even though tabulated momentum transfer data range from 0 to 10^{17} cm^{-1}, the fit is not made on the whole range of data. We only fit the values:

$$FF^2 \geq 10^{-6} \cdot Z^2$$

where Z is the atomic number, which is also the maximal value of form factors for a specific element (for momentum transfer ≤ $10^5 cm^{-1}$).
- Form factors of some elements cannot be better parameterized than previous fit does, because at high momentum transfers, the fact of having more points disturbs the fit. We perceived that by comparing the relative difference of fitted form factors (**square of form factors**) compared to tabulated data respectively using previous and new fitting parameters at the same time, an example is shown in Fig. 12. Note that:
    - in the legend, Geant4 fit means previous fit
    - the first momentum transfer – form factor point is not plotted in the graph, because it is a fixed point : the momentum transfer value is fixed to 0 and the corresponding form factor value is fixed to Z value. Therefore, we only plotted the graph from the second point (q = 10^5 cm^{-1}).

  For this reason, if the relative difference using new fitting parameters does not show an obvious improvement, we chose to keep the previous fitting parameters. Thus, the previous fitting parameters need to be read by this macro as well.
- To optimize the fit, artificial error bars are specified for each momentum transfer – form factor point increasingly with the momentum transfer. In low range of momentum transfer, the errors are much smaller than in high range of momentum transfer.

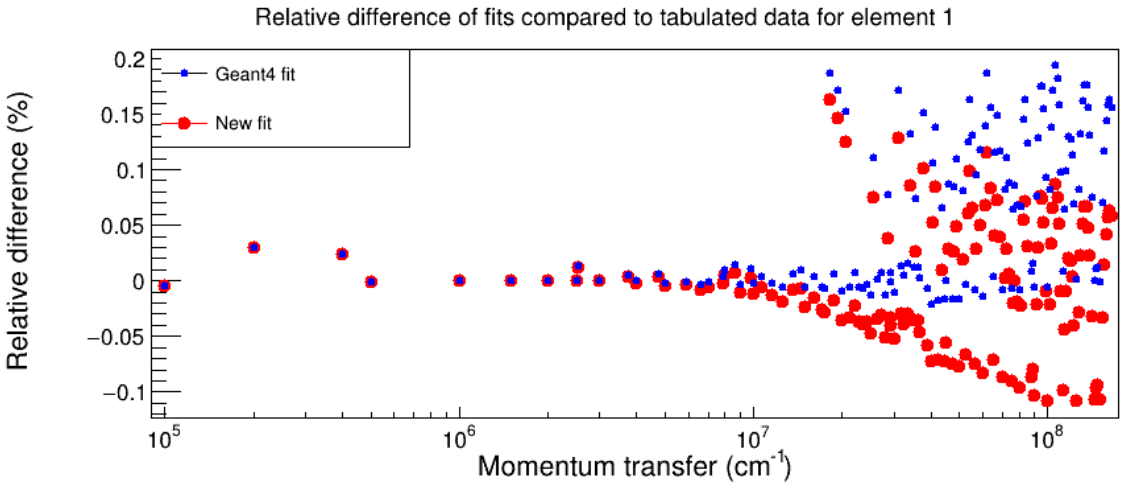

Fig. 12. Relative difference of fits compared to tabulated data for Hydrogen

To sum up, you can make the fit of form factors by using ***fit_formFactor_2017.c***, once you have prepared the following files:

- The form factor data files as explained in section 5.1
- 9 previous fitting parameter files named ***PPi.dat***, where i indicates the index of fitting parameters, varying from 0 to 8, because we have 9 fitting parameters for one element. For example see Fig. 13, ***PP0.dat*** contains 100 values, which are the first fitting parameter for 100 elements (Z: 1-100), demonstrated in the Fig. 13.

PP0.dat

```
0 2. 5.21459 10.2817 3.66207 3.63903 3.71155 36.5165 3.43548 3.40045
2.87811 3.35541 3.21141 2.95234 3.02524 126.146 175.044 162 296.833 300.994
373.186 397.823 430.071 483.293 2.14885 335.553 505.422 644.739 737.017 707.575
3.8094 505.957 4.10347 574.665 15.5277 10.0991 4.95013 16.3391 6.20836 3.52767
2.7763 2.19565 12.2802 965.741 1011.09 2.85583 3.65673 225.777 1.95284 15.775
39.9006 3.7927 64.7339 1323.91 3.73723 2404.54 28.3408 29.9869 217.128 71.7138
255.42 134.495 3364.59 425.326 449.405 184.046 3109.04 193.133 3608.48 152.967
484.517 422.591 423.518 393.404 437.172 432.356 478.71 455.097 495.237 417.8
3367.95 3281.71 3612.56 3368.73 3407.46 40.2866 641.24 826.44 3579.13 4916.44
930.184 887.945 3490.96 4058.6 3068.1 3898.32 1398.34 5285.18 1 872.368
```

Fig. 13. PP0.dat file of previous fit containing 100 values first fitting parameters for 100 elements

We observed that the relative difference of fit of form factors (**square of form factors**) varies depending on the momentum transfer, in a way that the relative difference is strongly higher at high momentum transfer, which corresponds to low form factor values. So, it would be misleading to plot the ***maximal difference*** obtained for each element, according to Z, as previously done for Compton effect (Technical note 2), since this maximal difference is not representative. For this reason, we turn to compare the ***average difference*** between previous and new fit.

After the fitting process, you will obtain the file:

AbsoluteAverageDiffereceOfFits_newFitUsing2017_oldFitUsing2017_oldFitUsing2014.dat,

which contains the absolute average ratio of fit.

Then using the ***plotAverageRatio.c***, you can plot the comparison of average difference according to Z values so as to evaluate the quality of fits, shown in Fig. 14.

On average for all elements, the new fit improves the precision by a factor of 1.3. Improved precision (IP) is calculated according to the following formula:

$$\mathrm{IP} = \frac{\sum_{Z=1}^{Z=100} \left| \frac{R_{old}(Z)}{R_{new}(Z)} \right|}{100}$$

where $R_{new}(Z)$ and $R_{old}(Z)$ are the average of absolute difference of new fit and previous fit of form factors for the element Z.

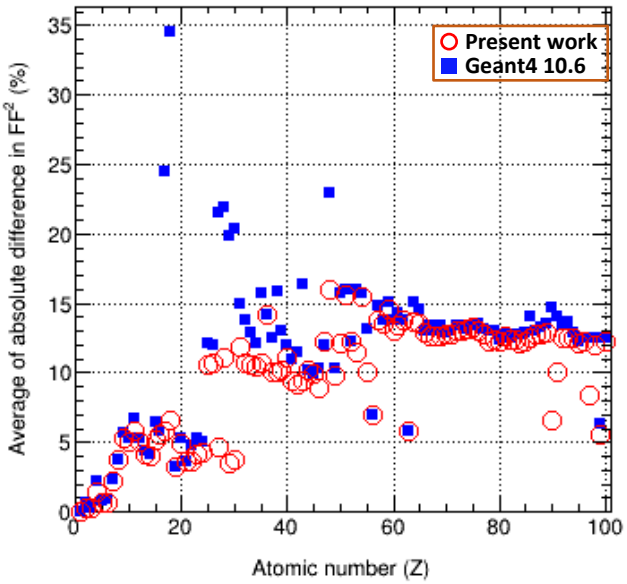

Fig. 14. Average absolute difference of previous fit and new fit according to Z values

In the end, you will obtain the following files by running this macro:

- Figures representing relative difference of fitted form factors compared to tabulated data respectively using previous and new fitting parameters for all the elements, an example is shown in Fig. 12
- 9 files in which new fitting parameters are written, named FF2017_PPi (i: 0-8)
- Average absolute difference of fits according to Z values as shows in Fig. 14

Command

To use the ***fit_formFactor_2017.c*** macro, make sure that

- the form factor data files have been extracted and prepared as explained in section 5.1
- the ***PPi.dat*** files (i: 0-8) containing the previous fitting parameters have been prepared

Then just type the following command in the Terminal.

```
root fit_FormFactor_2017.c
```

List of macro files

The ROOT macro files that we mentioned above are:

1. ***generate_re_csE2_2017.c***, generating "cross section" data files from ***EPDL2017.ALL***
2. ***generate_ce_csE_2014.c***, generating "cross section" data files from ***EPDL2014.ALL***
3. ***plot_ce.c***, plotting the comparison of cross section data between EPICS2017 and Livermore
4. ***generate_formFactor_2017.c***, generating form factor data files from ***EPDL2017.ALL***
5. ***generate_formFactor_97.c***, generating form factor data files from ***EPDL97.DAT***
6. ***plot_formFactor.c***, plotting the comparison of form factor data between EPICS2017 and Livermore
7. ***plotMaximalDifferenceOfFormFactorBetween2014And2017WithZ_2017_2014.c***, plotting the maximal difference of form factors of EPIC2017 compared to Livermore
8. ***fit_formFactor.c***, making a new fit for form factors of EPICS2017

Reference

[1] Cullen DE. A simple model of photon transport. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms. 1995;101:499-510.