Technical note 4: photoelectric process

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Introduction

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

- Section 1: description of Livermore cross section data format for photoelectric process
- Section 2: format of original EPICS2017 data library relating to photoelectric process
- Section 3: implementation of cross sections for Geant4 11.0
- Section 4: plots and comparison

1. Livermore model for photoelectric process

1.1. G4LivermorePhotoelectricModel model class

For the sprocess in Geant4, the ***G4LivermorePhotoelectricModel*** 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 previous version of Geant4, the Livermore total cross section data files that the class reads are contained in the directory:

> ***$G4LEDATA/livermore/phot_epics2014***

The previous work is accomplished by Marilena Bandieramonte, based on EPICS2014 data (EPDL2014).

Her work could be referred to from the repository: *https://gitlab.cern.ch/mbandier/epics2017*

While for the implementation of EPICS2017, the new data will be placed in ***$G4LEDATA/epics2017/phot***

1.3. Files in database

There are 5 types of files relating to total or subshell cross section data of photoelectric process in the ***$G4LEDATA/livermore/phot_epics2014***

- ***pe-cs-Z.dat***, total cross sections **above** K shell binding energy for element Z
- ***pe-le-cs-Z.dat***, total cross section **below** K shell binding energy for element Z
- ***pe-high-Z.dat***, high fitting parameters for subshell cross sections of element Z
- ***pe-low-Z.dat***, low fitting parameters for subshell cross sections of element Z
- ***pe-ss-cs-Z.dat***, subshell cross sections for element Z

where Z is the atomic number of elements.

The format of these files are given in the following section.

The calculation of total cross section is done according to 4 intervals, depending on the energy of the incident gamma E_γ, low fit limit, high fit limit and K binding energy.

1) If $E_\gamma \geq$ high fit limit:
$$\sigma(E) = \frac{a_1}{E} + \frac{a_2}{E^2} + \frac{a_3}{E^3} + \frac{a_4}{E^4} + \frac{a_5}{E^5} + \frac{a_6}{E^6}$$

2) If low fit limit $\leq E_\gamma <$ high fit limit:
$$\sigma(E) = \frac{b_1}{E} + \frac{b_2}{E^2} + \frac{b_3}{E^3} + \frac{b_4}{E^4} + \frac{b_5}{E^5} + \frac{b_6}{E^6}$$

3) If K binding energy $\leq E_\gamma <$ low fit limit: use tabulated values above K binding energy

4) If $E_\gamma < K$ binding energy: use tabulated values below K binding energy

1.3.1. Total cross sections **above** K shell binding energy

The total cross section above K shell binding energy is tabulated in **pe-cs-Z.dat** when the energy of incident gamma is higher than the binding energy, but lower than the low limit, which depends on the atomic number.

 A **pe-cs-Z.dat** file is composed of **two header lines** and **a series of "cross section" data lines** (energy – "cross section" points[1])

Fig. 1 represents an example of a part of total "cross section" data file **pe-cs-1.dat** for Hydrogen.
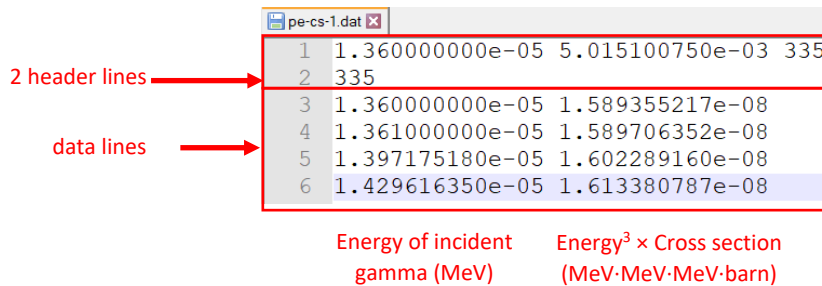
Fig. 1. Example of the beginning of the pe-cs-1.dat file for Hydrogen

1.3.2. Total cross section **below** K shell binding energy

The total cross section below K shell binding energy is tabulated in **pe-le-cs-Z.dat** when the energy of incident gamma is lower than the binding energy.

Fig. 2 displays an example of a part of total "cross section" data file **pe-le-cs-5.dat** for Boron.
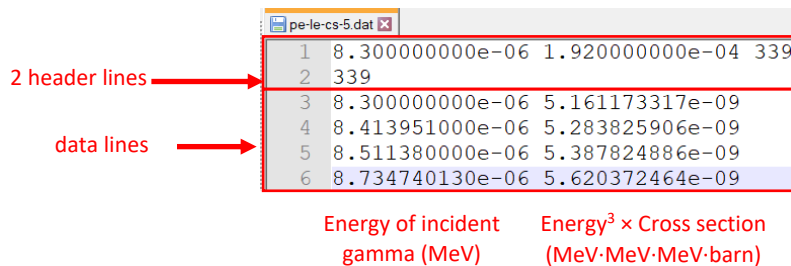

Fig. 2. Example of the beginning of the pe-le-cs-5.dat file for Boron

1.3.3. High fitting parameters for subshell cross sections

When the energy of incident gamma is higher than the high fit limit, **each subshell** cross section value is parameterized as follows, depending on the energy of incident gamma:

$$\sigma(E) = \frac{a_1}{E} + \frac{a_2}{E^2} + \frac{a_3}{E^3} + \frac{a_4}{E^4} + \frac{a_5}{E^5} + \frac{a_6}{E^6}$$

Where a_1, a_2, a_3, a_4, a_5, a_6 are fitting parameters which are indicated in the **pe-high-Z.dat** file.

A **pe-high-Z.dat** file is composed of a header line and fitting parameter lines. Here we take **pe-high-5.dat** of Boron as a specific example to explain the format, shown in Fig. 3.

The header line includes two times of the number of subshells for Boron, namely 4, followed by the high fit limit 0.0367282 MeV.

As for the fitting parameter lines, they are composed of 7 columns. The first column indicates the binding energy for subshells, starting from K subshell. The 6 following columns are cumulative fitting

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

parameters. For instance, the last 6 values of line 3 are sum of fitting parameters of the first two subshells. The value calculated using these 6 fitting parameters is the sum of subshell "cross sections" of the first two subshells. Similarly, the 6 parameters of last line (line 5) correspond to the sum of all subshells' fitting parameters. In other words, they correspond to the total "cross section" parameters.
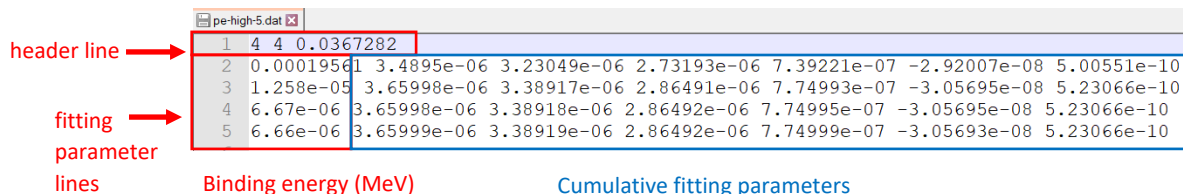

Fig. 3. pe-high-5.dat file for Boron

1.3.4. Low fitting parameters for subshell cross sections

Low fitting parameter files (**pe-low-Z.dat**) share the same format as high fitting parameter files, except that the last number in the header line, which represents the low fit limit. When the energy of incident gamma is higher than low fit limit and lesser than high fit limit, the calculation of cross section will be made using low fitting parameters.

1.3.5. Subshell cross sections

Subshell "cross sections" are provided too in the case of sampling ionized subshell in the method **G4LivermorePhotoelectricModel::SampleSecondaries()**.

We explain the format using the example of Boron. The file **pe-ss-cs-5.dat** contains the 4 subshells "cross section" data, each subshell "cross sections" starts with a header line, indicating the minimal and maximal energies of tabulated data, the number of data points as well as the index of the given subshell. For instance, Fig. 4 illustrates the beginning of the K subshell, whose index equals to 0.
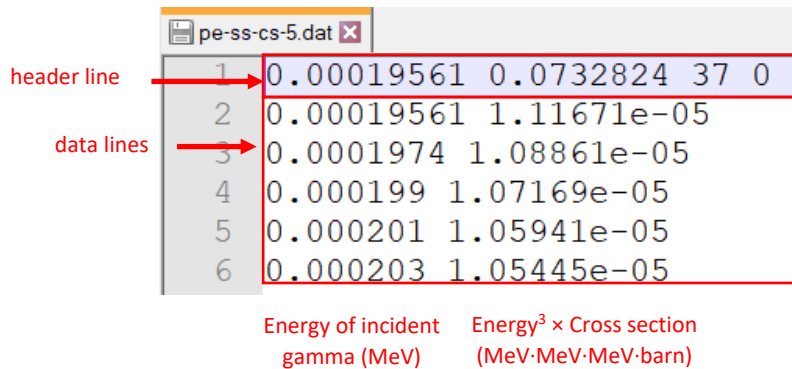

Fig. 4. Beginning of pe-ss-cs-5.dat file for Boron

2. Format of photoelectric data in *EPICS2017*

In **EPDL2017.ALL**, as introduced in Technical note 1, original data relevant to photoelectric are categorized under two processes that are more specific:

- total photoelectric process
- photoelectric process by subshell

However both can be located by specifying **73** for the reaction descriptor in the second header line (Fig. 5, line 2).

2.1. Total photoelectric process

There are four kinds of data relevant to total photoelectric process:

1) cross section (Fig. 5)

2) average energy to the residual atom

3) average energy of the secondary photons

4) average energy of the secondary electrons

Since we are only interested in the cross section data in this technical note for the purpose of updating the Geant4 database, we will not spare time on the other data here.

Fig. 5 represents an example of a part of **cross section data table relevant to the total photoelectric** process for Hydrogen.

In this example:

- In the first header line:
  $Z = 1$
  $A = 000$
  $Y_i = 7$, means the incident particle is photon
  $Y_o = 0$, means that the given information is not about the secondary particles
- In the second header line:
  $C = 73$, means the reaction is about photoelectric
  $I = 0$, means that the data lines below are the cross section data

Fig. 5. Example of total cross section data relevant to the total photoelectric process for Hydrogen in EPDL2017.ALL

2.2. Photoelectric process by subshell

Just as total photoelectric process, four kinds of data are available for photoelectric by subshell:

1) subshell cross section (Fig. 6)

2) average energy to the residual atom

3) average energy of the secondary photons

4) average energy of the secondary electrons

Only format of subshell cross sections is explained here.

Fig. 6 shows an example of a part of **K subshell cross section data** for Boron.

In this example:

- In the first header line:

Z = 1
A = 000
Yi = 7, means the incident particle is photon
Yo = 0, means that the given information is not about the secondary particles
- In the second header line:
C =73, means the reaction is about photoelectric
I = 0, means that the data lines below are the cross section data
S = 91, means X1 filed data required
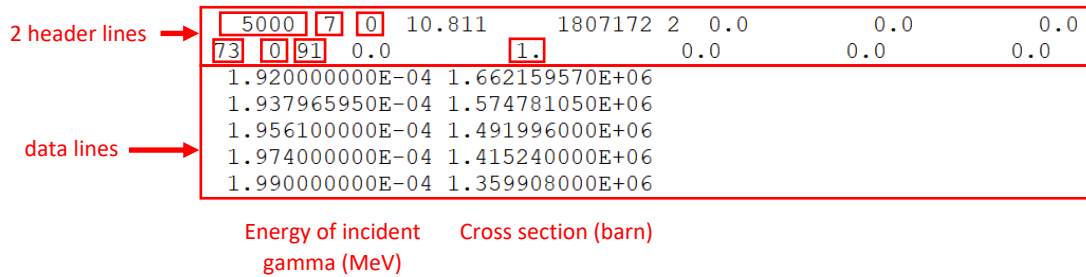X1: subshell designator, X1 = 1, means it is K subshell

*Fig. 6. Example of K subshell cross section data
for Boron in EPDL2017.ALL*

2.3. Units

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

Cross section is in **barn**.

3. Implementation of cross sections in Geant4

3.1. *Preliminary preparation of files*

To start with, we need to make preliminary preparation of some files by running the following macros:

- *generate_ss_cs_2017.c* generates subshell cross section files, which will be read by *fitForSubshellCS2017.c*
- *generate_bindingEnergy_2017.c* generates **binding.dat** file containing binding energies for all the elements
- *generate_pe_cs_2017.c* generates total cross section data files, which will be read by *generate_outputs.c* to generate final total cross section data files for Geant4 database

3.1.1. *generate_ss_cs_2017.c* macro

*generate_ss_cs_2017.*c is used to read subshell cross sections from **EPDL2017.ALL** and generate output files:

pe-ss-cs-Z.dat, where *Z* is the atomic number of the element ,

They are saved in **epics2017/phot_preliminary** folder.

Format
For a given element, the **pe-ss-cs-Z.dat** contains all the subshell cross section data of this element. The energy – cross section data points start with a header line in which, the first value indicates the binding energy of a specific subshell while the second is always 0. Furthermore, each subshell data are separated by -1 -1.
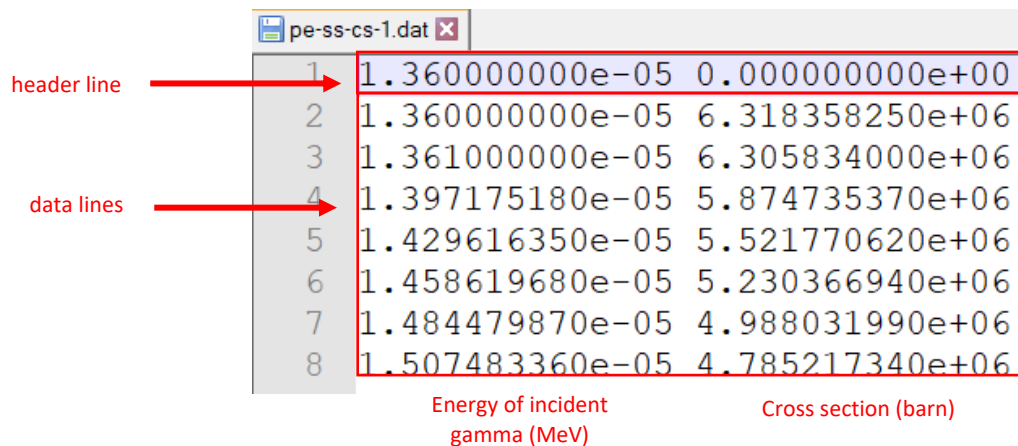
Fig. 7 shows a part of *pe-ss-cs-1.dat* file:

Fig. 7. A part of pe-ss-cs-1.dat file

Command

To use the ***generate_ss_cs_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_ss_cs_2017.c
```

Note that ***generate_ss_cs_2014.c*** is available to extract subshell cross sections data from ***EPDL2014.ALL***

Anomaly in the initial data

We would like to mention that for subshell cross section data, there are some completely repeated points in in terms of both energy and cross section for some elements in ***EPDL2017.ALL.*** For example, for Chlorine (Z = 17), L1 (2s1/2) subshell (Fig. 8), the point (2.77e-4, 3.2529e+5) is repeated, which is not necessarily needed.

It is worthwhile to mention that such anomaly did not exist in ***EPDL2014.ALL***.
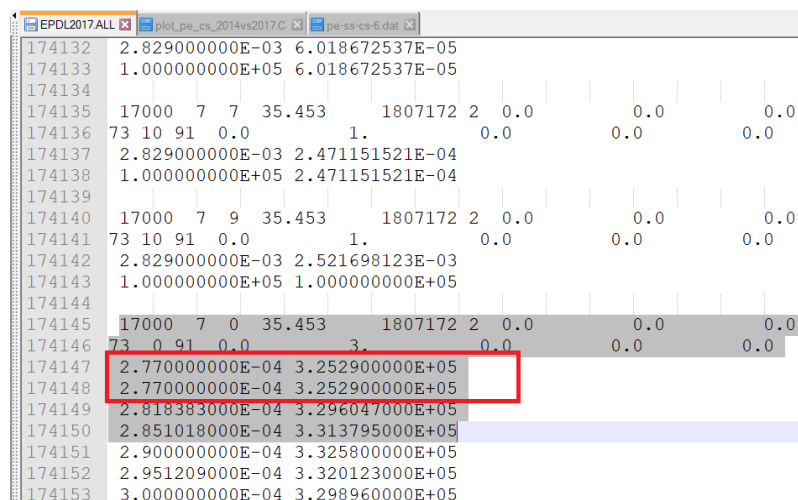

Fig. 8. Repeated point for L1 subshell of Chlorine

Fig. 9 gives a summary of all these anomalous data, indicating the atomic number, index of the subshell and the repeated point as well.

```
Z = 17 subshell_3 (2.770000000e-04 3.252900000e+05) Completely repeated
Z = 19 subshell_16 (4.340000000e-06 3.495570000e+04) Completely repeated
Z = 24 subshell_8 (8.000000000e-05 3.254940000e+05) Completely repeated
Z = 29 subshell_6 (9.380000000e-04 3.632548000e+05) Completely repeated
Z = 34 subshell_10 (1.730000000e-04 1.282578000e+05) Completely repeated
Z = 39 subshell_11 (3.040000000e-04 4.369319000e+05) Completely repeated
Z = 40 subshell_11 (3.350000000e-04 4.130496000e+05) Completely repeated
Z = 41 subshell_10 (3.820000000e-04 1.787200000e+05) Completely repeated
Z = 46 subshell_10 (5.650000000e-04 1.432930000e+05) Completely repeated
Z = 47 subshell_18 (6.900000000e-05 7.668200000e+05) Completely repeated
Z = 48 subshell_11 (6.210000000e-04 2.892732000e+05) Completely repeated
Z = 69 subshell_30 (3.000000000e-05 2.092136000e+07) Completely repeated
Z = 70 subshell_21 (2.000000000e-04 3.532884000e+05) Completely repeated
Z = 70 subshell_22 (1.900000000e-04 5.294202000e+05) Completely repeated
Z = 71 subshell_22 (2.020000000e-04 3.632028000e+05) Completely repeated
Z = 79 subshell_32 (1.250000000e-05 4.780320000e+06) Completely repeated
Z = 86 subshell_29 (1.670000000e-04 3.673120000e+05) Completely repeated
Z = 86 subshell_30 (1.340000000e-04 6.456240000e+05) Completely repeated
Z = 87 subshell_30 (1.470000000e-04 5.957080000e+05) Completely repeated
Z = 91 subshell_46 (6.000000000e-06 3.900920000e+06) Completely repeated
Z = 100 subshell_32 (1.600000000e-04 8.098800000e+05) Completely repeated
```

Fig. 9. A summary of all completely repeated points for subshell cross sections

3.1.2. *generate_bindingEnergy_2017.c* macro

generate_bindingEnergy_2017.c is used to read binding energies from *EADL2017.ALL* and generate the output file:

   binding.dat, which contains the binding energies for all the elements.

It is saved in *epics2017/phot_preliminary/bindingEnergy* folder.

Format
In Fig. 10, we can see the binding energies for the first four elements separated by -1 -1.

First column indicates the subshell designator[], the second is the binding energy value.

Subshell designator   Binding energy (MeV)

Fig. 10. A part of binding.dat file

Command
To use the *generate_bindingEnergy_2017.c* macro, firstly you should place this macro and the *EADL2017.ALL* file in the same directory. Secondly, type the following command in the Terminal:

```
root generate_bindingEnergy_2017.c
```

Note that *generate_bindingEnergy_2014.c* is available to extract binding energies from *EADL2014.ALL*

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3.1.3. *generate_pe_cs_2017.c* macro

generate_pe_cs_2017.c is used to read total cross sections from *EPDL2017.ALL* and generate the output files:

> *pe-cs-Z.dat*, where *Z* is the atomic number of the element

They are saved in *epics2017/phot_preliminary* folder.

Format

For a given element, the *pe-cs-Z.dat* is composed of two header lines and energy – cross section data points.

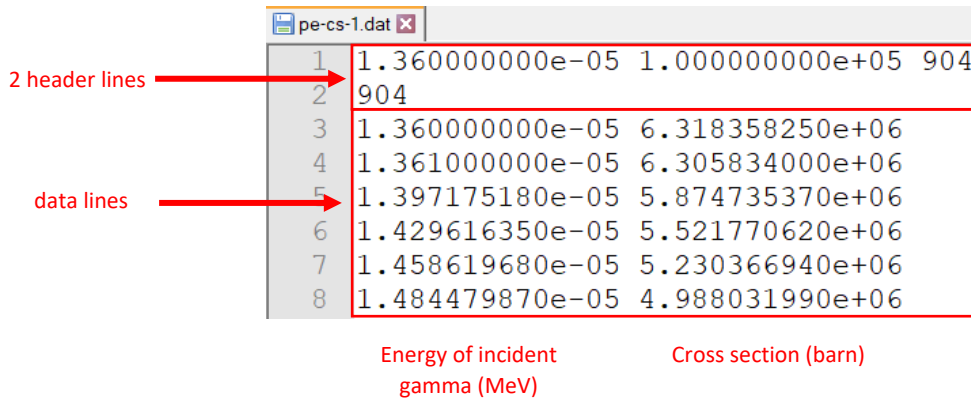Fig. 11 displays a part of *pe-cs-1.dat* file:

Fig. 11. A part of pe-cs-1.dat file

Command

To use the *generate_pe_cs_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_pe_cs_2017.c
```

Note that *generate_pe_cs_2014.c* is available to extract binding energies from *EPDL2014.ALL*

3.2. *fitForSubshellCS2017.c* macro

As explained in section 1.3, for each subshell, cross-sections are parameterized in two different intervals ("low fit" and "high fit"), using a fitting function as follows:

$$\sigma(E) = \frac{a_1}{E} + \frac{a_2}{E^2} + \frac{a_3}{E^3} + \frac{a_4}{E^4} + \frac{a_5}{E^5} + \frac{a_6}{E^6}$$

fitForSubshellCS2017.c reads subshell cross section data files extracted according to section 3.1.1 and calculates fitting parameters for both low fit and high fit in the same time. A special attention was paid to avoid discontinuity at the junction of two consecutive regions

Command

To use the *fitForSubshellCS2017.c* macro, make sure you have followed the steps explained in section 3.1, then type the following command in the Terminal:

```
root fitForSubshellCS2017.c
```

After running this macro, we will obtain the following output files:

- *low_high_limits.dat* contains energy limits of low fit and high fit intervals for all the elements

It is composed of three columns. The first column indicates the atomic number; the last two are respectively low energy limit and high energy limit for this element. Fig. 12 shows the first 5 elements of ***low_high_limits.dat***.

Fig. 12. A part of low_high_limits.dat file

- ***lowFittingParams.dat*** contains low fitting parameters for all subshells
  It is composed of 8 columns, the first two are atomic number of element and subshell index starting from 0, as illustrated in Fig. 13.

Fig. 13. A part of lowFittingParams.dat file

- ***highFittingParams.dat*** contains high fitting parameters for all subshells
  The format of ***highFittingParams.dat*** is the same as ***lowFittingParams.dat***.
- ***MaxDifferenceForTwoFitsOfSubshellsUsingNewParametersFor2017.dat*** contains maximal difference of fitted subshell cross section values compared with tabulated subshell cross sections for both low fit and high fit, which is meant to be used later in section 4.4.1.
  It is composed of 4 columns. The first two are atomic number and subshell index starting from 0. The last two gives the maximal difference of low fit and high fit for a given subshell. Fig. 14 displays the first 5 elements of this file.

Fig. 14. A part of MaxDifferenceForTwoFitsOfSubshellsUsingNewParametersFor2017.dat file

- *AverageDifferenceForTwoFitsOfSubshellsUsingNewParametersFor2017.dat* contains the average of absolute relative difference of fitted subshell values compared with tabulated subshell cross sections for both low fit and high fit, which is meant to be used later in section 4.4.1.
  The format of this file is similar to *MaxDifferenceForTwoFitsOfSubshellsUsingNewParametersFor2017.dat*.

In the meantime, figures showing the difference of fitted values compared with tabulated values are also plotted after running *fitForSubshellCS2017.c* macro. They are automatically saved in *epics2017/fit* directory. More information are given in section 4.5.1.

3.3. *generate_outputs.c* macro

Once you finish the fit process by running *fitForSubshellCS2017.c*, you can now generate the final outputs, which are about to be placed in Geant4 database and employed by Geant4 applications.

generate_outputs.c macro reads the following files:

- *pe-ss-cs-Z.dat*
- *binding.dat*
- *pe-cs-Z.dat*
- *low_high_limits.dat*
- *lowFittingParams.dat*
- *highFittingParams.dat*

Then, it finally generates 5 types of files, as follows:

- *pe-cs-Z.dat*, total cross sections **above** K shell binding energy for element Z
  Energy interval included in the file: [K binding energy; the closest energy point higher than low fit limit]
- *pe-le-cs-Z.dat*, total cross section **below** K shell binding energy for element Z
  Energy interval included in the file: [minimal tabulated energy; K binding energy]
- *pe-high-Z.dat*, high fitting parameters for subshell cross sections of element Z
- *pe-low-Z.dat*, low fitting parameters for subshell cross sections of element Z
- *pe-ss-cs-Z.dat*, subshell cross sections for element Z
  Energy interval included in the file: [minimal tabulated energy; the closest energy point higher than high fit limit]

These files are automatically saved in the folder ***epics2017/phot***

Command

To use the ***generate_outputs.c*** macro, make sure you have prepared all the files that need to be read by this macro, then type the following command in the Terminal:

```
root generate_outputs.c
```

4. Plots and comparison

4.1. Comparison of total cross sections

plot_pe_cs.c macro is capable to compare total cross section data from ***EPDL2017.ALL*** with that from ***EPDL2014.ALL*** by reading data extracted according to section 3.1.3. It finally generates a figure composed of two graphs for each element:

- the top graph is the comparison of total cross sections between EPDL2017 and EPDL2014
- the bottom is the relative difference of total cross sections of EPDL2017 compared to that of EPDL2014, only points with same energies are taken into account

All the figures are saved automatically in ***plots/totalCS_comparison***

Fig. 15 shows an example for element Boron.

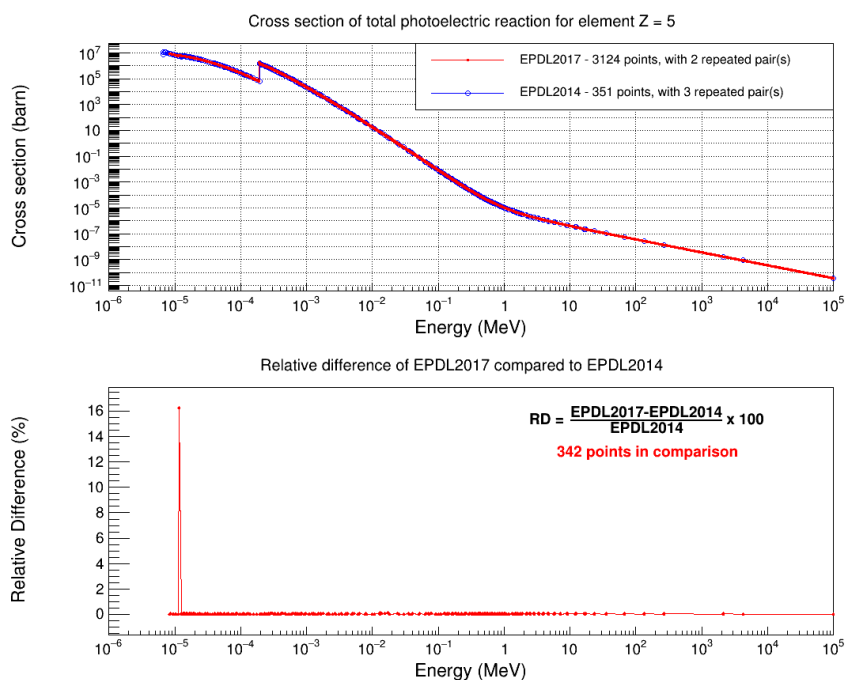The energy edge is represented as "repeated pair(s)".

Fig. 15. Comparison of total cross sections between EPDL2017 and EPDL2014 for Boron

Command

To use the ***plot_pe_cs.c*** macro, make sure you have prepared total cross section files that need to be read by this macro, then type the following command in the Terminal:

```
root plot_pe_cs.c
```

4.2. Comparison of subshell cross sections

plot_ss_cs.c macro is capable to compare subshell cross section data from ***EPDL2017.ALL*** with that from ***EPDL2014.ALL*** by reading data extracted according to section 3.1.1. It finally generates a figure composed of two graphs for each subshell:

- the top graph is the comparison of subshell cross sections between EPDL2017 and EPDL2014
- the bottom is the relative difference of subshell cross sections of EPDL2017 compared to that of EPDL2014, only points with same energies are taken into account

All the figures are saved automatically in ***plots/subshellCS_comparison***

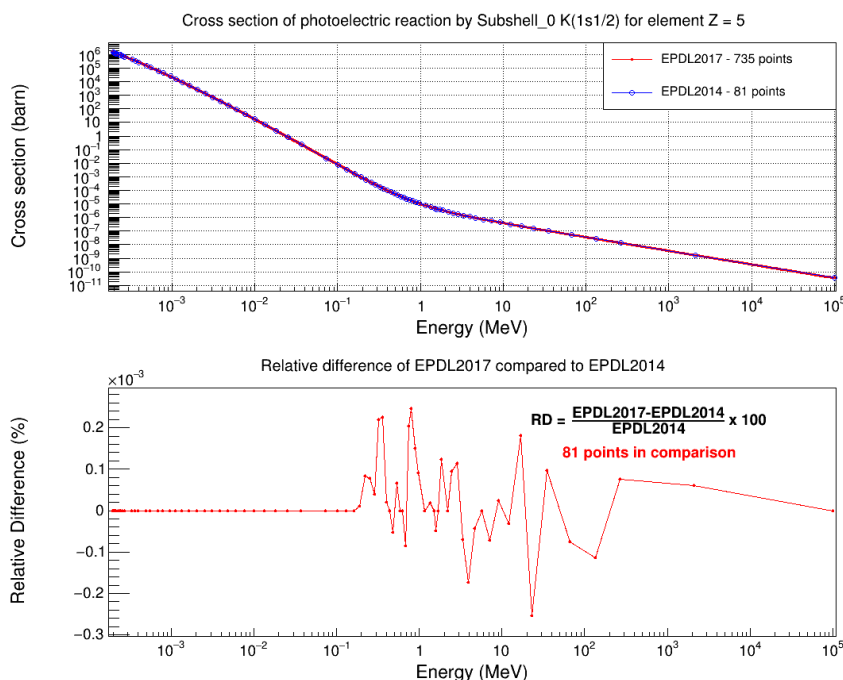Fig. 16 shows an example for the K subshell of Boron.

Fig. 16. Comparison of K subshell cross sections between EPDL2017 and EPDL2014 for Boron

Command
To use the ***plot_ss_cs.c*** macro, make sure you have prepared subshell cross section files that need to be read by this macro, then type the following command in the Terminal:

```
root plot_ss_cs.c
```

4.3. Comparison of binding energies

plot_bindingEnergy.c is used to plot the difference of binding energies between EADL2017 and EADL2014. It generates a figure composed of two graphs for each element:

- the top graph is the comparison of binding energies
- the bottom is the relative difference of binding energies of EADL2017 compared to that of EADL2014

All the figures are saved automatically in ***plots/bindingEnergy_comparison/2014VS2017***

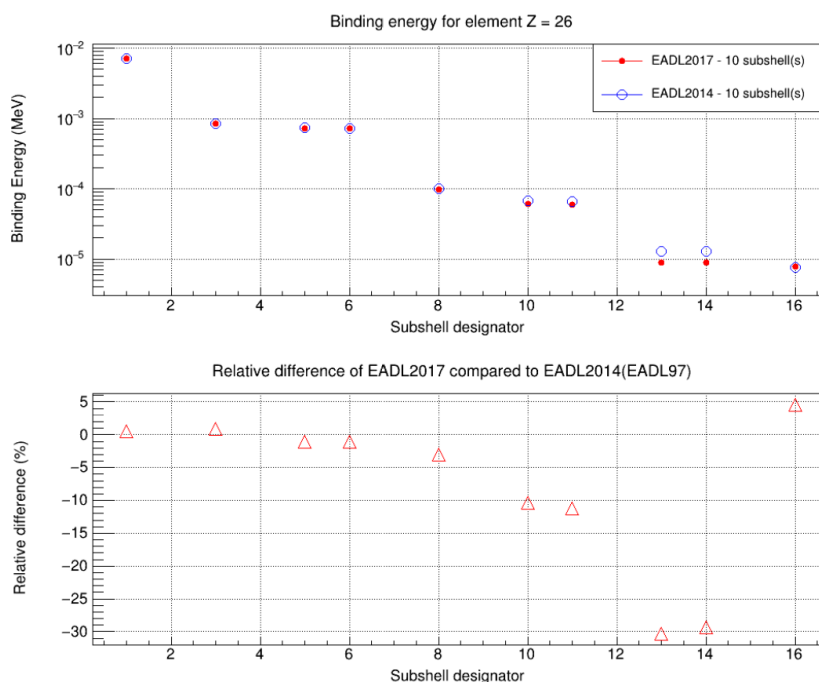Fig. 17 demonstrates the comparison of binding energies for Iron.

Fig. 17. Comparison of binding energies between EADL2017 and EADL2014 for Iron

Moreover, in the end of running this macro, ***ratioMax_ratioAverage_ForBindingEnergy_2014_2017.dat*** will be created, which contains

- maximal difference of binding energies of EADL2017 compared with EADL2014 for each element
- absolute average difference of binding energies of EADL2017 compared with EADL2014 for each element

These values can be read and plotted by ***plot_MaximalDifference_AverageDifference_BindingEnery_2014_2017_WithZ.c***

Besides, there are three kinds of available binding energy data in Geant4 database:

- ***$G4LEDATA/fluor/binding.dat***
- ***$G4LEDATA/fluor_Bearden/binding.dat***
- ***$G4LEDATA/fluor_XDB_EADL/binding.dat***

We have studied that binding energies in ***$G4LEDATA/fluor/binding.dat*** and ***$G4LEDATA/fluor_Bearden/binding.dat*** are the same, they both come from EADL97 (EADL2014).

While binding energies in ***$G4LEDATA/fluor_XDB_EADL/binding.dat*** are combinations of different sources, which are well illustrated in ***$G4LEDATA/README*** file.

Here we also provide a macro ***plot_bindingEnergy_XDB_EADL.c*** to achieve the comparison of binding energies between ***fluor_XDB_EADL*** and EADL2017.

It generates a figure composed of two graphs for each element:

- the top graph is the comparison of binding energies amongst EADL2014, EADL2017 and XDB_EADL
- the bottom is the relative difference of binding energies of XDB_EADL compared to that of EADL2014 and EADL2017

All the figures are saved automatically in ***plots/bindingEnergy_comparison/XDB_EADL***

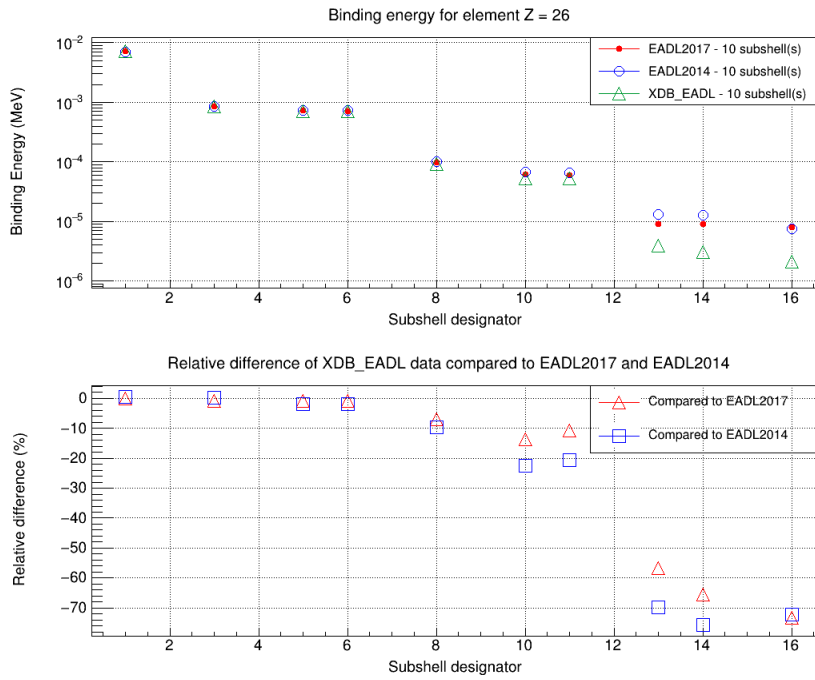Fig. 18 demonstrates the comparison of binding energies for Iron.

Fig. 18. Comparison of binding energies between EADL2017, EADL2014 and XDB_EADL for Iron

Command

To use the **plot_bindingEnergy.c** or **plot_bindingEnergy_XDB_EADL.c** macro, make sure you have prepared binding energy files that need to be read by this macro, then type the following command in the Terminal:

```
root plot_bindingEnergy.c  // or plot_bindingEnergy_XDB_EADL.c
```

4.4. Comparison of between fitted total cross sections and tabulated total cross sections

In order to evaluate the performance of new fitting parameters for total cross sections, we offered several ROOT macros to plot the relative difference of fitted total cross section values compared to the tabulated values in three cases:

- case 1: EPDL2017 data using new fitting parameters
- case 2: EPDL2017 data using existing[2] fitting parameters
- case 3: EPDL2014 data using existing fitting parameters

4.4.1. EPDL2017 data with new fitting parameters

plot_pe_fittedTotalCSUsingNewFitParameters2017.c reads EPDL2017 data and fitting parameters generated in section 3.2 in order to compare the values of fitted total cross sections with the tabulated values. It generates at last:

- one figure of comparison for each element, saved in **plots/fittedTotalCSUsingNewParameters**
- **ratioMaxForFittedTotalCSUsingNewParams2017_plotting.dat**, contains the maximal difference values of low fit and high fit for all the elements

Fig. 19 represents a part of this file, for the first 5 elements

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[2] "existing fitting parameters" refer to the those in **$G4LEDATA/Livermore/phot_epics2014** of Geant4 version 10.7. We recall that existing fitting parameters were obtained based on EPDL2014 data, which are the same as EPDL97

Fig. 19. A part of *ratioMaxForFittedTotalCSUsingNewParams2017_plotting.dat file*

An example of Hydrogen is given in Fig. 20.

Fig. 20. Relative difference of fitted total cross sections for low fit and high fit based on EPDL2017 data and EPDL2017 fitting parameters

4.4.2. EPDL2017 data with existing fitting parameters

plot_pe_fittedTotalCSUsingExistingFitParameters_2017.c reads EPDL2017 data and existing fitting parameters. You need to make sure this macro has access to existing fitting parameters (***$G4LEDATA/livermore/phot_epics2014***). It enables to compare the values of fitted total cross sections using existing fitting parameters with the tabulated values. It generates at last:

- one figure of comparison for each element, saved in ***plots/fittedTotalCSUsingExistingParameters***
- ***ratioMaxForFittedTotalCSUsingExistingParametersFor2017_plotting.dat***, contains the maximal difference values of low fit and high fit for all the elements. The format is the same to ***ratioMaxForFittedTotalCSUsingNewParams2017_plotting.dat*** explained in 4.4.1

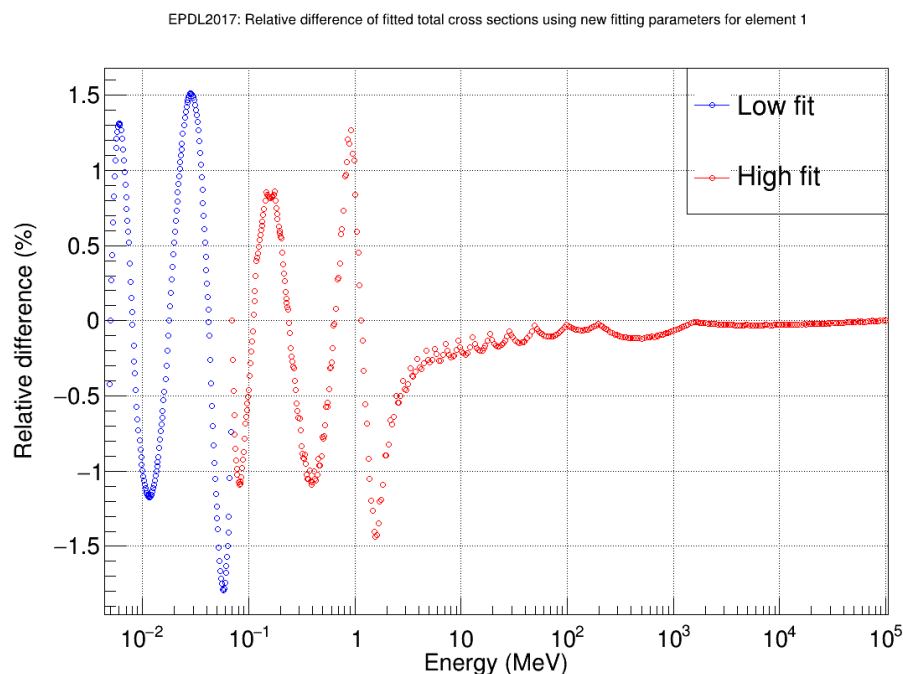Fig. 21 shows the comparison for Hydrogen.

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Fig. 21. Relative difference of fitted total cross sections for low fit and high fit based on EPDL2017 data and existing fitting parameters

4.4.3. EPDL2014 data with existing fitting parameters

plot_pe_fittedTotalCSUsingExistingFitParameters_2014.c reads EPDL2014 data and existing fitting parameters. It compares the values of fitted total cross sections using existing fitting parameters with the tabulated values. It generates at last:

- one figure of comparison for each element, saved in ***plots/ fittedTotalCSUsingExistingParameters_2014***
- ***ratioMaxForFittedTotalCS2014_plotting.dat***, contains the maximal difference values of low fit and high fit for all the elements. The format is the same to ***ratioMaxForFittedTotalCSUsingNewParams2017_plotting.dat*** explained in 4.4.1

Fig. 22 shows the comparison for Hydrogen.

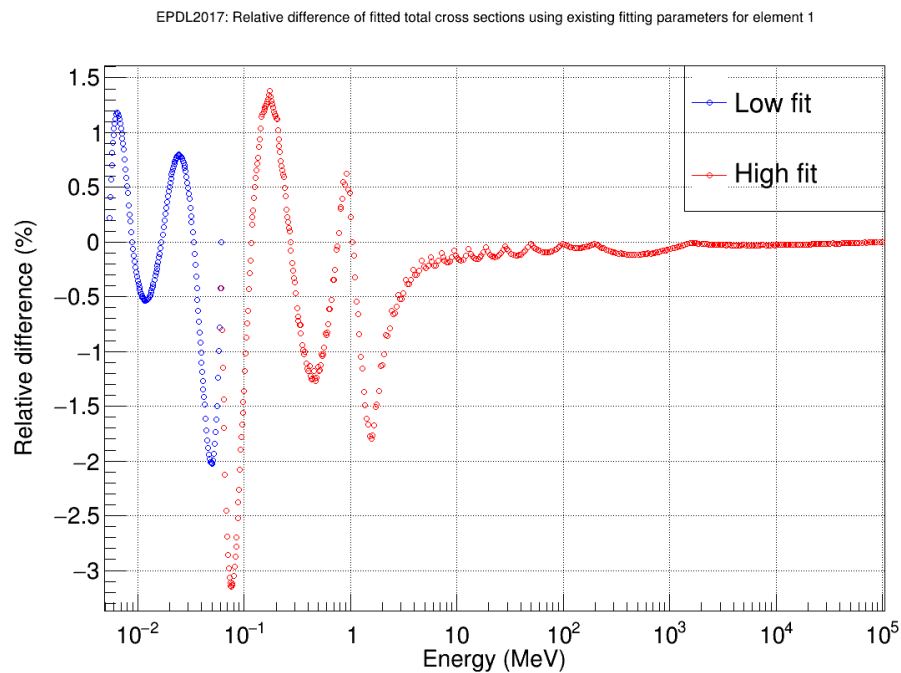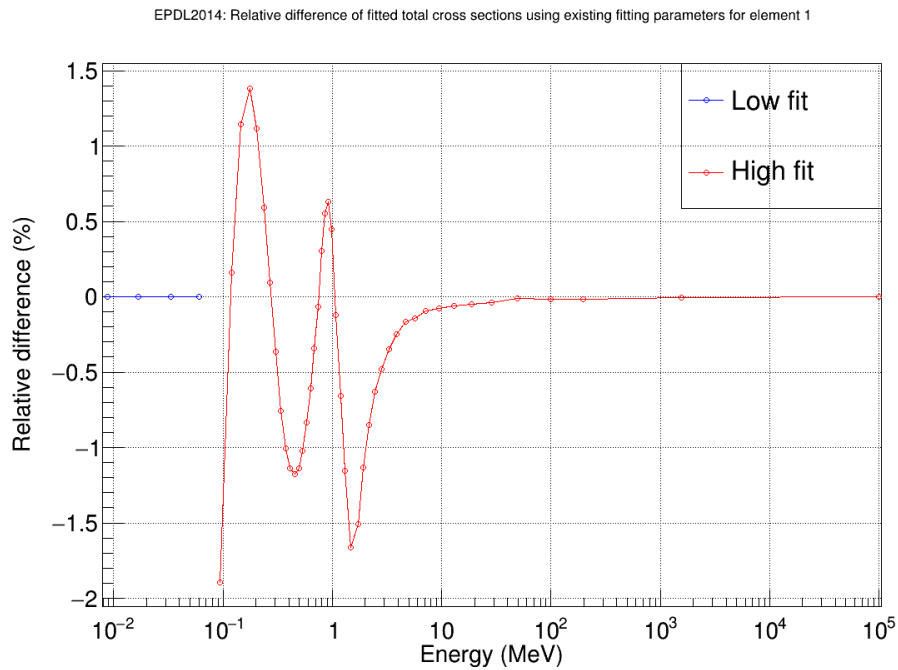EPDL2014: Relative difference of fitted total cross sections using existing fitting parameters for element 1

Fig. 22. Relative difference of fitted total cross sections for low fit and high fit based on EPDL2014 data and existing fitting parameters

4.4.4 Comparison of maximal difference of fitted total cross sections according to Z

plot_compare_MaximalDifferenceOfFittedTotalCS_2014_2017.c is able to read maximal difference of fitted values compared with tabulated values according to Z in the three cases mentioned above:

- fitted total cross sections VS tabulated values for EPDL2017 data using new fitting parameters
- fitted total cross sections VS tabulated values for EPDL2017 data using existing fitting parameters
- fitted total cross sections VS tabulated values for EPDL2014 data using existing fitting parameters

It then plots the comparison respectively for low fit and high fit according to Z, as shown in Fig. 23.
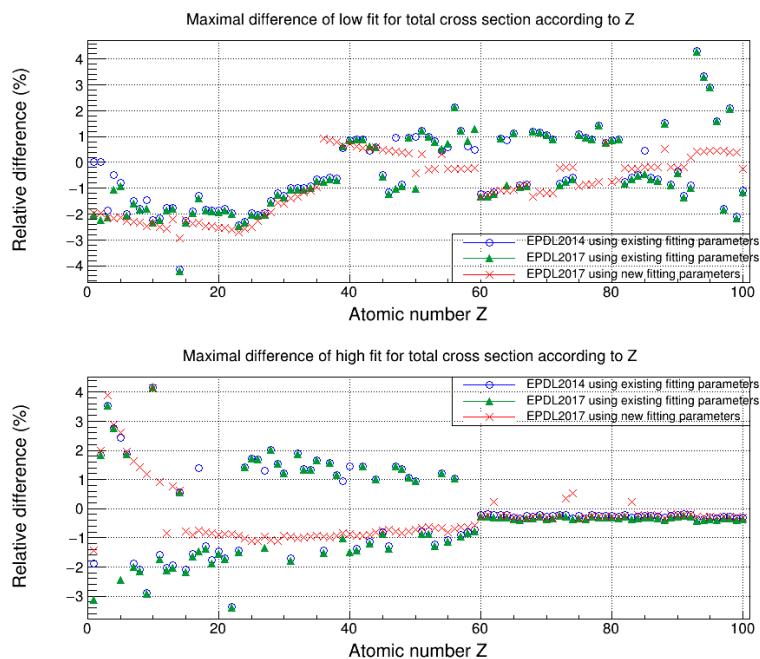
Fig. 23. Comparison of maximal difference of fitted total cross sections according to Z for the three cases

Based on the absolute maximal difference values, we can calculated the improved precision (IP) according to the following formula:

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

where $R_{new}(Z)$ and $R_{old}(Z)$ are the maximal relative difference of new fit and previous fit of scattering functions for the element Z.

For low energy fit, IP = 1.9, case 1 VS case 3;

For high energy fit, IP = 1.3, case 1 VS case 3.

4.5. Comparison between fitted subshell cross sections and tabulated subshell cross sections

Similarly, the comparison for subshell cross sections is also discussed in three cases.

4.5.1. EPDL2017 data with new fitting parameters

It is mention in section 3.2 that figures showing the difference of fitted values compared with tabulated values are generated simultaneously while running ***fitForSubshellCS2017.c***. These figures are saved in ***plots/fit/Histo_low_high***.

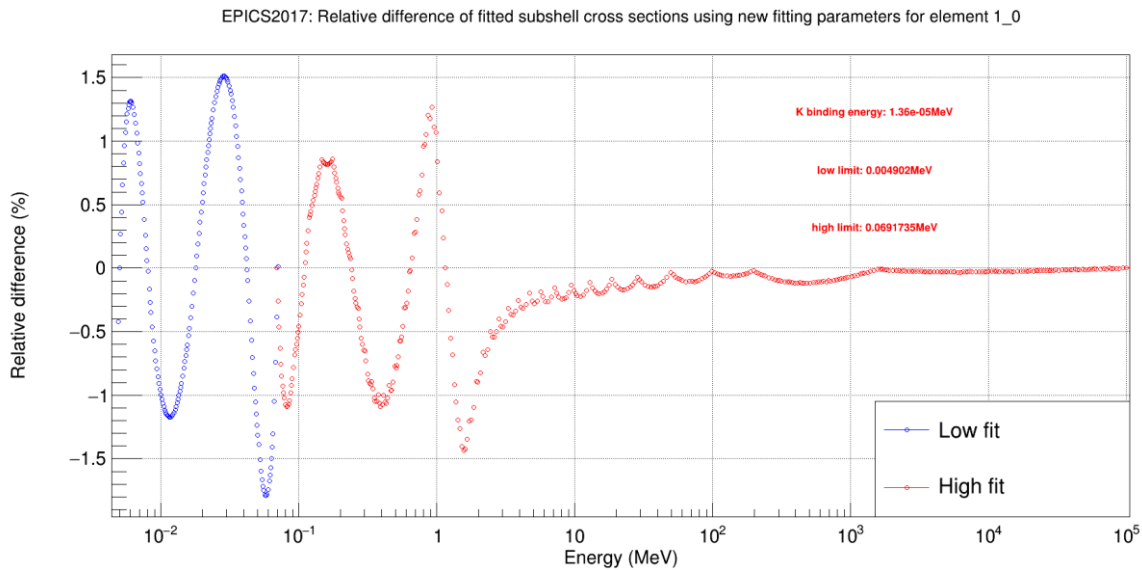An example of Hydrogen is displayed in Fig. 24.

Fig. 24. Relative difference of fitted subshell cross sections for low fit and high fit based on EPDL2017 data and new fitting parameters

4.5.2. EPDL2017 data with existing fitting parameters

plot_pe_fittedSubshellCSUsingExistingFitParameters_2017.c is able to plot the relative difference of fitted subshell cross sections for EPDL2017 data using existing fitting parameters. This object requires fitting parameters of each single subshell, which we successfully reproduced by using the macro ***fitPhotoelectricEffect.c***, left by Marilena Bandieramonte. See section 4.5.3.

In the end of running this macro, the following files will be created:

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- ***MaxDifferenceForTwoFitsOfSubshellsUsingExistingParameters_2017.dat*** contains maximal difference of fitted subshell cross section values compared with tabulated subshell cross sections for both low fit and high fit.
  Its format is similar to ***MaxDifferenceForTwoFitsOfSubshellsUsingNewParametersFor2017.dat*** in the section 3.2.
- ***AverageDifferenceForTwoFitsOfSubshellsUsingExistingParameters_2017.dat*** contains the average absolute difference of fitted subshell cross sections values compared with tabulated values for both low fit and high fit.
  Its format is similar to ***AverageDifferenceForTwoFitsOfSubshellsUsingNewParametersFor2017.dat*** in the section 3.2.
- Figures of relative difference of fitted subshell cross sections compared to tabulated values
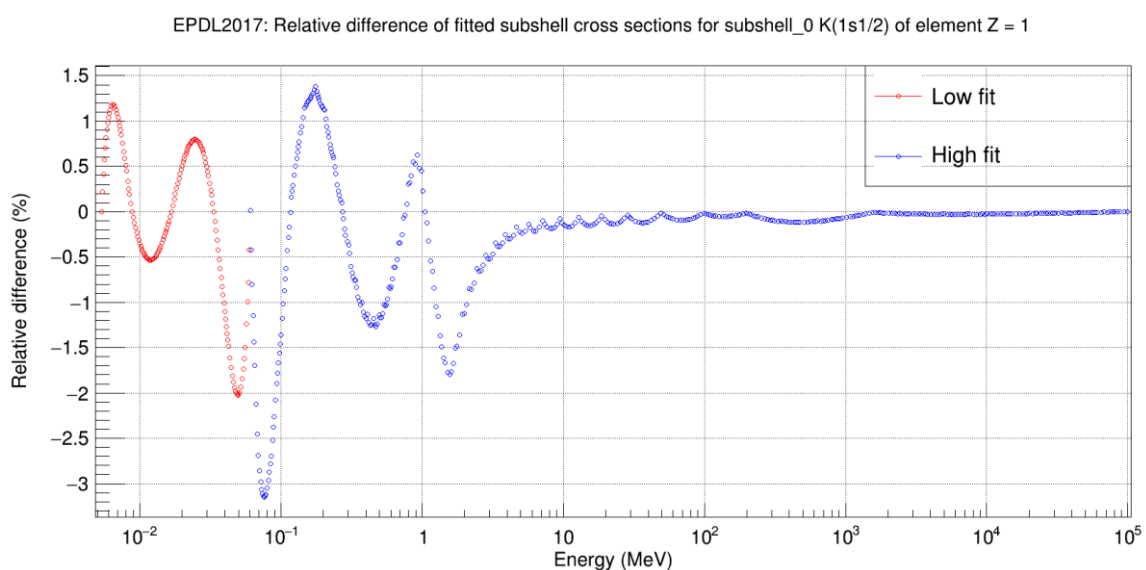
An example for Hydrogen is given Fig. 25.

Fig. 25. Relative difference of fitted subshell cross sections for low fit and high fit based on EPDL2017 data and existing fitting parameters

4.5.3. EPDL2014 data with existing fitting parameters

If you want to get the same type of figures, at first place, you should run the macro ***fitPhotoelectricEffect.c***, left by Marilena Bandieramonte. It can reproduce the exact fitting parameters as those in Geant4 database. With appropriate modifications, it eventually performs in the same way as ***fitForSubshellCS2017.c*** does. It is placed in ***epics2017-master/fitPhotoelectricEffect***.

After running this macro, we will obtain the following output files:

- ***low_high_limits.dat***
- ***lowFittingParams.dat***
- ***highFittingParams.dat***
- ***MaxDifferenceForTwoFitsOfSubshellsUsingExistingParametersFor2014***
- ***AverageDifferenceForTwoFitsOfSubshellsUsingExistingParametersFor2014.dat***
- Figures of relative difference of fitted subshell cross sections compared to tabulated values

Information that is more precise is given in section 3.2.

Fig. 26 illustrates the relative difference of low fit and high fit for Hydrogen.
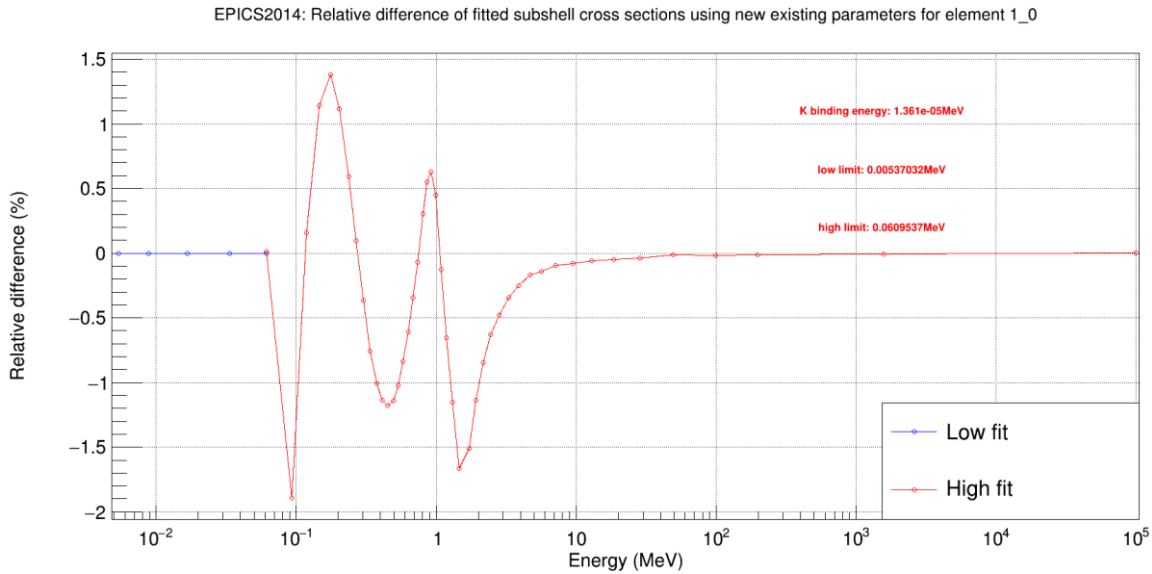
Fig. 26. Relative difference of fitted subshell cross sections for low fit and high fit based on EPDL2014 data and the existing parameters

4.5.4 Comparison of maximal difference of fitted subshell cross sections according to Z

Once we have possessed the following three files, we could make use of ***plot_compare_MaximalDifferenceOfSubshellsWithZ_2014_2017.c*** to plot the comparison of maximal difference of low fit and high fit according to Z:

- ***MaxDifferenceForTwoFitsOfSubshellsUsingNewParametersFor2017.dat***
- ***MaxDifferenceForTwoFitsOfSubshellsUsingExistingParameters_2017.dat***
- ***MaxDifferenceForTwoFitsOfSubshellsUsingExistingParametersFor2014***

The macro ***plot_compare_MaximalDifferenceOfSubshellsWithZ_2014_2017.c*** is about to read these three files to plot the maximal difference of low fit and high fit according to Z, see in the Fig. 27.
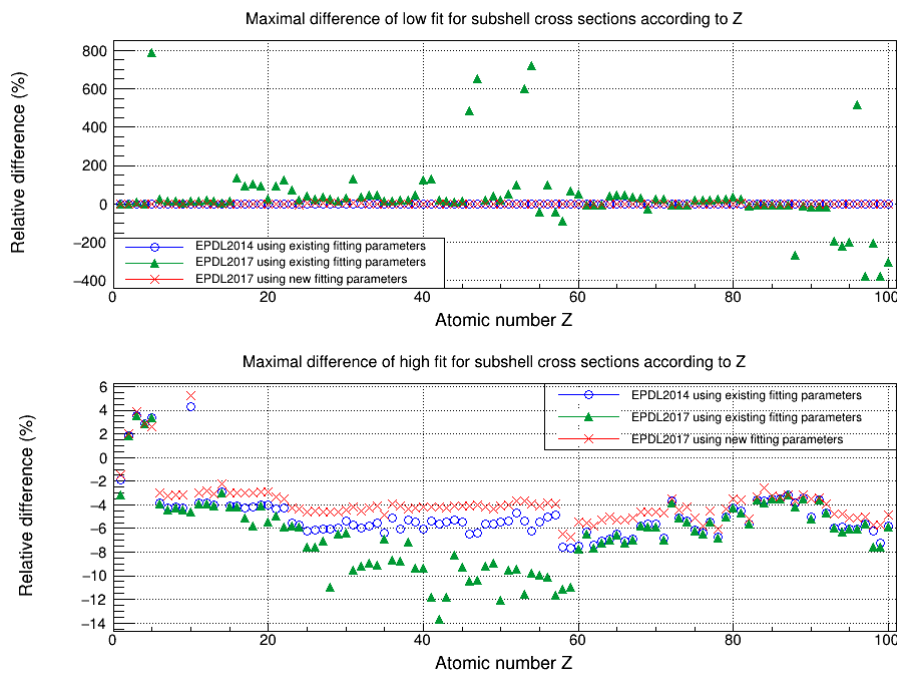

Fig. 27. Comparison of maximal difference of fitted subshell cross sections according to Z for the three cases

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Since there are several relatively higher values (for instance close to 800%) in the case of EPDL2017 data using existing fitting parameters, we can not better see the distribution of the other two cases. So Fig. 28 only represents the other two cases.
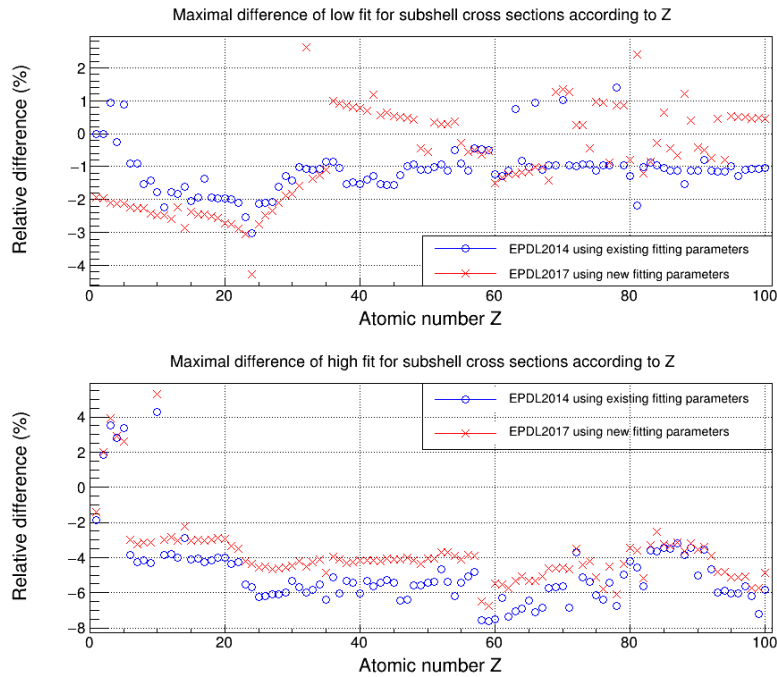

Fig. 28. Comparison of maximal difference of fitted subshell cross sections according to Z for two cases

4.5.5 Comparison of average difference according to Z

As a complementary information, we also compared the average absolute difference of fitted subshell cross sections for the three cases by using the macro *plot_compare_AverageDifferenceOfSubshellsWithZ_2014_2017.c*. It reads the following three files:

- *AverageDifferenceForTwoFitsOfSubshellsUsingNewParametersFor2017.dat*
- *AverageDifferenceForTwoFitsOfSubshellsUsingExistingParameters_2017.dat*
- *AverageDifferenceForTwoFitsOfSubshellsUsingExistingParametersFor2014.dat*

The output graph is represented in Fig. 29

Fig. 29. Comparison of average difference of fitted subshell cross sections according to Z for the three cases

A comparison without EPDL2017 using existing fitting parameters is also shown in Fig. 30.

Fig. 30. Comparison of average difference of fitted subshell cross sections according to Z for two cases

It should be noted that these there files contain the average of absolute relative difference (a_i) for all subshells. For a given Z, the real average difference (AD) that we used in Fig. 29 and Fig. 30 is calculated on all the subshells:

$$AD(Z) = \frac{1}{n} \cdot \sum_{i=0}^{i=n-1} a_i\,(Z)$$

Where a_i is the average of absolute relative difference of subshell i for the given element Z.

List of macro files

The ROOT macro files that we mentioned above are:

1. *generate_ss_cs_2017.c*, generates subshell cross section data files from *EPDL2017.ALL*
2. *generate_ss_cs_2014.c*, generates subshell cross section data files from *EPDL2014.ALL*
3. *generate_bindingEnergy_2017.c*, generates binding energy files from *EADL2017.ALL*
4. *generate_bindingEnergy_2014.c*, generates binding energy files from *EADL2014.ALL*
5. *generate_pe_cs_2017.c*, generates total cross section files from *EPDL2017.ALL*
6. *generate_pe_cs_2014.c*, generates total cross section files from *EPDL2014.ALL*
7. *fitForSubshellCS2017.c*, performs fit process based on EPDL2017
8. *generate_outputs.c*, generates final output files
9. *plot_pe_cs.c*, plots the comparison of total cross section data between EPDL2017 and EPDL2014
10. *plot_ss_cs.c*, plots the comparison of subshell cross section data between EPDL2017 and EPDL2014
11. *plot_bindingEnergy.c*, compares the binding energies between EADL2017 and EADL214
12. *plot_bindingEnergy_XDB_EADL.c*, compares the binding energies between EADL2017 and *fluor_XDB_EADL*
13. *plot_pe_fittedTotalCSUsingNewFitParameters2017.c*, compares the fitted total cross sections with the tabulated values, based on EPDL2017 data and new fitting parameters
14. *plot_pe_fittedTotalCSUsingExistingFitParameters_2017.c*, compares the fitted total cross sections with the tabulated values, based on EPDL2017 data and existing fitting parameters
15. *plot_pe_fittedTotalCSUsingExistingFitParameters_2014.c*, compares the fitted total cross sections with the tabulated values, based on EPDL2014 data and existing fitting parameters
16. *plot_compare_MaximalDifferenceOfFittedTotalCS_2014_2017.c*, plots maximal difference of fitted total cross sections according to Z in three cases
17. *plot_pe_fittedSubshellCSUsingExistingFitParameters_2017.c*, plots relative difference of fitted subshell cross sections, based on EPDL2017 data and existing fitting parameters
18. *plot_compare_MaximalDifferenceOfSubshellsWithZ_2014_2017.c*, plots maximal difference of fitted subshell cross sections according to Z in three cases
19. *plot_compare_AverageDifferenceOfSubshellsWithZ_2014_2017.c*, plots average difference of fitted subshell cross sections according to Z in three cases