Interpolate_DCS – a program for interpolating differential cross sections of bremsstrahlung from BremsLib v2.0

v1.0

User's Manual

by Andrius Poškus

(Vilnius University, Institute of Chemical Physics)

2025-03-01

E-mail: andrius.poskus@ff.vu.lt or andrius.poskus@live.com
Web: https://web.vu.lt/ff/a.poskus/brems/

Contents

1. Introduction

Interpolate_DCS is a set of Fortran-90 codes for interpolating the double- and single differential cross sections of bremsstrahlung stored in the data library BremsLib v2.0 for each atomic number Z of the target atom (from $Z = 1$ to $Z = 100$) with respect to three physical parameters: incident electron energy T_1, bremsstrahlung photon energy k, and photon emission angle θ. The energy range of the incident electron is from 10 eV to 30 MeV at $k \neq 0$, or from 10 eV to 100 MeV in the soft-photon limit ($k = 0$). Results of interpolation of the double differential cross section (DDCS) corresponding to a particular combination of Z and T_1 are output either as a set of values of the DDCS corresponding to one value of k and a set of values of θ, or as a set of values of the DDCS corresponding to one value of θ and a set of values of k. Results of interpolation of the single differential cross section (SDCS) are output as a set of values of the SDCS corresponding to a set of values of k.

Interpolate_DCS was written by Andrius Poškus (Vilnius University, Faculty of Physics, Institute of Chemical Physics). Interpolate_DCS is distributed under the GNU General Public License 3.

Interpolate_DCS is included in the BremsLib v2.0 distribution package, which can be downloaded from https://web.vu.lt/ff/a.poskus/brems/.

2. Methods of interpolation implemented in Interpolate_DCS

Any practical application of tables of differential cross sections requires interpolating between the tabulated values ("grid points"). The optimal interpolation techniques depend on density of grid points. In the limit of very high density of points, interpolation is usually linear or exponential (which is the same as linear interpolation on a logarithmic scale). If linear or exponential interpolation is not sufficiently accurate, other methods must be chosen. Thus, discussion of interpolation methods that are suitable for a particular dataset must be based on the density of grid points in it. In the case discussed, each value of DDCS corresponds to a particular combination of four physical parameters Z, T_1, k / T_1, and θ. Each value of SDCS corresponds to a triplet of values of Z, T_1, and k / T_1. Interpolation with respect to Z is not required, because BremsLib v2.0 includes the data for each value of Z from 1 to 100.

Interpolation with respect to θ is linear, because the interval between adjacent grid values of θ is sufficiently small. This interval is defined for four intervals of values of T_1 separately. For example, when 4 MeV $\leq T_1 \leq$ 30 MeV, the mentioned angular interval is equal to 0.1° at $\theta < 10°$, and to 0.5° at $\theta > 10°$. This interval decreases with increasing T_1. The mentioned linear interpolation with respect to θ is performed before any other kind of interpolation. If there are multiple values of θ, for which the interpolated values of DDCS have to be calculated, then the mentioned linear interpolation with respect to θ yields multiple sets of grid values of DDCS on a fixed two-dimensional grid formed by available grid values of T_1 and k / T_1. Each such two-dimensional set of grid points corresponds to one final value of θ (which is typically different from the original grid values of θ).

The mentioned linear interpolation with respect to θ is followed by interpolation with respect to T_1, which is based on cubic spline fitting. The grid points correspond to $T_1 = (1, 1.2, 1.5, 2, 2.5, 3, 4, 5, 6, 8) \times 10^n$ MeV, where $n = -5, -4, -3, -2, -1, 0, 1$, and the last grid point corresponds to $T_1 = 100$ MeV (the last five grid points from 40 MeV to 100 MeV are used only in the case $k = 0$). Interpolation with respect to T_1 is illustrated in Fig. 1. It has to be performed for every grid value of k / T_1, because it is followed by interpolation with respect to k / T_1. Since the interpolation with respect to T_1 is based on fitting, it modifies the values at all the grid points, too (in addition to providing intermediate values). The changes of values at the grid points are typically not significant (i.e., less than computational uncertainties of the original estimates of the SDCS or DDCS at the grid points). If the grid values are distorted by numerical errors, then fitting is preferable to "pure" interpolation (when the interpolating function passes exactly through each grid point), because fitting tends to smooth out irregularities of the original data caused by numerical
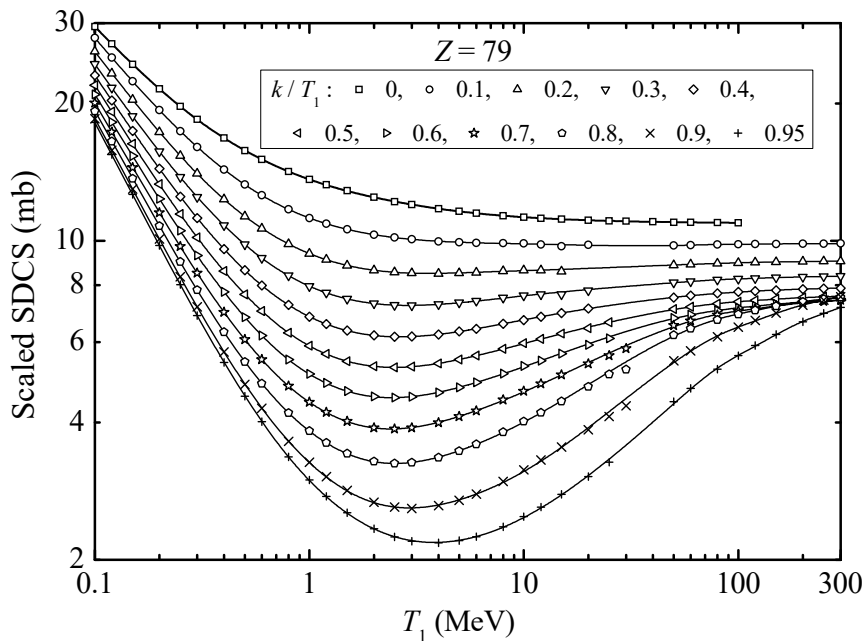
Fig. 1. The calculated dependences of the SDCS on T_1 when $Z = 79$ and the Kohn-Sham potential is used, for 11 values of the ratio k / T_1. Logarithmic scale is used on both axes. At $T_1 \leq 30$ MeV, the scatter plots corresponding to $k \neq 0$ show the results of the partial-wave calculations. At $T_1 \geq 50$ MeV, the same scatter plots show the SDCS calculated by integrating the analytical expression of triple differential cross section based on Sommerfeld-Maue wave functions with the next-to-leading-order correction, and with the screening correction of the DDCS. The scatter plot corresponding to $k = 0$ shows the results obtained using a more accurate partial-wave method based on the Low theorem. Each scatter plot defines a set of "grid points", which is used for constructing an interpolating function. The eleven curves have been obtained by cubic spline fitting of log(SDCS) with respect to log(T_1). The set of abscissas of breakpoints of each spline function consists of every fourth grid value, so that the number of breakpoints is equal to 1/4 of the number of original grid points. The points with relative computational uncertainty (Δ) greater than 0.05 are not shown and not used for the mentioned spline fitting. The contribution of points with $0.01 < \Delta \leq 0.05$ to the sum of squared residuals, which is minimized during the spline fitting, has been weighted by the factor $(0.01/\Delta)^2$.

errors (in contrast, pure spline interpolation may "amplify" the mentioned irregularities, causing unphysical oscillations of the interpolating spline function between grid points). It should be noted here that Fig. 1 illustrates not *usage* of the final grid data, but *generation* of missing SDCS grid data at 10 MeV $< T_1 \leq 30$ MeV and $T_2 > 3$ MeV. In the case of Fig. 1, the final grid points corresponding to missing original data lie on the curves showing the spline functions. Thus, there are no missing data in the final grid (which is stored in BremsLib v2.0), and some of the final grid points are by definition well approximated by cubic splines, so that the density of breakpoints ("knots") of the spline function used for subsequent interpolation may be increased in comparison with Fig. 1. In the range of values of T_1 corresponding to Fig. 1, this density is by default increased by a factor of 2, i.e., the set of abscissas of breakpoints of each interpolating spline function by default consists of every other grid value, so that the number of breakpoints used for spline fitting and interpolation with respect to T_1 is equal to half the number of original grid points (the corresponding spline functions would be visually indistinguishable from the curves of Fig. 1, if plotted in the same graph).

Interpolation with respect to k / T_1 is performed last. In the case of SDCS, it has to be performed only once (if there are several final values of k / T_1, then they correspond to several values of a single interpolating function of k / T_1). In the case of DDCS, the interpolation with respect to k / T_1 is performed for each final value of θ separately. This interpolation is in general more prone to errors than the mentioned interpolation with respect to θ and T_1, because the density of grid values of k / T_1 in BremsLib v2.0 is relatively small. There are thirteen grid values of k / T_1: ten equidistant values from 0 to 0.9, followed by 0.95, 0.975, and 1. Since the partial-wave DDCS and SDCS ("DCS" for both) sharply drop to zero at $k / T_1 = 1$, the last grid value of k / T_1 is actually slightly less than 1. It has been chosen so that it is just before the mentioned sharp drop of DCS to zero: (a) if $T_1 \leq 5$ keV, then it is equal to 0.99, (b) if 5 keV $< T_1 \leq 500$ keV, then the last grid value

of k / T_1 is equal to $1 - (50 \text{ eV} / T_1)$, which means that the final electron energy is $T_2 = 50$ eV, (c) if $T_1 > 500$ keV, then the last grid value of k / T_1 is equal to 0.9999. As shown in Fig. 2b and Fig. 2c, the dependence of the DDCS on k / T_1 at large angles and large values of T_1 (of the order of 1 MeV or greater) is characterized by an especially large curvature between the first two grid points (here, the term "curvature" refers to the *relative* rate of change of the first derivative as a function of k / T_1). Consequently, a simple spline fitting or interpolation typically causes relative errors greater than 10 % when k / T_1 is of the order of 0.01 (and the results of linear interpolation are even less accurate). As illustrated by the top two curves in Fig. 2f, the mentioned curvature can be reduced significantly if the values of the partial-wave DDCS ("PW DDCS") at the grid values of k / T_1 are replaced by the values of the ratio $DDCS / DDCS_{Born}$, where "$DDCS_{Born}$" denotes the screened Born-approximation DDCS (with the nuclear form factor and the Elwert factor), calculated using the same screening function as the partial-wave DDCS. The criterion for the validity of the Born approximation is

$$\beta >> Z\alpha, \tag{2.1}$$

where β is the ratio of the electron speed to the speed of light (this condition must be satisfied both for the initial and the final electron). Because of the mentioned smaller curvature of the dependence of $DDCS / DDCS_{Born}$ on k / T_1 at $k / T_1 < 0.1$, accuracy of spline-fitting of the ratio $DDCS / DDCS_{Born}$ is significantly better than accuracy of spline-fitting of the original DDCS (especially at small values of Z and at energies corresponding to condition (2.1), when $DDCS / DDCS_{Born}$ is close to 1 at all values of θ). Thus, the spline fitting with respect to k / T_1 should be done in three steps:

 (a) all grid values of the DDCS are replaced by the ratio $DDCS / DDCS_{Born}$,
 (b) the set of ratios is fitted by a cubic spline function,
 (c) the result of the fitting corresponding to each k / T_1 of interest is multiplied by the corresponding value of $DDCS_{Born}$, yielding the final interpolated value of the DDCS.

The last step requires availability of $DDCS_{Born}$ for any value of k / T_1 in the interval $0 \leq k / T_1 < 1$. In order to avoid repeated evaluation of the relatively complex expression of the screened Born-approximation DDCS, the value of $DDCS_{Born}$ can be calculated by spline interpolation, albeit with a much greater density of points in the interval $0 \leq k / T_1 < 0.1$, so as to avoid the mentioned problems caused by large curvature of the dependence of $DDCS_{Born}$ on k / T_1 inside this interval. In BremsLib v2.0, this is achieved by insertion of ten additional grid points of $DDCS_{Born}$, which correspond to $k / T_1 = 0.005, 0.01, 0.02, \ldots, 0.09$. The remaining ten grid points of $DDCS_{Born}$ correspond to ten equidistant values of k / T_1 from 0 to 0.9. Thus, the spline function used for interpolation of $DDCS_{Born}$ is defined in the interval $0 \leq k / T_1 \leq 0.9$, using a set of 20 pre-calculated grid values of $DDCS_{Born}$ (shown in Fig. 2a–d by solid circles) for every combination of grid values of Z, $T_1 \geq 1$MeV, and θ (at $T_1 < 1$ MeV, the dependence of DDCS on k / T_1 does not have regions of such high curvature as in Fig. 2c, hence simple spline fitting of the original grid values of the DDCS is sufficiently accurate at all values of k / T_1 and θ). The interval where the final DDCS is calculated by the mentioned three steps is $0 \leq k / T_1 \leq 0.7$. Inside the interval $0.7 < k / T_1 < 1$, the final DDCS is calculated by simple cubic spline fitting of the original grid values of the DDCS, using a spline function defined in the interval $0.4 \leq k / T_1 < 1$. Interpolation of $DDCS_{Born}$ with respect to θ and T_1 is performed using the same techniques as the mentioned interpolation of the partial-wave DDCS with respect θ and T_1, with only a minor difference during interpolation with respect to T_1: in the case of $DDCS_{Born}$, this is "pure" interpolation (not fitting), because fitting is needed only in the presence of computational uncertainties, which are negligible in the case of $DDCS_{Born}$. The method of fitting SDCS with respect to k / T_1 is exactly the same as the method of fitting DDCS, which was described above (i.e., 20 pre-calculated grid values of Born-approximation SDCS are used for every combination of grid values of Z and $T_1 \geq 1$MeV, etc.).

Uncertainties of the interpolated values of DCS are affected by uncertainties of grid values of the DCS and by uncertainties inherent in any interpolation procedure. The latter type of uncertainty will be further called "interpolation error". It is largest approximately midway between
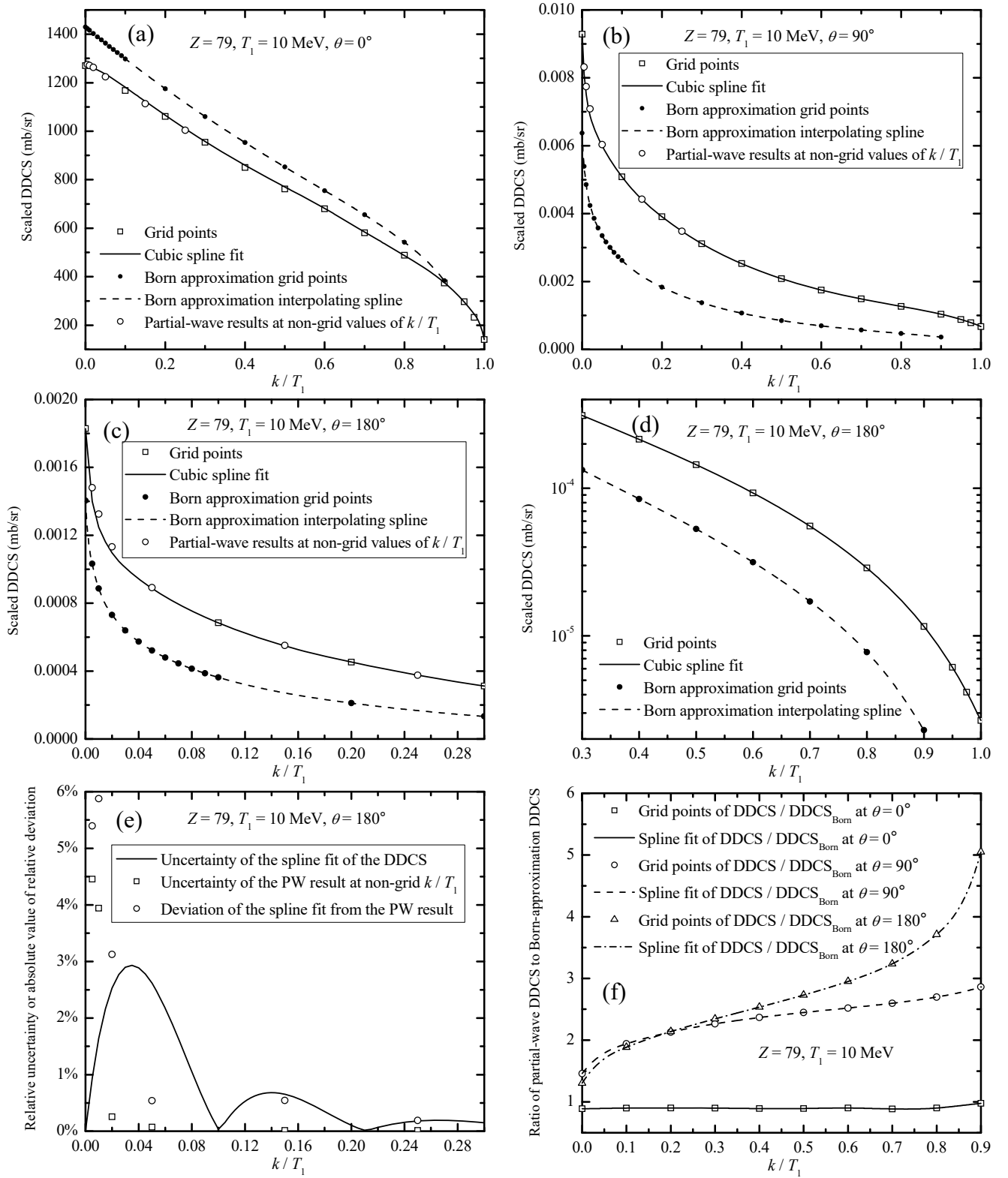
Fig. 2. (a) – (d) Grid points of the dependence of the scaled partial-wave DDCS and the Born-approximation DDCS on k/T_1, the corresponding cubic spline fit of the PW DDCS and cubic spline interpolating function of the Born-approximation DDCS, and the PW DDCS calculated at six non-grid values of k/T_1 (0.005, 0.01, 0.02, 0.05, 0.15, and 0.25), for three values of θ (0°, 90°, and 180°). (e) Estimate of relative uncertainty of the cubic spline fit of the DDCS (solid curve), estimates of relative uncertainties at six non-grid values of k/T_1 (squares), and absolute values of relative deviation of the spline fit from the PW DDCS at the same six values of k/T_1 (circles). (f) Values of the ratio of PW DDCS to Born DDCS at the grid points (scatter plots), and the corresponding cubic spline fits for three values of θ (0°, 90°, and 180°).

grid points. Interpolate_DCS evaluates the interpolation error by redoing the spline fitting (or spline interpolation) with a different set of breakpoints of the spline function and then using the relative difference of the interpolation results as the estimate of the relative interpolation error. After that, it is added in quadrature to the linearly interpolated relative uncertainty of the grid values (which possibly includes the interpolation error of the previous interpolation step), yielding the total relative uncertainty of the current interpolation step. Thus, interpolation errors tend to accumulate if there are multiple spline interpolation steps (in the case discussed, there are two such steps: spline fitting of log(DCS) with respect to log(T_1), and spline fitting of DCS with respect to k / T_1). The solid curve in Fig. 2e shows the total relative uncertainty of the cubic spline function shown in Fig. 2c. In this case, uncertainties of the grid values of the DDCS are relatively small, hence the total uncertainty is mainly the interpolation error, except very close to the grid values of k / T_1. Fig. 2e also shows the absolute values of the relative deviations of the interpolated DDCS from the independently calculated partial-wave DDCS at six non-grid values of k / T_1 (0.005, 0.01, 0.02, 0.05, 0.15, and 0.25). In the case of the two smallest mentioned values of k / T_1 (0.005 and 0.01), those relative deviations (shown by circles in Fig. 2e) are much greater than the total uncertainty, but this is a result of large uncertainty of the PW DDCS (shown by squares in Fig. 2e). I.e., the mentioned two largest deviations are caused by inaccuracy of the PW DDCS, and not by inaccuracy of the spline interpolation. In the case of the remaining four mentioned values of k / T_1 (0.02, 0.05, 0.15, and 0.25), the relative deviations shown in Fig. 2e are either of the same order of magnitude as the total uncertainty or less, as they should be if the estimate of total uncertainty is correct.

3. Overview of the calculation process and the codes included in Interpolate_DCS

The source code of Interpolate_DCS is written in Fortran-90 and consists of the following four files:

1) file "Interpolate_DCS.f90" with the source code of the main program and subroutines,
2) file "Spline_fit.f90" with subroutines for spline fitting and spline interpolation,
3) file "DMINV.FOR" with the code of subroutine DMINV from the IBM System/360 Scientific Subroutine Package (SSP),
4) file "DGELS.f" with the code of subroutine DGELS from SSP.

The latter three files are in subfolder "Spline_fit". The distribution package also includes compiled 64-bit executables for Windows and Linux. The Linux executable is in subfolder "Linux_exe". Both these executable files are named "Interpolate_DCS.exe". The folder "Linux_exe" also contains the file "Compile.sh" with the complete set of Linux shell ("bash") commands that must be entered in order to compile the mentioned executable on Linux.

Each parameter of the calculation process may be specified either on the command line, or in a file (the "parameter file"), using the format "<parameter_name>=<parameter_value>" (there must be no spaces before or after the equality sign). For example, "Z=1" specifies the atomic number of the target atom. There are 90 user-adjustable parameters in total. If a parameter value is not specified on the command line or in the parameter file, then a default value will be used. There are only three parameters that do not have default values: atomic number Z, incident electron energy T_1, and one or more values of photon energy k. Those parameters must be specified by the user. In the simplest case, the command line of Interpolate_DCS looks like this:

```
Interpolate_DCS.exe Z=79 T1=10 k=7
```

In this example, no parameter file would be used, and the program would calculate the SDCS when $Z = 79$, $T_1 = 10$ MeV, and $k = 7$ MeV (the input energy values must be specified in MeV). The results would be written to file "SDCS.txt". In order to calculate the DDCS (in addition to the SDCS), at least one value of the photon emission angle must be specified, for example,

```
Interpolate_DCS.exe Z=79 T1=10 k=7 theta=1
```

In this example, one value of the DDCS corresponding to $Z = 79$, $T_1 = 10$ MeV, $k = 7$ MeV, $\theta = 1°$ would be calculated and written to file "Z=79_T1=1.000E+01MeV_k=7.000E+00MeV.txt". A range of values of k can be specified as follows:

```
Interpolate_DCS.exe Z=79 T1=10 k_min=2 k_max=9.9 nk=80 theta=1
```

5

In this example, values of the DDCS corresponding to 80 equidistant values of *k* from 2 MeV to 9.9 MeV would be calculated and written to file "Z=79_T1=1.000E+01MeV_theta=1.000deg.txt". The set of values of *k* or θ can also be loaded from a file, for example,

```
Interpolate_DCS.exe Z=79 T1=10 k=7 theta_fileName=theta.txt
```

In this example, the program would read the values of θ from file "theta.txt" and write the calculated values of the DDCS to file "Z=79_T1=1.000E+01MeV_k=7.000E+00MeV.txt" (the first line in file "theta.txt" would be assumed to be a header line, and it would be skipped).

If some of the parameters have to be loaded from a parameter file or from several parameter files, then the names of those parameter files must be specified on the command line after the keyword "in=", for example:

```
Interpolate_DCS.exe Z=79 T1=10 in=k_theta.inp in=ExpErr.inp
```

In this example, two parameter files "k_theta.inp" and "ExpErr.inp" would be used. If a parameter value is specified both on the command line and in a parameter file, then the value specified on the command line takes priority (in such a case, a corresponding message is displayed before starting the calculation process). If a parameter is defined in two or more parameter files, then the program quits with an error message. The parameter names are case-sensitive. There must be no more than one parameter per line in a parameter file. One-line comments (starting with the exclamation mark '!' or the forward slash '/'), empty lines, and additional "in=" directives are allowed in a parameter file. If a parameter value is a character string containing '/' or a space, then this string must be enclosed by single quotes (along with the parameter name and the equality sign).

In addition to using individual parameter names, Interpolate_DCS allows using parameter "aliases", which replace the names of two or more related parameters. For example, the alias "k" refers to parameters "k_min" and "k_max". Consequently, specifying "k=7" on the command line or in a parameter file would be equivalent to two directives: "k_min=7" and "k_max=7". For convenience, all aliases together with the corresponding parameter names are listed in Section 6.

4. Descriptions of input parameters of Interpolate_DCS

In this section, names and default values of all parameters of Interpolate_DCS are given, along with short explanation of the meaning of each parameter. The default value is written after the equality sign, which follows the parameter name. Names and values of parameters that have the meaning of character strings (such as the prefix or suffix of a data file name) are enclosed by single quotes. Each parameter name is preceded by its number (the parameter numbers are used only to facilitate references to parameters in this document, and those numbers are different from the parameter numbers defined in the code of Interpolate_DCS).

1. **Z** – atomic number (must be specified by the user). It must be an integer number from 1 to 100.

2. **T1** – kinetic energy of the incident electron (MeV) (must be specified by the user).

3. **'prefix_lib**=../BremsLib_v2.0/' – overall prefix of the input file names (library folder name).

4. **'prefix_DCS**=DDCS/' – prefix of the DDCS input file name (inserted after prefix_lib and before "DDCS").

5. **'prefix_CS**=SDCS/' – prefix of the SDCS input file name (inserted after prefix_lib and before "SDCS").

6. **'suffix_DCS**=' – suffix of the DDCS input file name (inserted after "DDCS").

7. **'suffix_CS**=' – suffix of the SDCS input file name (inserted after "SDCS").

> If prefix_CS ends with the period '.', then suffix_CS must contain the complete SDCS input file name (in this case, the prefixes given by prefix_lib and prefix_CS are not included in the file name).

The next 11 parameters define the spline function used for interpolation or fitting of ln(DDCS) or ln(SDCS) as a function of ln(T_1) when $T_1 \geq$ T1_thr (see also the description of parameter No. 30).

8. **T1_spline_min_DCS**=0.01 – minimum grid value of T_1 (i.e., first breakpoint of a spline) for spline fitting of ln(DDCS) as a function of ln(T_1) when $k > 0$.

9. **T1_spline_max_DCS**=30 – maximum grid value of T_1 (i.e., last breakpoint of a spline) for spline fitting of ln(DDCS) as a function of ln(T_1) when $k > 0$.

10. **T1_spline_min_CS**=0.01 – minimum grid value of T_1 (i.e., first knot of a spline) for spline fitting of ln(SDCS) as a function of ln(T_1) when $k > 0$.

11. **T1_spline_max_CS**=30 – maximum grid value of T_1 (i.e., last knot of a spline) for spline fitting of ln(SDCS) as a function of ln(T_1) when $k > 0$.

12. **T1_spline_min_0_DCS**=0.01 – minimum grid value of T_1 (i.e., first knot of a spline) for spline fitting of ln(DDCS) as a function of ln(T_1) when $k = 0$.

13. **T1_spline_max_0_DCS**=100 – maximum grid value of T_1 (i.e., last knot of a spline) for spline fitting of ln(DDCS) as a function of ln(T_1) when $k = 0$.

14. **T1_spline_min_0_CS**=0.01 – minimum grid value of T_1 (i.e., first knot of a spline) for spline fitting of ln(SDCS) as a function of ln(T_1) when $k = 0$.

15. **T1_spline_max_0_CS**=100 – maximum grid value of T_1 (i.e., last knot of a spline) for spline fitting of ln(SDCS) as a function of ln(T_1) when $k = 0$.

16. **T1_spline**=2 – defines the spline function used for interpolation (0 or 1) or fitting (≥ 2) of the dependence of ln(DDCS) or ln(SDCS) on ln(T_1):

    0 – use the "natural" interpolating spline (zero second derivative at the endpoints),

    1 – use the "not-a-knot" condition for the spline interpolation (continuity of the third derivative at the second and next-to-last grid points),

    ≥ 2 – the average number of grid points between adjacent knots of the spline function used for spline fitting.

17. **T1_spline_test1**=1 – defines the spline function used for "test" spline interpolation or fitting No. 1. The meaning is the same as for parameter "T1_spline" (see above). The test interpolation is performed in order to evaluate the interpolation error, which is determined on the basis of the difference of the spline functions corresponding to different sets of spline breakpoints (see also Section 2). If this parameter is negative, then the test spline function No. 1 will not be used.

18. **T1_spline_test2**=0 – defines the spline function used for "test" spline interpolation or fitting No. 2. The meaning is the same as for parameters "T1_spline" and "T1_spline_test1" (see above). If this parameter is negative, then the test spline function No. 2 will not be used.

The next 11 parameters define the spline function used for interpolation or fitting of ln(DDCS) or ln(SDCS) as a function of ln(T_1) when $T_1 <$ T1_thr (see also the description of parameter No. 30).

19. **T1_spline0_min_DCS**=1e-5 – minimum grid value of T_1 (i.e., first knot of a spline) for spline fitting of ln(DDCS) as a function of ln(T_1) when $k > 0$.

20. **T1_spline0_max_DCS**=0.1 – maximum grid value of T_1 (i.e., last knot of a spline) for spline fitting of ln(DDCS) as a function of ln(T_1) when $k > 0$.

21. **T1_spline0_min_CS**=1e-5 – minimum grid value of T_1 (i.e., first knot of a spline) for spline fitting of ln(SDCS) as a function of ln(T_1) when $k > 0$.

22. **T1_spline0_max_CS**=0.1 – maximum grid value of T_1 (i.e., last knot of a spline) for spline fitting of ln(SDCS) as a function of ln(T_1) when $k > 0$.

23. **T1_spline0_min_0_DCS**=1e-5 – minimum grid value of T_1 (i.e., first knot of a spline) for spline fitting of ln(DDCS) as a function of ln(T_1) when $k = 0$.

24. **T1_spline0_max_0_DCS**=0.1 – maximum grid value of T_1 (i.e., last knot of a spline) for spline fitting of ln(DDCS) as a function of ln(T_1) when $k = 0$.

25. **T1_spline0_min_0_CS**=1e-5 – minimum grid value of T_1 (i.e., first knot of a spline) for spline fitting of ln(SDCS) as a function of ln(T_1) when $k = 0$.

26. **T1_spline0_max_0_CS**=0.1 – maximum grid value of T_1 (i.e., last knot of a spline) for spline fitting of ln(SDCS) as a function of ln(T_1) when $k = 0$.

27. **T1_spline0**=1 – defines the spline function used for interpolation (0 or 1) or fitting (≥ 2) of the dependence of ln(DDCS) or ln(SDCS) on ln(T_1):

    0 – use the "natural" interpolating spline (zero second derivative at the endpoints),

    1 – use the "not-a-knot" condition for the spline interpolation (continuity of the third derivative at the second and next-to-last grid points),

    ≥ 2 – the average number of grid points between adjacent knots of the spline function used for spline fitting.

28. **T1_spline0_test1**=0 – defines the spline function used for "test" spline interpolation or fitting No. 1. The meaning is the same as for parameter "T1_spline0" (see above). The test interpolation is performed in order to evaluate the interpolation error, which is determined on the basis of the difference of the spline functions corresponding to different sets of spline breakpoints (see also Section 2). If this parameter is negative, then the test spline function No. 1 will not be used. If this parameter is negative, then the test spline function No. 1 will not be used.

29. **T1_spline0_test2**=-1 – defines the spline function used for "test" spline interpolation or fitting No. 2. The meaning is the same as for parameters "T1_spline0" and "T1_spline0_test1" (see above). If this parameter is negative, then the test spline function No. 2 will not be used.

30. **T1_thr**=0.03 – the threshold value of T1 (MeV), which determines the choice among two sets of 11 spline-fitting parameters (see above) and the set of knots of k / T_1 to be used (see below).

31. **T1_spline_wt_thr**=0.01 – the threshold value of the relative uncertainty of a grid point value of DDCS or SDCS, which must be exceeded in order to apply an additional weight factor less than 1 to the corresponding term in the sum of squared residuals, which is minimized during the spline fitting of the dependence of ln(DDCS) or ln(SDCS) on ln(T_1). The mentioned factor is in such a case equal to the squared ratio of T1_spline_wt_thr and the mentioned relative uncertainty. If T1_spline_wt_thr = 0, then the mentioned factor is not applied.

32. **k_spline_wt_thr**=0.01 – the threshold value of the relative uncertainty of a grid point value of DDCS or SDCS, which must be exceeded in order to apply an additional weight factor less than 1 to the corresponding term in the sum of squared residuals, which is minimized during the spline fitting of the dependence of DDCS or SDCS (or of the ratio of DDCS or SDCS to the "reference" Born-approximation DDCS or SDCS) on k / T_1 when the number of spline knots is less than the number of grid points by three or more (i.e., when the number of degrees of freedom is greater than zero). The mentioned factor is in such a case equal to the squared ratio of k_spline_wt_thr and the mentioned relative uncertainty. If k_spline_wt_thr = 0, then the mentioned factor is not applied.

The next four parameters define the set of values of k corresponding to the output values of DDCS and SDCS.

33. **k_min**=0 – minimum photon energy (MeV) in the set of equidistant values of k corresponding to the output values of DDCS and SDCS. A negative value of this parameter is interpreted as opposite to the minimum ratio k / T_1.

34. **k_max**=0 – maximum photon energy (MeV) in the set of equidistant values of k corresponding to the output values of DDCS and SDCS. A negative value of this parameter is interpreted as opposite to the maximum ratio k / T_1.

35. **nk**=0 – number of equidistant values of k corresponding to the output values of DDCS and SDCS (if nk = 1, then k = k_min). If nk $\leq$ 0 and k_min is specified by the user, then nk is automatically set to 1, whereas k_max is automatically set equal to k_min. Similarly, if nk $\leq$ 0 and k_max is specified by the user but k_min is not specified, then nk is automatically set to 1, whereas k_min is automatically set equal to k_max.

36. **'k_fileName**=' – name of the file with the list of values of k corresponding to the output values of DDCS and SDCS (will not be used if empty). Negative values are interpreted as opposite to the ratio k / T_1. This file must start with a header line. The final set of values of k is obtained by merging the set of values in the file with the set of equidistant values defined by parameters No. 33 – 35.

The next three parameters are used only when T_1 < T1_thr (see also the description of parameter No. 30).

37. **'k_T1_knots0_fileName**=' – name of the file with the subset of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of DDCS or SDCS as a function of k / T_1 at a fixed value of T_1 < T1_thr. If this file name is an empty string, then linear interpolation of DDCS or SDCS with respect to k / T_1 will be performed instead.

38. **'k_T1_knots0_fn_test1**=k_T1_knots0_test1.txt' – name of the file with the "test" subset No. 1 of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of DDCS or SDCS as a function of k / T_1 at a fixed value of T_1 < T1_thr. If this file name is an empty string, then the test spline interpolation No. 1 of DDCS or SDCS with respect to k / T_1 will not be performed.

39. **'k_T1_knots0_fn_test2**=k_T1_knots0_test2.txt' – name of the file with the "test" subset No. 2 of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of DDCS or SDCS as a function of k / T_1 at a fixed value of T_1 < T1_thr. If this file name is an empty string, then the test spline interpolation No. 2 of DDCS or SDCS with respect to k / T_1 will not be performed.

The next six parameters are used only when $T_1 \geq$ T1_thr (see also the description of parameter No. 30). Parameters No. 40 – 42 are used when T_1 < T1_min_useRef, and parameters No. 43 – 45 are used when $T_1 \geq$ T1_min_useRef (see also the description of parameter No. 46).

40. **'k_T1_knots1_fileName**=k_T1_knots1.txt' – name of the file with the subset of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of DDCS or SDCS as a function of k / T_1 at a fixed value of T_1 < T1_min_useRef. If this file name is an empty string, then linear interpolation of DDCS or SDCS with respect to k / T_1 will be performed instead.

41. **'k_T1_knots1_fn_test1**=k_T1_knots1_test1.txt' – name of the file with the "test" subset No. 1 of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of DDCS or SDCS as a function of k / T_1 at a fixed value of T_1 < T1_min_useRef. If this file name is an empty string, then the test spline interpolation No. 1 of DDCS or SDCS with respect to k / T_1 will not be performed.

42. **'k_T1_knots1_fn_test2**=k_T1_knots1_test2.txt' – name of the file with the "test" subset No. 2 of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of DDCS or SDCS as a function of k / T_1 at a fixed value of T_1 < T1_min_useRef. If this file name is an empty string, then the test spline interpolation No. 2 of DDCS or SDCS with respect to k / T_1 will not be performed.

43. **'k_T1_knots_fileName**=k_T1_knots.txt' – name of the file with the subset of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of DDCS or SDCS as a function of k / T_1 at a fixed value of $T_1 \geq$ T1_min_useRef. If this file name is an empty string, then linear interpolation of DDCS or SDCS with respect to k / T_1 will be performed instead.

44. **'k_T1_knots_fn_test1**=k_T1_knots_test1.txt' – name of the file with the "test" subset No. 1 of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of DDCS or SDCS as a function of k / T_1 at a fixed value of $T_1 \geq$ T1_min_useRef. If this file name is an empty string, then the test spline interpolation No. 1 of DDCS or SDCS with respect to k / T_1 will not be performed.

45. **'k_T1_knots_fn_test2**=k_T1_knots_test2.txt' – name of the file with the "test" subset No. 2 of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of DDCS or SDCS as a function of k / T_1 at a fixed value of $T_1 \geq$ T1_min_useRef. If this file name is an empty string, then the test spline interpolation No. 2 of DDCS or SDCS with respect to k / T_1 will not be performed.

46. **T1_min_useRef**=1 – the starting point of the interval of T_1 where the ratio DDCS / DDCS_ref or SDCS / SDCS_ref is spline-fitted as a function of k / T_1 (in addition to spline fitting of DDCS or SDCS as a function of k / T_1, which is controlled by parameters No. 43 – 45). Notation "DDCS_ref" or "SDCS_ref" will be further used to denote the "reference" DDCS or SDCS, which is by default calculated according to the screened Born approximation (with the nuclear form factor and the Elwert factor).

The next eleven parameters are used only when $T_1 \geq$ T1_min_useRef.

47. **'prefix_ref_DCS**=DDCS/Born_appr/' – prefix of the reference DDCS input file name (inserted after the prefix defined by parameter No. 3 "prefix_lib" and before "DDCS").

48. **'prefix_ref_CS**=SDCS/Born_appr/' – prefix of the reference SDCS input file name (inserted after the prefix defined by parameter No. 3 "prefix_lib" and before "SDCS").

49. **'suffix_ref_DCS**=_Born' – suffix of the reference DDCS input file name (inserted after "DDCS").

50. **'suffix_ref_CS**=_Born' – suffix of the reference SDCS input file name (inserted after "SDCS").

51. **T1_spl_min_ref**=1 – minimum grid value of T_1 (i.e., first knot of a spline) for spline interpolation of ln(DDCS_ref) or ln(SDCS_ref) as a function of ln(T_1).

52. **T1_spl_max_ref**=30 – maximum grid value of T_1 (i.e., last knot of a spline) for spline interpolation of ln(DDCS_ref) or ln(SDCS_ref) as a function of ln(T_1).

53. **k_T1_max_useRef**=0.7 – the endpoint of the interval of k / T_1 where the final DDCS is calculated by spline-fitting of DDCS / DDCS_ref or SDCS / SDCS_ref as a function of k / T_1 and then multiplying the result by DDCS_ref or SDCS_ref (provided that $T_1 \geq$ T1_min_useRef). The starting value of this interval is always equal to 0.

54. **k_T1_spl_max_ref**=0.9 – the endpoint of the interval of k / T_1 used for constructing the optimal spline functions for the dependences of DDCS_ref, SDCS_ref, DDCS / DDCS_ref and SDCS / SDCS_ref on k / T_1. The starting value of this interval is always equal to 0.

55. **'k_T1_knots_ref_ratio_fileName**=k_T1_knots_ref_ratio.txt' – name of the file with the subset of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of the ratio DDCS / DDCS_ref or SDCS / SDCS_ref as a function of k / T_1 at a fixed value of T_1. If this file name is an empty string, then linear interpolation of the ratio DDCS / DDCS_ref or SDCS / SDCS_ref with respect to k / T_1 will be performed instead.

56. **'k_T1_knots_ref_ratio_fn_test1**=k_T1_knots_ref_ratio_test1.txt' – name of the file with the "test" subset No. 1 of grid values of k / T_1 corresponding to knots of the spline function for

10

spline fitting of the ratio DDCS / DDCS_ref or SDCS / SDCS_ref as a function of k / T_1 at a fixed value of T_1. If this file name is an empty string, then the test spline interpolation No. 1 of the ratio DDCS / DDCS_ref or SDCS / SDCS_ref with respect to k / T_1 will not be performed.

57. **'k_T1_knots_ref_ratio_fn_test2**=k_T1_knots_ref_ratio_test2.txt' – name of the file with the "test" subset No. 2 of grid values of k / T_1 corresponding to knots of the spline function for spline fitting of the ratio DDCS / DDCS_ref or SDCS / SDCS_ref as a function of k / T_1 at a fixed value of T_1. If this file name is an empty string, then the test spline interpolation No. 2 of the ratio DDCS / DDCS_ref or SDCS / SDCS_ref with respect to k / T_1 will not be performed.

58. **DDCS_exp_corrFactor**=0 – positive when experimental values of DDCS and their relative uncertainties are available, and indicates the factor to be applied in order to convert units of the experimental DDCS to cm^2/sr/MeV.

59. **SDCS_exp_corrFactor**=0 – positive when experimental values of SDCS and their relative uncertainties are available, and indicates the factor to be applied in order to convert units of the experimental SDCS to cm^2/MeV.

The experimental DDCS or SDCS and their relative uncertainties must be given as additional entries after each value of k or θ in the file defined by parameter No. 36 "k_fileName" (in this case, parameter nk must be zero) or No. 77 "theta_fileName" (ntheta=0). If both DDCS and SDCS are present, then the experimental value of DDCS must precede the experimental value of SDCS. The experimental uncertainty of DDCS or SDCS must be specified immediately after the corresponding experimental value of DDCS or SDCS. If both nk and ntheta are zero, then the experimental values must be in the file where the number of non-empty lines is greater than 1. If both files have one non-empty line, then the experimental values may be in any of them.

The next seven parameters define the relative experimental uncertainties of DDCS.

60. **exp_err_available_DCS**=1 – non-zero when a column with relative experimental uncertainties of DDCS is present in the file defined by parameter No. 36 "k_fileName" or No. 77 "theta_fileName". This column must be immediately after the column with experimental DDCS.

61. **exp_err_ignore_DCS**=0 – non-zero when the column with relative experimental uncertainties of DDCS must be ignored if present in the file defined by parameter No. 36 "k_fileName" or No. 77 "theta_fileName".

62. **exp_err_calculate_DCS**=0 – non-zero when experimental uncertainties of DDCS must be calculated using the next four parameters. If the uncertainties are also specified in the mentioned file, then the calculated uncertainties will be added in quadrature to those from the file.

The next four parameters define up to four components of the relative experimental uncertainty of DDCS, which are added up in quadrature.

63. **exp_err0_DCS**=0 – a constant component of the relative experimental uncertainty of DDCS.

64 – 66. **'exp_err_bp_file1_DCS**=', **'exp_err_bp_file2_DCS**=', **'exp_err_bp_file3_DCS**=' – names of three files, each defining a two-dimensional grid containing breakpoints of the relative experimental uncertainty of DDCS with respect to k / T_1 and θ. If a file name is the empty string, then it will not be used. Each of those files must start with a line containing the number of breakpoints of θ. The corresponding values of θ must be listed in ascending order in the second line (if there is only one breakpoint of θ, then it may be set equal to any number). Each subsequent line must start with a value of a breakpoint of k / T_1 (these breakpoints must be listed in ascending order). The remaining entries on the same line must be equal to the corresponding values of the relative uncertainty for each breakpoint of θ. The

final experimental uncertainty of DDCS is calculated by linear interpolation of the squared uncertainty with respect to both k / T_1 and θ, followed by calculation of the square root.

The next seven parameters define the relative experimental uncertainties of SDCS.

67. **exp_err_available_CS**=1 – non-zero when a column with relative experimental uncertainties of SDCS is present in the file defined by parameter No. 36 "k_fileName" or No. 77 "theta_fileName". This column must be immediately after the column with experimental SDCS.

68. **exp_err_ignore_CS**=0 – non-zero when the column with relative experimental uncertainties of SDCS must be ignored if present in the file defined by parameter No. 36 "k_fileName" or No. 77 "theta_fileName".

69. **exp_err_calculate_CS**=0 – non-zero when experimental uncertainties of SDCS must be calculated using the next four parameters. If the uncertainties are also specified in the mentioned file, then the calculated uncertainties will be added in quadrature to those from the file.

The next four parameters define up to four components of the relative experimental uncertainty of SDCS, which are added up in quadrature.

70. **exp_err0_CS**=0 – a constant component of the relative experimental uncertainty of SDCS.

71 – 73. **'exp_err_bp_file1_CS**=', **'exp_err_bp_file2_CS**=', **'exp_err_bp_file3_CS**=' – names of three files, each containing breakpoints of the relative experimental uncertainty of SDCS with respect to k / T_1. If a file name is the empty string, then it will not be used. Format of each of these files is the same as in the case of DDCS (see the descriptions of parameters No. 64 – 66). The first two lines are ignored, because SDCS can be interpolated only with respect to k / T_1 (but not with respect to θ). Each line starting with the third one must begin with a value of a breakpoint of k / T_1 (in ascending order). The second entry on the same line must be equal to the corresponding value of the relative uncertainty of SDCS. If there are more entries on the same line, then they will be ignored. The final experimental uncertainty of SDCS is calculated by linear interpolation of the squared uncertainty with respect to k / T_1, followed by calculation of the square root.

The next four parameters define the set of values of θ corresponding to the output values of DDCS and SDCS.

74. **theta_min**=0 – minimum angle (degrees) in the set of equidistant values of θ corresponding to the output values of DDCS

75. **theta_max**=0 – maximum angle (degrees) in the set of equidistant values of θ corresponding to the output values of DDCS

76. **ntheta**=0 – number of equidistant values of θ corresponding to the output values of DDCS (if ntheta = 1, then θ = theta_min) If ntheta ≤ 0 and theta_min is specified by the user, then ntheta is automatically set to 1, whereas theta_max is automatically set equal to theta_min. Similarly, if ntheta ≤ 0 and theta_max is specified by the user but theta_min is not specified, then ntheta is automatically set to 1, whereas theta_min is automatically set equal to theta_max.

77. **'theta_fileName**=' – name of the file with the list of values of θ corresponding to the output values of DDCS (will not be used if empty). This file must start with a header line. The final set of values of θ is obtained by merging the set of values in the file with the set of equidistant values defined by parameters No. 74 – 76. However, only the values of θ in the file are used for numerical angular integration of the DDCS when parameter int_DCS is non-zero (see the description of parameter No. 81), or for numerical integration of the shape

function when parameter normalize_SF is non-zero (see the description of parameter No. 84).

Note: The total number of values of k and the total number of values of θ cannot both be greater than 1. That is to say, only one of them can be greater than 1.

78. **use_point_nucleus**=0 – non-zero when the point-nucleus approximation is required. Otherwise, the finite-nucleus approximation will be used (if the corresponding data are available). If the point-nucleus approximation is required, then the program will check if the DDCS data files have an additional column with values of the ratio of the DDCS corresponding to the point-nucleus and finite-nucleus approximations. If this column is present, then it is assumed that the second column contains the values of the finite-nucleus DDCS, and the point-nucleus DDCS will be obtained by multiplication of the mentioned ratio with the value of the finite-nucleus DDCS. If the mentioned additional column is absent, then the value of the DDCS in the second column will be processed regardless of the value of this parameter.

79. **SDCS_pn_fn_ratio_available**=1 – non-zero when the SDCS data files have additional columns with values of the ratio of the SDCS corresponding to the point-nucleus and finite-nucleus approximations.

The next 11 parameters define the format of the output data of Interpolate_DCS.

80. **output_k_T1_first**=0 – non-zero if the first column of the DDCS output file must contain the values of the ratio k / T_1, and the second column must contain the values of k (otherwise, these two columns are interchanged).

81. **int_DCS**=0 – non-zero if the SDCS must be calculated by integration of the DDCS with respect to solid angle. In order to enable the mentioned angular integration, the following three additional conditions must be satisfied simultaneously: **(a)** a file with values of θ must be specified using parameter No. 77 ("theta_fileName"), **(b)** the first and last values of θ in the mentioned file must be equal to 0° and 180°, respectively, **(c)** the largest interval between adjacent values of θ in the mentioned file must not exceed 1°. If int_DCS has been set to a non-zero value and at least one of the mentioned additional conditions is not satisfied, then the program will exit with an error message. If int_DCS is not specified by the user and all three additional conditions are satisfied, then int_DCS will be automatically reset to 1.

Note: If prefix_CS (parameter No. 5) does not end with the period '.', or suffix_CS (parameter No. 7) is not an empty string, then ntheta and int_DCS may be zero, and theta_fileName may be an empty string.

82. **Brems_DDCS_lib_format**=0 – non-zero if format of the DDCS output file must be the same as format of DDCS data files in BremsLib v2.0.

83. **SF**=0 – non-zero for an additional entry equal to the value of the shape function, or 0 if it is not needed. The shape function (SF) is defined as follows:

$$\mathrm{SF}(\theta) = \frac{\mathrm{DDCS}(\theta)}{\int \mathrm{DDCS} \cdot \mathrm{d}\Omega} = \frac{\mathrm{DDCS}(\theta)}{2\pi \int\limits_{0}^{\pi} \mathrm{DDCS}(\theta) \sin\theta \, \mathrm{d}\theta} . \qquad (3.1)$$

The integral in the denominator of Eq. (3.1) is calculated only when parameter "int_DCS" (No. 81) is non-zero. Since this integral is either equal or very close to the estimate of the SDCS, it is replaced with the latter estimate when int_DCS = 0. Furthermore, Eq. (3.1) (or its approximate form, where the denominator is replaced with the estimate of the SDCS) is applied only at the grid values of k / T_1, after performing the spline fitting of ln(DDCS) and ln(SDCS) with respect to ln(T_1) (see also Section 2). Thus, the grid values of the DDCS are replaced by the grid values of SF. If the "reference" DDCS (i.e., the Born-approximation DDCS) is used, then the same replacement is also applied to the grid values of DDCS_ref,

resulting in grid values of reference SF, which will be further denoted SF_ref. After that, the grid values of SF and SF_ref are used for interpolation with respect to k / T_1 in exactly the same manner as the grid values of DDCS and DDCS_ref (see Section 2), yielding interpolated values of the SF.

84. **normalize_SF**=1 – if the three parameters normalize_SF, SF and int_DCS are simultaneously non-zero, then values of the shape function (SF) will be "normalized" by dividing them by the integral of the SF with respect to the solid angle of the photon emission (the result of this operation is given by Eq. (3.1), where "DDCS" is replaced by "SF"). This may be needed because the SF, which is calculated as described above (see the description of parameter No. 83), is in general not normalized (i.e., its angular integral is not exactly equal to 1), since Eq. (3.1) is applied to the *grid* values of the DDCS rather than to the final values of the DDCS. However, even without this normalization, the angular integral of the SF is very close to 1 (deviation of the mentioned integral from 1 is typically less than 0.001 in absolute value).

85. **Schiff**=0 – non-zero for an additional entry calculated according the Schiff formula, or 0 if it is not needed. The expression of the DDCS according to the Schiff formula is

$$\text{DDCS}_{\text{Schiff}} = \frac{2}{\pi} \frac{Z^2 r_0^2}{137 k} E_1^2 \left\{ \frac{16 y^2 E_2}{(y^2+1)^4 E_1} - \frac{(E_1+E_2)^2}{(y^2+1)^2 E_1^2} + \left[\frac{E_1^2 + E_2^2}{(y^2+1)^2 E_1^2} - \frac{4 y^2 E_2}{(y^2+1)^4 E_1} \right] \ln M(y) \right\},$$

(3.2)

$$y = E_1 \theta, \qquad \frac{1}{M(y)} = \left(\frac{k}{2 E_1 E_2} \right)^2 + \left(\frac{Z^{1/3}}{111(y^2+1)} \right)^2,$$

where E_1 and E_2 are the total relativistic energies of the incident and final electron, respectively, and r_0 is the classical radius of the electron (if the relativistic units are used, then $r_0 = \alpha$). The Schiff formula is known as an easy-to-calculate substitute for the exact screened Born approximation. If the Born approximation condition (2.1) is satisfied, then the prediction of the Schiff formula at a sufficiently small value of θ is typically very close to the Born-approximation result.

86. **ln_Y0**=0 – non-zero when the DDCS and SDCS must be replaced with ln(DDCS) and ln(SDCS), respectively, during spline fitting with respect to k / T_1 at a fixed value of $T_1 <$ T1_thr (at greater values of T_1, this parameter has no effect, and the logarithm is never used).

87. **verbose**=0 – non-zero if the values of k, θ and the breakpoint values of k / T_1 loaded from files must be listed.

88. **'suffix_out_DCS**=' – suffix of the name of the output file with the DDCS data.

89. **'suffix_out_CS**=' – suffix of the name of the output file with the SDCS data.

90. **overwrite**=1 – non-zero if an existing output file with the DDCS data must be overwritten.

5. Output data of Interpolate_DCS

Interpolate_DCS creates or updates up to two human-readable ASCII files. Their names end with extension ".txt". Each file starts with a header line, which is followed by multiple columns of numbers of fixed width. One of the mentioned two files contains the values of the interpolated DDCS for the user-specified set of values of k or θ, and the other file contains the values of the interpolated SDCS for the user-specified set of values of k. Both these files are created in the current folder. The name of the DDCS output file begins with the values of Z, T_1 and k or θ, followed by the suffix defined by parameter No. 88 ("suffix_out_DCS"). Examples of the name of the DDCS output file are given in Section 3. The name of the SDCS output file begins with the string "SDCS", followed by the suffix defined by parameter No. 89 ("suffix_out_CS"). Each run of Interpolate_DCS ends by overwriting the DDCS output file and by appending a line to the SDCS output file for every value of k.

14

It is possible to create or update only one of the mentioned two files. In order to update only the SDCS output file, neither the set of equidistant values of θ (defined by parameters No. 74 – 76), nor the input file with the values of θ (defined by parameter No. 77) must be specified by the user. In order to create only the DDCS output file, parameter "int_DCS" must be set to zero, and the input SDCS grid data file must not be used (this is achieved by setting parameter "prefix_CS" to the period '.', and parameter "suffix_CS" to an empty string).

The format of the DDCS output file depends on whether it contains the values of the DDCS for a set of values k at a fixed θ, or the values of the DDCS for a set of values of θ at a fixed k. In the former case, the first and second columns contain the values of k and k / T_1, respectively (these two columns may be interchanged, depending on the value of parameter "output_k_T1_first"). In the other case, the first column (with the header "theta(deg)") contains the values of θ (in degrees). The remaining columns have the same meaning in both cases. The explanation of the meaning of each column, which is presented below, pertains to the first case (with fixed θ). In order to apply it to the second case (when k is fixed), the numbers of all columns starting from column No. 3 must be reduced by 1. Each line written to the DDCS output file contains the following entries:

(1) Energy of the bremsstrahlung photon in MeV (column header "**k(MeV)**"),

(2) ratio of the previous entry to energy of the incident electron ("**k/T1**"),

(3) scaled theoretical DDCS (the scaling factor is k / Z^2) in units of mb/sr ("**DDCS_scaled(mb/sr)**"),

(4) non-scaled theoretical DDCS in units of cm^2/sr/MeV ("**DDCS(cm^2/sr/MeV)**"), or the same DDCS multiplied by photon energy k in units of cm^2/sr ("**DDCS*k(cm^2/sr)**") if the first value of k is equal to 0 (this column is present only when parameter "Brems_DDCS_lib_format" is zero),

(5) relative computational uncertainty of the theoretical DDCS ("**relErr**").

The next five columns are present only when parameter No. 58 ("DDCS_exp_corrFactor") is positive and experimental values of the DDCS are available (see the paragraph after the description of parameter No. 59):

(6) Experimental value of the scaled DDCS ("**DDCS_exp_scaled(mb/sr)**"),

(7) non-scaled experimental DDCS ("**DDCS_exp(cm^2/sr/MeV)**"), or the same DDCS multiplied by photon energy k in units of cm^2/sr ("**DDCS_exp*k(cm^2/sr)**") if the first value of k is equal to 0,

(8) relative uncertainty of the experimental DDCS, or zero if experimental uncertainties are not available ("**exp_relErr**"),

(9) relative deviation of the theoretical DDCS from the experimental DDCS ("**relDiff**"),

(10) ratio of the relative deviation given in the previous column to the absolute uncertainty of the same relative deviation ("**diffErrRatio**"). The latter absolute uncertainty is calculated by multiplying the ratio of the theoretical DDCS to the experimental DDCS by the relative uncertainty of the same ratio. The latter relative uncertainty is calculated by adding up the relative uncertainties of the two DDCS in quadrature.

The next two columns are present only when calculation of the shape function has been requested (option "SF=1"):

(11) Theoretical shape function ("**ShapeFn**"),

(12) relative uncertainty of the theoretical shape function ("**SF_relErr**").

The next column is present only when calculation of the Schiff DDCS has been requested (option "Schiff=1"):

(13) Value of the DDCS calculated according the Schiff formula, Eq. (3.2) (column header "**DDCS_Schiff**").

Each line written to the SDCS output file contains the following 19 entries:

(1)   Atomic number Z of the target atom (column header "**Z**"),

(2)   kinetic energy T_1 of the incident electron in MeV ("**T1(MeV)**"),

(3)   energy k of the bremsstrahlung photon in MeV ("**k(MeV)**"),

(4)   ratio k / T_1 ("**k/T1**"),

(5)   scaled theoretical SDCS (the scaling factor is k / Z^2) in units of mb ("**SDCS_scaled(mb)**"),

(6)   non-scaled theoretical SDCS in units of cm^2/MeV, or the same SDCS multiplied by photon energy k in units of cm^2 if the first value of k in a given sequence of values is equal to 0 (column header "**SDCS(cm^2/MeV)**"),

(7)   relative computational uncertainty of the theoretical SDCS ("**SDCS_relErr**"),

The next five entries are non-zero only when parameter No. 59 ("SDCS_exp_corrFactor") is positive and experimental values of the SDCS are available (see the paragraph after the description of parameter No. 59):

(8)   Experimental value of the scaled SDCS in units of mb ("**SDCS_exp_scaled(mb)**"),

(9)   non-scaled experimental SDCS in units of cm^2/MeV, or the same SDCS multiplied by photon energy k in units of cm^2/sr if the first value of k in a given sequence of values is equal to 0 (column "("**SDCS_exp(cm^2/MeV)**")

(10)   relative uncertainty of the experimental SDCS, or zero if experimental uncertainties are not available ("**exp_relErr**"),

(11)   relative deviation of the theoretical SDCS from the experimental SDCS ("**expRelDiff**"),

(12)   ratio of the mentioned relative deviation (given in the previous column) to the absolute uncertainty of the same relative deviation ("**diffErrRatio**"). The latter absolute uncertainty is calculated by multiplying the ratio of the theoretical SDCS to the experimental SDCS by the relative uncertainty of the same ratio. The latter relative uncertainty is calculated by adding the relative uncertainties of the two SDCS in quadrature.

The next six entries are non-zero only when parameter No. 81 ("int_DCS") is non-zero:

(13)   Value of the scaled angular integral of the final theoretical DDCS (denominator in Eq. (3.1)) in units of mb, calculated using the 10th-order Newton-Cotes formula (column header "**DDCS_int_scaled**"),

(14)   non-scaled angular integral of the final theoretical DDCS in units of cm^2/MeV, calculated using the 10th-order Newton-Cotes formula, or the same integral multiplied by photon energy k in units of cm^2 if the first value of k in a given sequence of values is equal to 0 (column header "**DDCS_int(cm^2/MeV)**"),

(15)   relative deviation of the angular integral of the final theoretical DDCS (calculated using the 10th-order Newton-Cotes formula) from the final estimate of the theoretical SDCS ("**rel_diff**"),

(16)   Value of the scaled angular integral of the final theoretical DDCS (denominator in Eq. (3.1)) in units of mb, calculated using the trapezoidal rule (column header "**DDCS_int2_scaled**"),

(17)   non-scaled angular integral of the final theoretical DDCS in units of cm^2/MeV, calculated using the trapezoidal rule, or the same integral multiplied by photon energy k in units of cm^2 if the first value of k in a given sequence of values is equal to 0 (column header "**DDCS_int2(cm^2/MeV)**"),

(18) relative deviation of the angular integral of the final theoretical DDCS calculated using the trapezoidal rule from the similar integral calculated using the 10th-order Newton-Cotes formula ("**rel_diff2**"),

The last entry is non-zero only when parameters No. 81 and No. 83 (int_DCS and SF) are non-zero:

(19) angular integral of the final theoretical shape function (before normalization), calculated using the 10th-order Newton-Cotes formula ("**ShapeFn_integral**").

6. List of parameter aliases used in Interpolate_DCS

In the code of Interpolate_DCS, some parameters are grouped into small groups consisting of 2 – 4 parameters, all of which can be assigned a value using a single directive, where the parameter name is replaced by its "alias". For example, the alias "theta" is associated with parameters "theta_min" and "theta_max". Consequently, specifying "theta=2.5" on the command line or in the parameter file would be equivalent to two directives: "theta_min=2.5" and "theta_min=2.5". There are 37 aliases in total. The list of all aliases and the associated parameter names is presented in the following table.

No.	Alias	I parameter	II parameter	III parameter	IV parameter
1	k	k_min	k_max		
2	theta	theta_min	theta_max		
3	T1_spline_min	T1_spline_min_DCS	T1_spline_min_CS		
4	T1_spline_max	T1_spline_max_DCS	T1_spline_max_CS		
5	T1_spline_min_0	T1_spline_min_0_DCS	T1_spline_min_0_CS		
6	T1_spline_max_0	T1_spline_max_0_DCS	T1_spline_max_0_CS		
7	T1_spl_min	T1_spline_min_DCS	T1_spline_min_CS	T1_spline_min_0_DCS	T1_spline_min_0_CS
8	T1_spl_max	T1_spline_max_DCS	T1_spline_max_CS	T1_spline_max_0_DCS	T1_spline_max_0_CS
9	T1_spline_test	T1_spline_test1	T1_spline_test2		
10	T1_spline0_min	T1_spline0_min_DCS	T1_spline0_min_CS		
11	T1_spline0_max	T1_spline0_max_DCS	T1_spline0_max_CS		
12	T1_spline0_min_0	T1_spline0_min_0_DCS	T1_spline0_min_0_CS		
13	T1_spline0_max_0	T1_spline0_max_0_DCS	T1_spline0_max_0_CS		
14	T1_spl0_min	T1_spline0_min_DCS	T1_spline0_min_CS	T1_spline0_min_0_DCS	T1_spline0_min_0_CS
15	T1_spl0_max	T1_spline0_max_DCS	T1_spline0_max_CS	T1_spline0_max_0_DCS	T1_spline0_max_0_CS
16	T1_spline0_test	T1_spline0_test1	T1_spline0_test2		
17	T1_min	T1_spline_min_DCS	T1_spline_min_CS	T1_spline0_min_DCS	T1_spline0_min_CS
18	T1_max	T1_spline_max_DCS	T1_spline_max_CS	T1_spline0_max_DCS	T1_spline0_max_CS
19	T1_min_0	T1_spline_min_0_DCS	T1_spline_min_0_CS	T1_spline0_max_DCS	T1_spline0_max_CS
20	T1_max_0	T1_spline_max_0_DCS	T1_spline_max_0_CS	T1_spline0_max_0_DCS	T1_spline0_max_0_CS
21	T1_test	T1_spline_test1	T1_spline_test2	T1_spline0_test1	T1_spline0_test2
22	k_T1_knots0_fn_test	k_T1_knots0_fn_test1	k_T1_knots0_fn_test2		
23	k_T1_knots1_fn_test	k_T1_knots1_fn_test1	k_T1_knots1_fn_test2		
24	k_T1_knots_fn_test	k_T1_knots_fn_test1	k_T1_knots_fn_test2		
25	k_T1_knots_fn_ref_ratio_test	k_T1_knots_ref_ratio_fn_test1	k_T1_knots_ref_ratio_fn_test2		
26	exp_err_available	exp_err_available_DCS	exp_err_available_CS		
27	exp_err_ignore	exp_err_ignore_DCS	exp_err_ignore_CS		
28	exp_err_calculate	exp_err_calculate_DCS	exp_err_calculate_CS		
29	exp_err0	exp_err0_DCS	exp_err0_CS		
30	exp_err_bp_file1	exp_err_bp_file1_DCS	exp_err_bp_file1_CS		
31	exp_err_bp_file2	exp_err_bp_file2_DCS	exp_err_bp_file2_CS		
32	exp_err_bp_file3	exp_err_bp_file3_DCS	exp_err_bp_file3_CS		
33	prefix	prefix_CS	prefix_DCS		
34	suffix	suffix_CS	suffix_DCS		
35	prefix_ref	prefix_ref_DCS	prefix_ref_CS		
36	suffix_ref	suffix_ref_DCS	suffix_ref_CS		
37	suffix_out	suffix_out_DCS	suffix_out_CS		

7. Sample files included in the distribution package of Interpolate_DCS

In addition to the code files mentioned in Section 3, the installation folder of Interpolate_DCS contains eleven files with breakpoint values of the ratio k / T_1 for cubic spline fitting under various conditions. Those files have the default names (starting with "k_T1_knots") mentioned in the descriptions of parameters No. 38 – 45 and No. 55 – 57. There is also file "theta.txt" with the complete set of grid values of θ corresponding to the energy range $4\text{ MeV} \leq T_1 \leq 30\text{ MeV}$ (at $T_1 \leq 3\text{ MeV}$, the grid values of θ are a subset of values in this file). The sample parameter file "Default_parameters.inp" contains the default values of all parameters of Interpolate_DCS (the same default values are also mentioned in the descriptions of parameters in Section 4).

Subfolder "Samples" contains the files needed to calculate the DDCS corresponding to the physical parameters used in the measurements of [1] and [2], as well as four output files created by Interpolate_DCS. The calculations were performed for $Z = 79$, $T_1 = 2.5$ MeV, $\theta = 10°$ using the data of [1], and for $Z = 79$, $T_1 = 9.66$ MeV, $\theta = 0°$ using the data of [2]. The main parameter values are in two parameter files "Rester_and_Dance_1967_Fig16_Z=79_T1=2.5MeV_theta=10deg.inp" and "Starfelt_and_Koch_1956_Fig9a_Z=79_T1=9.66MeV_theta=0deg.inp", respectively. The experimental values of k and DDCS are in files "k_79_2.5MeV_10deg.txt" and "k_79_9.66MeV_0deg.txt", respectively. The experimental uncertainties were calculated according to the "breakpoint" values of relative experimental errors defined in the mentioned two works (those data were taken into account using appropriate values of parameters No. 60 – 66). Additional information about the experimental errors is provided by comments in the six *.inp files whose names start with "Calculate_exp_err". The same calculations can be redone using the Windows batch file "Comparison_with_experiment.bat".

Subfolder "Linux_exe/Samples" contains the same sample files as subfolder "Samples" described above, but the mentioned Windows batch file is replaced with the file "Comparison_with_experiment.sh" containing two Linux "bash" commands that must be entered in order to redo the same calculations on Linux. The four output files in this subfolder were created by running the mentioned two commands on Ubuntu running on the Linux subsystem for Windows.

References

[1] D. H. Rester and W. E. Dance, "Bremsstrahlung cross-section measurements at incident electron energies of 1.0, 1.7, and 2.5 MeV," *Phys. Rev.*, vol. 161, pp. 85–93, 1967.

[2] N. Starfelt and H. W. Koch, "Differential cross-section measurements of thin-target bremsstrahlung produced by 2.7- to 9.7-Mev electrons," *Phys. Rev.*, vol. 102, pp. 1598–1612, 1956.