BremsLib v2.0

Library of double- and single differential cross sections of electron-atom bremsstrahlung
at electron energies from 10 eV to 30 MeV

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BremsLib v2.0 is a library of double- and single differential cross sections of electron-atom bremsstrahlung. It is a major update of BremsLib v1.0.5, which was published in 2019. BremsLib v2.0 contains the data for 86300 combinations of three physical parameters: atomic number Z, incident electron energy T_1, and bremsstrahlung photon energy k. All values of Z from 1 to 100 are represented. The range of variation of T_1 is from 10 eV to 30 MeV for $k \neq 0$, or from 10 eV to 100 MeV for $k = 0$. The range of variation of k / T_1 is from 0 to 0.9999. The library data were calculated by the relativistic partial-wave method. The target atom is described by Kohn-Sham interaction potential. Radial dependence of positive charge density inside the nucleus is modeled by the Fermi distribution.

In comparison with BremsLib v1.0.5, the high-energy endpoint of the incident electron energy range has been increased from 3 MeV to 30 MeV, all the previously-published data have been recalculated, and an additional grid value of the radiated photon energy (equal to 97.5 % of the incident electron energy) has been inserted at all values of the incident electron energy. Although the changes in the values of the previously-published cross sections are insignificant, their uncertainties have been made more reliable. In the soft-photon limit, those uncertainties have been in some cases reduced by several orders of magnitude because of a more efficient calculation method based on the Low theorem, which has been applied in the case of zero photon energy at all values of the incident electron energy up to 100 MeV.

The library data corresponding to $k \neq 0$ were generated using the code BREMS. The current version of BREMS (v1.5.8.8) is included in the BremsLib v2.0 distribution package (this version of BREMS would produce identical results to BREMS v1.5.8.7, which was used for generation of library data). The data corresponding to $k = 0$ were generated using a different code, which has not been published yet.

The distribution package of BremsLib v2.0 is split in two .ZIP files, which contain three folders:

- main library data folder "BremsLib_v2.0" with the values of scaled double- and single differential cross sections of bremsstrahlung corresponding to 86300 combinations of the physical parameters Z, T_1 and k / T_1,
- folder "Interpolate_DCS" with the code and documentation of the program "Interpolate_DCS", which can be used for data retrieval and interpolation,
- folder "Brems" with the code and documentation of the program BREMS (v1.5.8.8), which was used for generation of the library data at $k \neq 0$.

The first .ZIP archive contains the library data for $1 \leq Z \leq 50$, and the latter two folders. The second .ZIP archive contains the library data for $51 \leq Z \leq 100$. Both .ZIP files must be unpacked to the same folder. This PDF file is included in both .ZIP archives. Consequently, the user will be prompted to either overwrite it or skip it when unpacking the second .ZIP archive.

The library data files are in subfolders "DDCS" and "SDCS" of the main library folder "BremsLib_v2.0". All data files are human-readable ASCII files with name extension ".txt". The

data in all files are arranged as columns of numbers of fixed width, preceded by a line with column headers. Subfolder "DDCS" contains grid values and computational uncertainties of scaled double differential cross sections (DDCS) of electron-atom bremsstrahlung (with the scaling factor k / Z^2) in units of mb/sr, whereas subfolder "SDCS" contains grid values and computational uncertainties of scaled single differential cross sections (SDCS) in units of mb. The values of DDCS for each combination of the three physical parameters Z, T_1 and k are stored in a separate file, whose name has the format "DDCS_Z_T.TE±XX_k.kkkE±YY.txt", where "Z" is the atomic number Z, "T.TE±XX" is the kinetic energy T_1 of the incident electron (MeV) rounded to 2 significant digits in scientific notation, and "k.kkkE±YY" is the energy k of the bremsstrahlung photon (MeV) rounded to 4 significant digits in scientific notation ("E±XX" and "E±YY" are the decimal exponents). For example, file "DDCS_79_3.0E+01_2.400E+01.txt" corresponds to $Z = 79$, $T_1 = 30$ MeV, and $k = 24$ MeV. All values of Z from 1 to 100 are represented in the library. The "grid" values of T_1 and k / T_1 are the following:

- $T_1 = (1, 1.2, 1.5, 2, 2.5, 3, 4, 5, 6, 8) \times 10^n$ 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 $k = 0$),

- $k / T_1 = 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 0.95, 0.975, 1$. The last value of k / T_1 is actually slightly less than 1: (a) if $T_1 \le 5$ keV, then it is equal to 0.99, (b) if 5 keV $< T_1 \le 500$ keV, then it is equal to $1 - (50 \text{ eV} / T_1)$, which means that $T_2 = 50$ eV, (c) if $T_1 > 500$ keV, then the last grid value of k / T_1 is equal to 0.9999.

Thus, the total number of combinations of Z, T_1 and k is equal to 86300. This is the number of DDCS data files.

Each DDCS data file contains three or four columns of numbers (the first line contains headers of the columns). The first three entries in each line have the meaning of the photon emission angle θ in degrees, the corresponding value of scaled DDCS, and its relative computational uncertainty, respectively. The fourth entry is present only when the ratio of the reduced wavelength of the incident electron $\lambdabar_1$ to the mean radius of the nucleus R_n is less than 40, and this entry has the meaning of the ratio of the point-nucleus DDCS to the finite-nucleus DDCS. In such a case, the second entry in each line has the meaning of the *finite*-nucleus DDCS, and the point-nucleus DDCS can be obtained by multiplying the second and fourth entries. If $\lambdabar_1 / R_n > 40$, then the second entry has the meaning of the *point*-nucleus DDCS, and the fourth entry is missing (in this case, the finite-nucleus DDCS would not be significantly different from the point-nucleus DDCS).

Each SDCS data file contains all grid values of SDCS for a particular value of Z. The name of each SDCS data file has the format "SDCS_Z.txt", where "Z" is the atomic number. For example, "SDCS_79.txt" corresponds to $Z = 79$. Thus, there are 100 SDCS data files. The values of SDCS in each file are stored as a two-dimensional grid, with different lines corresponding to different values of T_1, which are listed in the first column (values of T_1 are in units of MeV). The subsequent entries in each line are equal to the SDCS, its relative computational uncertainty, and the ratio of the point-nucleus SDCS to the finite-nucleus SDCS for each of the mentioned 13 values of k / T_1. Thus, there are forty entries in each line. If the mentioned ratio (i.e., the third entry in a triplet of entries) is exactly equal to 1, this means that the preceding value of the SDCS (i.e., the first entry in a triplet of entries) was calculated using the point-nucleus approximation. Otherwise, the preceding value of the SDCS was calculated using the Fermi distribution of proton density. The range of values of T_1 in each SDCS data file is 10 eV $\le T_1 \le 300$ MeV. At $T_1 > 30$ MeV, some data are missing (the missing data are indicated by zeroes). There are no missing data at $T_1 \le 30$ MeV. The values of SDCS corresponding to $k / T_1 \ge 0.1$ and $T_1 \ge 50$ MeV were calculated by integrating the analytical triple differential cross section (TDCS) based on the Sommerfeld-Maue wave functions with the next-to-leading-order correction, and including the screening correction of the DDCS (in this case, the finite size of the nucleus is taken into account in the expression of the

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mentioned screening correction, whereas the analytical expression of the unscreened TDCS corresponds to the point-nucleus approximation).

Folder "SDCS" has subfolder "DDCS_int" with values of the angular integral of the scaled DDCS, calculated using the 10th order Newton-Cotes formula. The files in this subfolder are named "DDCS_int_Z.txt", where "Z" is the atomic number, and their format is similar to the format of the SDCS files. The main difference is in the meaning of the second entry for each value of k/T_1: in the "DDCS_int" files, it is equal to the relative deviation of the angular integral of the DDCS from the corresponding value of the SDCS. In addition, the maximum value of T_1 in the "DDCS_int" files is equal to 100 MeV, and the only available (i.e., non-zero) entries are those that correspond to existing DDCS data files for the same pair of T_1 and k/T_1. The values of the mentioned angular integral can be used to calculate shape functions corresponding to each pair of grid values of T_1 and k/T_1: the shape function is defined as the ratio of the DDCS to its angular integral.

Folders "DDCS" and "SDCS" have subfolder "Born_appr" with the grid values of the Born-approximation DDCS or SDCS, which is needed for cubic spline interpolation with respect to k/T_1. The names of the corresponding data files have the characters "_Born" inserted after "DDCS" or "SDCS". The grid values of T_1 and k/T_1 corresponding to the Born approximation are the following:

- T_1 = (1, 1.2, 1.5, 2, 2.5, 3, 4, 5, 6, 8, 10, 12, 15, 20, 25, 30) MeV,
- k/T_1 = 0, 0.005, 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9.

Format of the data in those files is similar to format of the files in the parent folder, with the only difference in the absence of columns with relative computational uncertainties. Thus, "DDCS_Born" files have three or two columns (depending on whether the finite-nucleus or point-nucleus approximation is used), whereas "SDCS_Born" files have 41 columns (two entries for each of 20 grid values of k/T_1) and 17 lines (header line and 16 lines corresponding to 16 grid values of T_1).