BREMS – a program for calculating spectra and angular distributions of bremsstrahlung at electron energies less than 3 MeV

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User‘s Manual

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1. Introduction

BREMS is a set of Fortran-90 codes for calculating the energy spectra and angular distributions of photons emitted due to atomic-field bremsstrahlung when fast electrons interact with neutral atoms. The approximate energy range of the incident electron is from 10 eV to 3 MeV. BREMS was written by Andrius Poškus (Vilnius University, Faculty of Physics, Institute of Chemical Physics). BREMS is distributed under the GNU General Public License 3.

BREMS can be downloaded from http://web.vu.lt/ff/a.poskus/brems/ or http://www.apsoftware.org/BREMS/.

1.1. The theoretical basis

The theory and some of the numerical methods used in BREMS were developed in [1], [2]. The atom is described as a static spherically symmetrical charge distribution of infinite mass. The elementary process of bremsstrahlung is described as a one-electron transition in the field of the neutral atom with a point-like nucleus. The atom is described by a central potential. The electron continuum wave functions are calculated by solving the Dirac equation with one of several possible types of the interaction potential. The wave functions are expanded in partial wave series and the radial integrals are calculated numerically. The relativistic partial-wave formulation is currently the best available theory for calculating the cross sections of unpolarized atomic-field bremsstrahlung.

BREMS allows selection of one of three central potentials:

1) the point-Coulomb potential (the unscreened nucleus),
2) the Thomas-Fermi-Csavinszky (TFC) potential [1], [3],
3) the Kohn-Sham (KS) potential [4], [5] in tabular format.

An arbitrary radial potential function $V(r)$ of the form $\bar{V}(r)/r$, where $\bar{V}(r)$ is any smooth negative-valued monotonous function that decays exponentially in the limit $r \to \infty$ and is equal to $-\alpha Z$ at $r = 0$, may be specified by the user in tabular format (either by replacing the data files used with the choice No. 3 above, or by adding an option to use another set of data files in the code).

The relativistic units will be used throughout this text, i.e., the reduced Planck's constant, the speed of light and the electron's rest mass will be assumed to be equal to 1, and the elementary charge squared will be assumed to be equal to the fine-structure constant α. The partial waves constituting the initial and final states of the electron will be labeled by the quantum number κ, which is defined in terms of the orbital angular momentum (quantum number l) and the total angular momentum (quantum number j) as follows [6]:

$$\kappa = \begin{cases} l & \text{for } j = l - \frac{1}{2}, \\ -l-1 & \text{for } j = l + \frac{1}{2}. \end{cases} \tag{1.1}$$

The incident and final electron states will be labeled with the subscripts "1" and "2", respectively. Energies and momenta will be denoted as follows:

E – total relativistic energy of the electron,
T – kinetic energy of the electron,
$p = |\boldsymbol{p}|$ – modulus of the momentum of the electron ($\boldsymbol{p}$ is the momentum vector),
$k = |\boldsymbol{k}|$ – energy of the bremsstrahlung photon and modulus of its momentum vector $\boldsymbol{k}$.

The coordinate system is centered on the atomic nucleus, with the z-axis along $\boldsymbol{k}$, y-axis along $\boldsymbol{k} \times \boldsymbol{p}_1$, and x-axis in the $(\boldsymbol{k}, \boldsymbol{p}_1)$ plane. The angles defining the direction of emission of the bremsstrahlung photon will be denoted as follows:

θ – angle between the directions of the emitted photon and the incident electron,
ϕ – azimuth angle,
Ω_k – solid angle.

The expressions of the "doubly differential" cross section (proportional to the joint probability density of the direction and energy of bremsstrahlung photons) and of the photon energy spectrum (the "singly differential" cross section, defined as the integral of the doubly differential cross

section with respect to the solid angle of photon emission), which were derived in [1], [7], are presented below:

$$\frac{k}{Z^2}\frac{\mathrm{d}\sigma}{\mathrm{d}k\mathrm{d}\Omega_k} \equiv \sigma(k,\theta) = \lambda_0 \sum_{\kappa_1\bar{\kappa}_1\kappa_2} (-1)^{l_1+\bar{l}_1} \cos(\delta_{\kappa_1} - \delta_{\bar{\kappa}_1}) \sum_{m\equiv|m_2|} [A_+^+(m)\bar{A}_+^+(m) + A_+^-(m)\bar{A}_+^-(m) + A_-^+(m)\bar{A}_-^+(m) + A_-^-(m)\bar{A}_-^-(m)] \tag{1.2}$$

(in mb/sr),

$$\frac{k}{Z^2}\frac{\mathrm{d}\sigma}{\mathrm{d}k} \equiv \sigma(k) = \lambda_0 \sum_{\kappa_2,\kappa_1,m\equiv|m_2|} \{[R^+_{\kappa_2\kappa_1}(m)]^2 + [R^-_{\kappa_2\kappa_1}(m)]^2\} \tag{1.3}$$

(in mb), where the set of values of the indices $\bar{l}_1$ and $\bar{\kappa}_1$ is the same as that of l_1 and κ_1, respectively, m_2 is the magnetic quantum number corresponding to the partial wave κ_2,

$$\lambda_0 = [(3.86144)^2 \times 10^5]\frac{32\alpha}{Z^2 p_1} E_1 E_2 p_2 k^2, \tag{1.4}$$

$$A_\pm^+(m) = C^\pm_{\kappa_1,m-1} y_{l_1,m-1\mp\frac{1}{2}}(\theta) R^+_{\kappa_2\kappa_1}(m), \tag{1.5}$$

$$A_\pm^-(m) = C^\pm_{\kappa_1,m+1} y_{l_1,m+1\mp\frac{1}{2}}(\theta) R^-_{\kappa_2\kappa_1}(m), \tag{1.6}$$

$C^\pm_{\kappa,m}$ is the Clebsch-Gordan coefficient:

$$C^\pm_{\kappa,m} = C(l\,\tfrac{1}{2}\,j; m\mp\tfrac{1}{2}, \pm\tfrac{1}{2}), \tag{1.7}$$

$y_{lm}(\theta)$ is the preexponential factor of the spherical harmonic $Y_{lm}(\theta, \phi)$:

$$Y_{lm}(\theta,\phi) = y_{lm}(\theta)\mathrm{e}^{\mathrm{i}m\phi}, \tag{1.8}$$

the bar over $A_\pm^\pm$ corresponds to the replacement of κ_1 and l_1 with $\bar{\kappa}_1$ and $\bar{l}_1$ in (1.5) and (1.6),

$$R^\pm_{\kappa_2\kappa_1}(m) = \sum_{n=1}^{2} Q_n^\pm(m) \sum_l P_n^\pm(m) S_n, \tag{1.9}$$

and δ_κ is the electron phase shift for the partial wave κ. In equation (1.9) the index l runs from $|l_2' - l_1|$ to $(l_2' + l_1)$ in steps of 2 for $n = 1$, and from $|l_2 - l_1'|$ to $(l_2 + l_1')$ in steps of 2 for $n = 2$. Here

$$l' = l + \eta_\kappa, \qquad \eta_\kappa = -\kappa/|\kappa|, \tag{1.10}$$

$$Q_1^\pm(m) = \eta_{\kappa_2}(-1)^{m\mp1/2}[(2l_2'+1)(2l_1+1)]^{1/2} C^\pm_{-\kappa_2,m} C^\mp_{\kappa_1,m\mp1}, \tag{1.11}$$

$$Q_2^\pm(m) = -\eta_{\kappa_1}(-1)^{m\mp1/2}[(2l_2+1)(2l_1'+1)]^{1/2} C^\pm_{\kappa_2,m} C^\mp_{-\kappa_1,m\mp1}, \tag{1.12}$$

$$P_1^\pm(m) = (-1)^{(l_2'+l_1+l)/2} T(l_2', l_1, l; m\mp\tfrac{1}{2}), \tag{1.13a}$$

$$P_2^\pm(m) = (-1)^{(l_2+l_1'+l)/2} T(l_2, l_1', l; m\mp\tfrac{1}{2}), \tag{1.13b}$$

$$T(l_2,l_1,l;m) = (2l+1)\begin{pmatrix} l_2 & l_1 & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & l_1 & l \\ -m & m & 0 \end{pmatrix}, \tag{1.14}$$

where the last two factors are the Wigner 3j coefficients, and

$$S_1 = \int_0^\infty j_l(kr) g_{\kappa_1}(r) f_{\kappa_2}(r)\mathrm{d}r, \tag{1.15a}$$

$$S_2 = \int_0^\infty j_l(kr) g_{\kappa_2}(r) f_{\kappa_1}(r)\mathrm{d}r. \tag{1.15b}$$

In equations (1.15a,b), j_l is the spherical Bessel function of the first kind, order l, and the functions g_κ and f_κ are defined as the radial continuum wave functions multiplied by r. Those functions satisfy the coupled radial Dirac equations

$$\frac{\mathrm{d}g_\kappa}{\mathrm{d}r} = [E + 1 - V(r)] f_\kappa(r) - \frac{\kappa g_\kappa(r)}{r}, \tag{1.16a}$$

$$\frac{\mathrm{d}f_\kappa}{\mathrm{d}r} = -[E - 1 - V(r)] g_\kappa(r) + \frac{\kappa f_\kappa(r)}{r}, \tag{1.16b}$$

where V is the central potential used to describe the target atom. The ratio of the screened and unscreened potentials is called the screening factor. It will be denoted $\tilde{V}(r)$:

$$\tilde{V}(r) \equiv \frac{V(r)}{-Z\alpha / r}. \tag{1.17}$$

In the case of a neutral atom, $\tilde{V}(r)$ tends to zero when $r \to \infty$.

If r is sufficiently large, the following asymptotic expressions may be used to approximate the solution of (1.16a,b) [1]:

$$\begin{aligned} g_\kappa(r) &= r\sqrt{\frac{E+1}{2E}} A_\kappa [\cos\bar{\delta}_\kappa j_\kappa(pr) - \sin\bar{\delta}_\kappa y_\kappa(pr)], \\ f_\kappa(r) &= r\sqrt{\frac{E-1}{2E}} A_\kappa [\cos\bar{\delta}_\kappa j_{\kappa-1}(pr) - \sin\bar{\delta}_\kappa y_{\kappa-1}(pr)], \end{aligned} \tag{1.18}$$

where $\bar{\delta}_\kappa$ is the phase shift and y_κ is the spherical Bessel function of the second kind, order κ (this notation differs from the notation of the spherical harmonic y_{lm} by the number of subscripts). The wave functions are normalized by setting $A_\kappa = 1$. Those expressions define the phase-shifted free-field solution of the Dirac equation for the case of screening factors that tend to zero when $r \to \infty$. The phase shift $\bar{\delta}_\kappa$, which is used in (1.18), is related to the phase shift δ_κ, which appears in (1.2), as follows [1]:

$$\delta_\kappa = \bar{\delta}_\kappa + (l-\kappa)\tfrac{1}{2}\pi = \begin{cases} \bar{\delta}_\kappa & \text{if } \kappa > 0, \\ \bar{\delta}_\kappa - (\kappa + \tfrac{1}{2})\pi & \text{if } \kappa < 0. \end{cases} \tag{1.19}$$

In the limit $k \to 0$, the values of the S integrals (1.15) grow indefinitely as $1/k$, whereas the factor λ_0 (1.4) approaches zero due to the presence of k^2 in the expression of λ_0. As a result, an indeterminate form of the type $0 \times \infty$ appears in (1.2) and (1.3). Consequently, the definition of the factor λ_0 (1.4) in the case $k = 0$ must be modified by removing the factor k^2, and the definition of the R factors (1.9) must be modified by replacing S_1 and S_2 with $\lim_{k\to 0}(kS_1)$ and $\lim_{k\to 0}(kS_2)$, respectively. In order to calculate the mentioned limits, only the values of the electron energy $E = E_1 = E_2$ and the phase shifts corresponding to that energy are needed, and numerical integration is not required (an analytical formula is used instead). The expression of the mentioned limits is the following [8]:

$$\begin{aligned} \lim_{k\to 0}(kS_1) = -\lim_{k\to 0}(kS_2) = \frac{\sqrt{\pi}}{2^{l+3}} \frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})} \frac{1}{E^2} \left(1 - \frac{1}{E^2}\right)^{\frac{l}{2}} F\left(\frac{l+2}{2}, \frac{l+1}{2}; l+\frac{3}{2}; 1-\frac{1}{E^2}\right) \\ \times \cos\left(\bar{\delta}_{\kappa 1} - \bar{\delta}_{\kappa 2} + (\kappa_2 - \kappa_1 + l)\frac{\pi}{2}\right), \end{aligned} \tag{1.20}$$

where F is the hypergeometric function.

In order to apply Eq. (1.18) in the case of the point-Coulomb field (i.e., unscreened nucleus), one should add a logarithmic term depending on r to the definition of the phase shift $\bar{\delta}_\kappa$ [6]:

$$\bar{\delta}_\kappa = \tilde{\bar{\delta}}_\kappa + \nu \ln 2pr, \tag{1.21}$$

where

$$\nu \equiv \frac{Z\alpha E}{p}, \tag{1.22}$$

and $\tilde{\bar{\delta}}_\kappa$ is a constant whose analytical expression can be obtained, for example, from Eq. (5.75) in [6]. This expression is reproduced below in a form consistent with Eq. (1.18):

$$\tilde{\bar{\delta}}_\kappa = -\arg(\Gamma(\gamma + \mathrm{i}\nu)) + \eta - \tfrac{1}{2}\pi\gamma + (\kappa+1)\frac{\pi}{2}, \tag{1.23}$$

$$\gamma \equiv (\kappa^2 - \alpha^2 Z^2)^{1/2}, \tag{1.24}$$

$$e^{2i\eta} = -\frac{\kappa - i\nu/E}{\gamma + i\nu}. \tag{1.25}$$

The left-hand sides of (1.2) and (1.3) will be further referred to as the "scaled" differential cross sections (due to the presence of the scaling factor k / Z^2).

1.2. The numerical methods

When $k \neq 0$, the process of calculating the S integrals (1.15) is the most time-consuming part of the calculation. By default, the system (1.16) of ordinary differential equations (ODEs) is solved by expanding the functions g_κ and f_κ in powers of the radial coordinate r at discrete values of r (the power-series coefficients are calculated using the recurrence relations derived from the coupled Dirac equations (1.16a,b) and from the power-series expansion of the screening factor (1.17), similarly to the approach applied in [9], [10], [11]). This system is solved simultaneously for the entire range of values of κ_1 and κ_2 specified by the user (i.e., multiple systems of ODEs corresponding to both values of E and all values of κ are solved simultaneously). If $k \neq 0$, then the S integrals (1.15) are calculated (i.e., incremented in predefined steps of r) for the user-specified range of values of κ_1, κ_2 and l simultaneously with the process of solving the ODEs. The solutions of (1.16) are periodically compared with the asymptotic form (1.18). As proposed in [2], the range of validity of the asymptotic expressions (1.18) can be extended to smaller values of r by assuming that A_κ and $\overline{\delta}_\kappa$ are not constants, but are functions of r instead, tending to constant values at $r \to \infty$ if $|V(r)|$ decreases faster than $1 / r$. These functions have a well-defined form, making it possible to determine the limiting values of A_κ and $\overline{\delta}_\kappa$ without excessive computation time, which would be needed for numerical integration of the system of equations (1.16a,b) to large values of r, where A_κ and $\overline{\delta}_\kappa$ become practically constant. In addition, the assumption that $\overline{\delta}_\kappa$ is a function of r makes it possible to use (1.18) in the case of unscreened point-Coulomb potential, too, by choosing an appropriate form of $\overline{\delta}_\kappa(r)$ (see (1.21)). Both A_κ and $\overline{\delta}_\kappa$ include a constant term and an oscillating term with the oscillation period equal to π / p and the oscillation amplitude tending to zero with increasing r [2] (the average value of the oscillating term is zero). In addition, $\overline{\delta}_\kappa$ includes a monotonously increasing term Q, which is called the "phase correction integral" [2]:

$$\overline{\delta}_\kappa = \tilde{\delta}_\kappa + Q(r), \tag{1.26}$$

where

$$Q(r) = \begin{cases} \nu \ln 2pr & \text{for point-Coulomb field,} \\ -\nu \int_r^\infty \dfrac{\tilde{V}(w)}{w} \mathrm{d}w & \text{for screened fields.} \end{cases} \tag{1.27}$$

Further on, notation $\tilde{\delta}_\kappa$ will be used to mean the average value of the first term in (1.26), i.e., its value at large r, where the oscillation amplitude has decayed to zero (for screened potentials, thus defined $\tilde{\delta}_\kappa$ is equal to the limiting value of $\overline{\delta}_\kappa$, because in this case $\lim_{r\to\infty} Q(r) = 0$). Similarly, notation A_κ will be used to mean the constant term in the oscillating factor $A_\kappa(r)$ in (1.18), i.e., the average value of that factor. When it is determined that the asymptotic form has been attained for a particular combination of values of E and κ (i.e., when the range of variation of the estimates of A_κ and $\tilde{\delta}_\kappa$ over the last 10 "test" points becomes less than the predefined tolerances), the value of $\tilde{\delta}_\kappa$ is stored in the array of phase shifts, the corresponding wave function is normalized by multiplying it (and the S integrals using it) by $1 / A_\kappa$, and the program switches from the numerical solution algorithm to the expressions (1.18) for calculation of the corresponding wave function (the factor A_κ cancels out, because the wave function is multiplied by $1 / A_\kappa$). The algorithm used for calculating the spherical Bessel functions in (1.18) depends on the value of their argument (pr). When $pr \leq 5000$, the spherical Bessel functions are estimated using the algorithms based on backward

recursion (for j_l) or forward recursion (for y_l), which are stable [12], [13]. At argument values greater than 5000, the explicit formulas (1.30a,b) are used.

The integrals are calculated using the 10th order Newton-Cotes (NC) formula (as in [1]). The default initial step size of the NC integration is $\Delta r_{\mathrm{NC}} = \min(0.1/p_1, 0.1)$. This step size is based on a trade-off between accuracy and performance (the indicated NC integration step size is approximately the same as in [1], where it was $\pi/(32p_1)$). It may be modified by the user. A decrease of the step size would make the numerical integration more accurate, but also proportionally longer. As reported in [1], variation of the NC integration step from $\pi/(128p_1)$ to $\pi/(16p_1)$ caused fluctuation of the results by $O(0.1\%)$ for $\sigma(k)$, $O(1\%)$ for $\sigma(k, \theta)$ with small and large photon angles, and $O(0.1\%)$ for intermediate photon angles (here, "$O(x)$" means the order of x).

The first part of the integration ends after all wave functions attain the asymptotic form (1.18) and (in the case of screened interaction potentials) after the absolute values of both phase correction integrals Q (corresponding to energies E_1 and E_2) become less than the predefined small value (10^{-8} by default). It is also possible to end the first part of the integration at a user-specified value of $r = r_0$. In the case of the point-Coulomb field, $Q(r)$ does not have a limiting value. This is one of the reasons why the point-Coulomb interaction potential usually has to be "truncated", i.e., set to zero for $r > R_{\mathrm{a}}$. A judicious choice of the truncation radius R_{a} may cause a significant decrease of the processing time without a significant effect on the accuracy of the results (not only in the case of the point-Coulomb potential, but also in the case of screened potentials). If $r_0 \geq R_{\mathrm{a}}$, then the iterative phase matching described above becomes unnecessary: if $r \geq R_{\mathrm{a}}$, the expressions (1.18) are exact and the values of A_κ and $\bar{\delta}_\kappa$ do not oscillate, hence they are determined from the values of g_κ and f_κ at $r = R_{\mathrm{a}}$. However, in some cases the asymptotic form (1.18) can be reached at a value of r less than R_{a}. Consequently, BREMS applies the method of iterative phase matching in the region of space where $V \neq 0$ regardless of whether the interaction potential is truncated or not. In the case of a truncated potential, the phase correction integral in (1.26) has to be calculated as follows:

$$Q(r)\big|_{r<R_{\mathrm{a}}} = \begin{cases} \nu \ln \dfrac{r}{R_{\mathrm{a}}} & \text{for truncated point-Coulomb field,} \\ -\nu \displaystyle\int_r^{R_{\mathrm{a}}} \frac{\tilde{V}(w)}{w}\,\mathrm{d}w & \text{for truncated screened fields,} \end{cases} \tag{1.28}$$

and $Q(r) \equiv 0$ when $r \geq R_{\mathrm{a}}$. [The second expression of (1.27) is obtained by taking the limit $R_{\mathrm{a}} \to \infty$ in the second expression of (1.28). Conversely, the exact point-Coulomb phase correction integral, which is given by the first expression of (1.27), cannot be obtained by taking the limit $R_{\mathrm{a}} \to \infty$ in the first expression of (1.28). If R_{a} is very large (such that the contribution of the region $r > R_{\mathrm{a}}$ to the interaction cross section is negligible), then the replacement of (1.27) with (1.28) in the case of the point-Coulomb potential shows up only as a constant term $\nu \ln(2pR_{\mathrm{a}})$ added to the phase shifts of all partial waves corresponding to a given energy of the electron. A change of all phase shifts by adding a constant term does not alter the physical state of the electron, hence the values of the cross sections calculated using the truncated point-Coulomb potential in the limit $R_{\mathrm{a}} \to \infty$ are the same as the values calculated using the exact point-Coulomb potential.]

In addition to the mentioned method of the power-series solution, two other (more conventional) methods are optionally available for solving the system of first-order ODEs (1.16): the Hamming's fourth-order modified predictor-corrector (P-C) method [14, p. 95–109], [15], and the method based on the Runge-Kutta formula pair (7,8), except in the vicinity of $r = 0$, where the power-series solution (based on the Taylor series expansion of the screening factor $\tilde{V}(r)$) is always applied. The method of the power-series solution at small r is similar to the method used in [2] and [1]. However, the default method of the iterative solution of the system of ODEs (1.16a,b) at larger values of r, which is implemented in BREMS, is different from the method used in [2] and [1], where the fourth-order Runge-Kutta method was preferred in the case of the interaction potentials

defined in tabular format (such as the Kohn-Sham potential, whose expression is given in Section 7).

All three mentioned methods of solving the system of ODEs (1.16a,b) are essentially equivalent in terms of accuracy, but the default method (based on the power-series expansion of the wave function) is usually faster than the other two methods, because it is specifically tailored for solving the system of ODEs (1.16). The Runge-Kutta method is the least efficient of the mentioned methods, because the P-C methods for solving the systems of ODEs are in general more efficient than the Runge-Kutta methods in terms of the balance between speed and accuracy [16], and the Hamming's method in particular was demonstrated to be superior to the other popular P-C methods (such as the Adams P-C method) [17]. Testing has shown that in the case of the exact (not truncated) point-Coulomb field the phase shifts calculated using BREMS converge to the exact phase shifts given by (1.23), whereas the normalization factors A_κ converge to their exact value (it is equal to 1 due to the choice of the initial values of $r^{-\gamma}g$ and $r^{-\gamma}f$, which are finite at $r = 0$, for the solution of the system of ODEs (1.16a,b) in BREMS).

The result of the first part of the integration is a set of the initial parts of S integrals (1.15), i.e., the values of the integrals from 0 to a certain value r_0. Further on, those integrals will be called "numerical integrals" in order to distinguish them from the second part (integration from r_0 to ∞), which is based on the analytical expressions presented below.

The integration from r_0 to ∞ relies on the assumption that the coefficients $\cos\bar{\delta}_\kappa$ and $\sin\bar{\delta}_\kappa$ in (1.18) are constant, i.e., that the phase correction integrals (1.27) are zero. This means that the interaction potential is either "truncated" at $r = R_a \le r_0$ (i.e., that $V(r) \equiv 0$ at $r > r_0$), or at least negligibly small at $r > r_0$. Then each of the integrals from r_0 to ∞ is equal to a linear combination of four integrals of this general form:

$$S_{11} \equiv \int_{r_0}^{\infty} j_l(kr) j_{N_1}(p_1 r) j_{N_2}(p_2 r) r^2 \mathrm{d}r\,,\ S_{12} \equiv \int_{r_0}^{\infty} j_l(kr) j_{N_1}(p_1 r) y_{N_2}(p_2 r) r^2 \mathrm{d}r\,,$$
$$S_{21} \equiv \int_{r_0}^{\infty} j_l(kr) y_{N_1}(p_1 r) j_{N_2}(p_2 r) r^2 \mathrm{d}r\,,\ S_{22} \equiv \int_{r_0}^{\infty} j_l(kr) y_{N_1}(p_1 r) y_{N_2}(p_2 r) r^2 \mathrm{d}r\,. \tag{1.29}$$

The mentioned linear combinations are obtained after substituting (1.18) into the definition of the S integrals (1.15a,b) with the lower bound replaced by r_0. The spherical Bessel functions of negative orders, which appear in (1.18) when $\kappa < 0$, are expressed via the spherical Bessel functions of non-negative orders N_1 and N_2 by making use of the "reflection identities" [18, Eq. 10.47.3 and Eq. 10.47.4]. In order to calculate the integrals (1.29), the three spherical Bessel functions in the integrand are replaced by their explicit expressions in terms of powers of $1/r$. The explicit formulas for calculating the spherical Bessel functions of non-negative order are given below (see also [18, Eq. 10.49.1, Eq. 10.49.2 and Eq. 10.49.4]):

$$j_l(z) = \sum_{n=0}^{l} \sin(z - \tfrac{1}{2}(l-n)\pi) \frac{a_n(l+\frac{1}{2})}{z^{n+1}}, \tag{1.30a}$$

$$y_l(z) = -\sum_{n=0}^{l} \cos(z - \tfrac{1}{2}(l-n)\pi) \frac{a_n(l+\frac{1}{2})}{z^{n+1}}, \tag{1.30b}$$

where

$$a_n(l+\tfrac{1}{2}) = \begin{cases} \dfrac{(l+n)!}{2^n n!(l-n)!}, & n = 0,1,...,l, \\ 0, & n = l+1, l+2,... \end{cases} = \begin{cases} 1, & n = 0, \\ \dfrac{(l-n+1)\cdot...\cdot(l+n)}{2^n n!}, & n = 1,...,l, \\ 0, & n = l+1, l+2,... \end{cases} \tag{1.31}$$

After replacing the spherical Bessel functions in (1.29) by the corresponding explicit expressions (1.30a,b), each of the integrals (1.29) is expressed as a sum of such terms:

$$\pm\frac{1}{4}a_{n_1}(N_1+\tfrac{1}{2})a_{n_2}(N_2+\tfrac{1}{2})a_{n_3}(l+\tfrac{1}{2})p_1^{-n_1-1}p_2^{-n_2-1}k^{-n_3-1}\int_{r_0}^{\infty}\frac{\sin p'r}{r^{n'}}\mathrm{d}r = CI_1(p'r_0,n') \tag{1.32a}$$

or

$$\pm\frac{1}{4}a_{n_1}(N_1+\tfrac{1}{2})a_{n_2}(N_2+\tfrac{1}{2})a_{n_3}(l+\tfrac{1}{2})p_1^{-n_1-1}p_2^{-n_2-1}k^{-n_3-1}\int_{r_0}^{\infty}\frac{\cos p'r}{r^{n'}}\mathrm{d}r = CI_2(p'r_0,n'), \tag{1.32b}$$

where p' is one of the four values

$$p' \equiv p_1 \pm p_2 \pm k \tag{1.33}$$

(the sign "±" in (1.33) is not correlated with the sign "±" in (1.32a,b)),

$$n' \equiv n_1 + n_2 + n_3 + 1, \tag{1.34}$$

$$C \equiv \pm\frac{1}{4}a_{n_1}(N_1+\tfrac{1}{2})a_{n_2}(N_2+\tfrac{1}{2})a_{n_3}(l+\tfrac{1}{2})p_1^{-n_1-1}p_2^{-n_2-1}k^{-n_3-1}p'^{n'-1}, \tag{1.35}$$

and $I_{1,2}$ are the integrals defined below:

$$I_1(p'r_0,n') \equiv \int_{p'r_0}^{\infty}\frac{\sin z}{z^{n'}}\mathrm{d}z, \tag{1.36a}$$

$$I_2(p'r_0,n') \equiv \int_{p'r_0}^{\infty}\frac{\cos z}{z^{n'}}\mathrm{d}z. \tag{1.36b}$$

Each of the terms (1.32a,b) is a result of multiplying r^2 and three factors proportional to $\sin(z)/z^n$ or $\cos(z)/z^n$, where $z = p_{1,2}r$ or kr, $n = n_{1,2}$ or n_3 respectively, the sign "±" in (1.32a,b) and (1.35) appears due to eliminating the term $-\frac{1}{2}(l-n)\pi$ from the argument of the sine and cosine functions in (1.30a,b), and summing is done over all values of n_1, n_2 and n_3 from 0 to N_1, N_2 and l, respectively. All the integrals that appear in (1.32a,b) can be calculated beforehand, once the value of r_0 is known. If the maximum value of n' is $n_{\max}$, then the maximum number of those integrals is $8n_{\max}$. Here, the factor 8 reflects the fact that there are two types of the I integral (sine and cosine) and four values of p' (1.33), i.e., four values of the lower bound in (1.36a,b). The values of I_1 and I_2 corresponding to $n' > 1$ are expressed in terms of the sine and cosine integrals

$$\mathrm{si}(p'r_0) = -I_1(p'r_0, 1), \tag{1.37a}$$

$$\mathrm{ci}(p'r_0) = -I_2(p'r_0, 1) \tag{1.37b}$$

using the known formulas [19, p. 219, Section 2.639]. This means that there are actually only 8 trigonometric integrals that have to be calculated numerically. All other I integrals are expressed analytically in terms of those 8 integrals. Thus, apart from the standard methods for calculating the sine and cosine integrals (1.37a,b), the integration from r_0 to ∞ does not require any specialized numerical algorithms. This second part of the integration will be therefore called "analytical integration".

In the case $k = 0$, the values of $\lim_{k\to 0}(kS_1)$ and $\lim_{k\to 0}(kS_2)$ are calculated instead of S_1 and S_2. Since the mentioned limits are given by the analytical formula (1.20), the numerical integration is not required. Thus, the value of r corresponding to transition from the "numerical" part of the calculation to the "analytical" part should be defined in the case $k = 0$ as the point where all needed phase shifts can be evaluated with sufficient accuracy, i.e., where all wave functions have attained the asymptotic form (1.18). Since the values of the phase shifts are stored in the files with the S integral data, it is possible to skip the stage of the numerical solution of the system (1.16a,b) in the case $k = 0$ by loading the phase shifts corresponding to an earlier calculation with the same Z, E_1 and interaction potential, but with $k \neq 0$.

1.3. The use of multiple-precision arithmetic and the methods of improving the performance

A problem that must be solved for an accurate analytical integration of a product of r^2 and three spherical Bessel functions from r_0 to ∞ when $k \neq 0$ is a strong cancellation of terms in the resulting alternating series. If this cancellation is almost exact, the final result may be dominated by

rounding errors. This problem is solved in BREMS by using multiple-precision (MP) arithmetic [20], [21], whereby the number of significant digits is increased beyond the "native" double precision (DP) of the compiler (the double precision corresponds to 15–17 significant digits, typically 16). Since the calculations using the available MP systems are extremely slow (slower by a factor of more than 100 than the equivalent calculations using DP) and may require a prohibitive amount of computer memory, BREMS uses the quadruple precision (QP) [22] when the required number of significant digits is between 18 and 38 (the calculations using QP are slower by a factor of 6–10 than the equivalent calculations using DP, and usually do not require much more memory).

In order to determine if the current precision level is sufficient, the capability of the MP system to change the precision level at runtime is employed. In addition, the known fact that the S integrals corresponding to the largest absolute values of the indices κ_1, κ_2 and l are the ones that are most susceptible to the cancellation errors is employed (this is because the number of terms of the type (1.32a,b) in the expressions of those S integrals is largest). Thus, if accurate values of the analytical integrals are obtained for the largest κ_1, κ_2 and l, then one can be certain that the current precision level is sufficient to obtain accurate values of all needed analytical integrals. In order to test the current precision level, the values of the four integrals (1.29) corresponding to the largest value of the sum $N_1 + N_2 + l$ are calculated at a different precision level. If the relative difference of the values obtained at both precision levels is less than 10^{-13}, this means that the current precision is sufficient. By repeating this procedure at different precision levels, it is possible to "optimize" the precision level, i.e., to find the lowest precision level needed to obtain the values of the analytical integrals with the first 12 significant digits guaranteed to be not affected by the rounding errors. This makes it possible to decrease the calculation time. When the number of significant digits is of the order of 100, the time of the analytical integration is roughly proportional to the precision level. At lower precision levels, the dependence of the calculation time on the precision level becomes weaker.

Since the "I" integrals (1.36a,b) are calculated before starting the mentioned optimization procedure, this method will work only if the I integrals are sufficiently accurate. In order to ensure the accuracy of the I integrals, they are calculated at the precision level of 3000 digits (or 4000 digits in the case of the sine and cosine integrals (1.37a,b)), keeping track of the rounding errors accumulated in their calculation procedure. If the maximum accumulated relative uncertainty of I_1 and I_2 is greater than 10^{-n_d}, where n_d is the required number of significant digits, the program quits with an error message. In the case of the sine and cosine integrals (1.37a,b), $n_d = 3000$. In the case of the higher-degree I_1 and I_2 integrals (1.36a,b), n_d is equal to the initial precision level of the analytical integration (300 or 100 by default).

The calculation time may also be reduced by decreasing the number of l values included in the sum (1.9), i.e., by decreasing the number of the S integrals calculated for each pair of values of κ_1 and κ_2. The absolute values of the S integrals decrease with increasing l, so that the S integrals corresponding to the largest l usually have no significant influence on the final values of the cross sections. However, at the stage of calculating the S integrals it is not possible to determine how this truncation of the sum with respect to l will affect the accuracy of the final values of the cross sections. Consequently, this is determined later by calculating the cross sections with two different values of l_{max} (i.e., the maximum value of l) in (1.9). Since the sum with respect to l has a finite number of terms, and since it is known that the terms corresponding to larger l have a progressively weaker influence on the magnitude of the sum, the estimate of the mentioned truncation error can be obtained by comparing the values of the cross sections obtained with two values of l_{max}. In addition to reducing the number of S integrals that have to be calculated, the decrease of l causes a decrease of the optimal precision level.

Yet another method of improving the performance is based on decomposing the sums in (1.2) and (1.3) into terms that are smooth functions of $|\kappa_1|$ or $|\kappa_2|$ (or l_1 or l_2). Then it may be sufficient to calculate only some of those terms exactly, and the missing terms may be obtained by interpolation. This method is called the "partial-wave interpolation method". It was applied in [23], where the singly differential cross section (SDCS) (1.3) was expressed as

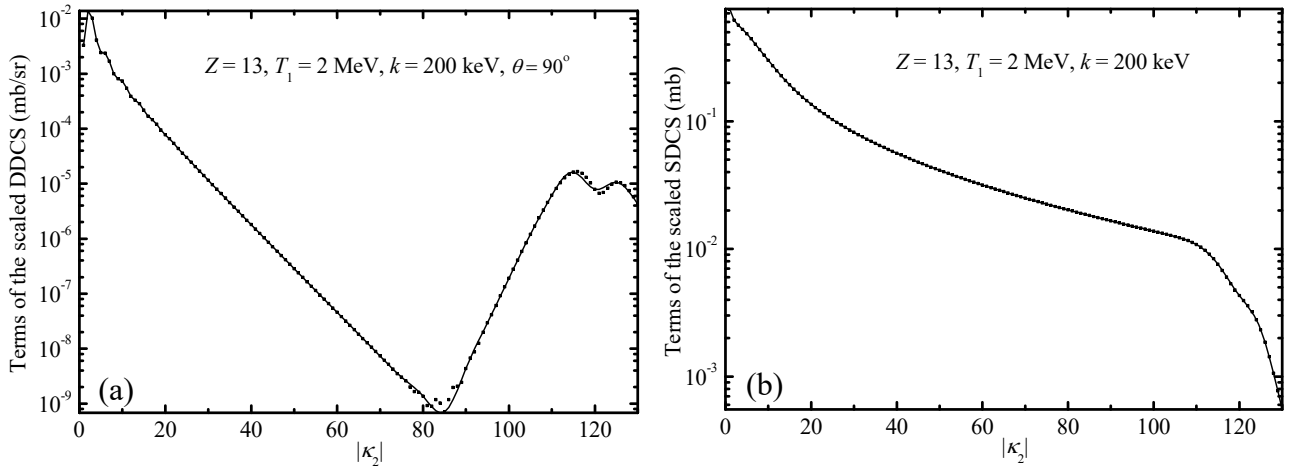

Fig. 1. Values of the first 130 terms of the expression of (a) scaled doubly differential cross section (DDCS) and (b) scaled singly differential cross section (SDCS), where the summation is done with respect to $|\kappa_2|$. The physical parameters are indicated in the graphs. The scaled cross sections have been calculated using (1.2) and (1.3), where the summation indices κ_1 and $\bar{\kappa}_1$ run from −130 to +130, and the sum (1.9) is truncated at $l = 130$. The exact values of the terms are shown by squares. Starting from the term No. 31, the solid line shows the values obtained by cubic spline interpolation between the exact values of the logarithm of the terms with sequence numbers from 30 to 130 in increments of 5.

$$\sigma(k) = \sum_{l_1, l_2} \sigma_{l_1, l_2}(k) = \sum_{l_1} \sigma_{l_1}(k) \,. \tag{1.38}$$

However, the interpolation with respect to l_1 (or $|\kappa_1|$) cannot be applied to the expression of the doubly differential cross section (DDCS) (1.2), because the latter expression includes a double sum with respect to the values of κ_1 (the corresponding summation indices are denoted κ_1 and $\bar{\kappa}_1$ in (1.2)). The terms of the mentioned double sum are not smooth functions of $|\kappa_1|$ and $|\bar{\kappa}_1|$ (or l_1 and $\bar{l}_1$), hence such interpolation would cause a significant loss of accuracy of the resulting sum. Conversely, the sum with respect to κ_2 is simple (not double) both in the expression of the DDCS (1.2) and in the expression of the SDCS (1.3). In addition, as shown in Fig. 1a and Fig. 1b, after replacing the sum with respect to κ_2 by the sum with respect to $|\kappa_2|$ (i.e., treating each pair of terms corresponding to opposite values of κ_2 as a single term), the terms of both those sums become smooth functions of $|\kappa_2|$. Consequently, BREMS allows "skipping" some of the values of κ_2 when calculating the set of the S integrals (1.15a,b). The values of the logarithm of the missing terms in the sums of (1.2) and (1.3) are subsequently calculated by cubic spline interpolation. By default, this method is applied in BREMS only when $|\kappa_2|_{\max} \geq 80$ (if $k \neq 0$), or when $|\kappa_2|_{\max} \geq 120$ (if $k = 0$), and the first skipped value of $|\kappa_2|$ is equal to 31 (i.e., the starting value of $|\kappa_2|$ for the mentioned interpolation is equal to 30). The default difference of the adjacent retained values of $|\kappa_2|$ in the interval $30 \leq |\kappa_2| \leq |\kappa_2|_{\max}$ is constant and equal to 5 (possibly excluding the last two values of $|\kappa_2|$, whose difference will be less than 5 if $|\kappa_2|_{\max}$ is not a multiple of 5). In addition, there is an option to use a set of values of $|\kappa_2|$ whose differences increase in an arithmetic progression.

A method of decreasing the computation time based on "truncation" of the interaction potential $V(r)$ should also be mentioned. The truncation radius R_a (or "atomic radius"), which is defined as the value of the radial coordinate where V drops to zero (i.e., $V(r) \equiv 0$ when $r > R_a$), can be calculated using the known fact that in momentum space the largest contribution to the radiation cross section originates from the region where the momentum transfer $\boldsymbol{q} = \boldsymbol{p}_2 + \boldsymbol{k} - \boldsymbol{p}_1$ is smallest [24]. In coordinate space, this corresponds to a distance from the nucleus of the order

$$r = 1/|\boldsymbol{q}_{\min}| \,, \tag{1.39}$$

where $|\boldsymbol{q}_{\min}|$ is the minimum momentum transfer, which is equal to

$$|\boldsymbol{q}_{\min}| = |\boldsymbol{p}_1| - |\boldsymbol{p}_2| - |\boldsymbol{k}| \equiv p_1 - p_2 - k = \sqrt{E_1^2 - 1} - \sqrt{E_2^2 - 1} - k \,. \tag{1.40}$$

It is reasonable to expect that if the value of R_a exceeds the value of r (1.39) by a factor of 10 or more, then the mentioned truncation will not have a significant effect on the values of the DDCS and the SDCS. However, the decrease of the computation time caused by the truncation of the potential function may be quite dramatic, because the value of the truncation radius R_a may be much less than the radius r_0 where the asymptotic form would be attained without this truncation (this is usually the case when the kinetic energy of the incident electron is of the order of 1 MeV or greater). The asymptotic expression of the wave function (1.18) (with constant values of the phase shift $\bar{\delta}_\kappa$ and the normalization factor A_κ) is known to be exact in the region of space where $V(r) \equiv 0$. Consequently, by truncating the potential function, one can decrease the region of the numerical integration and thus shorten the processing time. By default, BREMS calculates R_a by multiplying the value of (1.39) by 20 when $T_1 < 1$ MeV, or by 13 when $T_1 \geq 1$ MeV, and if the radius obtained in this way is less than $R_{a,min} = \max(800, 126/p_2)$ (i.e., either approximately six Bohr radii or twenty periods of the final electron wave function, whichever is greater), then R_a is set equal to $R_{a,min}$. When $k = 0$, the interaction potential is not truncated. This default behavior may be modified by the user.

Since each integral from r_0 to ∞ (the "analytical" integral) is expressed as a linear combination of the four integrals defined by (1.29), it is possible to decrease the total time of analytical integration by reusing the values of those four integrals for different values of Z, if a fixed set of values of T_1 and k is used for all Z. The values of the mentioned four integrals depend on T_1, k and r_0, but do not depend on Z explicitly. If the values of the radial coordinate corresponding to the transition from the numerical integration to the analytical integration (i.e., the lower integration bound r_0 in (1.29)) are also defined independently of Z (for example, if $r_0 = R_a$, where the truncation radius R_a is calculated as described above), then it is possible to reuse the values of the mentioned four integrals and thus to skip the stage of the analytical integration for some combinations of Z, T_1 and k. In such a case, a change of Z requires only recalculating the coefficients of the mentioned linear combination, which depend on the phase shifts calculated by numerical solution of the system of ODEs (1.16a,b). As a result, the total time of the analytical integration is decreased by a factor equal to the number of chemical elements, for which the cross sections are computed. For example, if BREMS is used for generation of a data library for all Z from 1 to 100, then the total time of the analytical integration can be reduced to the point where it will be only a small fraction of the total processing time.

1.4. The numerical errors

The errors in the final values of the cross sections are caused by the inaccuracies of the numerical methods used to evaluate the expressions presented in Section 1.1. The sources of errors are the following:

1) errors of the numerical solution of the system of ODEs (1.16a,b),
2) errors of the numerical integration due to the finite step size,
3) errors caused by truncation of the series (1.2) and (1.3) at finite values of κ_1 and κ_2.

The combined effect of the errors of the first and second types on the numerical integrals is estimated by calculating the so-called "test" numerical integrals, i.e., by redoing the numerical integration with all tolerances and step sizes increased by a factor of two. The output data files created at the stage of calculating the S integrals contain not only the values of the total integrals (from 0 to ∞), but also the values of both numerical integrals (corresponding to the initial numerical integration from 0 to r_0 and the test integration with the same bounds). The difference of the latter two integrals serves as the estimate of the error of the numerical integration. The uncertainty of the phase shifts $\tilde{\delta}_\kappa$ caused by errors of the first type affects the accuracy of the analytical integrals, too, because the asymptotic expressions of the radial wave functions (1.18) depend on the mentioned phase shifts. In the case of screened (exponentially decaying) or "truncated" interaction potentials, the effect of the uncertainty of the phase shifts on the analytical integrals is estimated by calculating three estimates of each analytical integral:

1) the one corresponding to the original (i.e., average) phase shifts $\tilde{\delta}_{\kappa_1}$ and $\tilde{\delta}_{\kappa_2}$,
2) the one obtained after incrementing $\tilde{\delta}_{\kappa_1}$ by the uncertainty of $\tilde{\delta}_{\kappa_1}$,
3) the one obtained after incrementing $\tilde{\delta}_{\kappa_2}$ by the uncertainty of $\tilde{\delta}_{\kappa_2}$.

The "uncertainty of $\tilde{\delta}_{\kappa}$" mentioned above is the range of variation (i.e., the difference of the maximum and minimum values) of $\tilde{\delta}_{\kappa}$ over the last 10 "test" points (see also Section 1.2). If the test integration has been performed, then the overall range of variation of $\tilde{\delta}_{\kappa}$ is obtained by combining the ranges of variation corresponding to the original integration and to the test integration. The absolute value of the maximum difference of these three estimates of the analytical integral serves as the estimate of the error of the analytical integral due to uncertainty of the phase shift. In the case of the exact (non-truncated) point-Coulomb potential, the phase shift $\overline{\delta}_{\kappa}$ in (1.18) is unknown due to an undefined value of the phase correction integral (see (1.26) and (1.27)). Consequently, the uncertainty of the *S* integrals caused by the uncertainty of the phase shift is estimated in this case as twice the absolute value of the largest of the four integrals (1.29), multiplied by the product of the two corresponding square-root factors before the brackets in (1.18), i.e., by $\sqrt{(E_1+1)(E_2-1)/(4E_1E_2)}$ for S_1 integrals, or by $\sqrt{(E_1-1)(E_2+1)/(4E_1E_2)}$ for S_2 integrals.

The mentioned errors of the analytical integrals caused by the uncertainty of the phase shift are also included in the *S* integral data files. The overall error (i.e., uncertainty) of each *S* integral is obtained by combining the error of the numerical integration and the error of the analytical integral caused by uncertainty of the phase shifts (these two errors are assumed to be independent, hence they are combined by adding them in quadrature). It should be noted that the overall relative errors of the *S* integrals are usually greater than the relative errors of the separate numerical and analytical integrals by several orders of magnitude due to a strong cancellation of those two integrals.

The effect of the truncation of the series (1.2) and (1.3) may be ameliorated by extrapolation as described in Section 1.5.

1.5. Refining the estimates of cross sections by extrapolation and smoothing

In the following text, the cross section that is differential in photon energy and angle (1.2) will be called simply "differential cross section" (DCS), and the cross section that is differential in photon energy only (1.3) will be called simply "cross section" (CS). It has been noticed that if the truncation error is not too large and if the summation in the truncated series (1.2) and (1.3) is symmetrical with respect to positive and negative values of the summation indices κ_1 and κ_2 (i.e., if for every term corresponding to a particular pair of indices (κ_1, κ_2) there are two terms corresponding to the pairs of indices ($-\kappa_1$, κ_2) and (κ_1, $-\kappa_2$)), then the dependence of both the DCS and the CS on the maximum value of $|\kappa_1|$ and $|\kappa_2|$ used in the sum may be approximated by the following five-parameter expression:

$$\mathrm{(D)CS} = c_\infty \pm \exp(a + b \cdot \kappa_{\max}^{d+h\kappa_{\max}}), \tag{1.41}$$

where $b < 0$, $d > 0$, $h \geq 0$, and $\kappa_{\max}$ is the largest value of $|\kappa_1|$ and $|\kappa_2|$ included in the series (1.2) and (1.3), i.e., the "truncation value" of $|\kappa|$:

$$\kappa_{\max} \equiv \max(|\kappa_1|, |\kappa_2|), \tag{1.42}$$

As it follows from (1.41), the CS (or the DCS) approaches the limiting value c_∞ as a stretched exponential of $\kappa_{\max}$, with the stretching exponent depending on $\kappa_{\max}$ linearly. Approximation (1.41) is applicable when the magnitude of the truncation error corresponding to a given value of $\kappa_{\max}$ (i.e., the absolute value of the relative deviation of the value of the truncated series (1.2) or (1.3) from the value corresponding to $\kappa_{\max} \to \infty$) is less than approximately 30 % and the shape of the actual dependence of the CS or DCS on $\kappa_{\max}$ is consistent with Eq. (1.41), i.e., a monotonous increase or decrease, with the first derivative asymptotically approaching zero.

Equation (1.41) defines a prescription for improving the accuracy of the final estimates of CS and DCS: the dependence of CS and DCS on $\kappa_{\max}$ must be fitted by the nonlinear function (1.41) in the range of values of $\kappa_{\max}$ where the CS or DCS is sufficiently close to the saturation value. The optimal value of c_∞ (i.e., the value obtained by nonlinear fitting) is the estimate of the CS or the DCS. The fitting is performed by minimizing the sum of squared differences between the fitting function (1.41) and the actual values over the last N_{fit} values of $\kappa_{\max}$, i.e., in the range $K - N_{\text{fit}} < \kappa_{\max} \leq K$, where K is the absolute maximum value of $|\kappa_1|$ or $|\kappa_2|$ represented in the available S integral data:

$$K \equiv \max(\kappa_{\max}). \tag{1.43}$$

In the case of the DCS, this fitting is performed independently for each value of the photon emission angle θ. If the partial-wave interpolation method described in Section 1.3 is applied, then the logarithmic cubic spline interpolation mentioned in Section 1.3 must be done for each value of $\kappa_{\max}$ independently, because a change of $\kappa_{\max}$ causes not only the change of the number of terms retained in the sums with respect to $|\kappa_2|$, but also a change of values of all terms in those sums (due to the change of the limits of summation with respect to κ_1 and $\bar{\kappa}_1$).

By default, the fitting mentioned above is done twice using two values of N_{fit}:

$$N_{\text{fit}} = \frac{K}{4} + 1.2\sqrt{K} \tag{1.44a}$$

and

$$N_{\text{fit}} = \frac{K}{8} + 0.6\sqrt{K}\,. \tag{1.44b}$$

The (D)CS is calculated as the arithmetic average of the two corresponding values of c_∞. This choice of N_{fit} is largely arbitrary. If the fitting model defined by (1.41) was perfectly accurate, then one should fit the values of (D)CS corresponding to all values of $\kappa_{\max}$ from 1 to K. However, the fitting equation becomes less accurate with decreasing $\kappa_{\max}$, hence the number of fitted data points N_{fit} is chosen on the basis of an empirical tradeoff between the accuracy of the fitting model and the rounding errors during the calculation of the original data and during the fitting procedure (the mentioned rounding errors tend to decrease with increasing N_{fit}).

For any triplet of values of parameters c_∞, d and h, the optimal values of parameters a and b are calculated by linear least squares fitting of $\ln|(\text{D})\text{CS} - c_\infty|$ as a function of $\kappa_{\max}^{d+h\kappa_{\max}}$. Thus, parameters a and b are expressed analytically in terms of parameters c_∞, d and h, so that the latter three parameters are the only ones that have to be varied during the iterative fitting procedure.

The overall error of the final estimates of the CS or DCS obtained by applying the extrapolation technique described above is usually less than the original truncation error at least by an order of magnitude. However, in the case of the DCS, the applicability of the approximation (1.41) is limited by the fact that the dependence of the DCS on $\kappa_{\max}$ at a fixed non-zero value of θ is sometimes oscillatory in a wide interval of values of $\kappa_{\max}$, when those values are insufficiently large. The mentioned oscillations are especially pronounced in the case of large values of T_1 (> 3 MeV) and k / T_1 (> 0.6). Those oscillations manifest themselves as wiggles in the angular dependence of the final DCS. As $\kappa_{\max}$ is increased, the amplitude of those oscillations decreases and eventually the DCS becomes a monotonous function of $\kappa_{\max}$, which is approximately described by Eq. (1.41). The approximation (1.41) can be applied only when the dependence of the DCS on $\kappa_{\max}$ is not oscillatory, or when the largest investigated values of $\kappa_{\max}$ are well outside the oscillatory interval. If the largest value of $\kappa_{\max}$ belongs to the oscillatory interval, then it is better to skip the nonlinear fitting, i.e., to use the original (unfitted) value of the DCS instead of the fitted value. BREMS checks the shape of the dependence of the DCS on $\kappa_{\max}$ before the nonlinear fitting, and if it is determined that it is not consistent with Eq. (1.41), then the fitting is not performed, i.e., the final value of the DCS is set equal to the original value.

At high electron energies, or when k / T_1 is very close to 1, the values of the DCS at large angles are less by several orders of magnitude than at small and intermediate angles, and those

values are especially sensitive to the truncation of the sums (1.2) and (1.9) with respect to $|\kappa_1|$, $|\kappa_2|$ and l. The nonlinear fitting described above is not always successful in eliminating the distortions of the function DCS(θ) at large values of θ. As a result, the angular dependence of the fitted DCS at large angles ($\theta > 160°$) is sometimes non-monotonous when T_1 is of the order of 1 MeV or greater, or when k / T_1 is greater than 0.99 (at those conditions, the correct angular dependence of the DCS at large angles is a monotonous decrease with increasing θ). In such a case, BREMS calculates a polynomial of degree 2 – 6 for extrapolation of the angular dependence of the fitted DCS at $\theta > 160°$, using the following equation:

$$\mathrm{DCS}(\theta) = c_0 + c_2(180° - \theta)^2 + c_3(180° - \theta)^3 + \ldots + c_6(180° - \theta)^6 , \tag{1.45}$$

where θ is expressed in degrees (this equation does not have the term that is linear in $180° - \theta$, because $\mathrm{d(DCS)}/\mathrm{d}\theta|_{\theta = 180°} = 0$, as it follows from the properties of the spherical harmonics in (1.2)). The coefficients $c_0 - c_6$ in (1.45) are calculated by least squares fitting of the DCS (obtained after performing the fitting of the dependence on $\kappa_{\max}$) in the angular interval $140° \le \theta \le 160°$. If the degree of the extrapolating polynomial is less than 6, then some of the last coefficients in (1.45) are zero. The optimal degree of the extrapolating polynomial (1.45) is determined on the basis of two requirements: (1) the polynomial (1.45) should be a monotonous function in the interval $120° \le \theta \le 180°$, (2) among all polynomials that satisfy the first requirement, the optimal polynomial should correspond to the smallest value of the maximum absolute deviation from the fitted DCS in the angular interval $120° \le \theta < 140°$.

The Nelder-Mead simplex method [25] is used in BREMS for minimizing the sum of squared differences between the fitting function (1.41) and the original (unfitted) CS or DCS, as well as between the extrapolating polynomial (1.45) and the fitted DCS.

In addition to the extrapolation mentioned above, BREMS applies smoothing to the CS and DCS data. Both the dependence on $\kappa_{\max}$ and the dependence on θ (for the DCS) are smoothed. The smoothing with respect to $\kappa_{\max}$ is implemented by replacing each value of the CS or DCS with the average of several values corresponding to consecutive values of $\kappa_{\max}$, where the last value is the current one. If a fitting error occurs, the averaging period is increased by 1 and the fitting is redone. This process is repeated until the fitting error does not occur or the maximum value of the averaging period is reached. The order of processing steps after calculating the truncated sums (1.2) and (1.3) is the following:

(1) smoothing with respect to $\kappa_{\max}$ (optional),
(2) extrapolation to $\kappa_{\max} \to \infty$ (i.e., the nonlinear fitting of the dependence on $\kappa_{\max}$),
(3) smoothing of the fitted DCS with respect to θ (optional),
(4) if necessary, the angular extrapolation of the (smoothed) fitted DCS to the range $\theta > 160°$.

1.6. Calculation of the uncertainties of the fitted singly and doubly differential cross sections

The calculation of the confidence interval of c_∞ in BREMS follows the standard procedure adopted in nonlinear least squares fitting (see, for example, [26]). It involves calculation of the matrix of second partial derivatives of the sum of squared differences (SSD) between the fitting function and the actual values SSD($\boldsymbol{p}$), where $\boldsymbol{p}$ denotes the set of varied parameters (the "parameter vector"). The mentioned second derivatives are calculated at the "optimal" parameter values ($\boldsymbol{p} = \boldsymbol{p}_0$), which correspond to the minimum value of SSD, which will be denoted SSD_0. Elements of that matrix are

$$G_{ij} = \frac{1}{2} \frac{\partial^2 \mathrm{SSD}}{\partial p_i \partial p_j}\bigg|_{\boldsymbol{p} \,=\, \boldsymbol{p}_0} , \tag{1.46}$$

where i and j are the sequence numbers of the parameters. If the theoretical model (i.e., the fitting function) is correct (i.e., unbiased) and if the differences between the theoretical and actual values are independent and distributed normally, then the distributions of the least squares estimates of the varied parameters are normal, and the estimate of the standard deviation of parameter No. i is equal to

$$s_i = \sqrt{\| G^{-1} \|_{ii} \, \mathrm{SSD}'_0} = \sqrt{\| G^{-1} \|_{ii} \, \mathrm{SSD}_0 / (n-m)} \,, \tag{1.47}$$

where n is the number of fitted points (denoted N_{fit} in Section 1.5), m is the number of varied parameters, and G^{-1} is the inverse of the matrix defined by (1.46) (the matrix G^{-1} is called the variance-covariance matrix). SSD'_0 is the reduced sum of squared deviations (here, the term "reduced" means divided by the number of degrees of freedom $n - m$).

In BREMS, Eq. (1.47) is used to estimate the uncertainty ("standard error") of the least squares estimate of c_∞ in (1.41). Since the fitting function (1.41) is not perfectly accurate, the mentioned assumptions of independence and normal distribution of the differences between the theoretical and actual values are not satisfied in the case discussed. This makes the estimate of the standard error (1.47) very inaccurate. It may be used only as an indicator of the order of magnitude of the uncertainty of c_∞ at best. However, this estimate has another useful property: it helps to keep the number of varied parameters reasonably small, because otherwise (when the theoretical model is "overparameterized") the standard deviations (1.47) become excessively large (sometimes exceeding the least squares estimates of the varied parameters). Consequently, a fitting function that provides a better fit inside the fitting interval (due to a larger number of varied parameters) can sometimes be safely rejected on the grounds of large standard deviations of varied parameters (because large values of (1.47) usually indicate large differences between the fitting function and the true values *outside* of the fitting interval). If, on the other hand, the inclusion of an additional varied parameter causes a significant decrease of the estimates of the standard deviations (1.47), this can usually be interpreted as an improvement of the fitting function. For this reason, (D)CS is fitted in BREMS twice: once with $h = 0$ and once with h varied, and if the difference of the two estimates of c_∞ obtained in both cases is less than the larger of the two standard errors, then the fitting mode corresponding to the smaller standard error is preferred. Otherwise, the fitting mode with $h > 0$ is preferred.

Since two widths of the fitting interval are used (see Eqs. (1.44a) and (1.44b)), two additional measures of the uncertainty of the fitted (D)CS become available: the value of (1.47) corresponding to the other value of N_{fit}, and the difference of the two least squares estimates of (D)CS corresponding to each of the two values of N_{fit}. In BREMS, the uncertainty of the fitted (D)CS is calculated by combining the three mentioned measures of the uncertainty as follows:

$$\Delta c_\infty = \frac{1}{2} \sqrt{\left(\min(\Delta c_\infty^{(1)}, | c_\infty^{(1)} - c_\infty^{(2)} |) \right)^2 + \left(\max(\Delta c_\infty^{(2)}, | c_\infty^{(1)} - c_\infty^{(2)} |) \right)^2} \,, \tag{1.48}$$

where $c_\infty^{(1)}$ and $c_\infty^{(2)}$ are the least squares estimates of (D)CS corresponding to each of the two values of N_{fit} (the superscript "(2)" corresponds to the wider fitting interval), and $\Delta c_\infty^{(1)}$ and $\Delta c_\infty^{(2)}$ are the corresponding uncertainties (calculated according to (1.47)). Functions "min" and "max" are used in (1.48), because the uncertainty of c_∞ corresponding to the narrower interval ($\Delta c_\infty^{(1)}$) is sometimes overestimated by a large factor, whereas the uncertainty corresponding to the wider interval ($\Delta c_\infty^{(2)}$) is frequently underestimated. The value of (1.48) is always of the order of $| c_\infty^{(1)} - c_\infty^{(2)} |$ or greater. If the relative range of variation of the unfitted (D)CS inside the narrower interval is less than 0.1 %, then the second term in the square root of (1.48) is replaced with $(c_\infty^{(1)} - c_\infty^{(2)})^2$, because it has been noticed that under those conditions the value of $\Delta c_\infty^{(2)}$ is also sometimes overestimated by a very large factor.

By default, c_∞ is calculated in BREMS using five values of the endpoint of the fitting interval (from $K - 4$ to K). The final estimate of the fitted DCS is the arithmetic average of the five corresponding least squares estimates. For each value of the mentioned endpoint, the CS is additionally estimated by integrating the fitted DCS with respect to the solid angle Ω. The latter integral will be denoted $\int \mathrm{DCS} \mathrm{d}\Omega$. This integral is calculated by numerical quadrature, and it is approximately equal to the least squares estimate of the CS (the difference between the two is

caused only by numerical errors, including the possible bias due to inaccuracy of the fitting function (1.41), because the CS and the values of the DCS for each angle θ are fitted independently). The final estimate of the fitted CS is the arithmetic average of ten values: five least squares estimates of c_∞, and five corresponding values of $\int \mathrm{DCS} \mathrm{d}\Omega$. The final estimate of the uncertainty of the fitted (D)CS (i.e., ΔCS or ΔDCS) is equal to the square root of the sum of (a) the average of the five values of $(\Delta c_\infty)^2$ corresponding to each of the five endpoints of the fitting interval (Δc_∞ is calculated according to (1.48)), (b) the empirical variance of the fitted (D)CS (the empirical variance is calculated using the same five or ten estimates of the (D)CS that are used to calculate the average (D)CS), (c) the squared angular integral of the uncertainty of the fitted DCS, i.e., $(\int \Delta\mathrm{DCS} \mathrm{d}\Omega)^2$. The latter term is added only when calculating the uncertainty of the fitted CS, and only when the angular interval is from 0° to 180°, whereas the angular grid is sufficiently dense for accurate estimation of the latter integral (i.e., the maximum angular step is not greater than 1°).

A similar approach is used to calculate the uncertainty of the fitted shape function (SF). The fitted SF is defined as the ratio of the fitted DCS and the mentioned angular integral of the same DCS (since the latter integral is approximately equal to the fitted CS, the fitted DCS can be calculated by multiplying the values of the fitted CS and the fitted SF). The final estimate of the fitted SF is the average of the five values of the mentioned ratio (DCS / $\int \mathrm{DCS} \mathrm{d}\Omega$) corresponding to each of the five endpoints of the fitting interval. The absolute uncertainty of the SF is calculated as the square root of the sum of two terms: the empirical variance of the ratio DCS / $\int \mathrm{DCS} \mathrm{d}\Omega$, and the average squared value of (1.48), divided by the average value of $\int \mathrm{DCS} \mathrm{d}\Omega$ squared. The relative uncertainty of the CS, DCS or SF is equal to the ratio of the corresponding absolute uncertainty and the corresponding estimate of the CS, DCS or SF.

When T_1 is sufficiently small or k / T_1 is sufficiently large, the extrapolation described in Section 1.5 becomes unnecessary, because the number of terms in the truncated series for the (D)CS (Eq. (1.2) or (1.3)) is sufficient to practically reach the saturation value. The minimum relative range of variation of the (D)CS inside the fitting interval (needed for the extrapolation to be performed) is 0.1 %. If the relative range is less, then the value of the corresponding relative uncertainty of the (D)CS or the SF is replaced by the relative range of variation with the minus sign.

2. Overview of the calculation process and the codes included in BREMS

The process of calculating the CS and DCS for a particular combination of Z, T_1 and k, and for a chosen interaction potential $V(r)$ consists of three stages:

1) calculation of the phase shifts and S integrals (1.15a,b),
2) calculation of the truncated series (1.2) and (1.3) for a set of values of $\kappa_{\max}$ in increments of 1,
3) improvement of the accuracy of the results by extrapolation and smoothing (see Section 1.5).

Each of those stages is performed by a separate subroutine, called from the main program:

Stage 1: S_integrals
Stage 2: Bremsstrahlung
Stage 3: Brems_fit

The main program and all subroutines are written in Fortran-90. The code of the main program is in the file “Brems.f90”. The names of the main source code file for each of the three mentioned subroutines are “S_integrals.f90”, “Bremsstrahlung.f90” and “Brems_fit.f90”, respectively. The subroutine “S_integrals” creates a binary file with the values of phase shifts (denoted $\tilde{\delta}_\kappa$ in Section 1.1), normalization factors (denoted A_κ in (1.18)), S integrals and the system parameters (the S integrals are written to file only when $k \neq 0$). This file is subsequently read by “Bremsstrahlung”, which creates the files with the values of the CS, DCS and the shape function (defined as the ratio DCS/CS) for each value of $\kappa_{\max}$, which is defined as the maximum value of $|\kappa_1|$ or $|\kappa_2|$ in the series (1.2) and (1.3). Finally, “Brems_fit” reads the values of CS and DCS from the files created by “Bremsstrahlung” and performs the nonlinear fitting described in Section 1.5. The

source codes of the main program and of the three mentioned subroutines, and the compiled executable "Brems.exe" are in the folder "Brems". In addition, there is a program "Read_S_integrals.f90", which displays the values of all phase shifts and the S integrals corresponding to the user-specified values of κ_1 and κ_2. The file "Read_S_integrals.f90" and the compiled executable "Read_S_integrals.exe" are in the subfolder "Read_S_integrals" of the folder "Brems". Those executables are 64-bit Windows console applications (the Windows console is opened by running the Windows command-line interpreter "cmd.exe"). They were compiled using the Intel Fortran compiler. The Linux versions of the files Brems.exe and Read_S_integrals.exe are in the subfolder "Linux_executables". They were compiled using GNU Fortran on Ubuntu running on the Windows Subsystem for Linux. All executables were compiled with optimization for speed enabled. The folder "Linux_executables" also contains the file "Compile.sh" with the complete set of Linux shell ("bash") commands that must be entered in order to compile both mentioned executables on Linux.

Since the results of the previous stage of a calculation are stored in a file, it is possible to redo only stage 2 or 3 of a calculation, if the data files with the results of the previous stage are available. Examples of such a situation include a resuming of an interrupted calculation process, or a recalculation of the DCS for a different set of values of the angle θ (the values of θ are required only in stages 2 and 3). There is also an option to delete all data files of the previous stage automatically upon a successful completion of the current stage (this is the default behavior).

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, "IV=1" specifies that the point-Coulomb potential $V(r) = -\alpha Z / r$ (corresponding to the unscreened nucleus) should be used when solving the system of ODEs (1.16a,b). There are 98 parameters in total, allowing great flexibility in the process of calculating the CS and DCS, in the amount of additional data (such as error estimates) calculated by the program, and in the number of files created (such as the files with intermediate data). 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: the atomic number Z, the incident electron energy T_1, and the photon energy k. Those parameters must be specified by the user. In the simplest case, the command line of BREMS looks like this:

```
Brems.exe Z=13 T1=0.001 Ep=6e-4
```

In this example, no parameter file would be used, and the program would calculate the CS and DCS for the case when $Z = 13$, $T_1 = 1$ keV, and $k = 600$ eV (the input energy values must be specified in MeV). The values of the control parameters and the scaled CS calculated in stage 2 (before extrapolation of its dependence on κ_{max}) would be written to the file "CS.txt", the extrapolated value of the scaled CS would be written to the file "CS_fitted.txt", and the values of the scaled DCS and the shape function would be written to the two files whose names start with "DCS_fitted_" and "ShapeFn_fitted_", respectively (the remaining part of the file name indicates the values of Z, T_1 and k). The scaled CS and DCS are defined as the left-hand sides of (1.3) and (1.2), respectively, and their values are expressed in the units indicated after (1.3) and (1.2). By default, the values of the DCS and the shape function are calculated for 181 equidistant values of θ from 0° to 180°. If some of the parameters have to be loaded from a parameter file, then its name must be specified on the command line after the keyword "in=", for example:

```
Brems.exe Z=13 T1=0.001 Ep=6e-4 in=Brems.inp
```

If a parameter value is specified both on the command line and in the 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). The parameter names are case-sensitive. There must be no more than one parameter per line in the parameter file. One-line comments (starting with the exclamation mark '!') and empty lines are allowed in the parameter file.

The default values of all parameters for the case when $T_1 = 100$ keV and $k = 10$ keV are given in the BREMS parameter file "Brems_defaults.inp".

The subfolder “V” contains the subfolder “Kohn-Sham”, which, in turn, contains the text files with the values of the Kohn-Sham potential function in tabular format. There is one file for each value of Z from 1 to 100 (the value of Z is indicated in the name of the corresponding file). Each of those files contains two columns of numbers with the values of the radial coordinate r and the interaction potential $V(r)$. Both r and V are specified in relativistic units (see Section 1.1). If the Kohn-Sham potential is required, then the mentioned folder “V” must be either a subfolder of the current folder when starting Brems.exe, or a subfolder of the folder where Brems.exe is located, or it must be explicitly specified using the parameter “dir_V” (see the description of parameter No. 44 in Section 3).

The files with the S integral data contain up to four entries for each S integral: the value of the total integral, the values of the two numerical integrals corresponding to the two sets of numerical tolerances and step sizes, and the value of the error caused by the uncertainty of the phase shifts. The latter three entries are needed for estimating the numerical errors (see Section 1.4). After the numerical integration, a temporary file containing only the numerical integrals is created. Further on, this file will be called the “_n” file (because its name ends with the suffix “_n”). If the subsequent analytical integration fails and the final file is not created (for example, due to insufficient maximum precision level requested by the user), then the “_n” file may be reused for another integration attempt (if the “_n” file exists, then it is possible to load the numerical integrals from it). Since the final (complete) file also contains the numerical integral data, it may also be used for skipping the stage of numerical integration and redoing the analytical integration with a different precision level (see also Section 1.3).

The subfolder “Test_runs” contains two Windows batch files “Brems_79_100keV_KS.bat” and “Brems_79_100keV_TFC.bat”, which perform the entire mentioned set of calculations for the case when the target is gold, incident electron energy is 100 keV and the photon energy is 10 keV or 0. The mentioned two files use the Kohn-Sham (KS) and the Thomas-Fermi-Csavinszky (TFC) potentials, respectively. The batch file “Read_S_integrals_79_100keV_10keV_KS.bat” can be used to display some of the data in the binary file with the S integral data created by the first mentioned batch file. All ASCII files created by running the Windows batch file “Brems_79_100keV_KS.bat”, as well as the file “Screen_output_Z=79_T1=0.1_Ep=0.01.txt” with the complete text that is displayed on the screen during the first call to Brems.exe in the mentioned batch file, are also in the subfolder “Test_runs” (those files were created by executing the mentioned batch file on a notebook computer with an Intel Core i5-8300H processor, 8 GB RAM, and Windows 10, without any other processor-intensive tasks being run at the same time). The subfolder “Linux_executables” contains three bash scripts for performing the same calculations on Linux (“Brems_79_100keV_KS.sh”, “Brems_79_100keV_TFC.sh” and “Read_S_integrals_79_100keV_10keV_KS.sh”, respectively).

The third-party open-source codes, which are needed for compiling Brems.exe and Read_S_integrals.exe, are in the subfolder “AuxiliaryPrograms” of the folder “Brems”. The complete list and descriptions of the third-party Fortran codes are below.

1) The routines and data structures of the multiple precision package are in two files “mpfun90.f90” and “mpmod90.f90” [20].
2) The routines and data structures of the quadruple precision package are in the file “quad_df.f90” [22].
3) Subroutine DHPCG from the IBM System/360 Scientific Subroutine Package (SSP) is used for solving the system of ODEs (1.16a,b) by the Hamming’s modified predictor-corrector method (it may be optionally used instead of the default method of the power-series solution). This subroutine is in the file “DHPCG.F”.
4) The suite of Runge-Kutta codes RKSUITE (Release 1.0, November 1991), which may also be optionally used for solving the system of ODEs (1.16a,b), is in the file “rksuite.f”.
5) The codes used to calculate the exponential integral (needed for calculation of the phase correction integral (1.27)) are in the files “de1.f”, “DCSEVL.f”, “INITDS.f”, “D1MACH.f”.

6) Subroutine PFQ for calculating the hypergeometric series [27] is in the file "acpa.f". This subroutine is used for calculating the exact radial wave functions at the stage of initial power-series solution (i.e., at small r) when the point-Coulomb potential is used.

7) Subroutines DLOGAM and CLOGAM (in files "DLOGAM.f" and "CLOGAM.f") are used for calculating the natural logarithm of the absolute value of the gamma function of real and complex arguments, respectively.

8) The routines and data for calculating the spherical Bessel functions of the first and second kinds at argument values less than 5000 are in the files "SphBes.f90" and "types.f90". Subroutine SPHJ (or its quadruple-precision version SPHJ_QP) estimates j_l using the Miller's method (based on the backward recursion), which does not have the stability problems [12], [13]. Subroutine SPHY estimates y_l using the forward recursion, which is also stable. At argument values greater than 5000, the explicit formulas (1.30a,b) are used.

9) Subroutine F3J and its QP and MP versions are used for calculating the 3j coefficients in (1.14). Those subroutines are in the files "F3J.f", "F3J_QP.f" and "F3J_MP.f", respectively. The code of the F3J subroutine has been copied from [28]. As pointed out in the title of [28], F3J is not suitable when at least one of the numbers l_1, l_2 and l in (1.14) is greater than 80. In the latter case, the quadruple-precision version F3J_QP is used if $l_1, l_2 \le 160$, and the multiple-precision version F3J_MP (with precision level of 100 digits) is used if l_1 or l_2 is greater than 160.

10) Subroutines SPLINE and SPLINT are used for the cubic spline interpolation mentioned in Section 1.3 and for the cubic spline interpolation of the screening factor defined in tabular format. Those subroutines are in the files "SPLINE.f90" and "SPLINT.f90", respectively.

11) Subroutine GOLDEN is used for optimizing parameter h in (1.41) by the golden section search method, which may be optionally used instead of the default three-parameter simplex method (the minimized function is the absolute value of the difference of the least squares estimates of parameter c_∞ corresponding to two different fitting intervals, with the condition that the value of h is the same for both intervals). This subroutine is in the file "golden.f90".

12) The random number generator RAND from [29] is used for random modification of the S integrals (by randomly adding or subtracting their uncertainties) in order to test sensitivity of the cross sections to the numerical errors of the S integrals. This Fortran subroutine is in the file "RAND.f".

13) Subroutine DSG13 from the IBM System/360 Scientific Subroutine Package (SSP) is used for additional smoothing of the fitted DCS, if multiple smoothing cycles are requested by the user. This subroutine is in the file "DSG13.F".

14) Subroutine DMINV from the IBM System/360 Scientific Subroutine Package (SSP), converted to quadruple-precision arithmetic ("DMINV_QP"), is used for inversion of a matrix of second partial derivatives of the sum of squared deviations for estimation of uncertainties of the parameter values obtained by nonlinear fitting. This subroutine is in the file "DMINV_QP.f90".

The code for calculating the Kohn-Sham potential is not included in the BREMS distribution package, because the Kohn-Sham potential functions for all values of Z from 1 to 100 are stored in tabular format in the folder "V/Kohn-Sham/". Those data were calculated using the Fortran program described in [5]. The source codes of the latter program and of the mentioned subroutines PFQ and CLOGAM were downloaded from the Computer Physics Communications Program Library [30]. In order to improve the accuracy of the Kohn-Sham potential function, the program described in [5] was modified by converting it from single-precision arithmetic to double precision, decreasing the accuracy criteria for convergence and for eigenvalues (variables "DELRVR" and "DEL",

respectively) by 3 orders of magnitude in comparison with the default values, and increasing the density of the radial grid.

Although there is no explicit limitation on the value of the incident electron energy T_1 in the code of BREMS, it is currently applicable only at electron energies that are not greater than approximately 3 MeV. This is because an increase of the electron energy requires a larger number of terms in the series (1.2) and (1.3), accompanied by an increase of the computation time and the memory requirements. The maximum absolute value of κ_1 and κ_2 that is currently allowed is 500. However, when $k \neq 0$, the recommended upper limit of $\max(\max|\kappa_1|, \max|\kappa_2|)$ for calculation of cross sections is approximately 200 (at larger values of $|\kappa_1|$ and $|\kappa_2|$, the calculation time and the memory requirements would become prohibitive). For sufficiently large values of k / T_1 (greater than approximately 0.7), acceptable accuracy can be achieved even at $T_1 = 10$ MeV. For example, the accuracy at $T_1 = 10$ MeV and $k = 7.5$ MeV is approximately the same as at $T_1 = 3$ MeV and $k = 0.3$ MeV, if the same values of $|\kappa_1|_{\max}$, $|\kappa_2|_{\max}$ and $l_{\max}$ are used in both cases (in order to achieve accuracy of the DCS better than 5 % for all values of θ in this example, $|\kappa_1|_{\max}$, $|\kappa_2|_{\max}$ and $l_{\max}$ should be at least 200). The times of the numerical integration can be also made approximately equal for both values of T_1 by ensuring that the ratio of the truncation radii (R_a) for both values of T_1 is equal to the reciprocal ratio of the corresponding values of p_1. When the kinetic energy of the incident electron is of the order of 1 MeV or greater, the double or quadruple precision is usually sufficient for the analytical integration. This is fortunate, because using multiple precision for the calculation of the entire set of S integrals with large values of $|\kappa_1|_{\max}$, $|\kappa_2|_{\max}$ and $l_{\max}$, which are needed at the mentioned high energies, would result in prohibitive memory requirements. The amount of memory required by BREMS in MP mode (i.e., at a precision level of 38 or more significant digits) does not depend on the precision level used. For example, if $|\kappa_1|_{\max} = |\kappa_2|_{\max} = l_{\max} = 100$ and the other parameters are equal to the default values, then BREMS would allocate approximately 5 GB of memory for calculating all S integrals using MP, and if $|\kappa_1|_{\max} = |\kappa_2|_{\max} = l_{\max} = 150$, then approximately 15 GB of memory would be needed in MP mode. It should be noted that the minimum precision level, which is sufficient for the analytical integration, decreases with increasing truncation radius R_a.

At the low-energy end of the spectrum, the single-electron approximation may not be sufficiently accurate due to an increased importance of the many-electron effects at electron energies of the order of 100 eV or lower. It should also be noted that the choice of the self-consistent central potential in the energy range $T_1 < 1$ keV is more important than in the energy range 1 keV $< T_1 <$ 10 MeV, where that choice has a relatively weak influence on the angular distribution of bremsstrahlung. The final electron energy T_2 is not allowed to be less than 0.1 eV, which means that the photon energy cannot be greater than $T_1 - 0.1$ eV.

BREMS can be run on modern personal computers, with processing times from several minutes to several hours, depending on the user-specified values of Z, T_1, and k and on the accuracy requested. BREMS is a single-threaded application. Consequently, in order to use all computing power of a multiprocessor or multicore system, several instances of BREMS should be run simultaneously. This is a natural approach for calculation of the cross sections for different sets of the physical parameters Z, T_1 and k, because the instances of BREMS using different sets of those parameters are completely independent. However, this approach can also be applied in the case of a single set of physical parameters. In the latter case, the computation of the S integrals may be broken into several parts, differing by the range of variation of l (see (1.9)), or by the type of the integrals computed (numerical or analytical). After the data files with the total S integrals (from 0 to ∞) have been created, the computation should be started from stage 2 (BREMS has the capability to merge the S integral data loaded from multiple files). If the numerical and analytical parts of the S integrals (from 0 to r_0 and from r_0 to ∞, respectively) have been calculated separately, then the computation should be again started from stage 1, but this time with the parameters specifying that the numerical and analytical integrals must be loaded from files rather than calculated.

Most of the input parameters of BREMS are used as arguments of the three mentioned subroutines “S_integrals”, “Bremsstrahlung” and “Brems_fit”. Some of the parameters (such as the

physical parameters Z, T_1 and k) are "shared", i.e., required by all three subroutines, and the other parameters are used by only one or two subroutines (for example, the values of the angle θ are used only by Bremsstrahlung and Brems_fit, and the numerical tolerance for nonlinear fitting is used only by Brems_fit). Descriptions of all those parameters will be given in the next three sections. There are also several parameters that are used only by the main program in order to determine the default values of some other parameters and the sequence of stages that has to be executed. The names, descriptions and default values of the parameters used only by the main program are given below (the parameter numbers are used only to facilitate references to them in this document, and those numbers are different from the parameter numbers defined in the code of BREMS):

Parameter No. 1 ("accuracy_level") is the number 0, ±1, or ±2, specifying the "accuracy level" to be used. If this number is 1 or 2, then several other parameters that have the largest effect on the accuracy and the computation time (such as the limits of κ_1 and κ_2) will be set to the default values corresponding to the lower or higher accuracy, respectively, unless those parameters have been explicitly specified by the user. If the accuracy level is specified with the minus sign, then all those parameters will be assigned the values corresponding to the given accuracy level, even if they have been explicitly set to other values by the user. "accuracy_level" affects 20 parameters: "tol_A", "tol_delta", "j_QP", "Q_last", "Kmax1", "Kmax2", "lmax", "lmax_MP", "lmax_MP_ratio", "vary_h_CS", "vary_h_DCS", "Kmin1", "Kmin2", "isAbs_K1", "isAbs_K2", "k2_breakpoint1", "k2_step0", "k2_step_last", "pr_transition2", and "R_atom". The default values of parameters "Kmax1" and "Kmax2" depend on the chosen accuracy level only when $T_1 > 0.1$ MeV. Otherwise, the default values of those parameters are the same for both accuracy levels (those values depend on the physical parameters T_1, k / T_1, and Z). The default values of the last nine parameters (starting with "Kmin1") are also the same for both accuracy levels (and do not depend on the physical parameters). If the user-specified value of accuracy_level is 0, or if this parameter is not specified by the user, then accuracy_level will be set equal to the default value (1).

Parameter No. 2 ("firstStage") is the number 1, 2 or 3, indicating the first stage to be executed. The default value of this parameter is 1.

Parameter No. 3 ("lastStage") is the number 1, 2 or 3, indicating the last stage to be executed. The default value of this parameter is 3.

Parameter No. 4 ("overwrite") is a "switch" (1 or 0), indicating whether the existing data files should be overwritten or not. This parameter is used as a substitute for three parameters: parameter "iSkip" of subroutine "S_integrals" (in stage 1), parameter "iCalculate" of subroutine "Bremsstrahlung" (in stage 2), and parameter "iFit" of subroutine "Brems_fit" (in stage 3), which tell each of the mentioned subroutines if the data files of the corresponding stage should be overwritten. If any of the mentioned three parameters is explicitly specified by the user, then the specification of the parameter "overwrite" will take priority (a corresponding warning will be displayed in such a case). If this parameter is set equal to −1 (the default value), then it will be ignored, i.e., the mentioned individual switches for each of the three stages will be used instead.

In the next three Sections, the remaining parameters of BREMS will be described in the same order as they appear in the list of formal parameters of each of the mentioned three subroutines "S_integrals", "Bremsstrahlung" and "Brems_fit". Those descriptions provide information about some details of the calculation process, too. The names of almost all parameters are either exactly the same as the names of the corresponding variables in the source code, or they can be transformed into the latter by enclosing the trailing number "1" or "2" with parentheses (this indicates that the variable is an array element).

3. Calculating the *S* integrals

Subroutine "S_integrals" is used for the first stage of the calculation process (see Section 2). The names, descriptions and default values of the formal parameters of S_integrals that can be modified by the user are given below.

Parameter No. 1 ("Z") is the atomic number of the target material (Z).

Parameter No. 2 ("T1") is the kinetic energy of the incident electron (T_1) in MeV.

Parameter No. 3 ("T2") is the kinetic energy of the outgoing electron (T_2) in MeV, or the opposite of the ratio T_2 / T_1. T_2 cannot be less than 0.1 eV. This means that the value of parameter No. 3 must be between −1 and T_1, excluding the range $-0.1\text{ eV}/T_1 < T_2 < 0.1$ eV (the values −1 and T_1 are allowed). ***Note***: this parameter cannot be specified together with parameter No. 4 (see below).

Parameter No. 4 ("Ep") is either the energy of the bremsstrahlung photon (k) in MeV, or the opposite of the ratio k / T_1. The value of parameter No. 4 must be between $-(1 - 0.1\text{ eV}/T_1)$ and $T_1 - 0.1$ eV. ***Note***: this parameter cannot be specified together with parameter No. 3 (see above).

Parameter No. 5 ("IV") is an integer number indicating the type of the interaction potential that must be used. Three types of the interaction potential are currently allowed:

1 – the point-Coulomb potential (unscreened nucleus),

2 – the Thomas-Fermi-Csavinszky (TFC) potential,

3 – the Kohn-Sham (KS) potential.

The default value of parameter "IV" is 3.

Parameter No. 6 ("nterms_max") is the maximum order of the power-series expansion of the wave function, i.e., the maximum number of terms in that expansion, excluding the term of the order 0. The default value of this parameter is 100.

Parameter No. 7 ("pr_transition") is the value of $p_i r$ (i = 1, 2) where the transition from the power series solution in the vicinity of $r = 0$ to the solution method specified by parameter No. 13 ("method") occurs. This transition occurs independently for both i. When negative, this parameter is opposite to the value of r where the transition occurs for the final electron energy ("r_transition"). An additional factor that can cause the transition earlier is a failure for the power series to converge. If IV = 3 (Kohn-Sham potential in tabular format) and pr_transition = 0, then r_transition is set equal to the first value of r in the $V(r)$ data table (this is the recommended option for the case IV = 3). In the case IV = 1 or 2, the recommended value of this parameter is between 5 and 10 (the value of zero is not allowed in this case). If IV = 3 and pr_transition ≠ 0, then r_transition must be less than the first value of r in the $V(r)$ data table. The default value of this parameter is 0 in the case IV = 3, and 10 in the case IV = 2 or IV = 1.

Note: When the final kinetic energy of the electron is of the order of 1 MeV or greater and this parameter is positive, r_transition may become less than 20 × r_incr_max, where "r_incr_max" is the maximum allowed increment of r for numerical quadrature (parameter No. 11). Then the mentioned increment would be decreased automatically, making the numerical integration longer (see also the description of parameter No. 11). In order to avoid this increase of the computation time, pr_transition should be increased, or r_transition should be specified instead.

Parameter No. 8 ("iExact") is an integer number 0, 1 or 2 indicating whether the exact wave function (expressed in terms of the confluent hypergeometric function) should be used at $r <$ r_transition in the case of the point-Coulomb field (this parameter is ignored when IV > 1). If IV = 1 and iExact = 0, then in the range of values of r corresponding to $r <$ r_transition the wave function will be expressed in terms of the power series with the coefficients calculated using the recurrence relations derived from (1.16a,b) (this approach is always applied for

IV > 1). If IV = 1 and iExact ≠ 0, then the wave function at $r <$ r_transition will be calculated using its exact expression (see [6, Eq. (5.76) and Eq. (5.77)]). [The exact expression of the wave function is not used for greater values of r, because the evaluation of the confluent hypergeometric function is sufficiently fast and accurate only for relatively small argument values.] If IV = 1 and iExact = 2, then, in addition to the above, the exact phase shift (1.23) will be used in the asymptotic expression of the wave function (1.18). [The value of $\tilde{\delta}_\kappa$ calculated according to (1.23) is adjusted by adding $2\pi n$, where n is an integer number, so that the final value of $\tilde{\delta}_\kappa$ is between $-\pi$ and π.] Since the values of the phase shifts are sufficient to calculate $\lim_{k\to 0}(kS_1)$ and $\lim_{k\to 0}(kS_2)$ (see the end of Section 1.2), the availability of the simple analytical expression of the exact phase shifts means that it is not necessary to solve the system of differential equations (1.16a,b) numerically in the case $k = 0$, IV = 1, iExact = 2. In the case $k \neq 0$, IV = 1, iExact = 2, the mentioned system is solved (because the functional form of the wave functions is needed in the entire integration range of the numerical integrals), and the exact value of the phase shift is used as an additional "test" point for evaluating the range of the phase shifts. This causes an increase of the effective range if the exact phase shift is outside of the true range of the values of $\tilde{\delta}_\kappa$ obtained from the analysis of the wave functions. The default value of parameter "iExact" is 0.

Parameter No. 9 ("step1") is the increment of $p_1 r$ for solution of the differential equations using the Hamming's modified predictor-corrector algorithm (i.e., when the option "method=1" is used). The recommended value of this parameter is $\leq 10^{-3}$, and the default value is 10^{-3}.

Parameter No. 10 ("pr_incr") is the increment of $p_1 r$ for numerical quadrature using the 10^{th} order Newton-Cotes formula. pr_incr should exceed step1 at least by a factor of 2. The recommended value is ≤0.1. If this parameter is specified with the minus sign, then the value of r_0 (the point of transition from the numerical integration to the analytical integration) will be "rounded up" i.e., the region of the numerical integration will be extended up to the value of the radial coordinate equal to 10^n, $2 \cdot 10^n$ or $5 \cdot 10^n$ in relativistic units, where n is an integer number. This option is useful for creating a library of cross sections for multiple chemical elements, because the integral from r_0 to ∞ (the "analytical" integral) is expressed as a linear combination of the four integrals (1.29), and each of the latter four integrals depends only on r_0, T_1 and k (but not on the atomic number Z). Thus, if the values of r_0, T_1 and k are exactly the same for different Z, then it will be possible to reuse the values of the mentioned four integrals and thus to skip the stage of the analytical integration for some combinations of Z, T_1 and k (in such a case, a change of Z would require only to recalculate the coefficients of the mentioned linear combination, which depend on the phase shifts). The default value or parameter "pr_incr" is 0.1.

Parameter No. 11 ("r_incr_max") is used to define the maximum allowed increment of r for numerical quadrature. This increment may be either specified explicitly or calculated from the rate of decrease of the screening factor (1.17) near $r = 0$:

(a) If r_incr_max is positive, then it is interpreted as the mentioned maximum allowed increment of r. r_incr_max must be chosen so that the relative change of the interaction potential over this distance is much less than 1 (otherwise the numerical quadrature may be insufficiently accurate). An additional requirement is that r_incr_max cannot be greater than 0.05 × r_transition, where "r_transition" is the mentioned point of transition from the power-series solution in the vicinity of $r = 0$ to the algorithm specified by parameter No. 13 ("method") for the final electron energy (see the description of parameter No. 7). If r_incr_max does not conform to this requirement, then it is decreased to 0.05 × r_transition, and pr_incr is decreased proportionally (if pr_incr becomes less than 2 × step1, then step1 is set equal to 0.5 × pr_incr). The actual increment of r is subsequently set equal to r_incr = min(pr_incr/p_1, r_incr_max). If r_incr is decreased in comparison with pr_incr/p_1 (i.e., if

r_incr_max is less than pr_incr/p_1), then both pr_incr and step1 are decreased proportionally. The recommended initial value of this parameter is ≤ 0.1.

(b) A negative value of parameter "r_incr_max" is interpreted as the opposite of the maximum allowed relative decrease of the screening factor (delta_V_series_max) near $r = 0$, which should be used for calculating the initial value of the integration step size and also for its automatic adjustment inside the interval of power-series solution in the vicinity of $r = 0$, i.e., at $r <$ r_transition, where "r_transition" is the value of the radial coordinate corresponding to the transition from the power-series solution in the vicinity of $r = 0$ to the algorithm specified by parameter No. 13 ("method"). In this case, the maximum allowed initial value of the integration step (r_incr_max) is initially set to pr_incr_init/p_1, where "pr_incr_init" is the initial value of parameter No. 10 ("pr_incr"), and then r_incr_max is doubled or halved iteratively until the optimum value is found. This value of r_incr_max is subsequently used to set the initial value of the integration step size "r_incr": if r_incr (which is initially set to pr_incr_init/p_1) is greater than r_incr_max, then the initial value of r_incr will be set equal to r_incr_max. Afterwards, the value of r_incr may be increased automatically, because this increase is capped only by the value of pr_incr_init*iRun/p_1 and (at $r <$ r_transition) by the value of 0.05*r_transition*iRun, where "iRun" is equal 1 or 2 for the initial or "test" numerical integration, respectively. The mentioned automatic increase of r_incr is controlled by parameter No. 32 ("delta_V_max") at $r >$ r_transition, or by the value of delta_V_series_max at $r <$ r_transition (in the latter case, the function whose decrease is being checked is the screening factor rather than the interaction potential).

The default value of parameter "r_incr_max" is –0.01.

Parameter No. 12 ("nPoints") is the maximum number of points used for the numerical integration. Normally, the numerical integration should end when all wave functions have attained their asymptotic form (1.18) and (for IV > 1 or R_atom ≠ 0) the absolute values of both phase correction integrals become less than the user-specified tolerance. This should happen before the maximum number of points is reached, because otherwise the analytical integration will be insufficiently accurate or will not be performed at all. Consequently, nPoints should be set to any sufficiently large number (for example, 100 000 000, which is the default value).

Parameter No. 13 ("method") controls the method of the numerical solution of the system of ODEs (1.16). In the case "method=1", the Hamming's modified predictor-corrector method is used. In the case "method=2", the Runge-Kutta formula pair (7,8) is used. In the case "method=3", the power-series solution method is used. The default value of this parameter is 3. ***Note***: All these methods are essentially equivalent in terms of the accuracy. The power-series solution method is usually the fastest, and the Runge-Kutta method is the slowest. The Runge-Kutta and the power-series solution methods are less likely to cause a premature termination of the solution routine due to a numerical error when κ_1 and κ_2 is too large. Sometimes, this is a disadvantage, because such an error condition is used by the program to reduce the maximum value of κ_1 or κ_2 and thus to reduce the total calculation time (due to a reduction of the number of S integrals and of the number of terms in the truncated series (1.2) and (1.3)). In the case "method=1", such an error occurs when the number of bisections of the initial increment becomes greater than 10.

Parameter No. 14 ("pr_Bessel") is the value of $p_2 r$ that must be exceeded in order to start checking periodically if the wave functions have attained the asymptotic form (1.18). If $p_2 r <$ pr_Bessel, then the numerical solution of the differential equations (1.16a,b) will continue without calculating the factor A_κ and the phase shift $\tilde{\delta}_\kappa$ (see (1.18) and (1.26)). If pr_Bessel < 0, then it is interpreted as the opposite of the value of r that must be exceeded in order to start calculating A_κ and $\tilde{\delta}_\kappa$. Normally, this parameter should be 0 (this is the default value).

Parameters No. 15 – 17 ("Kmin1", "Kmax1" and "isAbs_K1", respectively) are the minimum and maximum values of κ_1, and a "switch" indicating if those values should be interpreted as

absolute values. If isAbs_K1 = 1, then both Kmin1 and Kmax1 must be positive, and the program will calculate the S integrals for two ranges of κ_1: $-\text{Kmax1} \le \kappa_1 \le -\text{Kmin1}$ and $\text{Kmin1} \le \kappa_1 \le \text{Kmax1}$. If isAbs_K1 = 0, then only the latter range of the values of κ_1 will be used (in this case, Kmin1 and Kmax1 may be either positive or negative). The absolute values of Kmin1 and Kmax1 cannot be greater than the integer parameter "sz" defined by the "parameter" statement in "Brems.f90" (at the time of this writing, sz = 500). The latter parameter is used in declarations of several static arrays. Normally, Kmin1 = 1 and isAbs_K1 = 1. This is the recommended (and default) setting if the S integrals are to be used for calculation of bremsstrahlung cross sections. The default value of Kmax1 is calculated by interpolation between 32 tabulated values of Kmax1 corresponding 8 values of T_1 (10 eV, 100 eV, 1 keV, 10 keV, 100 keV, 1 MeV, 3 MeV, 10 MeV) and 4 values of k / T_1 (0, 0.1, 0.4, 0.95). The interpolation with respect to T_1 is linear-log (logarithmic in T_1), and the interpolation with respect to k / T_1 is linear-linear. If $T_1 > 0.1$ MeV, then the interpolated value of Kmax1 is rounded to the nearest multiple of 5 (when $k \ne 0$, this rounding is needed to facilitate reusing the values of the integrals S_{11}, S_{12}, S_{21} and S_{22} defined by (1.29) at default values of parameters, when the method of partial-wave interpolation is applied). The mentioned tabulated values corresponding to T_1 = 1 MeV, 3 MeV and 10 MeV depend on the chosen accuracy level (1 or 2) defined by parameter No. 1 of the main program ("accuracy_level"), which is described in Section 2. For $Z \le 7$, those values depend on Z, too (in this interval of values of Z, the default value of Kmax1 increases linearly with decreasing Z). If $k = 0$ and $T_1 > 0.1$ MeV, the interpolation with respect to T_1 and Z is performed using a different set of tabulated values than in the case $k \ne 0$ (the tabulated values of Kmax1 corresponding to $k = 0$ are greater than in the case $k \ne 0$).

Parameters No. 18 – 20 ("Kmin2", "Kmax2" and "isAbs_K2", respectively) are the minimum and maximum values of κ_2, and a "switch" indicating if those values should be interpreted as absolute values. Their interpretation and the limiting values are the same as in the case of the parameters No. 15 – 17. Normally, Kmin2 = 1 and isAbs_K2 = 1. This is the recommended (and default) setting if the S integrals are to be used for calculation of bremsstrahlung cross sections. The default value of Kmax2 is the smaller of these two numbers: the default value of Kmax1 corresponding to the current values of T_1 and k / T_1 (see above), and the default value of Kmax1 corresponding to $T_1 = T_2$ and $k = 0$.

Parameters No. 21 – 23 ("k2_breakpoint1", "k2_step0" and "k2_step_last", respectively) control the application of the partial-wave interpolation method described in Section 1.3. They are used for defining the set of values of κ_2 that have to be "skipped" in order to reduce the number of the S integrals to be calculated and the number of the systems of ODEs (1.16a,b) corresponding to the final electron energy to be solved. If the partial-wave interpolation method is applied, then the subroutine Bremsstrahlung (called in stage 2) will subsequently calculate the terms corresponding to the skipped values of κ_2 in the expressions of the cross sections (1.2) and (1.3) by logarithmic cubic spline interpolation as explained in Section 1.3. In stage 1 (subroutine S_integrals), this skipping of values of κ_2 is possible only when isAbs_K2 = 1 (otherwise, these three parameters are ignored and no values of κ_2 are skipped). In stage 2 (subroutine Bremsstrahlung), the condition for the partial-wave interpolation is more restrictive: Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1. "k2_breakpoint1" is the initial point of the range of values of $|\kappa_2|$ where the mentioned removal of points should be applied. If $\text{k2\_breakpoint1} \ge \text{Kmax2}$ or $\text{k2\_breakpoint1} < 1$, then no values of κ_2 will be skipped and parameters No. 22 and No. 23 will be ignored. "k2_step0" is the increment to obtain the next value ("breakpoint") of $|\kappa_2|$ that should be retained (i.e., k2_breakpoint2 is equal to k2_breakpoint1 + k2_step0). "k2_step_last" is the approximate interval between the last two breakpoints of $|\kappa_2|$. k2_step_last cannot be less than k2_step0. If $\text{k2\_step\_last} > \text{k2\_step0}$, then the intervals between the retained values of $|\kappa_2|$ will approximately form an arithmetic progression. If $\text{k2\_step\_last} = \text{k2\_step0}$, then all intervals will be equal to each other, except

possibly for the last interval, which in this case may be less than k2_step0 (this happens when Kmax2 – k2_breakpoint1 is a not multiple of k2_step0). In any case, the last breakpoint is equal to Kmax2. For example, if k2_breakpoint1 = 30, k2_step0 = k2_step_last = 5 and Kmax2 = 70, then the set of retained values of $|\kappa_2|$ will be 1 – 30, 35, 40, 45, 50, 55, 60, 65, 70. If the latter set of parameters is modified by increasing Kmax2 to 72, then the value 72 will be added to the mentioned set of values of $|\kappa_2|$ (i.e., the difference of the last two breakpoints of κ_2 in this case would be 2). Another example with an increasing set of the intervals: k2_breakpoint1 = 40, k2_step0 = 5, k2_step_last = 10 and Kmax2 = 130. In this case, the set of retained values of $|\kappa_2|$ would be the following: 1 – 40, 45, 50, 56, 63, 70, 77, 85, 93, 101, 110, 120, 130. If the photon energy (parameter "Ep") is non-zero and parameter Kmax2 is greater than or equal to 80, or if Ep = 0 and parameter Kmax2 is greater than or equal to 120, then the default values of these three parameters are the following: k2_breakpoint1 = 30, k2_step0 = 5, k2_step_last = 5. Otherwise, k2_breakpoint1 = 0 (i.e., the partial-wave interpolation is not applied).

Parameter No. 24 ("lmin") is the minimum value of l in (1.9). Normally, lmin = 0. This is the recommended (and default) minimum value of l if the S integrals are to be used for calculation of bremsstrahlung cross sections.

Parameters No. 25 and No. 26 ("lmax" and "lmax_MP", respectively) are the two alternative maximum values of l (l_{max}) in (1.9). If optimization of the precision level is not requested (see the description of parameter No. 35 below), then lmax_MP will be used if the requested number of significant digits is greater than 21 (i.e. if the quadruple or multiple precision is required), and lmax will be used if the requested number of significant digits is less than 22 (i.e., if the double precision is required). The value of lmax cannot be less than lmax_MP. Two alternative values of l_{max} are used because it is known that the contribution of an S integral to the sum (1.9) decreases rapidly with increasing l (especially at low photon energies). However, it is not known beforehand which value of l_{max} is necessary for a sufficiently accurate estimation of cross sections. Since the sensitivity of the cross sections to the value of l_{max} is tested during the next stage (by the subroutine Bremsstrahlung), the user may wish to risk using a smaller value of l_{max} and thus decrease the time of calculating the S integrals. If it later turns out that l_{max} is too small, the S integrals may be recalculated using a larger value of l_{max}. In such a case, the previously-calculated set of numerical integrals may be reused, because the numerical integrals are always calculated for all values of l up to lmax (if the total integrals are calculated using a smaller set of the values of l and if lastStage = 1 or del_S_int = 0, then the "_n" file is not deleted after the analytical integration). Since the calculations using MP and QP are much slower than the calculations using DP, one should take a greater "risk" in the case of MP or QP than in the case of DP (hence lmax_MP ≤ lmax). If optimization of the precision level is requested and lmax_MP < lmax, then the value of l_{max} is also optimized. In such a case, the parameters lmax_MP and lmax are treated as the limits of variation of l_{max} (for a more detailed explanation, see the description of parameter No. 35). If one does not wish to truncate the sum in (1.9), then both lmax_MP and lmax should be set equal to max(|Kmin1|,|Kmax1|)+max(|Kmin2|,|Kmax2|)+1, or to any larger number. If Kmin1=Kmin2=1, isAbs_K1=isAbs_K2=1 and Kmax1=Kmax2 (or, equivalently, Kmin1 = –Kmax1 = Kmin2 = –Kmax2 and isAbs_K1=isAbs_K2=0), then the range of variation of l in (1.9) is from 0 to 2*Kmax1. In the case "accuracy_level=1", the default value of lmax is equal to $\max(|\kappa_1|_{max},|\kappa_2|_{max})$. In the case "accuracy_level=2", the default value of lmax is equal to $\max(|\kappa_1|_{max},|\kappa_2|_{max}) + (\min(|\kappa_1|_{max},|\kappa_2|_{max}) / 4)$. The default value of lmax_MP is equal to lmin + (lmax –lmin) * lmax_MP_ratio, where the parameter "lmax_MP_ratio" is described below.

Parameter No. 27 ("lmax_MP_ratio") is interpreted as the ratio (lmax_MP – lmin) / (lmax – lmin). If lmax_MP is not specified by the user or if lmax_MP_ratio is non-zero, then the value of lmax_MP will be calculated using the values of lmax and lmax_MP_ratio (if lmax_MP is not specified by the user and lmax_MP_ratio is zero, then lmax_MP_ratio will be reset to the

default value). If lmax_MP is specified by the user and lmax_MP_ratio is zero, then the user-specified value of lmax_MP will be used. By default, the value of lmax_MP_ratio is linearly interpolated with respect to k / T_1 from a predefined value at $k / T_1 = 0$ to 1 at $k / T_1 \geq 0.95$. This interpolation has been implemented because it was noticed that in the case of a strongly peaked angular distribution of bremsstrahlung photons the values of the DCS corresponding to large angles ($\theta > 150°$) are especially sensitive to the truncation of the series (1.9) with respect to l, and this effect becomes more pronounced with increasing k / T_1. The mentioned predefined value of lmax_MP_ratio at $k / T_1 = 0$ is equal to 1/3. If lmax – lmin < 80, then a linear interpolation with respect to lmax – lmin is applied in addition to the mentioned interpolation with respect to k / T_1, with the value obtained by the latter interpolation used as the minimum value of lmax_MP_ratio (it corresponds to lmax – lmin = 80), and with the maximum value of lmax_MP_ratio equal to 1 (it corresponds to lmax = lmin). Since the default value of lmax_MP is equal to lmin + (lmax – lmin) * lmax_MP_ratio, the mentioned linear interpolation of lmax_MP_ratio with respect to lmax – lmin causes a quadratic dependence of the default value of lmax_MP on lmax – lmin. If this dependence has a maximum at lmax – lmin < 80, then it is additionally "capped" by reducing it to the value corresponding to lmax – lmin = 80. This is done in order to prevent the default value of lmax_MP from increasing after lmax is reduced.

Parameters No. 28 and No. 29 ("tol_A" and "tol_delta", respectively) are the maximum allowed relative range of the last 10 calculated values of the normalization factor A_κ and the phase shift $\tilde{\delta}_\kappa$ needed to switch from the numerical solution using the algorithm specified by parameter No. 13 ("method") to the approximate phase-shifted free-space solution (1.18), respectively. The parameter tol_delta may be negative. Then it will be interpreted as the opposite of the maximum allowed absolute range of $\tilde{\delta}_\kappa$ (in radians). If parameter No. 31 ("R_atom") is zero, then the recommended value of tol_A is from $2 \cdot 10^{-9}$ to 10^{-7}, and the recommended value of tol_delta is from $-2 \cdot 10^{-9}$ to -10^{-7} (a smaller value of tol_A or tol_delta may cause numerical difficulties, resulting in a failure to attain the asymptotic form (1.18)). If parameter "R_atom" is non-zero and parameter No. 13 ("method") is equal to 3, then both tol_A and tol_delta are equal to zero by default. If R_atom is zero, or if "method" is not equal to 3, and the photon energy ("Ep") is non-zero, then the default value of tol_A is 10^{-7} or $2 \cdot 10^{-9}$, depending on the chosen accuracy level (1 or 2, respectively) defined by parameter No. 1 of the main program ("accuracy_level"), which is described in Section 2. The corresponding default value of tol_delta is -10^{-7} or $-2 \cdot 10^{-9}$, respectively. If R_atom is zero, or if "method" is not equal to 3, and the photon energy ("Ep") is zero, then the default values of parameters tol_A and tol_delta do not depend on the accuracy level and are equal to $2 \cdot 10^{-9}$ and $-2 \cdot 10^{-9}$, respectively.

Note: The number of roughly equidistant values of r where A_κ and $\tilde{\delta}_\kappa$ are calculated is stored in the integer variable "ntest", and the approximate interval between the adjacent values of $p_1 r$ corresponding to the mentioned "test" values of r (i.e., the period of updating A_κ and $\tilde{\delta}_\kappa$) is stored in the integer variable "d_pr_test0" (at the time of this writing, ntest = 10 and d_pr_test0 = 50). These "test" values of r are the same for all wave functions. The updates of the average values of the normalization factors A_κ and the phase shifts $\tilde{\delta}_\kappa$ and the calculation of their ranges of variation are done at two alternating intervals of the radial coordinate r: each odd-numbered update is done after an interval of $(n_1 + 0.5)\pi/p_1$, and each even-numbered update is done after an interval of $(n_2 + 0.5)\pi/p_2$, where n_1 and n_2 are integers, which are chosen so that both those intervals are approximately equal to d_pr_test0 / p_1 = 50 / p_1. Those values of the update periods have been chosen in order to maximize the cancellation of the oscillating term in the normalization factors and the phase shifts (see Section 1.2), and thus to improve the accuracy of the mentioned average values (the radial period of the mentioned oscillations is equal to π / p).

Parameter No. 30 ("pr_transition2") is the minimum value of $p_2 r$ corresponding to transition to analytical integration. If pr_transition2 < 0, then it will be interpreted as the opposite of the minimum value of r where the transition occurs ("r0_min"). When all wave functions attain their asymptotic form and (for IV > 1 and R_atom ≤ r0_min) the absolute values of both phase correction integrals decrease below the tolerance defined by parameter No. 34, the program will end the numerical integration if the current value of $p_2 r$ is greater than pr_transition2. Otherwise, the numerical integration will continue up to the point r = r0_min = pr_transition2 / p_2. The value of r0_min may be optionally "rounded up" as explained in the description of parameter No. 10. The default value of this parameter depends on whether parameter No. 31 ("R_atom", indicating the atomic radius) has been explicitly specified by the user and on whether the photon energy is non-zero. If R_atom has not been specified and the photon energy is non-zero, then the default value of pr_transition2 is $-\max(800, 126/p_2)$ (i.e., r0_min is equal to either 800 or twenty periods of the final electron wave function, whichever is greater). Otherwise, the default value of pr_transition2 is 0. If R_atom > r0_min (i.e., the potential function is truncated, and the truncation radius is greater than r0_min), then the point of transition to analytical integration coincides with R_atom.

Parameter No. 31 ("R_atom") is the "atomic radius", defined as the value of the radial coordinate where the interaction potential $V(r)$ becomes zero, i.e., is "truncated". If this parameter is zero, then the interaction potential will not be truncated. Although the results obtained in the latter case may be more accurate (provided that the absolute value of parameter No. 34 is small enough), the computation time may become prohibitively long if the electron energy is greater than 1 MeV and the decrease of the screening factor is very slow. Besides, it is usually possible to achieve a negligibly small difference between the results obtained with R_atom = 0 and with R_atom ≠ 0 by a judicious choice of the value of R_atom. It should be much greater than the typical distance from the nucleus to the point where the interaction event occurs. The latter distance is approximately equal to the inverse of the minimum momentum transfer [24], which is equal to $q_{\min} = p_1 - p_2 - k$ (see also Section 1.3). For example, if $1 / q_{\min}$ is of the order of 10, then the value R_atom = 500 should be sufficient to achieve acceptable accuracy. If this parameter is negative, then it is interpreted as the opposite of the factor that must be used for multiplying the inverse minimum momentum transfer in order to calculate the value of R_atom. In the latter case, the previous parameter (r0_min) "doubles up" as the minimum allowed value of R_atom (i.e., if the calculated value of R_atom is less than r0_min, then R_atom is set equal to r0_min). The default value of this parameter is –20 if $T_1 < 1$ MeV, and –13 if $T_1 \geq 1$ MeV.

Notes: **1)** If this parameter is non-zero, then the phase correction integrals will be calculated only for $r <$ R_atom (according to (1.28)). **2)** Even if the wave function has not attained the asymptotic form at r = R_atom, the numerical solution algorithm is terminated anyway. In such a case, the phase shift and the normalization factor are calculated on the basis of the values of g_κ and f_κ at the first point satisfying the condition $r \geq$ R_atom, and the corresponding uncertainties (range widths) are set to zero. **3)** If r0_min < R_atom, then, as mentioned in the description of parameter No. 30, the point of transition to analytical integration (r_0) is set equal to R_atom. Consequently, at electron energies greater than 1 MeV, the judicious choice of R_atom (see above) usually results in a significant reduction of r_0 in comparison with the case when the potential function is not truncated (R_atom = 0). Since a decrease of r_0 may cause an increase of the precision level needed to compute the analytical integrals to an acceptable accuracy (and hence a significant increase of the time of the analytical integration), it may be advantageous to specify a value of r0_min greater than R_atom (or to increase R_atom) when the electron energy is greater than 1 MeV (see the description of parameter No. 30).

Parameter No. 32 ("delta_V_max") controls the option of doubling the size of the integration step automatically if it is less than 0.5*pr_incr_init*iRun/p_1, where "pr_incr_init" is the initial value of parameter No. 10 ("pr_incr") and "iRun" is equal 1 or 2 for the initial or "test" numerical

integration, respectively, and also less than half of the distance corresponding to a predefined value of the relative decrease of the interaction potential $V(r)$. Enabling this option causes a reduction of the time of numerical integration at low energies (especially in the case of the point-Coulomb potential). The value of parameter "delta_V_max" is interpreted as the mentioned maximum relative decrease of $V(r)$. This parameter is used only outside of the interval of the initial power-series solution, i.e., in the range of values of r where the wave functions corresponding to all values of κ_1 and κ_2 are calculated either by iterative solution of the coupled radial Dirac equations (using the method specified by parameter No. 13) or by evaluating the asymptotic expressions (1.18). If delta_V_max is zero, then the integration step will be fixed outside of the interval of the initial power-series solution. Inside the interval of the initial power-series solution, the size of the integration step is controlled using parameter No. 11 "r_incr_max" (see above). The default value of parameter "delta_V_max" is 0.01.

Parameter No. 33 ("j_QP") is an integer number 0, 1, or 2, which defines the way the quadruple-precision (QP) arithmetic should be used during the numerical quadrature when calculating the spherical Bessel function of the first kind $j_l(kr)$, which is used as a factor in the integrands of the S integrals (1.15). If j_QP=0, then QP will not be used, except when $kr > 5000$ and the required accuracy of the explicit formula (1.30a) cannot be achieved with double precision. If j_QP=1, then, in addition to the above, QP will be used for calculating $j_l(kr)$ at $kr \leq 5000$ (where $j_l(kr)$ is calculated by backward recursion). If j_QP=2, then, in addition to the above, QP will always be used for calculating $j_l(kr)$ at $kr > 5000$. By default, j_QP=0 in the case "accuracy_level=1", and j_QP=2 in the case "accuracy_level=2".

Parameter No. 34 ("Q_last") is the value of the phase correction integrals "Q(1)" and "Q(2)" that must be exceeded for the transition to analytical integration to occur. In the case of screened or truncated potentials (IV > 1 or R_atom ≠ 0), Q is negative and approaches zero when r is increased (see (1.27) and (1.28)). Consequently, Q_last should be the opposite of the maximum absolute value of Q(1) and Q(2). In the case of the Coulomb potential (IV = 1 and R_atom = 0), the values of Q(1) and Q(2) are never used for determining the point of transition to analytical integration, because in this case Q does not have a limiting value. In order to similarly ignore Q(1) and Q(2) when IV > 1 or R_atom ≠ 0, Q_last should be set to zero. When R_atom = 0 and Q_last = 0, the truncation radius of the potential function is determined "dynamically", based on the magnitudes of the ranges of variation of the normalization factor "A" and the phase shift "delta" (given by parameters No. 28 and No. 29). In this case, the truncation radius is equal to the value of the radial coordinate where the mentioned ranges of variation for all values of κ_1 and κ_2 and for both energies of the electron become less than the specified tolerances "tol_A" and "tol_delta", and the asymptotic expressions of the wave functions (in terms of the spherical Bessel functions) are never used for calculating the S integrals before the truncation radius is reached (even if the ranges of variation of the estimates of the normalization factors and phase shifts for a particular pair of values of E and κ are less than the corresponding tolerances "tol_A" and "tol_delta").

In the case of a non-zero photon energy, the recommended value of Q_last is from -10^{-10} to -10^{-8}. A larger value of Q_last may have to be used if the electron energy is greater than 1 MeV, or if the decay of the screening factor $\tilde{V}(r)$ is very slow, in order to reduce the time of numerical integration, especially if the interaction potential is not "truncated" (see the description of parameter No. 31). In the case of a non-zero photon energy, the default value of this parameter is -10^{-8} or -10^{-10}, depending on the chosen accuracy level (1 or 2, respectively) defined by parameter No. 1 of the main program ("accuracy_level"), which is described in Section 2. In the case of zero photon energy, the default value of this parameter is zero.

Parameter No. 35 ("ndp") is the approximate number of significant digits used for calculation of the analytical integrals. When ndp < 0, it is the opposite of the initial number of digits, and the program will attempt to "optimize" the precision level as explained in Section 1.3, i.e., it will attempt to reduce the number of significant digits without affecting the final values of the

analytical integrals rounded to 12 significant digits. In addition, if lmax_MP < lmax, the value of l_{max} will be optimized, too, i.e., it will be decreased in steps of max(0.1(l_{max}–l_{min}), 5) starting with "lmax" until double precision becomes sufficient, or until a user-specified minimum value of l_{max} ("lmax_MP") is reached (the previously mentioned optimization of the precision level will be performed for each value of l_{max}). If ndp = 0, then the analytical integration will not be performed, and only the file with the numerical integrals (file name suffix "_n") will be created. In order to extract the numerical integral data from an existing complete file and to create the corresponding "_n" file, the options ndp = 0 and iSkip = –2 should be used (see the description of parameter No. 37 below). If ndp > 0, then the specified precision level will be used. When ndp is positive, it cannot be less than 15 or greater than 1000. When ndp is negative, it cannot be greater than –22 or less than –1000. When min($T_1 - k$, k) ≤ 100 keV, the default value of this parameter is –300. Otherwise, the default value of this parameter is –100.

Note: In the case of large values of |Kmax1|, |Kmax2| and |lmax|, multiprecision calculations may require a prohibitive amount of memory (this amount does not depend on the precision level used, as long as the latter corresponds to the MP mode, i.e., more than 37 significant digits). For example, if |Kmax1| = |Kmax2| = |lmax| = 100 and the other parameters are equal to the default values, then approximately 5 GB of memory will be needed for calculating all S integrals using MP, and if |Kmax1| = |Kmax2| = |lmax| = 150, then approximately 15 GB of memory would be needed in MP mode. The smallest absolute value of ndp corresponding to the MP mode is 44. Consequently, in order to ensure that the program never attempts to allocate such amount of memory and quits with an error message after determining that quadruple precision is not sufficient, ndp should be set equal to –44.

Parameter No. 36 ("iTestRun") indicates if the mentioned test numerical integration (with all tolerances and step sizes increased by a factor of 2) should be performed. If this parameter is positive, then the test integration will be performed, and if it is 0 or negative, then the test integration will not be performed (see also Section 1.4). In addition, this parameter is used for creating a file with the integrals of the products of three spherical Bessel functions and r^2 from r_0 to ∞ (the integrals S_{11}, S_{12}, S_{21} and S_{22}, defined by (1.29)), and for loading the values of those integrals from an existing file. Unless changed by the user, the name of this file is formed by combining the prefix "S_integrals_" and the values of the incident electron energy (T_1), bremsstrahlung photon energy (k), the lower bound of the integrals (r_0) and the suffix "_a". Consequently, this file will be called the "_a" file. In order to skip the numerical integration and create the "_a" file, this parameter must be set equal to –2. In order to calculate the second part of the S_1 and S_2 integrals by combining the values of the S_{ij} integrals (i, j = 1, 2) loaded from an existing "_a" file, this parameter must be set equal to 2 or –1 (in the first case, the test numerical integration will be performed, and in the second case it will not be performed). The name of an existing "_a" file is defined using the parameters No. 41 – 43.

In the case k = 0, only the options "iTestRun=0" and "iTestRun=1" are allowed. Since the S integrals are not calculated numerically in the case k = 0 (see the end of Section 1.2), the option "iTestRun=1" is applied in this case only to the process of solving the coupled radial Dirac equations (1.16a,b). I.e., when iTestRun=1, the system of ODEs is solved using two sets of computational tolerances and step sizes. Thus, two sets of phase shifts and normalization factors are obtained. The differences of the corresponding phase shifts and normalization factors in the mentioned two sets are used for estimating their uncertainties.

The default value of parameter "iTestRun" is 1.

Parameter No. 37 ("iSkip") defines the actions that must be taken when a data file with the current name already exists. The allowed values of this parameter are 0, ±1, ±2, and –3. If this parameter is equal to 0 and a file with the current name already exists, then the output file name will be modified by appending a suffix "_1", or "_2", …, or "_999". A value of 1 indicates that processing should be skipped after determining that a data file with the original name already exists (this applies both to the complete file and to the file with the numerical integrals, i.e., the

"_n" file). A value of 1 is useful for resuming an interrupted batch run. A value of −1 indicates that the data file must be overwritten if it exists. A value of 2 indicates that the numerical integral data must be loaded from the existing "_n" files if there are no existing complete files (otherwise it is equivalent to 1, i.e., no processing). A value of −2 is equivalent to +2 if there is no existing complete file, otherwise it indicates that the complete file must be overwritten after extracting the numerical integrals from the existing "_n" file or from the complete file if there is no "_n" file. In order to extract the numerical integral data from an existing complete file and to create the corresponding "_n" file, the options ndp = 0 and iSkip = −2 should be used ("ndp" is set by parameter No. 35). The option "iSkip=-3" differs from "iSkip=-2" in that an existing complete file is not overwritten. Instead, a new file with an additional suffix "_1", "_2", etc is created (as in the case "iSkip=0"). If there is no complete file, then the option "iSkip=-3" is equivalent to "iSkip=-2" or "iSkip=2". If iSkip is equal to −3, then, in order to load the numerical integrals from files, the "_n" file or the complete file without the subscript ("_1", "_2", etc.) in the file name must exist (otherwise, the numerical integrals will be calculated instead of being loaded from files, even when the "_n" files or the complete files with subscripts "_1", "_2", etc. are available). In the case of zero photon energy, iSkip cannot be equal to ±2 or −3 (in this case, the name of the file with the phase shift data must be specified using parameters No. 40, No. 42, and No. 43). If the numerical *S* integral data have to be loaded from existing files and there are several files with names differing from the specified name only by the suffix "_1", "_2", …, "_999" at the end, then the data will be read from all those files, too. The default value of this parameter is −1.

Parameters No. 38 and No. 39 ("prefix" and "suffix", respectively) are the character strings that should be inserted at the beginning and at the end of the name of the file with the *S* integral data. The file name suffix does not include the extension (the file name extension is always ".dat"). The file name prefix may include the folder name (folder names must be terminated with the slash '/'). If parameter No. 38 is an empty string (specified by writing a space after "prefix=") then no prefix will be used, and the file with the *S* integral data will be created in the current folder. If parameter No. 39 is an empty string, then no suffix will be used. In order to specify an arbitrary name, parameter No. 38 must be the period '.', and parameter No. 39 must be the name of the file (possibly with the folder name and without the extension ".dat"). If parameter No. 38 is not the period '.', then the default name (with the optional prefix and suffix) will be used. In absence of the prefix or the suffix, the default name has the following format: "S_integrals_Z_T.TE±XX_k.kkkE±YY.dat", where "Z" is the atomic number consisting of 1, 2 or 3 digits, "T.TE±XX" is the kinetic energy of the incident electron (MeV) rounded to 2 significant digits in scientific notation, and "k.kkkE±YY" is the kinetic energy of the bremsstrahlung photon (MeV) rounded to 4 significant digits in scientific notation ("E±XX" and "E±YY" are the respective decimal exponents). If parameter No. 36 ("iTestRun") is equal to −2, then the default name format is "S_integrals_T.TE±XX_k.kkkE±YY_r.rE±PP_a.dat", where "r.rE±PP" is the lower bound of the integrals (1.29) rounded to 2 significant digits in scientific notation ("E±PP" is the decimal exponent). By default, parameters "prefix" and "suffix" are equal to empty strings.

Parameters No. 40 – 43 ("Ep00", "r_fileName", "prefix0" and "suffix0", respectively) are needed only in the case of zero photon energy, when the phase shifts have to be loaded from a data file corresponding to an earlier calculation rather than calculated by solving the system of ODEs (1.16a,b), or when the integrals from r_0 to ∞ must be calculated by combining the values of the S_{ij} integrals ($i, j = 1, 2$) defined by (1.29), which are stored in an existing "_a" file. Those four parameters define the name of the phase shift data file or the "_a" file. In the case of zero photon energy, parameter No. 40 is the photon energy (MeV) used for creating the phase shift data file, or the opposite of its ratio to the incident electron energy. If $k = 0$ and parameter No. 40 has not been explicitly specified, then the program will calculate the phase shifts by solving the system of ODEs (1.16a,b) instead of loading the phase shifts from file. Otherwise, it

will be assumed that the atomic number, incident electron energy and the type of the interaction potential used for creating the phase shift data file are the same as specified by parameters No. 1, No. 2, and No. 5. In the case of non-zero photon energy and iTestRun = 2 or −1 (i.e., when these parameters define the name of an existing "_a" file), parameter No. 41 is the value of the lower integration bound (r_0) that must be used to form the name of the "_a" file (assuming that it is formed in the default manner). If this parameter is zero, then the file name will be formed using the actual value of r_0, which may be calculated by the program or specified by parameter No. 30. If the name of the phase shift data file or the "_a" file has been formed in the default manner (see the description of parameters No. 38 and No. 39), then parameters No. 42 and No. 43 are used to specify those prefix and suffix, respectively. They are interpreted in the same way as parameters No. 38 and No. 39 described above. In particular, if parameter No. 42 is the period '.', then parameter No. 43 must specify the full name of the phase shift data file or the "_a" file (parameter No. 40 or No. 41 is ignored in this case). There is only one difference in treatment of parameters No. 42 and No. 43 in comparison with treatment of parameters No. 38 and No. 39: if the name of the output file is formed in the default manner, then the default values of parameters No. 42 and No. 43 are equal to the specified values of parameters No. 38 and No. 39, respectively (rather than to the empty strings). Otherwise, the default values of parameters No. 42 and No. 43 are equal to the empty strings. The default value of parameter r_fileName is 0.

Parameter No. 44 ("dir_V") is the name of the folder with the data files defining the interaction potentials in tabular format. If the specified folder name is incomplete, i.e., if it does not start with the forward slash '/' or the backslash '\' and does not contain the colon ':', then it is assumed to be a subfolder either of the BREMS installation folder or of the current folder, depending on whether the path to the BREMS executable file has been specified before its name on the command line or not. The default value of this parameter is 'V/Kohn-Sham'.

Parameter No. 45 ("start_suffix") is an integer number from 0 to 999 indicating the starting value of the additional suffix "_<number>" that is automatically appended to the name of the output file (a value of 0 means that there will be no additional suffix; see also the description of parameter No. 37). The default value of this parameter is 0.

Parameter No. 46 ("del_S_int") is a "switch" (1 or 0) indicating if the file with the numerical integration data (the "_n" file) should be deleted after a successful calculation of the total S integrals (from 0 to ∞). The value "1" of this parameter (indicating deletion of the "_n" file) will have an effect only if the numerical integrals were calculated in the current run, rather than loaded from an existing file. The default value of this parameter is 1. ***Note***: This parameter is also used by the subroutine Bremsstrahlung, where it has a different meaning (see the description of parameter No. 28 in Section 4).

As mentioned, the recommended values of Kmin1, isAbs_K1, Kmin2 and isAbs_K2 (i.e., parameters No. 15, No. 17, No. 18, and No. 20) are the following: Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1. Although mathematically this set of parameters is equivalent to Kmin1 = –Kmax1, Kmin2 = –Kmax2 and isAbs_K1 = isAbs_K2 = 0, the former set is the recommended one, because only in that case the program will automatically decrease Kmax1 or Kmax2 if the user-specified value does not correspond to the available data, or if a difficulty is encountered during the numerical solution of the system of ODEs (1.16a,b). If another set of the mentioned parameters is used and if such an abnormal situation occurs, processing will be terminated immediately with an error message. This remark applies both to Brems.exe and to Read_S_integrals.exe.

During execution of stage 1, the subroutine S_integrals displays some real-time information about the calculation process. To avoid text wrapping (which would reduce readability of the output data on the screen), the screen buffer width must be at least 235 (in Windows this can be achieved, e.g., by entering "mode 235" at the command prompt in the console window before starting the

calculation). At the start of the calculation, the total number of S integrals is displayed. Since the analytical integration is performed by calculating the integrals of products of three spherical Bessel functions and r^2 (1.29) and then combining them according to (1.15) and (1.18), the number of the latter integrals is displayed, too. In addition, the total number of terms of the form (1.35) that have to be added up during calculation of the coefficients of the linear combinations of the integrals (1.36a,b) is shown (it is denoted "nterms_tot"). The total time of the analytical integration is roughly proportional to the latter number (another factor that strongly affects the time of the analytical integration is the precision level used). After this preliminary information, the process of the numerical integration begins. During this process, a line with the current values of several variables is printed on the screen every 5 seconds. This line contains the following information:

- the current time of the numerical integration (in seconds),
- the sequence number of the last step of the numerical quadrature ("i"),
- the current value of the radial coordinate r ("r"),
- the percentage done, i.e., the ratio of the current value of r and the limiting radius (this entry is present only if the limiting radius has been defined, i.e., when the interaction potential is "truncated", i.e., when R_atom $\neq 0$, or during the "test" numerical integration, or when pr_transition2 $\neq 0$ and $r <$ pr_transition2 / p_2),
- the current values of $p_1 r$ and $p_2 r$ ("p(1)*r" and "p(2)*r", respectively),
- the number of wave functions that have not attained the asymptotic form yet ("Nasymp"),
- the current values of the S integrals ("S1" and "S2") corresponding to the largest absolute values of κ_1, κ_2 and l (with an additional condition that $\kappa_2 \neq \kappa_1$),
- the maximum ranges of variation of A_κ and $\tilde{\delta}_\kappa$ over the last 10 "test" points ("A_range" and "delta_range").

If the photon energy is zero, then the values of the S integrals are not displayed, because the numerical integration in this case involves only the solution of the coupled radial Dirac equations (1.16a,b) (for the same reason, the numerical integration is much faster in the case $k = 0$ than in the case $k \neq 0$). If A_range and delta_range have not been calculated yet, then they are equal to -1. A_range is the maximum relative range of A_κ, i.e., $\max((A_{\max} - A_{\min}) / \langle A \rangle)$, where $A_{\max}$ and $A_{\min}$ are the maximum and minimum values of A_κ over the last set of "test" points for a given value of κ and a given electron energy, $\langle A \rangle$ is the average value of A_κ over the same set of points, and the overall maximum is calculated over both energies and all values of κ_1 and κ_2. The variable delta_range may be either the maximum relative range of $\tilde{\delta}_\kappa$ or the maximum absolute range depending on the sign of parameter No. 29 (see above), and it is defined similarly to A_range (just replace "A" with "$\tilde{\delta}$" in the previous sentence). When "Nasymp" is non-zero, the values of the numerical integrals that are displayed during the numerical integration may have been calculated using unnormalized wave functions and may therefore differ from the final values by an order of magnitude or more. If all wave functions have attained the asymptotic form (1.18), i.e., if "Nasymp" is zero, but the other conditions for terminating the numerical integration are not satisfied yet, then the last two entries of the output line change: "A_range" and "delta_range" are replaced by the values of the two phase correction integrals ("Q(1)" and "Q(2)").

The indices of the displayed S integrals are indicated in parentheses after "S1" or "S2" in this order: κ_1, κ_2, l.

During the analytical integration, feedback is provided to the user every 10 seconds in the form of messages indicating the percentage of the terms of the type (1.35) calculated.

The information that is displayed after terminating the numerical and analytical integration is mostly self-explanatory. It includes the values of the S integrals and their uncertainties corresponding to the largest absolute values of κ_1, κ_2 and l (with the additional condition that $\kappa_2 \neq \kappa_1$), and the corresponding values of the factors $A_{\kappa 1}$ and $A_{\kappa 2}$ in (1.18) and the phase shifts $\tilde{\delta}_{\kappa_1}$

and $\tilde{\delta}_{\kappa_2}$ (the values of $\tilde{\delta}_{\kappa_1}$ and $\tilde{\delta}_{\kappa_2}$ are adjusted by adding $2\pi n$, where n is an integer number, so that the final values of the phase shifts are between $-\pi$ and π), as well as some overall statistics, such as the maximum change of the numerical S_1 and S_2 integrals after increasing the computational tolerances and step sizes by a factor of 2 (the maximum absolute change is denoted "S1_num_maxDiff_abs" and "S2_num_maxDiff_abs", and the maximum relative change is denoted "S1_num_maxDiff_rel" and "S2_num_maxDiff_rel"), and the maximum change of the total S_1 and S_2 integrals after changing the phase shift by the value of the corresponding range (the maximum absolute change is denoted "S1_maxDiff_abs" and "S2_maxDiff_abs", and the maximum relative change is denoted "S1_maxDiff_rel" and "S2_maxDiff_rel"). In the case IV = 1 (unscreened point-Coulomb potential) and iExact = 0 or 1, when the exact values of A_κ and $\tilde{\delta}_\kappa$ are known ($A_\kappa = 1$, and $\tilde{\delta}_\kappa$ are given by (1.23–1.25)) but not used, the exact values of $\tilde{\delta}_\kappa$ are displayed along with the values estimated numerically, so that the accuracy of the numerical solution of the system of differential equations (1.16a,b) can be evaluated if the point-Coulomb field has not been truncated (R_atom = 0). If the point-Coulomb field has been truncated (R_atom $\neq$ 0), then the empirical values of $\tilde{\delta}_\kappa$ should not be expected to be close to the values given by (1.23), but this difference should be approximately the same for all κ if R_atom is sufficiently large (see the remark after (1.28) in Section 1.2). The difference between the value of $\tilde{\delta}_\kappa$ calculated numerically and the exact value given by (1.23) is also displayed (it is denoted "difference", and the difference obtained after the additional subtraction of the term $\nu \ln(2pR_a)$ is denoted "difference2").

If the photon energy is zero, then there are some differences between the format of the data that are displayed during the execution of subroutine S_integrals and the data that are described above due to significant differences of the calculation procedure.

4. Calculating the cross sections

Subroutine "Bremsstrahlung" is used for the second stage of the calculation process (see Section 2). The names, descriptions and default values of the formal parameters of Bremsstrahlung that can be modified by the user are given below.

Parameters No. 1 – 4 are the same as parameters No. 1 – 4 of S_integrals (see Section 3), i.e., they specify the atomic number, initial electron energy, final electron energy, and photon energy.

Parameters No. 5 – 13 have the same meaning as parameters No. 15 – 23 of S_integrals (see Section 3). However, if the calculation starts from stage 2, then those parameters are not required to be exactly equal to the corresponding parameters of the subroutine S_integrals used in stage 1. The set of values of κ_1 and κ_2 defined on the command line or in the parameter file is required only to be contained inside the set of values of κ_1 and κ_2 corresponding to the specified files with the S integral data. If it is not so and if Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1, then Kmax1 or Kmax2 will be reduced automatically to make them equal to the corresponding values of the S integral data.

Parameters No. 14 and No. 15 ("lmin" and "lmax") are the minimum and maximum values of l in (1.9). Normally, lmin = 0. If lmax exceeds the corresponding value of the S integral data and if Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1, then lmax will be reduced. The default values of those parameters are the same as the default values of parameters No. 24 and No. 25 of S_integrals (see Section 3).

Parameter No. 16 ("k2_excl_last") is a "switch" (0 or 1) indicating whether the last value of $|\kappa_2|$ should be excluded from the set of the breakpoints used to calculate the cubic spline coefficients for the partial-wave interpolation (see Section 1.3). In the case "k2_excl_last=1", the interpolated values between the last two breakpoints of $|\kappa_2|$ are calculated using the same spline coefficients as between the previous two breakpoints. This parameter was added after noticing that in the case "IV=1" and at low electron energies (of the order of 10 eV or lower)

there is a discontinuity at the last value of $|\kappa_2|$ in the dependences of the terms of the CS and DCS on $|\kappa_2|$ (the last term is much less than the smoothly extrapolated value). Consequently, if the last value of $|\kappa_2|$ is not exluded from the calculation of the spline coefficients, the interpolating curve has an oscillatory character between the last several pairs of breakpoints of $|\kappa_2|$, causing large errors in the cross sections. The default value of this parameter is 1 in the case "IV=1", and 0 otherwise.

Parameter No. 17 ("lmax_decr") is a non-positive increment of lmax that must be applied for testing the sensitivity of the cross sections to the value of l_{max} and to the uncertainties of the S integrals. If lmax_decr < 0, then both mentioned error tests will be performed. If lmax_decr = 0, then only the sensitivity to the uncertainties of the S integrals will be tested. If lmax_decr > 0, then there will be no error testing of any kind. Regardless of the value of lmax_decr, the error testing will be performed only if Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1. The default value of this parameter is –max(1,min(10,lmax/10)).

Parameters No. 18 – 20 ("theta_min", "theta_max1" and "np1", respectively) define the set of equidistant values of the photon emission angle θ that should be used for calculating the differential cross section (DCS). theta_min and theta_max1 are the minimum and maximum angles, respectively (in degrees), and np1 is the number of values of θ. Normally, theta_min = 0 and theta_max1 = 180, unless two values of the angular increment are used (see below). By default, theta_min = 0, theta_max1 = 180, and np1 = 181.

Parameters No. 21 and No. 22 ("theta_max2" and "np2", respectively) define the second set of equidistant values of the photon emission angle θ that should be used for calculating the DCS. It is assumed that the starting angle of this set is equal to the upper bound of the first angular range "theta_max1", which is defined by parameter No. 19 (see above). "theta_max2" is the overall maximum value of θ, and "np2" is the number of values of θ in the second set, excluding the mentioned starting value ("theta_max1"). If np2 ≤ 0, then the second angular range will not be used. By default, theta_max2 = 180 and np2 = 0 (i.e., the second angular range is not used).

Note: The integration of the DCS is done in the two angular ranges defined by the parameters No. 18 – 22 independently, using the 10^{th}-order Newton-Cotes formula. Consequently, it is recommended to set the number of angular integration steps in each of those two ranges (i.e., np1 – 1 and np2) equal to a multiple of 10.

Parameter No. 23 ("iCalculate") indicates whether the cross section files with the data for different κ_{max} should be regenerated. If iCalculate=0, then the cross sections will be calculated only when the output data files do not exist, or when the parameters Kmin(1,2) or isAbs_K(1,2) do not satisfy the mentioned requirement Kmin1 = Kmin2 = 1, isAbs_K1 = isAbs_K2 = 1. If iCalculate=1, then the cross sections will be always calculated, and the output data files will be overwritten if they exist. If iCalculate=–1 and the output files with the cross section data already exist, then Bremsstrahlung will not calculate the cross sections and will regenerate only the files with the shape function data (the required the CS and DCS data will be loaded from the existing files). In the latter case, if neither of parameters No. 18 – 22 is explicitly specified by the user, then all angles will be read from the first line of the existing file with the DCS data. If iCalculate=–1 and at least one of parameters No. 18 – 22 is specified explicitly, then the set of angles will be constructed as explained in the descriptions of parameters No. 18 – 22, and the program will attempt to locate the corresponding columns in the existing file with the DCS data. If the data for at least one of the angles is not available, then the program will quit with an error message. The numerical integration of the angular dependence of the DCS (which is needed for calculating the shape functions) is performed using the final set of angles (i.e., if some of the angles, for which the DCS data are available, have been skipped due to the user-specified values of parameters No. 18 – 22, then the skipped DCS data will not be used for the mentioned integration). The default value of parameter "iCalculate" is 1.

Parameters No. 24 and No. 25 ("prefix" and "suffix", respectively) have the same meaning as parameters No. 38 and No. 39 of S_integrals (see Section 3), i.e., they define the names of the input files with the *S* integral data. For more information, see the description of parameters No. 38 and No. 39 in Section 3 (in order to make that description applicable to Bremsstrahlung, the sequence numbers of the parameters must be reduced by 14).

Parameter No. 26 ("suffix2") is the additional suffix to be inserted at the end of the names of some output files. If this parameter is an empty string (specified by writing a space after "suffix2="), then no additional suffix will be used. By default, this parameter is equal to an empty string.

Parameter No. 27 ("dir_3j") is the name of the folder where the binary files with the Wigner 3j coefficient data are located. If the specified folder name is incomplete, i.e., if it does not start with the slash '/' or '\' and does not contain the colon ':', then it is assumed to be a subfolder either of the BREMS installation folder or of the current folder, depending on whether the path to the BREMS executable file has been specified before its name on the command line or not. If the specified folder does not exist, then it will be created. If the folder name has a non-trailing slash, then one should keep in mind that Windows uses backslashes '\' for file paths, whereas Linux uses forward slashes '/'. If the folder name contains a forward slash and no backslash, then on Windows the attempt to create that folder will fail (however, if the folder already exists, then the attempt to open a 3j data file will succeed). The default value of this parameter is '3j'.

Parameter No. 28 ("del_S_int") is a "switch" (1 or 0) indicating if the S integral data files created in the previous stage (by the subroutine S_integrals) should be deleted after a successful calculation of the cross sections. The value "1" of this parameter (indicating deletion of the S integral data files) will have an effect only if firstStage = 1. The default value of this parameter is 1. ***Note***: This parameter is also used by the subroutine S_integrals, where it has a different meaning (see the description of parameter No. 46 in Section 3).

Parameter No. 29 ("additionalFiles_CS") is a "switch" (1 or 0) indicating if the files "system_parms.txt" and "err_test.txt" should be updated (those files belong to the third group of the output files of Bremsstrahlung, which are described further in this section). The default value of this parameter is 0 (i.e., the mentioned two files are not updated).

The calculation process in Bremsstrahlung starts with creation of the array of the Wigner 3j coefficients, which are used in (1.14). The 3j coefficients may be calculated or loaded from binary files, depending on the maximum absolute value of κ_1 and κ_2 used in the calculation:

$$K \equiv \max(\max|\kappa_1|, \max|\kappa_2|). \tag{4.1}$$

The maximum value of K that is required for the 3j coefficients to be calculated (rather than loaded from files) is stored in the variable "kmax_3j". At the time of this writing, kmax_3j = 80. I.e., Bremsstrahlung will attempt to load the 3j coefficients from files if $K > 80$. Only the values of the 3j coefficients corresponding to $l_1 \le l_2$ are stored (the values corresponding to $l_1 > l_2$ are calculated using the symmetry properties of the 3j coefficients). A separate file is used for each value of $l_2 > 80$. Those files are loaded (or created) during the calculation of the R factors (1.9) when a given value of l_2 becomes needed for the first time. All 3j files are in a separate folder, whose name is specified using parameter No. 27 ("dir_3j"); file names have the format "3j_⟨l_2⟩.dat". If the mentioned folder does not exist, or if there is no required file in it, then the coefficients will be calculated and the file will be created. The maximum number of the 3j coefficients that may be calculated or loaded from files during a single run of BREMS is equal to

$$\text{nCoefs} = \frac{1}{6}(K^4 + 7K^3 + 17K^2 + 17K) + 1. \tag{4.2}$$

All these coefficients would be needed only when both κ_1 and κ_2 vary from $-K$ to K, and l varies from 0 to $2K$. If the range of variation of κ_1, κ_2 or l is narrower, or if the partial-wave interpolation method described in Section 1.3 is applied, then some of those coefficients will not be used during the calculation of the cross sections. The maximum allowed absolute value of κ_1 and κ_2 is given by the parameter "sz", which is defined by the "parameter" statement in the file "Brems.f90". At the

time of this writing, sz = 500. However, when $k \neq 0$, the recommended upper limit of K for calculation of cross sections is approximately 200 (at larger values of K, the calculation time and the memory requirements would become prohibitive). If $K = 160$, then the value of nCoefs, which follows from (4.2), is approximately 1.1×10^8. The time needed to calculate this number of 3j coefficients is slightly greater than 2 min on a computer with an Intel Core i7-4930K processor and Windows 10. Loading them from files takes only a few seconds.

Bremsstrahlung creates or updates up to 12 human-readable ASCII files. Their names end with extension ".txt". The most complete set of files is created when Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1 and lmax_decr < 0. The description of the output data that is presented below pertains only to the latter case.

It is convenient to define the following three groups of files according to their purpose:

I. Seven files with the dependences of the CS, DCS and shape function on κ_{max}. The names of those files include the name of the input file with the S integral data. If those files already exist, then they may be overwritten or not, depending on the value of parameter No. 23.

II. Two files with the DCS and shape function for the last (greatest) value of κ_{max}. I.e., those files contain a subset of the data contained in the files of I group. Their format (two columns of numbers, with values of θ in Column 1) is convenient for plotting the angular dependence of the DCS or the shape function. The names of those files are formed by appending the two suffixes defined by parameters No. 25 and No. 26 ("suffix" and "suffix2") to a fixed sequence of characters. These files are overwritten during each run of Bremsstrahlung, except when parameter No. 23 is equal to 0 and the files with the CS and DCS data already exist.

III. Three files with the values of the physical and control parameters and some data for a possible statistical analysis in the future. The names of those three files are fixed. A line of text is appended to each of those files after each calculation of cross sections, i.e., after creating the files with the CS and DCS data.

All files created in stage 2 contain two or more columns of numbers with fixed width and with a header above each column. The values of the CS and DCS in the output data are defined as the left-hand sides of (1.3) and (1.2), respectively, i.e., they are equal to the true cross sections multiplied by k / Z^2 (the units are indicated after (1.3) and (1.2)). Further on, when referring to numerical values of the cross sections, the scaled CS and DCS (with the scaling factor k / Z^2 and with units indicated after (1.3) and (1.2)) will be always implied. This note also applies to the output of the subroutine Brems_fit.

The names of the files of the first group are formed by adding the prefix "_CS_", "DCS_" or "ShapeFn_" and the suffix defined by "suffix2" to the S integral data file name. The mentioned prefixes replace the prefix defined by parameter No. 24, which is used for forming the name of the files with the S integral data, whereas "suffix2" is appended to the suffix defined by parameter No. 25. In addition, if the full error testing has been requested (i.e., if lmax_decr < 0), two files with an additional suffix "_test" and two files with an additional suffix "_test2" are created. The names of the latter four files also start with the prefix "_CS_" and "DCS_". The two files whose names end with "_test" contain the values of CS and DCS calculated using a set of modified S integrals and the same range of values of l in (1.9) as the two "_CS_" and "DCS_" files whose names do not end with "_test" or "_test2" (the values of S integrals are modified by randomly adding or subtracting their uncertainties). In addition, the first line of the "_CS_…_test.txt" file contains the initial value of the number of cycles in stage 2, which is used in stage 3 (see the description of parameter No. 5 in Section 5). The two files whose names end with "_test2" contain the values of CS and DCS calculated using a reduced value of l_{max} and the same set of unmodified S integrals as the two "_CS_" and "DCS_" files whose names do not end with "_test" or "_test2" (if lmax_decr = 0, then l_{max} is not reduced and those two files are not created). The format of this line is "ncycles0 = ⟨number⟩". The three files whose names start with "_CS_" contain four columns of numbers. The number of columns in the three "DCS_" files and the "ShapeFn_" file is greater than

the number of values of θ by 1. The first column in all files of this group contains the values of κ_{max} (column header "kmax"). The second, third and fourth columns of the three "_CS_" files contain the values of the CS ("CS"), the angular integral of the DCS ("DCS_integral"), and the relative difference of the previous two values ("rel_diff"). All columns starting from the second one in the "DCS_" and "ShapeFn_" files contain the values of the DCS or the shape function corresponding to a given value of θ (the latter value is indicated in the header of the column).

The files of group 2 are "DCS1⟨suffix⟩⟨suffix2⟩.txt" and "ShapeFn1⟨suffix⟩⟨suffix2⟩.txt". Each of them contains two columns of numbers. The first column contains the values of θ (in degrees). The second column contains the values of the DCS or the shape function.

The names of the files of the third group are "CS.txt", "system_parms.txt" and "err_test.txt". The file "CS.txt" contains a line with several physical and control parameters, as well as the values of the CS, angular integral of the DCS and their relative difference for every calculation of bremsstrahlung cross sections. The entries in each line of this file have the following meaning:

- the atomic number of the target material (column header "Z"),
- the kinetic energy of the incident electron in MeV ("T1(MeV)"),
- the energy of the bremsstrahlung photon in MeV ("Ep(MeV)"),
- the type of the interaction potential ("IV"),
- the number of cycles ("nCyc"). If the dependence of the CS and DCS on κ_{max} was not calculated (i.e., the condition Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1 is not satisfied), then nCyc = 1. Otherwise, it is less than or equal to K defined by (4.1). The number of cycles may be less than K if the subroutine Bremsstrahlung determines that the relative range of variation of the CS and the DCS for the last N_{fit} values of κ_{max} and for all values of the angle θ is less than 0.1% (the meaning of N_{fit} is explained in Section 1.5). In such a case, stage 2 is terminated and nCyc is set equal to the last value of κ_{max}, which may be less than K.
- the minimum value of κ_1 ("kmin1"),
- the maximum value of κ_1 ("kmax1"),
- the number 1 or 0 indicating whether the limits of variation of κ_1 are defined in terms of its absolute value ("k1abs"),
- the minimum value of κ_2 ("kmin2"),
- the maximum value of κ_2 ("kmax2"),
- the number 1 or 0 indicating whether the limits of variation of κ_2 are defined in terms of its absolute value ("k2abs"),
- the value of the first breakpoint of κ_2 ("k2_bp1"),
- the interval between the first two breakpoints of κ_2 ("dk2_1"),
- the interval between the last two breakpoints of κ_2 ("dk2_n"),
- the value of parameter No. 16 "k2_excl_last" ("k2excl"),
- the minimum value of l ("lmin"),
- the maximum value of l ("lmax"),
- the value of the CS ("CS"),
- the value of the angular integral of the DCS calculated using the 10^{th}-order Newton-Cotes formula ("DCS_integral"),
- the relative difference of the previous two values ("rel_diff"),
- the time of calculating the numerical integrals with the bounds of integration equal to 0 and r_0 in stage 1 (this time is expressed in seconds; the column header is "t[0_to_r0]"),
- the time of calculating the analytical integrals with the bounds of integration equal to r_0 and ∞ in stage 1 (this time is expressed in seconds; the column header is "t[r0_to_Inf]"),
- the total duration of stage 2 in seconds ("t[CS_DCS]"),
- the total duration of the current run of BREMS in seconds ("total_time").

If firstStage = 2, or if stage 1 is skipped due to presence of the files with the *S* integral data, then the times of the numerical and analytical integration (in columns "t[0_to_r0]" and "t[r0_to_Inf]") are copied from the last loaded binary file with the *S* integral data. If the numerical or analytical integrals were loaded from files in stage 1, then the corresponding time of the numerical or analytical integration, which is written to the output file with the *S* integral data in stage 1, is copied from the last loaded binary file with the corresponding data.

The file "system_parms.txt" contains a line with several physical and control parameters for every calculation of the dependence of the CS and DCS on κ_{max} (i.e., when the condition Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1 is satisfied). The mentioned parameters are the following:

- the atomic number of the target material (column header "Z"),
- the kinetic energy of the incident electron in MeV ("T1(MeV)"),
- the energy of the bremsstrahlung photon in MeV ("Ep(MeV)"),
- the type of the interaction potential ("IV"),
- the number of cycles ("nCyc"),
- the maximum value of κ_1 ("kmax1"),
- the maximum value of κ_2 ("kmax2"),
- the value of the first breakpoint of κ_2 ("k2_bp1"),
- the interval between the first two breakpoints of κ_2 ("dk2_1"),
- the interval between the last two breakpoints of κ_2 ("dk2_n"),
- the value of parameter No. 16 "k2_excl_last" ("k2excl"),
- the maximum value of l ("lmax").

If the interval between the last two breakpoints of κ_2 is less than the interval between the first two breakpoints of κ_2 ("dk2_1"), then the value of the latter interval is repeated in column "dk2_n".

The file "err_test.txt" contains a line for every calculation of bremsstrahlung cross sections when the error testing was performed (see the description of parameter No. 17). Each line has 16 entries. The first twelve entries are the values of the same parameters as in the file "system_parms.txt" (see above). The remaining entries are the following:

- the reduced value of l_{max} (column header "test"), which was used for calculating the alternative set of the CS and DCS;
- the maximum "scaled" absolute difference between the original set of values of the CS (obtained with the original l_{max} and unmodified *S* integrals) and the alternative set of values of the CS (obtained with the original l_{max} and with the *S* integrals randomly incremented or decremented by the magnitude of the corresponding uncertainty). Is defined as the maximum absolute difference of the original and alternative cross sections divided by the maximum value of the original cross section. The maximum is calculated over the entire set of used values of κ_{max} (i.e., κ_{max} = 1, 2, ..., *K*, where *K* is defined by (4.1)). The header of this column is "max|relDiff_CS|";
- the maximum "scaled" absolute difference between the original set of values of the DCS and the alternative set of values of the DCS (obtained with the original l_{max} and with the *S* integrals randomly incremented or decremented by the magnitude of the corresponding uncertainty). Is defined in the same way as the maximum scaled absolute difference of the CS (see above). The maximum is calculated over all values of κ_{max} and θ. The header of this column is "max|relDiff_DCS|".
- the numbers in columns "max|relDiff2_CS|" and "max|relDiff2_DCS|" differ from the previous two numbers only in the definition of the alternative set of cross sections (in this case, the alternative cross sections are calculated using the reduced l_{max} and the original *S* integrals). If lmax_decr = 0, then those two entries are absent.

During the calculation of the scaled CS and DCS ((1.3) and (1.2), respectively), Bremsstrahlung displays the same data that are included in the "_CS_" file (see the description of the files of the first group above). The intermediate values of the scaled CS and DCS are written every 5 seconds to the temporary files (their names are formed by appending the suffix "_tmp" to the original filenames). If the calculation is interrupted, the temporary files may be used instead of the final files as the input files for stage 3. At the end of the calculation, Bremsstrahlung displays the value of the scaled CS (1.3) corresponding to the last (greatest) value of κ_{max} (i.e., to $\kappa_{max} = K$).

If the dependence of the CS and DCS on κ_{max} is not calculated (i.e., if the condition Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1 is not satisfied), then only 5 files are updated in stage 2: the file "CS.txt", the two files of the second group, and the files "DCS.txt" and "ShapeFn.txt". After the cross sections are calculated, a line with the physical and control parameters and the values of the DCS and the shape function is appended to each of the latter two files. The first 17 columns in the latter two files contain the same data as the first 17 columns in the file "CS.txt" (see above).

5. Extrapolating the cross sections as a function of κ_{max}

Subroutine "Brems_fit" is used for the third stage of the calculation process (see Section 2). The names, descriptions and default values of the formal parameters of Brems_fit that can be modified by the user are given below.

Parameters No. 1 – 4 are the same as parameters No. 1 – 4 of S_integrals and Bremsstrahlung (see Section 3), i.e., they specify Z, T_1, T_2, and k, respectively.

Parameter No. 5 ("kmax_fit") is the upper limit on the value of κ_{max} in the input files with the cross section data. If this parameter is less than 1, then all available cross section data will be used. The default value of this parameter is −1.

Parameter No. 6 ("kmin_fit") is used when the value of κ_{max} is reduced in Brems_fit due to large differences between the original and test cross sections (see the descriptions of parameters No. 34 and No. 35). If the reduced value of κ_{max} is less than kmin_fit, this is treated as a terminal error. If there is no additional reduction of κ_{max} in Brems_fit, then this test is not performed. If the user-specified value of kmin_fit is non-positive, then kmin_fit is reset in the program to ncycles0 / 2 before starting stage 3 (if firstStage = 3, then the value of ncycles0 is read from the first line of the file "_CS_…_test.txt", which is created in stage 2 when the parameter "lmax_decr" is non-positive). If firstStage = 3 and the line with the value of ncycles0 is absent (old format of the file "_CS_..._test.txt"), then in the case kmin_fit ≤ 0 the mentioned test will not be performed (i.e., any reduction of κ_{max} will be allowed in stage 3). The default value of parameter "kmin_fit" is 1 (i.e., any reduction of κ_{max} is allowed in stage 3).

Parameters No. 7 – 11 are the same as parameters No. 18 – 22 of Bremsstrahlung (see Section 4), i.e., they specify the limits of variation of the photon emission angle θ and the number of values of θ. If the calculation process starts from stage 3 ("firstStage=3") and neither of these five parameters is explicitly specified by the user, then all angles will be read from the first line of the file with the DCS data created in stage 2 (by subroutine "Bremsstrahlung"). If the calculation process starts from stage 3 and at least one of these parameters is specified explicitly, then the set of angles will be constructed as explained in the descriptions of parameters No. 18 – 22 of Bremsstrahlung (see Section 4), and the program will attempt to locate the corresponding columns in the input file with the DCS data. If the data for at least one of the angles is not available, then the program will quit with an error message.

Parameters No. 12 – 14 ("tol1", "tol2", and "tol3", respectively) are the tolerances of the three parameters c_∞, d, and h of the nonlinear fitting function (1.41), respectively. The iterative fitting procedure is terminated when the change of the values of c_∞, d, and h between two iterations becomes less than the corresponding tolerances (if the absolute changes are greater than the specified tolerances, then fitting will be terminated if the relative changes are less than the

relative tolerances defined by parameters No. 15 – 17). The recommended value of parameters tol1 and tol2 is 10^{-6} or greater, and the recommended value of tol3 is 10^{-10} or greater. Smaller values may cause a very slow decrease of the sum of squared deviations, resulting in an apparent "lock-up" of the program. The default values of those three parameters are 10^{-6}, 10^{-6} and 10^{-9}, respectively.

Parameters No. 15 – 17 ("rtol1", "rtol2", and "rtol3", respectively) are the relative tolerances of the three parameters c_∞, d, and h of the nonlinear fitting function (1.41), respectively. To be more precise, rtol1 is the relative tolerance of the maximum difference between c_∞ and the unfitted CS or DCS in the fitting interval of κ_{max}. The relative change of a varied parameter is checked only if the absolute change is greater than the absolute tolerance defined by one of the parameters No. 12 – 14. The default value of those three parameters is equal to 10^{-9}.

Parameter No. 18 ("tol_range_max") is the maximum relative range of CS or DCS allowed for skipping the nonlinear fitting (note that the CS and DCS, which are called "original" or "unfitted" in the following descriptions of the parameters, may have been optionally smoothed with respect to κ_{max} as explained in Section 1.5). If the range of relative variation of CS or DCS in the current range of values of κ_{max} is less than the variable "tol_range", then the fitting will not be performed, i.e., the final CS or DCS will be set equal to the one obtained by truncating the series at the last (greatest) value of κ_{max}. Otherwise, the fitting will be performed and the final CS or DCS will be set equal to the value of c_∞ returned by the fitting procedure. If the dependence of CS or DCS on κ_{max} is not suitable for fitting (i.e., non-monotonous or with a wrong curvature or, in the case of the DCS, out-of-sequence with respect to the one corresponding to the previous value of θ), or if the fitted value is incorrect (i.e., it is on the wrong side of the range of variation of the CS or DCS, or negative, or exceeds the original value by a factor greater than 20, or differs from the original value by more than 200 widths of the range of variation in the case of the DCS or by more than 25 widths of the range of variation in the case of the CS), then tol_range will be increased by a factor of 2 or 2.5 and the entire fitting process will be restarted. This is done until the mentioned error condition does not occur or until tol_range exceeds tol_range_max. In the latter case, the fitting procedure is terminated with an error message. The CS is fitted before the DCS. The starting value of tol_range for fitting the DCS is the same as the final value of tol_range after fitting the CS. If an error occurs during fitting of the DCS, then the CS is not fitted again. The starting value of tol_range for fitting the CS is 10^{-3}, and the default value of parameter "tol_range_max" is 0.05.

One of the criteria used for determining if the DCS as a function of κ_{max} at a given value of θ and in a given range of values of κ_{max} may be fitted by the function (1.41) is whether the direction and rate of change of the DCS with increasing κ_{max} are correct as compared to the DCS corresponding to the previous value of θ. Further on, the mentioned direction will be specified using the term "sign": the sign is negative ("–1") when the DCS decreases with decreasing rate, zero ("0") when there is no significant change (i.e., when the relative range of the DCS in a given range of κ_{max} is less than the mentioned variable tol_range), positive ("+1") when the DCS increases with decreasing rate, and undefined ("+2") when the DCS is a non-monotonous function of κ_{max} or when its curvature is not consistent with a tendency to saturation (i.e., when the absolute value of the first derivative is not decreasing). The correct sequence of signs of the DCS corresponding to a set of increasing values of θ is the following:

1) a range of values of θ where all DCS have the sign +1,
2) a range of values of θ where all DCS have the sign 0,
3) a range of values of θ where all DCS have the sign –1.

One or two of these ranges may be absent, but their sequence may not be reversed. In short, the "sign" may not increase with increasing θ, and the sign "+2" is not allowed. However, smoothing of the angular dependence of the fitted DCS (mentioned in the description of parameter No. 36) may eliminate some types of deviations from this rule. In particular, a

sequence of DCS with sign 0 interspersed with DCS with sign −1 is sometimes observed at large values of T_1 and k / T_1, and the resulting "dips" in the angular dependence of the fitted DCS are eliminated by the mentioned smoothing. Consequently, only two cases are treated as an error: (1) a non-monotonous dependence of CS or DCS on κ_{max} (or a dependence that does not show a tendency to saturation), and (2) a DCS with sign −1 followed by a DCS with sign +1 (any number of DCS with sign 0 may be in between). In those cases, the variable "tol_range" is increased and the fitting procedure is restarted as explained above.

Parameter No. 19 ("tol_err_test") is the maximum allowed relative difference of the original (unfitted) CS and the extrapolated (i.e., fitted) CS for performing the error test. If the absolute value of the mentioned difference is less than tol_err_test, then the error test will be performed, otherwise it will not be performed. The error test is performed by redoing the fitting (i.e., recalculating the extrapolated CS) at several smaller values of the endpoint of the range of values of κ_{max} where the fitting is performed and then comparing the values of c_∞ returned by the fitting procedure with the original ("optimal") value, which corresponds to the absolute maximum of the mentioned endpoint (defined by (4.1)). The main purpose of the error test is determining the degree of correlation between two quantities related to the accuracy of extrapolation:

1) the relative difference between the fitted value of c_∞ and the original value of CS,
2) the relative difference between the fitted value of c_∞ and the exact value of CS.

Since the exact value of CS (corresponding to $\kappa_{max} \to \infty$) is not always available, the fitted value corresponding to $\kappa_{max} = K$ is used in its place if the relative correction of CS due to the extrapolation is small enough (i.e., less than tol_err_test). If the correlation between the mentioned two quantities is strong enough, then it may become possible to formulate a simple rule (for example, multiplication by a constant factor) for determining an approximate upper bound of the relative uncertainty of the final estimate of the CS obtained by extrapolation, given the value of the first quantity, which is the one that is observed directly. The default value of parameter "tol_err_test" is 0 (i.e., the error test is not performed).

Parameter No. 20 ("fitMode") is an integer number equal to 0, ±1 or 2. If fitMode ≠ 0, then both the CS and the DCS data will be processed. If fitMode = 0, then only the CS will be fitted. If fitMode = −1, then the nonlinear fitting of the DCS as a function of κ_{max} will not be performed; only the optional smoothing and the polynomial approximation (1.45) of this dependence at $\theta > 120°$ will possibly be performed. If fitMode > 0, then the mentioned nonlinear fitting of the DCS will be performed (possibly followed by smoothing and polynomial extrapolation of the angular dependence of the fitted DCS). The cases fitMode = 1 and fitMode = 2 differ only in treatment of irrecoverable errors during this fitting (see the description of parameter No. 38). The default value of parameter "fitMode" is 1.

Parameters No. 21 and No. 22 ("vary_h_CS" and "vary_h_DCS", respectively) indicate the method of calculating parameter h when fitting the CS or the DCS, respectively: (1) if vary_h_(D)CS=0, h will be equal to zero; (2) if vary_h_(D)CS=-1, h will be calculated by minimizing the absolute difference between the least squares estimates of c_∞ corresponding to two different fitting intervals – the original one and the alternative one, whose endpoint coincides with the center of the original fitting interval, with the condition that the value of h is the same for both these fitting intervals; (3) if vary_h_(D)CS > 0, h will be calculated as the value corresponding to the smallest sum of squared absolute deviations after performing the fitting vary_h_(D)CS times with quasi-random initial values and quasi-random initial increments of parameters d and h. The latter method is the default one. By default, vary_h_CS=50, vary_h_DCS=5 in the case "accuracy_level=1", and vary_h_CS=100, vary_h_DCS=10 in the case "accuracy_level=2".

Parameters No. 23 and No. 24 ("fitRange_CS" and "fitRange_DCS", respectively) control the width of the fitting interval when fitting the function CS(κ_{max}) or DCS(κ_{max}), respectively. The

number of points (i.e., values of κ_{max}) in the fitting interval (N_{fit}) is calculated according to (1.44a) when fitRange_(D)CS is equal to 2, or according to (1.44b) when fitRange_(D)CS is equal to 1. The calculated value of N_{fit} is rounded to the nearest integer. If fitRange_(D)CS is equal to 3, then both values of N_{fit} will be tried, and the fitted (D)CS will be calculated as the average of the least squares estimates corresponding to each of the two fitting intervals. Parameters fitRange_CS and fitRange_DCS must be either both equal to 3, or both different from 3 (they are equal to 3 by default).

Parameters No. 25 and No. 26 ("tol_corr_CS" and "tol_corr_DCS", respectively) are used to specify the threshold value of the relative correction of the CS or DCS due to nonlinear fitting, respectively, which must be exceeded in order to perform the five-parameter fitting (with parameter h varied). Before performing the five-parameter fitting of CS(κ_{max}) or DCS(κ_{max}) (i.e., optimizing parameter h), the four-parameter fitting with $h = 0$ is performed, and if the relative correction of the CS or DCS due to the fitting is less than parameter "tol_corr_CS" or "tol_corr_DCS" respectively, then the result of the four-parameter fitting is accepted without attempting the five-parameter fitting. The default value of those two parameters is 0.001. ***Note***: The five-parameter fitting is never attempted if the number of points in the fitting interval (N_{fit}) is less than the value of parameter No. 27 ("tol_Nfit").

Parameter No. 27 ("tol_Nfit") specifies the minimum number of values of κ_{max} in the fitting interval (N_{fit}) needed for the five-parameter fitting by the expression (1.41) to be possible (if N_{fit} is less than tol_Nfit, then the four-parameter fitting with $h = 0$ will be performed). The default value of this parameter is 10. ***Notes***: **1)** The five-parameter fitting is never attempted if the relative correction of the CS or DCS due to the four-parameter fitting is less than the value of parameter No. 25 ("tol_corr_CS") or No. 26 ("tol_corr_DCS"). **2)** Another factor determining the choice between the four- and five-parameter fitting is the value of the uncertainty of the optimal value of the varied parameter c_∞ returned by the fitting procedure. This uncertainty is calculated using Eq. (1.47). If the difference of the two least-squares estimates of the (D)CS (obtained using the four- and five-parameter fitting) is less than the larger of the two corresponding uncertainties multiplied by parameter No. 39 or No. 40 ("thr_ratio_h_CS" or "thr_ratio_h_DCS"), then the result with the smaller uncertainty is preferred, otherwise the estimate obtained by the five-parameter fitting is preferred.

Parameters No. 28 and No. 29 ("avg_period_min" and "avg_period_max", respectively) are equal to the minimum and maximum averaging period during the nonlinear fitting of the functions CS(κ_{max}) and DCS(κ_{max}) (see Section 1.5). If the partial-wave interpolation is applied, then the default value of avg_period_min is equal to parameter k2_step_last (i.e., the interval between the last two breakpoints of κ_{max} if k2_step_last > k2_step0, or the interval between the first two breakpoints of κ_{max} if k2_step_last = k2_step0). If the partial-wave interpolation is not applied, then the default value of avg_period_min is equal to 5 when $\max(\max|\kappa_1|, \max|\kappa_2|) \geq 80$, or to 1 otherwise.

Parameter No. 30 ("avg_period_max_ratio") is used for an alternative estimation of the maximum averaging period. It is equal to the ratio of the maximum averaging period and N_{fit} (the meaning of N_{fit} is explained in Section 1.5). The actual value of the maximum averaging period is equal to the smaller of two values: avg_period_max (described above) and avg_period_max_ratio*N_{fit}. In the case "avg_period_max_ratio=0", no averaging will be applied. The default (and maximum allowed) value of this parameter is 0.25.

Parameter No. 31 ("shift_k_max") is equal to the maximum shift of the endpoint of the fitting interval during the nonlinear fitting of the functions CS(κ_{max}) and DCS(κ_{max}) (see Section 1.5). The endpoint of the fitting interval is changed in increments of 1 for shift_k_max+1 fitting cycles. In each case, the starting point of the interval is recalculated (see the description of parameters No. 23 and No. 24), so that the entire interval is shifted in the direction of the decreasing κ_{max} relative to the original interval. The fitting is performed starting with maximum

negative shift (-shift_k_max) and ending with zero shift (i.e., the original fitting interval). In the case "fitRange_(D)CS=3", each "shift" corresponds to two fitting cycles differing by the width of the fitting interval but having the same endpoint. In this case, the fitted (D)CS corresponding to each shift is calculated as the arithmetic average of the two least squares estimates corresponding to each of the two widths of the fitting interval. After performing the fitting for all shift_k_max + 1 shifts, the arithmetic average of the optimal values of CS or DCS corresponding to all shifts is used as the optimal fitted CS or fitted DCS. The standard deviation of the average fitted CS or DCS over all shifts contributes to the estimate of the overall uncertainty of the fitted CS or DCS, except when the relative range of variation of the CS or DCS in the fitting interval corresponding to "shift 0" is less than 0.001 (i.e., 0.1 %), in which case the fitting is not performed (i.e., the final CS or DCS is set equal to the unfitted CS or DCS corresponding to the largest value of κ_{max}), and the standard deviation is set equal to the range of variation of the CS or DCS corresponding to shift 0. When the angular integral of the fitted DCS can be estimated with sufficient accuracy, i.e., when fitMode>0 and the limiting values of θ are 0 and 180° and the maximum angular increment is less than or equal to 1°, then the values of the fitted DCS integral are used, too, when calculating the optimal fitted CS and its standard deviation (i.e., the number of observations of the fitted CS is equal in this case to 2(shift_k_max+1)). The default value of this parameter is 4 (i.e., five fitting cycles are performed by default).

Parameter No. 32 ("shift_k_max_ratio") is used for an alternative estimation of the maximum shift of the endpoint of the fitting interval (see the description of parameter No. 31). It is equal to the ratio of the maximum shift and N_{fit} (the meaning of N_{fit} is explained in Section 1.5). The actual value of the maximum shift is equal to the smaller of two values: shift_k_max (described above) and shift_k_max_ratio*N_{fit}. The default (and maximum allowed) value of this parameter is 0.25.

Parameter No. 33 ("range_ratio_max") is the maximum allowed ratio of the ranges of variation of the CS in two "shifts" (see the description of parameter No. 31). All shifts where the absolute range of variation of the CS exceeded the minimum observed range of variation of the CS by a factor greater than "range_ratio_max" are excluded. The default value of this parameter is 10.

Parameter No. 34 ("maxRelErr") is the maximum acceptable relative error of the singly and doubly differential cross sections calculated by Bremsstrahlung due to uncertainties of the S integrals. If this parameter is positive, then the "original" and "test" cross sections (in the files whose names end with "_test") calculated by Bremsstrahlung will be compared, and the maximum value of κ_{max} will be reduced if their relative differences are greater than maxRelErr. The default value of this parameter is 0.01.

Parameter No. 35 ("maxRelErr2") is the maximum acceptable relative error of the singly and doubly differential cross sections calculated by Bremsstrahlung due to truncation of the sum (1.9) with respect to l. If this parameter is positive, then the "original" and "test" cross sections (in the files whose names end with "_test2") calculated by Bremsstrahlung will be compared, and the maximum value of κ_{max} will be reduced if their relative differences are greater than maxRelErr2. The default value of this parameter is 0.001.

Parameter No. 36 ("theta_interval_max") controls angular smoothing of the ratio of the fitted DCS and the original (unfitted) DCS. Its absolute value is equal to the maximum interval (in degrees) between adjacent inflection points (i.e., the points where the second derivative of the mentioned ratio changes sign). If two inflection points separated by an interval less than or equal to the specified maximum value are found and if the difference of the two consecutive relative increments of the mentioned ratio immediately before and after such a point is greater than 0.01, then the program will attempt to remove one or both of the mentioned inflection points by smoothing. If this parameter is zero, then the smoothing will not be performed. The sign of this parameter indicates the number of smoothing cycles. The minus sign indicates one smoothing cycle, and a positive value indicates additional smoothing cycles. The recommended (and

default) value of this parameter is 15. ***Note***: Since the smoothed function is the ratio of the fitted DCS and the original DCS, this type of smoothing will not eliminate the oscillations in the angular dependence of the original DCS; it may eliminate only the spurious peaks or "dips" caused by the fitting errors. For the same reason, this parameter has no effect on the final results when fitMode = −1, because in this case the fitted DCS is replaced by the original DCS, so that the smoothed ratio is exactly equal to 1.

Parameter No. 37 ("iFit") is a "switch" indicating whether the existing data files with the fitted DCS and shape function data should be overwritten. This parameter is ignored if fitMode = 0 (see the description of parameter No. 20). If iFit = 0 and processing of the DCS is requested (fitMode ≠ 0), then Brems_fit will process the DCS data only if there is no file with the fitted DCS data (otherwise no files will be updated, and the program will quit with a corresponding message). If iFit = 1, the DCS data will be always processed, and the existing files with the fitted DCS and shape function data will be overwritten. The default value of this parameter is 1.

Parameter No. 38 ("nErrMax") is the maximum allowed number of consecutive irrecoverable error points in the angular dependence of the fitted DCS. If the nonlinear fitting fails at a given value of θ and the number of consecutive irrecoverable errors (nErr) is less than nErrMax, then the fitted DCS at the current value of θ will be replaced by a value calculated without the nonlinear fitting. The replacement value depends on the value of parameter No. 20 ("fitMode"). If fitMode = 1, then the replacement value is equal to the original (unfitted) DCS. If fitMode = 2, then the replacement value is calculated by log-linear interpolation between the two values of the fitted DCS corresponding to the two closest "bracketing" values of θ where the fitting was successful. This replacement is done before the angular smoothing mentioned in the description of parameter No. 36. If nErrMax = 0, then the fitting procedure will be terminated after the first irrecoverable error. The default value of this parameter is 6.

Parameters No. 39 and No. 40 ("thr_ratio_h_CS" and "thr_ratio_h_DCS") control the condition to perform the comparison of the absolute uncertainties of the fitted (D)CS needed to determine which of the two fitting modes ($h = 0$ or $h > 0$) should be preferred. This parameter defines the threshold value of the ratio of the absolute difference between the two estimates of the fitted (D)CS and the larger of the two corresponding absolute uncertainties, which must be exceeded in order to use the result corresponding to $h > 0$ unconditionally (i.e., without the additional requirement for the uncertainty corresponding to $h > 0$ to be less than the uncertainty corresponding to $h = 0$). The default value is thr_ratio_h_(D)CS=1, which means that the additional requirement will be applied only when the larger of the two confidence intervals contains the value of the fitted (D)CS corresponding to the other fitting mode. If thr_ratio_h_(D)CS=0, then the result corresponding to $h > 0$ will always be used (i.e., the uncertainties corresponding to $h = 0$ and $h > 0$ will never be compared). If thr_ratio_h_(D)CS is set equal to an extremely large value, then the two uncertainties will always be compared, and the result corresponding to the smaller uncertainty will always be used. This parameter has an effect only when parameter "vary_h_CS" or "vary_h_DCS" is non-zero.

Parameters No. 41 and No. 42 ("wt_fitRange2_CS" and "wt_fitRange2_DCS") have the meaning of the ratio of the weight factors corresponding to the two possible widths of the fitting interval (defined by fitRange_(D)CS = 1 and fitRange_(D)CS = 2, as explained in the description of parameters No. 23 and No. 24). Those weights are used when calculating the average fitted (D)CS and its uncertainty in the case "fitRange_(D)CS=3". When wt_fitRange2_(D)CS < 1, a greater weight is assigned to the fitted (D)CS corresponding to the narrower fitting interval (corresponding to fitRange_(D)CS = 1). The default value of wt_fitRange2_(D)CS is 1, which corresponds to a simple arithmetic average. This parameter has an effect only when fitRange_(D)CS = 3.

Parameter No. 43 ("prefix_fit") is the name of the folder with the cross section data files created by Bremsstrahlung. Brems_fit reads the CS data from six files created by Bremsstrahlung: three files whose names start with "_CS_" and three files whose names start with "DCS_" (see the

description of the files of the first group in Section 4). The folder name must end with the slash '/'. If this parameter is an empty string (specified by writing a space after "prefix_fit="), then the mentioned six files must be in the current folder. This parameter is used only when firstStage = 3 and parameter No. 24 of the subroutine Bremsstrahlung ("prefix") is not '.'. In other cases, or if this parameter is not specified, Brems_fit will search for the cross section data files in the current folder. The default value of this parameter is an empty string.

Parameter No. 44 ("suffix3") is the suffix that is appended to the names of files "DCS_fitted_...", "ShapeFn_fitted_...", "DCS_alt_...", and "DCS_parms_...".

Parameter No. 45 ("del_CS") is a "switch" (1 or 0) indicating if the cross section data files created in stage 2 (by the subroutine Bremsstrahlung), excluding the files that were updated by appending a single line (i.e., "CS.txt", "system_parms.txt" and "err_test.txt"), should be deleted after a successful completion of stage 3. The value "1" of this parameter (indicating deletion of the cross section data files) will have an effect only if firstStage < 3. The default value of this parameter is 1.

Parameter No. 46 ("additionalFiles_CS") has the same meaning as parameter No. 29 of Bremsstrahlung (see Section 4), i.e., it indicates if the files "system_parms.txt" and "err_test.txt" were updated in the previous stage.

Parameter No. 47 ("additionalFiles_fit") is a "switch" (1 or 0) indicating if the file "DCS_alt_....txt" and the files of the second and third group of output files defined below should be updated. The default value of this parameter 0 (i.e., the mentioned files are not updated).

Brems_fit creates or updates up to 7 ASCII (human-readable) files. Each file starts with a header line, which is followed by multiple columns of numbers of fixed width. It is convenient to define 3 groups of the output files of "Brems_fit" according to their purpose and format:

I. Four files with the extrapolated values of the CS or the DCS (i.e., the values of the parameter c_∞ returned by the fitting procedure), and the corresponding values of the shape function (defined as the ratio DCS/CS). The mentioned values of the DCS may have been smoothed (see the description of parameter No. 36). The name of the file with the fitted CS data is "CS_fitted.txt". The names of the other three files start with the string "DCS_alt_", "DCS_fitted_" and "ShapeFn_fitted_", respectively, followed by the name of the input file with the cross section data. If the file "CS_fitted.txt" already exists, then a line will be appended to it. The other three files are overwritten after each fitting. The line of text written to the file "CS_fitted.txt" contains 29 entries, which have the following meaning:
    - the atomic number of the target material (column header "Z"),
    - the kinetic energy of the incident electron in MeV ("T1(MeV)"),
    - the energy of the bremsstrahlung photon in MeV ("Ep(MeV)"),
    - the original value of K defined by (4.1) ("kmax0"),
    - the value of K after the reduction on the basis of the restrictions on the maximum relative error ("kmax"); see the descriptions of parameters No. 34 and No. 35,
    - the value of parameter No. 21 ("vary_h_CS"),
    - the value of parameter No. 22 ("vary_h_DCS"),
    - the final value of parameter No. 31, taking into account parameter No. 32 ("shift_k"),
    - the number of observations of the fitted CS used for averaging and calculation of its standard deviation ("nObs"). If no "shifts" were excluded, then this number is equal either to shift_k_max+1 or to 2(shift_k_max+1), depending on whether the angular grid is suitable for accurate angular integration of the fitted DCS. If some shifts were excluded, then this number will be smaller (a shift may be excluded either because of

an irrecoverable fitting error, or because the range of variation of the CS corresponding to that shift exceeded the minimum observed range of variation by a factor greater than the value of parameter No. 33),

- the tolerance for the relative error caused by uncertainties of the S integrals ("maxRelErr"),
- the number 1 or 2 indicating one of the two possible widths of the fitting interval corresponding to a successful fitting of the dependence of CS on κ_{max} in shift 0 (see the description of parameters No. 23 and No. 24). If the option "fitRange_CS=3" is used and the fitting is successful for both fitting intervals, then the value of this entry is 3. The header of this column is "fitRange_CS";
- same as above for the DCS ("fitRange_DCS"),
- the tolerance for the relative error caused by truncation of the sum (1.9) with respect to l ("maxRelErr2"),
- the total number of the values of θ where an irrecoverable error occurred when fitting the dependence of the DCS on κ_{max} in the case of zero shift of the fitting interval ("nErrTot"),
- the maximum number of consecutive values of θ where an irrecoverable error occurred when fitting the dependence of the DCS on κ_{max} in the case of zero shift of the fitting interval ("nErr"). Note that "nErrTot" and "nErr" do not include the irrecoverable fitting errors that occurred in the angular extrapolation range ($\theta > 160°$);
- the original (unfitted) value of the CS calculated by Bremsstrahlung for $\kappa_{max} = K$ ("CS[kmax]"),
- the value of c_∞ ("CS_fitted[k->Inf]"), averaged over all fitting intervals as explained in the description of parameter No. 31;
- the estimate of the CS obtained by integrating the fitted DCS numerically with respect to $\cos(\theta)$ and multiplying by 2π (and averaging over all fitting intervals as explained in the description of parameter No. 31). This integration is performed using the 10^{th} order Newton-Cotes formula, and the bounds of this integral are equal to the parameters No. 7 and No. 8 (or No. 7 and No. 10) described above. If the DCS is not fitted (i.e., if parameter No. 20 is zero), then this integral is set to zero. The header of this column is "DCS_int(10th_order_NC)";
- the relative difference of the previous two values, i.e., the relative deviation of the numerical integral of the fitted DCS from the value of c_∞ ("rel_diff"),
- five columns with the corrections of the CS, DCS, and shape function due to fitting:
  - relative correction of the CS ("CS_relCorr"),
  - maximum relative correction of the DCS ("DCS_maxRelCorr"),
  - maximum scaled absolute correction of the DCS ("DCS_maxScaledCorr"),
  - maximum relative correction of the shape function ("SF_maxRelCorr"),
  - maximum scaled absolute correction of the shape function ("SF_maxScaledCorr").

  When calculating the "scaled" corrections, the product of $\sin(\theta)$ and the correction of the fitted DCS or fitted shape function is divided by the maximum value of the product of $\sin(\theta)$ and the original (unfitted) DCS or shape function. Thus, the scaled correction is the correction of the probability density function of θ, expressed in terms of the fraction of the maximum value of the original (unfitted) probability density function;
- five columns with the standard deviations of the CS, DCS, and shape function, reflecting the differences of the fitting results for different fitting intervals (see the

description of parameter No. 31), as well as the uncertainty of the parameter c_∞ associated with each shift:

- relative standard deviation of the CS ("CS_fitted_relSD"),
- maximum relative standard deviation of the DCS ("DCS_maxRelSD"),
- maximum scaled standard deviation of the DCS ("DCS_maxScaledSD"),
- maximum relative standard deviation of the shape function ("SF_maxRelSD"),
- maximum scaled standard deviation of the shape function ("SF_maxScaledSD").

If the nonlinear fitting was performed during a given shift, then the mentioned uncertainty of the parameter c_∞ associated with that shift is calculated according to (1.47). In the case "fitRange_(D)CS=3", the fitting is performed in two intervals having a common endpoint but with the width differing by a factor of 2 (see the description of parameter No. 31, and Eqs. (1.44a,b) in Section 1.5). In this case, the uncertainty of c_∞ is calculated according to (1.48).

If the fitting was not performed due to insufficient variation of the (D)CS inside the fitting interval, then the associated uncertainty is set equal to the range of variation of the (D)CS corresponding to that shift. The overall uncertainty (i.e., the standard deviation) of the (D)CS and of the SF is calculated by combining the uncertainties for different shifts as explained in Section 1.6. as the square root of the sum of the variance of the fitted (D)CS reflecting the differences between the shifts, and the average squared uncertainty associated with one shift. In the case of the CS, this estimate of the uncertainty is modified by adding it in quadrature with the angular integral of the absolute uncertainty of the fitted DCS. The relative uncertainty of the fitted CS, DCS or SF is equal to the ratio of the corresponding absolute uncertainty and the corresponding fitted CS, DCS or SF.

When calculating the "scaled" standard deviations, the product of $\sin(\theta)$ and the absolute standard deviation of the fitted DCS or fitted shape function is divided by the maximum value of the product of $\sin(\theta)$ and the same DCS or fitted shape function. Thus, the scaled standard deviation is the absolute standard deviation of the probability density function of θ, expressed in terms of the fraction of the maximum value of the same probability density function.

If the relative range of variation of the CS or DCS for "shift 0" is less than 0.001, then the final value of the corresponding standard deviation may be set equal to the range of variation of the CS or DCS in the fitting interval corresponding to shift 0. As an indication of this special case, the value of the mentioned standard deviation is output with the minus sign. In order for this to happen, there is an additional condition, which is different for the CS and the DCS: in the case of the CS, the difference between the CS and the DCS integral must be less than the range of variation of the CS, and in the case of the DCS, its uncertainty after the angular smoothing (which is applied both to the values of the DCS and to the values of the corresponding uncertainties) must not exceed the range of variation of the DCS more than twice, whereas the change of the DCS due to the smoothing must be less than the range of variation of the DCS.

Each line of text written to the "DCS_alt_" file contains five entries corresponding to zero shift of the fitting interval:

- the value of θ in degrees (column header "theta"),
- the corresponding original (unfitted) value of DCS calculated by Bremsstrahlung for $\kappa_{max} = K$ ("DCS[kmax]"),
- the value of c_∞ ("DCS_fitted0[k->Inf]") after optional angular smoothing (see the description of parameter No. 36). If the fitting has not been performed due to

insufficient variation of the original DCS in that range (see the description of parameter No. 18), then the value of the original DCS is repeated here;

- the value of the DCS obtained by the sixth-degree polynomial extrapolation of the angular dependence of the fitted DCS from the range of angles $\theta \leq 160°$ into the range of angles $\theta > 160°$ (see Section 1.5). The coefficients of the extrapolating polynomial (1.45) are calculated by least squares fitting of the fitted DCS in the range $140° \leq \theta \leq 160°$. The values corresponding to $\theta < 120°$ in this column are the same as in the previous column, and the values corresponding to $\theta \geq 120°$ are obtained by calculating the mentioned polynomial. The header of this column is "DCS_extrap(>=120deg)";
- the value of the DCS obtained by using the same extrapolating polynomial (1.45) and with the same values of its coefficients as described above, but in the angular range $\theta \geq 160°$ (the column header is "DCS_extrap(>=160deg)"). The values in this column corresponding to $\theta < 120°$ are the same as the values in the previous two columns. The values in this column corresponding to $\theta \geq 160°$ are the same as in the previous column. The values in this column corresponding to $120° \leq \theta \leq 160°$ are calculated as a weighted average of the previous two columns, with the weight coefficients equal to $(160° - \theta) / (40°)$ and $(\theta - 120°) / (40°)$, respectively. If the angular extrapolation is deemed necessary, then the values in this column are used as the values of the true fitted DCS.

Each line of text written to the "DCS_fitted_" file contains eight entries, which have the following meaning:

- the value of θ in degrees (column header "theta"),
- the corresponding original (unfitted) value of DCS calculated by Bremsstrahlung for $\kappa_{max} = K$ ("DCS[kmax]"),
- the fitted value of the DCS ("DCS_fitted") after optional angular smoothing (see the description of parameter No. 36). If the fitting has not been performed due to insufficient variation of the original DCS in that range (see the description of parameter No. 18), then the value of the original DCS is repeated here. The fitted DCS may be either the "original" fitted DCS (without any additional modifications apart from interpolation between the adjacent values in the case of an unrecoverable error, or the optional smoothing), or the fitted DCS with the additional polynomial extrapolation (1.45) applied at $\theta \geq 160°$ (in the "DCS_alt_" file, those two cases correspond to the columns "DCS_fitted0[k->Inf]" and "DCS_extrap(>=160deg)", respectively),
- relative correction of the DCS due to fitting ("DCS_relCorr"),
- scaled absolute correction of the DCS due to fitting ("DCS_scaledAbsCorr"),
- number of observations of the DCS used for averaging and calculation of its standard deviation ("nObs"), i.e., the number of "shifts" that were not excluded (a shift may be excluded either because the number of consecutive irrecoverable fitting errors exceeded the value of parameter No. 38, or because the range of variation of the DCS exceeded the minimum observed range of variation at the corresponding value of θ by a factor greater than the value of parameter No. 33),
- relative standard deviation of the fitted DCS ("DCS_relSD"), reflecting both the differences between the results for the different fitting intervals and the uncertainties of the value of parameter c_∞ associated with each fitting interval (the calculation of the latter uncertainties is explained in the description of file "CS_fitted.txt" above). If the angular extrapolation is deemed necessary, then this value for $\theta > 160°$ also includes the estimate of the extrapolation error,

- scaled absolute standard deviation of the fitted DCS ("DCS_scaledAbsSD"). If the angular extrapolation is deemed necessary, then this value for $\theta > 160°$ also includes the estimate of the extrapolation error.

Each line of text written to the "ShapeFn_fitted_" file contains eight entries, which have the following meaning:

- the value of θ in degrees (column header "theta"),
- the corresponding original value of the shape function (i.e., the ratio of the unfitted DCS and CS corresponding to the maximum κ_{max}),
- the fitted value of the shape function. The latter value is calculated as the ratio of the fitted DCS (given in column "DCS_fitted" of the file "DCS_fitted_....txt") and the numerical integral of the fitted DCS (given in column "DCS_int(10th_order_NC)" of the file "CS_fitted.txt"),
- relative correction of the shape function due to fitting ("SF_relCorr"),
- scaled absolute correction of the shape function due to fitting ("SF_scaledAbsCorr"),
- number of observations of the shape function used for averaging and calculation of its standard deviation ("nObs"), i.e., the number of "shifts" that were not excluded (a shift may be excluded either because the number of consecutive irrecoverable fitting errors exceeded the value of parameter No. 38, or because the range of variation of the DCS exceeded the minimum observed range of variation at the corresponding value of θ by a factor greater than the value of parameter No. 33),
- relative standard deviation of the fitted shape function ("SF_relSD"), reflecting both the differences between the results for the different fitting intervals and the uncertainties of the value of parameter c_∞ associated with each fitting interval (the calculation of the latter uncertainties is explained in the description of file "CS_fitted.txt" above). If the angular extrapolation is deemed necessary, then this value for $\theta > 160°$ also includes the estimate of the extrapolation error,
- scaled absolute standard deviation of the fitted shape function ("SF_scaledAbsSD"). If the angular extrapolation is deemed necessary, then this value for $\theta > 160°$ also includes the estimate of the extrapolation error.

The mentioned angular extrapolation error is taken into account by adding in quadrature the standard deviation defined above and a linear function of θ, which is equal to zero at $\theta = 160°$ and to the maximum value at $\theta = 180°$. The latter maximum value is assumed equal to the maximum absolute error of the extrapolating polynomial in the angular range $120° \leq \theta < 140°$.

II. Two files with the parameters of the fitting function (1.41) obtained after fitting the CS and the DCS for each value of θ. The name of the file with the CS fitting parameters is "CS_parms.txt". A line of text is appended to this file after each fitting. In addition to the values of parameters a, b, c_∞, d, and h in (1.41) obtained by fitting the dependence of the CS on κ_{max}, the file "CS_parms.txt" contains several parameters pertaining to the angular dependence of the fitted DCS. The name of the file with the DCS fitting parameters starts with the string "DCS_parms_" and includes the input file name. This file is overwritten after each fitting.

Each line of text written to the "CS_parms.txt" file contains the following 36 entries:

- the atomic number of the target material (column header "Z"),
- the kinetic energy of the incident electron in MeV ("T1(MeV)"),
- the energy of the bremsstrahlung photon in MeV ("Ep(MeV)"),
- the original value of K defined by (4.1) ("kmax0"),

- the value of K after the reduction on the basis of the restrictions on the maximum relative error ("kmax"); see the descriptions of parameters No. 34 and No. 35,
- the number 1 or 2 indicating one of the two possible widths of the fitting interval corresponding to a successful fitting of the dependence of CS on κ_{max} in shift 0 (see the description of parameters No. 23 and No. 24). If the option "fitRange_CS=3" is used and the fitting is successful for both fitting intervals, then the value of this entry is 3. The header of this column is "fitRange_CS";
- same as above for the DCS ("fitRange_DCS"),
- the tolerance for the relative error caused by uncertainties of the S integrals ("maxRelErr"),
- the tolerance for the relative error caused by truncation of the sum (1.9) with respect to l ("maxRelErr2"),
- the original (unfitted) value of the CS calculated by Bremsstrahlung for $\kappa_{max} = K$ ("CS[kmax]"),
- the value of c_∞ ("CS_fitted[k->Inf]") copied from file "CS_fitted.txt". If the fitting has not been performed due to insufficient variation of the original CS (see the description of parameter No. 18), then the value of the original CS is repeated here;
- the final value of the variable "tol_range" (see the description of parameter No. 18),
- the value of θ corresponding to the last occurrence of the DCS with sign +1 (the meaning of the term "sign" used here is explained in the description of parameter No. 18). If there are no values of θ corresponding to the DCS with sign +1, then the corresponding entry is −1. The header of this column is "theta_limit_1";
- the value of θ corresponding to the first occurrence of the DCS with sign −1 (the meaning of the term "sign" used here is explained in the description of parameter No. 18). If there are no values of θ corresponding to the DCS with sign −1, then the corresponding entry is −1. The header of this column is "theta_limit_2";
- the number "0" or "1" indicating if the polynomial extrapolation should be preferred to the original fitted DCS in the angular range $\theta > 160°$ ("extrap");
- the fitted values of the polynomial coefficients in (1.45) ("polynomial_coef[0]", "polynomial_coef[2]", "polynomial_coef[3]", …, "polynomial_coef[6]", respectively). If the degree of the extrapolating polynomial is less than 6, then some of the last coefficients are 0;
- the maximum absolute difference between the original fitted DCS and the one obtained from the polynomial equation (1.45) in the angular range $120° \le \theta < 140°$ ("max_abs_dev_120-140deg"). This value is used as an estimate of the maximum absolute error introduced by the angular extrapolation in the range $160° < \theta \le 180°$ (see the descriptions of the "DCS_fitted_" and "ShapeFn_fitted_" files of group I);
- the maximum relative difference between the original fitted DCS and the one obtained from the polynomial equation (1.45) in three angular ranges: $120° \le \theta < 140°$, $140° \le \theta \le 160°$ and $\theta > 160°$ ("max_rel_dev_120-140deg", "max_rel_dev_140-160deg" and "max_rel_dev_160-180deg", respectively),
- the total number of the values of θ where an irrecoverable error occurred when fitting the dependence of the DCS on κ_{max} ("nErrTot"),
- the maximum number of consecutive values of θ where an irrecoverable error occurred when fitting the dependence of the DCS on κ_{max} ("nErr"). Note that both "nErrTot" and "nErr" do not include the irrecoverable fitting errors that occurred in the angular

extrapolation range ($\theta > 160°$), unless this extrapolation was not necessary (in the latter case, there is a zero in the column "extrap");

- the lower limit of the range of values of κ_{max} where the average absolute residual error of the nonlinear fitting was smallest (the subsequent entries correspond to this range of κ_{max}). The heading of this column is "kStart";
- the final value of the averaging period "nAvg" when processing the CS data (see the description of parameter No. 30),
- the root mean square value of the residual of the nonlinear fitting of the CS ("rmsResidual"),
- the opposite of the sign before the exponent in the fitting equation (1.41) (if the fitting has not been performed, then this entry is zero). In other words, this is the "sign" of the dependence of the fitted CS on κ_{max} as defined in the description of parameter No. 18. The header of this column is "sign";
- the optimal values of the five coefficients a, b, c_∞, d, and h in (1.41). If the fitting has not been performed, then $a = b = d = h = 0$, and c_∞ is equal to the original (unfitted) value of the CS. The headers of those four columns are "a", "b", "c", "d", and "h".

All the data in the last 21 columns of the file "CS_parms.txt" (starting with "theta_limit_1") correspond to zero shift of the fitting interval only.

Each line of text written to the "DCS_parms_" file contains 10 entries with the fitting results in the case of zero shift of the fitting interval:

- the value of θ ("theta"),
- the lower limit of the range of values of κ_{max} where the average absolute residual error of the nonlinear fitting was smallest ("kStart"),
- the final value of the averaging period when processing the DCS data ("nAvg"),
- the root mean square value of the residual of the nonlinear fitting ("rmsResidual"),
- the opposite of the sign before the exponent in the fitting equation (1.41) (i.e., the "sign" of the dependence of the fitted DCS on κ_{max} as defined in the description of parameter No. 18),
- the optimal values of the varied parameters a, b, c_∞, d, and h (in that order).

If the fitting has not been performed due to insufficient variation of the original DCS in that range (see the description of parameter No. 18), then the entry in the column "sign" is zero, $a = b = d = h = 0$, and c_∞ is equal to the original (unfitted) value of the DCS. A zero value in the column "kStart" indicates that the fitting was terminated due to an unrecoverable error, and the corresponding value in the column "c" is either the value of the original DCS, or the value obtained by interpolation (see the description of parameter No. 38). The values of c_∞ written to this file coincide with the values of the DCS before the optional angular smoothing (see the description of parameter No. 36).

III. The file "Errors.txt". This file is created for the purpose of the future statistical analysis with the aim of determining the degree of correlation between several quantities related to the accuracy of the fitting (see also the description of parameter No. 19). Several lines of text are appended to this file after each error testing. Each line has 24 entries and corresponds to one of the intervals of κ_{max} where the fitting is performed (in decreasing order of the endpoints of these intervals). Each set of results contained in a single line of this file corresponds to complete processing of the data pertaining to a particular maximum value of κ_{max}, including the optional averaging of the results corresponding to the fitting intervals shifted by up to shift_k_max relative to the original interval (see the description of parameter No. 31). The meanings of all entries are explained below:

- the atomic number of the target material (column header “Z”),
- the kinetic energy of the incident electron in MeV (“T1(MeV)”),
- the energy of the bremsstrahlung photon in MeV (“Ep(MeV)”),
- the endpoint of the interval of κ_{max} where the fitting was performed (“kmax”),
- the number 1 or 2 indicating one of the two possible widths of the fitting interval corresponding to a successful fitting of the dependence of CS on κ_{max} in shift 0 (see the description of parameters No. 23 and No. 24). If the option “fitRange_CS=3” is used and the fitting is successful for both fitting intervals, then the value of this entry is 3. The header of this column is “fitRange_CS”;
- same as above for the DCS (“fitRange_DCS”),
- the value of parameter No. 19, i.e., the maximum allowed relative correction of the CS due to the nonlinear fitting for the error test to be performed (“tol_err_test”),
- the value of the unfitted (original) CS corresponding to the current value of the endpoint of the range of κ_{max} (“CS[kmax]”),
- the value of c_∞ obtained by nonlinear fitting (extrapolation) at the current value of the endpoint of the range of κ_{max} (“CS[k->Inf]”),
- the value of the angular integral of the fitted DCS, obtained by numerical quadrature using the 10^{th} order Newton-Cotes formula (“DCS_integral”),
- the relative difference of the fitted and unfitted CS, i.e.., the relative deviation of “CS[k->Inf]” from “CS[kmax]” (“1-CS[kmax]/CS[k->Inf]”),
- the relative deviation of the value of c_∞ obtained by nonlinear fitting at the current value of the endpoint of the range of κ_{max} from the value of the numerical integral of the fitted DCS corresponding to that endpoint. If the DCS is not fitted (i.e., if parameter No. 20 is zero), then this entry is equal to 1. The header of this column is “1-DCS_integral/CS[k->Inf]”,
- the relative deviation of the value of the unfitted CS corresponding to the current value of the endpoint of the range of κ_{max} from the value of c_∞ obtained by nonlinear fitting at the maximum (original) value of that endpoint (i.e., at the “optimal” fitting conditions) (“CS[kmax]/CS_fit_opt-1”),
- the relative deviation of the value of c_∞ obtained by nonlinear fitting at the current value of the endpoint of the range of κ_{max}, and the value of c_∞ obtained by nonlinear fitting at the maximum (original) value of that endpoint (i.e., at the “optimal” fitting conditions) (“CS[k->Inf]/CS_fit_opt-1”),
- the relative deviation of the value of the angular integral of the fitted DCS corresponding to the current value of the endpoint of the range of κ_{max}, and the value of the fitted DCS integral corresponding to the maximum (original) value of that endpoint (i.e., to the “optimal” fitting conditions) (“DCS_int/DCS_int_fit_opt-1”),
- four entries indicating the maximum differences between the fitted DCS or fitted shape function corresponding to the current value of the endpoint of the range of κ_{max}, and the same function corresponding to the maximum (original) value of that endpoint (i.e., to the “optimal” fitting conditions):
  - maximum relative difference of the fitted DCS (“DCS_maxRelDiff”),
  - maximum scaled absolute difference of the fitted DCS (“DCS_maxScaledDiff”),
  - maximum relative difference of the fitted shape function (“SF_maxRelDiff”),
  - maximum scaled difference of the fitted shape function (“SF_maxScaledDiff”).

When calculating the "scaled" differences, the product of sin(θ) and the difference of the fitted DCS or fitted shape function corresponding to the current value of the endpoint of the range of κ_{max} is divided by the maximum value of the product of sin(θ) and the fitted DCS or fitted shape function corresponding to the maximum (original) value of that endpoint. Thus, the scaled differences are the differences of the probability density functions of θ, expressed in terms of the fraction of the maximum value of the fitted probability density function corresponding to the maximum (original) value of the endpoint of the range of κ_{max};

- five entries equal to the standard deviations of the CS, DCS, and shape function, reflecting the differences of the fitting results for different fitting intervals (see the description of parameter No. 31) and the angular extrapolation errors at the current value of the endpoint of the range of κ_{max}:
  - relative standard deviation of the CS ("CS_fitted_relSD"),
  - maximum relative standard deviation of the DCS ("DCS_maxRelSD"),
  - maximum scaled standard deviation of the DCS ("DCS_maxScaledSD"),
  - maximum relative standard deviation of the shape function ("SF_maxRelSD"),
  - maximum scaled standard deviation of the shape function ("SF_maxScaledSD").

The first of the lines appended to the file "Errors.txt" after the fitting corresponds to the absolute maximum of κ_{max}, i.e., to the optimal fitting conditions. Consequently, the six entries in columns No. 12 – 17 ("CS[k->Inf]/CS_fit_opt-1" through "SF_maxScaledDiff") in this line are always zero, and the entry in column No. 11 ("CS[kmax]/CS_fit_opt-1") is an exact opposite of the entry in column No. 9 ("1-CS[kmax]/CS[k->Inf]").

As mentioned in the description of parameter No. 19, it is the possible correlation between the values of the relative differences in columns No. 9 and No. 12 ("1-CS[kmax]/CS[k->Inf]" and "CS[k->Inf]/CS_fit_opt-1", respectively) that would be most useful for defining a rule of estimating the upper bound of the relative uncertainty of the final estimate of the CS obtained by the extrapolation, given the magnitude of the relative correction of the CS due to the extrapolation (the entry in column No. 9).

If the fitting has not been performed at a particular value of the endpoint of the range of κ_{max} due to insufficient variation of the CS in that range, then the value of the relative difference in column No. 9 corresponding to that endpoint is zero (clearly, such cases cannot be used for estimating the mentioned correlation).

It should be noted that in the case when the partial-wave interpolation is applied at the maximum (optimum) value of κ_{max} (which will be denoted K), it will also be applied at all smaller ("test") values of κ_{max} that are greater than the starting point of the interpolation range (i.e., greater than the value of parameter "k2_breakpoint1", which is described in Section 3). It is possible that some of those values of κ_{max} are too small for the partial-wave interpolation to be effective, so that the corresponding cross sections may be too inaccurate. In the case of the default values of parameters that specify the conditions for the partial-wave interpolation (parameters No. 21 – 23 in Section 3), it is recommended to ignore the results corresponding to $30 < \kappa_{max} < 80$ when $|\kappa_2|_{max} \geq 80$ and the photon energy is non-zero, and the results corresponding to $30 < \kappa_{max} < 120$ when $|\kappa_2|_{max} \geq 120$ and the photon energy is zero.

At the start of the calculation, Brems_fit displays the unfitted value of the scaled CS (1.3) corresponding to the last (greatest) value of κ_{max} (i.e., to $\kappa_{max} = K$). After performing the initial fitting, the program displays the final value of the "tol_range" variable mentioned in the description of parameter No. 18, the values of θ corresponding to the change of the "sign" from 1 to 0 and from 0 to −1 ("theta_limits"; see also the descriptions of columns "theta_limit_1" and "theta_limit_2" in the file "CS_parms.txt", belonging to Group II of the output files defined above), the fitted

(extrapolated) value of the scaled CS, and the relative difference between the fitted CS and the unfitted CS. In addition, if the error test mentioned in the description of parameter No. 19 has been performed, then some of the information pertaining to each of the tested values of the endpoint of the fitting range is displayed, too.

6. Displaying the *S* integral data

The *S* integral data, the phase shifts, the normalization factors and the system parameters are stored in binary files created by the subroutine S_integrals (see Section 3). The program "Read_S_integrals.exe" displays some of these data on the screen. The displayed data include most of the parameters of S_integrals.exe that were used for generating the *S* integral data, as well as the values of all phase shifts, all normalization factors, and *S* integrals for any pair of values of κ_1 and κ_2 specified by the user. Unlike Brems.exe, Read_S_integrals.exe accepts input only as command-line arguments. The command-line arguments must be specified in the same way as for Brems.exe, i.e., using the format "<parameter_name>=<parameter_value>" (there must be no spaces before or after the equality sign). The names, descriptions, and default values of the command-line arguments are given below.

Parameters No. 1 – 15 have the same meaning as parameters No. 1 – 15 of Bremsstrahlung (see Section 4). The names and default values of those parameters are also the same.

Parameter No. 16 ("iDelta") is a "switch" ("0" or "1") indicating whether the values of the phase shifts and normalization factors should be displayed. The default value of this parameter is 1.

Parameters No. 17 and No. 18 ("k1" and "k2", respectively) are the values of κ_1 and κ_2, respectively, corresponding to the *S* integrals whose values must be displayed. If at least one of these two parameters is zero (the default value), then the table with the values of the *S* integrals will not be displayed (only the minimum and maximum values of the *S* integrals will be shown).

Parameters No. 19 and No. 20 ("prefix" and "suffix", respectively) have the same meaning as parameters No. 38 and No. 39 of S_integrals (see Section 3), i.e., they define the names of the input files with the *S* integral data. For more information, see the description of parameters No. 38 and No. 39 in Section 3 (in order to make that description applicable to Read_S_integrals.exe, the sequence numbers of the parameters must be reduced by 19). By default, parameters "prefix" and "suffix" are equal to empty strings.

Parameter No. 21 ("prefix_t") is a prefix used for creating a smaller file containing only the phase shifts and the total integrals (from 0 to ∞), without the numerical integrals and estimates of the uncertainties (its size is approximately 1/4 of the size of the complete file). The name of this file is formed by adding the specified prefix ("prefix_t") and the suffix "_t" to the original file name (here, "t" stands for "total integrals only"). prefix_t replaces the prefix of the original file name (specified by parameter No. 19), and the suffix "_t" is appended to the suffix of the original file name (specified by parameter No. 20). The "_t" file may also be used as an input file for the second stage (i.e. for the subroutine Bremsstrahlung). If this parameter is not specified, then the "_t" file will not be created.

Parameter No. 22 ("accuracy_level") has the same meaning as parameter No. 1 of the main program (it is described in Section 2). The default value of this parameter is 1.

Parameters No. 23 and No. 24 ("first" and "last", respectively) specify the first and last additional suffix in the names of the files to be loaded. The allowed values of those parameters are integer numbers from 0 to 999. "0" means no additional suffix, and a positive value means that the additional suffix is formed by concatenating the underscore and the specified number. The default value of parameter "first" is 0. The default value of "last" is 999.

Read_S_integrals.exe attempts to read all the data corresponding to the specified limits of κ_1, κ_2 and l from the specified files, and displays both some overall information about the loaded dataset and

the data corresponding to the user-specified pair of values of κ_1 and κ_2. The S integral data may be loaded from several files with names differing by the additional suffix "_1", "_2", …, "_999" (see also the description of parameter No. 37 of S_integrals in Section 3).

Before displaying the data stored in the indicated binary files, Read_S_integrals.exe displays the default values of several parameters, which were not explicitly specified by the user and which are used for defining the subset of *S* integrals to be analyzed. All the data displayed after this preliminary information is loaded from the files with *S* integral data. The list of all variables loaded from the mentioned files, whose values are displayed by Read_S_integrals.exe, is below:

- the maximum absolute values of κ_1, κ_2 and l in all files that were loaded ("Kmax1_file", "Kmax2_file", "lmax_file", respectively),
- the total number of the data files loaded;

most of the data defining the calculation parameters (i.e., the energies, numerical tolerances, precision level, etc.) from the last loaded file. The amount of this type of data in the *S* integral data file depends on the version number of the file (the latter number is not the same as the version number of the program). For example, most of it is absent in version 0 files (such as the "_t" files mentioned in the description of parameter No. 21). In the case of version number 12 (the maximum possible *S* integral data file version number at the time of this writing), this part of the displayed data consists of the following entries:

- the values of the parameters of S_integrals No. 1 – 14, 28 – 34, 36. The photon energy is denoted "Ep", and the notations of all other variables in this block of output data are the same as in the descriptions of the corresponding parameters of S_integrals (see Section 3), with the exception of "R_atom", which denotes the final value of the truncation radius of the potential function (the initial value of this parameter is denoted "R_atom_init"),
- the values of three processing times (in seconds): the time of the numerical integration (from 0 to r_0) "time [0 to r0]", the time of the analytical integration (from r_0 to ∞) "time [r0 to Inf]", and the total duration of stage 1 ("total time"),
- the initial and final precision levels, i.e., the approximate numbers of significant digits used for calculating the analytical parts of the *S* integrals ("ndp" and "n_digits", respectively),
- the final values of the six variables corresponding to the parameters No. 15 – 20 of S_integrals (using the same notations as in the descriptions of the corresponding parameters in Section 3). The final values of Kmax1 and Kmax2 may be less than their original (default or user-specified) values, because S_integrals may reduce them in some situations,
- if some of the values of κ_2 have been "skipped" (see Section 1.3), then the number of breakpoints of κ_2 and their values (for an example of a set of breakpoints of κ_2, see the description of the parameters No. 21 – 23 in Section 3),
- the minimum and maximum values of l for the set of calculated S_1 integrals ("lmin1" and "lmax1", respectively),
- the minimum and maximum values of l for the set of calculated S_2 integrals ("lmin2" and "lmax2", respectively),
- the value of the radial coordinate corresponding to the transition to analytical integration ("r0"). This variable coincides with r_0 from Section 1.2. If the numerical integration region has been extended (see the description of parameter No. 10 of S_integrals in Section 3), then both the original and the "extended" values of r_0 are displayed ("r0_original" and "r0_extended", respectively),
- the values of the two phase correction integrals at $r = r_0$ ("Q(1)" and "Q(2)"),
- the version number of the file ("version");

the next four lines characterize the complete loaded dataset (rather than the last loaded file) and answer the following questions:

- Do all the files contain the test numerical integral data? (see also the description of parameter No. 36 of S_integrals and Section 1.4),
- Did all wave functions attain the asymptotic form?
- Do all the files contain the total integrals (from 0 to ∞)? If at least one of the files contains the numerical integrals only (from 0 to r_0), then the answer to this question is "No",
- Do all the files contain the data needed for estimating the uncertainties of the *S* integrals?

The last line of text in the block specifying the calculation parameters displays the minimum version number of all loaded files with the *S* integral data.

The second part of the data displayed by Read_S_integrals.exe contains the values of the phase shifts, normalization factors and *S* integrals, as well as their uncertainties. First, if the display of the phase shifts has been requested (see the description of parameter No. 16), then the normalization factors ("A") and phase shifts ("delta"), well as their ranges of variation ("A_range" and "delta_range", respectively), which are stored in the *S* integral data files, are displayed for each energy and each value of κ (those ranges are defined as the differences of the maximum and minimum values of the normalization factors and phase shifts, respectively, calculated over the last 10 observations of those variables during the initial numerical integration and the last 10 observations during the "test" numerical integration). In addition, if the last loaded data file corresponds to IV = 1 (unscreened point-Coulomb potential) and iExact < 2 (numerical estimation of phase shifts), then the exact phase shifts (calculated according to (1.23–1.25)) are displayed, too. If the point-Coulomb field has been truncated (R_atom ≠ 0), then the values of $\tilde{\delta}_\kappa$ stored in the *S* integral data files should not be expected to be close to the values given by (1.23)), but this difference should be approximately the same for all κ if R_atom is sufficiently large (see the remark after (1.28) in Section 1.2). The values of the latter difference are shown in the column "difference". If R_atom > 0, then the difference obtained after the additional subtraction of the term $\nu \ln(2pR_a)$ is shown in the column "difference2" (the latter difference should approach zero when $R_a \to \infty$). Next, the maximum and minimum values of the S_1 and S_2 integrals ("S1" and "S2", respectively) are displayed along with their absolute uncertainties ("err_S1" and "err_S2", respectively). The indices of the displayed *S* integrals are indicated in parentheses after "S1" and "S2" in this order: κ_1, κ_2, l. After that, the two phase shifts corresponding to the values of κ_1 and κ_2 specified on the command line are displayed ("delta1" and "delta2", respectively, followed by the values of κ_1 and κ_2 in parentheses). Finally, a table of values of the S_1 and S_2 integrals corresponding to the values of κ_1 and κ_2 specified on the command line and their percent uncertainties is displayed. This table consists of 5 columns:

1) values of l,
2) values of the S_1 integrals,
3) relative uncertainties of the S_1 integrals (in percent, i.e., multiplied by 100),
4) values of the S_2 integrals,
5) relative uncertainties of the S_2 integrals (in percent, i.e., multiplied by 100).

This table will be displayed only if both values of κ specified by the parameters No. 17 and No. 18 are represented in the available data. If it is not so and if both κ_1 and κ_2 are non-zero, then a corresponding error message will be displayed at the beginning of the output data. If κ_1 or κ_2 is zero, then this error message will not be displayed.

7. The interaction potential

The interaction potential is defined by parameter No. 5 of S_integrals (see Section 3). The corresponding variable is denoted "IV" in the source code. At the time of this writing, three types of the interaction potential are allowed:

IV = 1: the point-Coulomb potential $V(r) = -\alpha Z / r$ (the unscreened nucleus),
IV = 2: the Thomas-Fermi-Csavinszky (TFC) potential,
IV = 3: the Kohn-Sham (KS) potential in tabular format.

An arbitrary radial potential function $V(r)$ of the form $\bar{V}(r)/r$, where $\bar{V}(r)$ is any smooth negative-valued monotonous function that decays exponentially in the limit $r \to \infty$ and is equal to $-\alpha Z$ at $r = 0$, may be specified by the user in tabular format (either by replacing the data files used with the choice No. 3 above, or by adding an option to use another set of data files in the code).

The most accurate of the mentioned potentials is the Kohn-Sham potential [4], [5], which was used for the calculations reported in [1] and in the subsequent works by Tseng and Pratt. According to the Kohn-Sham theory [4], the total potential acting upon an electron in an atom consists of three terms:

$$V(\boldsymbol{r}) = -\frac{\alpha Z}{r} + \alpha \int \frac{n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} \mathrm{d}\boldsymbol{r}' + \mu_x(n(\boldsymbol{r})), \tag{7.1}$$

where the first term is the potential due to the charge of the nucleus, the second term is the electrostatic potential due to all electrons of the atom (n is the electron density), and the third term is a local approximation to the exchange potential. As shown in [4] (using the variational principle), the assumption of a slowly varying electron density in conjunction with the approximation of an inhomogeneous electron gas leads to the following expression of the exchange potential:

$$\mu_x(n(\boldsymbol{r})) = -\alpha \frac{[3\pi^2 n(\boldsymbol{r})]^{1/3}}{\pi}. \tag{7.2}$$

An expression of the exchange potential differing from (7.2) only by an additional factor of 3/2 had been earlier obtained by Slater [31] on the basis of the Hartree-Fock equations, using the approximation of free electron gas and the concept of an "exchange hole" (a decrease of the number of electrons with the same spin orientation as the investigated electron in the vicinity of the latter). It was proved in [4] formally that usage of the expression (7.2) for the estimation of the self-consistent potential $V(\boldsymbol{r})$ by iterative solution of the one-electron wave equation (or, equivalently, by applying the variational principle) gives the exchange correction of the electron density that is more accurate than that obtained using the expression by Slater.

Due to the spherical symmetry of $n(\boldsymbol{r})$, Eq. (7.1) may be rewritten as follows:

$$V(r) = -\frac{\alpha Z}{r} + 4\pi\alpha \left[\frac{1}{r} \int_0^r n(r') r'^2 \mathrm{d}r' + \int_r^\infty n(r') r' \mathrm{d}r' \right] + \mu_x(n(r)). \tag{7.3}$$

Apart from the differences in notations and units, this expression coincides with Eq. (3.1d) in [1] (where the Kohn-Sham potential was referred to as the "modified Hartree-Fock-Slater" potential).

For comparison with the KS potential, the Thomas-Fermi-Csavinszky (TFC) potential [3] will be used (in [1], it was referred to as the "modified Thomas-Fermi" potential). The TFC potential is intended as a replacement for the Thomas-Fermi (TF) potential [32], [33], [34]. In the Thomas-Fermi atomic model, the electrons are regarded as forming an ideal gas satisfying the Fermi statistics and occupying the region of phase space of lowest energy. This region of phase space is assumed to be saturated, with two electrons with opposite spins in each unit volume, and the remainder is assumed to be empty. As noted in [3], a shortcoming of the TF theory is that it leads to a radial electron density which decreases as the inverse fourth power of the distance from the nucleus, whereas the quantum mechanics requires an exponential decrease. This shortcoming is overcome in [3] by replacing the TF differential equation for the screening factor $\tilde{V}(r)$ with an equivalent variational principle (i.e., defining a functional $L(\tilde{V})$ such that the corresponding Euler-Lagrange equation coincides with the TF equation), choosing a trial function subject to the requirement that it both satisfies the boundary conditions of the TF equation and has the desirable asymptotic behavior, and then extremalizing the functional with respect to the unknown parameters of the trial function subject to the subsidiary condition that the electron density is normalized. The trial function that satisfies the mentioned requirements is the following three-parameter function:

$$\tilde{V}(r) = [c_1 \mathrm{e}^{-c_2 a_0 r} + (1 - c_1)\mathrm{e}^{-c_3 a_0 r}]^2, \tag{7.4}$$

where

$$a_0 = 2(\tfrac{3}{4}\pi)^{-2/3} \alpha Z^{1/3}. \tag{7.5}$$

After substituting the values of the three parameters c_1, c_2 and c_3 that extremalize the mentioned functional subject to the subsidiary condition, the following expression of the screening factor is obtained [3]:

$$\tilde{V}(r) = (0.7111\mathrm{e}^{-0.175 a_0 r} + 0.2889\mathrm{e}^{-1.6625 a_0 r})^2, \tag{7.6}$$

so that the potential function is

$$V(r) \equiv -\frac{Z\alpha}{r}\tilde{V}(r) = -\frac{Z\alpha}{r}(0.7111\mathrm{e}^{-0.175 a_0 r} + 0.2889\mathrm{e}^{-1.6625 a_0 r})^2. \tag{7.7}$$

As shown in [3], the screening factor defined by (7.6) is within 5% of the exact solution $\tilde{V}_0(a_0 r)$ of the TF equation (the so-called "Thomas-Fermi universal function") at radii $r < 1.8 / a_0$, and within 15% at $r < 7.5 / a_0$. At greater radii, the exponential decrease of (7.6) becomes much faster than the decrease of $\tilde{V}_0(a_0 r)$. The simplicity of the functional form of the TFC potential function (7.7) makes it attractive from the computational point of view for solving the system of differential equations (1.16a,b). However, since it is an approximation to the simplified TF model of the atom, it is less accurate than the KS potential. Consequently, BREMS uses the KS potential by default.

Applications of the Thomas-Fermi and Kohn-Sham potentials for atomic systems often include a so-called "tail correction" [35], [36], [5], whose purpose is to take into account absence of the electrostatic self-interaction of the electron. This is achieved by changing the asymptotic form of the potential function at large radii, i.e., by making it go to zero as $-\alpha / r$ (i.e., as the potential function of a positive elementary charge) rather than exponentially. A modification of the Kohn-Sham variational method by addition of the tail correction was described in [36] and [5]. It consists in dividing the atom into two parts by a sphere centered on the nucleus, with the radius R chosen so that on the average there is one electron outside the sphere. Then the assumption of no self-interaction of the charge outside the sphere leads to the mentioned result (i.e., $V(r) = -\alpha / r$ when $r > R$). Clearly, the tail correction is not appropriate when describing interaction of an extraneous electron with a neutral atom (for example, in the case of the hydrogen atom, $R = 0$ and the tail correction becomes equivalent to a complete absence of screening). The program described in [5], which was used for generating the tables with the values of the KS potential used by BREMS, has an option to calculate either the original KS potential (7.3), or the potential with the tail correction (thus modified KS potential is called "new potential" in [36] and [5]). The KS potential used in BREMS, as well as the KS potential used in the works cited herein, was constructed according to the original definition (7.3) (which does not have the tail correction) by the relativistic (Dirac) self-consistent calculation with a local approximation to the exchange potential defined by (7.2).

Fig. 2 shows the KS and TFC screening factors ($\tilde{V}_{\mathrm{KS}}$ and $\tilde{V}_{\mathrm{TFC}}$, respectively) as functions of r for 8 values of Z from 1 to 92. In all cases excluding $Z = 1$, the relative difference of the two functions at $r < 200$ is less than 30 %, and in most of those cases the relative difference is less than 10 % at $r < 200$. Since r is expressed in units of αa_{B}, where a_{B} is the Bohr radius, the mentioned range of r approximately corresponds to $r < 1.5 a_{\mathrm{B}}$. At larger values of r, $\tilde{V}_{\mathrm{KS}} > \tilde{V}_{\mathrm{TFC}}$, except in the case $Z = 2$, when $\tilde{V}_{\mathrm{KS}} < \tilde{V}_{\mathrm{TFC}}$, and the ratio of the two functions increases exponentially with increasing r. The magnitude of this divergence increases with increasing Z. In the case $Z = 1$, the ratio $\tilde{V}_{\mathrm{KS}} / \tilde{V}_{\mathrm{TFC}}$ is roughly constant (between 2 and 3) when $r > 200$.

The $V(r)$ data tables are in subfolder "V/Kohn-Sham/". This folder contains the text files with the values of the Kohn-Sham potential function in tabular format. There is one file for each value of Z from 1 to 100 (the value of Z is indicated in the name of the corresponding file). Each of those files contains two columns of numbers with the values of the radial coordinate r and the interaction potential $V(r)$. Both r and V are specified in relativistic units (see Section 1.1). This

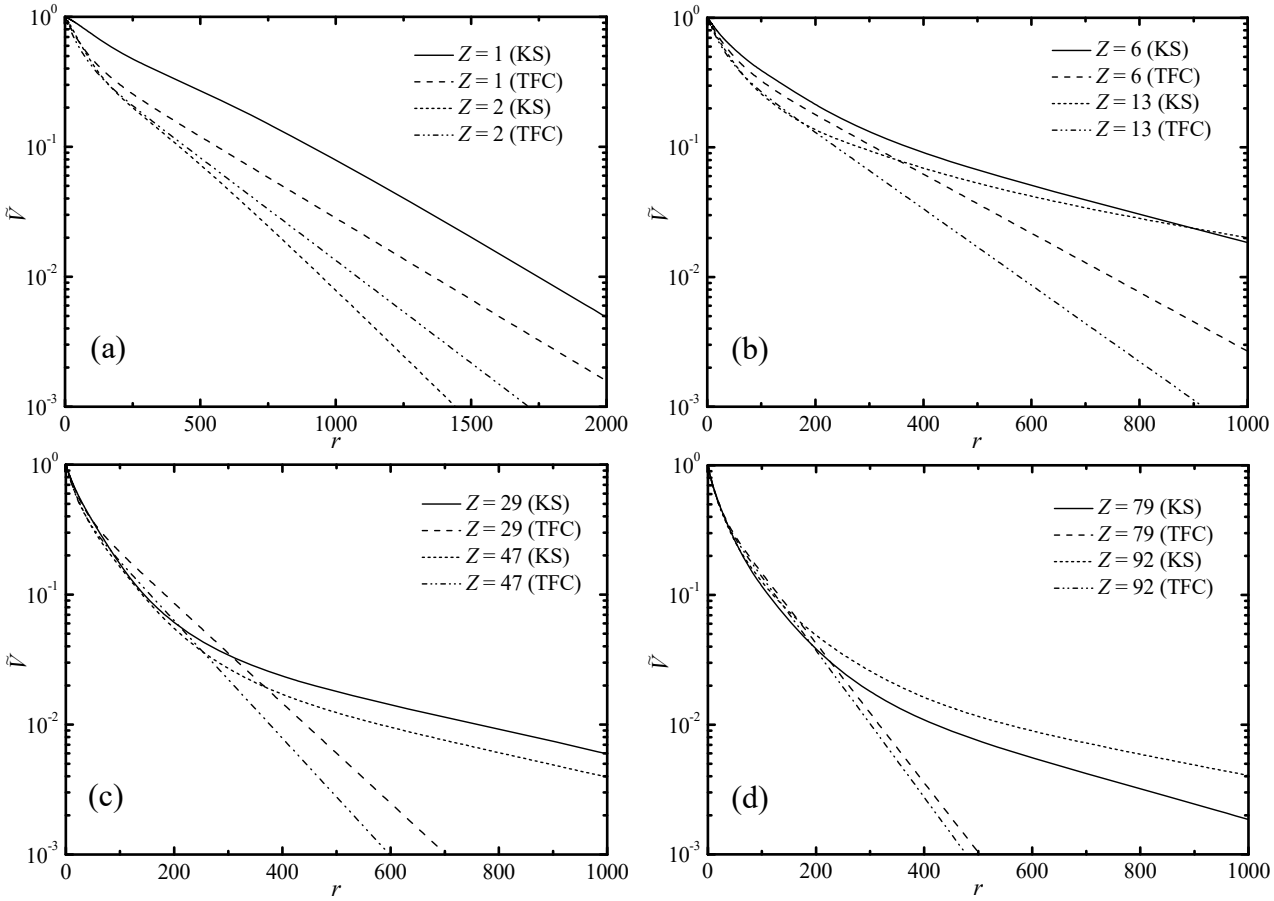

Fig. 2. Comparison of the Kohn-Sham (KS) and Thomas-Fermi-Csavinszky (TFC) screening factors for: (a) $Z = 1$ (hydrogen) and $Z = 2$ (helium), (b) $Z = 6$ (carbon) and $Z = 13$ (aluminum), (c) $Z = 29$ (copper) and $Z = 47$ (silver), (d) $Z = 79$ (gold) and $Z = 92$ (uranium).

means that r is specified in units of $\alpha a_B = 3.861592677 \times 10^{-13}$ m, where α is the fine-structure constant and a_B is the Bohr radius, and V is specified in units of the electron rest energy $m_0c^2 = 510.9989461$ keV. Cubic spline interpolation of the screening factor $\tilde{V}(r)$ (defined by (1.17)) is applied between the discrete values of r in the $V(r)$ data tables. In the interval $0 < r < r_1$, where r_1 is the first value of r in the $V(r)$ data table, the dependence of $\tilde{V}$ on r is approximated by an exponential function. Exponential extrapolation of the screening factor is applied in order to estimate $V(r)$ when r is greater than the last value of r in the data table. The slope and intercept of $\ln \tilde{V}(r)$ in this range of r are determined by linear least squares fitting over a set of 10 adjacent values of r, with an additional constraint requiring the fitted value of $\tilde{V}$ corresponding to the first point in the set to be equal to the corresponding value in the data table. The mentioned set of 10 data points is in the range containing the last 20 points of the data table, excluding the part of the data beginning with the first zero or positive value of V. 11 sets of 10 points are tried, and the one providing the best fit is chosen. After that, the first point of the chosen set of 10 values of r is treated as the last point of the data table (at greater values of r, the interaction potential is calculated using the known slope and intercept of $\ln \tilde{V}(r)$).

Any other interaction potential defined in tabular format may be used instead of the Kohn-Sham potential, with the condition that it is described by a positive-valued screening factor, which is a monotonous function equal to 1 at $r = 0$ and decaying exponentially when $r \to \infty$, and which can be approximated by a cubic spline between any two adjacent points of the data table. If the user does not wish to modify the file "S_integrals.f90" and recompile the program "Brems.exe", the $V(r)$ data tables corresponding to the user-specified interaction potential should replace the corresponding tables with the values of the KS potential (in subfolder "V/Kohn-Sham/"). This interaction potential will be used when parameter No. 5 of S_integrals is equal to 3. Alternatively,

the source code in the file "S_integrals.f90" could be modified to allow an additional type of the interaction potential (for example, corresponding to IV = 4). The maximum allowed number of the values of r in the $V(r)$ data table ("breakpoints") is 5000.

The value of r corresponding to the first point of the $V(r)$ data table (r_1) should not be too small, because it is used for setting the upper limits of the increment of r for numerical quadrature and of the step size of the Hamming's modified predictor-corrector algorithm (see the descriptions of the parameters No. 11 and No. 9 of S_integrals in Section 3). A very small value of r_1 may cause a decrease of the mentioned step sizes. This, in turn, would increase the calculation time.

In order to add an option to use a new interaction potential (tabular or analytic) in the code, one should modify subroutines POTENTIAL, PHASE_CORRECTION, and INITIALIZE, which are defined at the beginning of the file "S_integrals.f90", and the conditions of several "if" statements in the same file (the specific changes required in the case of a new tabular potential are described at the end of this section). Below are the descriptions of the mentioned subroutines.

Function POTENTIAL(R) returns the value of the interaction potential corresponding to the specified value of the radial coordinate (variable "R"). All parameters that are specific to a given type of potential must be passed to this function through a separate named block "COMMON". At the time of this writing, there are two such "COMMON" blocks: "const2" with the variables needed in the case IV = 2, and "const3" with the variables needed in the case IV = 3 (variables "exp1", "Q_factor", and "Q_factor_calculated", which belong to "const2", are needed in both these cases).

Subroutine PHASE_CORRECTION(r,p) calculates the phase correction integral defined by (1.27) for given values of the radial coordinate ("r") and the momentum ("p"). In the case of an exponentially decaying screening factor

$$\tilde{V}(r) = \tilde{V}_0 \mathrm{e}^{-zr} \quad (z > 0), \tag{7.8}$$

this calculation requires estimation of the integral in (1.27), which is equal to

$$\tilde{V}_0 \int_r^\infty \frac{\mathrm{e}^{-zw}}{w} \mathrm{d}w \equiv \tilde{V}_0 E_1(zr), \tag{7.9}$$

where E_1 is the exponential integral defined as

$$E_1(x) = \int_1^\infty \frac{\mathrm{e}^{-tx}}{t} \mathrm{d}t \tag{7.10}$$

(the latter integral is calculated by the function DE1(x)).

Subroutine INITIALIZE(dir_V) is used for initializing the calculation parameters needed for a given type of the interaction potential (these parameters should be passed to the mentioned subroutines POTENTIAL and PHASE_CORRECTION through a named "COMMON" block). In the case of an analytical interaction potential (such as used with IV = 2), this initialization mainly consists of calculating the coefficients of the Taylor series expansion of the screening factor (defined by (1.17)). This calculation is performed in the "if" block near the beginning of this subroutine. The Taylor series coefficients are stored in the one-dimensional array "ds". The index value of this array is equal to the order of the corresponding term of the series expansion. The number of coefficients that have to be calculated (i.e., the maximum order) is given by the value of the variable "nterms_max" (parameter No. 6 of the subroutine "S_integrals") and passed to INITIALIZE through the "COMMON" block "CONST0".

The above-mentioned Taylor series expansion is needed not only in the case of a purely analytical interaction potential, but also in the case of a potential defined in a tabular form, because in the latter case the Taylor series expansion is applied when $r < r_1$, where r_1 is the first value of the radial coordinate in the $V(r)$ data table. In the case IV = 3, the shape of $V(r)$ in this interval is exponential, and the coefficients of the corresponding Taylor series are calculated at the end of the subroutine INITIALIZE.

The remaining part of subroutine INITIALIZE performs initializations specific to the case of interaction potentials defined in tabular format. Those initializations are the following:

1) calculating the slope of the natural logarithm of the screening factor at $r < r_1$ (variable "exp1"),

2) calculating the slope of the natural logarithm of the extrapolating exponential function at large values of r (variable "slope_opt") and the corresponding preexponential factor (variable "f_opt"), and the sequence number of the starting point of this extrapolation (variable "nbp"),
3) calculating the arrays used for the cubic spline interpolation ("a1", "a2", and "a3") and for the calculation of the phase correction integral (1.27) ("V", "v1", "v2", "v3", and "Q_fact_terms").

The conditional statements that are used for checking the value of the variable "IV" in the source code are optimized for the case when all potentials corresponding to IV > 3 are defined using the same format as with IV = 3 (the Kohn-Sham potential in tabular format). The inclusion of a new tabular potential (corresponding to IV=4) requires only two changes in the file S_integrals.f90:

(1) the "if" operator with the header "if (IV.eq.3)" in the subroutine INITIALIZE, where the name of the $V(r)$ data file is assigned to the variable "fileName", should be expanded with an "else if" branch testing the condition "IV.eq.4" and assigning a value to "fileName" if IV=4;
(2) the "if" operator with the header "if (IV .lt. 1 .or. IV .gt. 3)" near the beginning of the subroutine S_integrals, where the validity of the user-specified value of IV is checked, should be replaced by the statement with the header "if (IV .lt. 1 .or. IV .gt. 4)".

A similar rule should be applied for all subsequent user-defined tabular potentials (corresponding to IV=5, IV=6, etc).

8. The test run

8.1. The description of the test run and the output files

In the subfolder "Test_runs" of the BREMS installation folder, there is the Windows batch file "Brems_79_100keV_KS.bat", which performs the entire set of calculations described in Section 2 for the case when the target is gold ($Z = 79$), incident electron energy is 100 keV, the photon energy is 10 keV or zero, and the Kohn-Sham (KS) interaction potential is used. All ASCII files created by running the mentioned batch file are in the same subfolder. There is also the file "Screen_output_Z=79_T1=0.1_Ep=0.01.txt" with the complete text that is displayed on the screen during the first call to Brems.exe in the mentioned batch file. Those output files were created by executing the mentioned batch file on a notebook computer with an Intel Core i5-8300H processor, 8 GB RAM, and 64-bit Windows 10 (no other processor-intensive tasks were being run at the same time). Explanations of the various parts of the screen output contained in the file "Screen_output_Z=79_T1=0.1_Ep=0.01.txt" are provided in Section 8.2. There is also the batch file "Read_S_integrals_79_100keV_10keV_KS.bat", which displays all the phase shifts, the normalization factors, and the values of the S integrals corresponding to $\kappa_1 = 14$ and $\kappa_2 = 15$, which are stored in the binary file with the S integral data created by the first mentioned batch file.

The file "Brems_79_100keV_KS.bat" contains two calls to the program Brems.exe, which perform the three steps of the calculation process described in Section 2. Since some of the stages of the calculation are relatively long, the program displays some intermediate data every few seconds in order to inform the user about the progress of the calculation. When $k \neq 0$, the longest stage of the calculation is the numerical integration. By default, BREMS calculates two sets of the numerical integrals: the one corresponding to the specified parameters, and the "test" set, which is calculated with all computational tolerances and step sizes greater by a factor of 2 (this is done in order to estimate the uncertainties of the S integrals). When $k = 0$, the numerical integration is much shorter (because in this case the S integrals are not calculated numerically; only the system of ODEs (1.16a,b) is solved at the stage of the numerical integration), and stage 2 is typically the longest stage of the calculation in this case. At the end of the calculation, the values of the scaled singly differential cross section and the extrapolated cross section are displayed. If the user does not request to keep the files with the intermediate data (such as the values of the S integrals and the values of the CS and the DCS for each value of κ_{max}) and does not request to create the additional files (such as the file with the comparison of the fitted values of the CS obtained at several values of

the endpoint of the fitting interval of κ_{max}), then the output data of Brems.exe are written to four ASCII files (file name extension ".txt"). A line of text with the values of the physical parameters, the main control parameters and the scaled CS calculated in stage 2 (before extrapolation of its dependence on κ_{max}) is appended to the file "CS.txt", and a line of text with the extrapolated value of the scaled CS is appended to the file "CS_fitted.txt" (in this file, the values of the original and fitted CS are in the columns with headers "CS[kmax]" and "CS_fitted[k->Inf]" respectively). The values of the scaled DCS and the shape function are written to the two files whose names start with "DCS_fitted_" and "ShapeFn_fitted_", respectively. The remaining part of the names of the latter two files indicates the values of Z, T_1 and k. This part of the file name has the format "Z_T.TE±XX_k.kkkE±YY_KS.txt", where "Z" is the atomic number consisting of 1, 2 or 3 digits, "T.TE±XX" is the kinetic energy of the incident electron (MeV) rounded to 2 significant digits in scientific notation, and "k.kkkE±YY" is the kinetic energy of the bremsstrahlung photon (MeV) rounded to 4 significant digits in scientific notation ("E±XX" and "E±YY" are the respective decimal exponents). The first three columns in the latter two files contain values of the angle θ in degrees, values of the original (unfitted) scaled DCS or shape function, and values of the extrapolated (fitted) scaled DCS or shape function. In all output files, the values of the scaled CS and DCS are given with 18-digit precision using scientific notation (the units are mb and mb/sr, respectively). By default, the values of the DCS and the shape function are calculated for 181 equidistant values of θ from 0° to 180°. If the mentioned batch file is executed repeatedly, then additional lines will be appended to the files "CS.txt" and "CS_fitted.txt", and the other two mentioned files will be overwritten.

The contents of the file "CS.txt" created during the test run:

Columns 1 to 10:

Z	T1(MeV)	Ep(MeV)	IV	nCyc	kmin1	kmax1	k1abs	kmin2	kmax2
79	1.0000000000000006E-01	1.0000000000000002E-02	3	80	1	80	1	1	80
79	1.0000000000000006E-01	0.0000000000000000E+00	3	100	1	100	1	1	100

Columns 11 to 19:

k2abs	k2_bp1	dk2_1	dk2_n	k2excl	lmin	lmax	CS	DCS_integral
1	30	5	5	0	0	32	2.8042200505786617E+01	2.8042244781088054E+01
1	0	0	0	0	0	100	2.9631737494515352E+01	2.9631737494515373E+01

Columns 20 to 24:

rel_diff	t[0_to_r0]	t[r0_to_Inf]	t[CS_DCS]	total_time
1.5788811E-06	53.562	169.859	21.000	249.672
6.6613381E-16	9.047	0.047	141.188	150.281

The contents of the file "CS_fitted.txt" created during the test run:

Columns 1 to 9:

Z	T1(MeV)	Ep(MeV)	kmax0	kmax	vary_h_CS	vary_h_DCS	shift_k	nObs
79	1.0000000000000006E-01	1.0000000000000002E-02	80	80	50	5	4	10
79	1.0000000000000006E-01	0.0000000000000000E+00	100	100	50	5	4	10

Columns 10 to 15:

fitRange_CS	fitRange_DCS	maxRelErr	maxRelErr2	nErrTot	nErr
3	3	1.0000000E-02	1.0000000E-03	0	0
3	3	1.0000000E-02	1.0000000E-03	0	0

Columns 16 to 19:

CS[kmax]	CS_fitted[k->Inf]	DCS_int(10th_order_NC)	rel_diff
2.8042200505786617E+01	2.8044196090124167E+01	2.8044879839736178E+01	2.4382722E-05
2.9631737494515352E+01	2.9671801938977534E+01	2.9671761517566711E+01	-1.3622837E-06

Columns 20 to 24:

CS_relCorr	DCS_maxRelCorr	DCS_maxScaledCorr	SF_maxRelCorr	SF_maxScaledCorr
7.1163614180E-05	7.4965702690E-04	3.3194628596E-04	6.5404132553E-04	2.7515909218E-04
1.3520788131E-03	2.6295380369E-03	1.6494380733E-03	1.2770978875E-03	6.0671398518E-04

Columns 25 to 29:

CS_fitted_relSD	DCS_maxRelSD	DCS_maxScaledSD	SF_maxRelSD	SF_maxScaledSD
2.87040496E-04	-9.81840186E-04	-9.32586211E-04	-9.81840186E-04	-9.32622063E-04
1.12260837E-04	1.50090946E-04	1.00154864E-04	1.44146973E-04	9.52002116E-05

The contents of the file "DCS_fitted_79_1.0E-01_0.000E+00_KS.txt" with the values of the scaled DCS calculated during the second call to Brems.exe in the mentioned batch file:

Columns 1 to 3:

```
                  theta                    DCS[kmax]                  DCS_fitted
 0.0000000000000000E+00      6.5266583633809058E+00      6.5438204598082876 4E+00
 1.0000000000000000E+00      6.5239903189691403 9E+00      6.5411364491474923 7E+00
 2.0000000000000000E+00      6.5159995013460161 3E+00      6.5330978604737737 2E+00
 3.0000000000000000E+00      6.5027257121656640 8E+00      6.5197448624222262 8E+00
…(174 lines removed)…
 1.7800000000000000E+02      1.1440885649361001 2E+00      1.1454505708914333 2E+00
 1.7900000000000000E+02      1.1438673012156845 8E+00      1.1452290464167067 5E+00
 1.8000000000000000E+02      1.1437935560623782 0E+00      1.1451552143503049 8E+00
```

Columns 4 to 8:

```
     DCS_relCorr     DCS_scaledAbsCorr    nObs         DCS_relSD   DCS_scaledAbsSD
 2.6295380369E-03      0.0000000000E+00       5    1.50090946E-04    0.00000000E+00
 2.6281660977E-03      1.1497873916E-04       5    1.50004512E-04    6.57128525E-06
 2.6240577711E-03      2.2928186482E-04       5    1.49733554E-04    1.31007129E-05
 2.6172332972E-03      3.4224266027E-04       5    1.49283729E-04    1.95470269E-05
…(174 lines removed)…
 1.1904724836E-03      1.8263931819E-05       5    7.15046771E-05    1.09690101E-06
 1.1904748038E-03      9.1316083945E-06       5    7.15052689E-05    5.48432505E-07
 1.1904755720E-03      6.4073004942E-20       5    7.15049788E-05    3.84812312E-21
```

The contents of the file "ShapeFn_fitted_79_1.0E-01_0.000E+00_KS.txt" with the values of the shape function calculated during the second call to Brems.exe in the mentioned batch file:

Columns 1 to 3:

```
                  theta                  ShapeFn[kmax]                ShapeFn_fitted
 0.0000000000000000E+00      2.0225905043860941 1E-01      2.2054034280662202 0E-01
 1.0000000000000000E+00      2.0216901034496169 6E-01      2.2044988607204613 1E-01
 2.0000000000000000E+00      2.1989933943468845 1E-01      2.2017896893574459 6E-01
 3.0000000000000000E+00      2.1945138091781751 8E-01      2.1972894516416099 9E-01
…(174 lines removed)…
 1.7800000000000000E+02      3.8610242316970570 8E-02      3.8604063675713604 1E-02
 1.7900000000000000E+02      3.8602775197620696 5E-02      3.8596597840744054 1E-02
 1.8000000000000000E+02      3.8600286475745378 1E-02      3.8594109546735505 5E-02
```

Columns 4 to 8:

```
      SF_relCorr      SF_scaledAbsCorr    nObs          SF_relSD    SF_scaledAbsSD
 1.2770978875E-03      0.0000000000E+00       5    1.44146973E-04    0.00000000E+00
 1.2757277995E-03      5.5811378901E-05       5    1.44061681E-04    6.31094617E-06
 1.2716250161E-03      1.1111057015E-04       5    1.43793659E-04    1.25810107E-05
 1.2648097505E-03      1.6539291862E-04       5    1.43348854E-04    1.87699216E-05
…(174 lines removed)…
-1.6002596426E-04     -2.4550784170E-06       5    6.89477825E-05    1.05767756E-06
 -1.6002364713E-04    -1.2274709845E-06       5    6.89484070E-05    5.28821836E-07
 -1.6002287998E-04    -8.6126477693E-21       5    6.89481159E-05    3.71052259E-21
```

Notes: **1.** The values of the scaled CS and DCS in the output data (including the data displayed on the screen) are defined as the left-hand sides of (1.3) and (1.2), respectively, i.e., they are equal to the true cross sections multiplied by k / Z^2 (the units are indicated after (1.3) and (1.2)). **2.** The values of the shape function are defined as the ratio of the DCS and the angular integral of the same DCS (the latter integral is calculated numerically). **3.** During the calculation, in order to avoid text wrapping (which would reduce readability of the output data on the screen), the screen buffer width must be at least 235. On Windows, this can be achieved, e.g., by entering "mode 235" at the command prompt in the console window before starting the calculation (this command is included in the mentioned batch file).

8.2. The screen output of the test run

Below is the complete screen output displayed during the first call to Brems.exe in the Windows batch file "Test_runs\Brems_79_100keV_KS.bat" (the corresponding command line is "Brems.exe Z=79 T1=0.1 Ep=0.01"), with explanations of each part of the output text (the screen output and its explanations are printed in different typefaces). The only omitted part of the displayed text is the version number, which is displayed immediately after starting BREMS. This output was produced using a notebook computer with an Intel Core i5-8300H processor, 8 GB RAM, and 64-bit Windows 10, without any other processor-intensive tasks being run at the same time. The complete text that is displayed on the screen during the mentioned call to Brems.exe is in

the file “Test_runs\Screen_output_Z=79_T1=0.1_Ep=0.01.txt”. The four ASCII files created during this run are also included in the BREMS distribution package.

1) At first, the values of several control parameters that were not explicitly specified by the user are displayed:

```
IV =                3
ndp =            -300
Kmax1 =            80
Kmax2 =            80
isAbs_K1 =          1
isAbs_K2 =          1
k2_breakpoint1 =   30
k2_step0 =          5
k2_step_last =      5
k2_excl_last =      0
lmax =             80
lmax_MP =          32
tol_A =          0.000000E+00
tol_delta =      0.000000E+00
Q_last =        -1.000000E-08
R_atom =        -2.000000E+01
pr_transition2 = -8.000000E+02
r_incr_max =    -1.000000E-02
delta_V_max =    1.000000E-02
j_QP =              0
maxRelErr =      1.000000E-02
maxRelErr2 =     1.000000E-03
nErrMax =           6
vary_h_CS =        50
vary_h_DCS =        5
fitRange_CS =       3
fitRange_DCS =      3
avg_period_min =    5
```

2) The next six lines display the total number of S integrals (1.15a,b), the total number of S_{ij} integrals ($i, j = 1, 2$) defined by (1.29), and the total number of terms of the form (1.35) that have to be added up during calculation of the coefficients of the linear combinations of the integrals (1.36a,b). It is denoted “nterms_tot”. The time of the analytical integration is proportional to the latter number (another factor that affects the time of the analytical integration is the precision level used). The alternative values of the same numbers to be used in QP or MP mode are shown with the suffix “MP”. Those numbers are less than the ones to be used in DP mode because of the smaller maximum value of l in the sum (1.9). In this example, the maximum value of $l_{\max}$ in DP mode is 80 (it is denoted “lmax” in the previous excerpt), but in QP or MP mode it is less by a factor of 2.5, i.e., 32 (denoted “lmax_MP” in the previous excerpt):

```
Number of S integrals          =   415000
Number of S integrals using MP =   127724

 Number of integrals of r*r*"j/y"[n1]*"j/y"[n2]*j[n3]          =      294404
 Number of integrals of r*r*"j/y"[n1]*"j/y"[n2]*j[n3] using MP =       84828

 nterms_tot    =            7138212801
 nterms_tot_MP =             789216035
```

3) After the preliminary information described above, the numerical integration begins. During the numerical integration, a line with the current values of several variables is printed on the screen every 5 seconds. This line contains the following information: (a) the current time of the numerical integration (in seconds), (b) the sequence number of the last step of the numerical quadrature (“i”), (c) the current value of the radial coordinate r (“r”), (d) the percentage done, i.e., the ratio of the current value of r and the limiting radius (this entry is present only if the limiting radius has been defined, i.e., when the interaction potential is “truncated”, i.e., when R_atom $\neq 0$, or during the “test” numerical integration, or when pr_transition2 $\neq 0$ and $r <$ pr_transition2 / p_2), (e) the current values of $p_1 r$ and $p_2 r$ (“p(1)*r” and “p(2)*r”, respectively), (f) the number of wave functions that have not attained the asymptotic form yet (“Nasymp”), (g) the current values of the S integrals (“S1” and “S2”) corresponding to the largest κ_1, κ_2 and l, with an additional condition that $\kappa_2 \neq \kappa_1$

(the indices of the displayed S integrals are indicated in parentheses after "S1" or "S2" in this order: κ_1, κ_2, l), (h) the maximum ranges of variation of A_κ and $\tilde{\delta}_\kappa$ over the last 10 "test" points ("A_range" and "delta_range"). If A_range and delta_range have not been calculated yet, then they are equal to −1. If all wave functions have attained the asymptotic form (1.18), i.e., if "Nasymp" is zero, but the other conditions for terminating the numerical integration are not satisfied yet, then the last two entries of the output line change: "A_range" and "delta_range" are replaced by the values of the two phase correction integrals ("Q(1)" and "Q(2)"). Since these lines are rather long (234 characters), some of the mentioned entries are omitted in the sample output, which is presented below. The omitted text is marked by an ellipsis (however, if the ellipsis is at the end of a line and is not preceded by a comma, then it is actually present in the text displayed by BREMS):

```
  Calculating the coefficients of the explicit formulas for the spherical Bessel functions...

  Calculating the continuum wave functions and the numerical integrals...
   Truncation radius of the potential function =   1187.20482202182
  The integration step became too large. Restarting the numerical integration...
        5.0 s:  i =      320, r = 1.372987E+01 ( 1.1%), … A_range=-1.000000E+00, delta_range=-1.000000E+00.
       10.0 s:  i =     1680, r = 2.105247E+02 (17.7%), … A_range=-1.000000E+00, delta_range=-1.000000E+00.
       15.1 s:  i =     3060, r = 4.210494E+02 (35.4%), … A_range=-1.000000E+00, delta_range=-1.000000E+00.
       20.1 s:  i =     4440, r = 6.315741E+02 (53.1%), … A_range=-1.000000E+00, delta_range=-1.000000E+00.
       25.2 s:  i =     5820, r = 8.420988E+02 (70.9%), … A_range= 1.077333E-01, delta_range= 8.171722E-02.
       30.2 s:  i =     7180, r = 1.049572E+03 (88.4%), … A_range= 7.150634E-05, delta_range= 4.201165E-04.
  Wave functions corresponding to energy No.1 attained asymptotic form at r <= 1.187205E+03, …
  The power-series solution algorithm terminated at r = 1.187205E+03, …
  Time of the initial numerical integration =      34.3 s

  r0 =   1.18720482202181779E+03, … Max|S1,2| = 1.057305E+01, Min|S1,2| = 2.962741E-39.

  Recalculating the continuum wave functions and the numerical integrals with the computational tolerances
and step sizes greater by a factor of 2...
  The integration step became too large. Restarting the numerical integration...
        5.0 s:  i =      880, r = 2.234918E+02 (18.8%), … A_range=-1.000000E+00, delta_range=-1.000000E+00.
       10.0 s:  i =     2240, r = 6.384391E+02 (53.7%), … A_range=-1.000000E+00, delta_range=-1.000000E+00.
       15.0 s:  i =     3590, r = 1.050335E+03 (88.4%), … A_range= 7.079209E-05, delta_range= 4.289608E-04.
  Wave functions corresponding to energy No.1 attained asymptotic form at r <= 1.187205E+03, …
  The power-series solution algorithm terminated at r = 1.187205E+03, …
  Time of the test numerical integration =      17.4 s

  Total time of the two numerical integrations =     53.6 s

  r0 =   1.18720482202181756E+03, … Max|S1,2| = 1.057305E+01, Min|S1,2| = 2.962736E-39.
```

4) The information that is displayed after terminating the numerical integration is mostly self-explanatory. It consists of the following items: (a) the maximum change of the numerical S_1 and S_2 integrals after increasing the computational tolerances and step sizes by a factor of 2 (the maximum absolute change is denoted "S1_num_maxDiff_abs" and "S2_num_maxDiff_abs", respectively, and the maximum relative change is denoted "S1_num_maxDiff_rel" and "S2_num_maxDiff_rel", respectively), (b) the values of the numerical S integrals and their uncertainties corresponding to the largest absolute values of κ_1, κ_2, and l (with the additional condition that $\kappa_2 \neq \kappa_1$), (c) the values of the factors $A_{\kappa 1}$ and $A_{\kappa 2}$ in (1.18) and the corresponding values of $\tilde{\delta}_{\kappa_1}$ and $\tilde{\delta}_{\kappa_2}$ for the same values of κ_1 and κ_2 (the values of $\tilde{\delta}_{\kappa_1}$ and $\tilde{\delta}_{\kappa_2}$ are adjusted by adding $2\pi n$, where n is an integer number, so that the final values of the phase shifts are between $-\pi$ and π), (d) the final values of the phase correction integrals corresponding to the two energies of the electron (in the case of a truncated interaction potential, the final values of the phase correction integrals are usually zero):

```
  The maximum change of the S1 integrals after increasing the computational tolerances and step sizes by a
factor of 2:
  S1_num_maxDiff_abs =  1.5035777844119025E-05, S1_num_maxDiff_rel =  2.1062178477348263E-05

  The maximum change of the S2 integrals after increasing the computational tolerances and step sizes by a
factor of 2:
  S2_num_maxDiff_abs =  1.5409783467035254E-05, S2_num_maxDiff_rel =  1.6975764524295426E-05

  S1(  80,  75,  80):
       Numerical integral =  -1.092983979632094E-035
```

```
       Test integral =       -1.092983979602492E-035
       Difference =          -2.960180463191960E-046
       Relative difference =  2.708347531487494E-011

  S2(  80,  75,  80):
       Numerical integral  =  9.921851823580044E-036
       Test integral =        9.921851823898637E-036
       Difference =          -3.185922170606347E-046
       Relative difference = -3.211015672532780E-011

  Energy No. 1: A(  80) = 3.5692967395530579E+00, delta(  80) = 1.0081397568729931E-01
  Energy No. 2: A(  75) = 3.7519177343203913E+00, delta(  75) = 1.0623641193469767E-01

  The final values of the phase correction integrals:
   Q(1) =  0.000000000000000E+000
   Q(2) =  0.000000000000000E+000
```

5) Before calculating the analytical part of the S integrals, the program attempts by default to determine the maximum value of $l_{\max}$ such that double precision is sufficient for the analytical integration and $l_{\max}$ belongs to the interval with the endpoints equal to the values of the two parameters "lmax" and "lmax_MP" mentioned above (thus, not only the precision level is optimized as described in Section 1.3, but also the value of $l_{\max}$ is optimized). If no such value of $l_{\max}$ is found, then the analytical integration will be performed using QP or MP, with $l_{\max}$ = lmax_MP. The precision level is optimized for each tested value of $l_{\max}$. In this example, the final precision level corresponds to QP, and $l_{\max}$ = 32. During the subsequent analytical integration, feedback is provided to the user every 10 seconds in the form of messages indicating the percentage of the terms of the type (1.35) calculated:

```
Performing analytical integration to infinity:

Calculating the trigonometric integrals...
     p_prime = p(1) + p(2) + p(3)
     p_prime = p(1) + p(2) - p(3)
     p_prime = p(1) - p(2) + p(3)
     p_prime = p(1) - p(2) - p(3)

Optimizing the precision level...
Precision level of   87 digits required with lmax =  80. Calculating with lmax =  72...
Precision level of   73 digits required with lmax =  72. Calculating with lmax =  65...
Precision level of   66 digits required with lmax =  65. Calculating with lmax =  59...
Precision level of   58 digits required with lmax =  59. Calculating with lmax =  53...
Precision level of   44 digits required with lmax =  53. Calculating with lmax =  48...
Precision level of   44 digits required with lmax =  48. Calculating with lmax =  43...
Precision level of   37 digits required with lmax =  43. Calculating with lmax =  38...
Precision level of   29 digits required with lmax =  38. Calculating with lmax =  33...
Precision level of   22 digits required with lmax =  33. Calculating with lmax =  32...
Precision level set to   22 digits.

Quadruple precision will be used.

 kmax(1)    =          80
 kmax(2)    =          80
 kmax(3)    =          32
 kmax_tot   =         192

 nterms_tot =             789216035

 Number of S integrals =      127724
 Number of integrals of r*r*"j/y"[n1]*"j/y"[n2]*j[n3] =       84828

      10.0 s:  15.9% of terms calculated.
      20.0 s:  32.5% of terms calculated.
      30.1 s:  49.5% of terms calculated.
      40.1 s:  66.7% of terms calculated.
      50.1 s:  84.3% of terms calculated.
```

6) After terminating the analytical integration, the maximum change of the total S_1 and S_2 integrals, when the phase shift is changed by the value of the corresponding range of $\tilde{\delta}_\kappa$, is displayed (the maximum absolute change is denoted "S1_maxDiff_abs" and "S2_maxDiff_abs", respectively, and the maximum relative change is denoted "S1_maxDiff_rel" and "S2_maxDiff_rel", respectively). The last piece of information displayed after terminating the analytical integration and before

exiting subroutine "S_integrals" (i.e., before ending stage 1) consists of the final values of the total S integrals (from 0 to ∞) corresponding to the largest absolute values of κ_1, κ_2, and l (with the additional condition that $\kappa_2 \neq \kappa_1$), their uncertainties due to the uncertainty of the phase shift, and the total uncertainties. The total uncertainties are calculated by combining the errors of the numerical integration with the errors caused by the uncertainty of the phase shift (the latter two errors are assumed to be independent, hence they are combined in quadrature):

```
The maximum change of S1 integrals after changing the phase shift:
S1_maxDiff_abs =  1.2639464657999751E-13, S1_maxDiff_rel =  6.2715290019544848E-03

The maximum change of S2 integrals after changing the phase shift:
S2_maxDiff_abs =  1.2797095434328897E-13, S2_maxDiff_rel =  1.2298409366273294E-03

Analytical integrals calculated in     169.9 s

S1(  80,  75,  32):
      Total integral:               -1.055494028184595E-009
      Change after modifying delta:  9.980936588936583E-017
      Relative change:               9.456175328725802E-008
      Total absolute uncertainty:    6.179129674190528E-014
      Total relative uncertainty:    5.854253562020023E-005

S2(  80,  75,  32):
      Total integral:                1.207714274500417E-009
      Change after modifying delta:  1.096531569426547E-016
      Relative change:               9.079395620128259E-008
      Total absolute uncertainty:    6.451786093802440E-014
      Total relative uncertainty:    5.342146093678726E-005

Subroutine S_INTEGRALS: elapsed time =     228.7 s
```

7) At the beginning of stage 2, subroutine "Bremsstrahlung" loads the S integral data from the binary files created in stage 1 by subroutine "S_integrals". If the values of $|\kappa_1|_{\max}$, $|\kappa_2|_{\max}$ or $l_{\max}$ in the available data are less than the values indicated by the input parameters, the latter parameters will be reduced and a corresponding message will be displayed (this is the case in the current example: the original value of $l_{\max}$ is 80, but its value after the mentioned optimization in stage 1 is 32). After that, the "R factors" (defined by Eq. (1.9)) and the spherical harmonics are calculated, and the messages indicating the duration of each of those two stages are displayed. Those two times are usually a small fraction of the total duration of stage 2, but only if the pre-computed values of the Wigner 3j coefficients in Eq. (1.14) are available, or if the maximum values of l_1 and l_2 do not exceed 160. The Wigner 3j coefficients corresponding to $l_{1,2} > 80$ are loaded from the files located in the subfolder "3j", and if those files are not available, then the mentioned 3j coefficients will be calculated and those files will be created. If the maximum value of l_1 or l_2 is greater than 160, then some of the 3j coefficients will be calculated using multiple precision (at the precision level of 100 digits), which may cause a significant increase of the total processing time:

```
Values of     287276 S integrals are missing.

 lmax reduced to             32

 Number of R factors =       665600
R factors calculated in       2.4 s

Calculating spherical harmonics...
Spherical harmonics calculated in       2.0 s
```

8) After calculating the R factors and the spherical harmonics, the calculation of the truncated series (1.2) and (1.3) begins. The terms of those two series are grouped into sets of terms having the same value of $|\kappa_1|$, $|\bar{\kappa}_1|$ or $|\kappa_2|$. This makes it possible to calculate the values of the mentioned series corresponding to a sequence of increasing values of $\kappa_{\max} = \max(|\kappa_1|, |\kappa_2|)$. The corresponding values of the scaled CS (1.3) are displayed every 5 seconds or at longer intervals (depending on the time needed to process one value of $\kappa_{\max}$), together with the value of the angular integral of the corresponding truncated DCS, calculated using the 10^{th} order Newton-Cotes formula, and the relative difference of the latter two values. The angular integration is performed using the values of

the DCS calculated according to (1.2) on the angular grid defined by the corresponding input parameters of BREMS (by default, 181 equidistant values of θ from 0 to 180° are used). Stage 2 is terminated after processing all values of κ_{max} up to max($|\kappa_1|_{max}$, $|\kappa_2|_{max}$), or after determining that the relative range of variation of the CS and the DCS for the last N_{fit} values of κ_{max} and for all values of the angle θ is less than 0.1% (the value of N_{fit} used for this test depends on the current value of κ_{max} and is calculated using one of the two formulas (1.44a) and (1.44b) in Section 1.5, with "K" replaced by "κ_{max}"):

```
Calculating cross sections...
       5.2 s:  kmax =  55,  CS =  2.8018791936278610 4E+01,  DCS integral =  2.8018710030516846 4E+01,  rel.
diff. = -2.9232439E-06
      10.4 s:  kmax =  69,  CS =  2.8037938552113313 8E+01,  DCS integral =  2.8038003369248688 3E+01,  rel.
diff. =  2.3117654E-06
      15.6 s:  kmax =  78,  CS =  2.8041781917160289 3E+01,  DCS integral =  2.8041778919852951 9E+01,  rel.
diff. = -1.0688719E-07

Cross sections calculated in      16.4 s

CS =  2.8042200505786617 3E+01,  DCS integral =  2.8042244781088054 9E+01,  rel. diff. =  1.5788811E-06

Subroutine BREMSSTRAHLUNG: elapsed time =      21.0 s (total time =      249.7 s)
```

9) The text that is displayed during stage 3 consists of at least six lines. The first line repeats the value of κ_{max} and CS from stage 2. The first entry in the second line ("tol_range") is the tolerance for the relative range of variation of the DCS in the fitting interval of κ_{max}. If the range of variation of the DCS as a function of κ_{max} for a particular value of θ is less than this tolerance, then BREMS will assume that there is no significant change, and the nonlinear fitting will not be performed for that angle. The second and third entries in the second line are the two limiting values of the angle θ ("theta_limits") where the dependence of the DCS on κ_{max} changes its direction. The first limit is the last value of θ where the mentioned dependence is a monotonous increase, and the second limit is the first value of θ where the mentioned dependence is a monotonous decrease (the range of variation of the DCS in the fitting interval is greater than tol_range in both cases). If the value of a limit is equal to −1, this means that the DCS does not belong to the corresponding category at any value of θ. The third and fourth lines contain the value of the fitted CS and its relative deviation (in percent) from the original (unfitted) value of the CS. The fifth line contains the angular integral of the fitted DCS and its relative deviation from the fitted CS. The last line contains the duration of stage 3 and the total duration of the current run of BREMS:

```
  kmax =          80 ,   CS =   28.0422005057866
  tol_range = 1.0E-03,  theta_limits =  61.00 and  -1.00

  Fitted CS =                  2.8044196090124167 1E+01
  Correction due to fitting =  7.1164E-03 %
  Fitted DCS integral =        2.8044798839736178 E+01 (deviation from the fitted CS =  2.4383E-03 %)

  Subroutine BREMS_FIT: elapsed time =       0.3 s (total time =      250.0 s)
```

It should be noted that some variation in the format and quantity of the information that is displayed and written to files is possible, depending on the values of some input parameters. For example, if the photon energy is zero, then the format of the information that is displayed in stage 1 is different from the above example due to significant differences of the calculation procedure.

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