

# G-value calculation program

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## 1 Compton effect

Following [1], we derive a differential cross section as a function of the electron energy  $T$  from the differential cross section per unit solid angle  $\theta$  given by Klein and Nishina

$$\frac{d\sigma}{d\Omega} = \frac{r_0^2}{2} \frac{1}{(1 + \alpha(1 - \cos\theta))^2} \left( 1 + \cos^2\theta + \frac{\alpha^2(1 - \cos\theta)^2}{(1 + \alpha(1 - \cos\theta))} \right), \quad (1)$$

where  $r_0 = e^2/(mc^2)$ ,  $\alpha = h\nu/(mc^2)$ ,  $e$  is the elementary charge,  $m$  is the electron mass,  $c$  is the speed of light and  $h\nu$  is the energy of  $\gamma$ -ray. The solid angle is  $d\Omega = \sin\theta d\theta d\varphi$ . From the conservation laws, the electron energy  $T$  is written in terms of the photon deflection angle  $\theta$ ,

$$T = h\nu \left( 1 - \frac{1}{1 + \alpha(1 - \cos\theta)} \right). \quad (2)$$

Using the electron energy, we obtain

$$\frac{d\sigma}{d\Omega} = \frac{r_0^2}{2} \left( \frac{h\nu - T}{h\nu} \right)^2 \left[ 1 + \left( 1 - \frac{T}{\alpha(h\nu - T)} \right)^2 + \frac{T^2}{(h\nu - T)h\nu} \right]. \quad (3)$$

By taking the derivative of  $T$  with respect to  $\theta$ , we have

$$\frac{dT}{d\theta} = h\nu \frac{\alpha \sin\theta}{(1 + \alpha(1 - \cos\theta))^2}. \quad (4)$$

Therefore, the differential cross section per unit energy  $T$  becomes

$$\frac{d\sigma(T)}{dT} = \frac{d\sigma}{d\Omega} \left( 2\pi \sin\theta \frac{d\theta}{dT} \right) = \frac{\pi r_0^2}{\alpha h\nu} \left[ 1 + \frac{T^2}{(h\nu - T)h\nu} + \left( 1 - \frac{T}{\alpha(h\nu - T)} \right)^2 \right]. \quad (5)$$

Figure 1 shows the differential cross section per unit energy for three primary photon energies,  $\alpha = 1, 2.35, 5.403$ . The figure completely reproduces the result given in Fig. 49 of [1]. Figure 2 shows the differential cross section per unit energy for  $^{60}\text{Co}$   $\gamma$ -ray energy,  $h\nu = 1.17, 1.33$  [MeV]. The graph looks similar to Fig. 1 of [4], but the vertical axis differs. **But, I don't understand what  $f(T)$  is and its unit.**

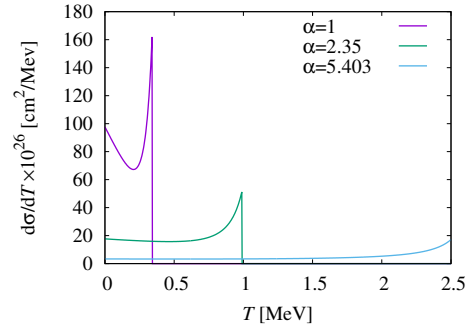


Figure 1: The differential cross section per unit energy for three primary photon energies,  $\alpha = 1, 2.35, 5.403$ .

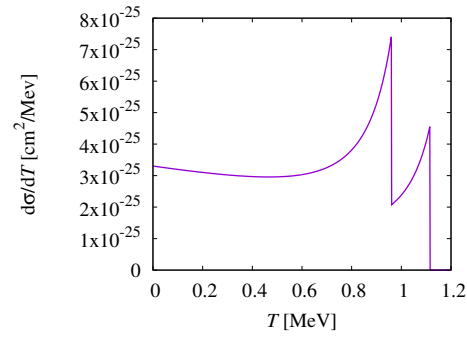


Figure 2: The differential cross section per unit energy for  $^{60}\text{Co}$   $\gamma$ -ray energy,  $h\nu = 1.17, 1.33$  [MeV].

## 2 Cross section

The differential cross section<sup>1</sup> per unit of energy for the energy loss  $E$  of the incident electron with the energy  $T$  is given by

$$\sigma_E(T) = \sigma_{E,d} + \sigma_{E,e}, \quad (6)$$

where the direct excitation and excitation induced by the exchange between the incident electron and an atomic electron are respectively given by

$$\sigma_{E,d}(T) = \frac{\pi e^4}{T + I_i + E_i} \left( \frac{1}{E^2} + \frac{4E_i}{3E^3} \right), \quad (7)$$

$$\sigma_{E,e}(T) = \frac{\pi e^4}{T + I_i + E_i} \left( \frac{1}{(T + I_i - E)^2} + \frac{4E_i}{3(T + I_i - E)^3} \right) \quad (8)$$

for  $T + I_i - E \geq 0$ . The subscript  $i = 1, 2, 3, \dots$  signifies the shell ( $i = 1$  is the outermost shell.)  $E_i$  and  $I_i$  are the average kinetic energy and the binding energy of the atomic electron under consideration. If the atomic electron is in the outermost shell of the atom,  $I_i$  is the ionization potential of the atom  $I$  ( $I_1 = I$ ).

## 3 Total cross section

### 3.1 Ionization

The total cross section for ionization is

$$Q_{\text{ion},i} = \frac{1}{2} \int_{I_i}^T \sigma_E dE = \int_{I_i}^{(T+I_i)/2} \sigma_E dE = \int_{I_i}^T \sigma_{E,d} dE. \quad (9)$$

The factor of 1/2 arises because we cannot distinguish whether the scattered electron is originally incidental or atomic. The second and third equalities are proven by using  $E' = T + I_i - E$ . We integrate  $\sigma_E$  over  $E \in [I_i, (T + I_i)/2]$ ,

$$\begin{aligned} \int_{I_i}^{(T+I_i)/2} \sigma_E dE &= \frac{\pi e^4}{T + I_i + E_i} \int_{I_i}^{(T+I_i)/2} \left( \frac{1}{E^2} + \frac{4E_i}{3E^3} \right) dE \\ &\quad + \frac{\pi e^4}{T + I_i + E_i} \int_{I_i}^{(T+I_i)/2} \left( \frac{1}{(T + I_i - E)^2} + \frac{4E_i}{3(T + I_i - E)^3} \right) dE \\ &= \frac{\pi e^4}{T + I_i + E_i} \int_{I_i}^{(T+I_i)/2} \left( \frac{1}{E^2} + \frac{4E_i}{3E^3} \right) dE \\ &\quad + \frac{\pi e^4}{T + I_i + E_i} \int_T^{(T+I_i)/2} \left( \frac{1}{E'^2} + \frac{4E_i}{E'^3} \right) (-dE') \\ &= \int_{I_i}^T \sigma_{E,d} dE. \end{aligned} \quad (10)$$

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<sup>1</sup>The unit of the differential cross section is  $[\text{charge}]^4/[\text{Energy}]^3 = [\text{dyn}^2 \text{ cm}^4/\text{erg}^3] = [\text{cm}^2/\text{erg}] = [\text{s}^2/\text{g}]$ .

Similarly, we evaluate the integral of  $\sigma_{E,e}$ .

$$\begin{aligned}
\int_{I_i}^T \sigma_{E,e} dE &= \frac{\pi e^4}{T + I_i + E_i} \int_{I_i}^T \left( \frac{1}{(T + I_i - E)^2} + \frac{4E_i}{(T + I_i - E)^3} \right) dE \\
&= \frac{\pi e^4}{T + I_i + E_i} \int_T^{I_i} \left( \frac{1}{E'} + \frac{4E_i}{E'^3} \right) (-dE') \\
&= \int_{I_i}^T \sigma_{E,d} dE.
\end{aligned} \tag{11}$$

Therefore, (9) is proven.

Now, we evaluate (9).

$$\begin{aligned}
Q_{\text{ion},i} &= \int_{I_i}^T \sigma_{E,d} dE = \frac{\pi e^4}{T + I_i + E_i} \int_{I_i}^T \left( \frac{1}{E^2} + \frac{4E_i}{3E^3} \right) dE \\
&= \frac{\pi e^4}{T + I_i + E_i} \left[ -\frac{1}{E} - \frac{2E_i}{3E^2} \right]_{I_i}^T \\
&= \frac{\pi e^4}{T + I_i + E_i} \left[ \left( \frac{1}{I_i} - \frac{1}{T} \right) + \frac{2E_i}{3} \left( \frac{1}{I_i^2} - \frac{1}{T^2} \right) \right].
\end{aligned} \tag{12}$$

Figure 3 shows the total ionization cross section of hydrogen with  $I_1 = 16.0[\text{eV}]$  and  $E_1 = 31.96[\text{eV}]$ . As in [3], the dissociative ionization and excitation are also considered. We are not able to reproduce the result of [3].

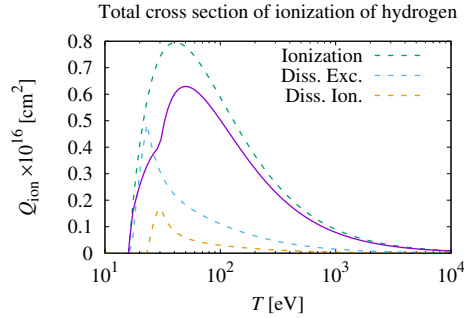


Figure 3: The total ionization cross section of hydrogen with  $I_1 = 16.0[\text{eV}]$ ,  $E_1 = 31.96[\text{eV}]$ .

### 3.2 Singlet and Triplet

The cross section of excitations are given by

$$Q_{\text{snl},i} = Q_{\text{de},i} + \frac{1}{2}Q_{\text{ee},i}, \quad (13)$$

$$Q_{\text{trpl},i} = \frac{1}{2}Q'_{\text{ee},i} \quad (14)$$

$$Q_{\text{de},i}(T \geq I_i) = \int_{E_{s,i}}^{I_i} \sigma_{E,\text{d}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[ \left( \frac{1}{E_{s,i}} - \frac{1}{I_i} \right) + \frac{2E_i}{3} \left( \frac{1}{E_{s,i}^2} - \frac{1}{I_i^2} \right) \right], \quad (15)$$

$$Q_{\text{de},i}(E_{s,i} \leq T < I_i) = \int_{E_{s,i}}^T \sigma_{E,\text{d}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[ \left( \frac{1}{E_{s,i}} - \frac{1}{T} \right) + \frac{2E_i}{3} \left( \frac{1}{E_{s,i}^2} - \frac{1}{T^2} \right) \right], \quad (16)$$

$$Q_{\text{de},i}(T < E_{s,i}) = 0, \quad (17)$$

$$Q_{\text{ee},i}(T \geq I_i) = \int_{E_{s,i}}^{I_i} \sigma_{E,\text{e}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[ \left( \frac{1}{T} - \frac{1}{T + I_i - E_{s,i}} \right) + \frac{2E_i}{3} \left( \frac{1}{T^2} - \frac{1}{(T + I_i - E_{s,i})^2} \right) \right], \quad (18)$$

$$Q_{\text{de},i}(E_{s,i} \leq T < I_i) = \int_{E_{s,i}}^T \sigma_{E,\text{e}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[ \left( \frac{1}{I_i} - \frac{1}{T + I_i - E_{s,i}} \right) + \frac{2E_i}{3} \left( \frac{1}{I_i^2} - \frac{1}{(T + I_i - E_{s,i})^2} \right) \right], \quad (19)$$

$$Q_{\text{ee},i}(T < E_{s,i}) = 0, \quad (20)$$

$$Q'_{\text{ee},i}(T \geq I_i) = \int_{E_{t,i}}^{I_i} \sigma_{E,\text{e}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[ \left( \frac{1}{T} - \frac{1}{T + I_i - E_{t,i}} \right) + \frac{2E_i}{3} \left( \frac{1}{T^2} - \frac{1}{(T + I_i - E_{t,i})^2} \right) \right], \quad (21)$$

$$Q'_{\text{ee},i}(E_{t,i} \leq T < I_i) = \int_{E_{t,i}}^T \sigma_{E,\text{e}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[ \left( \frac{1}{I_i} - \frac{1}{T + I_i - E_{t,i}} \right) + \frac{2E_i}{3} \left( \frac{1}{I_i^2} - \frac{1}{(T + I_i - E_{t,i})^2} \right) \right], \quad (22)$$

$$Q'_{\text{ee},i}(T < E_{t,i}) = 0, \quad (23)$$

$E_{s,i}$  and  $E_{t,i}$  are the energies of the singlet and triplet levels of  $i$ -th shell, respectively.

## 4 Stopping power

The stopping power of the medium consists of a single kind of atom<sup>2</sup> is expressed as

$$S(T) = \sum_i S_i(T), \quad (24)$$

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<sup>2</sup>The unit of the stopping power is [cross sec.][Energy]<sup>2</sup>/[Volume]=[cm/dyn erg<sup>2</sup>/cm<sup>3</sup>]=[dyn].

where

$$S_i(T \geq I_i) = Nn_i \left[ \int_{I_i}^{(T+I_i)/2} E\sigma_E dE + \int_{E_{s,i}}^{I_i} E\sigma_E dE + \frac{1}{2} \int_{E_{t,i}}^{E_{s,i}} E\sigma_{E,e} dE \right], \quad (25)$$

$$S_i(E_{s,i} \leq T < I_i) = Nn_i \left[ \int_{E_{s,i}}^T E\sigma_E dE + \frac{1}{2} \int_{E_{t,i}}^{E_{s,i}} E\sigma_{E,e} dE \right], \quad (26)$$

$$S_i(T < E_{s,i}) = Nn_i \frac{1}{2} \int_{E_{t,i}}^T E\sigma_{E,e} dE. \quad (27)$$

$N$  is the number of atoms in a unit volume<sup>3</sup>,  $n_i$  the number of electrons in the  $i$ -th shell and  $E_{s,i}$ ,  $E_{t,i}$  are, respectively, the energies of the lowest singlet and triplet levels of the  $i$ -th shell. We analytically evaluate the integral. The indefinite integrals to be evaluated are

$$\begin{aligned} \int \frac{E}{(T+I_i-E)^2} dE &= \int \frac{-(T+I_i-E) + (T+I_i)}{(T+I_i-E)^2} dE \\ &= - \int \frac{1}{T+I_i-E} dE + (T+I_i) \int \frac{1}{(T+I_i-E)^2} dE \\ &= \ln(T+I_i-E) + \frac{T+I_i}{T+I_i-E}. \end{aligned} \quad (28)$$

$$\begin{aligned} \int \frac{E}{(T+I_i-E)^3} dE &= \int \frac{-(T+I_i-E) + (T+I_i)}{(T+I_i-E)^3} dE \\ &= - \int \frac{1}{(T+I_i-E)^2} dE + (T+I_i) \int \frac{1}{(T+I_i-E)^3} dE \\ &= -\frac{1}{T+I_i-E} + \frac{T+I_i}{2(T+I_i-E)^2}, \end{aligned} \quad (29)$$

$$\int \frac{E}{E^2} dE = \ln E, \quad (30)$$

$$\int \frac{E}{E^3} dE = -\frac{1}{E}. \quad (31)$$

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<sup>3</sup>At the standard temperature and pressure (0°C and 1atm=101.325kPa; the former IUPAP definition until 1982), the molar volume of a gas is 22.4 litre. Then,  $N = 6.02 \times 10^{23} / (22.4 \times 10^3) = 0.269 \times 10^{20} \text{ [cm}^{-3}\text{]}$ . For a solid,  $N = d/(M/N_A)$  with  $d$ ,  $M$ ,  $N_A \equiv 6.02 \times 10^{23}$  being the density, molecular weight and Avogadro number, respectively.

For  $T < E_{s,i}$ , we obtain

$$\begin{aligned}
S_i(T < E_{s,i}) &= N \frac{n_i}{2} \int_{E_{t,i}}^T E \sigma_{E,e} dE \\
&= N \frac{n_i}{2} \frac{\pi e^4}{T + I_i + E_i} \left[ \ln(T + I_i - E) + \frac{T + I_i}{T + I_i - E} \right. \\
&\quad \left. + \frac{4E_i}{3} \left( -\frac{1}{T + I_i - E} + \frac{T + I_i}{2(T + I_i - E)^2} \right) \right]_{E_{t,i}}^T
\end{aligned} \tag{32}$$

$$\begin{aligned}
&= N n_i \frac{\pi e^4}{T + I_i + E_i} \left[ \frac{1}{2} \ln \frac{I_i}{T + I_i - E_{t,i}} + \frac{1}{2} \frac{T + I_i}{I_i} - \frac{1}{2} \frac{T + I_i}{T + I_i - E_{t,i}} \right. \\
&\quad \left. + \frac{2E_i}{3} \left( -\frac{1}{I_i} + \frac{1}{T + I_i - E_{t,i}} + \frac{T + I_i}{2I_i^2} - \frac{T + I_i}{2(T + I_i - E_{t,i})^2} \right) \right].
\end{aligned} \tag{33}$$

For  $E_{s,i} \leq T < I_i$ , we obtain

$$\begin{aligned}
S_i(E_{s,i} \leq T < I_i) &= N n_i \int_{E_{s,i}}^T E \sigma_E dE + N \frac{n_i}{2} \int_{E_{t,i}}^{E_{s,i}} E \sigma_{E,e} dE \\
&= N n_i \frac{\pi e^4}{T + I_i + E_i} \left[ \ln E - \frac{4E_i}{3E} \right]_{E_{s,i}}^T \\
&\quad + N n_i \frac{\pi e^4}{T + I_i + E_i} \left[ \ln(T + I_i - E) + \frac{T + I_i}{T + I_i - E} \right. \\
&\quad \left. + \frac{4E_i}{3} \left( -\frac{1}{T + I_i - E} + \frac{T + I_i}{2(T + I_i - E)^2} \right) \right]_{E_{s,i}}^T \\
&\quad + N \frac{n_i}{2} \frac{\pi e^4}{T + I_i + E_i} \left[ \ln(T + I_i - E) + \frac{T + I_i}{T + I_i - E} \right. \\
&\quad \left. + \frac{4E_i}{3} \left( -\frac{1}{T + I_i - E} + \frac{T + I_i}{2(T + I_i - E)^2} \right) \right]_{E_{t,i}}^{E_{s,i}} \\
&= N n_i \frac{\pi e^4}{T + I_i + E_i} \left[ \ln \frac{T}{E_{s,i}} + \ln \frac{I_i}{T + I_i - E_{s,i}} + \frac{1}{2} \ln \frac{T + I_i - E_{s,i}}{T + I_i - E_{t,i}} \right. \\
&\quad - \frac{4E_i}{3} \left( \frac{1}{T} - \frac{1}{E_{s,i}} \right) + \frac{T + I_i}{I_i} - \frac{T + I_i}{T + I_i - E_{s,i}} \\
&\quad + \frac{4E_i}{3} \left( -\frac{1}{I_i} + \frac{1}{T + I_i - E_{s,i}} + \frac{T + I_i}{2I_i^2} - \frac{T + I_i}{2(T + I_i - E_{s,i})^2} \right) \\
&\quad + \frac{1}{2} \frac{T + I_i}{T + I_i - E_{s,i}} - \frac{1}{2} \frac{T + I_i}{T + I_i - E_{t,i}} \\
&\quad \left. + \frac{2E_i}{3} \left( -\frac{1}{T + I_i - E_{s,i}} + \frac{1}{T + I_i - E_{t,i}} + \frac{T + I_i}{2(T + I_i - E_{s,i})^2} - \frac{T + I_i}{2(T + I_i - E_{t,i})^2} \right) \right] \\
&= N n_i \frac{\pi e^4}{T + I_i + E_i} \left[ \frac{1}{2} \ln \frac{T^2 I_i^2}{E_{s,i}^2 (T + I_i - E_{s,i})(T + I_i - E_{t,i})} \right. \\
&\quad + 1 + \frac{T}{I_i} - \frac{T + I_i}{2(T + I_i - E_{s,i})} - \frac{T + I_i}{2(T + I_i - E_{t,i})} \\
&\quad + \frac{E_i}{3} \left( -\frac{4}{T} + \frac{4}{E_{s,i}} - \frac{4}{I_i} + \frac{2}{T + I_i - E_{s,i}} + \frac{2}{T + I_i - E_{t,i}} \right) \\
&\quad \left. + \frac{E_i}{3} (T + I_i) \left( \frac{2}{I_i^2} - \frac{1}{(T + I_i - E_{s,i})^2} - \frac{1}{(T + I_i - E_{t,i})^2} \right) \right]. \tag{34}
\end{aligned}$$



For  $T > I_i$ , we first evaluate the singlet and triplet excitations using the previous result.

$$\begin{aligned}
\int_{E_{s,i}}^I E \sigma_E dE + \frac{1}{2} \int_{E_{t,i}}^{E_{s,i}} E \sigma_{E,e} dE &= \frac{\pi e^4}{T + I_i + E_i} \left[ \ln \frac{I_i}{E_{s,i}} + \ln \frac{T}{T + I_i - E_{s,i}} + \frac{1}{2} \ln \frac{T + I_i - E_{s,i}}{T + I_i - E_{t,i}} \right. \\
&\quad - \frac{4E_i}{3} \left( \frac{1}{I_i} - \frac{1}{E_{s,i}} \right) + \frac{T + I_i}{T} - \frac{T + I_i}{T + I_i - E_{s,i}} \\
&\quad + \frac{4E_i}{3} \left( -\frac{1}{T} + \frac{1}{T + I_i - E_{s,i}} + \frac{T + I_i}{2T^2} - \frac{T + I_i}{2(T + I_i - E_{s,i})^2} \right) \\
&\quad + \frac{1}{2} \frac{T + I_i}{T + I_i - E_{s,i}} - \frac{1}{2} \frac{T + I_i}{T + I_i - E_{t,i}} \\
&\quad \left. + \frac{2E_i}{3} \left( -\frac{1}{T + I_i - E_{s,i}} + \frac{1}{T + I_i - E_{t,i}} + \frac{T + I_i}{2(T + I_i - E_{s,i})^2} - \frac{T + I_i}{2(T + I_i - E_{t,i})^2} \right) \right] \\
&= \frac{\pi e^4}{T + I_i + E_i} \left[ \frac{1}{2} \ln \frac{I_i^2 T^2}{E_{s,i}^2 (T + I_i - E_{s,i})(T + I_i - E_{t,i})} \right. \\
&\quad + 1 + \frac{I_i}{T} - \frac{T + I_i}{2(T + I_i - E_{s,i})} - \frac{T + I_i}{2(T + I_i - E_{t,i})} \\
&\quad + \frac{E_i}{3} \left( -\frac{4}{I_i} + \frac{4}{E_{s,i}} - \frac{4}{T} + \frac{2}{T + I_i - E_{s,i}} + \frac{2}{T + I_i - E_{t,i}} \right) \\
&\quad \left. + \frac{E_i}{3} (T + I_i) \left( \frac{2}{T^2} - \frac{1}{(T + I_i - E_{s,i})^2} - \frac{1}{(T + I_i - E_{t,i})^2} \right) \right]. \tag{35}
\end{aligned}$$

The first term becomes

$$\begin{aligned}
\int_{I_i}^{\frac{(T+I_i)}{2}} E \sigma_E dE &= \frac{\pi e^4}{T + I_i + E_i} \left[ \ln E - \frac{4E_i}{3E} \right]_{I_i}^{(T+I_i)/2} \\
&\quad + \frac{\pi e^4}{T + I_i + E_i} \left[ \ln(T + I_i - E) + \frac{T + I_i}{T + I_i - E} \right. \\
&\quad \left. + \frac{4E_i}{3} \left( -\frac{1}{T + I_i - E} + \frac{T + I_i}{2(T + I_i - E)^2} \right) \right]_{I_i}^{(T+I_i)/2} \\
&= \frac{\pi e^4}{T + I_i + E_i} \left[ \ln \frac{T + I_i}{2I_i} + \ln \frac{T + I_i}{2T} - \frac{4E_i}{3} \left( \frac{2}{T + I_i} - \frac{1}{I_i} \right) \right. \\
&\quad \left. + 2 - \frac{T + I_i}{T} + \frac{4E_i}{3} \left( -\frac{2}{T + I_i} + \frac{1}{T} + \frac{2}{T + I_i} - \frac{T + I_i}{2T^2} \right) \right] \\
&= \frac{\pi e^4}{T + I_i + E_i} \left[ \ln \frac{(T + I_i)^2}{4TI_i} + 1 - \frac{I_i}{T} + \frac{4E_i}{3} \left( \frac{1}{I_i} + \frac{1}{2T} - \frac{2}{T + I_i} - \frac{I_i}{2T^2} \right) \right]. \tag{36}
\end{aligned}$$

Combining the terms, we finally obtain

$$S_i(T \geq I_i) = Nn_i \frac{\pi e^4}{T + I_i + E_i} \left[ \frac{1}{2} \ln \frac{(T + I_i)^4}{16E_{s,i}^2(T + I_i - E_{s,i})(T + I_i - E_{t,i})} \right. \\ \left. + 2 - \frac{T + I_i}{2(T + I_i - E_{s,i})} - \frac{T + I_i}{2(T + I_i - E_{t,i})} \right. \\ \left. + \frac{2E_i}{3} \left( \frac{2}{E_{s,i}} - \frac{4}{T + I_i} + \frac{1}{T + I_i - E_{s,i}} + \frac{1}{T + I_i - E_{t,i}} - \frac{T + I_i}{2(T + I_i - E_{s,i})^2} - \frac{T + I_i}{2(T + I_i - E_{t,i})^2} \right) \right]. \quad (37)$$

## 5 Degradation spectrum

The degradation spectrum of the incident electron is expressed as

$$y_1(T) = \frac{1}{S(T)}. \quad (38)$$

To describe the degradation spectrum of secondary electrons, we modify the differential cross section of ionization by replacing  $T$  by  $T_1$  and  $E$  by  $T_2 + I_i$ ,

$$\sigma(T_1, T_2) = \frac{\pi e^4}{T_1 + I_i + E_i} \left[ \frac{1}{(T_2 + I_i)^2} + \frac{4E_i}{3(T_2 + I_i)^3} + \frac{1}{(T_1 - T_2)^2} + \frac{4E_i}{3(T_1 - T_2)^2} \right], \quad (39)$$

for  $T_1 \geq T_2$ , where  $T_1$  is the energy of incident electron,  $T_2$  is the energy of secondary electron. The degradation spectrum of the secondary electrons is

$$y_2(T) = \frac{N}{S(T)} \sum_i n_i \int_T^{(T_{\text{in}} - I_i)/2} \int_{2T_2 + I_i}^{T_{\text{in}}} y_1(T_1) \sigma(T_1, T_2) dT_1 dT_2. \quad (40)$$

The integration range is shown in Fig. 4. The generated energy by collisions  $T_2$  cannot exceed  $(T_{\text{in}} - I_i)/2$  with  $T_{\text{in}}$  being the incident electron energy by definition. The incident electron energy for the secondary is  $T_{\text{in}}$ , that for the tertiary is the maximum energy of the secondary  $(T_{\text{in}} - I_i)/2$ , and so on. The energy of incident electron  $T_1$  must be greater than  $2T_2 + I_i$  because the energy of the incident electron after the collision ( $T'_1$ ) must be greater than  $T_2$  while the relation  $T_1 = T'_1 + T_2 + I_i$  must hold. Similar to the secondary, the degradation spectrum for the tertiary electrons is given by

$$y_3(T) = \frac{N}{S(T)} \sum_i n_i \int_T^{(T_{\text{in}} - 3I_i)/4} \int_{2T_2 + I_i}^{(T_{\text{in}} - I_i)/2} y_2(T_1) \sigma(T_1, T_2) dT_1 dT_2. \quad (41)$$

And, similar equations can be constructed for the electrons in the later steps. The total degradation spectrum is the sum of the above:

$$y(T) = \sum_m y_m(T). \quad (42)$$

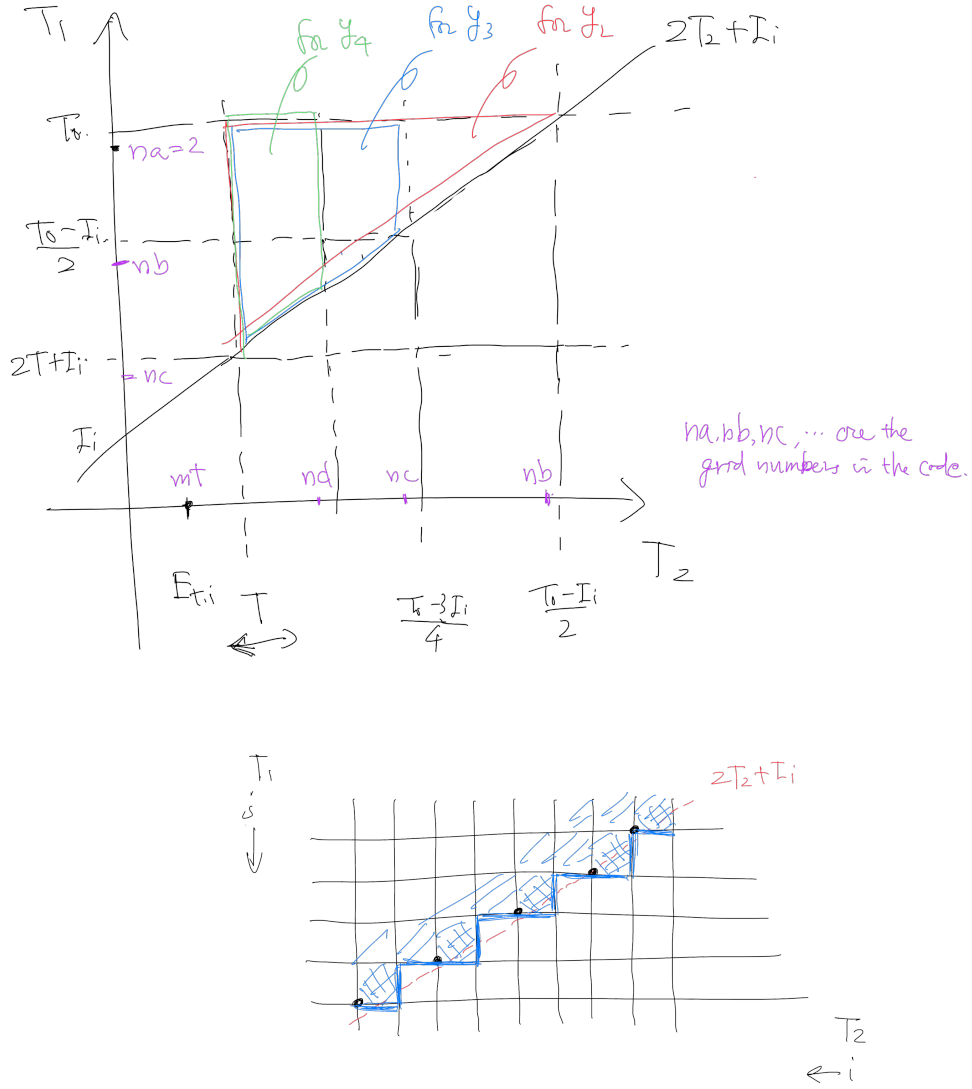


Figure 4: The integration range. The bottom figure shows the enlarged area along the  $T_1 = 2T_2 + I_i$  line.

## 5.1 Numerical evaluation

The energy grid is given by

$$\ln T_k = \ln T_{\text{in}} + (k - 1) \ln \Delta T \quad (43)$$

where  $\Delta T$  is chosen to be  $(1/2)^{1/N_{\text{div}}} < 1$  with  $N_{\text{div}}$  being an input parameter. Inversely, for a given energy  $T$ , the mesh point given by

$$k = \left\lceil \frac{\ln \frac{T}{T_{\text{in}}}}{\ln \Delta T} + 1 \right\rceil \quad (44)$$

means the smallest energy grid greater than  $T$  (i.e.,  $T_{k+1} < T \leq T_k$ )<sup>4</sup>. The mesh point of  $T_{\text{in}}$  is  $k = 1$ .

The integral is simply evaluated by

$$\int_T^{(T_{\text{in}} - I_i)/2} \int_{2T_2 + I_i}^{T_{\text{in}}} y_1(T_1) \sigma(T_1, T_2) dT_1 dT_2 \approx \sum_{k_1} \sum_{k_2} y_1(T_{k_1}) \sigma(T_{k_1}, T_{k_2}) (T_{k_1-1} - T_{k_1}) (T_{k_2-1} - T_{k_2}). \quad (45)$$

## 5.2 Results

We calculate the degradation spectrum for Helium. The parameters for Helium [5] are  $E_{s,1} = 21.2$ ,  $E_{t,1} = 19.8$ ,  $I_1 = 24.581$ ,  $E_1 = 38.74$  [eV],  $n_1 = 2$  is used. The incident electron energy is  $T_{\text{in}} = 10^5$  [eV]. The result is shown in Fig. 5, fully reproducing Fig. 1 of [5].

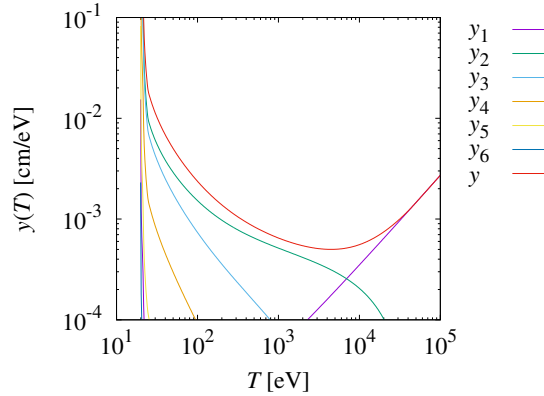


Figure 5: The degradation spectrum in Helium.

Figure 6 shows the degradation spectrum in water (gas phase) with the incident electron energy  $T_{\text{in}} = 10^5$  [eV]. The figure looks different from Fig. 5 of [4] probably because the electron distribution generated by <sup>60</sup>Co  $\gamma$ -ray is not taken into account here.

<sup>4</sup>The square bracket is the Gauss bracket denoting the smaller integer not exceeding its argument.

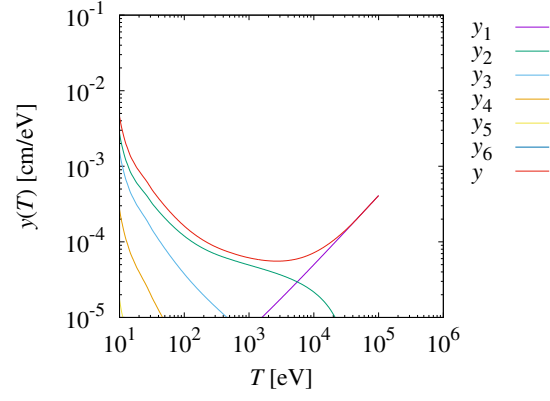


Figure 6: The degradation spectrum in water (gas phase).

Table 1: The parameters used for water [4].

Shell ( $i$ )	$I_i$	$E_i$	$E_{s,i}$	$E_{t,i}$	$n_i$
1	12.6	70.40	7.42	5.0	2
2	14.7	66.46	9.50	7.0	2
3	18.4	28.41	13.0	11.0	2
4	32.2	74.94	27.0	25.0	2
5	539.7	799.60	535.0	533.0	2

## 6 $G$ value

Once the degradation spectrum  $y(T)$  is obtained, the calculation of the yields of excitation and ionization per incident electron is straightforward. The number of the species produced in the process  $s$  is given by

$$\begin{aligned} N_{\text{ion}} &= N \sum_i n_i \int_{I_i}^{T_{\text{in}}} y Q_{\text{ion},i} dT + N \sum_i n_i \int_{I_i}^{T_{\text{in}}} y Q_{\text{snl},i} dT + N \sum_i n_i \int_{I_i}^{T_{\text{in}}} y Q_{\text{trpl},i} dT \\ &= N \sum_i n_i \int_{I_i}^{T_{\text{in}}} T y (Q_{\text{ion},i} + Q_{\text{snl},i} + Q_{\text{trpl},i}) d \ln T, \end{aligned} \quad (46)$$

$$N_{\text{snl}} = N \sum_i n_i \int_{E_{s,i}}^{I_i} T y Q_{\text{snl},i} d \ln T, \quad (47)$$

$$N_{\text{trpl}} = N \sum_i n_i \int_{E_{t,i}}^{I_i} T y Q_{\text{trpl},i} d \ln T. \quad (48)$$

The energy integral is evaluated by the trapezoidal rule<sup>5</sup>, e.g.

$$\int T y Q d \ln T \approx \left( \sum_k \frac{T_k y_k Q_{s,i,k} + T_{k-1} y_{k-1} Q_{s,i,k-1}}{2} \ln \Delta T \right). \quad (51)$$

The radiation yield (the  $G$  value) is the number of molecules formed per 100[eV] defined as

$$G_s = \frac{100 N_s}{T_{\text{in}}}, \quad (52)$$

where  $s$  signifies the process (ionization, singlet or triplet excitation).

Figure 7 is the  $TyQ$  plot showing the contribution of the electron slowing-down spectrum to the ionization and excitations for water in a gas phase. The  $G$  values are 2.91 (ionization), 3.72 (singlet) and 0.785 (triplet).

## 7 Range and mean free path

The mean free path is defined by

$$\lambda = \frac{1}{N \sum_s Q_s} \quad (53)$$

---

<sup>5</sup>For most cases, the smaller energy grid in the integration range is slightly above the exact values of the threshold energies ( $I_i$ ,  $E_s$ ,  $E_t$ ). For example, we consider the threshold energy  $E_{\text{th}} = I_i, E_s, E_t$  and let

$$k_{\text{max}} = \left\lceil \frac{\ln \frac{E_{\text{th}}}{T_{\text{in}}}}{\ln \Delta T} + 1 \right\rceil. \quad (49)$$

Then,  $T_{k_{\text{max}}} > E_{\text{th}}$ . Therefore, in the code, we define

$$\int_{E_{\text{th}}}^{T_{\text{in}}} f(T) d \ln T \approx \sum_{k=1}^{k_{\text{max}}} f(T_k) \ln \Delta T - \frac{1}{2} f(T_1) \ln \Delta T, \quad (50)$$

and do not subtract half of the contribution from  $k_{\text{max}}$ .

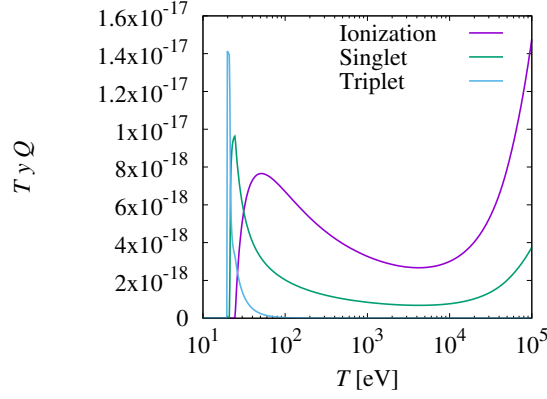


Figure 7: The  $T\gamma Q$  plot for Helium.

The stopping power is the rate by which the electron loose the energy per unit length,  $S = dT/dx$ . Then, the length that electron can travel (the range) is given by [6]

$$R = \int_0^R dx = \int_{T_{\text{in}}}^0 \frac{dT}{dT/dx} \sim \int_{T_{\text{in}}}^{\min(E_{t,i})} \frac{T}{S} d \ln T. \quad (54)$$

(Note that  $S$  is singular at  $T = E_t$  and the integral does not converge. This definition must be re-considered. We also show the range evaluated from the minimum energy above  $\min(E_{s,i})$  and  $\min(I_i)$ .)

Figure 8 shows the mean free path and range for helium with the incident electron energy  $T_{\text{in}} = 10^5 [\text{eV}]$ .

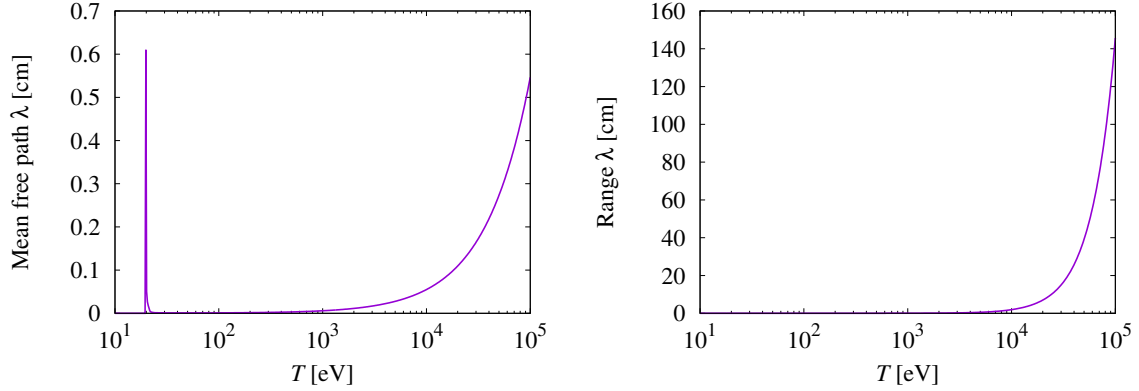


Figure 8: The mean free path and range for Helium.

## A Constants and units

Basic physical constants are given in Table 2. Table 3 summarizes the derived quantities. The classical electron radius is given by  $r_0 = e^2/(mc^2)$  with  $e$  given in the cgs-electrostatic unit, while  $r_0 = e^2/(4\pi\epsilon_0 mc^2)$  with  $e$  in the SI unit. The conversion of C to statC is given by  $1[\text{C}] = 10c[\text{statC}]$ .

Table 2: Numerical values of basic constants. Adapted from [2].

Symbol	Name	Value	Unit [esu]	Value	Unit [SI]
$e$	elementary charge	$4.8032 \times 10^{-10}$	statC	$1.6022 \times 10^{-19}$	C=A·s
$m$	electron masse	$9.1094 \times 10^{-28}$	g	$9.1094 \times 10^{-31}$	kg
$c$	speed of light	$2.9979 \times 10^{10}$	cm s <sup>-1</sup>	$2.9979 \times 10^8$	m s <sup>-1</sup>

Table 3: Derived quantities.

Symbol	Name	Value	
$mc^2$	electron rest mass energy	0.510999 [MeV]	$8.18711 \times 10^{-14}$ [J]
$r_0$	classical electron radius	$2.8179 \times 10^{-13}$ [cm]	$2.8179 \times 10^{-15}$ [m]

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