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 θ given by Klein and Nishina

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

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 γ-ray. The solid angle is $\mathrm{d}\Omega = \sin\theta\mathrm{d}\theta\mathrm{d}\varphi$. From the conservation laws, the electron energy T is written in terms of the photon deflection angle θ,

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

Using the electron energy, we obtain

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

By taking the derivative of T with respect to θ, we have

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

Therefore, the differential cross section per unit energy T becomes

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

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}Co γ-ray energy, $h\nu = 1.17, 1.33$ [MeV]. The graph looks similar to Fig. 1 of [5], but the vertical axis differs. But, I don't understand what $f(T)$ is and its unit.

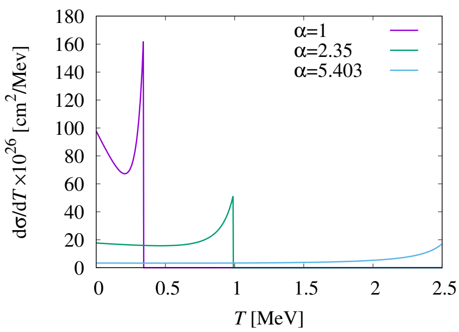


Figure 1: The differential cross section per unit energy for three primary photon energies, $\alpha = 1, 2.35, 5.403$.

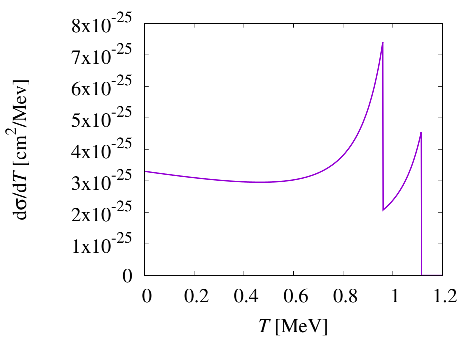


Figure 2: The differential cross section per unit energy for ^{60}Co γ-ray energy, $h\nu = 1.17, 1.33$ [MeV].

2 Cross section

The differential cross section[1] per unit of energy for the energy loss E of the incident electron with the energy T is given by

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

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

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

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

for $T + I_i - E \geq 0$. The subscript $i = 1, 2, 3, \ldots$ 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

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

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 σ_E over $E \in [I_i, (T + I_i)/2]$,

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

[1]The unit of the differential cross section is [charge]^4/[Energy]^3=[dyn^2 cm^4/erg^3]=[cm^2/erg]=[s^2/g].

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

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

Therefore, (9) is proven.

Now, we evaluate (9).

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

Figure 3 shows the total ionization cross section of hydrogen with $I_1 = 16.0$[eV] and $E_1 = 31.96$[eV]. As in [4], the dissociative ionization and excitation are also considered. We are not able to reproduce the result of [4].

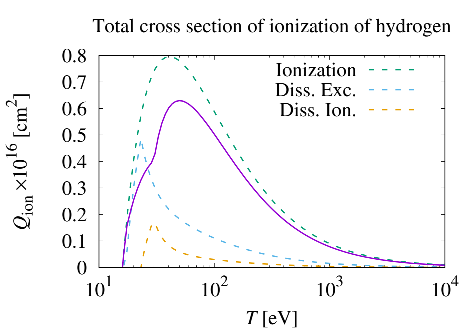


Figure 3: The total ionization cross section of hydrogen with $I_1 = 16.0$[eV], $E_1 = 31.96$[eV].

3.2 Singlet and Triplet

The cross section of excitations are given by

$$Q_{\mathrm{sngl},i} = Q_{\mathrm{de},i} + \frac{1}{2} Q_{\mathrm{ee},i}, \tag{13}$$

$$Q_{\mathrm{trpl},i} = \frac{1}{2} Q'_{\mathrm{ee},i} \tag{14}$$

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

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

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

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

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

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

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

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

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

$E_{s,i}$ 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[2] is expressed as

$$S(T) = \sum_i S_i(T), \tag{24}$$

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

where

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

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

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

N is the number of atoms in a unit volume[3], 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

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

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

$$\int \frac{E}{E^2} \mathrm{d}E = \ln E, \tag{30}$$

$$\int \frac{E}{E^3} \mathrm{d}E = -\frac{1}{E}. \tag{31}$$

[3] 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, $N = 6.02 \times 10^{23}/(22.4 \times 10^3) = 0.269 \times 10^{20}$ [cm^{-3}]. For a solid, $N = d/(M/N_\mathrm{A})$ with d, M, $N_\mathrm{A} \equiv 6.02 \times 10^{23}$ being the density, molecular weight and Avogadro number, respectively.

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

$$
\begin{aligned}
S_i(T < E_{s,i}) &= N\frac{n_i}{2}\int_{E_{t,i}}^{T} E\sigma_{E,\mathrm{e}}\mathrm{d}E \\
&= N\frac{n_i}{2}\frac{\pi e^4}{T+I_i+E_i}\left[\ln(T+I_i-E)+\frac{T+I_i}{T+I_i-E}\right. \qquad (32)\\
&\quad \left.+\frac{4E_i}{3}\left(-\frac{1}{T+I_i-E}+\frac{T+I_i}{2(T+I_i-E)^2}\right)\right]_{E_{t,i}}^{T} \\
&= Nn_i\frac{\pi e^4}{T+I_i+E_i}\left[\frac{1}{2}\ln\frac{I_i}{T+I_i-E_{t,i}}+\frac{1}{2}\frac{T+I_i}{I_i}-\frac{1}{2}\frac{T+I_i}{T+I_i-E_{t,i}}\right. \\
&\quad \left.+\frac{2E_i}{3}\left(-\frac{1}{I_i}+\frac{1}{T+I_i-E_{t,i}}+\frac{T+I_i}{2I_i^2}-\frac{T+I_i}{2(T+I_i-E_{t,i})^2}\right)\right]. \qquad (33)
\end{aligned}
$$

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

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

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

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

The first term becomes

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

Combining the terms, we finally obtain

$$
\begin{aligned}
S_i(T \geq I_i) = N n_i \frac{\pi e^4}{T+I_i+E_i} \Bigg[& \frac{1}{2} \ln \frac{(T+I_i)^4}{16 E_{s,i}^2 (T+I_i-E_{s,i})(T+I_i-E_{t,i})} \\
& + 2 - \frac{T+I_i}{2(T+I_i-E_{s,i})} - \frac{T+I_i}{2(T+I_i-E_{t,i})} \\
& + \frac{2E_i}{3} \left(\frac{2}{E_{s,i}} - \frac{4}{T+I_i} + \frac{1}{T+I_i-E_{s,i}} + \frac{1}{T+I_i-E_{t,i}} - \frac{T+I_i}{2(T+I_i-E_{s,i})^2} - \frac{T+I_i}{2(T+I_i-E_{t,i})^2} \right) \Bigg].
\end{aligned}
\tag{37}
$$

5 Degradation spectrum

The degradation spectrum of the incident electron is expressed as

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

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 $T_2 + I_i$,

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

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

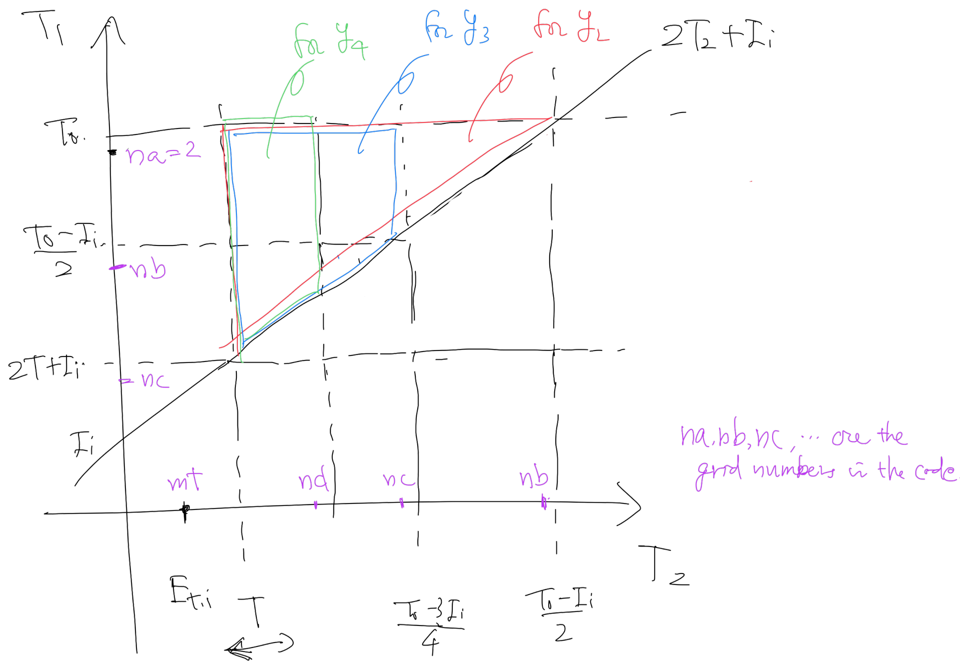
$$
y_2(T) = \frac{N}{S(T)} \sum_i n_i \int_T^{(T_{\text{in}}-I_i)/2} \int_{2T_2+I_i}^{T_{\text{in}}} y_1(T_1) \sigma(T_1, T_2) \mathrm{d}T_1 \mathrm{d}T_2. \tag{40}
$$

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_{in} being the incident electron energy by definition. The incident electron energy for the secondary is T_{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

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

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

$$
y(T) = \sum_m y_m(T). \tag{42}
$$



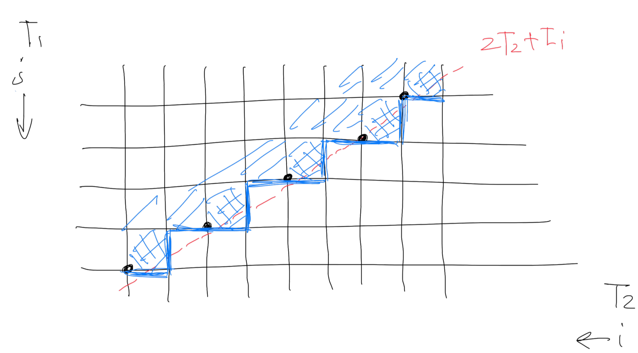


Figure 4: The integration range. The bottom figure shows the enlarged area along the $T_1 = 2T_2 + I_i$ line.

5.1 Numerical evaluation

The energy grid is given by

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

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

$$k = \left[\frac{\ln \frac{T}{T_{\rm in}}}{\ln \Delta T} + 1 \right] \tag{44}$$

means the smallest energy grid greater than T (i.e., $T_{k+1} < T \le T_k$)[4]. The mesh point of $T_{\rm in}$ is $k = 1$.

The integral is simply evaluated by

$$\int_T^{(T_{\rm in}-I_i)/2} \int_{2T_2+I_i}^{T_{\rm in}} y_1(T_1)\sigma(T_1,T_2)\mathrm{d}T_1\mathrm{d}T_2 \approx \sum_{k_1}\sum_{k_2} y_1(T_{k_1})\sigma(T_{k_1},T_{k_2})(T_{k_1-1}-T_{k_1})(T_{k_2-1}-T_{k_2}). \tag{45}$$

5.2 Results

We calculate the degradation spectrum for Helium. The parameters for Helium [6] 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 $T_{\rm in} = 10^5$[eV]. The result is shown in Fig. 5, fully reproducing Fig. 1 of [6].

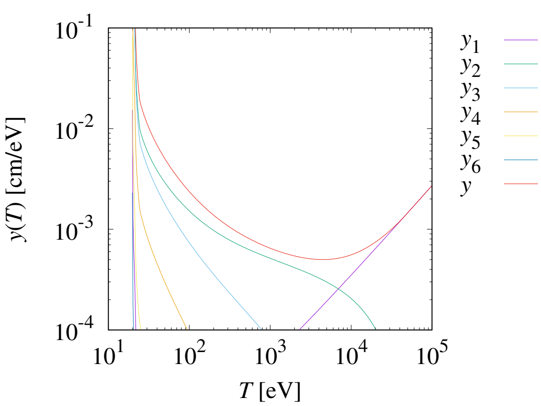


Figure 5: The degradation spectrum in Helium.

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

[4] The square bracket is the Gauss bracket denoting the smaller integer not exceeding its argument.

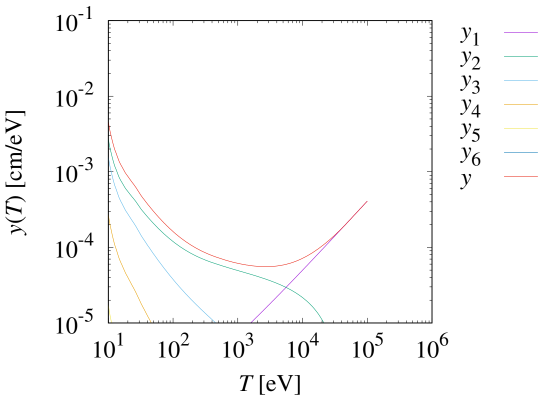


Figure 6: The degradation spectrum in water (gas phase).

Table 1: The parameters used for water [5].

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

$$
\begin{aligned}
N_{\text{ion}} &= N\sum_i n_i \int_{I_i}^{T_{\text{in}}} yQ_{\text{ion},i}\mathrm{d}T + N\sum_i n_i \int_{I_i}^{T_{\text{in}}} yQ_{\text{sngl},i}\mathrm{d}T + N\sum_i n_i \int_{I_i}^{T_{\text{in}}} yQ_{\text{trpl},i}\mathrm{d}T \\
&= N\sum_i n_i \int_{I_i}^{T_{\text{in}}} Ty(Q_{\text{ion},i} + Q_{\text{sngl},i} + Q_{\text{trpl},i})\mathrm{d}\ln T, \qquad (46)\\
N_{\text{sngl}} &= N\sum_i n_i \int_{E_{s,i}}^{I_i} TyQ_{\text{sngl},i}\mathrm{d}\ln T, \qquad (47)\\
N_{\text{trpl}} &= N\sum_i n_i \int_{E_{t,i}}^{I_i} TyQ_{\text{trpl},i}\mathrm{d}\ln T. \qquad (48)
\end{aligned}
$$

The energy integral is evaluated by the trapezoidal rule[5], e.g.

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

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

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

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

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

[5]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

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

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

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

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

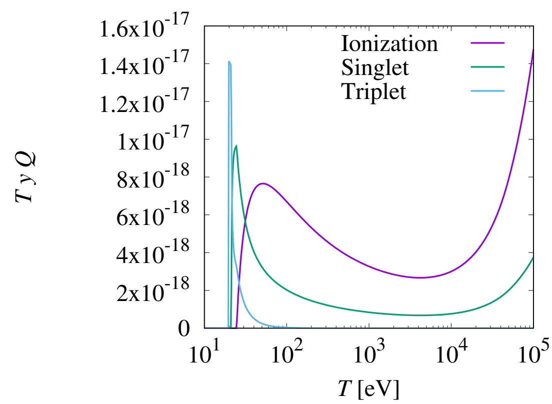


Figure 7: The TyQ plot for Helium.

The stopping power is the rate by which the electron loose the energy per unit length, $S = \mathrm{d}T/\mathrm{d}x$. Then, the length that electron can travel (the range) is given by [7]

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

(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 $T_{\mathrm{in}} = 10^5$[eV].

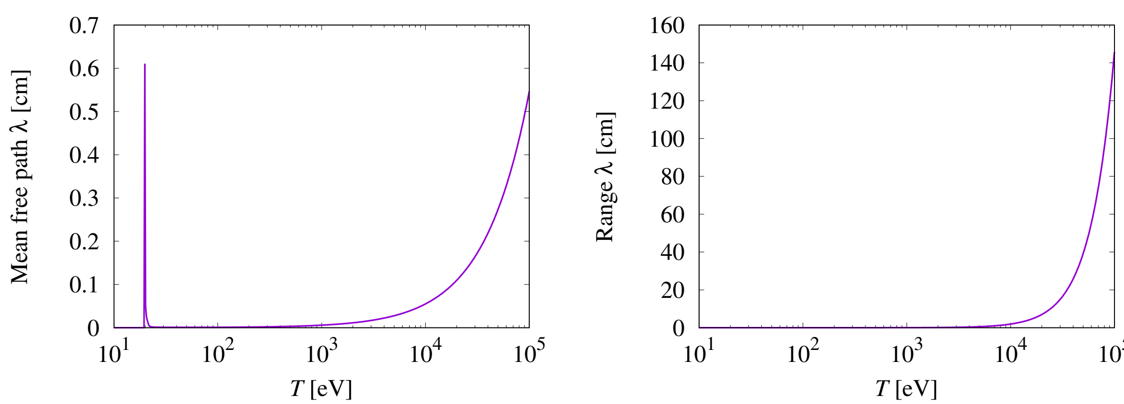


Figure 8: The mean free path and range for Helium.

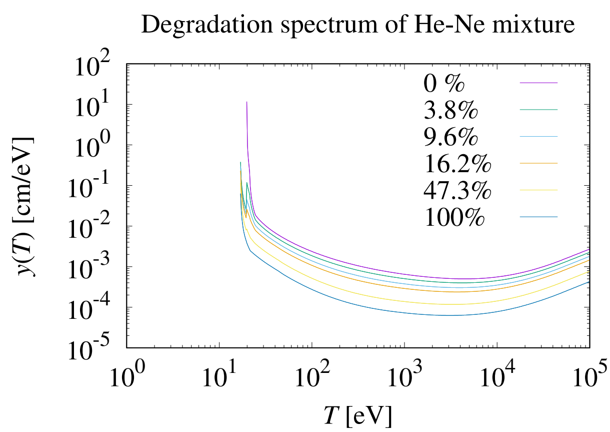


Figure 9: Degradation spectrum of He-Ne mixture with different Ne fractions.

8 Mixture of media

We consider a mixture of multiple media. The stopping power of the mixture is given by

$$S_{\mathrm{mix}}(T) = \frac{1}{\sum_j N_j} \sum_j N_j S_j(T), \tag{55}$$

where N_j, S_j are, respectively, the number density and stopping power of the media j. The degradation spectra are accordingly modified as

$$y_1(T) = \frac{1}{S_{\mathrm{mix}}(T)}, \tag{56}$$

$$y_2(T) = \sum_j \frac{N_j}{S_{\mathrm{mix}}(T)} \sum_i n_{i,j} \int_T^{(T_{\mathrm{in}}-I_{i,j})/2} \int_{2T_2+I_{i,j}}^{T_{\mathrm{in}}} y_1(T_1)\sigma_j(T_1,T_2)\mathrm{d}T_1\mathrm{d}T_2. \tag{57}$$

Similar modifications apply to the later generations.

The mean free path is modified as

$$\lambda_{\mathrm{mix}}(T) = \frac{1}{\sum_j N_j \sum_s Q_{s,j}(T)}. \tag{58}$$

For gases, the number of atoms per unit volume is proportional to the pressure at a constant temperature. The above definition of the mixture is consistent with the mixture of noble gases considered in [3].

Figure 9 shows the degradation spectrum of He-Ne mixture. The result fully reproduces that shown in [3].

9 Input parameters

There are two categories of namelist inputs: One is for the run parameters and the other is for the parameters of media (gases, compounds, etc.). The run parameters are given in the input file to be passed to the program.

The media parameters are given in the files defined by `file_medium`. The media parameter file can be generated by converting CSV using `generate_parameters.py` in `tools` directory. See help of the script.

9.1 Run parameters

Table 2: `param_calc`

name	meaning	default
`ngeneration`	Number of electron generations (Sec. 5)	6
`nmedia`	Number of media (Sec. 8)	1

Table 3: `param_medium`: List of media parameters. The size of list is defined by `nmedia`.

name	meaning	default
`file_medium`	Input file of orbital parameters	-
`number_density`	Number density	1.0

Table 4: `param_grid`

name	meaning	default
`nediv`	Number of energy grid division N_{div} (Sec. 5.1)	40
`egrid_max`	Incident photon energy T_{in} (Sec. 5.1)	10^5
`egrid_min`	Minimum of energy grid	1

9.2 Media parameters

A Constants and units

Basic physical constants are given in Table 7. Table 8 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 $1[\mathrm{C}] = 10c[\mathrm{statC}]$.

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Table 5: `param_orbital`

name	meaning	default
`name`	Name of medium	'unknown'

Table 6: `params_per_orbitals`: List of orbital parameters. The size of the list determines the number of orbitals (must be less than or equal to `norbital_max`=1000).

name	meaning	default
`energy_ionize`	Ionization energy per orbital	-
`energy_singlet`	Singlet excitation energy per orbital	-
`energy_triplet`	Triplet excitation energy per orbital	-
`energy_kinetic`	Kinetic energy per orbital	-
`number_electrons`	Number of electrons per orbital	-

Table 7: Numerical values of basic constants. Adapted from [2].

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

Table 8: Derived quantities.

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

K. M. Black, E. Blucher, R. Bonventre, R. A. Briere, A. Buckley, V. D. Burkert, M. A. Bychkov, R. N. Cahn, Z. Cao, M. Carena, G. Casarosa, A. Ceccucci, A. Cerri, R. S. Chivukula, G. Cowan, K. Cranmer, V. Crede, O. Cremonesi, G. D'Ambrosio, T. Damour, D. de Florian, A. de Gouvêa, T. DeGrand, S. Demers, Z. Demiragli, B. A. Dobrescu, M. D'Onofrio, M. Doser, H. K. Dreiner, P. Eerola, U. Egede, S. Eidelman, A. X. El-Khadra, J. Ellis, S. C. Eno, J. Erler, V. V. Ezhela, A. Fava, W. Fetscher, B. D. Fields, A. Freitas, H. Gallagher, T. Gershon, Y. Gershtein, T. Gherghetta, M. C. Gonzalez-Garcia, M. Goodman, C. Grab, A. V. Gritsan, C. Grojean, D. E. Groom, M. Grünewald, A. Gurtu, H. E. Haber, M. Hamel, S. Hashimoto, Y. Hayato, A. Hebecker, S. Heinemeyer, K. Hikasa, J. Hisano, A. Höcker, J. Holder, L. Hsu, J. Huston, T. Hyodo, Al. Ianni, M. Kado, M. Karliner, U. F. Katz, M. Kenzie, V. A. Khoze, S. R. Klein, F. Krauss, M. Kreps, P. Kriăn, B. Krusche, Y. Kwon, O. Lahav, L. P. Lellouch, J. Lesgourgues, A. R. Liddle, Z. Ligeti, C.-J. Lin, C. Lippmann, T. M. Liss, A. Lister, L. Littenberg, K. S. Lugovsky, S. B. Lugovsky, A. Lusiani, Y. Makida, F. Maltoni, A. V. Manohar, W. J. Marciano, J. Matthews, U.-G. Meißner, I.-A. Melzer-Pellmann, P. Mertsch, D. J. Miller, D. Milstead, K. Mönig, P. Molaro, F. Moortgat, M. Moskovic, N. Nagata, K. Nakamura, M. Narain, P. Nason, A. Nelles, M. Neubert, Y. Nir, H. B. O'Connell, C. A. J. O'Hare, K. A. Olive, J. A. Peacock, E. Pianori, A. Pich, A. Piepke, F. Pietropaolo, A. Pomarol, S. Pordes, S. Profumo, A. Quadt, K. Rabbertz, J. Rademacker, G. Raffelt, M. Ramsey-Musolf, P. Richardson, A. Ringwald, D. J. Robinson, S. Roesler, S. Rolli, A. Romaniouk, L. J Rosenberg, J. L. Rosner, G. Rybka, M. G. Ryskin, R. A. Ryutin, B. Safdi, Y. Sakai, S. Sarkar, F. Sauli, O. Schneider, S. Schönert, K. Scholberg, A. J. Schwartz, J. Schwiening, D. Scott, F. Sefkow, U. Seljak, V. Sharma, S. R. Sharpe, V. Shiltsev, G. Signorelli, M. Silari, F. Simon, T. Sjöstrand, P. Skands, T. Skwarnicki, G. F. Smoot, A. Soffer, M. S. Sozzi, C. Spiering, A. Stahl, Y. Sumino, F. Takahashi, M. Tanabashi, J. Tanaka, M. Taševsk'y, K. Terao, K. Terashi, J. Terning, U. Thoma, R. S. Thorne, L. Tiator, M. Titov, D. R. Tovey, K. Trabelsi, P. Urquijo, G. Valencia, R. Van de Water, N. Varelas, L. Verde, I. Vivarelli, P. Vogel, W. Vogelsang, V. Vorobyev, S. P. Wakely, W. Walkowiak, C. W. Walter, D. Wands, D. H. Weinberg, E. J. Weinberg, N. Wermes, M. White, L. R. Wiencke, S. Willocq, C. L. Woody, R. L. Workman, W.-M. Yao, M. Yokoyama, R. Yoshida, G. Zanderighi, G. P. Zeller, R.-Y. Zhu, S.-L. Zhu, F. Zimmermann, P. A. Zyla, J. Anderson, M. Kramer, P. Schaffner, and W Zheng. Review of particle physics. *Phys. Rev. D*, 110(3):030001, 2024.

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