Maxwellian rate coefficient

$$\mathcal{R}_{\alpha\beta} = \frac{n_\alpha n_\beta}{1+\delta_{\alpha\beta}} \langle \sigma(\upsilon)\upsilon \rangle \quad \left[\frac{1}{\mathrm{cm^3 s}} \right]$$ - reaction rate

$$R_{\alpha\beta} = \langle \sigma(\upsilon)\upsilon \rangle = \int \sigma(\upsilon)\upsilon f_\alpha(\mathbf{v}_\alpha) f_\beta(\mathbf{v}_\beta) d^3\mathbf{v}_\alpha d^3\mathbf{v}_\beta$$ - rate coefficient

$$\upsilon = \left| \mathbf{v}_\alpha - \mathbf{v}_\beta \right| = \sqrt{\left(\mathrm{v}_{\alpha x} - \mathrm{v}_{\beta x}\right)^2 + \left(\mathrm{v}_{\alpha y} - \mathrm{v}_{\beta y}\right)^2 + \left(\mathrm{v}_{\alpha z} - \mathrm{v}_{\beta z}\right)^2}$$

$$f_\alpha(\mathbf{v}_\alpha) = \left(\frac{m_\alpha}{2\pi T_\alpha} \right)^{3/2} e^{-\frac{m_\alpha \mathrm{v}_\alpha^2}{2T_\alpha}} \quad ; \quad f_\beta(\mathbf{v}_\beta) = \left(\frac{m_\beta}{2\pi T_\beta} \right)^{3/2} e^{-\frac{m_\beta \mathrm{v}_\beta^2}{2T_\beta}} \quad ;$$ assume $T_\alpha = T_\beta$

$$\frac{m_\alpha \mathrm{v}_\alpha^2}{2} + \frac{m_\beta \mathrm{v}_\beta^2}{2} = \frac{MV^2}{2} + \frac{\mu \upsilon^2}{2}$$, where $M = m_\alpha + m_\beta$, $\mu = \dfrac{m_\alpha m_\beta}{m_\alpha + m_\beta}$

Maxwellian rate coefficient (continued)

$$\mathbf{V} = \frac{m_\alpha \mathbf{v}_\alpha + m_\beta \mathbf{v}_\beta}{m_\alpha + m_\beta}$$ - velocity of the centre of mass

The integrand depends on the absolute values of the c.m. velocity and the relative velocity, and there is no angular dependence, therefore in spherical polar coordinates:

$$R_{\alpha\beta}^{(MM)} = 16\pi^2 \int_0^\infty V^2 dV \int_0^\infty \upsilon^2 d\upsilon \sigma(\upsilon)\upsilon \left(\frac{m_\alpha}{2\pi T_\alpha}\right)^{3/2} \left(\frac{m_\beta}{2\pi T_\beta}\right)^{3/2} e^{-\frac{\mu\upsilon^2}{2T} - \frac{MV^2}{2T}}$$

$$\int_0^\infty V^2 e^{-\frac{MV^2}{2T}} dV = \left[z = \sqrt{\frac{M}{2T}} V; \quad dz = \sqrt{\frac{M}{2T}} dV \right] = \left(\frac{2T}{M}\right)^{3/2} \int_0^\infty z^2 e^{-z^2} dz$$

$$= \left(\frac{2T}{M}\right)^{3/2} \int_0^\infty z^2 e^{-z^2} dz = \left[t = z^2 \right] = \frac{1}{2} \left(\frac{2T}{M}\right)^{3/2} \int_0^\infty t^{1/2} e^{-t} dt = \frac{1}{2} \left(\frac{2T}{M}\right)^{3/2} \Gamma\left(\frac{3}{2}\right) = \frac{\sqrt{\pi}}{4} \left(\frac{2T}{M}\right)^{3/2}$$

Maxwellian rate coefficient (continued)

$y = \frac{\upsilon^2}{\upsilon_0^2}$ - dimensionless variable ; υ_0 - atomic unit of velocity

CODATA internationally recommended 2018 values of the Fundamental Physical Constants:
https://physics.nist.gov/cuu/Constants/index.html

$\gamma = \frac{\mu \upsilon_0^2}{2T}$ - dimensionless parameter ;

$$R_{\alpha\beta}^{(MM)}\left(\mu/T\right) = \frac{2}{\sqrt{\pi}} \upsilon_0 \gamma^{3/2} \int_0^\infty \sigma(y) f(y) dy$$

$f(y) = y e^{-\gamma y}$; $f'(y) = \left(1 - \gamma y\right) e^{-\gamma y}$; $f'(y) = 0$ when $y = \frac{1}{\gamma}$