[振動分配関数]

$$q_{\mathrm{vib}}^{(1)} = \left[1 - \exp\left(-\frac{h\nu}{kT}\right)\right]^{-1} \qquad (7.4)$$

$$q_{\mathrm{vib\text{-}cl}}^{(1)} = \frac{kT}{h\nu} \qquad (7.4\text{-cl})$$

$$q_{\mathrm{vib}} = \prod_{i=1}^{n_{\mathrm{v}}}\left[1 - \exp\left(-\frac{h\nu_i}{kT}\right)\right]^{-1} \qquad (7.5)$$

[回転分配関数]

$$q_{\mathrm{rot}}^{2\mathrm{D}} = \int_0^{\infty} \rho_{\mathrm{rot}}^{2\mathrm{D}} \exp\left(-\frac{\varepsilon_J}{kT}\right) \mathrm{d}\varepsilon_J = \frac{kT}{\sigma B} \qquad (7.6)$$

σ: 回転対称数
= 2 (H_2, N_2, CO_2)
= 1 (HCl, N_2O)

$$q_{\mathrm{rot}}^{3\mathrm{D}} = \frac{n_{\mathrm{isom}}\pi^{1/2}}{\sigma}\left(\frac{kT}{A}\frac{kT}{B}\frac{kT}{C}\right)^{1/2} \qquad (7.7)$$

σ: 回転対称数
= 2 (H_2O, SO_2)
= 3 (NH_3)
:

n_{isom} : (光学)異性体の数

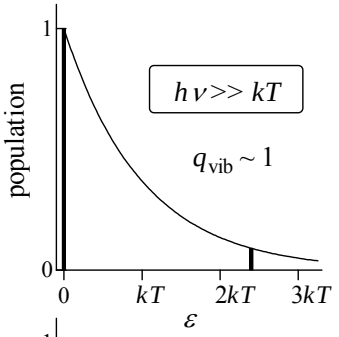
[並進分配関数]

$$q_{\mathrm{trans}}^{1\mathrm{D}} = \left(\frac{2\pi mkT}{h^2}\right)^{1/2} l \qquad (7.9)$$

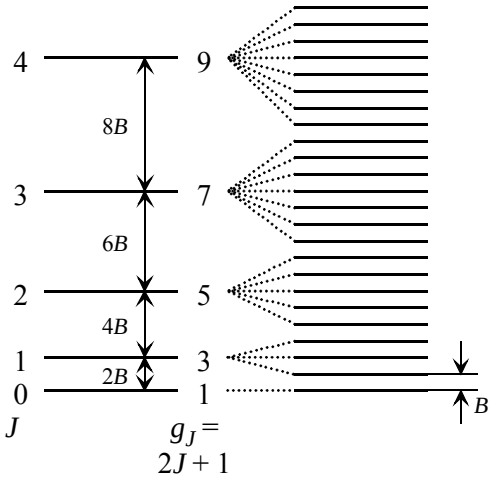
$$q_{\mathrm{trans}}^{3\mathrm{D}} = \left(\frac{2\pi mkT}{h^2}\right)^{3/2} l_x l_y l_z \qquad (7.10)$$

$$q_{\mathrm{trans}}^{\circ} = \left(\frac{2\pi mkT}{h^2}\right)^{3/2} \qquad (7.11)$$

$$q_{\mathrm{trans}}^{\circ} = \left(\frac{2\pi \mu kT}{h^2}\right)^{3/2} \qquad (7.12)$$



振動分配関数



二次元回転の状態密度 $\sim 1 / B$