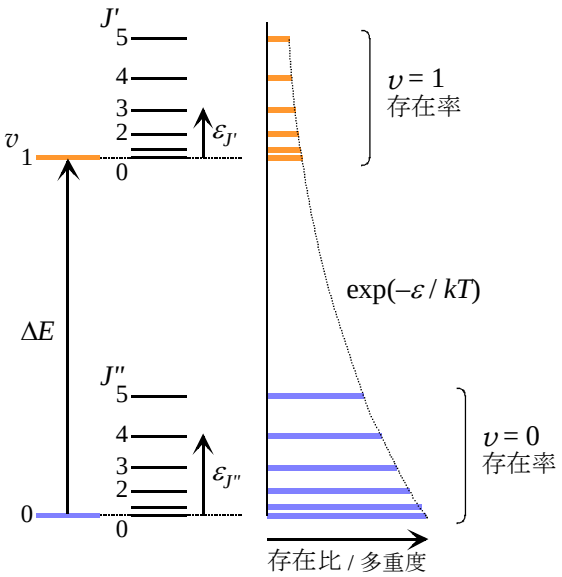
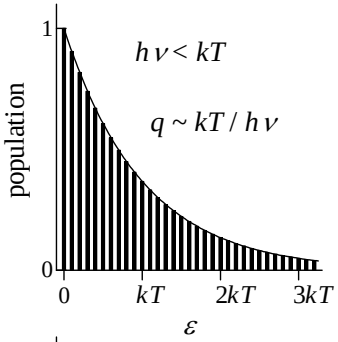
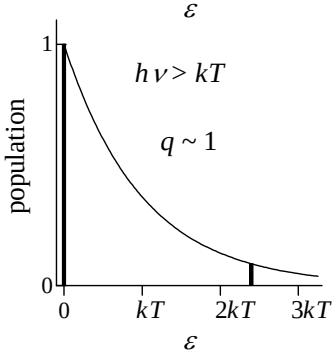



$$\frac{n(\upsilon=1)}{n(\upsilon=0)}=\frac{\sum_{J'} g(J')\exp\left(-\frac{\varepsilon_{J'}+\Delta E}{kT}\right)}{\sum_{J''} g(J'')\exp\left(-\frac{\varepsilon_{J''}}{kT}\right)}=\frac{q(\upsilon=1)}{q(\upsilon=0)}$$

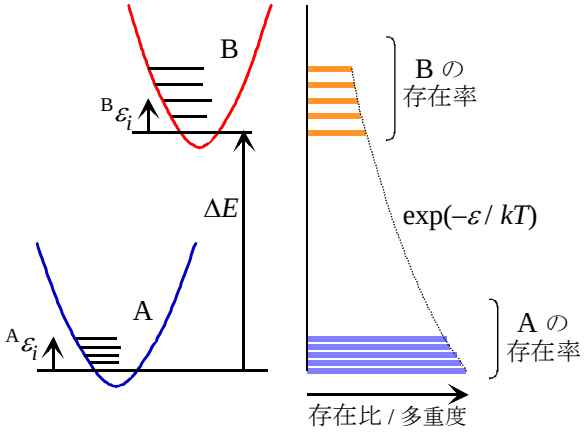
$$=\frac{\sum_{J'} g(J')\exp\left(-\frac{\varepsilon_{J'}}{kT}\right)}{\sum_{J''} g(J'')\exp\left(-\frac{\varepsilon_{J''}}{kT}\right)}\exp\left(-\frac{\Delta E}{kT}\right)=\frac{q'_{\mathrm{rot}}}{q''_{\mathrm{rot}}}\exp\left(-\frac{\Delta E}{kT}\right)$$

CO の振動回転準位分布




振動分配関数



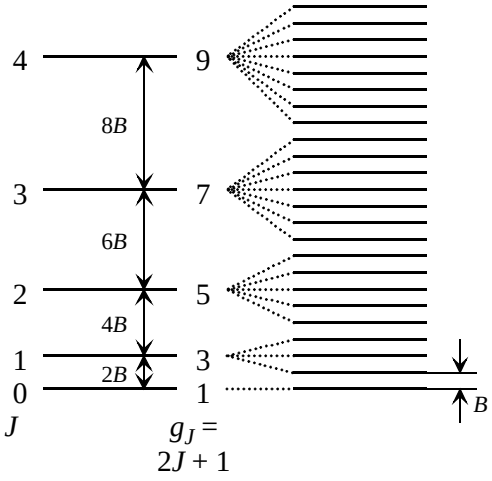

分子内準位分布と化学平衡

$$K_c=\frac{[\mathrm{B}]_\mathrm{e}}{[\mathrm{A}]_\mathrm{e}}=\frac{\sum_i {}^{\mathrm{B}}g_i\exp\left(-\frac{{}^{\mathrm{B}}\varepsilon_i+\Delta E}{kT}\right)}{\sum_i {}^{\mathrm{A}}g_i\exp\left(-\frac{{}^{\mathrm{A}}\varepsilon_i}{kT}\right)}$$

$$=\frac{\sum_i {}^{\mathrm{B}}g_i\exp\left(-\frac{{}^{\mathrm{B}}\varepsilon_i}{kT}\right)}{\sum_i {}^{\mathrm{A}}g_i\exp\left(-\frac{{}^{\mathrm{A}}\varepsilon_i}{kT}\right)}\exp\left(-\frac{\Delta E}{kT}\right)$$

$$K_c=\frac{q_\mathrm{B}}{q_\mathrm{A}}\exp\left(-\frac{\Delta E}{kT}\right)\qquad(7.1)$$

$$q=q_\mathrm{elec}q_\mathrm{trans}q_\mathrm{vib}q_\mathrm{rot}\qquad(7.2)$$




二次元回転の状態密度 ~ 1 / $B$