# FORMULAE IN ATOMIC PHYSICS (170314)

**Orbital radius Bohr**

$$r = \frac{\varepsilon_0 h^2}{\pi \mu e^2}\frac{n^2}{Z} \approx a_0 \cdot \frac{n^2}{Z},\ a_0 = 0,529\text{Å}$$

**Orbital velocity Bohr**

$$v = \frac{e^2}{4\pi\varepsilon_0 \hbar}\frac{Z}{n} \approx \frac{1}{137}\cdot c \cdot \frac{Z}{n}$$

**Rydberg formula**

$$\frac{1}{\lambda} = R_M \cdot Z^2 \cdot \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$R_M = \frac{e^4}{8\varepsilon_0^2 h^3 c}\cdot \mu,\ R_M = R_\infty \frac{M}{M+m}$$

$$R_\infty = 109737{,}31568\ \text{cm}^{-1}$$

1 eV = 1.602 $\cdot 10^{-19}$ J = 2.418 $\cdot 10^{14}$ Hz = 8066 $\text{cm}^{-1}$

**Angular momentum operators**

$$\mathbf{L} = \mathbf{r}\times\mathbf{p}$$

$$[L_x, L_y] = i\hbar L_z,\ [L_y, L_z] = i\hbar L_x$$

$$[L_z, L_x] = i\hbar L_y,\ [L^2, L_z] = 0$$

**Orbital angular momentum eigenfunctions**

$$\mathbf{L}^2 Y_{\ell,m_\ell}(\theta,\varphi) = \hbar^2 \ell(\ell+1) Y_{\ell,m_\ell}(\theta,\varphi)$$

$$\mathbf{L_z} Y_{\ell,m_\ell}(\theta,\varphi) = \hbar m_\ell Y_{\ell,m_\ell}(\theta,\varphi)$$

$$\ell = 0,1,2,3....\quad m_\ell = -\ell, -\ell+1, .....\ell$$

$$Y_{\ell,m_\ell}(\theta,\varphi) = \Theta(\theta)\cdot e^{im_\ell\varphi}$$

$$Y_{0,0}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,\pm1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\cdot e^{\pm i\varphi}$$

$$Y_{1,0}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

**Coupling of 2 angular momentum**

$$\Psi_{j_1,j_2,j,m} = \sum_{m_1} C(j_1, m_1, j_2, m-m_1 : j, m)\cdot \psi_{j_1,m_1}\psi_{j_2,m-m_1}$$

**Hamiltonian for one electron systems**

$$H = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{\mathbf{L}^2}{2\mu r^2} - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

**Schrödinger equation one electron systems**

$$H\Psi = E\Psi$$

$$\Psi_{n,\ell,m_\ell}(r,\theta,\varphi) = R_{n,\ell}(r)\cdot Y_{\ell,m_\ell}(\theta,\varphi)$$

Let $\rho = Zr/(na_0)$

$$R_{1,0}(\rho) = \left(\frac{Z}{a_0}\right)^{3/2}\cdot 2\cdot e^{-\rho}$$

$$R_{2,0}(\rho) = \left(\frac{Z}{2a_0}\right)^{3/2}\cdot 2(1-\rho)\cdot e^{-\rho}$$

$$R_{2,1}(\rho) = \left(\frac{Z}{2a_0}\right)^{3/2}\cdot \frac{2}{\sqrt{3}}\cdot \rho \cdot e^{-\rho}$$

**Magnetic moments**

$$E = -\boldsymbol{\mu}\cdot\mathbf{B}$$

$$\boldsymbol{\mu}_L = -\frac{e}{2m}\mathbf{L},\ \boldsymbol{\mu}_S = -2\frac{e}{2m}\mathbf{S},\ \boldsymbol{\mu}_I = +g_I\frac{e}{2m_p}\mathbf{I}$$

**Spin-orbit interaction, one electron systems**

$$E_{SO} = \beta_{n,\ell}\cdot\frac{1}{2}[j(j+1) - \ell(\ell+1) - s(s+1)]$$

$$\beta_{n,\ell} = R_M \cdot \frac{\alpha^2 Z^4}{n^3\cdot \ell(\ell+1/2)(\ell+1)}$$

**Total fine structure energy, one electron systems**

$$E_{n,j} = -R_M\cdot\left[\frac{Z^2}{n^2} + \frac{\alpha^2 Z^4}{4n^4}\left(\frac{4n}{j+1/2} - 3\right)\right]$$

**Hyperfine interaction**

$$E_{hfs} = A\cdot\frac{1}{2}[F(F+1) - J(J+1) - I(I+1)]$$

For an s-electron in one electron systems

$$A = \frac{2}{3}\mu_0 g_s \mu_B g_I \mu_N \frac{Z^3}{\pi a_0^3 n^3},\ g_s = 2$$

**Quantum defect**

$$T = R_M \frac{\zeta^2}{(n-\delta)^2}, \; T = E_{\text{ion}} - E_{\text{exc}},$$

$$\zeta = Z - N_{\text{core}}$$

**Zeeman effect**

$$E = \mu_B \cdot B \cdot g_J \cdot M_J$$

$$g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

**Paschen-Back effect**

$$E = (M_L + 2M_S)\mu_B B + \beta M_L M_S$$

**Selection rules E1**

$\Delta J$ = 0, ±1 not 0 to 0

Only one electron can change orbital

$\Delta\ell$ = ±1

$\Delta M_J$ = 0, ±1 not 0 to 0 if $\Delta J$ = 0

Under perfect LS-coupling

$\Delta S$ = 0

$\Delta L$ = 0, ±1 not 0 to 0

Under perfect jj-coupling

$\Delta j_1$ = 0

$\Delta j_2$ = 0, ±1 not 0 to 0

**Lifetime**

$$\tau_i = \frac{1}{\sum_f A_{if}}$$

**Intensity $i \rightarrow f$**

$I_{\text{if}} = \varepsilon_{\text{exp}} \cdot A_{\text{if}} \cdot N_{\text{i}}$

**Natural line width**

$$\Delta f_{\text{N}} = \frac{1}{2\pi}\left(\frac{1}{\tau_1} + \frac{1}{\tau_2}\right)$$

**Doppler line width**

$$\Delta f_{\text{D}} = C \cdot f_0 \cdot \sqrt{\frac{T}{M}}, \; \text{C} = 7.16 \cdot 10^{-7} \; (\text{g/mol})^{1/2}\text{K}^{-1/2}$$

**Boltzmann distribution**

$$\frac{N_1}{N_2} = \frac{g_1}{g_2} \cdot e^{-\Delta E/kT}$$

**Planck's radiation law**

$$\rho(f)df = \frac{8\pi h f^3}{c^3} \cdot \frac{1}{\text{e}^{hf/kT} - 1} df$$

**Radiation balance**

$$(A_{21} + \rho(f_{21})B_{21}) \cdot N_2 = \rho(f_{21})B_{12} \cdot N_1$$

**Einstein coefficients**

$$g_1 B_{12} = g_2 B_{21}$$

$$A_{21} = \frac{8\pi h f_{12}^3}{c^3} \cdot B_{21}$$

**Molecular energies**

$$E = E_{\text{electron}} + E_{\text{vib}} + E_{\text{rot}} =$$

$$E_{\text{electron}} + \hbar\omega_0(\nu + \frac{1}{2}) + \frac{\hbar^2}{2\mu r^2}\ell(\ell+1)$$