USEFUL CONSTANTS and FORMULAS

$1mW = 10^{-3}W = 10^{-3} \text{ J s}^{-1}$ $1nm = 10^{-9}m$ $1eV = 1.602 \times 10^{-19} \text{ J}$

$h = 6.63 \times 10^{-34} \text{ J s}$ $\hbar = 1.05 \times 10^{-34} \text{ J s}$ $c = 3.0 \times 10^{8} \text{ m s}^{-1}$

$hc = 2.0 \times 10^{-25} \text{ J m}$ $\varepsilon_0 = 8.854 \times 10^{-12} \, Cs^2 kg^{-1} m^{-3}$

$1 \text{ AMU} = 1.66 \times 10^{-27} \text{ kg}$ $m_e = 9.11 \times 10^{-31} \text{ kg}$ $e = 1.602 \times 10^{-19} \text{ C}$

$\lambda \nu = c$ $E = h\nu$ $\lambda = h/p$

$l_n = mrv = n\hbar$ $r_n = n^2 a_0$ $a_0 = 5.29 \times 10^{-11} \text{ m}$

Particle in a box:

$$E_n = \frac{n^2 h^2}{8ma^2} = \frac{n^2 \hbar^2 \pi^2}{2ma^2} \quad E_n = \frac{n^2 h^2}{8ma^2} = \frac{n^2 \hbar^2 \pi^2}{2ma^2} \qquad \psi_n \left(0 \le x \le a\right) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right)$$

Harmonic Oscillator:

$$E_n = \left(n + \frac{1}{2}\right)h\nu = \left(n + \frac{1}{2}\right)\hbar\omega \qquad \alpha = \frac{\sqrt{km}}{\hbar} = \frac{m\omega}{\hbar}, \qquad \tilde{\nu} = \frac{1}{2\pi c}\left(\frac{k}{\mu}\right)^{1/2}, \quad V = \tfrac{1}{2} m\omega^2 x^2$$

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}} \qquad \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}\frac{1}{2\alpha} \qquad \int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx = 2\frac{1\cdot 3 \cdot 5 \cdots (2n-1)}{2^{n+1} a^n}\sqrt{\frac{\pi}{\alpha}}$$

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} \qquad \psi_1(x) = \frac{1}{\sqrt{2}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(2\alpha^{1/2} x\right)e^{-\alpha x^2/2}$$

$$\psi_2(x) = \frac{1}{\sqrt{8}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(4\alpha x^2 - 2\right)e^{-\alpha x^2/2} \qquad \psi_3(x) = \frac{1}{\sqrt{48}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(8\alpha^{3/2} x^3 - 12\alpha^{1/2} x\right)e^{-\alpha x^2/2}$$

Raising and Lowering Operators:

$$a_{\pm} \equiv \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp ip + m\omega x\right)$$

$$\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(a_+ + a_-\right) \qquad \hat{p} = i\left(\frac{\hbar m\omega}{2}\right)^{1/2}\left(a_+ - a_-\right)$$

$$a_+ \psi_n = \left(n+1\right)^{1/2}\psi_{n+1} \qquad a_- \psi_n = n^{1/2}\psi_{n-1}$$

Angular Momentum Operators

$$\left[L_i, L_j\right] = i\hbar L_k \qquad i,j,k \Rightarrow x,y,z$$

$$L_+ = L_x + iL_y \qquad\qquad L_- = L_x - iL_y$$

Rigid Rotor

$$Y_0^0 = \frac{1}{(4\pi)^{1/2}} \qquad Y_1^0 = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\cos\theta \qquad Y_1^{\pm 1} = \left(\frac{3}{8\pi}\right)^{\frac{1}{2}}\sin\theta e^{\pm i\phi}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{\frac{1}{2}}\left(3\cos^2\theta - 1\right) \quad Y_2^{\pm 1} = \left(\frac{15}{8\pi}\right)^{\frac{1}{2}}\sin\theta\cos\theta e^{\pm i\phi} \quad Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{\frac{1}{2}}\sin^2\theta e^{\pm 2i\phi}$$

$$E_J = \frac{\hbar^2}{2I}J(J+1) \qquad B \equiv \frac{h}{8\pi^2 I} \quad \text{(Hz)} \qquad \bar{B} \equiv \frac{h}{8\pi^2 cI} \quad \text{(cm}^{-1}\text{)}$$

Hydrogen atom

Three-dimensional operators in spherical coordinates

$$\hat{H}(r,\theta,\phi) = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + V(r,\theta,\phi)$$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \qquad\qquad \hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$U = \frac{-Ze^2}{4\pi\varepsilon_0 r}, \qquad E_n = \frac{-Z^2 e^2}{8\pi\varepsilon_0 a_0 n^2} = \frac{-Z^2}{2n^2} \text{ (atomic units)} \quad n = 1,2,3,..., \qquad a_0 = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2}$$

$$\int_0^\infty x^n e^{x/a}dx = n!a^{n+1}$$

H atom spatial wavefunctions (where $\sigma = Zr/a_0$. In atomic units $a_0 = 1$ and $\sigma = Zr$.)

$$n = 1 \quad l = 0 \quad m = 0 \quad \psi_{100} = \psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$$

$$n = 2 \quad l = 0 \quad m = 0 \quad \psi_{200} = \psi_{2s} = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \left(2 - \sigma \right) e^{-\sigma/2}$$

$$l = 1 \quad m = 0 \quad \psi_{210} = \psi_{2p_z} = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos\theta$$

$$l = 1 \quad m = \pm 1 \quad \psi_{21\pm1} = \frac{1}{\sqrt{64\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin\theta \, e^{\pm i\phi}$$

$$n = 3 \quad l = 0 \quad m = 0 \quad \psi_{300} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \left(27 - 18\sigma + 2\sigma^2 \right) e^{-\sigma/3} = \psi_{3s}$$