

**Some equations and formulae that might or might not be useful:**

$$\Delta E = h\nu; \nu = \frac{c}{\lambda}; \lambda = \frac{h}{p}; \tilde{\nu} = \frac{1}{\lambda}$$

$$E_{kinet} = K = \frac{p^2}{2m}; \hat{p}_x = -i\hbar \frac{\partial}{\partial x}; \Delta p_x \cdot \Delta x \geq \frac{\hbar}{2}$$

$$E_n = \frac{h^2 n^2}{8ma^2}; \Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n}{a} x\right)$$

$$E_n = \left(n + \frac{1}{2}\right) h\nu; \Psi_n(x) = A_n H_n e^{-\alpha x^2/2}$$

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}; \alpha = \frac{\sqrt{k\mu}}{\hbar}; A_n = \frac{1}{\sqrt{2^n n!}} \left(\frac{\alpha}{\pi}\right)^{1/4}$$

$$E_{m_l} = \frac{\hbar^2}{2I} m_l^2; \Psi_{m_l}(\phi) = \frac{1}{\sqrt{2\pi}} e^{im_l \phi}$$

$$E_l = \frac{l(l+1)\hbar^2}{2I}; \Psi_{l,m_l} = Y_{l,m_l}(\theta, \phi);$$

$$|\vec{l}|^2 = l(l+1)\hbar^2; l_z = m_l \hbar$$

$$E_J = \frac{J(J+1)\hbar^2}{2I} = hcBJ(J+1); B = \frac{\hbar^2}{2hcI}$$

$$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 \hbar^2 n^2} = -\frac{\hbar^2}{2m_e a_0^2 n^2};$$

$$\Psi_{n,l,m_l} = R_{n,l}(r) Y_{l,m_l}(\theta, \phi);$$

$$a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2}; V = -\frac{e^2}{4\pi\varepsilon_0 r}$$

$$e = 1.6 \times 10^{-19} \text{ C};$$

$$\varepsilon_0 = 8.85 \times 10^{-12} \text{ m}^{-3} \text{ kg}^{-1} \text{ s}^4 \text{ A}^2$$

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}; \Delta A \times \Delta B \geq \frac{1}{2} \left| \langle [\hat{A}, \hat{B}] \rangle \right|$$

$$\text{For spin S: } |\vec{S}|^2 = S(S+1)\hbar^2; S_z = m_s \hbar$$

$$h = 6.62 \times 10^{-34} \text{ J s}; \hbar = h/(2\pi); c = 3 \times 10^8 \text{ m/s}$$

$$k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}; N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$$

$$R = N_A \times k_B = 8.31 \text{ J mol}^{-1} \text{ K}^{-1}$$

$$m_e = 9.1 \times 10^{-31} \text{ kg}; m_p = 1.67 \times 10^{-27} \text{ kg}$$

$$1 \text{ a.m.u.} = 1.66 \times 10^{-27} \text{ kg}$$

$$H_0 = 1; H_1 = 2\sqrt{\alpha x}; H_2 = 2(2\alpha x^2 - 1)$$

$$H_3 = 4\sqrt{\alpha x}(2\alpha x^2 - 3)$$

$$\mu = m_1 m_2 / (m_1 + m_2)$$

$$\hat{l}_z = -i\hbar \frac{\partial}{\partial \phi}; l_z = m_l \hbar; I = \mu r^2$$

$$Y_{0,0}(\theta, \phi) = 1/\sqrt{4\pi}; Y_{1,0}(\theta, \phi) = (3/4\pi)^{1/2} \cos\theta$$

$$Y_{1,\pm 1}(\theta, \phi) = \mp (3/8\pi)^{1/2} \sin\theta e^{\pm i\phi}$$

$$Y_{2,0}(\theta, \phi) = (5/16\pi)^{1/2} (3\cos^2\theta - 1)$$

$$Y_{2,\pm 1}(\theta, \phi) = \mp (15/8\pi)^{1/2} \cos\theta \sin\theta e^{\pm i\phi}$$

$$Y_{2,\pm 2}(\theta, \phi) = (15/32\pi)^{1/2} \sin^2\theta e^{\pm 2i\phi}$$

$$R_{1,0} = 2(1/a_0)^{3/2} e^{-r/a_0}$$

$$R_{2,0} = \frac{1}{\sqrt{8}} (1/a_0)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

$$R_{2,1} = \frac{1}{2\sqrt{6}} (1/a_0)^{3/2} \frac{r}{a_0} e^{-r/2a_0}$$

$$R_{3,0} = \frac{2}{81\sqrt{3}} (1/a_0)^{3/2} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$$

$$R_{3,1} = \frac{4}{81\sqrt{6}} (1/a_0)^{3/2} \left(6\frac{r}{a_0} - \frac{r^2}{a_0^2}\right) e^{-r/3a_0}$$

$$R_{3,2} = \frac{4}{81\sqrt{30}} (1/a_0)^{3/2} \frac{r^2}{a_0^2} e^{-r/3a_0}$$

$$\Delta p_x \cdot \Delta x \geq \frac{\hbar}{2}$$

For  $S = 1/2$ :

$$\hat{S}_z \alpha = \frac{\hbar}{2} \alpha; \quad \hat{S}_z \beta = -\frac{\hbar}{2} \beta; \quad [\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z; \quad \hat{S}_x \alpha = \frac{\hbar}{2} \beta; \quad \hat{S}_x \beta = \frac{\hbar}{2} \alpha; \quad \hat{S}_y \alpha = i\frac{\hbar}{2} \beta; \quad \hat{S}_y \beta = -i\frac{\hbar}{2} \alpha$$

$$\hat{S}^2 \alpha = \frac{3\hbar^2}{4} \alpha; \quad \hat{S}^2 \beta = \frac{3\hbar^2}{4} \beta; \quad \int \alpha^* \alpha d\sigma = 1; \quad \int \beta^* \beta d\sigma = 1; \quad \int \beta^* \alpha d\sigma = 0; \quad \int \alpha^* \beta d\sigma = 0$$

$$p_i = \frac{a_i}{N} = \frac{g_i e^{-\epsilon_i \beta}}{q}; \quad q = \sum_i g_i e^{-\epsilon_i \beta}$$

$$\beta = \frac{1}{k_B T}$$

$$q_{transl} = \frac{V}{\Lambda^3}; \quad \Lambda = h \left( \frac{\beta}{2\pi m} \right)^{1/2} = \frac{h}{\sqrt{2\pi m k_B T}}$$

$$E = -N \frac{\partial}{\partial \beta} \ln q = N k_B T^2 \frac{\partial}{\partial T} \ln q$$

$$e^{i\alpha} = \cos \alpha + i \sin \alpha$$

$$\cos \alpha = (e^{i\alpha} + e^{-i\alpha})/2$$

$$\sin \alpha = (e^{i\alpha} - e^{-i\alpha})/2i$$

$$\sin \alpha \sin \beta = [\cos(\alpha - \beta) - \cos(\alpha + \beta)]/2$$

$$\sin \alpha \cos \beta = [\sin(\alpha - \beta) + \sin(\alpha + \beta)]/2$$

$$\int_0^a \sin^2 \left( \frac{\pi m}{a} x \right) dx = \frac{a}{2}$$

$$\int_0^\infty e^{-ax^2} x^{2n} dx = \sqrt{\frac{\pi}{a}} \frac{1 \cdot 3 \cdot 5 \cdot \dots \cdot (2n-1)}{2^{n+1} a^n}; \quad (\text{for } n \geq 1); \quad \int_0^\infty e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}; \quad \int_0^\infty e^{-ax^2} x^2 dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}$$

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}; \quad n! = 1 \cdot 2 \cdot \dots \cdot n$$

$$W = \frac{N!}{a_0! a_1! a_2! \dots}$$

$$n! \approx \sqrt{2\pi n} n^{n+1/2} e^{-n}; \quad \ln n! \approx n \ln n - n \quad (\text{for } n \gg 1)$$

$$q_{rot} = \frac{1}{(\sigma) h c B \beta} \quad (\text{assuming } k_B T \gg h c B)$$

$$q_{vibr} = \frac{1}{1 - e^{-h\nu\beta}}; \quad q_{vibr} \approx \frac{1}{h\nu\beta} \quad (\text{when } k_B T \gg h\nu)$$

$$S = k_B \ln W; \quad S = \frac{E}{T} + k_B N \ln q$$

$$\sin 2\alpha = 2 \sin \alpha \cos \alpha$$

$$\cos 2\alpha = \cos^2 \alpha - \sin^2 \alpha$$

$$2 \sin^2 \alpha = 1 - \cos 2\alpha$$

$$2 \cos^2 \alpha = 1 + \cos 2\alpha$$

$$\cos \alpha \cos \beta = [\cos(\alpha - \beta) + \cos(\alpha + \beta)]/2$$