

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

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

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

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

$$E_n = \left(n + \frac{1}{2}\right)h\nu;$$

$$\Psi_n(x) = A_n H_n(\sqrt{\alpha}x) e^{-\alpha x^2/2};$$

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}; \alpha = \sqrt{k\mu} / \hbar;$$

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

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

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

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

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

$$a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2}; \Psi_{n,l,m_l} = R_{n,l}(r) Y_{l,m_l}(\theta, \phi)$$

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

$$\int \alpha^* \alpha d\sigma = 1; \int \beta^* \beta d\sigma = 1$$

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

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

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

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

$$c = 3 \times 10^8 \text{ m/s}; k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}$$

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

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

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

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

$$H_0(\xi) = 1; H_1(\xi) = 2\xi; H_2(\xi) = 4\xi^2 - 2;$$

$$H_3(\xi) = 8\xi^3 - 12\xi; \text{ here } \xi = \sqrt{\alpha}x \quad A_n = \frac{1}{\sqrt{2^n n!}} \left(\frac{\alpha}{\pi} \right)^{1/4};$$

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

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

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

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

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

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

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

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

$$\hat{I}_x \alpha = \frac{\hbar}{2} \beta; \hat{I}_x \beta = \frac{\hbar}{2} \alpha; \hat{I}_y \alpha = i \frac{\hbar}{2} \beta; \hat{I}_y \beta = -i \frac{\hbar}{2} \alpha;$$

$$\int \beta^* \alpha d\sigma = 0; \int \alpha^* \beta d\sigma = 0$$

$$\beta = \frac{1}{k_B T}; W = \frac{N!}{a_0! a_1! a_2! \dots}; \ln N! \approx N \ln N - N;$$

$$q_{rot} = \frac{1}{hcB\beta}; q_{vibr} = \frac{1}{1 - e^{-h\nu\beta}}$$

$$U - U(0) = - \left(\frac{\partial}{\partial \beta} \ln Q \right)_V = k_B T^2 \left(\frac{\partial}{\partial T} \ln Q \right)_V$$

$$Q = q^N \text{ or } q^N/N!$$

$$S = k_B \ln W; S = \frac{U - U(0)}{T} + k_B \ln Q;$$

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

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

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

$$\int_{-\infty}^{\infty} e^{-ax^2} x^{2n} dx = \sqrt{\frac{\pi}{a}} \frac{1 \cdot 3 \cdot 5 \cdot \dots \cdot (2n-1)}{2^n a^n};$$

$$\int_0^{\infty} e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}; \int_0^{\infty} e^{-ax^2} x^2 dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}$$

(for $n \geq 0$)

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

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