Basic Information

Constants and units

$$
\begin{aligned}
c &= 299\,792\,458\,\mathrm{m\,s^{-1}} \\
&\approx 3 \times 10^{8}\,\mathrm{m\,s^{-1}} \\
h &= 6.626 \times 10^{-34}\,\mathrm{J\,s} \\
\hbar &= \frac{h}{2\pi} = 1.055 \times 10^{-34}\,\mathrm{J\,s} \\
N_A &= 6.022 \times 10^{23}\,\mathrm{mol^{-1}} \\
k_B &= 1.381 \times 10^{-23}\,\mathrm{J\,K^{-1}} \\
&= 1.381 \times 10^{-16}\,\mathrm{g\,cm^2\,s^{-2}\,K^{-1}} \\
R &= 8.3145\,\mathrm{J\,K^{-1}\,mol^{-1}} \\
&= 0.082\,06\,\mathrm{L\,atm\,mol^{-1}\,K^{-1}} \\
101.3\,\mathrm{J} &= 1\,\mathrm{L\,atm} \\
&= 0.083\,145\,\mathrm{L\,bar\,mol^{-1}\,K^{-1}} \\
m_{e^-} &= 9.109 \times 10^{-31}\,\mathrm{kg} \\
e &= 1.602 \times 10^{-19}\,\mathrm{C} \\
m_{p^+} &= 1.673 \times 10^{-27}\,\mathrm{kg} \\
m_{n^0} &= 1.675 \times 10^{-27}\,\mathrm{kg} \\
a_0 &= 4\pi\varepsilon_0\hbar^2/m_e e^2 \\
&= 0.5292 \times 10^{-10}\,\mathrm{m} \\
\varepsilon_0 &= 8.8542 \times 10^{-12}\,\mathrm{C^2\,N^{-1}\,m^{-2}} \\
\gamma_{^1H} &= 2.675\,221 \times 10^{8}\,\mathrm{s^{-1}\,T^{-1}} \\
&= 42.577\,\mathrm{MHz\,T^{-1}} \\
R_H &= 1.097 \times 10^{5}\,\mathrm{cm^{-1}} \\
1\,\mathrm{N} &= 1\,\mathrm{kg\,m\,s^{-2}} \\
1\,\mathrm{J} &= 1\,\mathrm{N\,m} = 1\,\mathrm{kg\,m^2\,s^{-2}} \\
1000\,\mathrm{L} &= 1\,\mathrm{m^3} \\
1\,\mathrm{eV} &= 1.602 \times 10^{-19}\,\mathrm{J} \\
1\,\mathrm{cm^{-1}} &= 1.986 \times 10^{-23}\,\mathrm{J} \\
1\mathrm{u} &= 1.661 \times 10^{-27}\,\mathrm{kg}
\end{aligned}
$$

Math

$$
\begin{aligned}
a \ln X &= \ln\left(X^a\right) \\
\ln A + \ln B &= \ln\left(AB\right) \\
\ln A - \ln B &= \ln \frac{A}{B} \\
\ln N! &\approx N \ln N - N \\
\ln\left(M - N\right) &\approx \ln M \text{ if } M \gg N
\end{aligned}
$$

Trigonometry

$$
\begin{aligned}
\sin(2x) &= 2 \sin x \cos x \\
\cos(2x) &= \cos^2 x - \sin^2 x \\
\sin^2 x &= \frac{1 - \cos 2x}{2} \\
\cos^2 x &= \frac{1 + \cos 2x}{2} \\
\sin^2 x + \cos^2 x &= 1 \\
\sin x \sin y &= \frac{1}{2}\left[\cos(x-y) - \cos(x+y)\right] \\
\cos x \cos y &= \frac{1}{2}\left[\cos(x-y) + \cos(x+y)\right] \\
\sin x \cos y &= \frac{1}{2}\left[\sin(x+y) + \sin(x-y)\right]
\end{aligned}
$$

Determinants

$$
\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc
$$

$$
\psi\left(1, 2, 3, \ldots, n\right) = \frac{1}{\sqrt{n!}} \begin{vmatrix} u_1(1) & u_2(1) & \cdots & u_n(1) \\ u_1(2) & u_2(2) & \cdots & u_n(2) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(n) & u_2(n) & \cdots & u_n(n) \end{vmatrix}
$$

Integrals

$$\int_{-\infty}^{+\infty} f(x)\,dx = 0 \text{ for odd } f(x)$$

$$f(-x) = -f(x) \text{ for odd } f(x)$$

$$\int_{-\infty}^{+\infty} f(x)\,dx = 2\int_{0}^{+\infty} f(x)\,dx \text{ for even } f(x)$$

$$f(-x) = f(x) \text{ for even } f(x)$$

$$\int \sin(ax)\,dx = -\frac{1}{a}\cos(ax)$$

$$\int \cos(ax)\,dx = \frac{1}{a}\sin(ax)$$

$$\int \sin^2(ax)\,dx = \frac{x}{2} - \frac{\sin(2ax)}{4a}$$

$$\int \cos^2(ax)\,dx = \frac{x}{2} + \frac{\sin(2ax)}{4a}$$

$$\int x\sin^2(ax)\,dx = \frac{x^2}{4} - \frac{\cos(2ax)}{8a^2} - \frac{x\sin(2ax)}{4a}$$

$$\int x\cos^2(ax)\,dx = \frac{x^2}{4} + \frac{\cos(2ax)}{8a^2} + \frac{x\sin(2ax)}{4a}$$

$$\int x^2\sin^2(ax)\,dx = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin(2ax) - \frac{x}{4a^2}\cos(2ax)$$

$$\int x^2\cos^2(ax)\,dx = \frac{x^3}{6} + \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin(2ax) + \frac{x}{4a^2}\cos(2ax)$$

$$\int_0^\infty e^{-ax^2}dx = \left(\frac{\pi}{4a}\right)^{1/2}$$

$$\int_0^\infty x^{2n}e^{-ax^2}dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}$$

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

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

Thermodynamics and Kinetics

Thermodynamics

$$\Delta U = w + q$$
$$w = -p_{ext}\Delta V$$
$$w_{\text{iso-T}} = -\int_{V_1}^{V_2} \frac{nRT}{V} dV = -nRT \ln \frac{V_2}{V_1}$$
$$H = U + pV$$
$$\Delta H = q_p = \int dH = \int C_p(T) dT$$
$$C_V = \left(\frac{\partial U}{\partial T}\right)_V ; C_p = \left(\frac{\partial H}{\partial T}\right)_p$$
$$C_p = C_V + nR$$
$$\Delta S = \frac{q_{rev}}{T} = nR \ln \frac{V_2}{V_1} + C_V \ln \frac{T_2}{T_1}$$
$$\Delta S = \int \frac{C_p}{T} dT + \sum_i \frac{\Delta_{trs} H}{T}$$
$$\ulcorner \frac{S}{R} = \frac{7}{2} + \ln \left[\left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} \frac{V}{N} \right] + \ln \left[\frac{T}{\sigma \theta_{rot}} \right] \ldots$$
$$\ldots + \frac{\theta_{vib}}{T} \left(\frac{1}{e^{\theta_{vib}/T} - 1} \right) - \ln \left[1 - e^{-\theta_{vib}/T} \right] + \ln \left[g_{e1} \right] \lrcorner$$
$$\frac{p_2}{p_1} = \left(\frac{V_1}{V_2}\right)^\gamma$$
$$V_2 = \frac{V_1}{\gamma} \left[\gamma - 1 + \frac{p_1}{p_2} \right]$$
$$\gamma = C_p / C_V$$
$$A = U - TS$$
$$G = U - TS + pV = H - TS$$
$$\Delta G^\circ = -RT \ln K_{eq}$$
$$\Delta G = \Delta G^\circ + RT \ln Q$$
$$dU = TdS - pdV; \left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V$$
$$dH = TdS + Vdp; \left(\frac{\partial T}{\partial p}\right)_S = \left(\frac{\partial V}{\partial S}\right)_p$$
$$dA = -SdT - pdV; \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V$$
$$dG = -SdT + Vdp; \left(\frac{\partial S}{\partial p}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_p$$
$$\left(\frac{\partial \left(\Delta G / T\right)}{\partial T}\right)_p = -\frac{\Delta H}{T^2}$$

Statistical Mechanics

$$\frac{a_n}{a_m} = e^{-\beta \Delta E}; \beta = \frac{1}{k_B T}$$
$$p_j = \frac{e^{-\beta E_j}}{\sum_i e^{-\beta E_j}} = \frac{e^{-\beta E_j}}{Q}$$
$$Q\left(N, V, \beta\right) = \sum_i e^{-\beta E_i} = \frac{q^N}{N!}$$
$$q_{trans} = \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} V$$
$$q_{rot} \approx \frac{T}{\sigma \theta_{ROT}}; \theta_{ROT} = \frac{\hbar^2}{2 I k_B}, I = \mu r^2$$
$$q_{vib} = \frac{e^{-\theta_{VIB}/2T}}{1 - e^{-\theta_{VIB}/T}}$$
$$\theta_{VIB} = \frac{\hbar \left(\frac{k}{\mu}\right)^{1/2}}{k_B} = \frac{h\nu}{k_B}$$
$$\langle E \rangle = U = -\left(\frac{\partial \ln Q}{\partial \beta}\right)_{N,V}$$
$$= k_B T^2 \left(\frac{\partial \ln Q}{\partial T}\right)_{N,V}$$
$$\langle p \rangle = \frac{1}{Q\beta} \left(\frac{\partial Q}{\partial V}\right)_{N,T} = k_B T \left(\frac{\partial \ln Q}{\partial V}\right)_{N,T}$$
$$S = k_B \ln W = -k_B \sum_i p_i \ln p_i$$
$$S = k_B T \left(\frac{\partial \ln Q}{\partial T}\right)_{N,V} + k_B \ln Q$$
$$H = k_B T \left[T \left(\frac{\partial \ln Q}{\partial T}\right)_{N,V} + V \left(\frac{\partial \ln Q}{\partial V}\right)_{N,T} \right]$$
$$A = -k_B T \ln Q$$
$$G = k_B T \left[V \left(\frac{\partial \ln Q}{\partial V}\right)_{N,T} - \ln Q \right]$$
$$\mu = -RT \left(\frac{\partial \ln Q}{\partial N}\right)_{V,T}$$
$$W(M, N) = \frac{M!}{N!(M-N)!}$$

Equilibrium

$$\mu = \left(\frac{\partial G}{\partial n}\right)_{p,T}$$

$$\frac{dp}{dT} = \frac{\Delta S}{\Delta V} = \frac{\Delta H}{T\Delta V}$$

$$\ln\frac{p_2}{p_1} = -\frac{\Delta_{vap}H}{R}\left(\frac{1}{T_2}-\frac{1}{T_1}\right)$$

$$\ln\frac{K_p(T_2)}{K_p(T_1)} = -\frac{\Delta_{rxn}H}{R}\left(\frac{1}{T_2}-\frac{1}{T_1}\right)$$

$$\Delta_{rxn}G^\circ(T) = -RT\ln K_p(T)$$

$$\Delta_{rxn}G = \Delta_{rxn}G^\circ + RT\ln Q$$

$$Q = \frac{p_Y^{\nu_Y}p_Z^{\nu_Z}\cdots}{p_A^{\nu_A}p_B^{\nu_B}\cdots}$$

$$K_p = \left(\frac{p_Y^{\nu_Y}p_Z^{\nu_Z}\cdots}{p_A^{\nu_A}p_B^{\nu_B}\cdots}\right)_{eq}$$

$$K_c = \left(\frac{c_Y^{\nu_Y}c_Z^{\nu_Z}\cdots}{c_A^{\nu_A}c_B^{\nu_B}\cdots}\right)_{eq} = \frac{\left(\frac{q_Y}{V}\right)^{\nu_Y}\left(\frac{q_Z}{V}\right)^{\nu_Z}\cdots}{\left(\frac{q_A}{V}\right)^{\nu_A}\left(\frac{q_A}{V}\right)^{\nu_A}\cdots}$$

$$K_p = K_c\left(\frac{c^\circ}{p^\circ}RT\right)^{\nu_Y+\nu_Z+\cdots-\nu_A-\nu_B-\cdots}$$

$$\frac{q}{V} = \frac{q_{trans}}{V}q_{rot}q_{vib}q_{elec} = \frac{q^\circ}{V}e^{D_0/k_BT}$$

$$q_{vib}q_{elec} = \frac{1}{1-e^{-\theta/T}}\cdot g\cdot e^{D_0/RT}$$

$$\frac{q^\circ}{V} = \frac{N_Ap^\circ}{RT}e^{-\left(G^\circ-H_0^\circ\right)/RT}$$

Kinetics

$$k = Ae^{-\frac{E_a}{RT}}$$

$$t_{1/2} = \frac{\ln 2}{k}\ \text{first-order only}$$

$$v(t) = -\frac{1}{a}\frac{d[A]}{dt} = \cdots = -\frac{1}{V}\frac{d\xi}{dt}$$

$$K_c = \frac{k_1}{k_{-1}} = \frac{[B]_{eq}}{[A]_{eq}}$$

$$k = \frac{k_BT}{hc^\circ}e^{\frac{\Delta^\ddagger S^\circ}{R}}e^{-\frac{\Delta^\ddagger H^\circ}{RT}} = \frac{k_BT}{hc^\circ}e^2\cdot e^{\frac{\Delta^\ddagger S^\circ}{R}}e^{-\frac{E_a}{RT}}$$

$$E_a = \Delta^\ddagger H^\circ + 2RT$$

Kinetic Molecular Theory

$$\sigma = \pi d^2$$

$$\rho = \left(\frac{pN_A}{RT}\right)$$

$$z_{12} = \frac{N_2}{V}\sigma\left(\frac{8kT}{\pi\mu}\right)^{1/2}$$

$$\lambda = \frac{1}{\sqrt{2}\rho\sigma}$$

$$Z_{12} = \rho_1\rho_2\sigma\left(\frac{8kT}{\pi\mu}\right)^{1/2}$$

$$P(v) = 4\pi\left(\frac{M}{2\pi RT}\right)^{3/2}v^2e^{-Mv^2/2RT}$$

$$\langle v\rangle = \left(\frac{8RT}{\pi M}\right)^{1/2}$$

$$v_{rms} = \left(\frac{3RT}{M}\right)^{1/2}$$

$$v_{mp} = \left(\frac{2RT}{M}\right)^{1/2}$$

Molecular Transport

$$J(x) = -D\left[\frac{\partial c(x)}{\partial x}\right]$$

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2}$$

$$D = \frac{k_B T}{f}$$

$$f_{\text{sphere}} = 6\pi\eta r$$

$$f_{\text{disk, random}} = 12\eta r$$

$$\left\langle r^2 \right\rangle_{3D}^{1/2} = \sqrt{6Dt}$$

Quantum Mechanics and Spectroscopy

General QM

$$E = h\nu = \frac{hc}{\lambda}$$
$$\lambda = \frac{h}{p}$$
$$\Psi\left(x,t\right) = \psi\left(x\right) e^{-i(E/\hbar)t}$$
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\left(x,t\right)\right]\Psi\left(x,t\right) = i\hbar\frac{\partial\Psi\left(x,t\right)}{\partial t}$$
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\left(x\right)\right]\psi\left(x\right) = E\psi\left(x\right)$$
$$\hat{H}\psi_n\left(x\right) = E_n\psi_n\left(x\right)$$
$$\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$
$$\hat{x} = x$$
$$\hat{p_x} = -i\hbar\frac{\partial}{\partial x}$$
$$\int_{-\infty}^{+\infty}\Psi^*\left(x,t\right)\Psi\left(x,t\right)dx = 1$$
$$\langle a\rangle = \frac{\int_{-\infty}^{+\infty}\Psi^*\left(x,t\right)\hat{A}\Psi\left(x,t\right)dx}{\int_{-\infty}^{+\infty}\Psi^*\left(x,t\right)\Psi\left(x,t\right)dx}$$
$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$$
$$\left[\hat{A},\hat{B}\right] = -\left[\hat{B},\hat{A}\right]$$
$$\Delta p\Delta x \geq \frac{\hbar}{2}$$
$$E_{variational} = \frac{\int\Phi^*\hat{H}\Phi d\tau}{\int\Phi^*\Phi d\tau} \geq E_0$$

Particle in a Box

$$\psi_{1D}\left(x\right) = \left(\frac{2}{a}\right)^{1/2}\sin\left(\frac{n\pi x}{a}\right); n = 1,2,3\ldots$$
$$E_n = \frac{h^2n^2}{8ma^2}$$
$$\psi_{3D}\left(x,y,z\right) = \left(\frac{8}{abc}\right)^{1/2}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)\sin\left(\frac{n_z\pi z}{c}\right)$$
$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

Harmonic Oscillator

$$V\left(x\right) = \frac{1}{2}kx^2$$
$$x_{cm} = \frac{m_1x_1 + m_2x_2}{m_1m{+}_2}$$
$$\mu = \frac{m_1m_2}{m_1 + m_2}$$
$$\hat{H} = \left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2\right]$$
$$\psi_v\left(x\right) = A_vH_v\left(\alpha^{1/2}x\right)e^{-\frac{1}{2}\alpha x^2}$$
$$\psi_0\left(x\right) = \left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\frac{1}{2}\alpha x^2}$$
$$\psi_1\left(x\right) = \left(\frac{4\alpha^3}{\pi}\right)^{1/4}xe^{-\frac{1}{2}\alpha x^2}$$
$$\psi_2\left(x\right) = \left(\frac{\alpha}{4\pi}\right)^{1/4}\left(2\alpha x^2 - 1\right)e^{-\frac{1}{2}\alpha x^2}$$
$$\alpha = \sqrt{\frac{k\mu}{\hbar^2}}$$
$$E_v = \hbar\sqrt{\frac{k}{\mu}}\left(v + \frac{1}{2}\right) = h\nu\left(v + \frac{1}{2}\right); v = 0,1,2,3,\cdots$$
$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} = \tilde{\nu}c$$

Anharmonic Oscillator

$$V\left(x\right) = D_e\left(e^{-2ax} - 2e^{-ax}\right); a = \sqrt{\frac{k}{2D_e}}$$
$$E_v = h\nu\left(v + \frac{1}{2}\right) - \frac{(h\nu)^2}{4D_e}\left(v + \frac{1}{2}\right)^2$$
$$G\left(v\right) = \tilde{\nu}\left(v + \frac{1}{2}\right) - \tilde{x}\tilde{\nu}\left(v + \frac{1}{2}\right)^2; \tilde{x} = \frac{hc\tilde{\nu}}{4D_e}$$

Rigid Rotor

$$I = \mu r^2$$
$$L = I\omega$$
$$KE = \frac{1}{2}I\omega^2 = \frac{L^2}{2I}$$

2D

$$\hat{H} = -\frac{\hbar^2}{2\mu r_0^2}\frac{\partial^2}{\partial\phi^2}$$
$$\Phi_{m_l}(\phi) = \frac{1}{\sqrt{2\pi}}e^{im_l\phi}$$
$$m_l = 0, \pm1, \pm2, \cdots$$
$$E_{m_l} = \frac{\hbar^2 m_l^2}{2I}$$
$$\hat{L_z}\Phi_{m_l}(\phi) = m_l\hbar\Phi_{m_l}(\phi)$$

3D

$$\hat{H} = -\frac{\hbar^2}{2\mu r_0^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)_{r,\phi} + \frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)_{r,\theta}\right]$$
$$Y(\theta,\phi) = Y_l^{m_l}(\theta,\phi) = \Theta_l^{m_l}(\theta)\,\Phi_{m_l}(\phi)$$
$$E_l = \frac{\hbar^2}{2I}l(l+1)$$
$$l = 0, 1, 2, 3, \ldots$$
$$m_l = -l, -(l-1), \ldots, 0, \ldots, (l-1), l$$
$$E_J = hc\tilde{B}J(J+1)$$
$$\tilde{B} = \frac{h}{8\pi^2 c\mu r_0^2}$$
$$\hat{L_z}Y_l^{m_l}(\theta,\phi) = m_l\hbar Y_l^{m_l}(\theta,\phi)$$
$$\hat{L^2}Y_l^{m_l}(\theta,\phi) = \hbar^2 l(l+1)\,Y_l^{m_l}(\theta,\phi)$$
$$\hat{L}_{\substack{x\\y\\z}} = -i\hbar\left(\substack{y\\z\\x}\frac{\partial}{\partial \substack{z\\x\\y}} - \substack{z\\x\\y}\frac{\partial}{\partial \substack{y\\z\\x}}\right)$$
$$\left[\hat{L}_{\substack{x\\y\\z}}, \hat{L}_{\substack{y\\z\\x}}\right] = i\hbar\hat{L}_{\substack{z\\x\\y}}$$

Hydrogen atom

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$
$$V_{eff}(r) = \frac{\hbar^2 l(l+1)}{2m_e r^2} - \frac{e^2}{4\pi\varepsilon_0 r}$$
$$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 h^2 n^2} = -\frac{e^2}{8\pi\varepsilon_0 a_0 n^2}$$
$$a_0 = \frac{\varepsilon_0 h^2}{\pi m_e e^2}$$
$$n = 1, 2, 3, \cdots$$
$$l = 0, 1, 2, \cdots, n-1$$
$$m_l = 0, \pm1, \pm2, \cdots, \pm l$$

Radial functions

$$R_{nl}(r) = \cdots$$
$$R_{10}(r) = 2\left(\frac{1}{a_0}\right)^{3/2}e^{-r/a_0}$$
$$R_{20}(r) = \frac{1}{\sqrt{8}}\left(\frac{1}{a_0}\right)^{3/2}\left(2 - \frac{r}{a_0}\right)e^{-r/2a_0}$$
$$R_{21}(r) = \frac{1}{\sqrt{24}}\left(\frac{1}{a_0}\right)^{3/2}\frac{r}{a_0}e^{-r/2a_0}$$
$$R_{30}(r) = \frac{2}{81\sqrt{3}}\left(\frac{1}{a_0}\right)^{3/2}\left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$$
$$R_{31}(r) = \frac{4}{81\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}\left(6\frac{r}{a_0} - \frac{r^2}{a_0^2}\right)e^{-r/3a_0}$$
$$R_{32}(r) = \frac{4}{81\sqrt{30}}\left(\frac{1}{a_0}\right)^{3/2}\frac{r^2}{a_0^2}e^{-r/3a_0}$$
$$P_{nl}(r)\,dr = R_{nl}^2(r)\,r^2 dr$$

Full wavefunctions

$$\psi_{nlm_l}(r,\theta,\phi) = R_{nl}(r)\,Y_l^{m_l}(\theta,\phi) = R_{nl}(r)\,Y_{s,p,d,f,\ldots x,y,z}(\theta,\phi)$$

Term Symbols

$^{2S+1}L_J$

$L = \sum_i l_i, M_L = \sum_i l_{z,i}$

$S = \sum_i s_i, M_S = \sum_i s_{z,i}$

$J = L + S, L + S - 1, \ldots, |L - S|$

$^{2S+1}\Lambda_\Omega$ for molecules

Spherical Harmonics

Complex

$$Y_l^{m_l}(\theta, \phi) = \cdots$$
$$Y_0^0(\theta, \phi) = \left(\frac{1}{4\pi}\right)^{1/2}$$
$$Y_1^0(\theta, \phi) = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$
$$Y_1^{\pm 1}(\theta, \phi) = \mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$$
$$Y_2^0(\theta, \phi) = \left(\frac{5}{16\pi}\right)^{1/2} \left(3\cos^2\theta - 1\right)$$
$$Y_2^{\pm 1}(\theta, \phi) = \mp\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{\pm i\phi}$$
$$Y_2^{\pm 2}(\theta, \phi) = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$$

Real

$$p_z = Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$
$$p_x = \frac{-1}{\sqrt{2}}\left(Y_1^1 - Y_1^{-1}\right) = \sqrt{\frac{3}{4\pi}}\sin\theta\cos\phi$$
$$p_y = \frac{-1}{\sqrt{2}i}\left(Y_1^1 + Y_1^{-1}\right) = \sqrt{\frac{3}{4\pi}}\sin\theta\sin\phi$$
$$d_{z^2} = Y_2^0 = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$$
$$d_{xz} = \frac{-1}{\sqrt{2}}\left(Y_2^1 - Y_2^{-1}\right) = \sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\cos\phi$$
$$d_{yz} = \frac{-1}{\sqrt{2}i}\left(Y_2^1 + Y_2^{-1}\right) = \sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\sin\phi$$
$$d_{xy} = \frac{1}{\sqrt{2}i}\left(Y_2^2 - Y_2^{-2}\right) = \sqrt{\frac{15}{16\pi}}\sin^2\theta\sin 2\phi$$
$$d_{x^2-y^2} = \frac{1}{\sqrt{2}}\left(Y_2^2 + Y_2^{-2}\right) = \sqrt{\frac{15}{16\pi}}\sin^2\theta\cos 2\phi$$