Basic Quantum Chemistry Reference

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Particle in a Box

$$\psi_n = \sqrt{\frac{2}{l}}\sin\frac{n\pi x}{l}, \quad n = 1,2,3,\ldots$$

$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$E_n = \frac{h^2 n^2}{8ml^2} \qquad \Delta E_n = \frac{(2n+1)h^2}{8ml^2}$$

3-Dimensional Particle in a Box

$$\psi_n = \left(\sqrt{\frac{2}{l}}\right)^3 \sin\frac{n_x\pi x}{l}\sin\frac{n_y\pi y}{l}\sin\frac{n_z\pi z}{l}, \quad n_x, n_y, n_z = 1,2,3,\ldots$$

$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\nabla^2$$

$$E_n = \frac{h^2}{8m}\left(\frac{n_x{}^2}{l_x{}^2} + \frac{n_y{}^2}{l_y{}^2} + \frac{n_z{}^2}{l_z{}^2}\right)$$

Harmonic Oscillator

$$\psi_n = \sqrt{2^n n!}\left(\frac{\alpha}{\pi}\right)^{1/4} H_n(\sqrt{\alpha}\,x)e^{-\alpha x^2/2} \quad n = 0,1,2,\ldots \quad \alpha \equiv \frac{2\pi\nu m}{\hbar}$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}kx^2 = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2$$

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

Hermite Polynomials

$$H_n(x) = \sum_{m=0}^{m=n} c_m^{(n)} x^m$$

$$c_m^{(n)} = \frac{1}{\sqrt{m\hbar\omega}} e^{-i\pi/2}$$

$$H_n(x) = (-1)^n e^{x^2}\frac{\partial^n}{\partial x^n}e^{-x^2}$$

Ladder Operators

$$a^+ = (2m)^{-1/2}(\hat{p} + im\omega x);$$

$$a^- = (2m)^{-1/2}(\hat{p} - im\omega x);$$

$$\psi_n = \frac{1}{\sqrt{n!}}\left(\frac{a^+}{\sqrt{\hbar\omega}}\right)^n \psi_0(-i)^n = \frac{1}{\sqrt{n!\,(2\hbar\omega m)^n}}\left(-\hbar\frac{\partial}{\partial x} + \omega m x\right)^n \psi_0$$

The First Few Normalized Wave Functions

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

$$\psi_1 = \left(\frac{4\alpha^3}{\pi}\right)^{1/4} xe^{-\alpha x^2/2}$$

$$\psi_2 = \left(\frac{\alpha}{4\pi}\right)^{1/4}(2\alpha x^2 - 1)e^{-\alpha x^2/2}$$

Alternate General Form of the Wave Function

$$\psi_n = e^{-\alpha x^2/2} \sum_{m=0 or 1}^{n} c_m^{(n)} x^m$$

Note that only even or only odd terms are included in the sum

For n = even, $c_0^{(n)} = 1$

For n = odd, $c_1^{(n)} = 1$

$$c_{m+2}^{(n)} = \frac{2\alpha(m-n)}{(n+1)(n+2)} c_m$$

The entire wave function must be normalized after the summation

Rigid Rotor and Spherical Harmonics

$$\psi = Y_j^m(\theta, \phi)$$

$$\hat{H} = \frac{\hat{J}^2}{2I}$$

$$E_j = \frac{j(j+1)\hbar^2}{2I}$$

Spherical Harmonics

$$Y_j^m(\theta, \phi) = S_{j,m}(\theta) T_m(\phi)$$

$$T_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

$$S_{j,m}(\theta) = \left[\frac{(2j+1)[(j-|m|)!]}{2[(j+|m|)!]}\right]^{1/2} P_j^{|m|}(\cos\theta)$$

$$P_j^{|m|}(w) \equiv \frac{1}{2^j j!}(1-w^2)^{|m|/2} \frac{\partial^{j+|m|}}{\partial w^{j+|m|}}(w^2-1)^j$$

$\boldsymbol{S_{j,m}(\theta)}$		
$j = 0$	$m = 0$	$\frac{1}{2}\sqrt{2}$

$j=1$	$m=0$	$\frac{1}{2}\sqrt{6}\cos\theta$
	$m=\pm 1$	$\frac{1}{2}\sqrt{3}\sin\theta$
$j=2$	$m=0$	$\frac{1}{4}\sqrt{10}(3\cos^2\theta-1)$
	$m=\pm 1$	$\frac{1}{2}\sqrt{15}\sin\theta\cos\theta$
	$m=\pm 2$	$\frac{1}{4}\sqrt{15}\sin^2\theta$
$j=3$	$m=0$	$\frac{3}{4}\sqrt{14}\left(\frac{5}{3}\cos^3\theta-\cos\theta\right)$
	$m=\pm 1$	$\frac{1}{8}\sqrt{42}\sin\theta\,(5\cos^2\theta-1)$
	$m=\pm 2$	$\frac{1}{4}\sqrt{105}\sin^2\theta\cos\theta$
	$m=\pm 3$	$\frac{1}{8}\sqrt{70}\sin^3\theta$

Angular Momentum Operators

$$\hat{J}_z = -i\hbar\frac{\partial}{\partial\theta}$$

$$J_z = m\hbar$$

$$\hat{J}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

$$J^2 = j(j+1)\hbar^2$$

$$\hat{J}_x = y\hat{p}_z - z\hat{p}_y$$

$$\hat{J}_y = z\hat{p}_x - x\hat{p}_z$$

$$\hat{J}_z = x\hat{p}_y - y\hat{p}_x$$

$$[\hat{J}_x,\hat{J}_y] = i\hbar\hat{J}_z$$

$$[\hat{J}_y,\hat{J}_z] = i\hbar\hat{J}_x$$

$$[\hat{J}_z,\hat{J}_x] = i\hbar\hat{J}_y$$

$$\hat{J}_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta}+\cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$\hat{J}_y = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta}-\cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

Ladder Operators

$J_\pm = J_x \pm iJ_y$

$J_\pm Y_j^m(\theta,\phi) = \hbar\sqrt{j(j+1) - m(m\pm 1)}Y_j^{m+1}(\theta,\phi)$

Hydrogenic Atom

Wave Functions

$\psi = R_{n,l}(r)Y_l^m(\theta,\phi)$

$$\alpha_o = \frac{4\pi\varepsilon_o\hbar^2 n^2}{\mu e^2 Z}$$

$R_{n,l}(r)$		
$n=1$	$l=0$	$2\left(\frac{Z}{\alpha_o}\right)^{3/2} e^{-Zr/\alpha_o}$
$n=2$	$l=0$	$\frac{1}{\sqrt{2}}\left(\frac{Z}{\alpha_o}\right)^{3/2}\left(1-\frac{Zr}{2\alpha_o}\right)e^{-Zr/2\alpha_o}$
	$l=1$	$\frac{1}{2\sqrt{6}}\left(\frac{Z}{\alpha_o}\right)^{5/2} re^{-Zr/2\alpha_o}$
$n=3$	$l=0$	$\frac{2}{3\sqrt{3}}\left(\frac{Z}{\alpha_o}\right)^{3/2}\left(1-\frac{2Zr}{3\alpha_o}+\frac{2}{27}\left(\frac{Zr}{\alpha_o}\right)^2\right)e^{-Zr/3\alpha_o}$
	$l=1$	$\frac{8}{27\sqrt{6}}\left(\frac{Z}{\alpha_o}\right)^{5/2}\left(1-\frac{1}{6}\frac{Zr}{\alpha_o}\right)re^{-Zr/3\alpha_o}$
	$l=2$	$\frac{4}{81\sqrt{30}}\left(\frac{Z}{\alpha_o}\right)^{7/2} r^2 e^{-Zr/3\alpha_o}$

Complex Hydrogenic Wave Functions	
$1s$	$\frac{1}{\sqrt{\pi}}\left(\frac{Z}{\alpha_o}\right)^{3/2} e^{-Zr/\alpha_o}$
$2s$	$\frac{1}{\sqrt{\pi}}\left(\frac{Z}{2\alpha_o}\right)^{3/2}\left(1-\frac{Zr}{2\alpha_o}\right)e^{-Zr/2\alpha_o}$
$2p_0$	$\frac{1}{\sqrt{\pi}}\left(\frac{Z}{2\alpha_o}\right)^{5/2} re^{-Zr/2\alpha_o}\cos\theta$
$2p_{\pm 1}$	$\frac{1}{8\sqrt{\pi}}\left(\frac{Z}{\alpha_o}\right)^{5/2} re^{-Zr/2\alpha_o}\sin\theta\, e^{\pm i\phi}$

3s	$\frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{\alpha_o}\right)^{3/2}\left(27-18\frac{Zr}{\alpha_o}+2\left(\frac{Zr}{\alpha_o}\right)^2\right)e^{-Zr/3\alpha_o}$
$3p_0$	$\frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{Z}{\alpha_o}\right)^{5/2}\left(6-\frac{Zr}{\alpha_o}\right)re^{-Zr/3\alpha_o}\cos\theta$
$3p_{\pm1}$	$\frac{1}{81\sqrt{\pi}}\left(\frac{Z}{\alpha_o}\right)^{5/2}\left(6-\frac{Zr}{\alpha_o}\right)re^{-Zr/3\alpha_o}\sin\theta e^{\pm i\phi}$
$3d_0$	$\frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{\alpha_o}\right)^{7/2}r^2e^{-Zr/3\alpha_o}(3\cos^2\theta-1)$
$3d_{\pm1}$	$\frac{1}{81\sqrt{\pi}}\left(\frac{Z}{\alpha_o}\right)^{7/2}r^2e^{-Zr/3\alpha_o}\sin\theta\cos\theta\, e^{\pm i\phi}$
$3d_{\pm2}$	$\frac{1}{162\sqrt{\pi}}\left(\frac{Z}{\alpha_o}\right)^{7/2}r^2e^{-Zr/3\alpha_o}\sin^2\theta\, e^{\pm 2i\phi}$

Real Hydrogenic Wave Functions	
1s	$\frac{1}{\sqrt{\pi}}\left(\frac{Z}{\alpha_o}\right)^{3/2}e^{-Zr/\alpha_o}$
$2s$	$\frac{1}{\sqrt{\pi}}\left(\frac{Z}{2\alpha_o}\right)^{3/2}\left(1-\frac{Zr}{2\alpha_o}\right)e^{-Zr/2\alpha_o}$
$2p_z$	$\frac{1}{\sqrt{\pi}}\left(\frac{Z}{2\alpha_o}\right)^{5/2}re^{-Zr/2\alpha_o}\cos\theta$
$2p_x$	$\frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{\alpha_o}\right)^{5/2}re^{-Zr/2\alpha_o}\sin\theta\cos\phi$
$2p_y$	$\frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{\alpha_o}\right)^{5/2}re^{-Zr/2\alpha_o}\sin\theta\sin\phi$
3s	$\frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{\alpha_o}\right)^{3/2}\left(27-18\frac{Zr}{\alpha_o}+2\left(\frac{Zr}{\alpha_o}\right)^2\right)e^{-Zr/3\alpha_o}$
$3p_z$	$\frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{Z}{\alpha_o}\right)^{5/2}\left(6-\frac{Zr}{\alpha_o}\right)re^{-Zr/3\alpha_o}\cos\theta$
$3p_x$	$\frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{Z}{\alpha_o}\right)^{5/2}\left(6-\frac{Zr}{\alpha_o}\right)re^{-Zr/3\alpha_o}\sin\theta\cos\phi$
$3p_y$	$\frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{Z}{\alpha_o}\right)^{5/2}\left(6-\frac{Zr}{\alpha_o}\right)re^{-Zr/3\alpha_o}\sin\theta\sin\phi$

$3d_{z^2}$	$\frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{\alpha_o}\right)^{7/2} r^2 e^{-Zr/3\alpha_o}(3\cos^2\theta - 1)$
$3d_{xz}$	$\frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{Z}{\alpha_o}\right)^{7/2} r^2 e^{-Zr/3\alpha_o}\sin\theta\cos\theta\cos\phi$
$3d_{yz}$	$\frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{Z}{\alpha_o}\right)^{7/2} r^2 e^{-Zr/3\alpha_o}\sin\theta\cos\theta\sin\phi$
$3d_{x^2-y^2}$	$\frac{1}{81\sqrt{2\pi}}\left(\frac{Z}{\alpha_o}\right)^{7/2} r^2 e^{-Zr/3\alpha_o}\sin^2\theta\cos 2\phi$
$3d_{xy}$	$\frac{1}{81\sqrt{2\pi}}\left(\frac{Z}{\alpha_o}\right)^{7/2} r^2 e^{-Zr/3\alpha_o}\sin^2\theta\sin 2\phi$

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

$$V(r) = \frac{-Ze^2}{4\pi\varepsilon_o r} = \frac{-Ze'^2}{r}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2\partial}{r\partial r}\right) + \frac{1}{2mr^2}\hat{L}^2 - \frac{Ze^2}{4\pi\varepsilon_o r}$$

Energies

$$E_n = -\frac{Z^2e^2}{2n^2(4\pi\varepsilon_o)\alpha_o}$$

$$E_n = -\frac{Z^2\mu e^4}{2(4\pi\varepsilon_o)^2\hbar^2 n^2}$$

$$E_n \approx -13.606\frac{Z^2}{n^2}eV$$

Many Electron Atom

Wave Functions

Hamiltonian

$$\hat{H} = \hat{H}^o + \hat{H}_{rep} + \hat{H}_{S.O.}$$

$$\hat{H}^{o} = \sum_{i=1}^{n}\left(-\frac{\hbar^2}{2m}\nabla_i{}^2 - \frac{Ze'^2}{r_i}\right)$$

$$\hat{H}_{rep} = \sum_{i=1}^{n-1}\sum_{j>i}^{n}\frac{e'^2}{r_{ij}}$$

$$\hat{H}_{S.O.} = \sum_{i=1}^{n}\xi_i\hat{L}_i\cdot\hat{S}_i$$

Energies

Term Symbols for Equivalent Electrons	
Configuration	Terms
s^1	^2S
s^2; p^6; d^{10}	^1S
p^1; p^5	^2P
p^2; p^4	$^3P, {}^1D, {}^1S$
p^3	$^4S, {}^2D, {}^2P$
d^1; d^9	^2D
d^2 ; d^8	$^3F, {}^3P, {}^1G, {}^1D, {}^1S$
d^3 ; d^7	$^4F, {}^4P, {}^2H, {}^2G, {}^2F, {}^2D(2), {}^2P$
d^4 ; d^6	$^5D, {}^3H, {}^3G, {}^3F(2), {}^3D, {}^3P(2),$ $^1I, {}^1G(2), {}^1F, {}^1D(2), {}^1S(2)$
d^5	$^6S, {}^4G, {}^4F, {}^4D, {}^4P, {}^2I, {}^2H,$ $^2G(2), {}^2F(2), {}^2D(3)$, $^2P, {}^2S$
Term Symbols for Nonequivalent Electrons	
Configuration	Terms
s^1s^1	$^3S, {}^1S$
s^1p^1	$^3P, {}^1P$
s^1d^1	$^3D, {}^1D$
s^1f^1	$^3F, {}^1F$
p^1p^1	$^3D, {}^3P, {}^3S, {}^1D, {}^1P, {}^1S$
p^1d^1	$^3F, {}^3D, {}^3P, {}^1F, {}^1D, {}^1P$
p^1f^1	$^3G, {}^3F, {}^3D, {}^1G, {}^1F, {}^1D$
d^1d^1	$^3G, {}^3F, {}^3D, {}^3P, {}^3S,$ $^1G, {}^1F, {}^1D, {}^1P, {}^1S$
d^1f^1	$^3H, {}^3G, {}^3F, {}^3D, {}^3P,$

	$^1H, ^1G, ^1F, ^1D, ^1P$
f^1f^1	$^3I, ^3H, ^3G, ^3F, ^3D, ^3P, ^3S,$ $^1I, ^1H, ^1G, ^1F, ^1D, ^1P, ^1S$

$(N) indicates\ that\ the\ term\ occurs\ N\ times$

Variational Theory

$$\langle \widehat{\mathrm{H}} \rangle \equiv \frac{\langle \phi | \widehat{\mathrm{H}} | \phi \rangle}{\langle \phi | \phi \rangle} \geq \mathrm{E}_0$$

Linear Variational Theory

For a set of m trial functions:

$$\Psi_n = \sum_{i=1}^{m} c_i^{(n)} \ \phi_i$$

Energies

To find $\mathrm{E_n}$ solve for W in the secular equation:

$$\begin{vmatrix} \mathrm{H}_{11} - \mathrm{S}_{11}\mathrm{W} & \cdots & \mathrm{H}_{1m} - \mathrm{S}_{1m}\mathrm{W} \\ \vdots & \ddots & \vdots \\ \mathrm{H}_{m1} - \mathrm{S}_{m1}\mathrm{W} & \cdots & \mathrm{H}_{mm} - \mathrm{S}_{mm}\mathrm{W} \end{vmatrix} = 0$$

This gives m roots of W, corresponding to the upper bounds of the m lowest energy states.

Wave Functions

To find $c_i^{(n)}$ and Ψ_n solve this system of equations:

$$\sum_{i=1}^{i=m} (\mathrm{H_{1i}} - \mathrm{S_{1i}} \mathrm{W}_n) c_1^{(n)}$$

$$\sum_{i=1}^{i=m} (\mathrm{H_{2i}} - \mathrm{S_{2i}} \mathrm{W}_n) c_2^{(n)}$$

$$\vdots$$

$$\sum_{i=1}^{i=m} (\mathrm{H_{mi}} - \mathrm{S_{mi}} \mathrm{W}_n) c_m^{(n)}$$

Because the above system is not completely linearly independent (by one degree) we must finally normalize by:

$$\sum_{i=1}^{m} c_i^{(n)} = 0$$

Non-Degenerate Perturbation Theory

$$\psi_n^{(1)} = \sum_{i \neq n} \frac{\langle \psi_i^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_i^{(0)}} \psi_i^{(0)}$$

$\hat{H} = \hat{H}^o + \hat{H}'$ Where $\hat{H}^o$ is exactly solvable for $\psi_n^{(0)}$ and $\hat{H}'$ is a perturbation

$$E_n = E_n^{(0)} + E_n^{(1)} + \cdots$$

$$E_n^{(0)} \psi_n^{(0)} = \hat{H}^o | \psi_n^{(m-1)} \rangle$$

The First Few Degrees of Energy Correction

$$E_n^{(1)} = \langle \psi_n^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle$$

$$E_n^{(2)} = \sum_{i \neq n} \frac{\left| \langle \psi_i^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle \right|^2}{E_n^{(0)} - E_i^{(0)}}$$

Degenerate Perturbation Theory

$$\psi_n^{(1)} = \sum_{i \neq n} \frac{\langle \phi_i^{(0)} | \hat{H}' | \phi_n^{(0)} \rangle}{E_n^{(0)} - E_i^{(0)}} \psi_i^{(0)}$$

$$\phi_n^{(0)} = \sum_{i=1}^{d} c_i \, \psi_i^{(0)}, \quad 1 \leq n \leq d, d \text{ is the degeneracy}$$

Finding Correct Zero-Order Wave Functions

To find c_i, solve the secular equation:

$$\begin{vmatrix} H'_{11} - E_n^{(1)} & H'_{12} & \cdots & H'_{1d} \\ H'_{21} & H'_{22} - E_n^{(1)} & \cdots & H'_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ H'_{d1} & H'_{d2} & \cdots & H'_{dd} - E_n^{(1)} \end{vmatrix} = 0$$

The First Few Degrees of Energy Correction

$$E_n^{(1)} = \langle \phi_n^{(0)} | \hat{H}' | \phi_n^{(0)} \rangle$$

$$E_n^{(2)} = \sum_{i \neq n} \frac{\left| \langle \phi_i^{(0)} | \hat{H}' | \phi_n^{(0)} \rangle \right|^2}{E_n^{(0)} - E_i^{(0)}}$$

Definite and Indefinite Integrals

Remember that

$d\tau = r^2 \sin\theta \, dr d\theta d\phi$

$$\nabla^2 = \left(\frac{\partial^2}{\partial \theta^2} + \cot\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right)$$

$$\int x \sin bx \, dx = \frac{1}{b^2} \sin bx - \frac{x}{b} \cos bx$$

$$\int \sin^2 bx \, dx = \frac{x}{2} - \frac{1}{4b} \sin(2bx)$$

$$\int x \sin^2 bx \, dx = \frac{x^2}{4} - \frac{x}{4b} \sin(2bx) - \frac{1}{8b^2} \cos(2bx)$$

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

$$\int \sin ax \sin bx \, dx = \frac{\sin[(a-b)x]}{2(a-b)} - \frac{\sin[(a+b)x]}{2(a+b)}, \qquad a^2 \neq b^2$$

$$\int x e^{bx} dx = \left(\frac{x}{b} - \frac{1}{b^2} \right) e^{bx}$$

$$\int x^2 e^{bx} dx = \left(\frac{x^2}{b} - \frac{2x}{b^2} + \frac{2}{b^3} \right) e^{bx}$$

$$\int_0^\infty x^n e^{-bx} dx = \frac{n!}{b^{n+1}}, \quad n > -1, b > 0$$

$$\int_0^\infty e^{-bx^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{b}}, \quad b > 0$$

$$\int_0^\infty x^{2n} e^{-bx^2} dx = \frac{(2n)!}{2^{2n+1} n!} \sqrt{\frac{\pi}{b^{2n+1}}}, \quad b > 0, n = 1,2,3, \ldots$$

$$\int_t^\infty x^n e^{-bx} dx = \frac{n!}{b^{n+1}} e^{-bt} \left(1 + bt + \frac{b^2 t^2}{2!} + \cdots + \frac{b^n t^n}{n!} \right), \quad b > 0, n = 0,1,2, \ldots$$

Physical Constants and Conversions

Constant	Symbol	SI Value	Gaussian Value
Speed of Light in Vacuum	c	$2.99792458 * 10^8 \, ^{m}/_{s}$	$2.99792458 * 10^{10} \, ^{cm}/_{s}$

Proton Charge	e	$1.602177 * 10^{-19}\text{C}$	
″	e'		$4.803207 * 10^{-10}\text{statC}$
Vacuum Permittivity	ε_o	$8.8541878 * 10^{-12}\ {C^2}/{\text{N-m}^2}$	
Avogadro Constant	N_A	$6.02214 * 10^{-12}\text{mol}^{-1}$	$6.02214 * 10^{-12}\text{mol}^{-1}$
Electron Rest Mass	m_e	$9.1093897 * 10^{-31}\text{kg}$	$9.1093897 * 10^{-28}\text{g}$
Proton Rest Mass	m_p	$1.672623 * 10^{-27}\text{kg}$	$1.672623 * 10^{-24}\text{g}$
Neutron Rest Mass	m_n	$1.674929 * 10^{-27}\text{kg}$	$1.674929 * 10^{-24}\text{g}$
Planck Constant	h	$6.6260755 * 10^{-34}\text{J-s}$	$6.6260755 * 10^{-27}\text{erg-s}$
Reduced Planck Constant	$\hbar$	$1.0545727 * 10^{-34}\text{J-s}$	$1.0545727 * 10^{-27}\text{erg-s}$
Faraday Constant	F	$96485.3\ {C}/{\text{mol}}$	
Vacuum Permeability	μ_o	$4\pi * 10^{-7}\ {N}/{C^2\text{-s}^2}$	
Bohr Radius	α_o	$5.291772 * 10^{-11}\text{m}$	$5.291772 * 10^{-9}\text{cm}$
Bohr Magneton	β_e	$9.27402 * 10^{-24}\ {J}/{T}$	
Nuclear Magneton	β_N	$5.05079 * 10^{-27}\ {J}/{T}$	
Electron g Value	g_e	2.0023193044	2.0023193044
Proton g Value	g_p	5.585695	5.585695
Gas Constant	R	$8.3145\ {J}/{\text{mol-K}}$	$8.3145 * 10^7\ {\text{erg}}/{\text{mol-K}}$
Boltzmann Constant	k	$1.38066 * 10^{-23}\ {J}/{K}$	$1.38066 * 10^{-16}\ {\text{erg}}/{K}$
Gravitational Constant	G	$6.673 * 10^{-11}\ {m^3}/{\text{kg-s}^2}$	$6.673 * 10^{-8}\ {\text{cm}^3}/{\text{g-s}^2}$

Energy Conversion Factors
1 erg = 10^{-7}J
1 cal ≅ 4.184 J
1 eV $\cong 1.602177 * 10^{-19}\text{J} \cong 1.602177 * 10^{-12}\text{erg} \triangleq 23.0605\ {\text{kcal}}/{\text{mol}}$
1 hartree $\cong 4.35975 * 10^{-18}\text{J} \cong 27.2114\ \text{eV} \triangleq 627.510\ {\text{kcal}}/{\text{mol}}$

The symbol ≙ means "corresponds to"

<u>Notes and Acknowledgements:</u>

1. Spherical coordinates are represented in the way standard for chemists (which is different from the standard used by mathematicians). i.e. r = radius from origin, θ = angle with

the positive z axis, $\phi =$ angle between the positive x axis and the projection onto the x/y plane.

2. While I have worked hard to ensure that this document is correct, I assume no responsibility for the accuracy of the information here.

The following were used in compiling this reference:

1. http://panda.unm.edu/Courses/Finley/P262/Hydrogen/WaveFcns.html
2. Levine, Ira N. *Quantum Chemistry 6th ed.* Pearson Prentice Hall (Upper Saddle River, NJ) 2009.
3. Hollas, J. Michael. *Modern Spectroscopy.* John Wiley & Sons, Ltd. (Chichester, West Sussex, England) 2004.