Química Física I
Grado en Química

UNIVERSIDAD DE MURCIA

FORMULAS AND PHYSICAL CONSTANTS

Formulas

$\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$	$E_n = \frac{h^2 n^2}{8ml^2}$	$\psi_n(x) = \sqrt{\frac{2}{l}}\,\mathrm{sen}\left(\frac{n\pi x}{l}\right)\ ;\ n = 1, 2, \ldots$
$\hat{l}_z(\phi) = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$	$\hat{l}_z(\phi)\psi_m(\phi) = m\hbar\,\psi_m(\phi)$	$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}}\,e^{im\phi}$
$E_m = \frac{m^2\hbar^2}{2MR^2};\quad m = 0, \pm 1, \ldots$	$\hat{H}(\theta,\phi) = \frac{\hat{L}^2(\theta,\phi)}{2I} = \frac{\hat{L}^2(\theta,\phi)}{2mR^2}$	$\hat{L}^2(\theta,\phi) = -\hbar^2\left(\frac{1}{\mathrm{sen}^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\mathrm{sen}\theta}\frac{\partial}{\partial\theta}\mathrm{sen}\theta\frac{\partial}{\partial\theta}\right)$
$E_n = -\frac{ke^2}{2a_o}\frac{Z^2}{n^2} = -13.6\,\frac{Z^2}{n^2}\ \mathrm{eV}$	$dV = r^2\sin\theta\,dr\,d\theta\,d\phi$	$\hat{L}^2\psi_{l,m_l} = l(l+1)\hbar^2\,\psi_{l,m_l};\quad l = 0, 1, \ldots$
$< r >_{n,l} = \frac{a_o}{2Z}\left[3n^2 - l(l+1)\right]$		$\cos(\alpha\pm\beta) = \cos\alpha\,\cos\beta \mp \sin\alpha\sin\beta$
$\sin(2\alpha) = 2\,\sin\alpha\,\cos\alpha$	$\sin^2\alpha = \frac{1}{2}\,(1 - \cos\,2\alpha)$	$\sin(\alpha\pm\beta) = \sin\alpha\,\cos\beta \pm \cos\alpha\,\sin\beta$
$\int_0^\infty r^n e^{-br}dr = \frac{n!}{b^{n+1}}$	$\int_t^\infty z^n\,e^{-bz}\,dz = \frac{n!}{b^{n+1}}\,e^{-bt}\left(1 + bt + \frac{(bt)^2}{2!} + \frac{(bt)^3}{3!} + \ldots + \frac{(bt)^n}{n!}\right)$	
$\int_0^\infty e^{-bx^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{b}}$	$\int_0^\infty xe^{-bx^2}dx = \frac{1}{2b}$	$\int_0^\infty x^2e^{-bx^2}dx = \frac{\sqrt{\pi}}{4b^{\frac{3}{2}}}$
$\int_0^\infty x^4e^{-bx^2}dx = \frac{3\sqrt{\pi}}{8b^{\frac{5}{2}}}$	$\int x\sin(ax)dx = \frac{\sin(ax) - ax\cos(ax)}{a^2} + C$	

$$\int x\sin^2(ax)dx = -\frac{1}{8a^2}(2ax\sin(2ax) + \cos(2ax) - 2a^2x^2) + C$$

$$\int x^2\sin(ax)dx = \frac{2ax\sin(ax) + (2 - a^2x^2)\cos(ax)}{a^3} + C$$

$$\int x^2\sin^2(ax)dx = -\frac{1}{24a^3}\left((6a^2x^2 - 3)\sin(2ax) + 6ax\cos(2ax) - 4a^3x^3\right) + C$$

Physical constants

$R = 8.31$ J mol^{-1} K^{-1}	$R = 1.98$ cal mol^{-1} K^{-1}	$R = 0.082$ atm l mol^{-1} K^{-1}
$h = 6.62608\cdot 10^{-34}$ J s	$m_e = 9.10939\cdot 10^{-31}$ kg	$\epsilon_0 = 8.854\cdot 10^{-12}$ F m^{-1}
$e = 1.602\cdot 10^{-19}$ C	1 atm $= 1.013\cdot 10^5$ Pa	1 bar = 10^5 Pa
$a_0 = 5.292\cdot 10^{-11}$ m	$c = 2.9979\cdot 10^8$ m/s	1 uma = 1.66$\cdot 10^{-27}$ kg

Radial functions of the atomic orbitals

$R_{1s} = 2\left(\frac{Z}{a_o}\right)^{3/2} e^{-Zr/a_o}$
$R_{2s} = \frac{1}{\sqrt{2}}\left(\frac{Z}{a_o}\right)^{3/2}\left(1-\frac{Zr}{2a_o}\right) e^{-Zr/2a_o}$
$R_{2p} = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_o}\right)^{5/2} re^{-Zr/2a_o}$
$R_{3s} = \frac{2}{3\sqrt{3}}\left(\frac{Z}{a_o}\right)^{3/2}\left(1-\frac{2Zr}{3a_o}+\frac{2Z^2r^2}{27a_o^2}\right) e^{-Zr/3a_o}$
$R_{3p} = \frac{8}{27\sqrt{6}}\left(\frac{Z}{a_o}\right)^{3/2}\left(\frac{Zr}{a_o}-\frac{Z^2r^2}{6a_o^2}\right) e^{-Zr/3a_o}$

Spherical harmonics.

$Y_{l,m}(\theta,\phi) = \frac{1}{\sqrt{2\pi}} S_{l,m}(\theta) e^{im\phi}$

$\int_0^\pi |S_{l,m}|^2 \sin\theta d\theta = 1$

$l = 0:$	$S_{0,0} = \frac{1}{2}\sqrt{2}$
$l = 1:$	$S_{1,0} = \frac{1}{2}\sqrt{6}\cos\theta$
	$S_{1,\pm1} = \frac{1}{2}\sqrt{3}\sin\theta$
$l = 2:$	$S_{2,0} = \frac{1}{4}\sqrt{10}(3\cos^2\theta - 1)$
	$S_{2,\pm1} = \frac{1}{2}\sqrt{15}\sin\theta\cos\theta$
	$S_{2,\pm2} = \frac{1}{4}\sqrt{15}\sin^2\theta$
$l = 3:$	$S_{3,0} = \frac{3}{4}\sqrt{14}(\frac{5}{3}\cos^3\theta - \cos\theta)$
	$S_{3,\pm1} = \frac{1}{8}\sqrt{42}\sin\theta(5\cos^2\theta - 1)$
	$S_{3,\pm2} = \frac{1}{4}\sqrt{105}\sin^2\theta\cos\theta$
	$S_{3,\pm3} = \frac{1}{8}\sqrt{70}\sin^3\theta$

Harmonic oscillator eigenfunctions ($\alpha = \mu\omega/\hbar$)

$\psi_0 = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2/2}$
$\psi_1 = \sqrt{2\alpha}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} xe^{-\alpha x^2/2}$
$\psi_2 = \frac{1}{\sqrt{2}}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} (2\alpha x^2 - 1)e^{-\alpha x^2/2}$
$\psi_3 = \sqrt{3}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} (\frac{2}{3}\alpha^{3/2}x^3 - \alpha^{1/2}x)e^{-\alpha x^2/2}$
$\psi_4 = \frac{1}{\sqrt{6}}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} (2\alpha^2x^4 - 6\alpha x^2 + \frac{3}{2})e^{-\alpha x^2/2}$

Linear least squares ($y = ax + b$)

$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$	$\bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i$
$a = \frac{\sum_{i=1}^{N}(x_i-\bar{x})(y_i-\bar{y})}{\sum_{i=1}^{N}(x_i-\bar{x})^2}$	$b = \bar{y} - a\bar{x}$