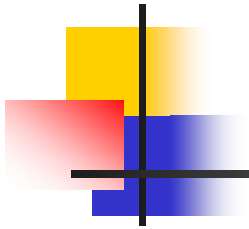


Liaison Chimique ‘09

Chap. I: The Hydrogen Atom

WebElements: the periodic table on the world-wide web

http://www.webelements.com/

1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
hydrogen 1 **H** 1.00794(7)																		helium 2 **He** 4.002602(2)
lithium 3 **Li** 6.941(2)	beryllium 4 **Be** 9.012182(3)												boron 5 **B** 10.811(7)	carbon 6 **C** 12.0107(8)	nitrogen 7 **N** 14.00674(7)	oxygen 8 **O** 15.9994(3)	fluorine 9 **F** 18.9984032(5)	neon 10 **Ne** 20.1797(6)
sodium 11 **Na** 22.989770(2)	magnesium 12 **Mg** 24.3050(6)												aluminium 13 **Al** 26.981538(2)	silicon 14 **Si** 28.0855(3)	phosphorus 15 **P** 30.973761(2)	sulfur 16 **S** 32.066(6)	chlorine 17 **Cl** 35.4527(9)	argon 18 **Ar** 39.948(1)
potassium 19 **K** 39.0983(1)	calcium 20 **Ca** 40.078(4)		scandium 21 **Sc** 44.955910(8)	titanium 22 **Ti** 47.867(1)	vanadium 23 **V** 50.9415(1)	chromium 24 **Cr** 51.9961(6)	manganese 25 **Mn** 54.938049(9)	iron 26 **Fe** 55.845(2)	cobalt 27 **Co** 58.933200(9)	nickel 28 **Ni** 58.6934(2)	copper 29 **Cu** 63.546(3)	zinc 30 **Zn** 65.39(2)	gallium 31 **Ga** 69.723(1)	germanium 32 **Ge** 72.61(2)	arsenic 33 **As** 74.92160(2)	selenium 34 **Se** 78.96(3)	bromine 35 **Br** 79.904(1)	krypton 36 **Kr** 83.80(1)
rubidium 37 **Rb** 85.4678(3)	strontium 38 **Sr** 87.62(1)		yttrium 39 **Y** 88.90585(2)	zirconium 40 **Zr** 91.224(2)	niobium 41 **Nb** 92.90638(2)	molybdenum 42 **Mo** 95.94(1)	technetium 43 **Tc** [97.9072]	ruthenium 44 **Ru** 101.07(2)	rhodium 45 **Rh** 102.90550(2)	palladium 46 **Pd** 106.42(1)	silver 47 **Ag** 107.8682(2)	cadmium 48 **Cd** 112.411(8)	indium 49 **In** 114.818(3)	tin 50 **Sn** 118.710(7)	antimony 51 **Sb** 121.760(1)	tellurium 52 **Te** 127.60(3)	iodine 53 **I** 126.90447(3)	xenon 54 **Xe** 131.29(2)
caesium 55 **Cs** 132.90545(2)	barium 56 **Ba** 137.327(7)	57-70 *	lutetium 71 **Lu** 174.967(1)	hafnium 72 **Hf** 178.49(2)	tantalum 73 **Ta** 180.9479(1)	tungsten 74 **W** 183.84(1)	rhenium 75 **Re** 186.207(1)	osmium 76 **Os** 190.23(3)	iridium 77 **Ir** 192.217(3)	platinum 78 **Pt** 195.078(2)	gold 79 **Au** 196.96655(2)	mercury 80 **Hg** 200.59(2)	thallium 81 **Tl** 204.3833(2)	lead 82 **Pb** 207.2(1)	bismuth 83 **Bi** 208.98038(2)	polonium 84 **Po** [208.9824]	astatine 85 **At** [209.9871]	radon 86 **Rn** [222.0176]
francium 87 **Fr** [223.0197]	radium 88 **Ra** [226.0254]	89-102 **	lawrencium 103 **Lr** [262.1097]	rutherfordium 104 **Rf** [261.1088]	dubnium 105 **Db** [262.1142]	seaborgium 106 **Sg** [266.1219]	bohrium 107 **Bh** [264.1247]	hassium 108 **Hs** [269.1341]	meitnerium 109 **Mt** [268.1388]	ununnilium 110 **Uun** [271.1461]	unununium 111 **Uuu** [272.1535]	ununbium 112 **Uub** [277]		ununquadium 114 **Uuq** [289]		ununhexium 116 **Uuh** [289]		ununoctium 118 **Uuo** [293]

Key:

element name
atomic number
symbol
1997 atomic weight (mean relative mass)

*lanthanoids	lanthanum 57 **La** 138.9055(2)	cerium 58 **Ce** 140.116(1)	praseodymium 59 **Pr** 140.90765(2)	neodymium 60 **Nd** 144.24(3)	promethium 61 **Pm** [144.9127]	samarium 62 **Sm** 150.36(3)	europium 63 **Eu** 151.964(1)	gadolinium 64 **Gd** 157.25(3)	terbium 65 **Tb** 158.92534(2)	dysprosium 66 **Dy** 162.50(3)	holmium 67 **Ho** 164.93032(2)	erbium 68 **Er** 167.26(3)	thulium 69 **Tm** 168.93421(2)	ytterbium 70 **Yb** 173.04(3)
**actinoids	actinium 89 **Ac** [227.0277]	thorium 90 **Th** 232.0381(1)	protactinium 91 **Pa** 231.03588(2)	uranium 92 **U** 238.0289(1)	neptunium 93 **Np** [237.0482]	plutonium 94 **Pu** [244.0642]	americium 95 **Am** [243.0614]	curium 96 **Cm** [247.0703]	berkelium 97 **Bk** [247.0703]	californium 98 **Cf** [251.0796]	einsteinium 99 **Es** [252.0830]	fermium 100 **Fm** [257.0951]	mendelevium 101 **Md** [258.0984]	nobelium 102 **No** [259.1009]

Element symbols and names: symbols, names, and spellings are those recommended by IUPAC (http://www.iupac.org/). After controversy, the names of elements 101-109 are now confirmed (Pure & Appl. Chem., 1997, 69, 2471–2473). Names have yet to be proposed for the elements 110–112, 114, 116, and 118, those used here are IUPAC's temporary systematic names (Pure & Appl. Chem., 1979, 51, 381–384). In the USA and some other countries, the spellings aluminum and cesium are normal while in the UK and elsewhere the usual spelling is sulphur.
Atomic weights (mean relative masses): Apart from the heaviest elements, these are IUPAC 1997 values (Pure & Appl. Chem., 1999, 71, 1593–1607). Elements for which values are given in brackets have no stable nuclides and are represented by 5-figure values for the longest-lived isotope. The elements thorium, protactinium, and uranium have characteristic terrestrial abundances and these are the values quoted. The last significant figure of each value is considered reliable to ±1 except where a larger uncertainty is given in parentheses.
Periodic table organisation: for a justification of the positions of the elements La, Ac, Lu, and Lr in the WebElements periodic table see W.B. Jensen, "The positions of lanthanum (actinium) and lutetium (lawrencium) in the periodic table", J. Chem. Ed., 1982, 59, 634–636.
Group labels: the numeric system (1–18) used here is the current IUPAC convention. For a discussion of this and other common systems see: W.C. Fernelius and W.H. Powell, "Confusion in the periodic table of the elements", J. Chem. Ed., 1982, 59, 504–508.

Quantum Mechanics

Classical Quantum Theory

- electron treated as particle
- interpretation of atomic spectra
- assignment of electronic configurations

- The Bohr Model

$$mvr = n\left(\frac{h}{2\pi}\right)$$

$$\Delta E = E_{n_2} - E_{n_1} = h\nu$$

n=principal quantum number
m=mass of electron
v=velocity of electron

h=Planck's constant
E=energy
ν=frequency of emitted radiation

Modern Wave Mechanics

- Electron treated as wave (wave-particle duality)

$$\lambda = \frac{h}{mv}$$ ← De Broglie relationship

- Probability of finding electron in given volume of space
  - due to uncertainty principle of Heisenberg we speak of probability
  - determined from Ψ^2, where Ψ is the wavefunction that describes behavior of electron-wave

Schrödinger Equation

(Erwin Schrödinger, 1926)

$$H\Psi = E\Psi$$

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$$

Ψ-wave function
E-total energy of particle
V-potential energy of particle
h-Planck's constant
m-mass of particle

Radial wave function Angular wave functions

$$\Psi(x, y, z) \equiv \Psi(r, \theta, \phi) = R(r) \cdot \Theta(\theta) \cdot \Phi(\phi)$$

- Wave function
  - Solution of Schrödinger equation (3 quantum numbers)
  - Contains detailed information about behavior of electron in region of space called atomic orbital
- Energy values associated with particular wave functions
- Quantization of energy levels

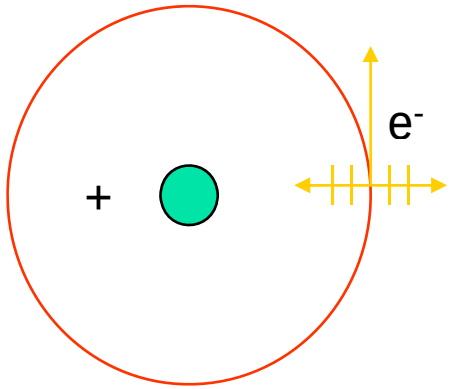
Hydrogen Atom (I)

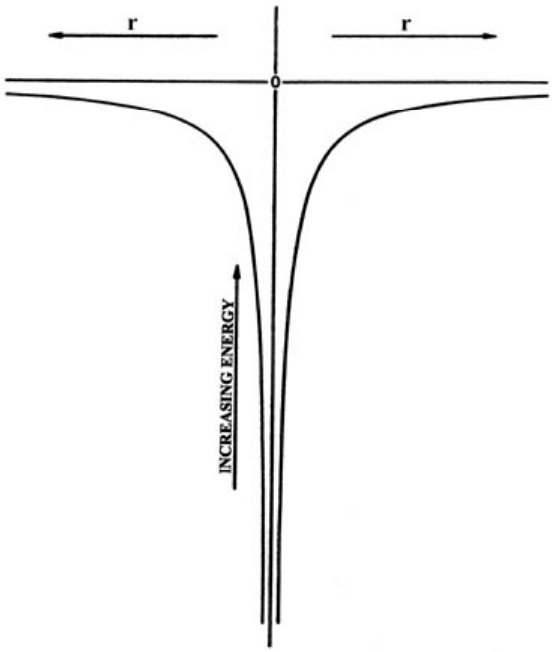
Why H?

- A simple « two body » problem, with an EXACT solution
- Prototype orbitals

A central force problem

$V=-e^2/r$





If the nucleus if « fixed » then ….

Hydrogen Atom (II)

In cartesian coordinates

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2m}{\hbar^2}(E-U)\psi=0$$

with

$$U=-\frac{e^2}{4\pi\varepsilon_0 r}$$

Spherical potential

cartesian coordinates (x , y , z) → spherical polar coordinates (r,θ,ϕ)

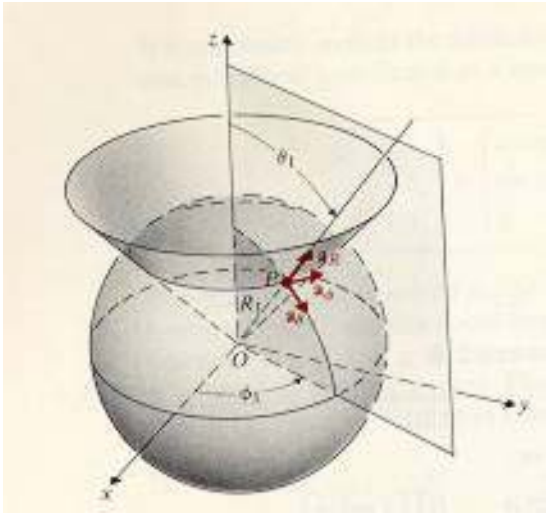
Hydrogen Atom (III)

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\theta = \cos^{-1} \frac{z}{\sqrt{x^2 + y^2 + z^2}}$$

$$\phi = \tan^{-1} \frac{y}{x}$$

$$\begin{cases} x = r \sin\theta \cos\phi \\ y = r \sin\theta \sin\phi \\ z = r \cos\theta \end{cases}$$



The Schrödinger equation becomes

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \psi}{\partial \theta}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial^2 \psi}{\partial \phi^2} + \frac{2m}{\hbar^2}(E - U)\psi = 0$$

or

$$\sin^2\theta \frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right) + \sin\theta \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \psi}{\partial \theta}\right) + \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2mr^2 \sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r} + E\right)\psi = 0$$

Hydrogen Atom (IV)

The wavefunctions as product of a radial and an angular part

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

and

$$\frac{\partial\psi}{\partial r} = \Theta\Phi\frac{\partial R}{\partial r}, \quad \frac{\partial\psi}{\partial\theta} = R\Phi\frac{\partial\Theta}{\partial\theta}, \quad \frac{\partial^2\psi}{\partial\phi^2} = R\Theta\frac{\partial^2\Phi}{\partial\phi^2}$$

The Schrödinger equation becomes

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \underbrace{\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}} + \frac{2mr^2\sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r} + E\right) = 0$$

$\rightarrow$ constant

$$-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = m_l^2$$

Hydrogen Atom (V)

The remain part

$$\underbrace{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)}_{\text{r-dependent}}=\underbrace{\frac{m_l^2}{\sin^2\theta}-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)}_{\theta\text{-dependent}}$$

r-dependent constant for variation of θ

θ-dependent constant for variation of r

Equal to a constant

$$\frac{m_l^2}{\sin^2\theta}-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)=l(l+1)$$

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)=l(l+1)$$

Hydrogen Atom (VI)

Finally

$$\begin{cases} \dfrac{1}{r^2}\dfrac{d}{dr}\left(r^2\dfrac{dR}{dr}\right)+\left[\dfrac{2m}{\hbar^2}\left(\dfrac{e^2}{4\pi\varepsilon_0 r}+E\right)-\dfrac{l(l+1)}{r^2}\right]R=0 \\ \dfrac{1}{\sin\theta}\dfrac{d}{d\theta}\left(\sin\theta\dfrac{d\Theta}{d\theta}\right)+\left[l(l+1)-\dfrac{m_l^2}{\sin^2\theta}\right]\Theta=0 \\ \dfrac{d^2\Phi}{d\phi^2}+m_l^2\Phi=0 \end{cases}$$

Hydrogen Atom (VII)

Solution for Θ

$$\frac{1}{\sin\theta}\frac{\boldsymbol{d}}{\boldsymbol{d}\theta}\left(\sin\theta\frac{\boldsymbol{d}\Theta}{\boldsymbol{d}\theta}\right)+\left[\boldsymbol{l}(\boldsymbol{l}+1)-\frac{\boldsymbol{m}_l^2}{\sin^2\theta}\right]\Theta=0$$

Put $\mu = \cos\theta$

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{d\Theta}{d\mu}\right]+\left[l(l+1)-\frac{m_l^2}{1-\mu^2}\right]\Theta=0$$

differential equation for associated Legendre functions

$$P_l^m(\mu)=(1-\mu^2)^{\frac{m_l}{2}}\frac{d^m P_l(\mu)}{d\mu^m}$$

Hydrogen Atom (VIII)

by normalizing

$$\Theta_{lm}(\theta) = N_{lm} P_l^m(\cos\theta)$$

when $$N_{em} = \left[\frac{(2l+1)(l-m)!}{2(l+m)!}\right]^{1/2}$$

$$\begin{cases} P_0^0 = 1 \end{cases}$$

$$\begin{cases} P_1^0 = \mu \\ P_1^1 = (1-\mu^2)^{1/2} \end{cases}$$

$$\begin{cases} P_2^0 = \frac{1}{2}(3\mu^2 - 1) \\ P_2^1 = 3\mu(1-\mu^2)^{1/2} \\ P_2^2 = 3(1-\mu^2) \end{cases}$$

$$\begin{cases} P_3^0 = \frac{1}{2}(5\mu^3 - 3\mu) \\ P_3^1 = \frac{3}{2}(5\mu^2 - 1)(1-\mu^2)^{3/2} \\ P_3^2 = 15\mu(1-\mu^2) \\ P_3^3 = 15(1-\mu^2)^{3/2} \end{cases}$$

Hydrogen Atom (IX)

Solution for R

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left[\frac{2m}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)-\frac{l(l+1)}{r^2}\right]R=0$$

put $\rho=\alpha_n r$

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right)+\frac{2mr^2}{\hbar^2}\left[\frac{E_n}{\alpha_n^2}+\frac{Ze^2}{4\pi\varepsilon_0\alpha_n\rho}-\frac{l(l+1)\hbar^2}{2m\rho^2}\right]R=0$$

$$\alpha_n^2=-\frac{8mE_n}{\hbar^2}\quad,\quad \lambda_n=\frac{Ze^2}{4\pi\varepsilon_0\hbar}\left(-\frac{m}{2E_n}\right)^{1/2}$$

$$\frac{d^2R}{d\rho^2}+\frac{2}{\rho}+\left[\frac{\lambda_n}{\rho}-\frac{1}{4}-\frac{l(l+1)}{\rho^2}\right]R=0 \qquad R(\rho)=e^{-\rho/2}F(\rho)$$

$$\frac{d^2F}{d\rho^2}+\left(\frac{2}{\rho}-1\right)\frac{dF}{d\rho}+\left[\frac{\lambda_n-1}{\rho}-\frac{l(l+1)}{\rho^2}\right]F=0$$

↳ associated Languerre polynomials

Hydrogen Atom (X)

if $\lambda_n = n$, $n > l$

$$R_{nl} = A_{nl}\, e^{-\rho/2}\, \rho^{l}\, L_{n+1}^{2l+1}(\rho)$$

$$A_{nl} = \left[\left(\frac{2Z}{na_0'} \right)^3 \frac{(n-l-1)!}{2n(n+l)!^3} \right]^{\frac{1}{2}}$$

Solution for Φ

$$\frac{d^2\Phi}{d\phi^2} + m_l^2 \Phi = 0 \qquad \Phi = Ae^{im_l\phi}$$

Quantum numbers (I)

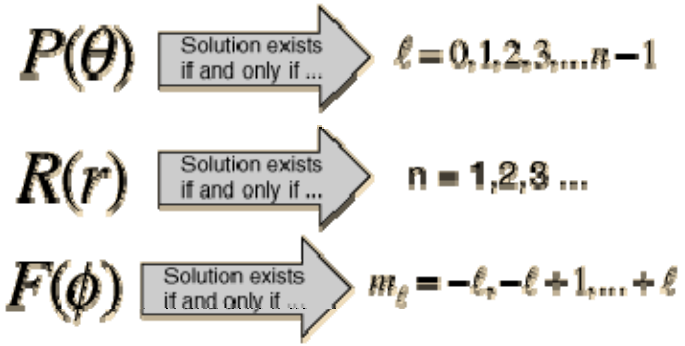
$$Ae^{im_l\phi} = Ae^{im_l(\phi+2\pi)} \rightarrow \quad m_l = 0 \ , \pm \text{ integer}$$

$m_l = 0, \pm 1, \pm 2, \pm 3 \cdots\cdots \pm l$; magnetic quantum number

$$l >> |m_l|$$

$$R_{nl} = A_{nl} e^{-\rho/2} \rho^l L_{n+1}^{2l+1}(\rho)$$

$$\Theta_{lm}(\theta) = N_{lm} P_l^m(\cos\theta)$$



$n = 1 \ , 2 \ , 3 \cdots\cdots$; principal quantum number

$l = 0 \ , 1 \ , 2 \ , \cdots\cdots (n-1)$; orbital quantum number

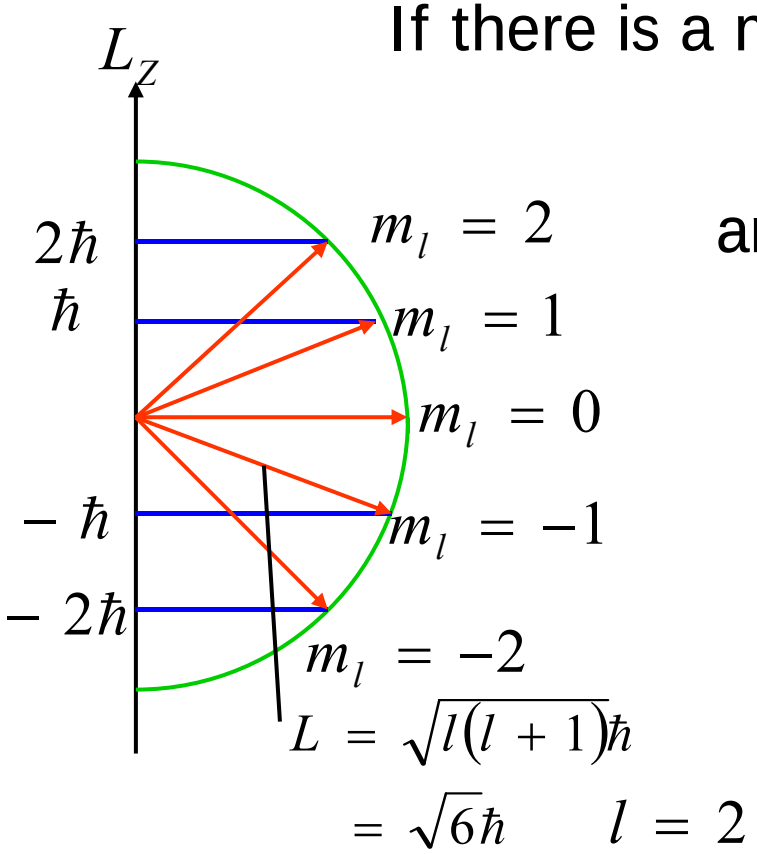
Quantum numbers (II)

- Designation of angular momentum states

=	0	1	2	3	4	5	6	•••
	s	p	d	f	g	h	i	
	(sharp)	(principal)	(diffused)	(fundamental)				

	l=0	1	2	3	4	5	
n=1	1s						
2	2s	2p					
3	3s	3p	3d				
4	4s	4p	4d	4f			
5	5s	5p	5d	5f	5g		
6	6s	6p	6d	6f	6g	6h	

Magnetic Quantum Number



If there is a magnetic field in Z-axis,

$$\vec{L} = \vec{r} \times \boldsymbol{m}\vec{v}$$

angular momentum orientation

is quantized

space quantization

$$L_Z = m_l \hbar$$

$$m_l = 0, \pm 1, \pm 2 \cdots\cdots \pm l$$

(magnetic quantum number)

$$L_Z = |m_l \hbar| < L$$

Ground state Energy

For the ground state (e.g. the state with the lowest energy)

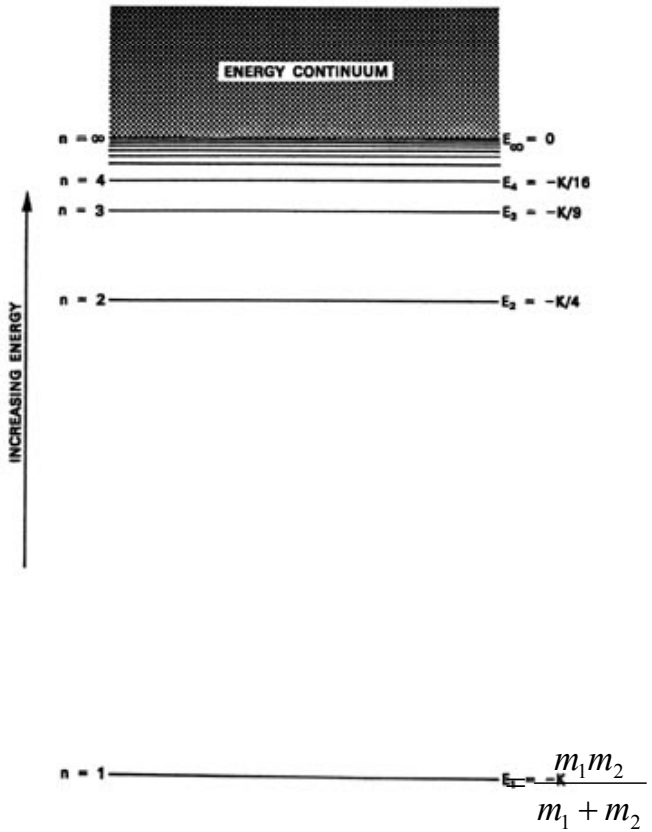
$$\psi(r,\theta,\phi) = R_{nl}\Theta_{lm_l}\Phi_{m_l} \qquad n = 1, l = 0, m_l = 0$$

$$R = \left(\frac{2}{a_0^{3/2}}\right)e^{-r/a_0} \qquad \psi = \frac{1}{\sqrt{\pi}}\frac{1}{a_0^{3/2}}e^{-r/a_0}$$

$$\left[\left(\frac{2}{a^{7/2}} + \frac{4mE_1}{\hbar^2 a_0^{3/2}}\right) + \left(\frac{me^2}{\pi\varepsilon_0\hbar a_0^{3/2}} - \frac{4}{a_0^{5/2}}\right)\frac{1}{r}\right]e^{-r/a_0} = 0$$

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \qquad \boldsymbol{E_1} = -\frac{\hbar^2}{2\boldsymbol{m}\boldsymbol{a_0}} = -\frac{\boldsymbol{me^4}}{32\pi^2\varepsilon_0^2\hbar^2}$$

Higher Energies



Two particle problem – nucleus and one electron (hydrogen or hydrogen-like atom)

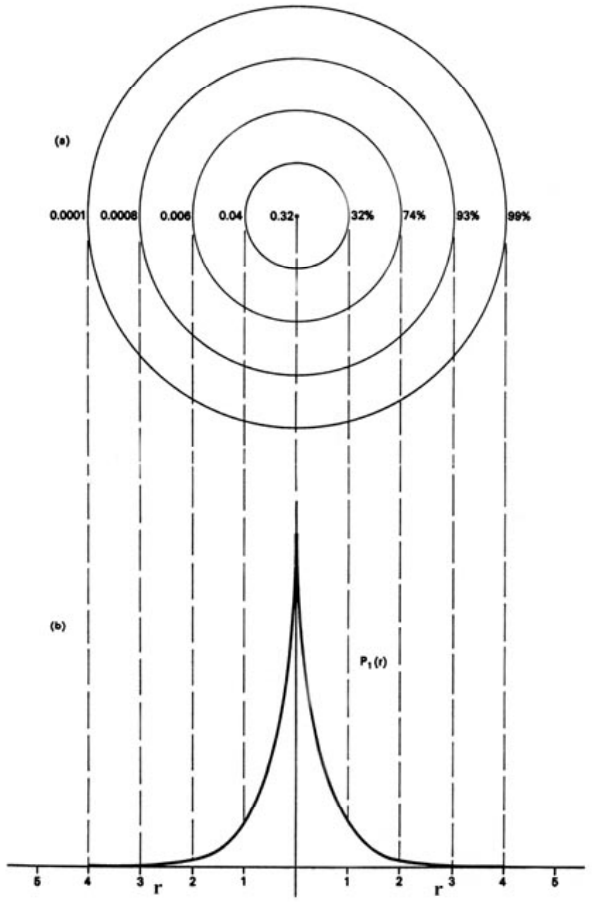
$$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 h^2 n^2} \qquad n = 1, 2, 3, \ldots$$

$$E_n = \frac{E_1}{n^2} \qquad (n = 1, 2, 3, \cdots)$$

- $E<0$ – electron in atom
- $E\geq 0$ – ionized atom

Degeneracy of orbitals

H ground state wavefunction



$$\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

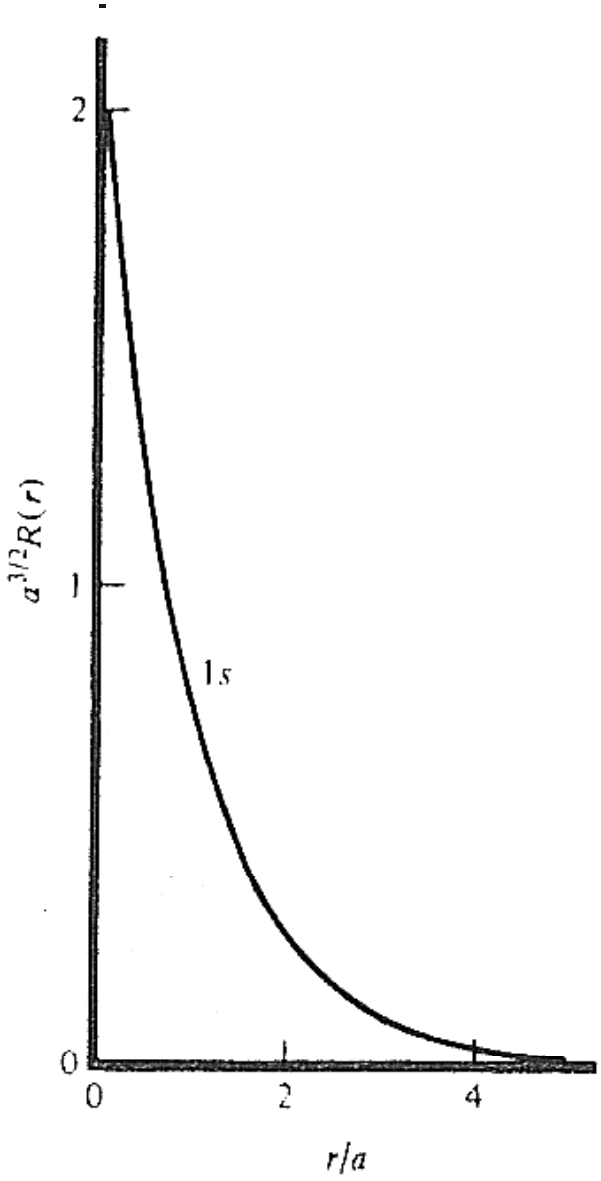
$$R_{10}(r) = \frac{2}{\sqrt{a^3}} b_0 e^{-r/a} .$$

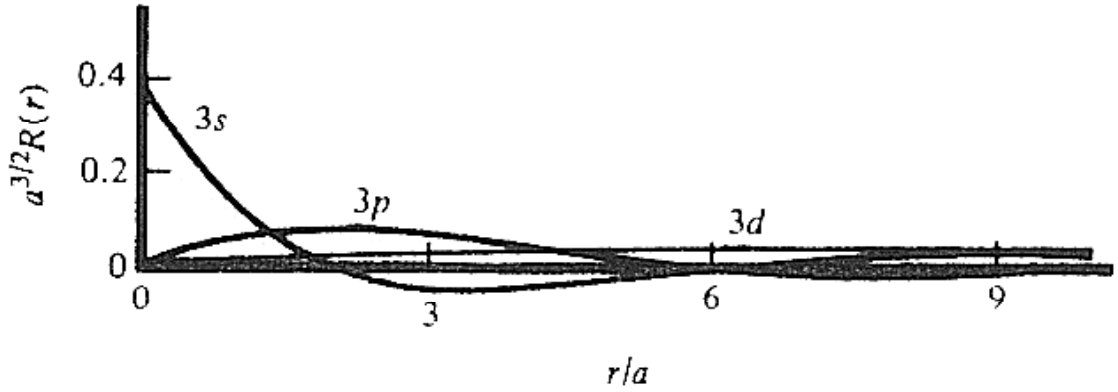
Radial Wave Functions for Hydrogen-like Orbitals

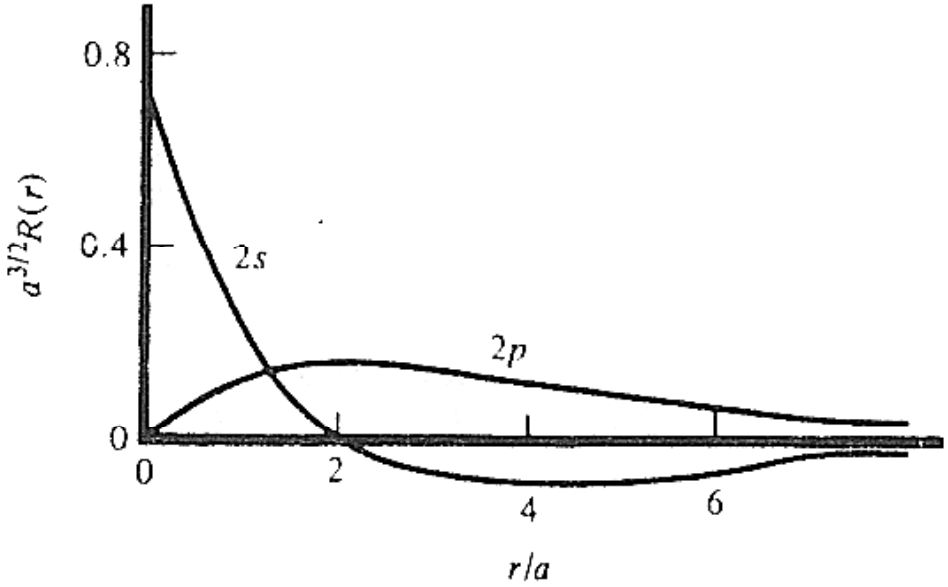
$n=1,\ l=0,\ m_l=0$	$R=2\left(\frac{Z}{a}\right)^{3/2}e^{-Zr/a}$	*1 s orbital*
$n=2,\ l=0,\ m_l=0$	$R=\frac{1}{\sqrt{2}}\left(\frac{Z}{a}\right)^{3/2}\left(2-\frac{Zr}{a}\right)e^{-Zr/2a}$	*2 s orbital*
$n=2,\ l=1,\ m_l=0$	$R=\frac{1}{\sqrt{24}}\left(\frac{Z}{a}\right)^{5/2}re^{-Zr/2a}$	*2 p orbital*

$$a=\frac{h^2}{4\pi^2\mu e^2}$$

Exponential Decay Functions







Angular Wave Functions for Hydrogen-like Atoms

$l = 0, m_l = 0$	$\Theta\Phi = \left[1/(4\pi) \right]^{1/2}$	*s orbital*
$l = 1, m_l = 0$	$\Theta\Phi = \left[3/(4\pi) \right]^{1/2} \cos\theta$	p_z *orbital*
$l = 2, m_l = 0$	$\Theta\Phi = \left[5/(16\pi) \right]^{1/2} (3\cos^2\theta - 1)$	d_{z^2} *orbital*

Real Hydrogen-like Wave Functions for $n=1$ and $n=2$

1 s orbital	$\Psi = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a}\right)^{3/2} e^{-Zr/a}$
2 s orbital	$\Psi = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a}\right)^{3/2}\left(2-\frac{Zr}{a}\right)e^{-Zr/2a}$
2 p_x orbital	$\Psi = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a}\right)^{5/2} re^{-Zr/2a}\sin\theta\cos\phi$
2 p_y orbital	$\Psi = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a}\right)^{5/2} re^{-Zr/2a}\sin\theta\sin\phi$
2 p_z orbital	$\Psi = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a}\right)^{5/2} re^{-Zr/2a}\cos\theta$

Electron probability density

$p(r, \theta, \phi) \longrightarrow$ has a meaning in quantum mechanics.

- the probability of density to find an electron:

$$|\psi|^2 = |R|^2 |\Theta|^2 |\Phi|^2$$

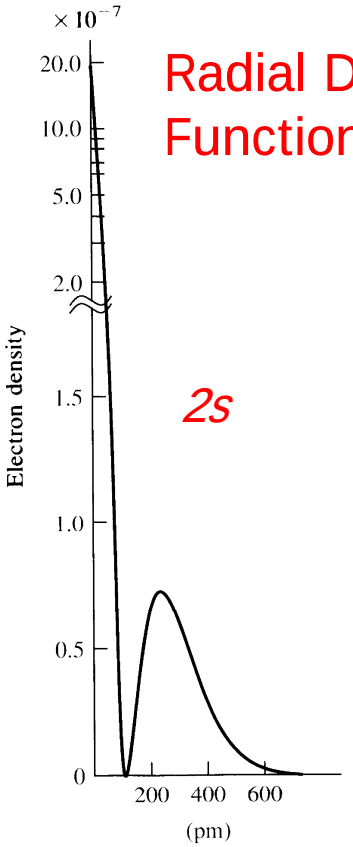
$$\Phi = Ae^{im_l \phi} \rightarrow |\Phi|^2 \text{ is symmetrical for } \phi$$

- radial part of probability

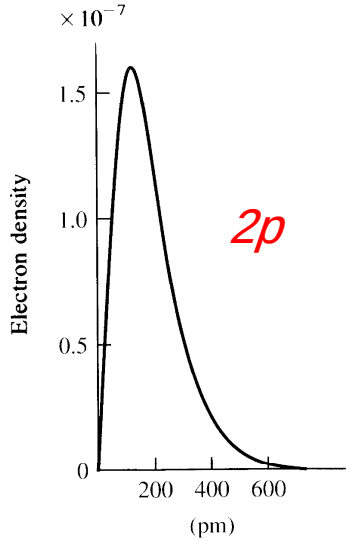
$$P(r)dr = r^2 |R|^2 dr \int_0^{\pi} |\Theta|^2 \sin\theta d\theta \int_0^{2\pi} |\Phi|^2 d\phi = r^2 |R|^2 dr$$

$$\because dV = (r\sin\theta d\phi)(d\theta) r dr$$

Radial Density Functions for H



2s



2p

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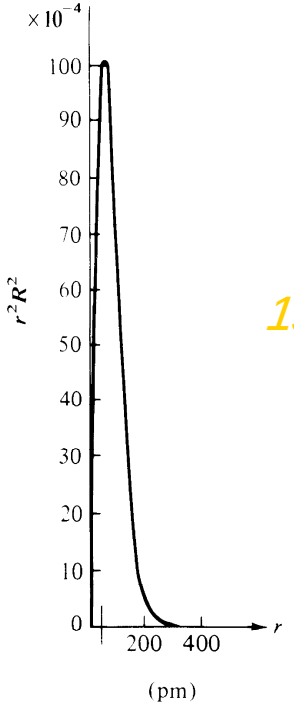
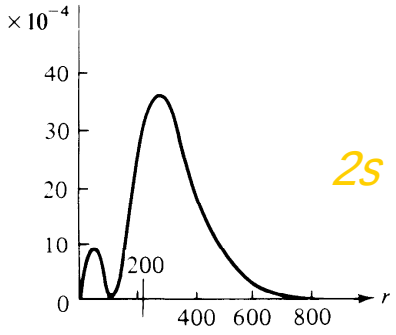
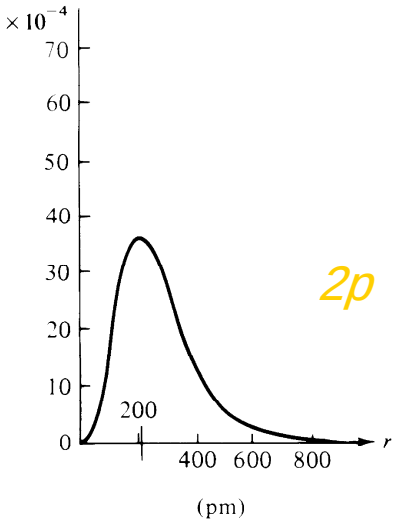


1s

Radial Probability Functions for H



2s



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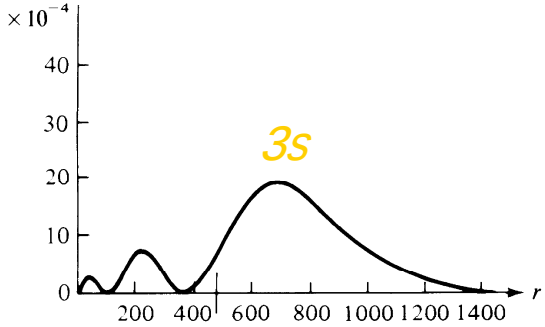
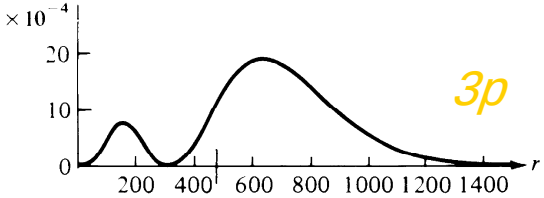


3s



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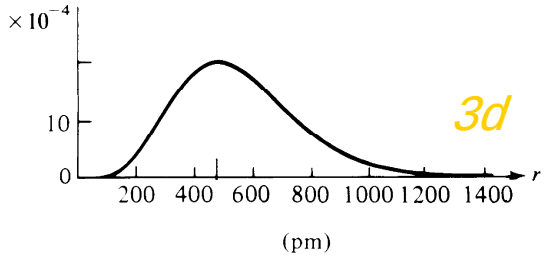
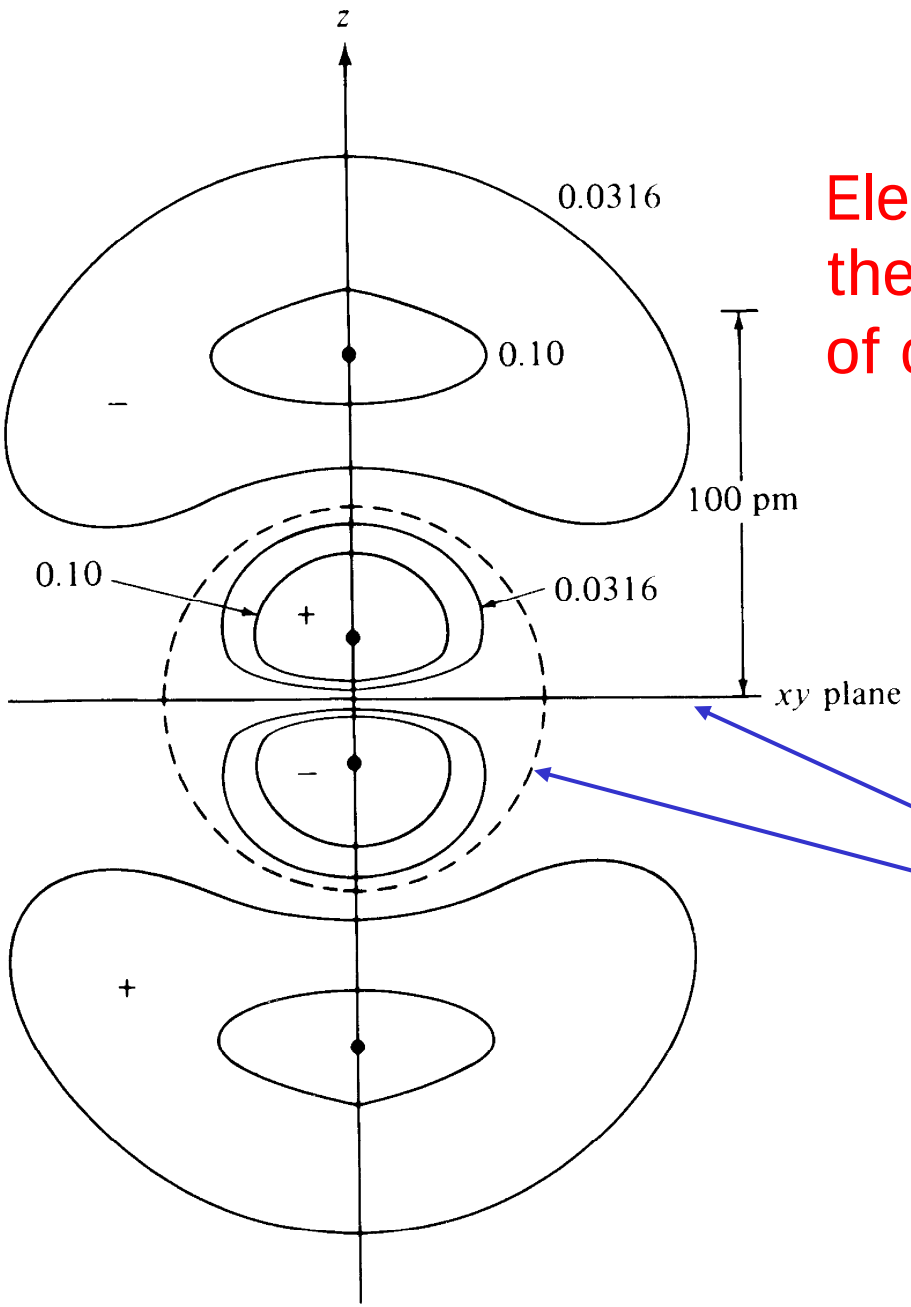


3d

Radial Nodes

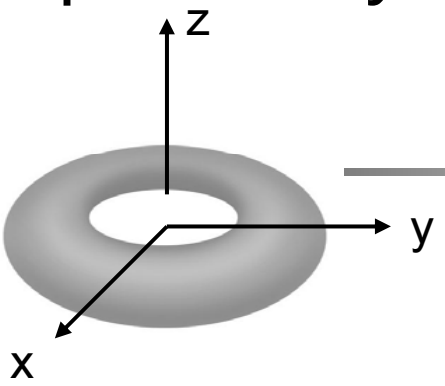
- Orbitals have n-l-1 radial nodes
- Probability of finding electron in this point in space is zero
- Particle-wave duality
- Effect of nodes and maxima on chemistry – orbital overlap
- Penetrating orbitals



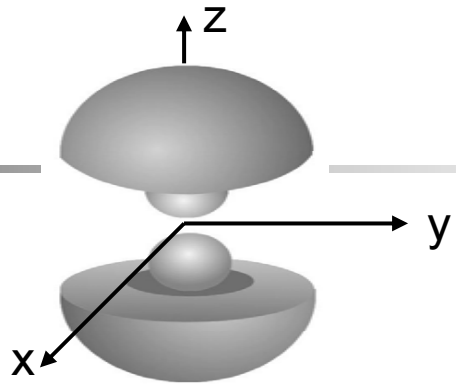
Electron density contours for the hydrogen-like $3p_z$ orbital of carbon

Nodal surfaces

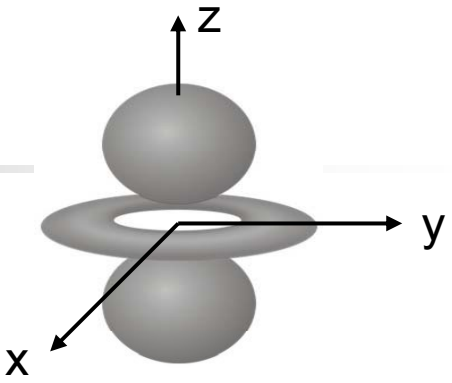
- probability densities



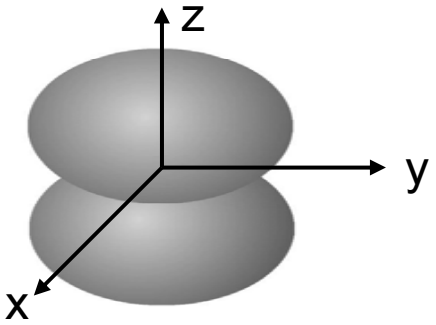
$|\psi_{2,1,1}|^2$



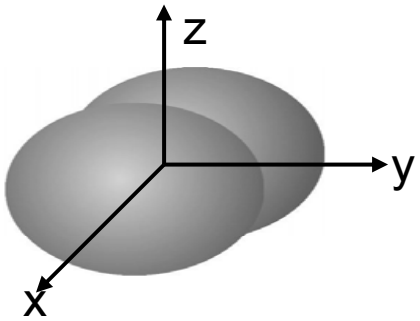
$|\psi_{3,1,0}|^2$



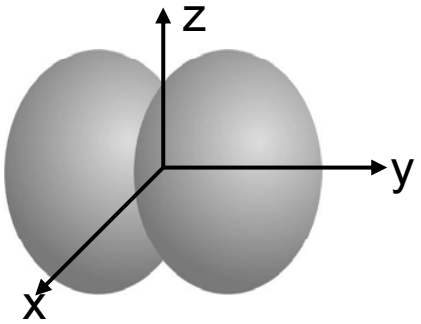
$|\psi_{3,2,0}|^2$



$2P_z$



$2P_x$



$2P_y$