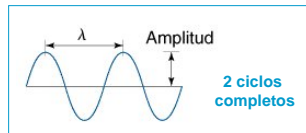


Ecuación de Schrödinger $\hat{H} \Psi = E \Psi$

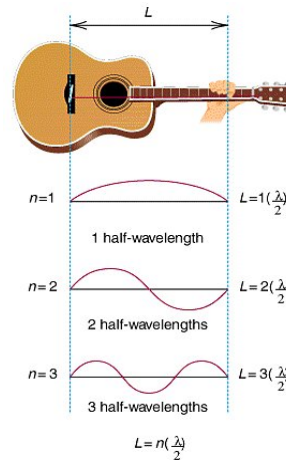
Ψ Función de onda



Propiedades de Ψ :

- Posee condiciones de frontera, ej. $\Psi=0$ para $r = \infty$ y $r = 0$ ($r = \text{dist e- nucl}$)
- Es continua y unievaluada
- Ψ^2 da la probabilidad de encontrar al e- en cierta región del espacio a un tiempo t.
- $\int \Psi^2 = 1$
- Posee nodos (superficies dde $\Psi=0$ y cambia de signo)
- Posee amplitudes y fases
- Dos o más Ψ interactúan constructiva o destructivamente

Ejemplo del mundo clásico:



Ecuación de Schrödinger $\hat{H} \Psi = E \Psi$

\hat{H} Operador Hamiltoniano Operador de la energía

$$E = T + V$$

$$= \frac{1}{2}mv^2 + V \quad p = mv \therefore v = \frac{p}{m}$$

$$= \frac{1}{2} \frac{p^2}{m} + V \quad \hat{p} = \frac{\hbar}{i} \frac{d}{dx}$$

$$E = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V$$

$$E\Psi = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi + V\Psi$$

$$E\Psi = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right) \Psi$$

$$\hat{H}$$

En un átomo la V tiene 2 componentes como resultado de las interacciones electrostáticas entre cargas de diferente signo:

- atracciones núcleo – electrón
- repulsiones electrón – electrón

$$V = -\sum_i \frac{Ze^2}{r_i} + \sum_{j>i} \frac{e^2}{r_{ij}}$$

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 - \sum_i \frac{Ze^2}{r_i} + \sum_{j>i} \frac{e^2}{r_{ij}}$$

$$\left(-\frac{\hbar^2}{2m} \nabla^2 - \sum_i \frac{Ze^2}{r_i} + \sum_{j>i} \frac{e^2}{r_{ij}} \right) \Psi = E\Psi$$

Ecuación de Schrödinger para el átomo de H

$$\left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{r_i} \right) \Psi = E\Psi$$

Las soluciones a esta ecuación están caracterizadas por 4 números cuánticos que caracterizan los orbitales atómicos:

	nombre	valores	determina	características
<i>n</i>	principal	# enteros	E y tamaño	n-1 sup. nodales
<i>l</i>	angular o azimutal	0, 1, ..., n-1	Forma	l sup. nod. no esféricas
<i>m</i>	magnético	-1 ... 0 ... +1	Orientación	
<i>s</i>	espín	-1/2 +1/2	Direcc. del spin	

l = 0 → orbital s

l = 1 → orbital p

l = 2 → orbital d

l = 3 → orbital f

Cada orbital atómico está caracterizado por 3 números cuánticos: *n*, *l* y *m*

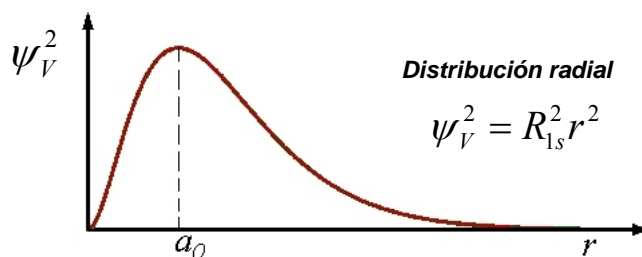
Y su máxima ocupación posible es de 2 e-
s(e1)=-1/2 s(e1)=+1/2

-Orbitales atómicos

Orbitales s 1s

$$\begin{aligned} \psi_{1s} &= R_{1s} \times Y_{1s} \\ &= 2Z^{3/2} e^{-\rho/2} \times (1/4\pi)^{1/2} \end{aligned}$$

Z = carga nuclear efectiva
e = carga del e-
r = radio atómico
 $\rho = 2Zr/n$



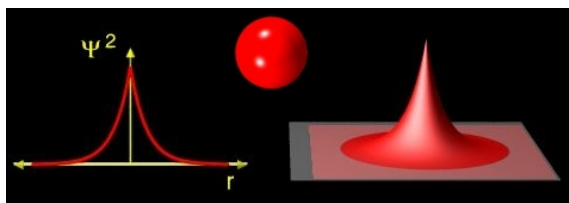
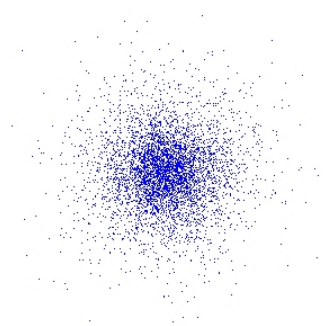
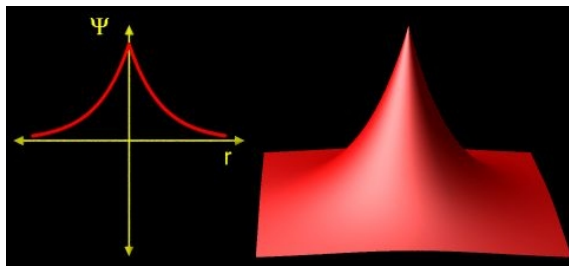
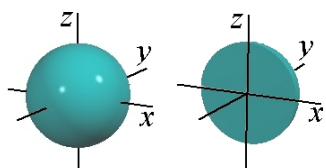
La distribución radial se obtiene integrando ψ^2 por unidad de volumen

a_0 para el orbital 1s del átomo de H define la unidad de radio atómico
 $a_0(H, 1s) = 1au = 52.9 pm$

-Orbitales atómicos

Química Cuántica

Orbitales s 1s



-Orbitales atómicos

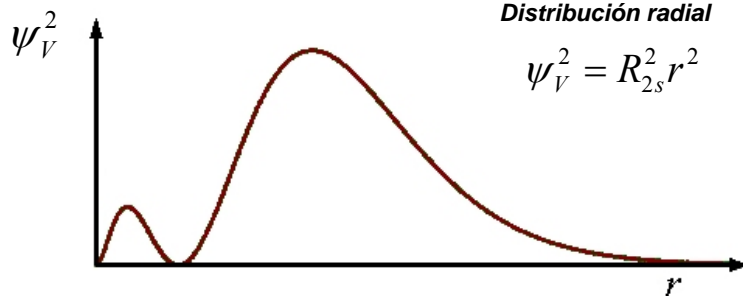
Química Cuántica

Orbitales s 2s

$$\psi_{2s} = R_{2s} \times Y_{2s}$$

$$R_{2s} = (1/2\sqrt{2}) \times (2 - \rho) \times z^{3/2} \times e^{-\rho/2}$$

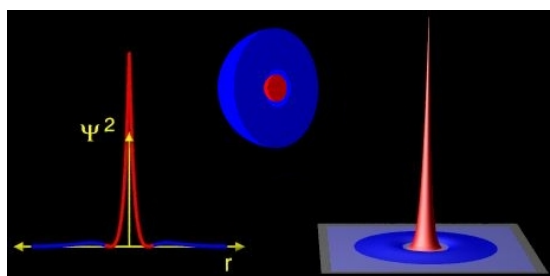
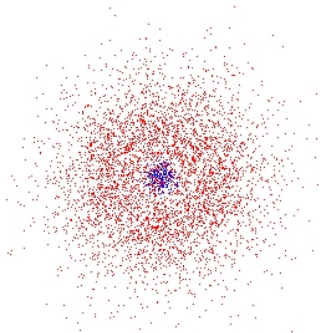
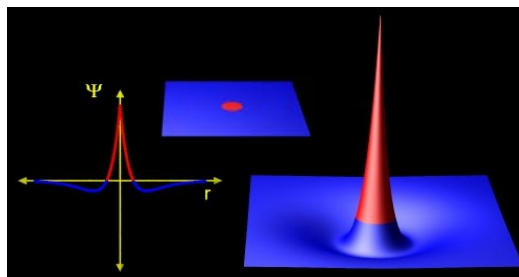
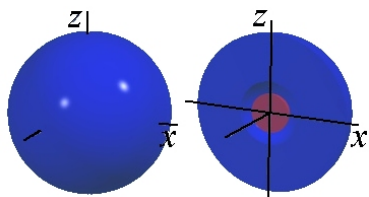
$$Y_{2s} = 1 \times (1/4\pi)^{1/2}$$



-Orbitales atómicos

Química Cuántica

Orbitales s **2s**



-Orbitales atómicos

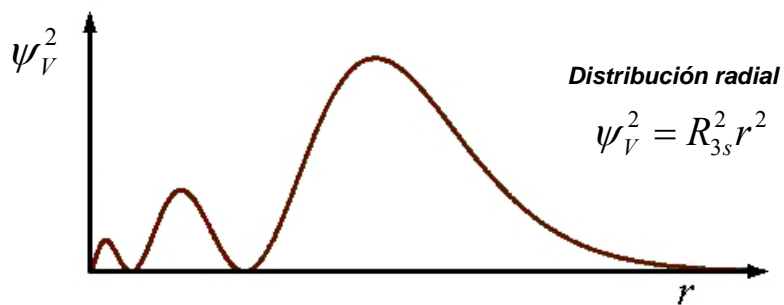
Química Cuántica

Orbitales s **3s**

$$\psi_{3s} = R_{3s} \times Y_{3s}$$

$$R_{3s} = (1/9\sqrt{3}) \times (6 - 6\rho + \rho^2) \times Z^{3/2} \times e^{-\rho/2}$$

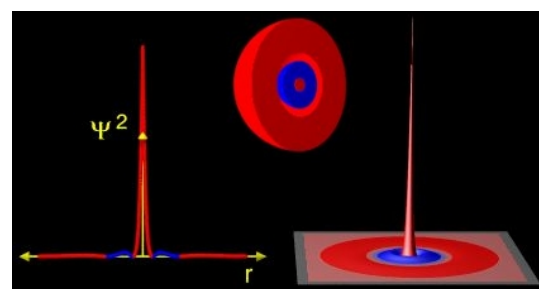
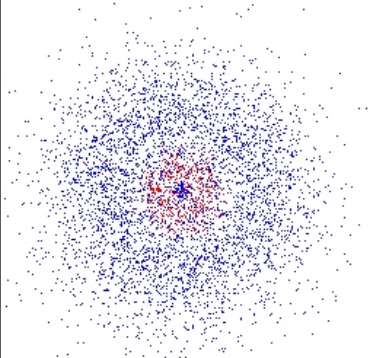
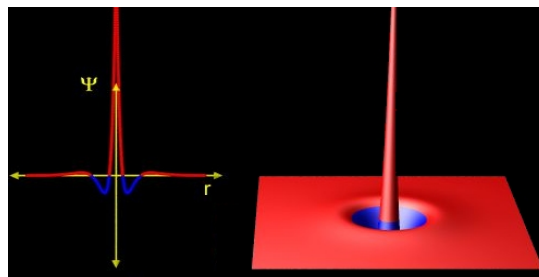
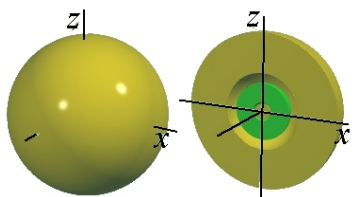
$$Y_{3s} = 1 \times (1/4\pi)^{1/2}$$



-Orbitales atómicos

Química Cuántica

Orbitales s 3s

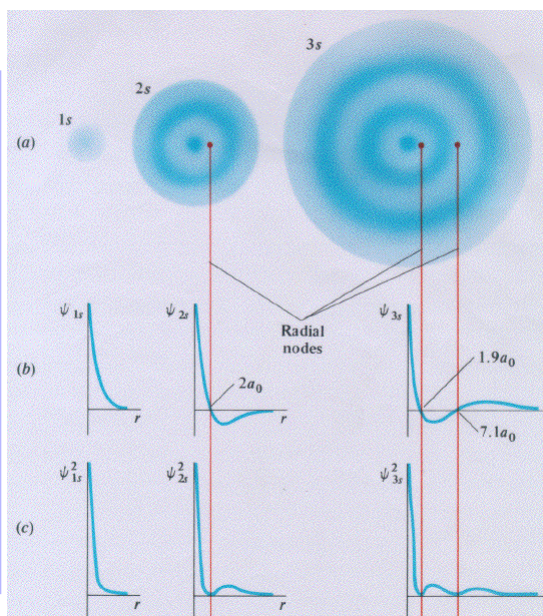


-Orbitales atómicos

Química Cuántica

Orbitales s

 1s	$n = 1$ $l = 0$ $m = 0$
 2s	$n = 2$ $l = 0, 1$ $m = 0, \pm 1$
 3s	$n = 3$ $l = 0, 1, 2$ $m = 0, \pm 1, \pm 2$



-Orbitales atómicos

Química Cuántica

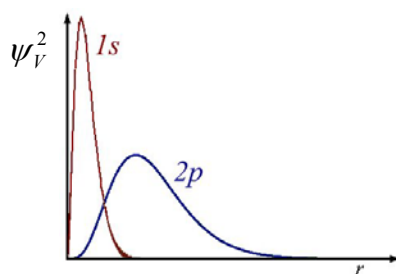
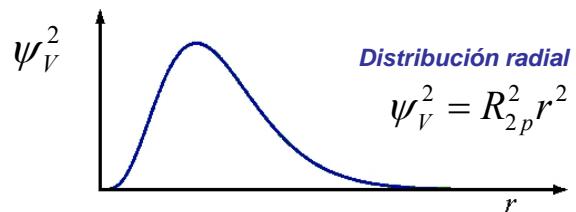
Orbitales p

2p

$$\psi_{2p_x} = R_{2p} \times Y_{2p_x}$$

$$R_{2p} = (1/2\sqrt{6}) \times \rho \times z^{3/2} \times e^{-\rho/2}$$

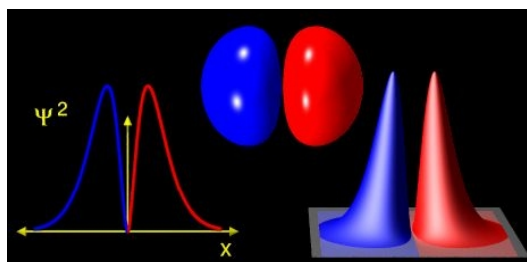
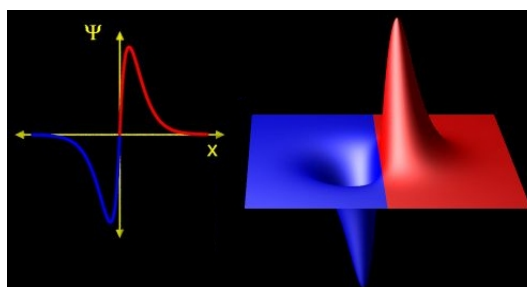
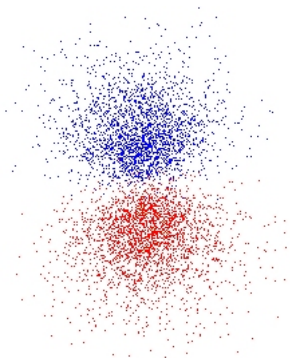
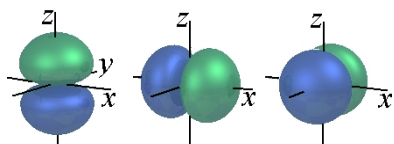
$$Y_{2p_x} = \sqrt{3}x/r \times (1/4\pi)^{1/2}$$



-Orbitales atómicos

Química Cuántica

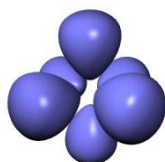
Orbitales p **2p**



-Orbitales atómicos

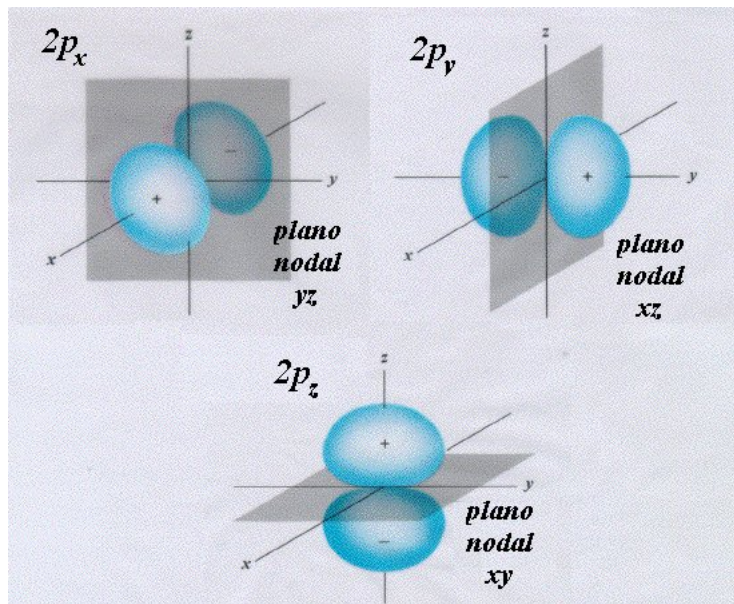
Química Cuántica

Orbitales p



2p

$n = 2$
$l = 1$
$m = -1$
0
$+1$



-Orbitales atómicos

Química Cuántica

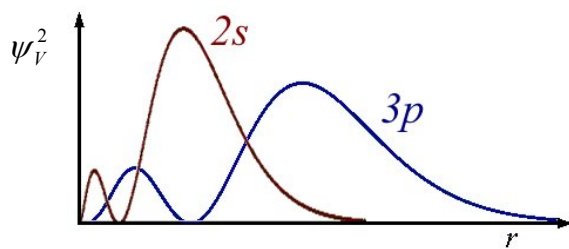
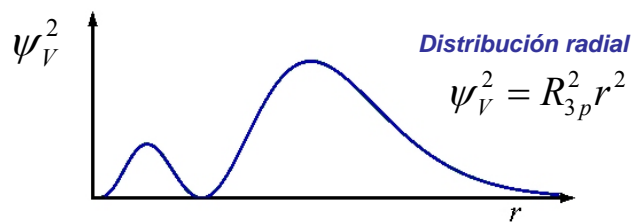
Orbitales p

3p

$$\psi_{3p_x} = R_{3p_x} \times Y_{3p_x}$$

$$R_{3p_x} = (1/9\sqrt{6}) \times \rho(4 - \rho) \times z^{3/2} \times e^{-\rho/2}$$

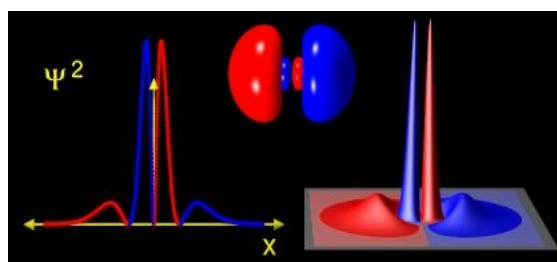
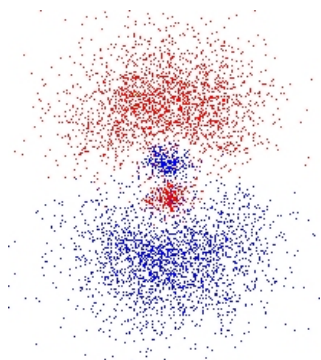
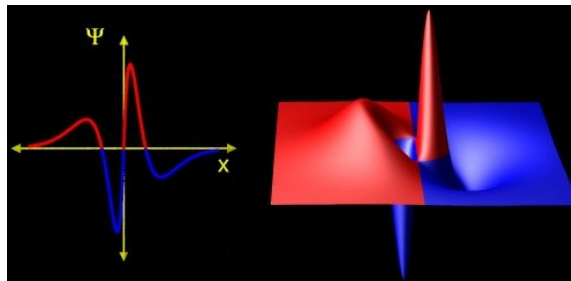
$$Y_{3p_x} = \sqrt{(3)x/r} \times (1/4\pi)^{1/2}$$



-Orbitales atómicos

Química Cuántica

Orbitales p **3p**



-Orbitales atómicos

Química Cuántica

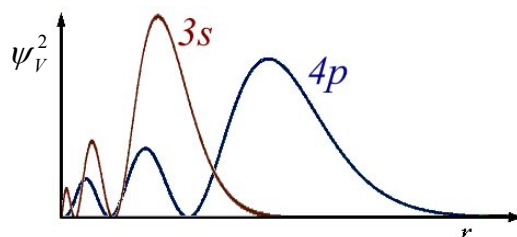
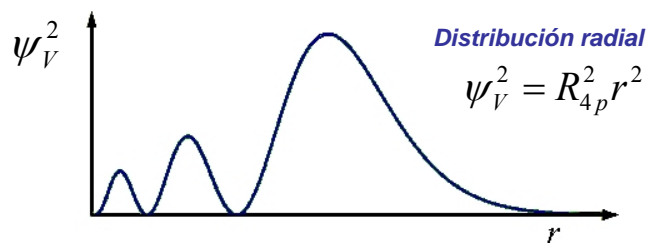
Orbitales p

4p

$$\psi_{4p_x} = R_{4p_x} \times Y_{4p_x}$$

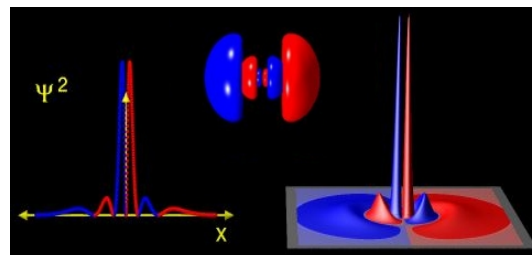
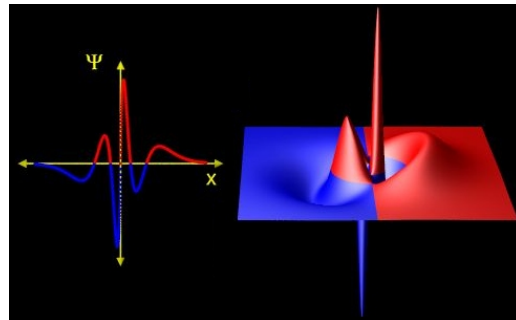
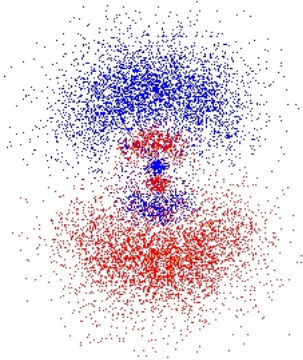
$$R_{4p_x} = (1/32\sqrt{15}) \times \rho(20 - 10\rho + \rho^2) \times z^{3/2} \times e^{-\rho/2}$$

$$Y_{4p_x} = \sqrt{3}x/r \times (1/4\pi)^{1/2}$$



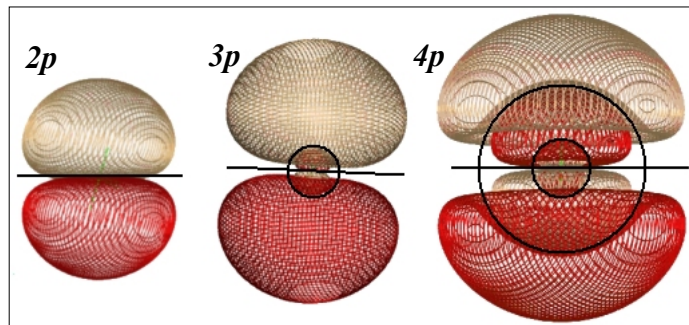
-Orbitales atómicos

Orbitales p 4p



-Orbitales atómicos

Orbitales p



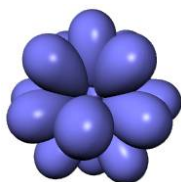
$n=2$
 $\ell=1$
 nodos tot. = $n-1=1$
 nodos no esf. = $\ell=1$
 nodos esf. = 0

$n=3$
 $\ell=1$
 nodos tot. = $n-1=2$
 nodos no esf. = $\ell=1$
 nodos esf. = 1

$n=4$
 $\ell=1$
 nodos tot. = $n-1=3$
 nodos no esf. = $\ell=1$
 nodos esf. = 2

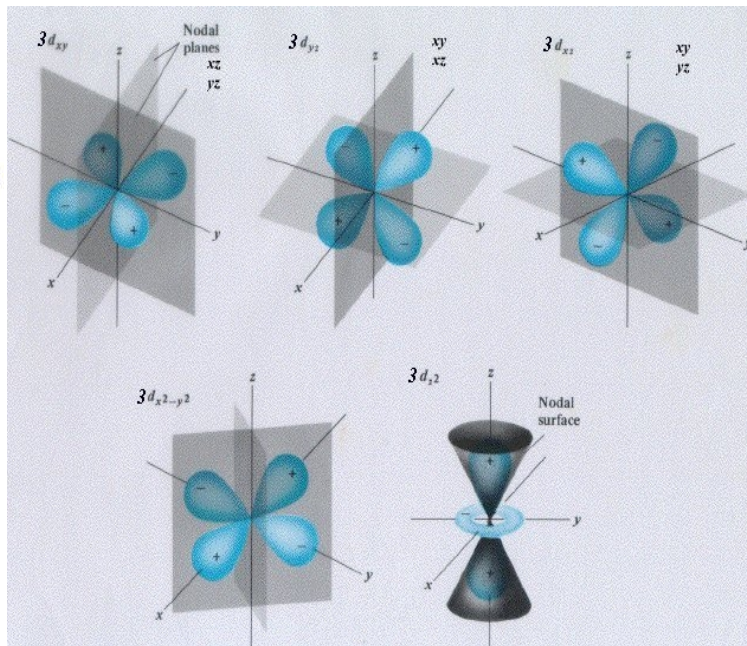
-Orbitales atómicos

Orbitales d



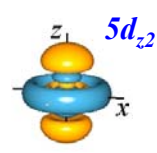
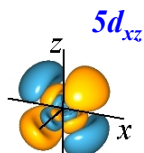
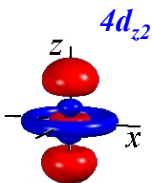
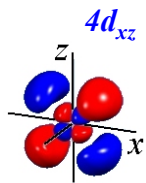
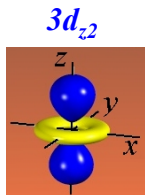
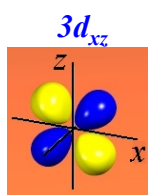
3d

$n = 3$
 $l = 2$
 $m = -2$
 -1
 0
 $+1$
 $+2$

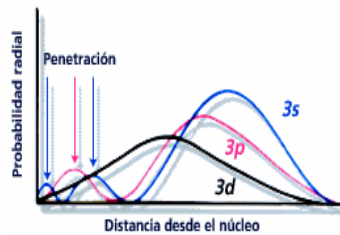


-Orbitales atómicos

Orbitales d



Extensión radial de los orbitales atómicos 3s, 3p, 3d



-Números Cuánticos

Los números cuánticos n y l determinan el tamaño del orbital (distancia promedio del e- al núcleo):

$$r = a_0 \frac{n^2}{Z} \left[\frac{3}{2} - \frac{l(l+1)}{2n^2} \right] \quad a_0 = 0.529 \text{ \AA}$$

La E de los diferentes orbitales hidrogenoides viene determinada únicamente por el número cuántico principal, n , según:

$$E_n = -R_H \frac{Z^2}{n^2}$$

∴ Para los diferentes orbitales hidrogenoides se cumple el siguiente orden de niveles energéticos:

$$1s < 2s=2p < 3s=3p=3d < 4s=4p=4d=4f < 5s \dots\dots$$

Sin embargo para átomos con más de 1 electrón, la repulsión electrónica modifica este orden de la siguiente manera:

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s$$

-Orbitales atómicos

Orden energético:

