

## A Closer Look at $\psi$

- Contains Information about the Probability of finding the Quantum Mechanical Entity in a Certain State
  - For atom, know energy so  $\psi$  is related to probability of finding electron at a certain point in space
- The Probability is not  $\psi$ , rather  $\psi^2$ 
  - Actually this is  $\psi^*\psi$

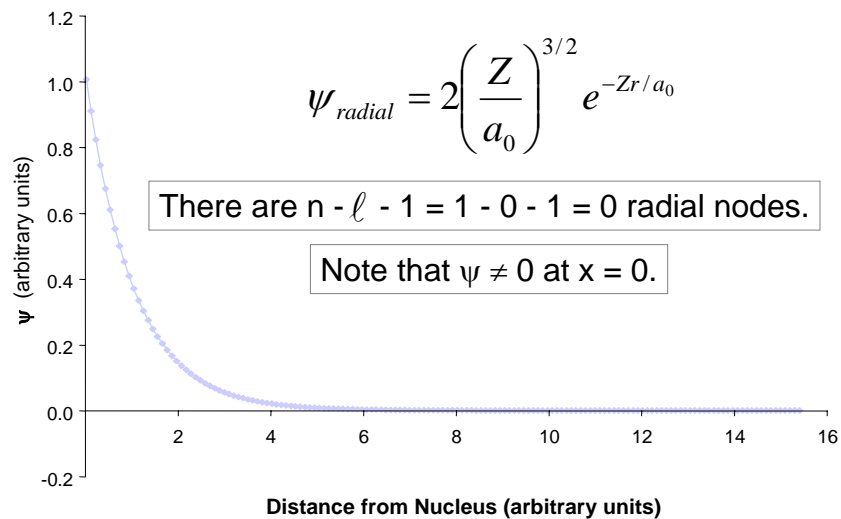
## More on Orbitals

- Wavefunctions for Atomic Orbitals can be divided into Two Parts
  - Radial (depends on distance from nucleus)
  - Angular (depends on angles  $\phi$  and  $\theta$ )
- For Chemistry Angular Part is (most) Important
  - Molecular shape
  - Bonding

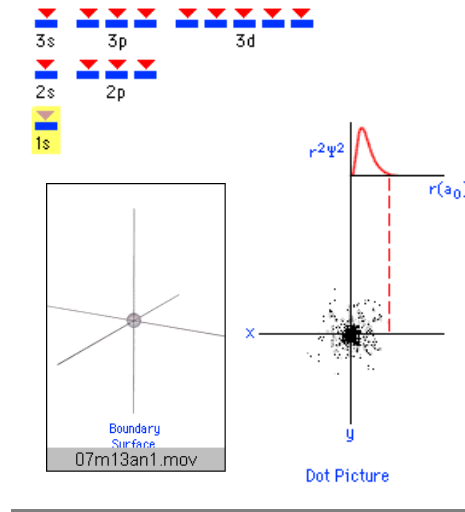
## Nodes

- Places where the Probability of finding the Electron is Zero ( $\psi = 0$  so  $\psi^2 = 0$ )
- When  $\psi_{\text{radial}}$  is zero, called a *radial* (or *spherical*) *node*
  - There are  $n - \ell - 1$  radial nodes
- When  $\psi_{\text{angular}}$  is zero, called an *angular node* (or a *nodal plane*)
  - There are  $\ell$  angular nodes

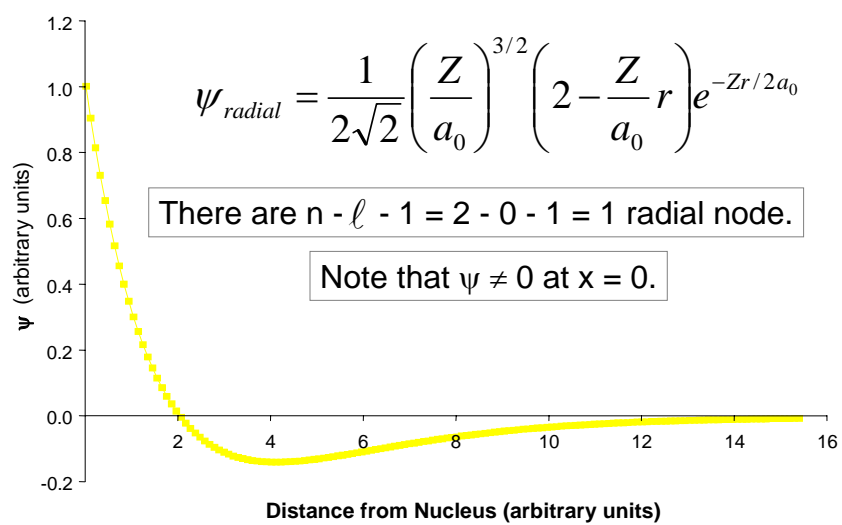
## 1s Radial Wavefunction



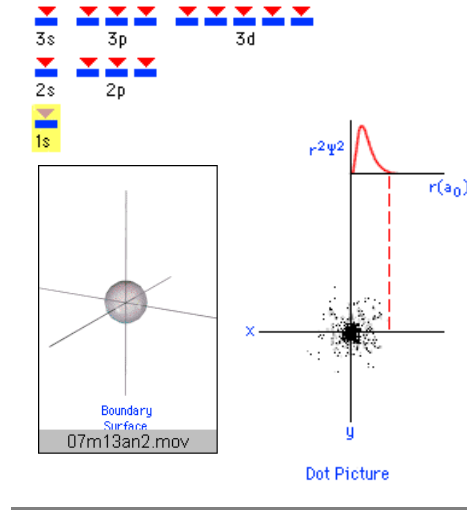
## 1s Orbital



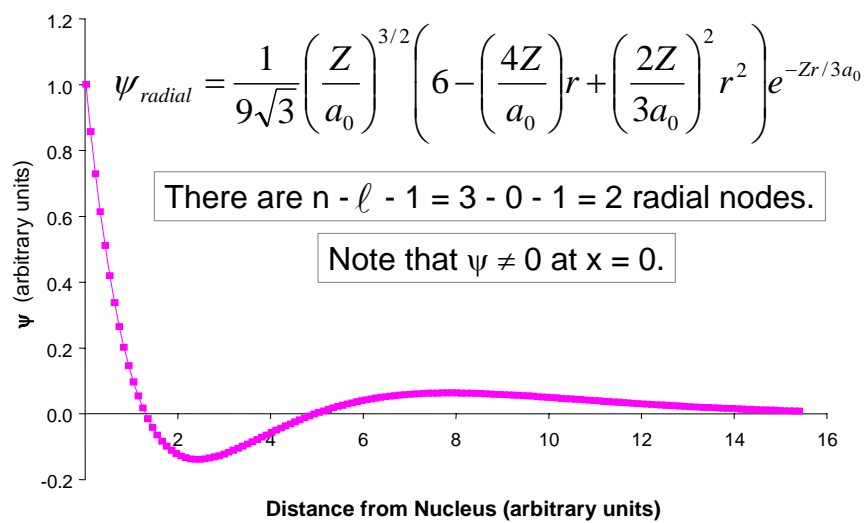
## 2s Radial Wavefunction



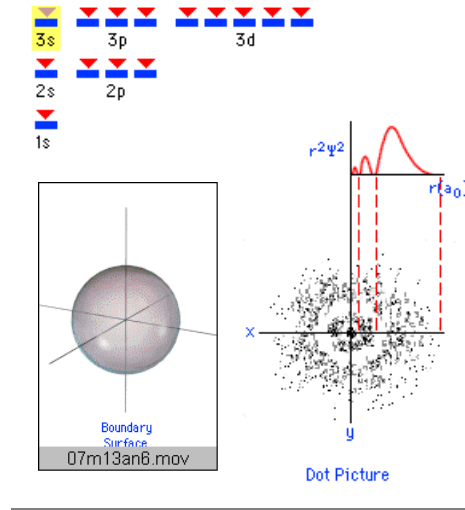
## 2s Orbital



## 3s Radial Wavefunction

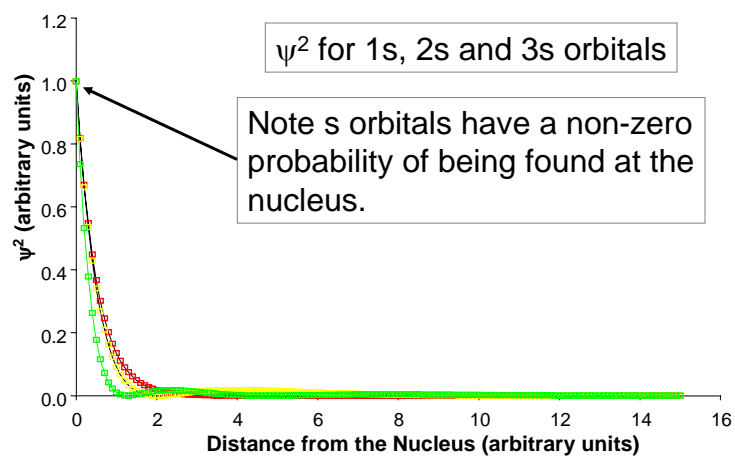


## 3s Orbital

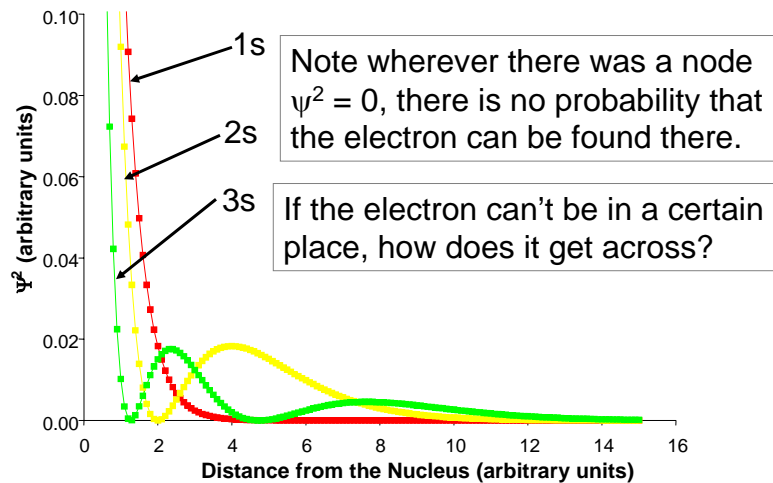


## Probability of Finding an Electron

- Remember  $\psi^2$ , not  $\psi$ , is Probability



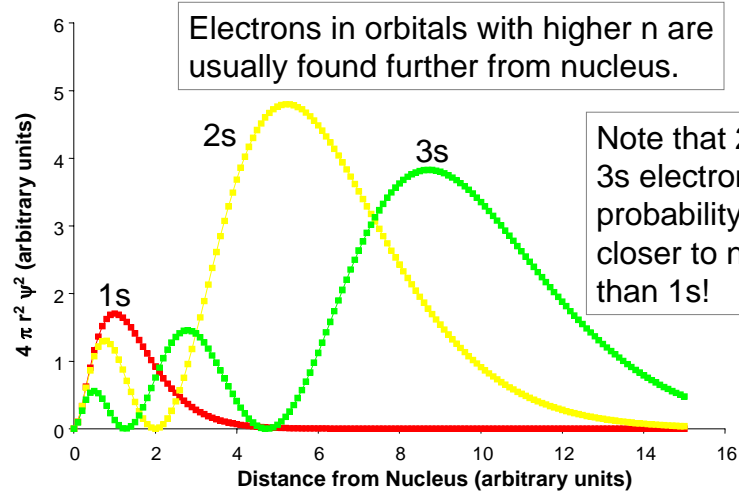
## Probability of Finding an Electron



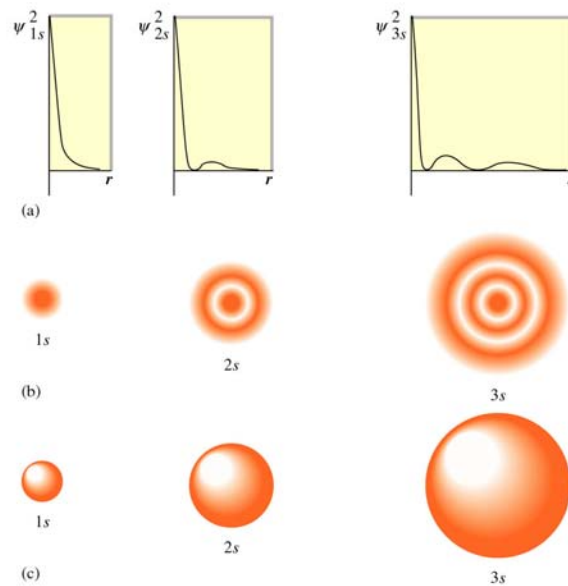
## Radial Distribution Function

- Problem with  $\psi^2$ , it over estimates Probability Close to Nucleus and under estimates it Further Out
- Correct by multiplying  $\psi^2$  by  $4\pi r^2$ 
  - Takes into account that a wedge is smaller toward the center than ends
  - This correction only works for s orbitals

## Radial Distribution Function

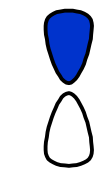


## 1s, 2s, and 3s orbitals

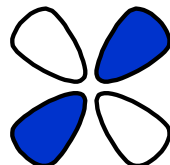


## Angular Part of Wavefunction

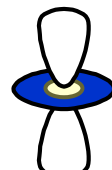
- Every Time  $\psi$  goes through a node *Sign* of Wavefunction changes
  - s orbital has same angular sign throughout
  - p orbital lobes have different signs
  - Lobes alternate signs in a d orbital
- Difference in *Phase*



p orbital



d orbital

 $d_{z^2}$  orbital

## p Orbitals

When  $n = 2$ , then  $\ell = 0$  and 1  
Therefore, in  $n = 2$  shell there are 2 types of orbitals (2 subshells)

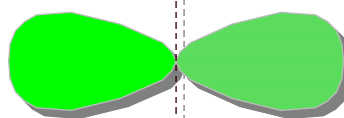
For  $\ell = 0$   $m_\ell = 0$

this is a s subshell

For  $\ell = 1$   $m_\ell = -1, 0, +1$

this is a p subshell  
with 3 orbitals

Typical p orbital

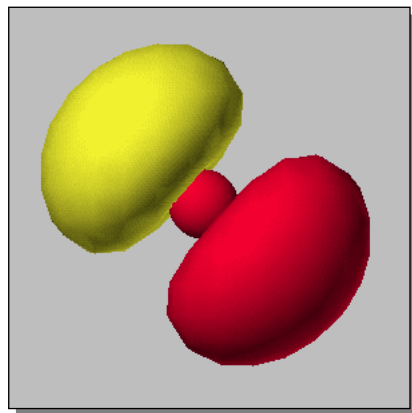


planar node

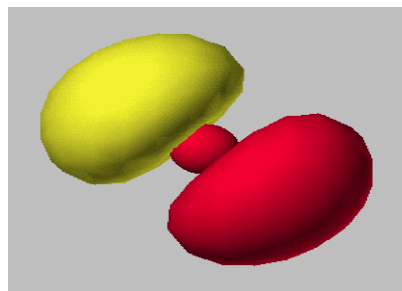
When  $\ell = 1$ , there is a **PLANAR NODE** thru the nucleus.



## p Orbitals



A p orbital



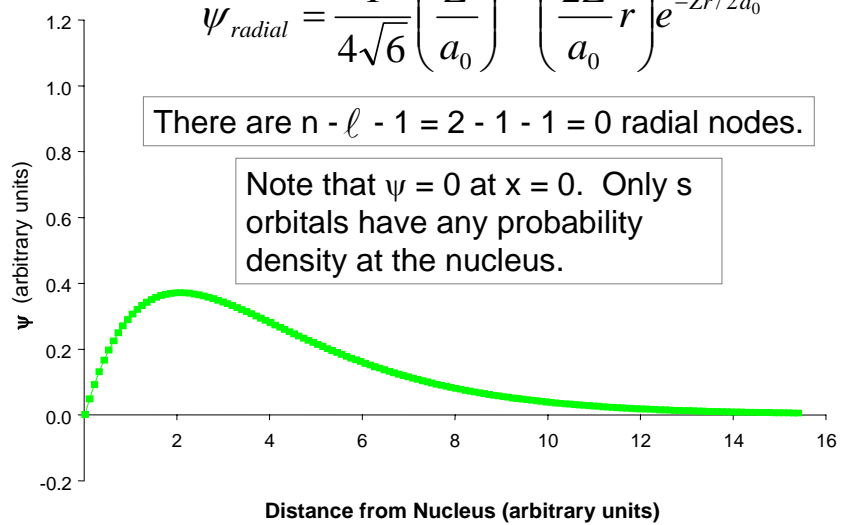
The three p orbitals lie 90° apart in space

## 2p Radial Wavefunction

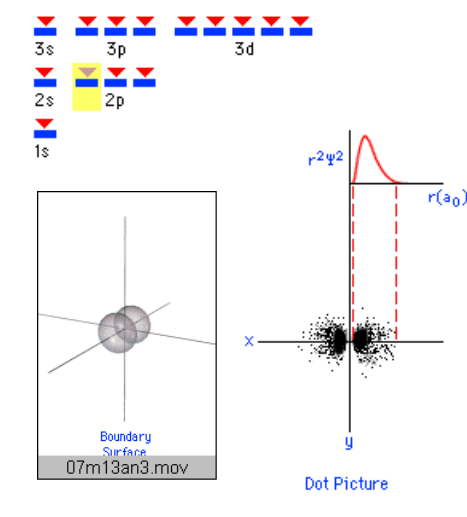
$$\psi_{radial} = \frac{1}{4\sqrt{6}} \left( \frac{Z}{a_0} \right)^{3/2} \left( \frac{2Z}{a_0} r \right) e^{-Zr/2a_0}$$

There are  $n - \ell - 1 = 2 - 1 - 1 = 0$  radial nodes.

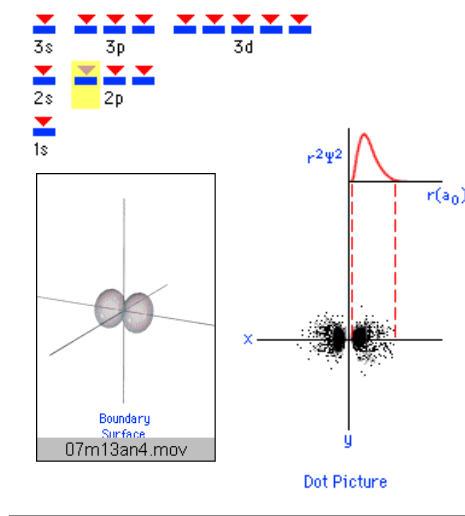
Note that  $\psi = 0$  at  $x = 0$ . Only s orbitals have any probability density at the nucleus.



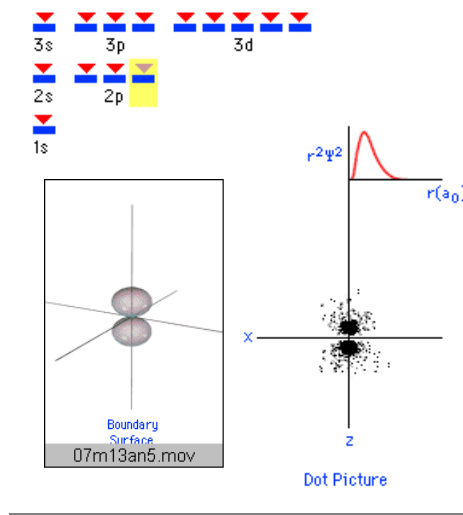
## 2p<sub>x</sub> Orbital



## 2p<sub>y</sub> Orbital

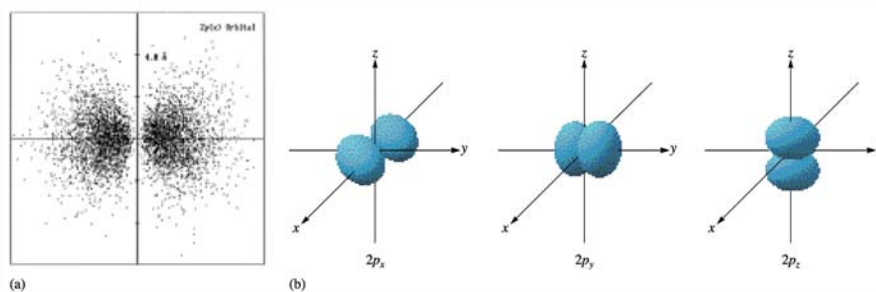


## 2p<sub>z</sub> Orbital

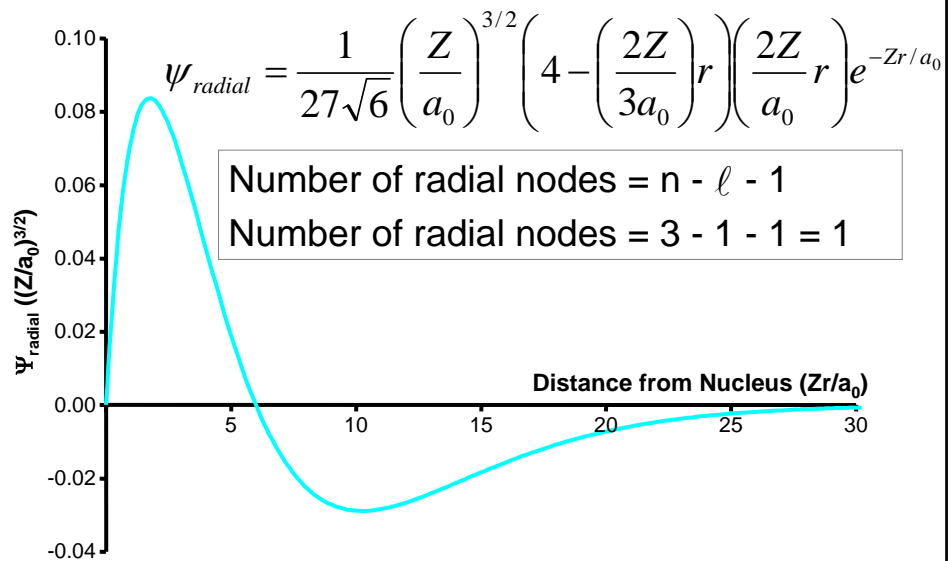


## Degenerate 2p Orbitals

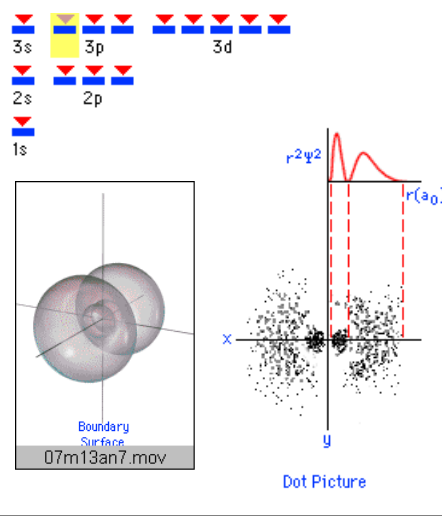
- All 3 orbitals have the same energy ( $n$  and  $\ell$ ), but differ in orientation ( $m_\ell$ )



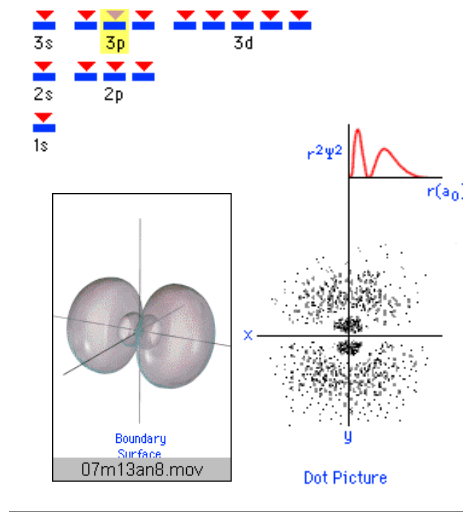
## 3p Radial Wavefunction



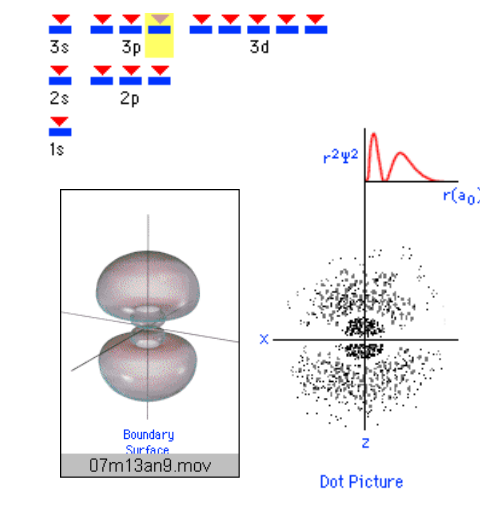
## 3p<sub>x</sub> Orbital



## 3p<sub>y</sub> Orbital



## 3p<sub>z</sub> Orbital



## d Orbitals

When  $n = 3$ , what are the values of  $\ell$ ?

$$\ell = 0, 1, 2$$

so there are 3 subshells in the shell.

For  $\ell = 0$ ,  $m_\ell = 0$

---> s subshell with single orbital

For  $\ell = 1$ ,  $m_\ell = -1, 0, +1$

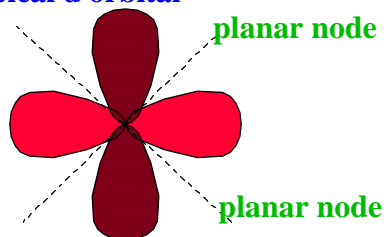
---> p subshell with 3 orbitals

For  $\ell = 2$ ,  $m_\ell = -2, -1, 0, +1, +2$

---> **d subshell with 5 orbitals**

## d Orbitals

typical d orbital

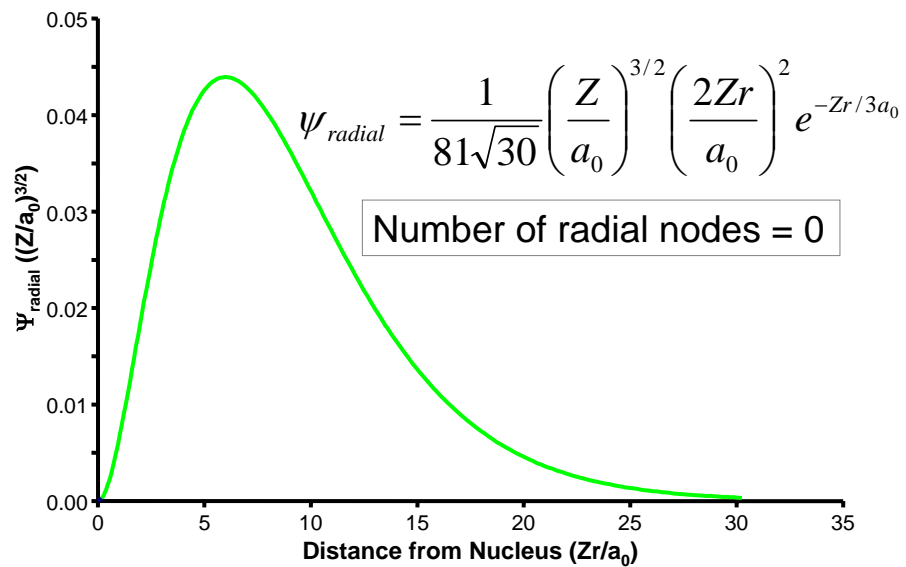


s orbitals have no planar nodes ( $\ell = 0$ ) and are spherical.

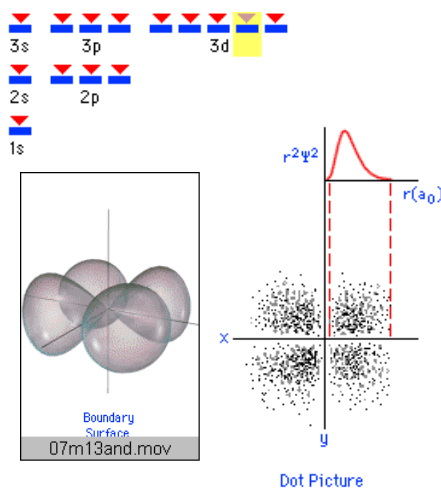
p orbitals have  $\ell = 1$ , have 1 planar node, and are “dumbbell” shaped.

This means d orbitals ( $\ell = 2$ ) have 2 planar nodes

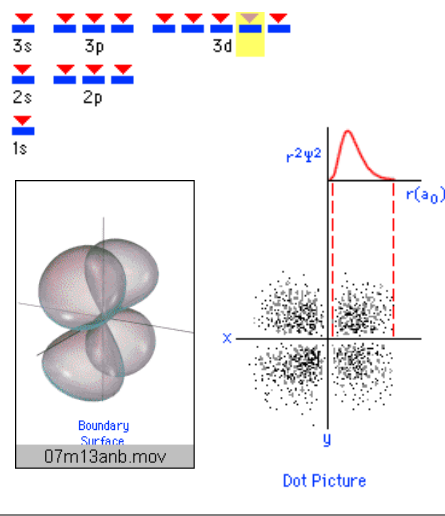
## 3d Radial Wavefunction



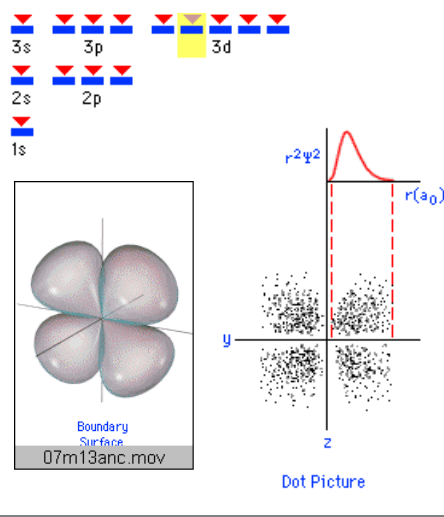
## 3d<sub>xy</sub> Orbital



## 3d<sub>xz</sub> Orbital

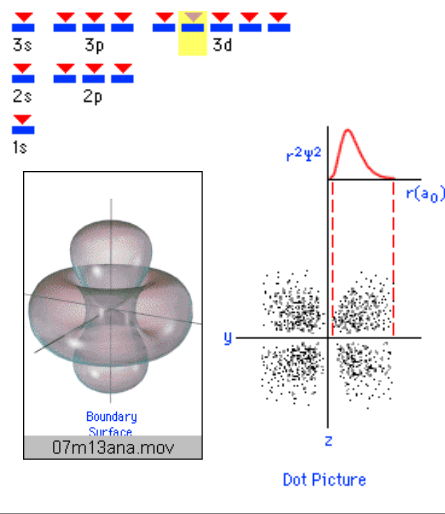


## 3d<sub>yz</sub> Orbital

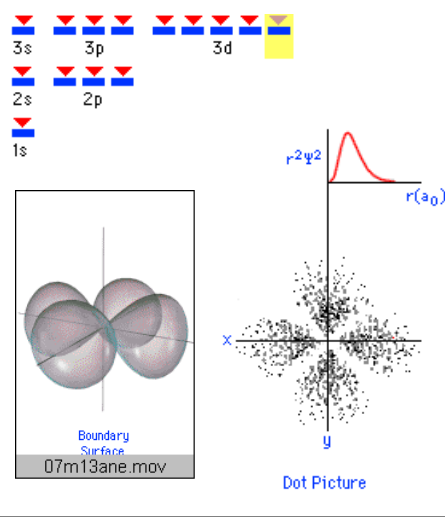




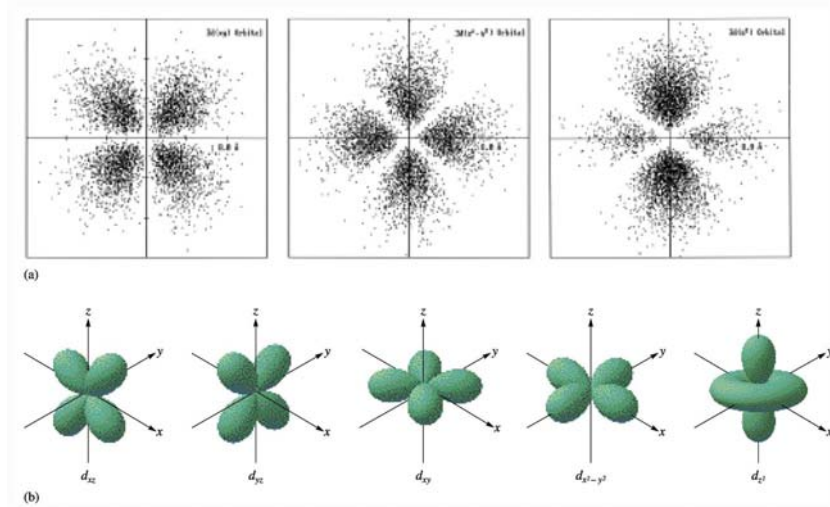
## 3d<sub>z<sup>2</sup></sub> Orbital



## 3d<sub>x<sup>2</sup>-y<sup>2</sup></sub> Orbital



## d Orbitals



## f orbitals

When  $n = 4$ ,  $\ell = 0, 1, 2, 3$  so there are 4 subshells in the shell.

For  $\ell = 0$ ,  $m_\ell = 0$

→ s subshell with single orbital

For  $\ell = 1$ ,  $m_\ell = -1, 0, +1$

→ p subshell with 3 orbitals

For  $\ell = 2$ ,  $m_\ell = -2, -1, 0, +1, +2$

→ d subshell with 5 orbitals

For  $\ell = 3$ ,  $m_\ell = -3, -2, -1, 0, +1, +2, +3$

→ **f subshell with 7 orbitals**

## f orbitals

